THE PREPARATION AND STUDY OF BIS(PYRIDYL-IMINE) AND MONOHELICAL SALEN-TYPE COMPLEXES OF IRON AND ZINC

by

ALEXANDER V. WIZNYCIA

B.S., Nottingham Trent University, 1998

AN ABSTRACT OF A DISSERTATION

submitted in partial fulfillment of the requirements for the degree

DOCTOR OF PHILOSOPHY

Department Of Chemistry
College of Arts and Sciences

KANSAS STATE UNIVERSITY
Manhattan, Kansas

2006

Abstract

In the field of asymmetric catalysis salens and related molecules occupy a unique position in the breath and scope of reactions facilitated. They, nonetheless, are characterized by several conformationally derived limitations. This work deals with applying the principles of helicity with the goal of remedying these shortcomings, thereby ultimately fashioning, better, more selective catalysts.

A series of novel ligands bearing phenanthryl and benz[a]anthryl side-arms attached to either a cyclohexyl or binaphthyl backbone bridging group, were prepared via multi-step synthesis. The ligands were subsequently metallated with zinc and iron salts to afford neutral helimeric complexes, that were characterized in the solution and solid states. The binaphthyl complexes were found via X-ray crystallographic analysis to afford exclusively *M*-helimers, while those incorporating a cyclohexyl bridge gave predominantly 1 : 1 *P* + *M* mixtures. A significantly greater degree of side-arm overlap was apparent where benz[a]anthryl side-arms were employed. ^{1}H NMR analysis, unfortunately, did not allow for solution phase helimer determination, and ECD spectroscopy was therefore utilized as an alternative. In conjunction with computational techniques the conformations were probed, and to a high degree of certainty the prevailing solution geometries of the cyclohexyl complexes predicted. Our results indicate that in solution the *M* configuration is the sole or dominant form.

Ionic zinc complexes based upon a tetradentate nitrogen donor motif and 8-isopropyl-2-quinolinecarboxaldehyde were also prepared. Structural characterization of the zinc complexes showed each to bind to two $ZnCl_2$ units, and as a consequence to form dinuclear helicates.

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CHAPTER 1

Introduction

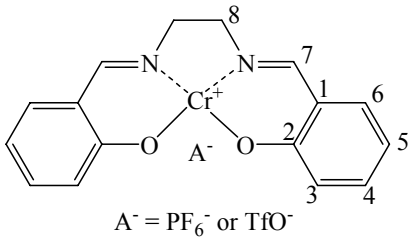
1.1 Synopsis

Metallo-salens, and related complexes have over the past two decades received much attention due to their ability to act as heterogeneous (and supported) catalysts for the chiral epoxidation of alkenes.[1] More recently, the catalytic scope has expanded to include various other chemical processes such as amination,[2] cyclopropanation,[3] sulfoxidation,[4] and epoxide ring-opening.[5] The ready synthesis of these systems and ease of introducing stereogenicity close to the coordinated metal has made them useful frameworks for chiral catalysis. Collectively, they constitute a "privileged class"[6] of molecules, able to promote reactivity and enantioselectivity across a diverse range of reactions and substrates.

Critical to the observed stereoselectivies is the active conformation of the catalyst during the chemical change. However, studies have shown that metallo-salens exhibit substantial conformational mobility,[7] hence methods of controlling this flux are necessary. One approach is to incorporate a secondary structure that restricts the range of motion, for example a helical motif. Such a helix would also act to amplify existing chiral elements within the structure. We therefore chose to prepare and study a series of novel metallo-salen and related tetradentate nitrogen complexes that incorporate helicity. This thesis details ongoing work on the synthesis and conformational properties of the aforementioned molecules.

1.2 Background

In 1985 Kochi and coworkers reported the stoichometric epoxidation of alkenes by achiral Cr(III)(salen) complexes (figure 1.1), for which an oxo Cr(V) intermediate was implicated as the active species.[8] In most cases moderate to good yields were obtained, although product yields were low for unfunctionalized acyclic alkenes. As evinced with the related metallo-porphyrin systems the addition of donor ligands such as pyridine-N-oxide increased observed conversion and reaction rates.[9]



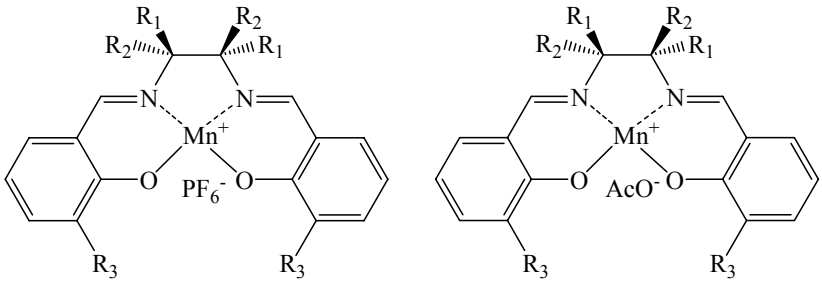
1. 3-8 = H
2. 8,8,8',8' = CH_3
3. 5,5' = Cl
4. 7,7' = CH_3
5. 7,7' = Ph
6. 5,5' = Cl, 8,8,8',8' = CH_3
7. 5,5' = OCH_3, 8,8,8',8' = CH_3
8. 4,4',6,6' = OCH_3, 8,8,8',8' = CH_3

Figure 1.1 Achiral Cr(salen) catalysts of Kochi and coworkers

In subsequent studies Kochi and coworkers found that Mn(salen)s also catalyzed alkene epoxidation.[10] In contrast to their Cr(salen) systems, Mn(salen)s were able to effectively epoxidize unfunctionalized acyclic alkenes. Enhanced reactivities and a greater substrate scope were also demonstrated. Due to the fleeting nature of the intermediate the active species was not directly observed, but was postulated to be an O=Mn(V)(salen)$^+$ complex.

This work set the stage for the development of chiral salen catalysts by Jacobson[11] and Katsuki.[12] In 1990, they independently reported asymmetric alkene epoxidations by a series of 3,3' and 8,8' substituted Mn(salen)s (figure 1.2). Subsituents at the 8,8' positions gave rise to the necessary catalyst chirality, while groups at the 3,3' positions if electron donating in nature,

enhanced the size of the enantiomeric excess. For Jacobsen's initial complex **11**, ee's were considerably higher than had been observed at that time for stereoselective epoxidations of unfunctionalized alkenes, ranging from 50-70% for mono- and tri-substituted alkenes, and 75-95% for *cis*-alkenes. The Mn(salen) complexes of Katsuki were less effective, 50% being the highest reported ee. The active intermediate was thought to be the same O=Mn(V)(salen)$^+$ complex as put forward by Kochi.[9]



9. R_1 = Ph, R_2 = H, R_3 = H
10. R_1 = H, R_2 = Ph, R_3 = H
11. R_1 = H, R_2 = Ph, R_3 = $C(CH_3)_3$

12. R_1 = Ph, R_2 = H, R_3 = (*S*)-$Ph(CH_3CH_2)CH$
13. R_1 = H, R_2 = Ph, R_3 = (*S*)-$Ph(CH_3CH_2)CH$
14. R_1 = Ph, R_2 = H, R_3 = CH_3

Figure 1.2 Initial Mn(salen) catalysts of Jacobson (left) and Katsuki (right)

Following this initial work, reports detailing metallo-salens containing various substituent groups at the 3-5 and 8 positions were published.[13-18] In one of these, the well known Jacobsen's catalyst (figure 1.3) was first described, [18] wherein, the inclusion of *t*-butyl groups at the 3,3' and 5,5' positions markedly improved enantioselectivities. It was suggested that the effect of the *t*-butyl groups was steric in nature. Recent *ab initio* calculations, however, have concluded that while the 3,3' *t*-butyl groups play mainly a steric role, the effect of those at the 5,5' positions is principally electronic.[19,20]

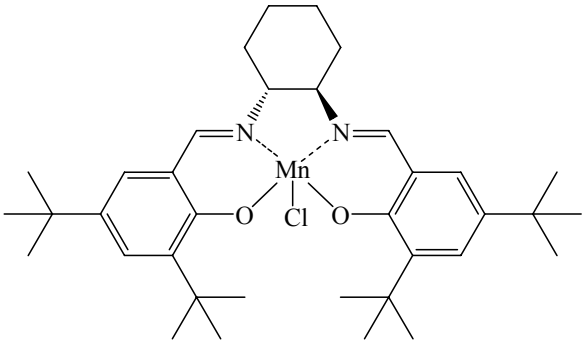


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Figure 1.3 Jacobson's catalyst

Since then numerous studies have been carried out, many focusing on Jacobsen's catalyst. It is not possible, however, due to the size and scope of this field to more than briefly mention a few of these studies, hence, only those with some relevance to this text will now be discussed.

1.3 Salen Catalyst Conformation

The conformation of a catalyst is often critical to its stereoselectivity, and this is indeed the case with salen-type systems.[8] The majority of metallo-salens incorporate a flexible *trans*-substituted ethylene bridge into the backbone of the molecule, that allows a significant degree of conformational mobility. This pliability is also present to some extent with 1,2-cyclohexane-diamine derived salens.[19] The flexibility and chirality of this ethylene bridge results in two 'stepped' conformers (figure 1.4). Of the two, steric factors favor the diequatorial structure, although in solution an equilibriating diaxial-diequatorial mixture will exist.[7] Small changes in ligand structure as well as in the metal, its oxidation state and/or counter ion can alter this

conformation, and the position of the equilibrium. In most instances this will result in a loss of stereochemical induction. Thus, conformational control of the metallo-salen is necessary.

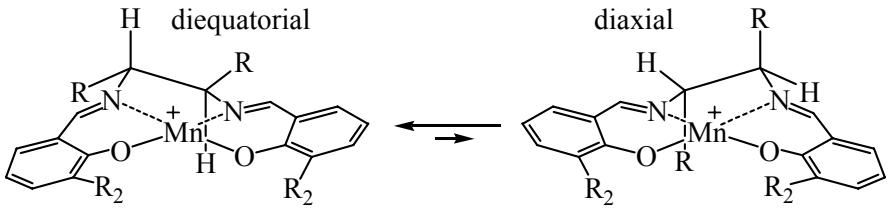


Figure 1.4 Diaxial-diequatorial equilibrium of salen complexes

For high stereoselectivity the favored conformer must also be able to transfer chirality to the incoming substrate, for which, one predominant trajectory of approach to the metal center is preferred. In this, the size and placement of substituent groups on the salen aromatic rings and on the substrate play a role. This is exemplified by Mn(salen) epoxidation of alkenes, where **a-d** (figure 1.5) are possible approach angles.[18,21-23]

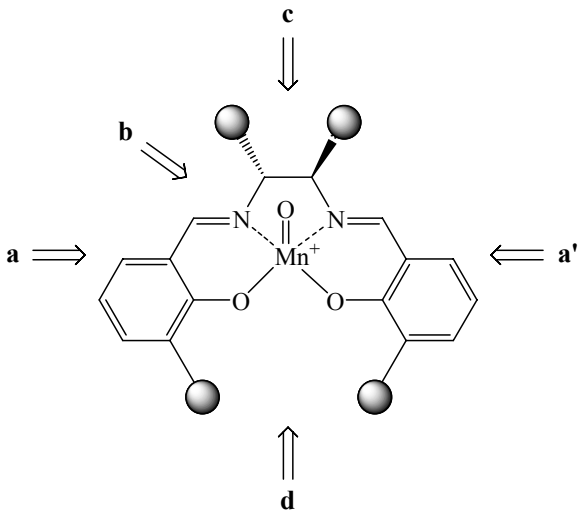


Figure 1.5 Approach trajectories for epoxidation of *cis*-alkenes

Trajectories **c** and **d** are unlikely in most Mn(salen) complexes due to the bulky groups that are usually present at the 3,3' and 8,8' positions. Furthermore, since chiral induction by the 8,8' substituents gives rise to non-planar structures, the approach trajectories **a** and **a'** are no longer equivalent. This issue is further complicated by the presence of both diaxial and diequatorial conformers. Thus, six possible modes result from **a**, **a'** and **b** (figure 1.6). In the

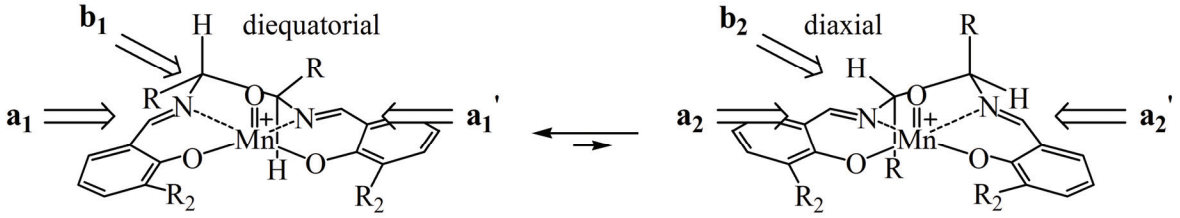


Figure 1.6 Analysis of approach trajectories $\mathbf{a_1}$ to $\mathbf{b_2}$

case of trajectories $\mathbf{a_1}$, $\mathbf{a_1}'$, $\mathbf{a_2}$ and $\mathbf{a_2}'$ if the sense of twist to the backbone is high, then $\mathbf{a_1}'$ and $\mathbf{a_2}$ will be partially occluded, and $\mathbf{a_1}$ and $\mathbf{a_2}'$ will be preferred. Since the equilibrium favors the equatorial conformer over the diaxial, $\mathbf{a_1}$ will be the dominant pathway of the two. The equilibrium will also favor pathway $\mathbf{b_1}$ over $\mathbf{b_2}$, and approach along the second N–Mn bond is unlikely due to blocking by the raised bulky R group. Although differentiating between pathways $\mathbf{a_1}$ and $\mathbf{b_1}$ is difficult, the available literature evidence is most supportive of $\mathbf{a_1}$.[8,19]

The steric role of the alkene and its attached substituents must also be considered. With the related porphyrin systems the incoming alkene is thought to orientate ~90° to the M=O bond (figure 1.7) to allow favorable orbital overlap.[23] The same general orientation of approach is predicted in salens also.[1,19] For a *trans*-alkene (figure 1.8) this would necessitate one of the substituents being directed downwards into the salen ligand; an unfavorable interaction. Differentiation due to sterics therefore is expected between the stereoselectivities of *cis*- and

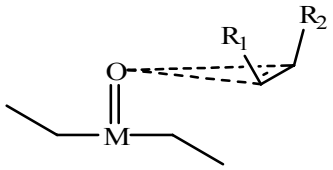


Figure 1.7 *Cis*-alkene approach

trans-alkenes, and this is indeed the case.[11,13] Cis-alkenes are in general observed to give higher ee's than the corresponding *trans*-alkene. However, if the salen were 'deeply twisted' or 'stepped' steric repulsion for *trans*-alkenes is minimized, allowing the preferred direction of approach. Higher ee's would therefore be expected, and in a few instances this has been observed.[25-27]

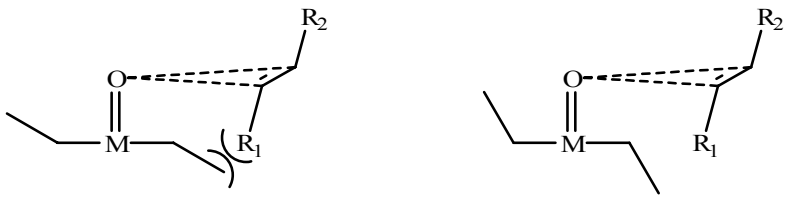


Figure 1.8 *Trans*-alkene approach to 'slightly' and 'deeply stepped' Mn(salen)s

As can be seen, the stereochemical outcome is complicated by many competing factors. Nonetheless, if the salen were constrained in some manner to assume only one 'deeply stepped' conformation many of these factors could be negated. A helical molecule can be thought of as adopting this single 'locked' conformation. The Mn(salen) structures discussed above are already in a sense 'pseudo-helical' (figure 1.9), and so it would only be necessary to extend the ligand arms to obtain a true helix. Interconversion between conformers would not be possible (figure 1.10), and a 'deeply stepped' structure is likely to result from steric repulsion between the

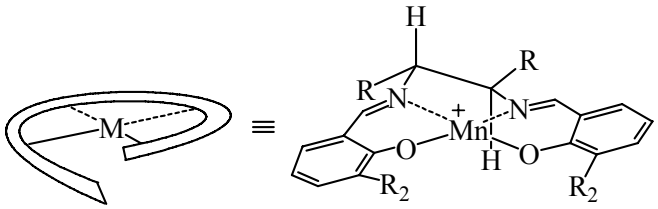


Figure 1.9 Pseudo-helicity of the Mn(salen) diequatorial conformer

overlapping ligand arms. As an added benefit a helical 'deeply stepped' structure may act to efficiently and stereoselectively epoxidize *trans*-alkenes. The chirality at C-8 and C-8' predetermines the directionality of this helix, where the chirality is transmitted and amplified throughout the metallo-salen. The usage of, for example, (*R,R)* stereochemistry (as in fig. 1.9)

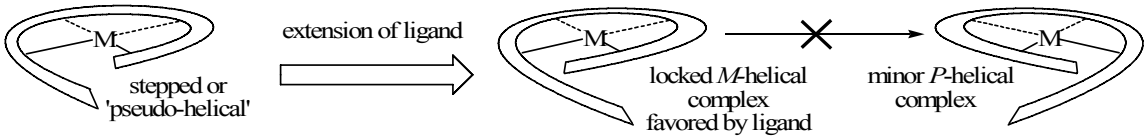


Figure 1.10 Extrapolation of ligand termini

biases the free ligand toward formation of the *M*-helix, thus, only one helical type is expected to form. However, creation of a limited quantity of the minor helical type cannot be ruled out.

For a helical metallo-salen, many trajectories to the catalytic center are partially or fully blocked by the ligand. Of the potential side approaches **e** (figure 1.11) is the most feasible. In this case, as one ligand arm passes under the other the resultant downward turn provides a route of access. The prospect of top-on approach to the metal, pathway **f**, is unlikely with respect to oxidation reactions due to absence of the necessary orbital overlap.[24] Depending on the exact salen structure there is the possibility of a combination of **a-f**, **b-f**, **c-f**, etc, to provide an angled

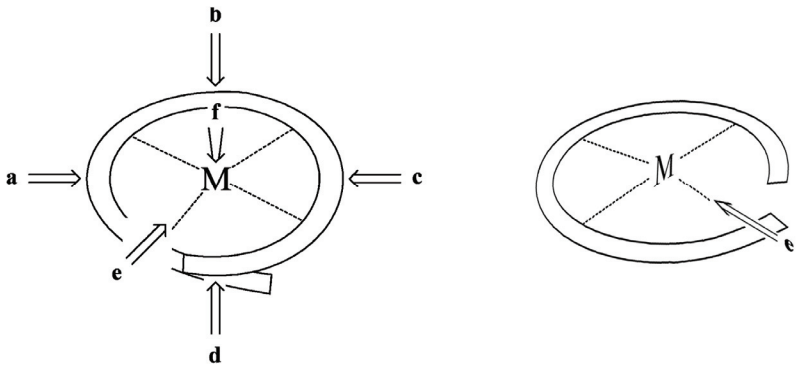


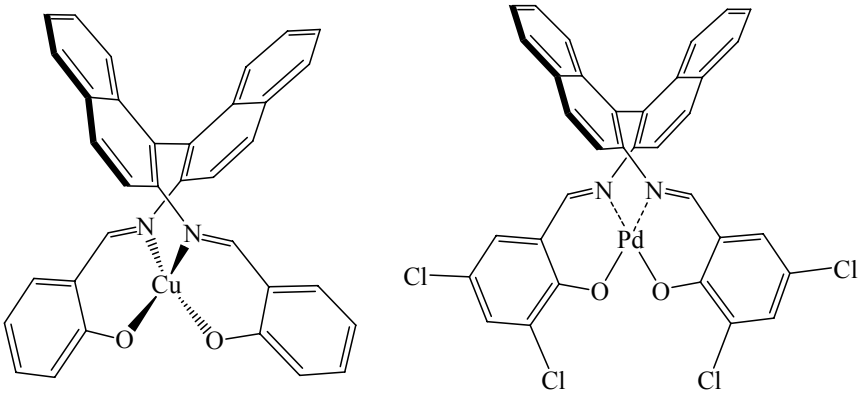
Figure 1.11 Front-view of approach trajectories for a helical complex (left) and side-view of the most feasible trajectory (right)

approach, although this decreases the extent of orbital interaction, making it a less probable trajectory than **e**. Overall therefore, the substrate path is regulated and there is the potential to act as a highly stereospecific catalyst.

1.4 Binap-Salen Catalyst Conformation

In comparison to ethylene bridged metallo-salens, relatively few have been examined where a binaphthyl moiety is incorporated as the backbone bridging group.[28] Thus, data on their conformational and catalytic properties is limited. Of the reported four-coordinate binap-M(salen)s the majority adopt a distorted tetrahedral geometry (figure 1.12) about the metal center.[29] Notable exceptions involve Pd(II) complexes that are almost square planar,[30] presumably due to the strong preference of palladium for this arrangement. The effect of penta- and hepta-coordination on binap-M(salen) complexes has also been studied, and found to afford distorted trigonal bypiramidal and octahedral geometries respectively.[31] No clear connection is

known regarding the relationship between conformation and stereoselectivity, although a few comparisons to the complexes discussed previously can be made.



16 **17**

Figure 1.12 Distorted tetrahedral and square planar binap-M(salen)s

Unlike the conformationally mobile ethylene bridged metallo-salens, the use of a binaphthyl backbone results in one main conformer. Rotational isomerism is not possible, and the steep energy well to rotation restricts the binaphthyl dihedral angle to ~60-130^{o}.[32] With the exception of the Pd(II) salens the structures that result are deeply 'stepped', leading to potential catalysts for *trans*-alkene epoxidation, although, to date, only one literature report has examined this possibility.[33] In that example, observed epoxidation ee's were low.

The catalytic center is sterically crowded by the large bulky binaphthyl group (figure 1.13), effectively shielding one facet of approach to the metal. A secondary effect is that axial coordination of donor ligands is also blocked. Substituents at the 3,3' positions of the phenyl rings can shield a second direction of approach, and, if too bulky, overcrowd the already hindered catalytic center. Additionally, substrates are likely to approach over one of the phenyl rings as a consequence of this hindrance.

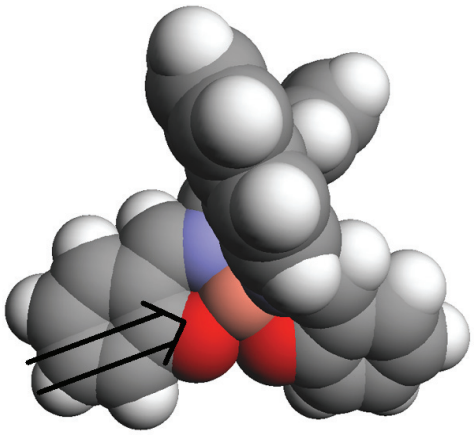


Figure 1.13 Substrate approach path for a binap-M(salen).
(space filling model of **16** is shown)

To obtain a helical binap-M(salen) the same methodology as discussed for the ethylene bridged complexes can be applied, i.e. extension of the ligand arms. This is likely to have several beneficial effects. Foremost, the degree of asymmetry at the metal center is maximized. The interlocking nature of the ligand arms also decreases the amount of conformational freedom available, although the rigidity of the binaphthyl moiety already precludes the formation of secondary conformers.

1.5 Monohelicies

Helical structures are ubiquitous in nature, and have gathered increasing interest as potential scaffolds for chiral catalysis.[34] The majority of studies have focused on helicates;[34,35] metal complexes containing one or more ligand strands and two or more metal centers. Stabilization of the resulting structures is typically facilitated by the multiple interactions (figure 1.14) and/or bonds that are involved. By contrast in monohelicies the overall co-operative forces

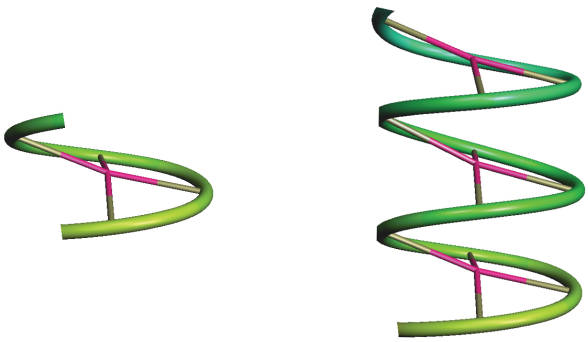
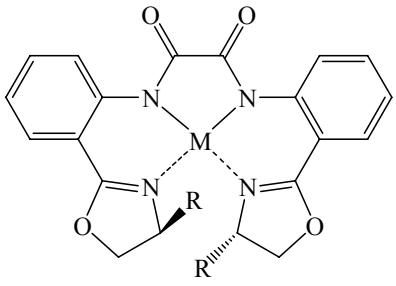


Figure 1.14 Single-stranded monohelical (left) and single-stranded helicate (right) structures.

stabilizing the superstructure are smaller, which can render a helical geometry unfavourable in comparison to other potential conformations. Moreover, if the ligand is flexible bridging across metal centers can occur, leading to dimer and trimer formation.[36] As a result, a variety of different arrangements and geometries are possible, only one of which is desired.

Of the helical complexes that have been studied perhaps the most relevant to this text are those of Pfaltz,[37] who has examined oxalamides **18**-**24** (figure 1.15). Steric repulsion arising



18. R = $CH(CH_3)_2$, M = Cu
19. R = $CH(CH_3)_2$, M = Ni
20. R = $CH(CH_3)_2$, M = Co
21. R = CH_3, M = Co
22. R = $C(CH_3)_3$, M = Co
23. R = Ph, M = Co
24. R = CH_2Ph, M = Co

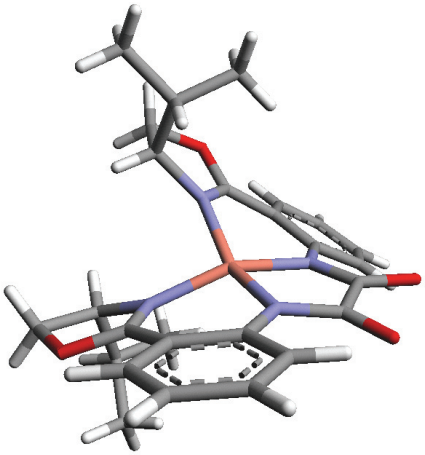
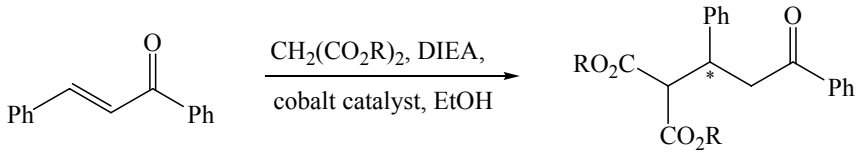


Figure 1.15 Oxalamide complexes of Pfaltz (left) and the crystal structure of **18** (right)

between the chirally substituted oxazoline groups results in adoption of a single monohelical conformer, as confirmed by the crystal structures of **18** and **19**. In the same study, the cobalt analogues **20**-**24** were employed as catalysts for the Michael additions of malonic acid esters to chalcone (figure 1.16). Notably, it was found that if the appended R-groups of the oxalamide



25 **26**

Figure 1.16 Cobalt catalyzed Michael additions of malonates to chalcone

were sterically large, such as in **22**, substantial increases in ee's were observed. A greater degree of selectivity in the substrate approach and orientation is likely occurring in these cases. The R-substituents of the reacting malonate esters also appeared to influence enantioselectivities, but to a lesser extent. In related work Pfaltz used monohelical ruthenium oxalamide complexes to epoxidize *cis*- and *trans*-alkenes.[38] However, oxidative cleavage was a significant problem, affording sizeable quantites of aldehyde by-products.

Other researchers that have worked in this field include Bermejo,[39] Kinoshita,[40] Zhang,[41] and Fabrbrizzi.[42] Bermejo[39] incorporated various transition metals into H_2FTs ligand **27** (figure 1.17), where, in the case of Ni(FTs) exclusively *P*-monohelicies were afforded. The formation from an achiral ligand of solely the *P*-helimeric form was attributed to chiral self-recognition, and subsequent induction during the complexation process. Solution spectroscopic studies suggested that M(FTs) complexes incorporating Cu, Zn, and Cd were also monohelical. Mixed *P*- and *M*-helimer systems formed from achiral ligands have additionally been examined by

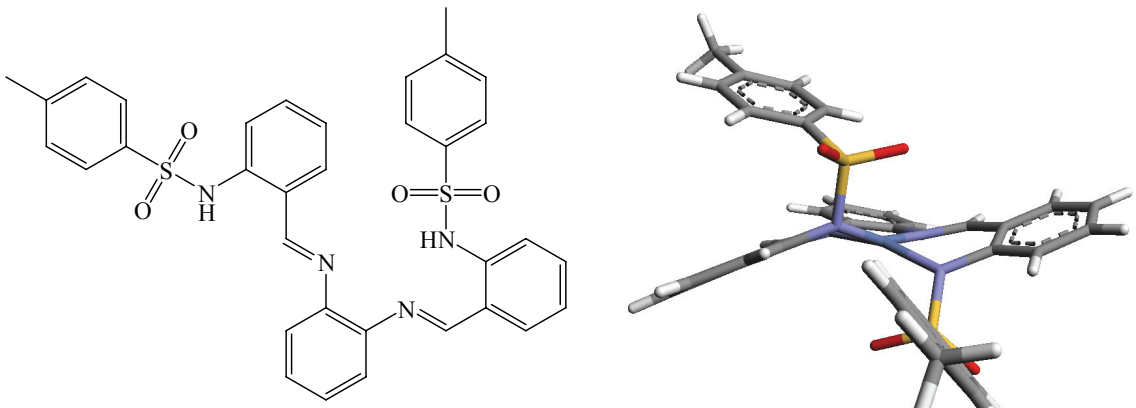


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Figure 1.17 Bermejo's H_2FTs ligand (left) and the structure of Ni(FTs) (right)

Bermejo,[43] but these cannot be used as enantioselective catalysts and so will not be discussed here. In the work of Zhang,[41] chiral titanium(IV) complexes were employed as catalysts for the alkylation of benzaldehyde. Highly stepped helical structures derived from MM2 calculations were used to explain the stereoselectivites encountered, although no crystallographic data to support their interpretations was presented. Fabbrizzi[42] and coworkers in their studies examined the geometries of two enantiomerically related bis-imine bis-quinoline copper complexes. In the

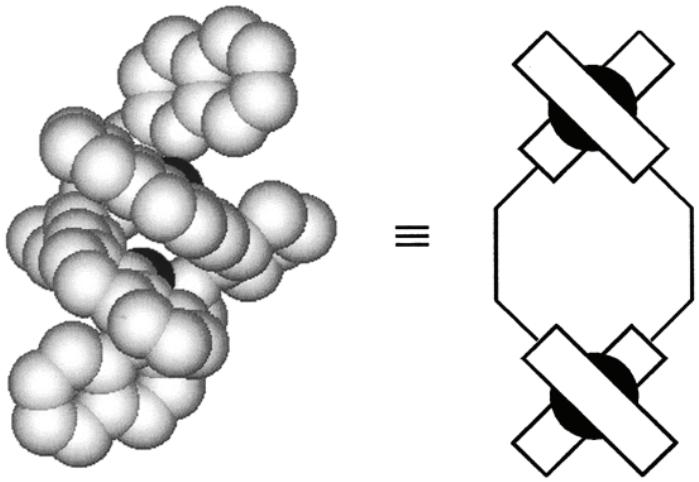

Figure 1.18 *M* handed dinuclear helicate of Fabbrizzi

solid state dinuclear helicates of *M* handedness were afforded from the *R*,*R*-enantiomer (figure 1.18), and ostensibly also in solution, though due to the difficulty inherent in characterizing solution states, here, the degree of certainty was lower. Similarly, the *S*,*S*-enantiomer afforded structures of *P* handedness. More recent studies by Kinoshita[40] probed mononuclear copper(II) complex **28** (figure 1.19). It was found that rapid conversion to a dicopper helicate occurred on the addition of base. Moreover, the process was reversible via HBr addition, with the overall sequence being governed by protonation-deprotonation.

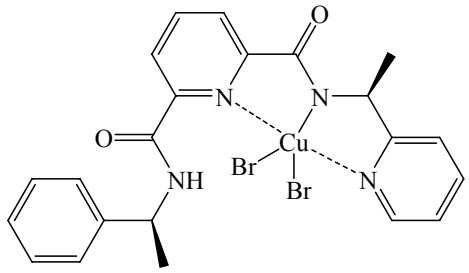

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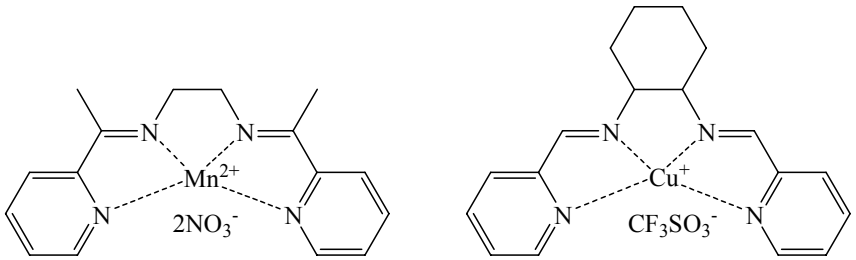
Figure 1.19 Mononuclear H[$CuBr_2$(*S*-PEPDAH]

1.6 Donor Groups and Atoms

The choice of donor groups and metal atom has a profound impact on structure and catalytic activity. For oxidation the electronic character of the ligating groups must be such that high valency intermediates are readily stabilized. If stabilities are low, poor enantioselectivity can result.[44] Anionic phenoxide donors such as those incorporated within salen complexes are useful for this purpose. However, highly stable intermediates may adversely affect reactivity and

turnover numbers, and for alkane hydroxylation it is likely that a high positive charge at the metal center is necessary.[45] Thus in some cases fewer anionic donors may be preferred.

A second major category of tetradentate ligand incorporates donors analogous to pyridine (figure 1.20), and in contrast to the dianionic salen ligands these pyridyl-imine chelates are uncharged. Several problems do exist with this type of complex however. The metal is less



29 **30**

Figure 1.20 Examples of pyridyl-imine complexes

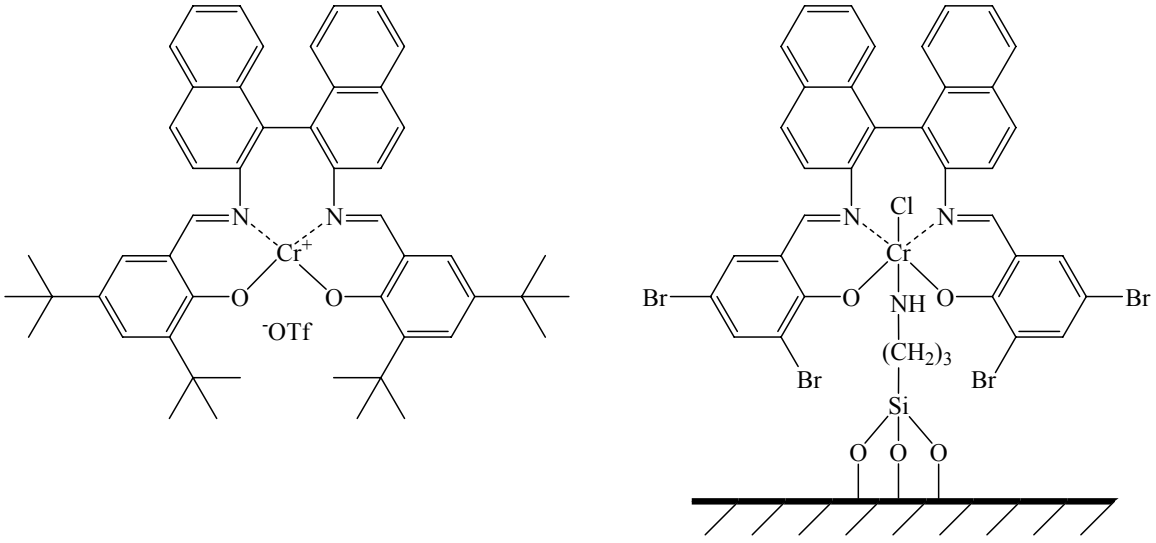
tightly bound, leading potentially to a bound-unbound equilibrium. Moreover, the molecular systems that result have a tendancy to form helicates[46] rather than discrete single complexes, and are significantly more difficult to prepare in a pure form. The analogous binap-M(pyridyl-imine) complexes also suffer from many of the same problems.

The properties of these systems bear some resemblance to that of metallo-salens, for example, the addition of donor ligands to pyridyl-imine catalysts increases conversion and reaction rates, and as with metallo-salens, metal-oxo (M=O) intermediates have been implicated in their usage for catalytic epoxidation.[47] Structurally they also exhibit similarity, one notable difference however is that the ligand arms are held closer to the metal, potentially giving a higher effective chirality at the coordination site.

1.7 Metal Ion Effects

Within the four ligand classes (salen, binap-salen, pyridyl-imine, and binap-pyridyl-imine) a variety of different metals in a range of oxidation states have been incorporated. For salens, manganese(III) has seen the most scrutiny due to the useful epoxidative properties of its complexes.[1] The related nitrogen transfer reaction aziridination has also been studied, and found to be effectively catalyzed by Mn(salen)s.[48] The applicability of any specific metal is highly dependant on the ligand, and as a consequence epoxidation reactions utilizing binap-Mn(salen)s and Mn(pyridyl-imine) complexes have generally yielded poor results.[33,47a,49] With these systems it is likely that the structural and/or electronic requirements for selective catalysis have, as yet, not been met.

To a lesser extent other *d*-block metals such as divalent and trivalent chromium and cobalt have been employed in salen catalysis. Cr(salen)s exhibit many of the same properties as the related manganese complexes and are particularly useful for mechanistic studies.[8] Cr-oxo (Cr=O) adducts unlike their manganese counterparts are isolatable, and so make it possible to more easily study active intermediates. For the related binap-Cr(salen)s few reports detailing their catalytic properties are available, although Diels-Alder and epoxidation reactions have been briefly studied. Rawal[50] has examined a series of related chromium complexes, and found **31** (figure 1.21) to be an effective catalyst for the enantioselective Diels-Alder reactions of 1,2-dihydropyridine, while in the work of Che[51] polymer supported complex **32** epoxidized alkenes with moderate stereoselectivity. To date, no studies on the properties of Cr(pyridyl-imine) and binap-Cr(pyridyl-imine) complexes have been reported.



31 **32**

Figure 1.21 Chromium catalysts for Diels-Alder (left) and epoxidation (right) reactions

In Co(salen) chemistry the ability to bind and activate molecular oxygen is perhaps the most important aspect, and has afforded an atom efficient method for the regioselective oxidation of phenols,[52] indoles,[53] and conjugated amines.[54] A square planar geometry is necessary to provide the appropriate electronic configuration for oxygen binding, hence binap-Co(salen) and binap-Co(pyridyl-imine) complexes do not exhibit this interesting property. Similar to Co(salen)s, square planar Co(pyridyl-imine) complexes can bind and utilize molecular oxygen.[47c,55] This process has been examined in detail by Iqbal and co-workers.[55] Their studies implicated a cobalt(IV)-oxo complex as the main oxidant species, although peroxide anion and peracid intermediates were proposed for oxygenations employing Co(pyridyl-imine) catalysts (figure 1.22). Not surprisingly Co(salen) complexes have seen the most use in this respect, and have subsequently been applied to the catalysis of other reaction types, such as the ring opening of epoxides[56] and cyclopropanation.[57]

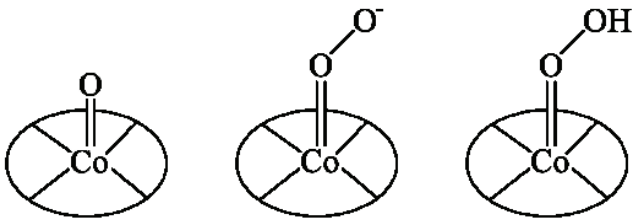


Figure 1.22 Oxo, peroxide anion, and peracid intermediates of cobalt oxygenation reactions

Of the remaining *d*-block metals iron is perhaps the most attractive for catalysis due to its significant abundance, low cost, and often high catalytic activity. Few catalytic applications using Fe(salen)s have been reported, although a large volume of literature is available on structural, electronic, and spectroscopic properties. Bryliakov has investigated the asymmetric oxidation of sulfides using Fe^{III}(salen)s.[58] Conversion rates to the corresponding sulfoxides were high, albeit with moderate stereoselectivity. Over oxidation to sulfones was in general minimal. The non-asymmetric version of this reaction has also been examined.[59] Other oxidative studies include those of Kobayashi,[60] who has employed Fe^{III}(salen) complexes in the preparation of phenolic polymers. Industrially this process requires the use of formaldehyde, a probable carcinogen, and consequently cleaner alternate methods are required. By employing Fe^{III}(salen) catalysts hydrogen peroxide can act as the oxidant, so that the need for formaldehyde is negated. The related Fe^{II}(salen)s have also seen some use in catalysis,[61] but their application has been hindered by the relative ease with which inactive μ-oxo dimers are formed.[61b,62] In the studies of Nguyen[61b] this problem was circumvented via *in situ* reduction of dimeric [Fe^{III}(salen)$_2$O] to the active Fe^{II}(salen) complex. The general applicability of this method to catalysis however is not known. With regards to the other ligand types under discussion within this text, binap-Fe(salen) and Fe(pyridyl-imine) complexes have been briefly examined catalytically. In the work of

Labinger[63] a binap-Fe(salen) was found to be inactive for hydrocarbon hydroxylation, while Agarwal[64] has studied the epoxidation of cyclic alkenes using a Fe(pyridyl-imine) catalyst.

1.8 Design Considerations

For the preparation of a monohelical salen or related monohelical complex it is desirable that certain criteria be met. Primarily, the ligand should incorporate groups that predispose the structure towards helix formation. This requirement can be partially fulfilled through the use of a chirally directing backbone, to provide a sense of 'handedness' or 'twist'. If at the same time the backbone group is relatively inflexible, the probability that unwanted arrangements and geometries will form is decreased. It is also desirable that sterically large ligand arms be employed, so as to yield slightly over one helical turn (see figure 1.14), in effect 'locking' the structure. Aryl rings typically comprise the arms of salen complexes, consequently this objective can be accomplished through either replacement with extended polyaromatic ring systems, and/or by appending on the appropriate substituents. Saturated rings are unattractive for use in

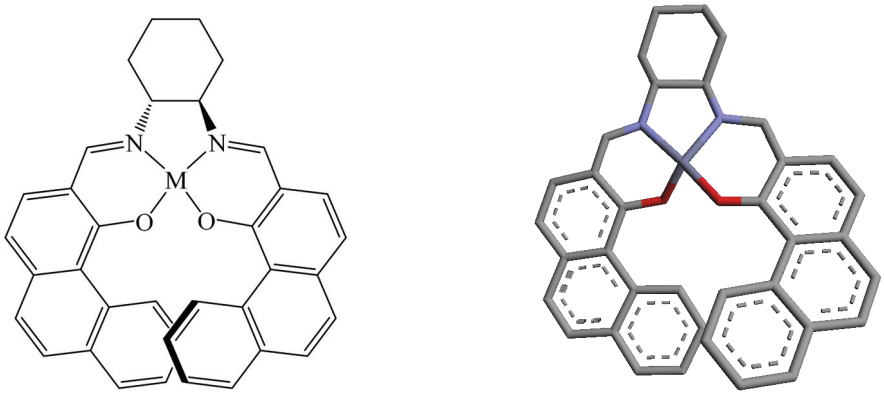
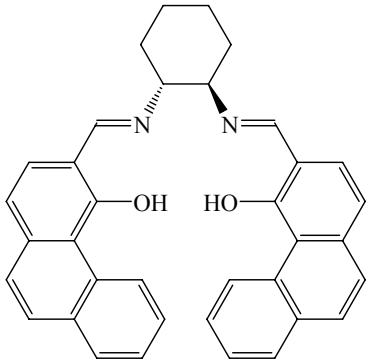


Figure 1.23 Idealized representations of a 'locked' helical salen

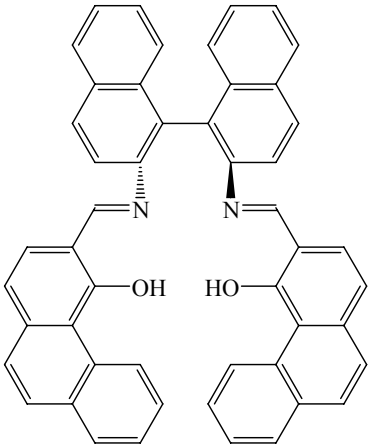
this respect due to their innate flexibility, and to the conformational mobility that subsequently results. Modeling studies indicate that both methodologies are feasible and that for polyaromatic arms, nonlinear, i..e curved polyaromatics, are required for the adoption of a 'locked' helix (figure 1.23). Additionally, if the second approach is to be followed, the appended substituents must be positioned on the inward side of the ligand arms close to the donor atoms, for 'locking' to take place.

In addition to the ligand, the metal must also be carefully selected. In this work there are three main considerations for the choice of metal; ease of characterization, ease of handling, and potential for high catalytic activity. Zinc(II) complexes are diamagnetic and so can be readily characterized via ^{1}H NMR spectroscopy. Furthermore, they are typically stable to air and consequently meet the second requirement also. For high catalytic activity potential metals include divalent and trivalent cobalt, iron, and manganese, where, in the context of salen and pyridyl-imine catalysis iron is the least studied. For metals in the 2+ oxidation state no counterions are present when two anionic donors are employed, as in M(salen) and M(binap-salen) complexes. Counterions can play a role if the metal has a 3+ or higher charge, or if the ligand incorporates less than two of these donors. The choice of counterion largely depends upon ligating ability, and on the electronic influence that strong/weak coordination exerts upon the metal. Typically, Cl^{-}, PF_6^{-}, BF_4^{-}, and ^{-}OTf are utilized as counterions.

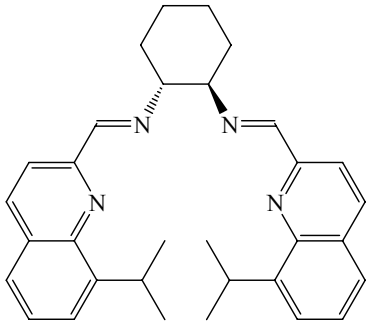
With the above considerations in mind it was decided to first prepare and examine (*R,R*)-**33** - (*R*)-**36** (figure 1.24), where iron and zinc were the metals to be incorporated. On the basis of the ensuing results, (*R,R*)-**37** and (*R*)-**38** were then investigated. In the following chapters this work is discussed.



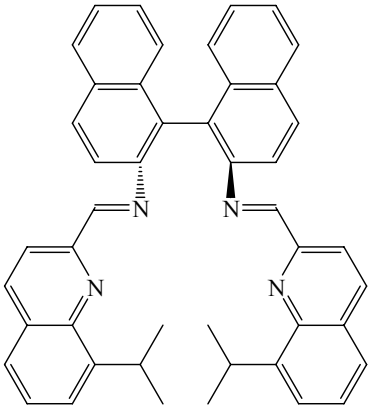
(*R,R*)-**33**



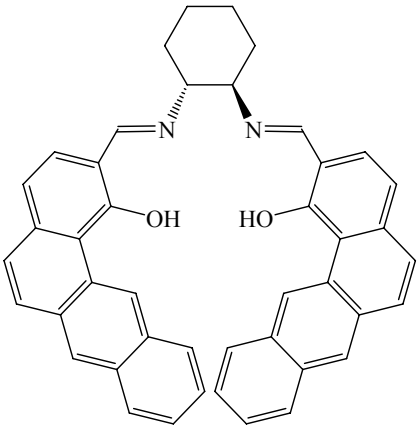
(*R*)-**34**



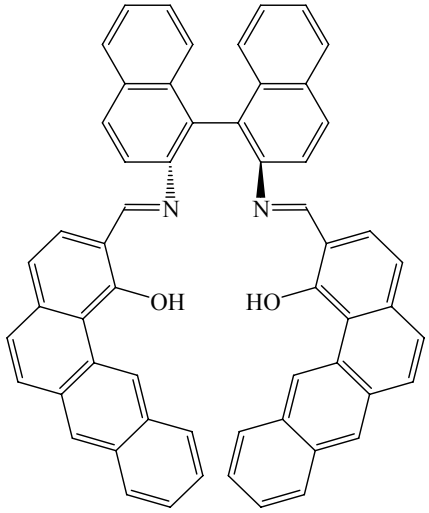
(*R,R*)-**35**



(*R*)-**36**



(*R,R*)-**37**



(*R*)-**38**

Figure 1.24 General structures of the ligands

CHAPTER 2

Synthesis, Characterization, and Study of Phenanthryl Derived Complexes

2.1 Synthesis

There are two steps almost universal to the preparation of a salen or related bis-imine containing complex (figure 2.1). The first involves condensation of a diamine with an appropriate aromatic aldehyde to afford the ligand. In the second, metallation provides the complex. This, of course, requires that the diamine and aldehyde be available, which, for many

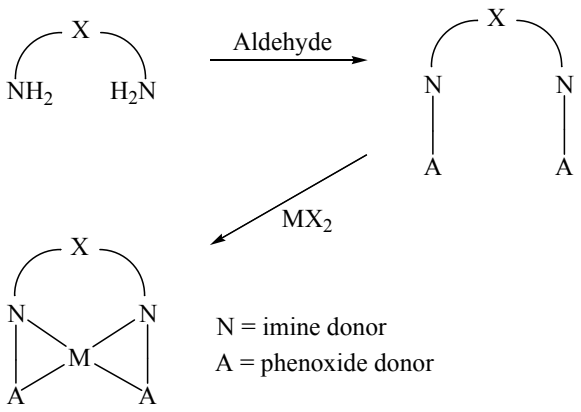


Figure 2.1 General methodology for complex formation

simple salens can be obtained from commercial sources. With regards to this work, the aldehydes (figure 2.2) although seemingly simple, are of sufficiently high complexity that they must instead be prepared. Nor, for these, do well established literature preparations exist. The chiral diamines, (1*R*,2*R*)-1,2-cyclohexanediamine (*R,R*)-**39** and (*R*)-[1,1'- binaphthalene]-2,2'-

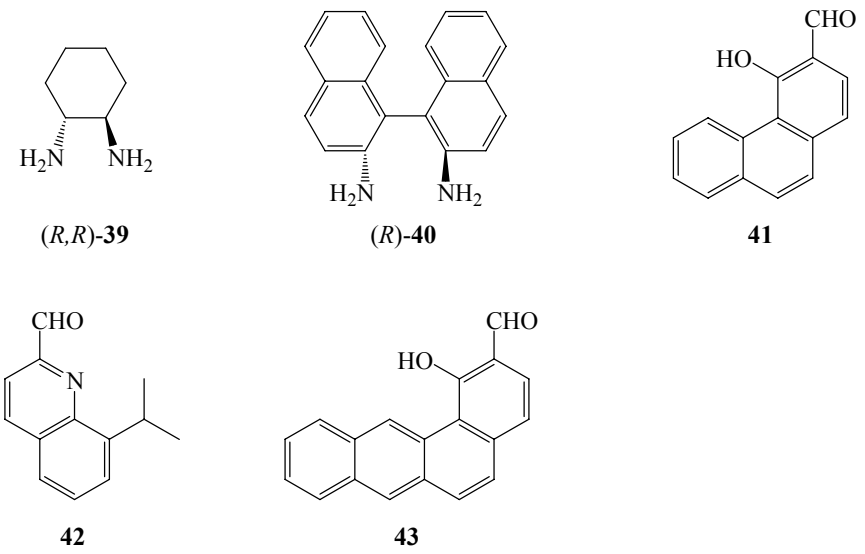


Figure 2.2 Synthetic precursors

diamine (*R*)-**40** are commercially available, but their cost, and the need for multi-gram quantities renders their synthesis necessary. (*R,R*)-**39** can be readily prepared via the procedure of Jacobsen.[65] Likewise, diamine (*R*)-**40** can be prepared via known methods.[66] As the syntheses of (*R,R*)-**39** and (*R*)-**40** are well documented in the literature and relatively straightforward, no further synthetic discussion of them will be made here. The (*S*)-enantiomeric forms of **39** and **40** can also be made via the above literature methods. The preparation of **42** and **43** will be included in later chapters.

To synthesize aldehyde **41**, naphthalene was employed as the starting reagent (figure 2.3). $AlCl_3$ catalyzed Friedel-Crafts acylation of **44** with succinic anhydride gave an approximately equal mixture of two regioisomers, **46** and **47**. Separation via established procedures[67] although yielding both compounds in high purity required multiple steps, thus an alternate purification route was desired. The discovery that **46** had considerably higher solubility in hot benzene than the sought after regiomer, **47**, allowed for facile separation of the two. In the next step conversion of the ketone moiety of **47** to a methylene via Wolf-Kishner reduction,[68]

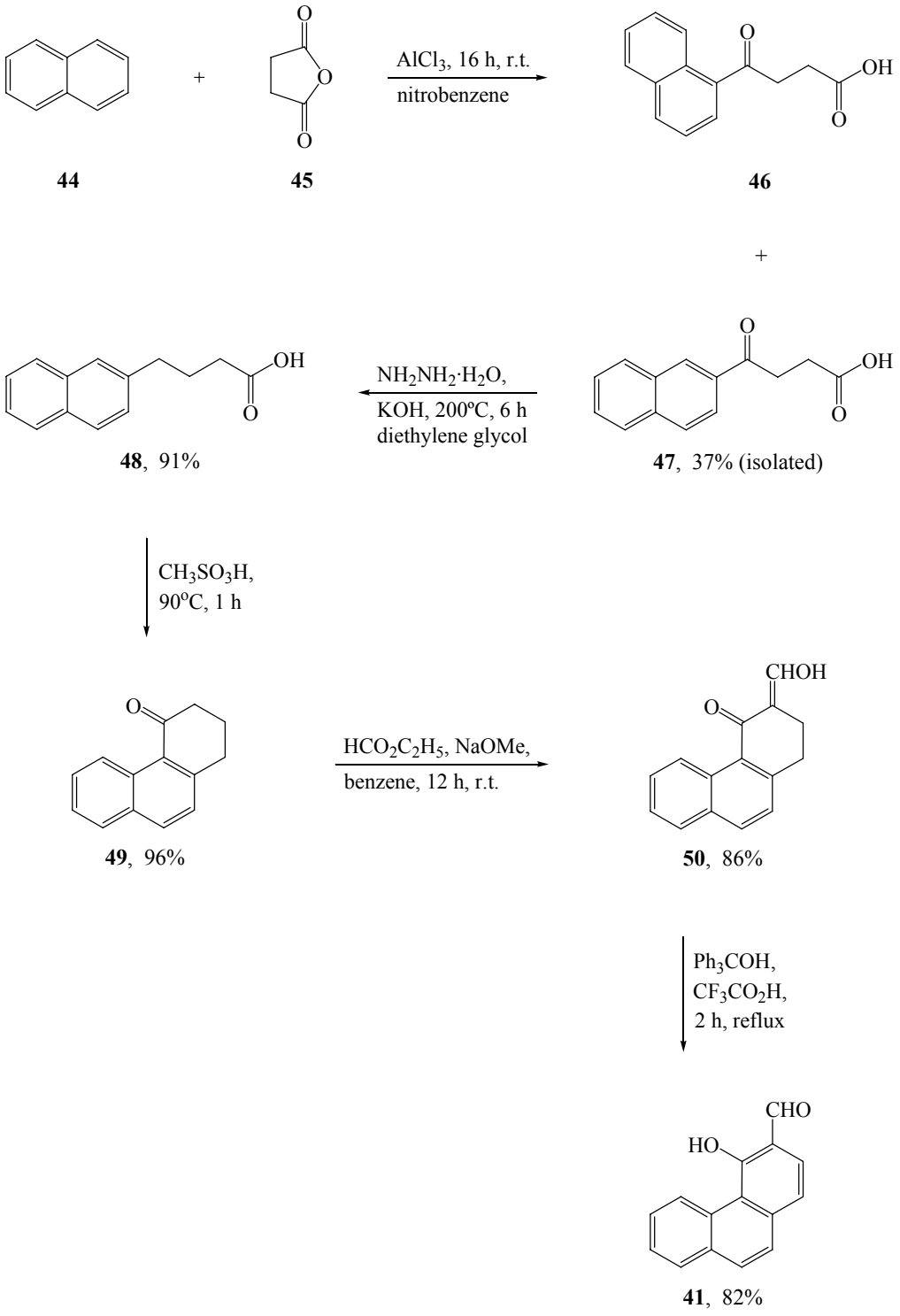
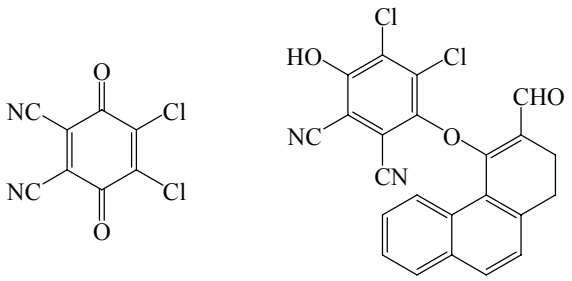


Figure 2.3 Synthesis of 4-hydroxy-3-phenanthrenecarboxaldehyde, **41**

afforded **48** in high yield. Indicative of its formation was the evolution of gas (N_2) during the reaction, and the appearance of a third multiplet in the ^{1}H NMR spectrum, due to the additional aliphatic protons. Cyclization of **48** catalyzed by methanesulfonic acid gave ketone **49**.[69] Ring closure with attack at the 1 position to furnish the 1,2-fused heterocycle, is kinetically favored with respect to cyclization across the 2-3 positions. Consequently, only minimal traces of the linear side-product formed, rendering the need for complicated purification measures unnecessary. In the second to last step **49** was condensed under basic conditions with ethyl formate to give **50**.[70] Initial attempts to oxidize **50** to **41** employed 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) as a stoichometric oxidant, however the highest obtainable yield was 42%.[70] ^{1}H NMR analysis of the reaction mixture indicated that to a large extent, **50** was converted to a single by-product, **52** (figure 2.4). Notable in the spectrum were two methylene triplets at 2.80 and 3.40 ppm, and an aldehyde singlet at 10.08 ppm. This was in addition to characteristic phenolic and aldehyde hydrogen signals at 10.05 and 15.04 ppm arising from the desired product. Although complete characterization of the impurity was not undertaken, isolation and analysis suggested it to be DDQ addition product **52**. The occurrence of cyano and hydroxyl bands in the IR spectrum confirmed the presence of the DDQ moiety. The ability of this to form addition products via one of its oxygen atoms has been documented in the

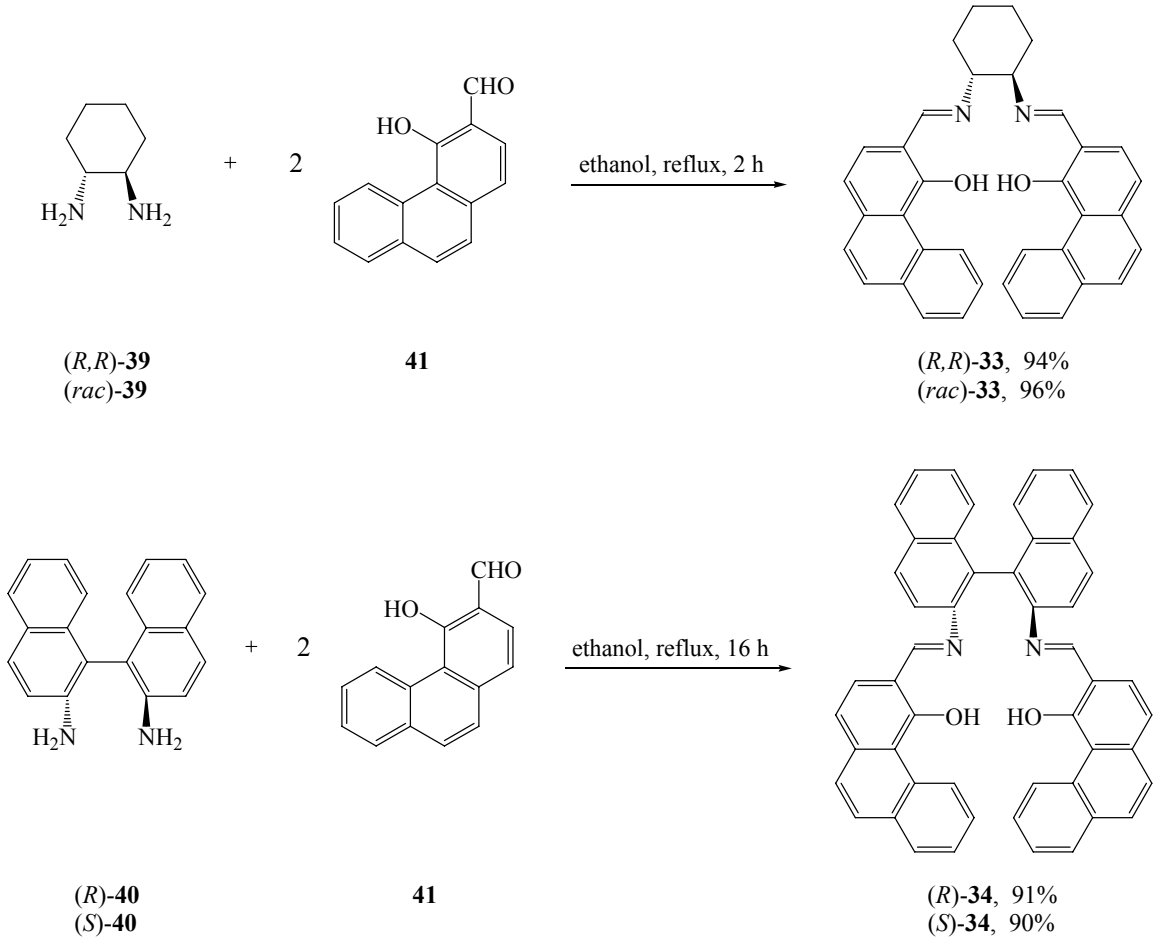


51 **52**

Figure 2.4 Structure of DDQ and of the proposed by-product

literature.[71] It was necessary therefore to find an alternate method, and for this reason we examined the use of triphenyl-methanol in trifluoroacetic acid (TFA), a protocol that has previously been applied to polycyclic aryl oxidiations.[72] The *in situ* generated trityl cations afforded conversion of **50** to **41** in 82% yield, and 23% over the five steps.

With the synthesis of the ligand arm completed, the chiral diamines (*R,R*)-**39** and (*R*)-**40**, were independently condensed with **41** in refluxing ethanol (figure 2.5). Utilizing the same



(*R,R*)-**39**
(*rac*)-**39**

41

(*R,R*)-**33**, 94%
(*rac*)-**33**, 96%

(*R*)-**40**
(*S*)-**40**

41

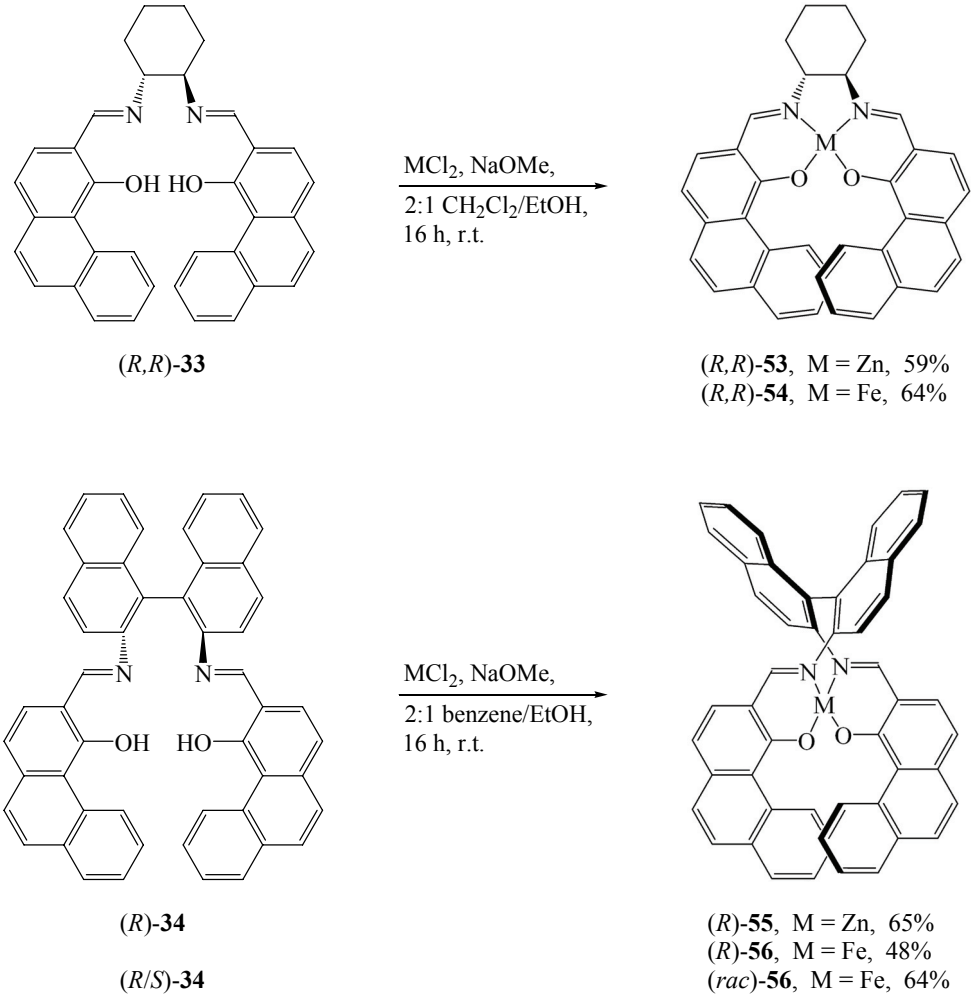
(*R*)-**34**, 91%
(*S*)-**34**, 90%

Figure 2.5 Ligand preparation

methodology (*rac*)-**33** (racemic, trans **33**), and enantiomerically pure (*S*)-**34** were also prepared. The formation of the Schiff bases is thermodynamically favored, and hence anhydrous forcing

conditions were not required. Longer reaction times were necessary with respect to condensation of (*R*)-**40** and (*S*)-**40** with **41**. This presumably results from the emergence of steric crowding on production of the mono-imine. Indeed, ^{1}H NMR spectroscopy suggests that the mono-imine is completely formed within the first two hours, whereas attachment of the second ligand 'arm' is considerably slower.

Metallation of salens typically requires that phenolic donor groups be deprotonated, and this is the case with (*R,R*)-**33**, and (*R*)- and (*S*)-**34** (figure 2.6). In attempting to incorporate zinc



(*R,R*)-**33**

(*R,R*)-**53**, M = Zn, 59%
(*R,R*)-**54**, M = Fe, 64%

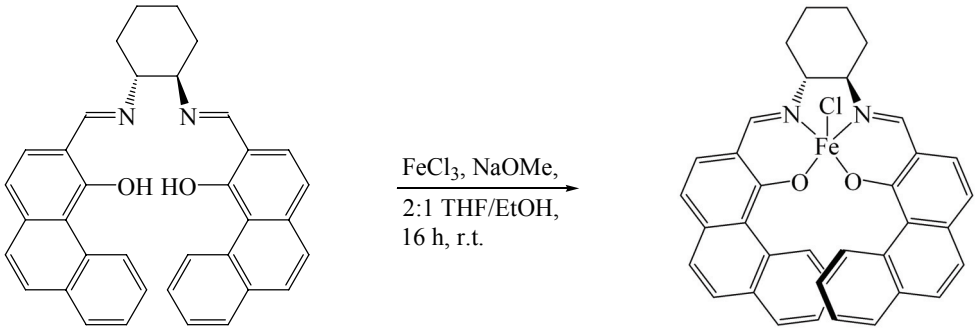
(*R*)-**34**

(*R*/*S*)-**34**

(*R*)-**55**, M = Zn, 65%
(*R*)-**56**, M = Fe, 48%
(*rac*)-**56**, M = Fe, 64%

Figure 2.6 Synthesis of Zn(II) and Fe(II) complexes

into (*R,R*)-**33** in the absence of base, only starting reagents were recovered. The addition of triethylamine gave the desired product, however removal of all traces of triethylamine and its hydrochloride salt proved difficult. The subsequent use of sodium methoxide enabled easier purification via filtration protocols, as the afforded neutralization products were methanol and insoluble sodium chloride. A polar/non-polar solvent mixture, for example, ethanol and THF, was also utilized. Their application was necessary to enhance the solubility, and consequently the reactivity, of the dianionic sodium salts of (*R,R*)-**33**, and (*R*)- and (*S*)-**34**.



(*R,R*)-**33** (*R,R*)-**57**, 24%

Figure 2.7 Fe^{III}(salen) preparation

In a manner similar to the synthesis of (*R,R*)-**53**, the iron(III) complex (*R,R*)-**57** was prepared (figure 2.7). A higher oxidation state affords a more closely bound metal that may increase the degree of ligand arm overlap, and (*R,R*)-**57** is therefore of interest. Curiously, the solubility of this complex in common organic solvents was substantially less than that of (*R,R*)-**54**, despite their almost identical structures. We attribute this difference to the loss of the solvent coordination site, which in (*R,R*)-**57** is occupied by a chloride moiety. Moreover, due to the lower solubility difficulties were encountered in the purification step. It proved necessary to use a large volume of THF to dissolve the complex prior to filtration, and even so, much of the

product remained unsolvated. This resulted in only partial product separation, and a low isolated yield.

2.2 NMR Spectroscopy of the Ligands & Diamagnetic Zinc Complexes

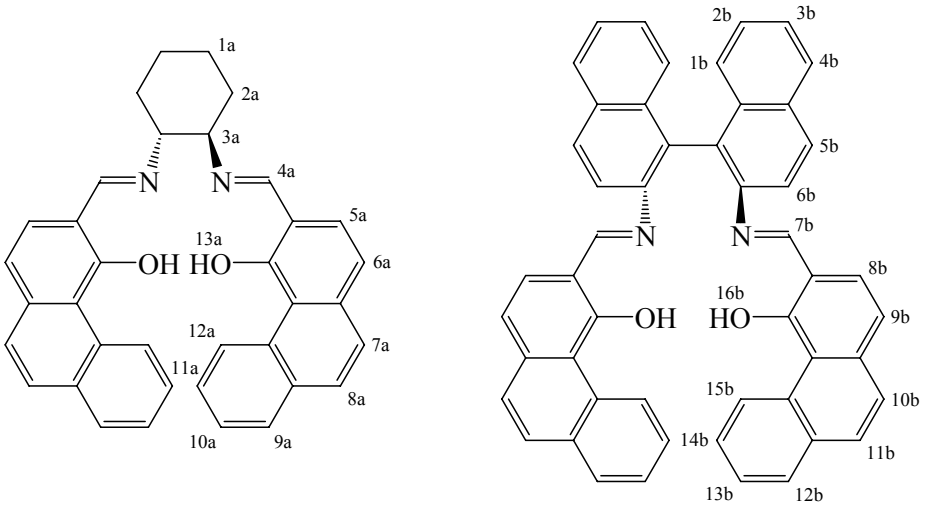
With the synthetic steps completed, ^{1}H and ^{13}C NMR spectroscopy were employed to characterize the prepared substances. Table 2.1 lists the ^{1}H NMR chemical shifts of the ligands and diamagnetic zinc(II) complexes. Absolute assignment of all signals was not attempted due to the intricacy of the spectrum, although those readily identifiable were assigned. The ^{13}C NMR spectrum are not included here due to the little additional structural/electronic information yielded by their analysis. For all compounds a single set of proton resonances was observed, suggesting the existence of only one discrete species in solution, and the absence of dinuclear

Table 2.1 Ligand and Zn(II) complex ^{1}H NMR chemical shifts[a]

	Chemical shifts, $\delta(^{3}J,^{4}J)$			
	Imine C─H	O··H··N	Aliphatic C─H	Aromatic C─H
(*R,R*)-**33**[b]	8.61(4.3)	15.97	1.34-1.50, 1.66-1.82, 2.02-2.13, 3.53-3.65	7.11(8.3), 7.32(8.3), 7.60-7.66, 7.77-7.83, 7.86(8.7), 7.96(7.9,1.3), 10.61(8.7)
(*R*)-**34**[c]	8.80	15.19		7.16(8.2), 7.25(8.2), 7.38-7.43, 7.50-7.60, 7.64-7.69, 7.75(8.6), 7.81-7.85, 8.12(8.2), 8.24(8.8), 9.44(8.6)
(*R,R*)-**53**[b]	8.63		1.20-1.34, 1.79, 2.31, 3.22	7.30(8.2), 7.57-7.66, 7.80-7.87, 7.96(8.6), 8.01(7.9), 11.79(8.5)
(*R*)-**55**[c]	8.57			6.95(8.5), 7.08(8.3), 7.21-7.26, 7.40-7.52, 7.60(8.7), 7.83-7.88, 7.90(8.2), 8.03(8.6), 10.50-10.56

[a]Since (*R*)- and (*S*)-enantiomers and their admixtures have identical spectra, only the data for the (*R*)-enantiomer is included. For (*rac*)-**33** and (*S*)-**34** see the relevant (*R*)-enantiomer chemical shifts. [b]Taken in pyridine-d_5. [c]Taken in $CDCl_3$.

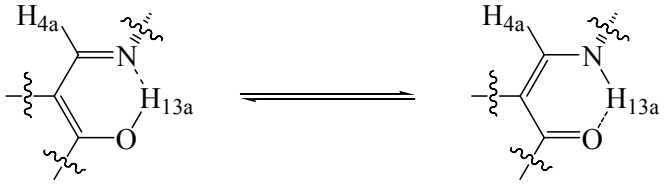
complexes (helicates) in the case of the zinc salens. The cyclohexyl proton signals of (*R,R*)-**33** and (*R,R*)-**53** exhibited some slight line broadening, this however is likely a result of minor ring fluctuations rather than the presence of multiple conformers. The number of resonances was half that possible in total, as is expected for C_2 symmetric molecules.



(*R,R*)-**33** (*R*)-**34**

Figure 2.8 Atom numbering

Notable at low field were the 15.97 and 15.19 ppm signals of (*R,R*)-**33** and (*R*)-**34**. These can be assigned respectively to H_{13a} and H_{16b} (figure 2.8), which on the NMR time scale are each observed as an average of two hydrogen bonded structures (figure 2.9). The far downfield shift



enol-imine *keto-amine*

Figure 2.9 Ligand tautomerism in (*R,R*)-**33**

seen is typical of intramolecularly H-bonded protons.[73] Similarly, at 8.61 and 8.80 ppm are bands that respectively correspond to the averaged H_{4a} and H_{7b} resonances. In the complexes (*R,R*)-**53** and (*R*)-**55** this tautomeric process cannot occur, and as such the 8.63 and 8.57 ppm signals, arise solely from H_{4a}/H_{7b} of the enol-imine tautomer.

Upon metallation of (*R,R*)-**33**, small to moderate (±0.2-0.5 ppm) shifts were apparent for the aliphatic proton signals of C_1, C_2, and C_3. Since, zinc cannot appreciably influence $H_{1ax/eq}$ and $H_{2ax/eq}$ over the distances involved, via inductive electron withdrawal, it is likely that the movement of these signals arises predominantly through conformational changes. In particular, the imine substituents are forced into equatorial positions by coordination, barring formation of the diaxial conformer. The minor ring perturbations that typically occur in flexible cyclohexyl systems, will also to some extent be inhibited. For the resonances in the aromatic region most undergo a downfield shift, indicating that the electropositive zinc exerts a deshielding influence. The aromatic protons in closest proximity to the coordinated metal appear to be affected the most, with H_{12a} particularly deshielded, and moved downfield by 1.18 ppm to 11.79 ppm. Though, as H_{12a} lies in the deshielding zone of the neighboring phenanthryl arm, this will be an additional factor contributing to the shift.

In the case of (*R*)-**34** the majority of signals are moved upfield on metallation. The sole exception is H_{15b}, which is shifted downfield by 1.06 ppm. This differentiation from the remaining signals likely relates to the through-space proximity of H_{15b} to the metal center, although induction and other processes (see discussion of H_{12a}) will also influence the resonance frequency. Regarding the general upfield movement that occurs, the cause most probably arises from reduced delocalization in the ligand framework, engendered by complexation (figure 2.17

& 2.18). Che[30] and Meunier[49] have documented the same effect for related M(binap-salen) complexes. They gave no explanation for the trend however.

2.3 NMR Spectroscopy of the Paramagnetic Iron Complexes

The ^{1}H NMR spectra of the iron complexes (*R,R*)-**54**, (*R*)-**56** and (*R,R*)-**57** were collected. The data is listed in table 2.2 (see fig 2.10 also). Iron(II) and iron(III) respectively have d^6 and d^5 electronic configurations, and often form complexes that are paramagnetic. As a consequence,

Table 2.2 Fe(II) & Fe(III) complex ^{1}H NMR chemical shifts

	Chemical shifts, δ
(*R,R*)-**54**[a]	−25.11, −11.69, −4.80, −3.28, 1.66, 5.26, 10.13, 10.90, 17.14, 24.61, 40.42
(*R*)-**56**[b]	−39.04, −15.27, −9.23, −7.60, 0.56, 1.28, 10.68, 11.68, 12.08, 13.71, 15.29 24.52, 60.63
(*R,R*)-**57**[c]	−36-−31, −30-−25, −1.6-−0.5, 1.0-1.8, 1.26, 3.17, 4.10, 5.35, 5.98, 6.80-7.80, 7.90-8.90, 9.40-15.60, 19-24, 26-32, 33-37, 49-56

[a]Taken in pyridine-d_5. [b]Taken in CD_2Cl_2. [c]Taken in DMSO-d_6.

large linewidths may result affording ^{1}H NMR signals that are broad and of low intensity. Furthermore, due to the large magnetic moment of the unpaired electrons, the signals are frequently shifted to regions outside of the normal diamagnetic range. Complete assignment of the proton spectrum is therefore difficult, although for the Fe(II) complexes included here, partial assignments were still possible. For our attempts to collect useful ^{13}C NMR data, the acquired spectra contained no discernable signals, a result which we ascribe to the paramagnetism.

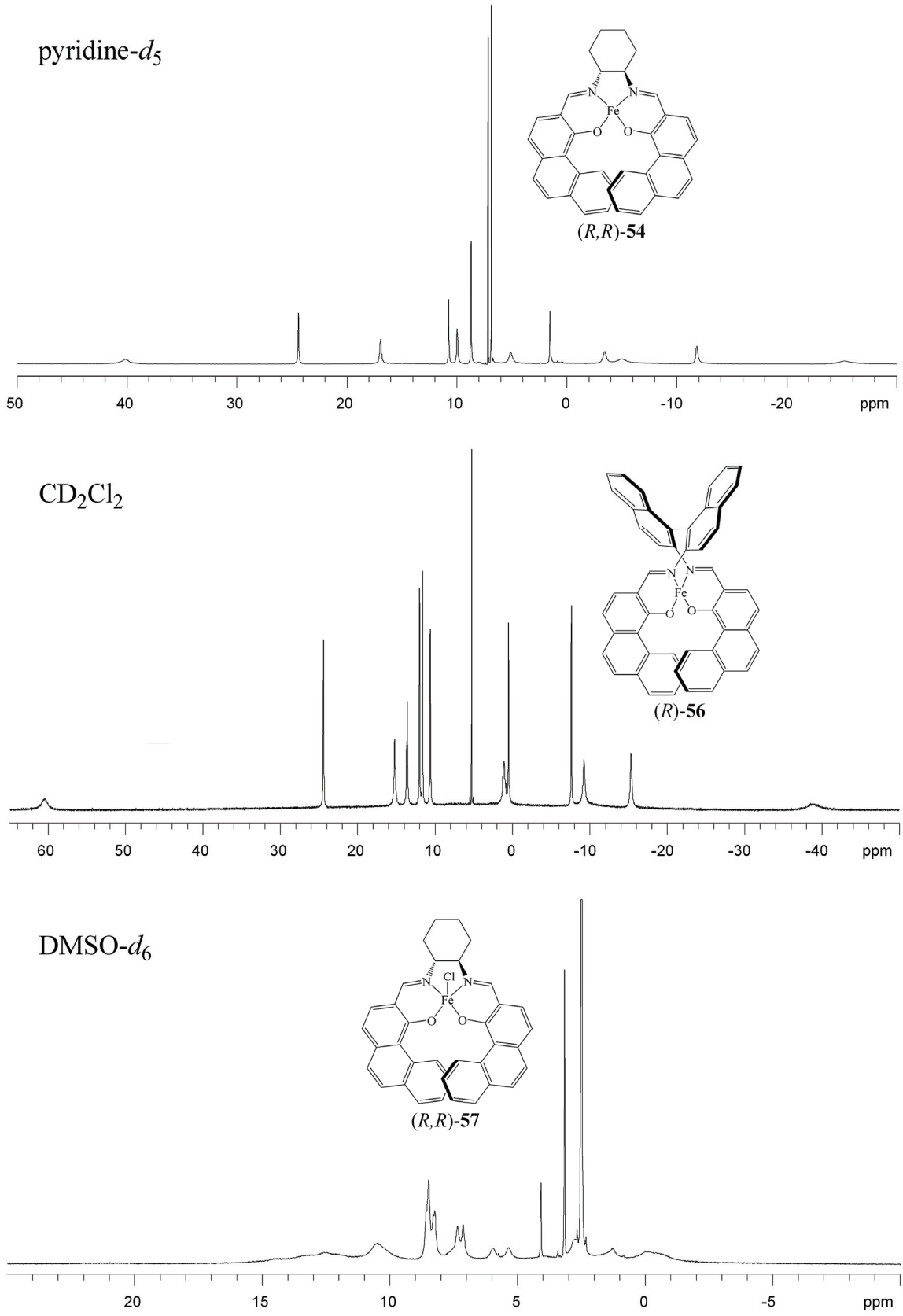


Figure 2.10 400MHz ^{1}H NMR spectra of (*R*,*R*)-**54**, (*R*)-**56** and (*R*,*R*)-**57**

The degree of line broadening for paramagnetic molecules predominately depends upon the electronic relaxation time, which for the unpaired spin states of Fe(II) is relatively short.[74] This leads to a low rate of nuclear relaxation, and correspondingly sharp signals in the spectra of (*R,R*)-**54** and (*R*)-**56**. The separation between the metal center and the resonating nuclei is also a factor, as the through-space (dipolar relaxation) and through-bond (contact relaxation) mechanisms that transmit spin information attenuate on distance. Hence the signals resulting from protons in close proximity are broadened to the greatest extent, where the more powerful dipolar relaxation mechanism will predominate. It is therefore likely that the broad signals of (*R,R*)-**54** at ⁻25.11, ⁻4.80, and 40.42 ppm are due to the H_{3a}, H_{4a} and H_{12a} resonances. Furthermore, in analogy**,** the ⁻39.04 and 60.63 ppm signals of (*R*)-**56** can be attributed to H_{7b} and H_{15b}. In both complexes the smaller linewidth signals are afforded by more distantly located nuclei.

Regarding the chemical shifts of (*R,R*)-**54** and (*R*)-**56**, their distribution pattern indicates that a spin polarization pathway is in operation, involving significant delocalization of unpaired spin density across the π orbital framework.[75] This leads to a series of alternating upfield and downfield shifted signals for protons on adjacent carbons. Unfortunately, the degree of shift is dependant upon the spin density localized onto each individual carbon atom, which cannot be easily predicted. It is generally true however that the lower the number of intervening bonds the greater the spin density, and therefore the larger the size of the shift.

For an iron(III) complex such as (*R,R*)-**57** three major spin configurations exist, with d^5 occupancy affording the possibility of either a high, intermediate, or low spin system. In high and intermediate spin complexes nuclear relaxation is rapid, resulting in extremely broad ^{1}H NMR signals for the most affected protons, i.e. those with short through-bond and through-space

proton-metal distances. A general examination of the spectrum of (*R,R*)-**57** indicates the presence of such spectral features, where between ⁻2 and 16 ppm a number of low-intensity high-linewidth bands are apparent. In addition, signals may lie outside of this range that are broadened beyond detection. The same distance mechanisms that were previously discussed apply here, influencing the linewidth size and chemical shifts. With regards to signal assignment, due to the extreme broadness no attempt was made.

2.4 Structural Studies of the M(salen) Ligands and Complexes

Single crystals suitable for X-ray analysis were grown of (*rac*)-**33**, and of the metallation products (*R,R*)-**53**, (*R,R*)-**54**, and (*R,R*)-**57**. Table 2.3 lists for each substance the solvents and methodology ultimately employed for crystallization. Enantiopure (*R,R*)-**33** gave only poly-

Table 2.3 Crystal growth conditions

	Method	Solvent A	Solvent B
(*rac*)-**33**	Diffusion	Methylene chloride	Hexanes
(*R,R*)-**53**	Slow cooling	Pyridine	
(*R,R*)-**54**	Diffusion	Pyridine	Methanol
(*R,R*)-**57**	Diffusion	Methylene chloride	Diethyl ether

crystalline material, and consequently the racemic ligand (*rac*)-**33** was utilized to prepare crystals of suitable quality. In those instances where a combination of solvents was employed, the compound was first dissolved into solvent A, and into this solvent B was then allowed to slowly diffuse. For more detailed information see the experimental section and appendix III.

In the crystal structure of (*rac*)-**33** each enantiomer adopts two distinct spatial arrangements, with the difference primarily arising due to rotation about the N–C single bonds. The geometries corresponding to the *R*,*R*-enantiomer are shown in figure 2.11, and relate to those of the *S*,*S*-configuration (not shown) as object to mirror image. Two phenanthryl group

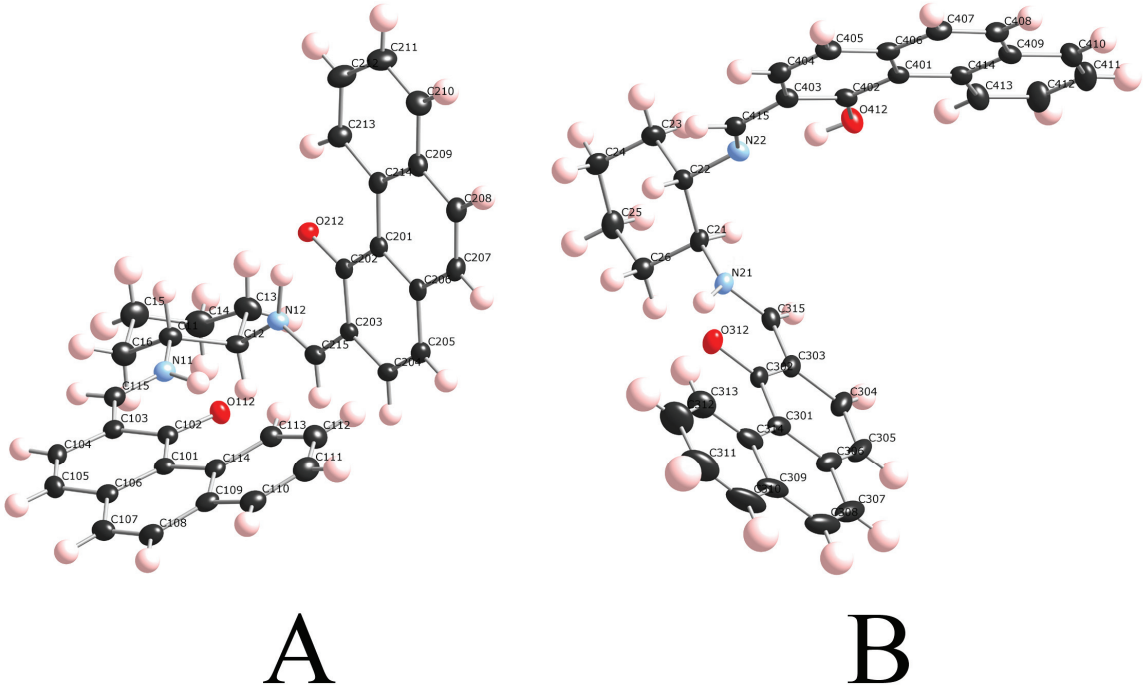


Figure 2.11 Thermal ellipsoid plots (50% probability) of *R*,*R*-**33** from (*rac*)-**33**

orientations exist within each enantiomeric A and B unit, where, the ligand arm is either perpendicular to the plane of the cyclohexyl ring, or orientated almost parallel. In all cases the imine moieties are coplanar with respect to the phenanthryl substituents, indicative of extended conjugation. The two structures also differ from one another in that they are tautomers, **A** incorporates two N–H groups, while **B** incorporates one N–H and one O–H group. The proximity of the imine nitrogen and the phenolic oxygen appears to facilitate rapid enol-imine to

keto-amine interconversion (and vice versa), as is shown in figure 2.9. The occurrence of such exchange processes is well documented in the literature for related phenolic imines.[73,76]

Metallation of (*R*,*R*)-**33** with Fe(II) and Zn(II) affords complexes that have almost identical molecular geometries, with only minimal differences between their respective atom positions (see figure 2.13). Moreover, both crystal structures contain a 1:1 mixture of *P*- and *M*-helimers that have the same orientation relative to each other, in addition to the same general unit cell packing. For the two helimers of each compound, the core difference lies in the spatial relationship between the phenanthryl moieties, and arises mainly from small variations in the

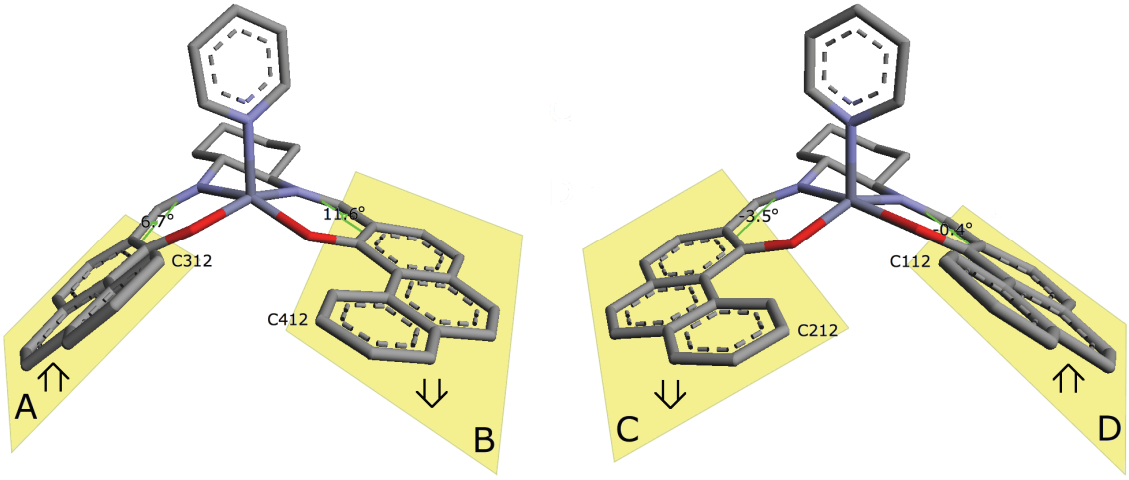


Figure 2.12 A comparison of the *P*- (left) and *M*-helimers (right) of (*R*,*R*)-**53**·py

N=C–C=C torsion angles. Evident in (*R*,*R*)-**53**·py, for example, from the *M* to the *P* form is a torsional angle increase from -3.5(8)° to 6.7(8)°, and from -0.4(9)° to 11.6(8)° (figure 2.12). A more positive value equates to an anticlockwise rotation of the ligand arms, and thus from *M* to *P*, to a decrease in the upward inclination of the 'right' phenanthryl group, and an increase in that of the 'left'. The differences between the two forms are further amplified by steric repulsion that

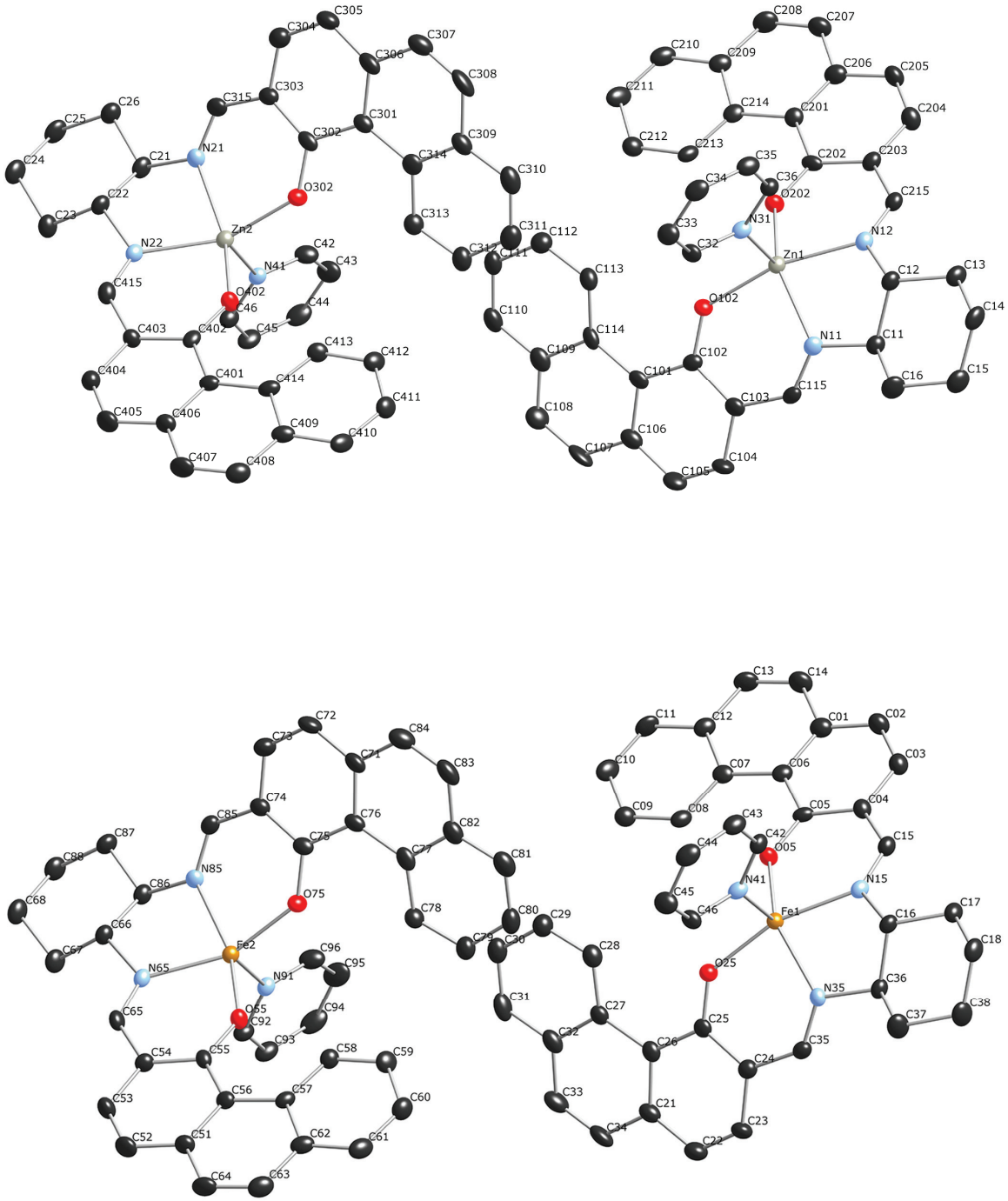


Figure 2.13 Thermal ellipsoid plots (50% probability) of the *P*- and *M*-helimers (left & right respectively) of the complexes (*R,R*)-**53**·py (top) and (*R,R*)-**54**·py (bottom)

forces twisting and curvature of the polyaryl rings. C112 and C312 for example, respectively lie 0.063 and 0.082 Å above the least-squares planes defined by the phenanthryl atoms, C101–C114 (plane D), and C301–C314 (plane A). In contrast, C212 and C412 are located 0.057 and 0.014 Å below the corresponding C201–C214 (C), and C401–C414 (B) planes. Overall therefore, helimers result in which the individual phenanthryl arms curve in opposite directions, effectively increasing the interval between the phenanthryl rings. Near identical positional and torsional variations were also observed for the Fe(II) analogue (*R*,*R*)-**54**·py.

The geometry around the metal center in the two M(II) systems is five-coordinate and slightly distorted from square-pyramidal, with in each case a pyridine molecule occupying the axial coordination site. The pyridine ligands lie near perpendicular to the mean N,N,O,O donor planes, and are orientated in a manner that minimizes unfavorable pyridine-salen steric

Table 2.4 Selected bond lengths, their averages, and metal atom displacements from the mean N,N,O,O donor planes for (*R,R*)-**53**·py, (*R,R*)-**54**·py, and (*R,R*)-**57**

		Bond lengths, Å						Displace-ments, Å
(*R,R*)-**53**·py	(*P*)	$Zn_2–N_{21}$	2.093(5)	$Zn_2–O_{302}$	1.973(4)	$Zn_2–N_{41}$	2.083(4)	0.432
		$Zn_2–N_{22}$	2.069(5)	$Zn_2–O_{402}$	1.982(4)			
	(*M*)	$Zn_1–N_{11}$	2.061(4)	$Zn_1–O_{102}$	1.995(4)	$Zn_1–N_{31}$	2.089(4)	0.355
		$Zn_1–N_{12}$	2.066(5)	$Zn_1–O_{202}$	1.978(4)			
	Av.		2.072		1.982		2.086	0.394
(*R,R*)-**54**·py	(*P*)	$Fe_2–N_{65}$	2.078(4)	$Fe_2–O_{55}$	1.965(3)	$Fe_2–N_{91}$	2.116(3)	0.348
		$Fe_2–N_{85}$	2.092(3)	$Fe_2–O_{75}$	1.953(3)			
	(*M*)	$Fe_1–N_{15}$	2.077(4)	$Fe_1–O_{05}$	1.943(3)	$Fe_1–N_{41}$	2.126(3)	0.315
		$Fe_1–N_{35}$	2.082(3)	$Fe_1–O_{25}$	1.966(3)			
	Av.		2.082		1.957		2.121	0.332
(*R,R*)-**57**	(*P*)	$Fe_2–N_{65}$	2.091(2)	$Fe_2–O_{55}$	1.906(2)	$Fe_2–Cl_2$	2.226(1)	0.492
		$Fe_2–N_{85}$	2.076(2)	$Fe_2–O_{75}$	1.889(2)			
	(*M*)	$Fe_1–N_{15}$	2.077(2)	$Fe_1–O_{25}$	1.901(2)	$Fe_1–Cl_1$	2.234(1)	0.516
		$Fe_1–N_{35}$	2.078(2)	$Fe_1–O_{05}$	1.888(2)			
	Av.		2.081		1.896		2.230	0.504

interactions. Listed in table 2.4 are the M–O and M–N distances, which appear to be in general agreement with the literature values for related Fe^{II} and Zn^{II}(salen) complexes.[77,78] Not surprisingly the M–N salen bonds are somewhat longer than the M–O bonds, being on average 0.090 Å longer in (*R*,*R*)-**53**·py, and 0.125 Å longer in (*R*,*R*)-**54**·py. The pyridine M–N interatomic distances are greater still, although the increase is less pronounced in the Zn^{II}(salen) complex. Presumably the high axial Lewis acidity of zinc renders solvent coordination more favorable relative to iron, and thus a stronger (shorter) bond results.[79] If the coordinate bond lengths are compared across the two complexes, the average M–O distance is found to be ~0.025 Å shorter for iron than for zinc. The inverse appears to be true in regards to the salen Fe–N and Zn–N bonds, with the Fe–N bond ~0.010 Å longer on average. Given that the ionic radii of five-coordinate Zn(II) is in fact less (~0.030 Å) than that of high-spin five-coordinate Fe(II), from a size standpoint the zinc bond lengths are expected to be smaller. As this is not the case, the differences in their relative lengths must therefore ensue from other factors. One possible cause relates to the apical ligand; to sterically accommodate the closer bound pyridine moiety of the zinc salen, an increase in the remaining bond lengths is likely necessary. A comparison of the metal atom displacements above the mean N,N,O,O donor planes further supports this reasoning. For (*R*,*R*)-**53**·py and (*R*,*R*)-**54**·py the average displacements are respectively 0.394 and 0.332 Å, indicating that in the complex containing the shorter pyridyl M–N bond, (*R*,*R*)-**53**·py, there is a greater degree of metal atom pyramidalization. A similar effect is seen in bis(acetylacetone)-ethylenediimine complexes, where the size of the apical group influences the distortion from planarity, and the lengths of the M–N and M–O bonds.[80]

The molecular structure of the Fe(III) complex (*R*,*R*)-**57** is depicted in figure 2.14, and consists of two helimeric forms that adopt a head to tail arrangement. As might be expected, the

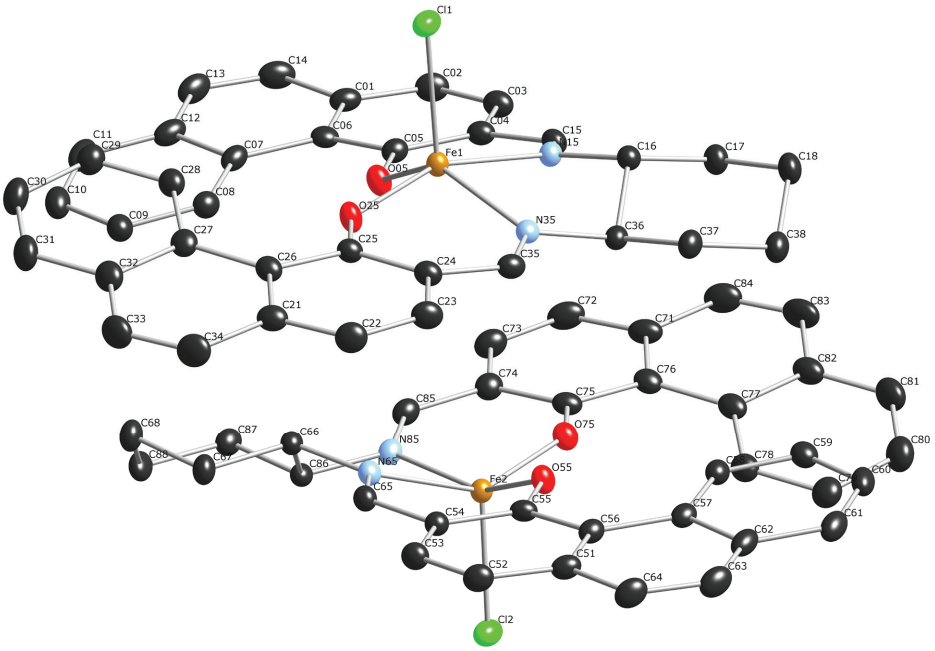


Figure 2.14 A thermal ellipsoid plot (50% probability) of (*R*,*R*)-**57** (*M* top, *P* bottom)

degree of similarity of the individual helimers to those that comprise (*R*,*R*)-**54**·py is high. Careful scrutiny however indicates that the tilt imparted to the ligand arms by the N=C–C=C torsions is somewhat smaller in (*R*,*R*)-**57** (figures 2.15 & 2.16), yielding an almost planar ligand arrangement near the metal. As a result, the terminal aryl rings are forced into close proximity, although this is partially counterbalanced by increased curvature of the polyaryl rings, thus reducing the occurrence of unfavorable steric interactions. The atoms C09, C29, C59, and C79,

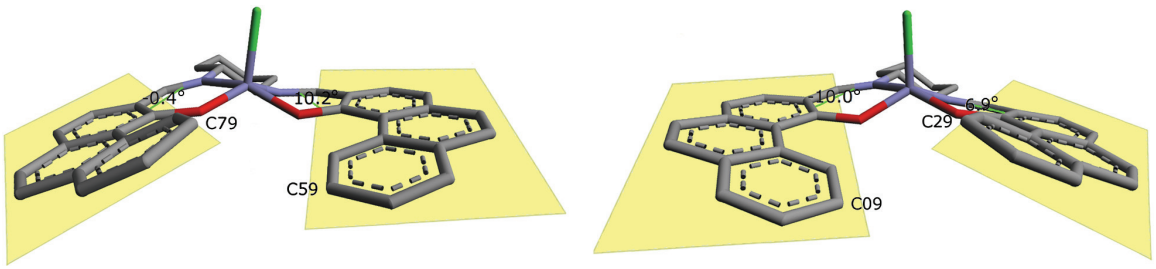


Figure 2.15 A comparison of the *P*- (left) and *M*-helimers (right) of (*R*,*R*)-**57**

for example, are displaced from the mean phenanthryl planes by 0.100 to 0.200 Å, a substantially larger deviation from planarity than is evident in the Fe(II) analogue. Also of importance in comparison to (*R*,*R*)-**54**·py, is the additional +1 charge carried by the metal atom. The most noticeable consequence that arises from this is the ligation of a chloride ion, which, by occupying the apical site prohibits solvent coordination. Furthermore, the M–O and M–N

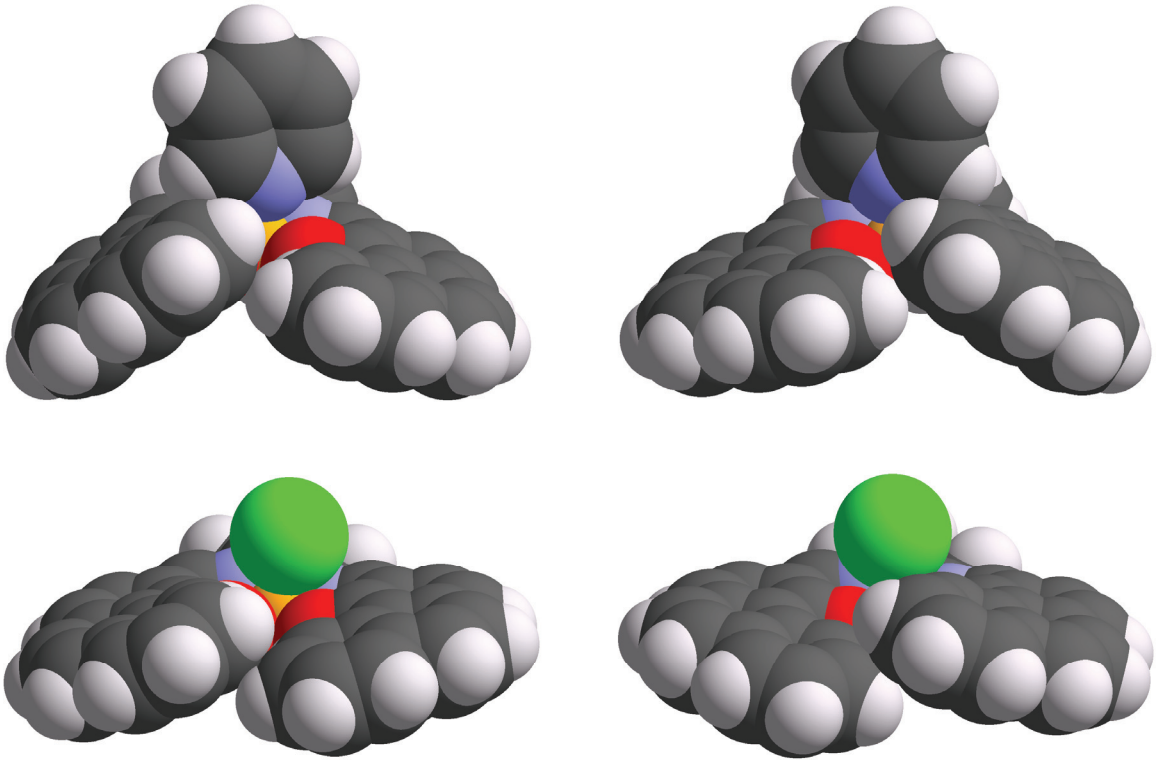


Figure 2.16 Space filling models representing *P* and *M* (*R*,*R*)-**54**·py (top left & right respectively), and *P* and *M* (*R*,*R*)-**57** (bottom left & right respectively)

lengths are affected, as is illustrated by the distances listed in table 2.4. A general decrease in the Fe-O interatomic distances is seen, with the Fe^{III}–O bonds being on average 0.061 Å shorter than the Fe^{II}–O bonds. An analysis of the Fe–N lengths, however, shows that here the average distance is decreased by only 0.001 Å, which is within the margin of error on the basis of the

individual bonds. The electronic effect of the increased iron oxidation state therefore predominates on the charged coordinating atoms, rather than on the Lewis-basic imine fragments. The stronger Fe^{III}–N and Fe^{III}–O binding also causes closer phenanthryl-phenanthryl contact, which leads to the greater degree of ligand distortion that is observed.

Concerning the deviation of the iron atoms from the N,N,O,O donor planes, a large difference is apparent between (*R*,*R*)-**54**·py and (*R*,*R*)-**57**. The displacement distances respectively increase by 0.144 and 0.201 Å for the *P* and *M* forms. Yet given that the Fe(III) ion has a considerably smaller radii than that of the Fe(II), on a size basis, a better 'fit' and smaller displacement is expected. Moreover, such an adjustment would increase the separation between the phenanthryl arms, and thereby minimize the amount of ligand distortion. Thus, processes that shape the coordination geometry are in operation that do not rely solely on metal atom size. Such effects have been previously suggested by Gerloch for a Fe^{III}(salen)Cl complex.[81]

2.5 Structural Studies of the binap-M(salen) Ligands and Complexes

Single crystals suitable for X-ray analysis were grown of the ligand (*R*)-**34**, and of the binap-M(salen) complexes (*R*)-**55** and (*rac*)-**56** via solvent diffusion. The use of enantiopure (*R*)-**56** resulted exclusively in precipitation of a fine powder, necessitating that for crystal growth the racemic analogue be employed. In table 2.5 are listed the crystallization solvents, depicting in column B the lower solubility solvents, and in A the primary solvent into which each substance was dissolved prior to layering.

Table 2.5 Crystal growth conditions

	Method	Solvent A	Solvent B
(*R*)-**34**	Diffusion	Methylene chloride	Hexanes
(*R*)-**55**	Diffusion	Methylene chloride	Methanol
(*rac*)-**56**	Diffusion	Methylene chloride	Methanol

The structure obtained for the ligand (*R*)-**34** is shown in figure 2.17. It consists of a single ligand molecule that can be divided into two roughly equivalent halves, bridged by a naphthyl-naphthyl bond. Comprising each of these is a phenanthryl and a naphthyl moiety that are approximately co-planar, with, in one half a phenanthryl-naphthyl dihedral angle of 7.6°, and in the other of 27.4°. From the aforesaid angles it can be inferred that there is significant delocalization across the co-planar groups, as is evident for other literature documented binap-salen ligands.[29a,82] Also apparent are hydrogen bonding contacts between the hydroxyl moieties and imine nitrogens, that further stabilize this arrangement. The somewhat larger inter-planar angle of 27.4° presumably results from crystal packing forces, which distort the molecular

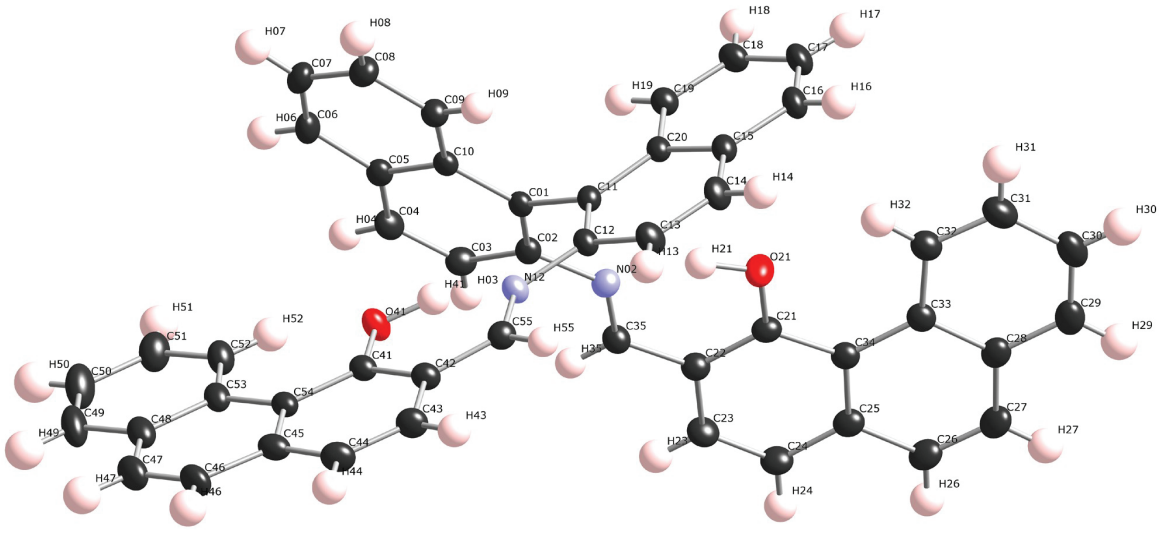


Figure 2.17 A thermal ellipsoid plot (50% probability) of (*R*)-**34**

geometry in order to maximize the filled volume. For (*R*)-**34** the naphthyl-naphthyl dihedral angle is 103.4°, whereas torsion about the bridging bond of 1,1'-binaphthyl has an energy minima located at approximately 90°.[32] The similarity between this and our value suggests that the phenanthryl groups do not greatly influence the geometry of the backbone, and although spatially large, engender little steric strain.

In figure 2.18 is shown the molecular structure of the Zn(II) complex (*R*)-**55**·MeOH. Clearly, only the *M*-helimer is present in the solid state, coordinating to a methanol solvent molecule through the zinc center. The co-planarity that was evinced by the ligand phenanthryl and naphthyl moieties in (*R*)-**34** is absent, though this change is not unexpected given the spatial demands of coordination, which requires reorientation of the ligand for suitable orbital overlap. The loss of co-planarity is further illustrated by the large aryl inter-plane angles of 63.9° and 76.1°, showing that there is little if any conjugation occurring across the two groups. An additional effect can be seen from the rotated ligand arms, in that the terminal aryl rings of the phenanthryl moieties overlap. As indicated by the space-filling model in figure 2.18, however, the extent is small. The dihedral angle between the naphthyl backbone fragments decreases upon metallation, with respective angles for the complex and the free ligand of 69.7(3)° and 103.1(3)°. This difference is attributable to the zinc ion which forces adoption of a smaller angle, although it still lies within the region where unfavorable naphthyl-naphthyl interactions are not significant.[32] It is likely that the associated energetic penalty is minimal.

The molecular structure of (*rac*)-**56** incorporates both *P* and *M*-helimers, a result of the use of the racemate for crystal growth. For each form there are two slightly different geometries (A and B), which vary mostly in the orientation of one of the phenanthryl arms. The *P*-helimers originate from the *S*-enantiomer, and analogously the *M*-helimers are afforded by the

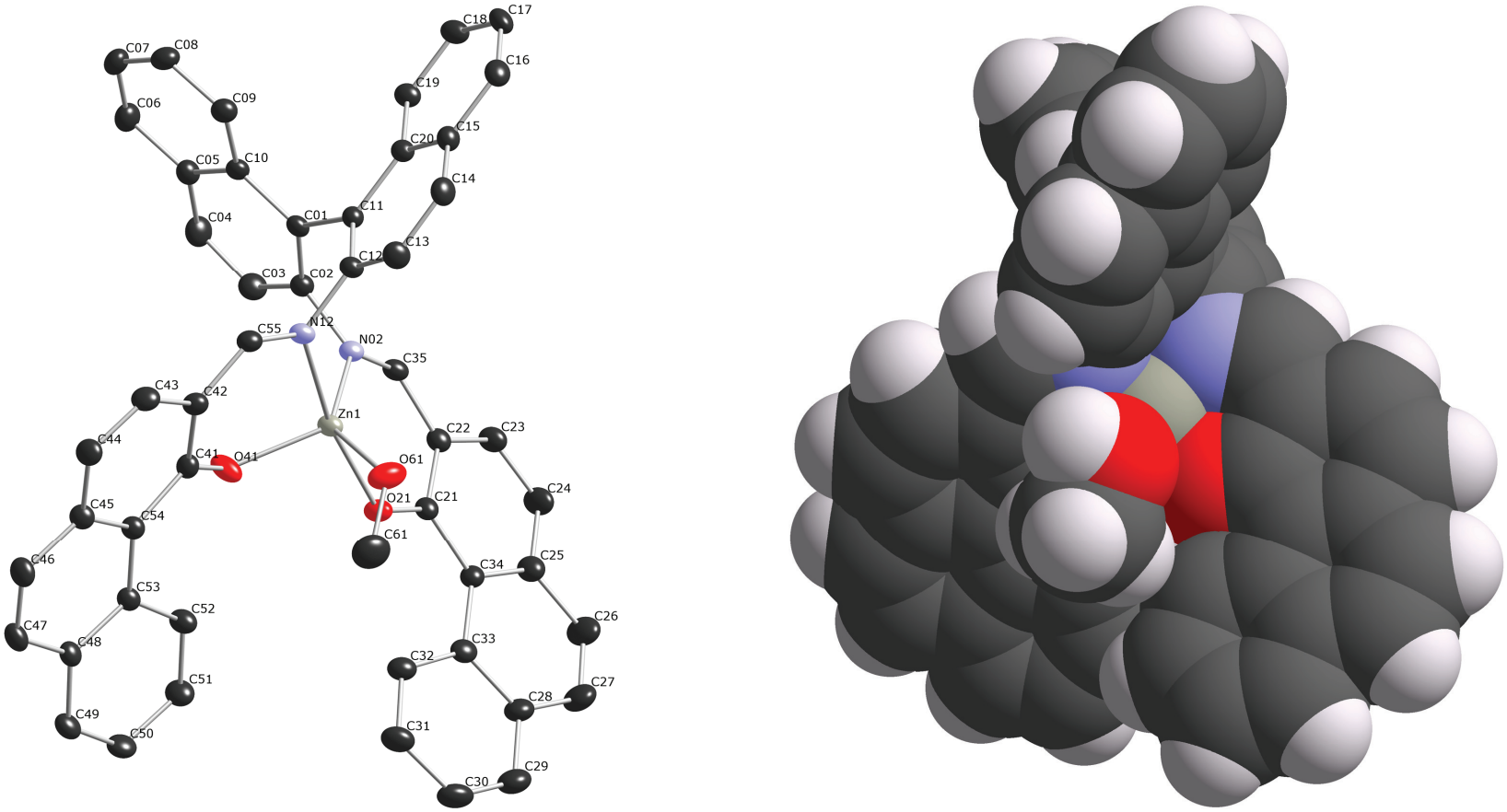


Figure 2.18 A thermal ellipsoid plot (50% probability) and space filling model for (*R*)-**55**·MeOH

R-enantiomer. Each *M* form relates to its *S* counterpart as object to mirror image. In figure 2.19 is depicted the overall molecular arrangement and in 2.20 one of the two *M* geometries; the other is not shown as the positional changes that differentiate the structures are minimal.

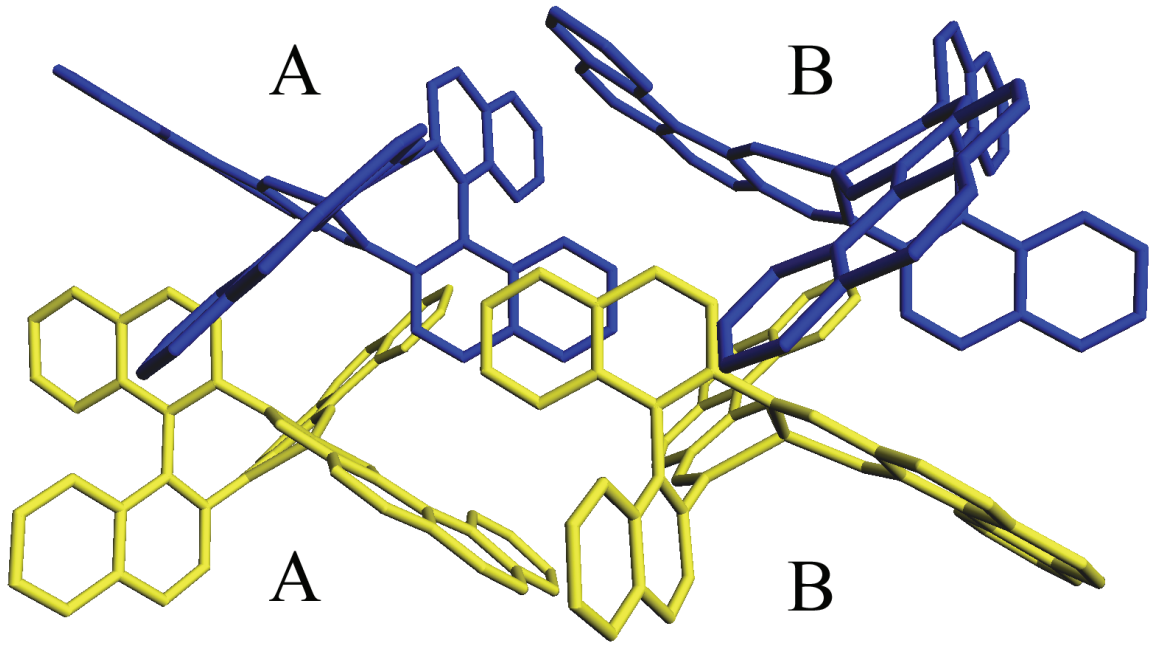


Figure 2.19 The molecular structure of (*rac*)-**56** (*M* yellow, *P* blue)

The *M* arrangement in figure 2.20 (hereafter termed (*R*)-**56A**) is structurally akin to the Zn(II) complex (*R*)-**55**·MeOH, albeit with some differences. Coordination of the iron atom by solvent does not occur, leading to a distorted tetrahedral geometry at the metal. In contrast, in the zinc analogue the configuration is five-coordinate and close to trigonal-bypiramidal. The ligand sidearms consequently differ in their respective orientations, with angles between the phenanthryl planes of 43.7° for (*R*)-**55**·MeOH, and 74.5° for (*R*)-**56A**. Some modest variation is also seen in the phenanthyl-naphthyl dihedral angles, wherein the inter-plane torsions are 67.9° and 79.9° for the iron structure, compared to 63.9° and 76.1° for the zinc system. The naphthyl-

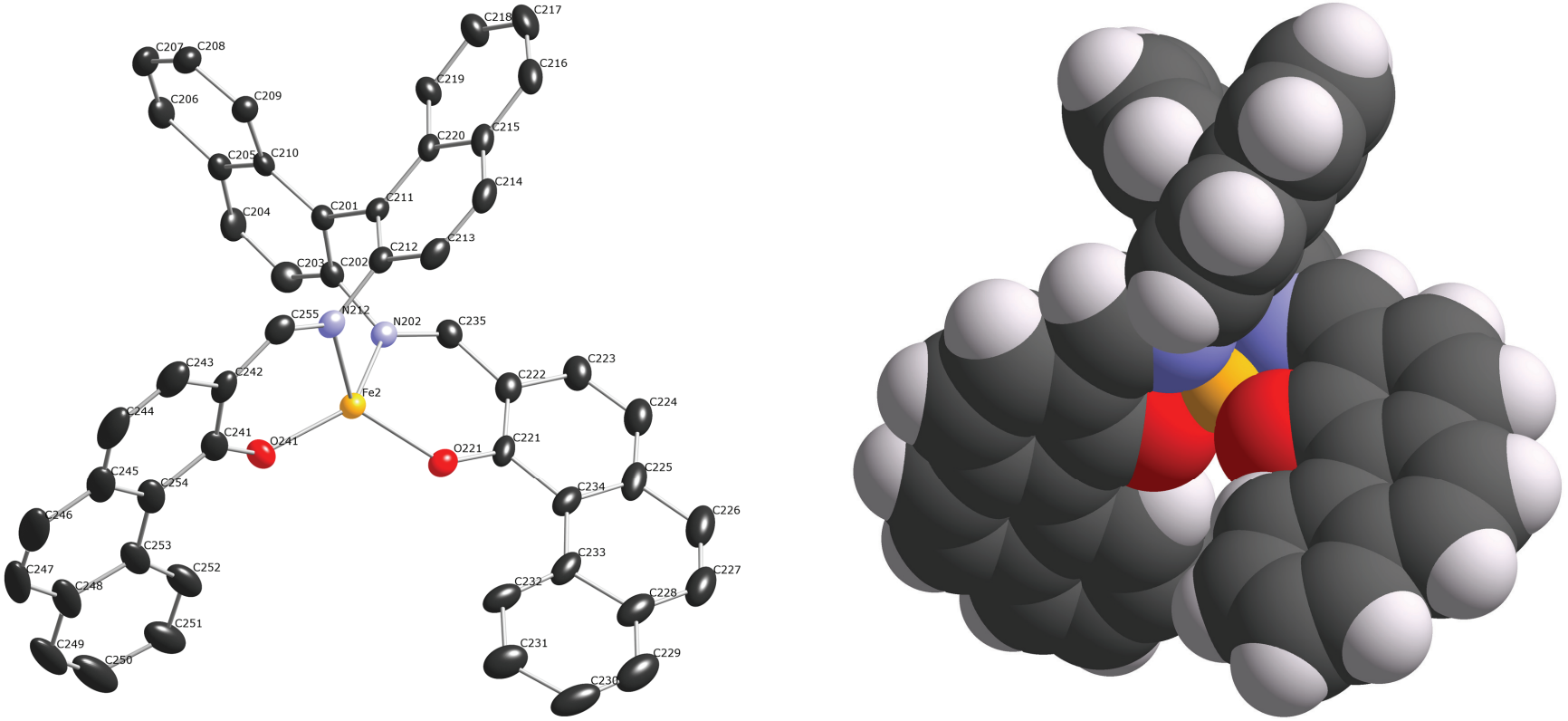


Figure 2.20 A thermal ellipsoid plot (50% probability) and space filling model for (*R*)-**56A** of (*rac*)-**56**

naphthyl dihedral angle is essentially unaffected by the change in coordination modes, with a value of 69.3(5)^{o} for (*R*)-**56A**, a 0.4^{o} decrease. The angles of the second *M*-helimer in the asymmetric unit vary by less than 4.0^{o}, from those of (*R*)-**56A** that are quoted here.

In table 2.6 are listed the binap-salen M–O and M–N bond lengths of (*R*)-**55**·MeOH, (*R*)-**56A**, and the second (*rac*)-**56** *M*-helimer (*R*)-**56B**. There is by and large little variation between the tabulated distances of the two (*rac*)-**56** *M* geometries, particularly if the average lengths are examined. If they are evaluated against (*R*)-**55**·MeOH however, a substantial difference can be

Table 2.6 Selected bond lengths and their averages for (*R*)-**55**·MeOH and (*R*)-**56A/B**

	Bond lengths, Å			
(*R*)-**55**·MeOH	Zn_1–N_{02}	2.071(2)	Zn_1–O_{21}	1.983(2)
	Zn_1–N_{12}	2.086(2)	Zn_1–O_{41}	1.955(2)
	Av.	2.079	Av.	1.969
(*R*)-**56A**	Fe_2–N_{202}	2.010(3)	Fe_2–O_{221}	1.907(3)
	Fe_2–N_{212}	2.022(3)	Fe_2–O_{241}	1.879(3)
	Av.	2.016	Av.	1.893
(*R*)-**56B**	Fe_1–N_{102}	2.008(3)	Fe_1–O_{121}	1.893(2)
	Fe_1–N_{112}	2.021(3)	Fe_1–O_{141}	1.894(3)
	Av.	2.015	Av.	1.894

seen. The Zn–N and Zn–O bonds are respectively, and on average, 0.063 and 0.076 Å longer. This trend generally mirrors the larger ionic radii of five-coordinate Zn(II) (~0.68 Å), as compared to that of high-spin four-coordinate Fe(II) (~0.63 Å). A result which is unlike that observed in the Fe^{II}/Zn^{II}(salen) case. One possible explanation for the difference lies in the high torsional flexibility of the binap-salen ligand.[32] Here, adoption of more favorable M–O and M–N bond lengths should be possible, without inducing steric crowding. Such steric effects are likely to influence the Fe^{II}/Zn^{II}(salen) coordinate bonds (p42).

2.6 Solid State vs Solution Structures

For the complexes so far discussed, the systems that incorporate a cyclohexyl backbone take on both *P* and *M*-helimeric arrangements in the solid state. It can be speculated that this derives from crystal packing forces, which seek to maximize the filled volume, and will favor the adoption of pseudo-racemic conformations. In comparison, our single point DFT calculations for (*R,R*)-**53**·py at the BL3YP/6-31G(d,p) level, indicate that the *M* form is 2.5 kcal/mol more stable than the *P*.[83] Thus, the solid state may not accurately reflect the conformations that are occurring in solution. Given that catalysts can act homogenously (solution phase) and/or heterogeneously (solid state), it is therefore beneficial to investigate the solution structure(s), to determine if indeed both helimers are present. Various methods can potentially yield the required information, and initially we focused on chiral shift reagents in combination with VT-NMR spectroscopy. However, it was found that VT-NMR alone yielded inconclusive results; slight line broadening was observed for (*R*,*R*)-**53** at -90^{o}C, while elevated temperatures afforded a spectrum that did not perceptibly differ from that taken at room temperature. Moreover, the complex proved too insoluble in the non-coordinating solvents ($CDCl_3$, C_6D_6, etc) necessary for proper chiral shift reagent use. We therefore turned to electronic circular dichromism (ECD) spectroscopy, a technique commonly used to examine the helicity of proteins, which we utilized in conjunction with UV-Vis.

ECD spectroscopy relies upon the difference in absorption of left- and right-handed circularly polarized light by chiral molecules.[84] This process in turn is governed by electrically and/or magnetically allowed transitions, from occupied orbitals of the absorbing chromophores, to those of the excited state. Where the chromophoric groups are achiral, as in our case, the

induced transitions directly correlate to the surrounding asymmetric environment. Thus, in theory, the spectrum contains all the information needed to derive the solution geometries. Although this is difficult to do in practice, a partial qualitative/empirical analysis is feasible and as such was attempted. We also decided to simulate the spectra to aid our interpretation, utilizing for this purpose the ADF software suite, and data from the (*R*,*R*)-**53** crystal structure. The Fe^{II}(salen) and Fe^{III}(salen)Cl spectra were not calculated owing to poor convergence of the SCF, which resulted in severe computational errors. Only the simulated spectra for the helimers of the closed shell zinc complex are shown. Detailed information on the computational parameters can be found in the appendixes.

In figure 2.21 are depicted the UV-Vis spectra of (*R*,*R*)-**33** and (*R*,*R*)-**53** in THF. Pyridine could not be used as the solvent due to its high molar absorptivity. There are several regions of interest in the spectra, arising from the various electron orbital-orbital transitions. Centered at 438 and 461 nm are two bands that originate from the (*R*,*R*)-**33** keto-amine tautomer (figure 2.9), and correspond to $\pi \rightarrow \pi*$ excitations. In analogy, the bands at 365 and at 383 nm can be assigned to the enol-imine tautomeric form.[73b,76c] The existence of two equilibrating species in solution is confirmed by variations in their relative intensities, with respect to the solvent system chosen. A non-polar solvent such as cyclohexane, results in less than 10% occurring as the keto-amine tautomer. The molecular orbitals responsible for these four low energy excitation bands, appear to be localized on both the phenanthrene and azomethine chromophores. A result analogous to that seen for salicylaldehyde derived salen ligands.[85] At 214 and 250 nm are signals that are primarily due to the phenanthryl moiety, and which are respectively classified as β` and β bands under Clar's[86] notational system. The peak shapes and their 2nd derivatives indicate the presence of multiple overlapped absorptions, where one is of

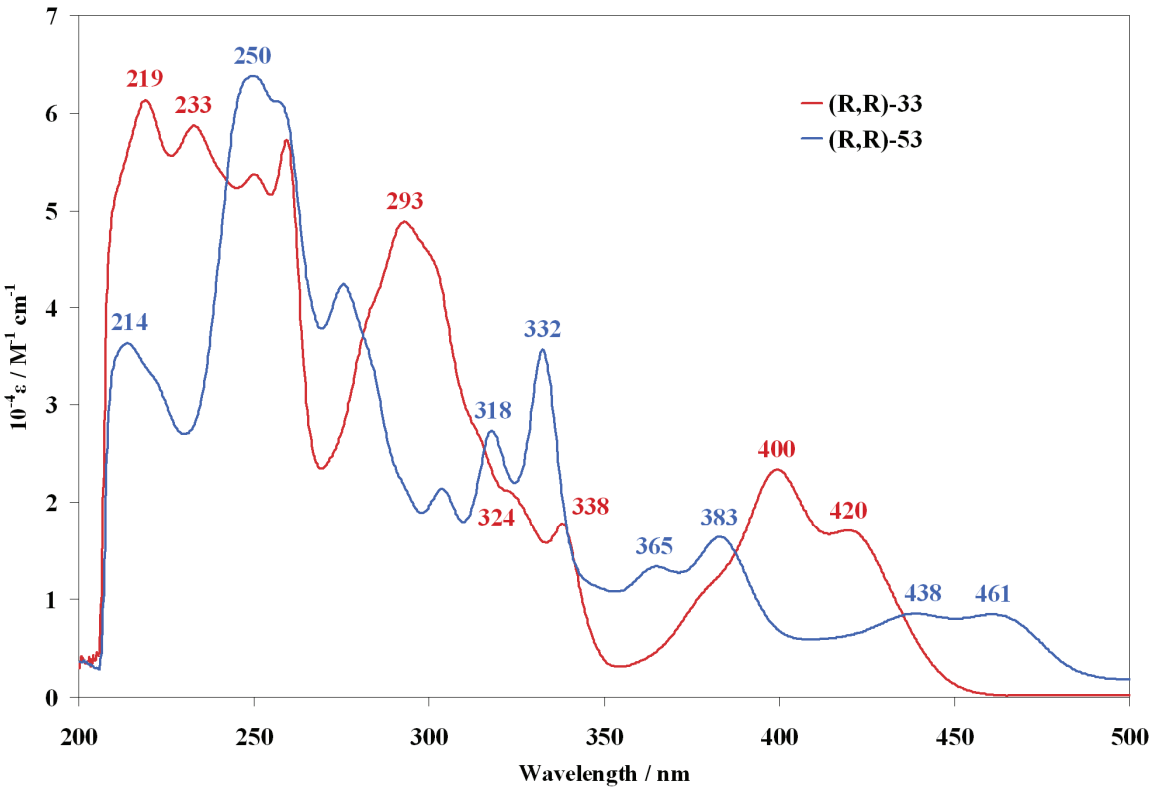


Figure 2.21 UV-Vis spectra of (*R*,*R*)-**33** and (*R*,*R*)-**53**

greater intensity than the others. The 332 nm signal is designated as the ρ band under Clar's notation, and it is likely that the 318 nm signal corresponds to this also. The signals at 214, 250, 318, and 332 nm, all arise from electron movements of the π→π* type.

For the spectrum of the zinc(II) complex (*R*,*R*)-**53** there are several substantial differences. The keto-amine tautomer can no longer form, and hence the associated excitations (438 & 461 nm) disappear. The two bands situated at 365 and 383 nm in the free ligand, and which originate from the enol-imine tautomer, are shifted to 400 and 420 nm by metallation. This long wavelength shift is attributable to increased planarity across the π network, and results from enhanced conjugation.[87] The bands at 324 nm - which appears as a shoulder - and at 338 nm occur at slightly longer wavelengths as compared to the ligand, shifted from 318 and 332 nm

respectively. Both change by the same value, giving credence that the two bands arise from the same or related transitions. A new broad intense signal is seen at 293 nm, appearing from the peak shape to be comprised of multiple overlapped absorption bands. For the signals visible in the 200-260 nm range, there is little difference in their relative wavelengths, although considerable variation is observed in their intensities. The band at 233 nm arises in the ligand spectrum as well as in that of the complex, but is of lower absorptivity for (*R*,*R*)-**33**, and can therefore only be distinguished in the spectrum via deconvolution techniques.[88]

Given that circular dichroism is a function of molecular structure, to correctly simulate ECD spectra requires that the solution structure(s) be accurately modeled. There are three main possibilities in this regard, either a) the *P*-helimer predominates, b) the *M*-helimer predominates, or c) in solution there is an approximately equal mixture of the two. The question of whether (*R*,*R*)-**53** is coordinated by THF must additionally be considered. For our spectral simulations we therefore first generated DFT minimized structures of *P* and *M* (*R*,*R*)-**53**, and *P* and *M* (*R*,*R*)-

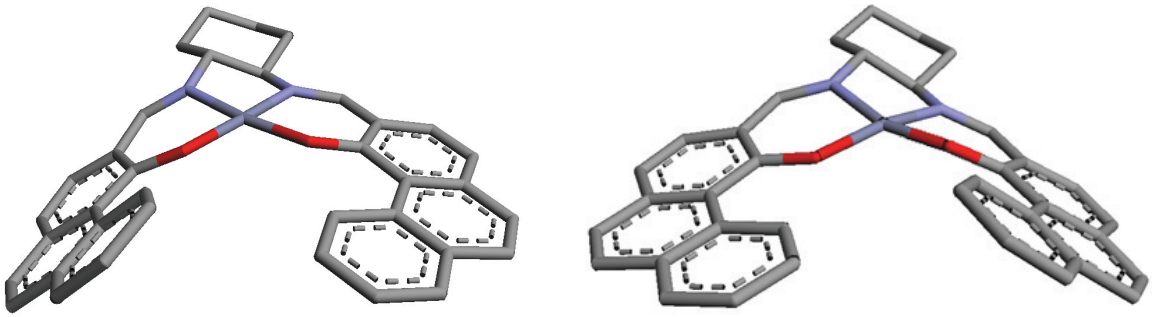


Figure 2.22 Minimized structures of *P* and *M* (*R*,*R*)-**53** (left & right respectively)

53·THF. The (*R*,*R*)-**53**·py crystal structure was used as the foundation for building, and subsequently minimizing the different molecular geometries. Those which resulted for (*R*,*R*)-**53** are depicted in figure 2.22. The chief difference to the THF bound structures was found to lie in

the degree of pyramidalization of the zinc atom, being substantially less for the solvent free salens. The zinc, as shown, is coplanar with respect to the N,N,O,O atoms, and displaced on average by only 0.004 Å from each donor plane. Some slight lessening in the upward tilts of the phenanthryl side-arms is also apparent. Thereafter, for each geometry, the excitation energies and rotational strengths were calculated. Gaussian shaped distributions were generated from the computed data, and spectral simulations obtained by superposition of the individual Gaussian curves. In figure 2.23 are compared the *P* and *M* (*R*,*R*)-**53** theoretical spectra, to the experimental. The simulations corresponding to (*R*,*R*)-**53**·THF are shown but will not be discussed (figure 2.24), as comparatively greater inaccuracies were seen relative to the experimental results. Evidently, the salen solution structures resemble those in figure 2.22 more so than the solvent bound analogues, which is consistent with rapid solvent movement between the two axial positions. It is important to note that the depicted empirical and computed rotational strengths are not comparable numerically. Their relative intensities and signs if predicted correctly, should, however, be meaningful.

An analysis of figure 2.23a indicates that there is little agreement between the simulated *P* and experimental spectra. For the *P* structure in the 400-435 nm range, for example, the Cotton effect is positive at lower energies (longer wavelength), and negative at higher energies. This conforms to exciton theory which predicts such a couplet shape for Λ (*P*) stereogenicity.[89] In contrast, despite a sizeable difference in magnitude, the opposite band shape is observed by experiment. There is likewise little resemblance at shorter wavelengths, although underestimation of the 247, 275, and 285 nm energies, could partially account for the divergence. Though given the other evident differences, it is substantially more probable that the *P*-helimer is not the predominant solution form.

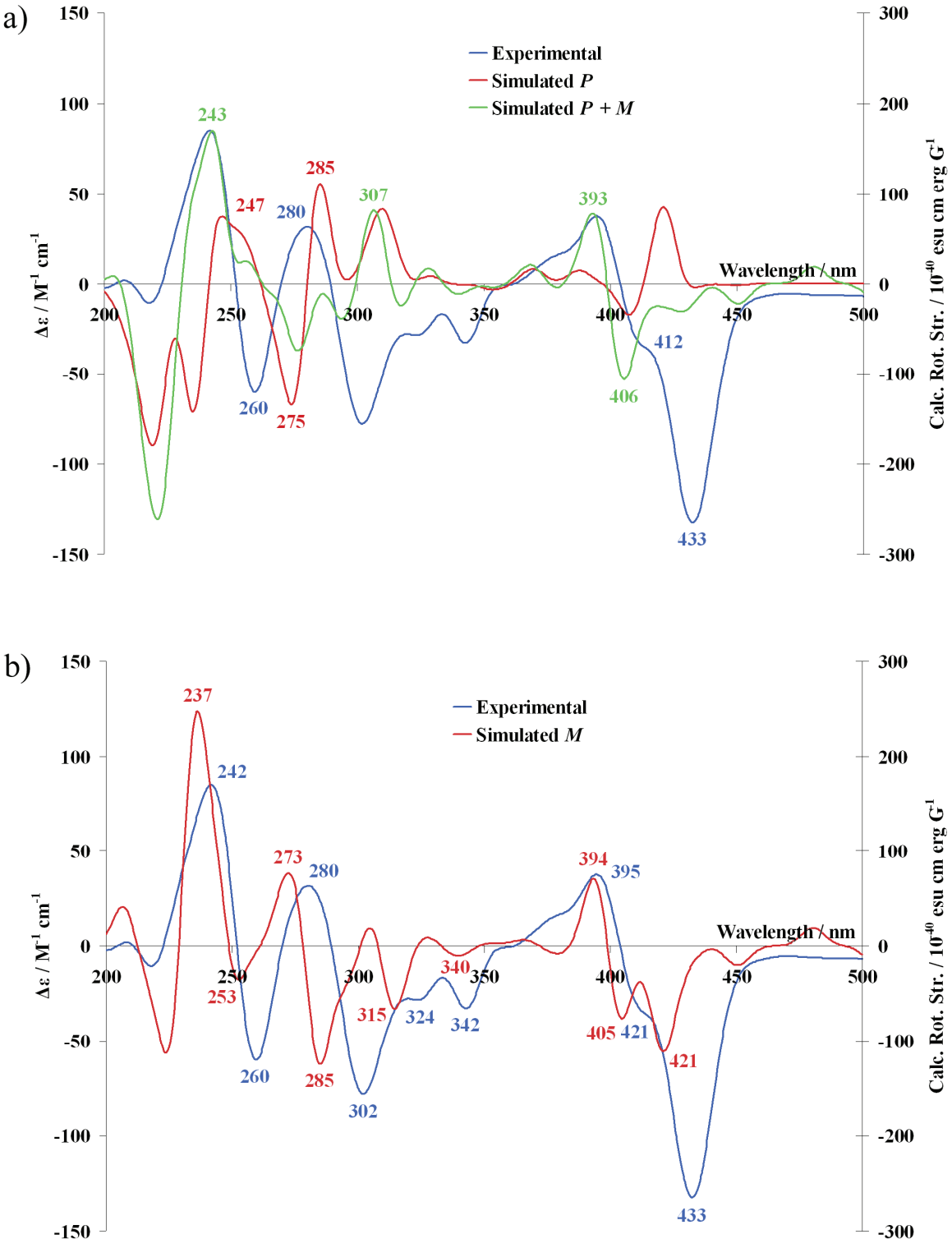


Figure 2.23 a) Simulated *P*, *P* + *M*, and experimental ECD spectra for (*R*,*R*)-**53**. b) Simulated *M* and experimental ECD spectra for (*R*,*R*)-**53**.

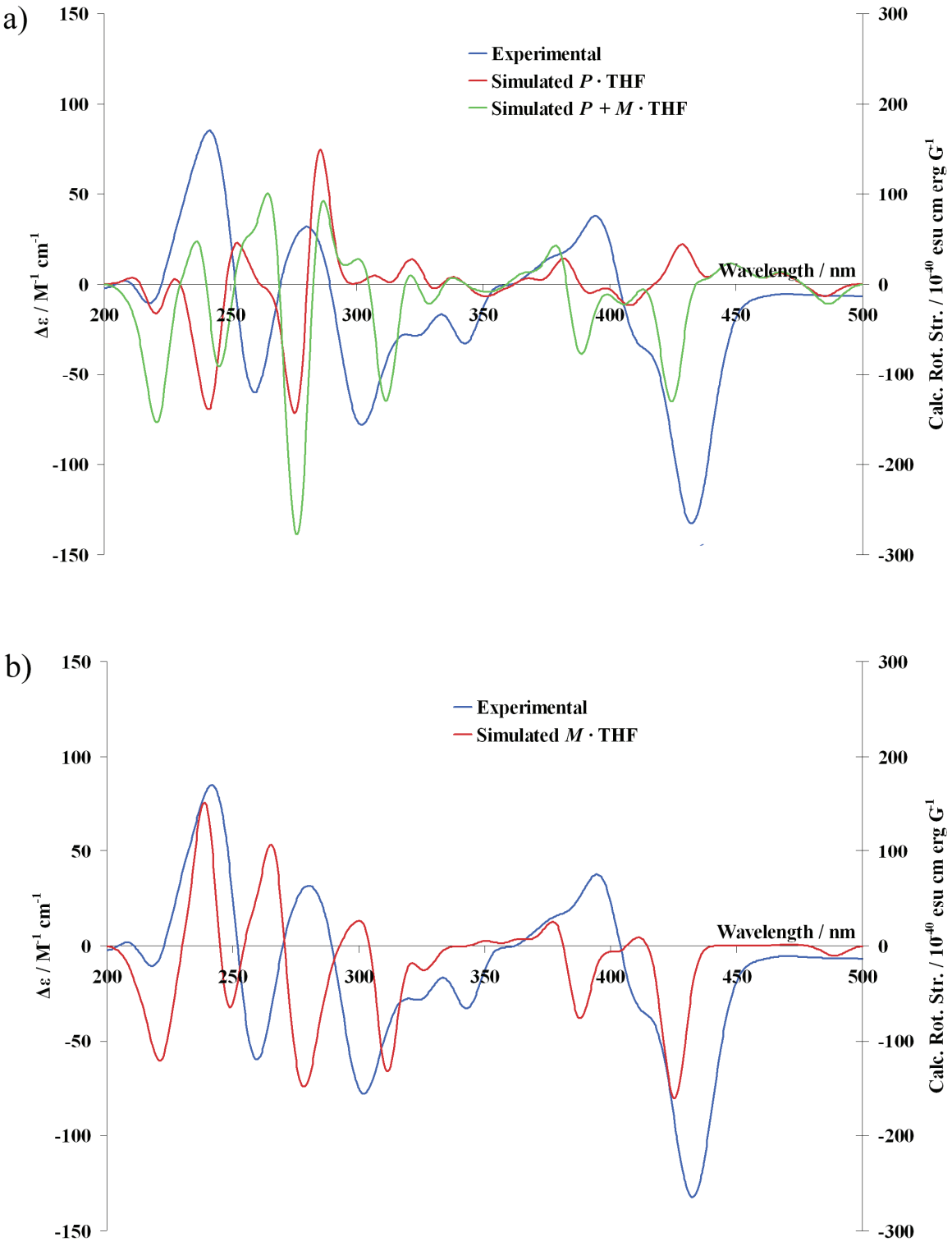


Figure 2.24 a) Simulated *P*, *P* + *M*, and experimental ECD spectra for (*R*,*R*)-**53**·THF. b) Simulated *M* and experimental ECD spectra for (*R*,*R*)-**53**·THF.

With regards to the 1 : 1 *P* + *M* spectrum, in some regions there appears to be good agreement between the theoretical and experimental results. The 243 and 393 nm bands in particular correlate well, and the 406 nm signal is closely aligned to the visible 412 nm shoulder. There are, nonetheless, major inconsistencies between 250 and 350 nm. More so than for the pure *P* spectrum. The band at 307 nm is of opposite sign to that expected, and no match or possible match exists, to the experimentally observed 260 and 280 nm maxima. The band at 433 nm is in addition poorly reproduced. These differences for the most part can be attributed to canceling of oppositely signed signals, which results in simulated bands that are of low intensity. On balance therefore, the evidence suggests that an equal *M* and *P* mixture is unlikely.

The final possibility and the possibility which the data favors, is the adoption of principally *M*-helices. The computed *M*-helical spectrum is shown and contrasted in figure 2.23b. From the overall appearance it is apparent that the signs and intensities of the bands, generally duplicate those determined by experiment. Unfortunately, it is also evident that the excitation energies are systematically overestimated, by between 0.01 to 0.24 eV (table 2.7). Whether this derives in some measure, from inaccuracies in the minimized geometry is not

Table 2.7 Comparison of the simulated *M* and experimental maxima

Simulated *M*, nm	Experimental, nm	Difference, nm (eV)
237	242	5 (0.11)
253	260	7 (0.13)
273	280	7 (0.11)
285	302	17 (0.24)
315	324	9 (0.11)
340	342	2 (0.03)
394	395	1 (0.01)
405	412	7 (0.05)
421	433	12 (0.08)

known. Given the approximations the employed LDA functional uses to decrease the computation time,[90] however, suggests that this is the source of the error. The *M*-helimer, nonetheless, affords the closest facsimile to the experimental spectrum. The 433 nm component of the 375-450 nm couplet is for instance replicated, whereas it is of opposite sign or absent in the *P* and *P* + *M* simulations. The causative orbitals are located on the 'raised' ligand arms (figure 2.22), and the transition density, i.e. the net displacement of charge, is inverted over the two structures. The electron density changes are thus related through a mirror image relationship, and the sign of the band accordingly inverts from the *M* to the *P*-helimer. Similarly, both the *P* and *P* + *M* simulations incorrectly predict the sign of the 302 nm band. Only the *M*-helimer 285 nm signal lies close enough in energy, and has the correct sign and intensity, to account for the experimentally observed excitation.

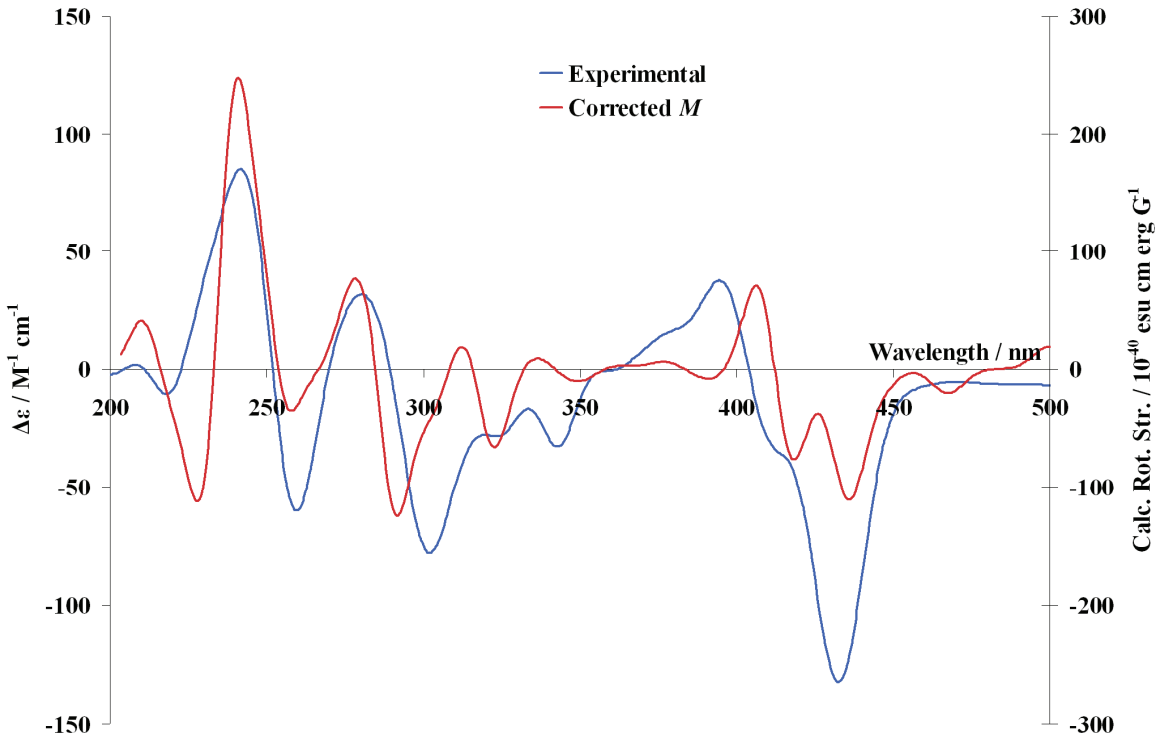


Figure 2.25 Comparison of the corrected *M* and experimental ECD spectra for (*R*,*R*)-**53**

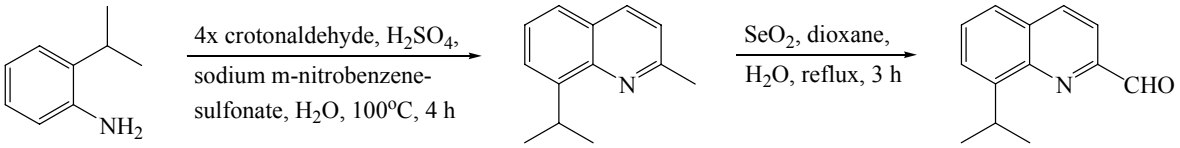
In view of the overestimated energies we subsequently applied a 0.1 eV correction, and plotted the adjusted values as depicted in figure 2.25. Overall there is a markedly better fit between the peaks in comparison to the uncorrected data. Notably, the level of agreement does not substantially improve for the *P* and *P* + *M* spectra, if these are likewise treated. Rather, the resemblance is greater in some respects, but worse in others. In conclusion we can therefore state that the *M*-helimer is the predominant or sole form occurring in solution. The percentage as the *P* form is not sufficient to affect the experimental ECD spectrum, at least to an extent that is detectable via our methods.

CHAPTER 3

Synthesis, Characterization, and Study of 8-Isopropylquinoline Derived Complexes

3.1 Synthesis

To generate our bis(pyridyl-imine) complexes necessitated that first the aldehyde **42** be prepared. This was relatively simple, requiring a two step procedure to complete (figure 3.1). In the first, 2-isopropylaniline and crotonaldehyde were reacted under strongly acidic oxidative conditions, via a modified Skraup's procedure,[91] to yield the dialkyl substituted quinoline **59**. The use of a large excess of crotonaldehyde was necessary, due to its low stability and rapid self-



58 **59**, 58% **42**, 84%

Figure 3.1 Synthesis of 8-isopropyl-2-quinolinecarboxaldehyde

polymerization in acidic media. Employment of a three fold surfeit effected approximately 75% conversion of the aniline (via ^{1}H NMR), to the desired end product. Larger quantities improved the conversion rate, but complicated the workup by further increasing the amount of polymeric contaminant. In the second step, the quinoline, **59**, was oxidized with selenium dioxide to afford **42**.[92] The yield after purification was respectively 58 and 84% for the first and second steps, and 49% overall.

With this precursor in hand, the ligands (*R,R*)-**35** and (*R*)-**36** were synthesized by the condensation of **42** with (*R,R*)-**39** and (*R*)-**40** (figure 3.2). Anhydrous conditions were necessary to prepare the imine products, since otherwise the equilibrium favored the starting reagents and no reaction occurred. To remove the *in situ* generated water and drive the equilibrium,

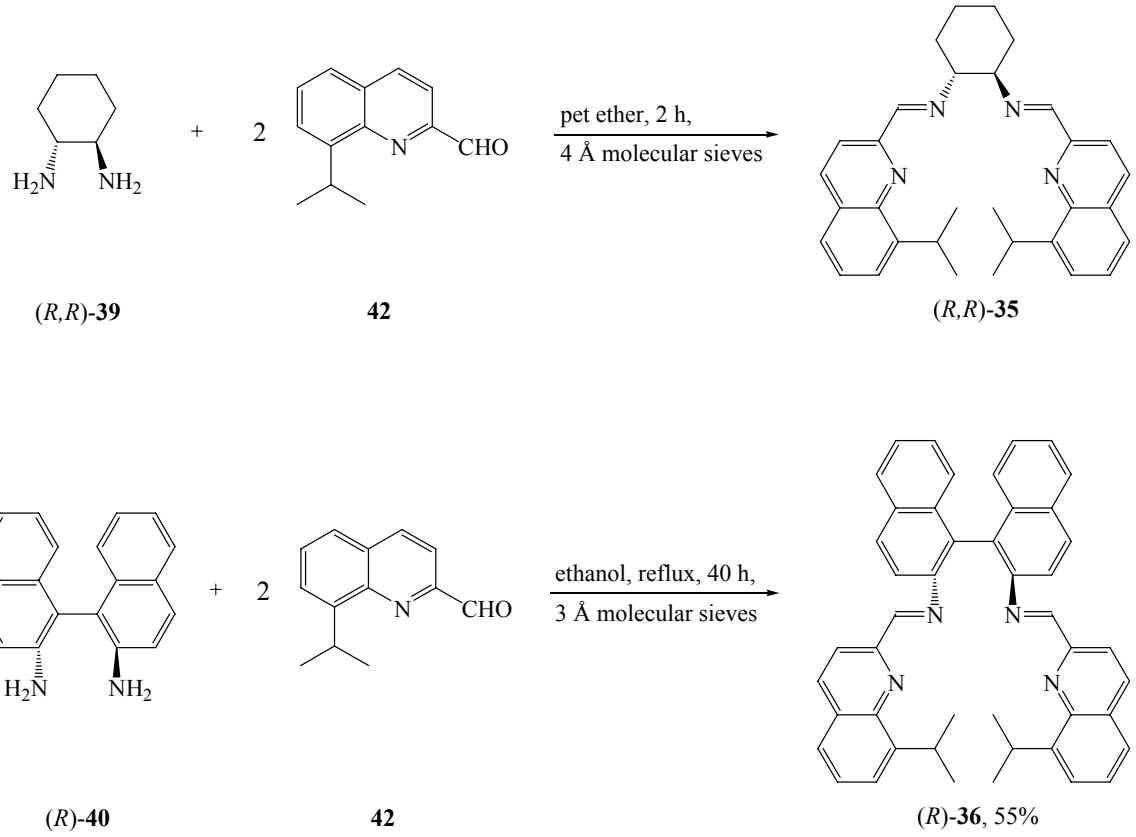


Figure 3.2 Ligand preparation

molecular sieves were added. The ligand (*R*)-**36** was isolated in high purity after workup, albeit in moderate yield. (*R,R*)-**35** on the other hand was afforded as a moisture sensitive oil, and as no straightforward purification was possible without simultaneously causing decomposition, was used as is. ^{1}H NMR analysis did, nonetheless, indicate (*R,R*)-**35** to be of greater than 90% purity.

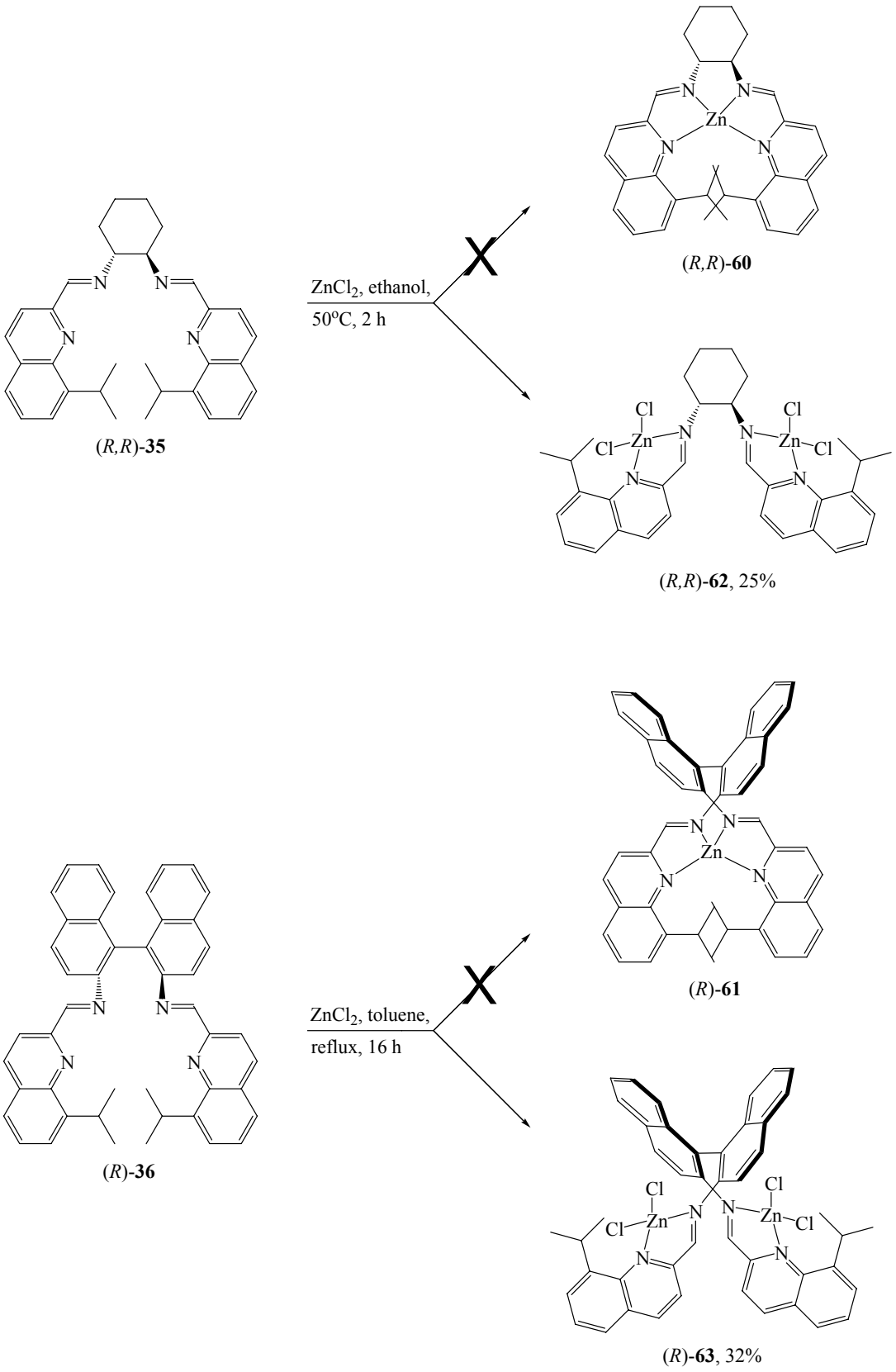


Figure 3.3 Zinc complex synthesis

The two ligands were then metallated using $ZnCl_2$, to give complexes which at that time were thought to be (*R,R*)-**60** and (*R*)-**61** (figure 3.3). Single crystal X-ray analysis later showed each ligand molecule to incorporate two $ZnCl_2$ units, and therefore (*R,R*)-**62** and (*R*)-**63** were in fact the prepared substances. The low product yields are mainly a consequence of stoichometric addition of $ZnCl_2$, rather than the use of two equivalents; we expected mono-metallation and not as shown dimetallation.

Following the formation of the zinc(II) complexes, we attempted to incorporate $Fe(CF_3SO_3)_2$ into (*R,R*)-**35** and (*R*)-**36**. The $CF_3SO_3^-$ ion was of interest to us due to its low ligating ability, which theoretically might facilitate monohelix formation. To our disappointment under the employed conditions the majority of the iron reagent (>90%) did not react. Moreover, it proved impossible to separate out the small quantity of organic paramagnetic material that formed, from the unreacted starting reagents. Whether this iron containing substance was the desired product is not known, owing to the difficulty inherent in interpreting paramagnetic ^1H NMR spectra, and the lack of an alternate facile characterization technique.

3.2 NMR Spectroscopy of the Ligands & Diamagnetic Zinc Complexes

The ligands (*R,R*)-**35** and (*R*)-**36**, and the zinc complexes (*R,R*)-**62** and (*R*)-**63**, were analyzed via ^1H NMR spectroscopy. Table 3.1 lists the ^1H chemical shifts. All aryl product peaks were well-resolved consisting of a single set of resonances, indicating the existence of one discrete molecular species in solution. The cyclohexyl ring proton signals were somewhat broadened, though as previously stated this is not unusual for cyclohexyl groups, and is attributable to ring motions. With regards to the complexes, although the number of bands and

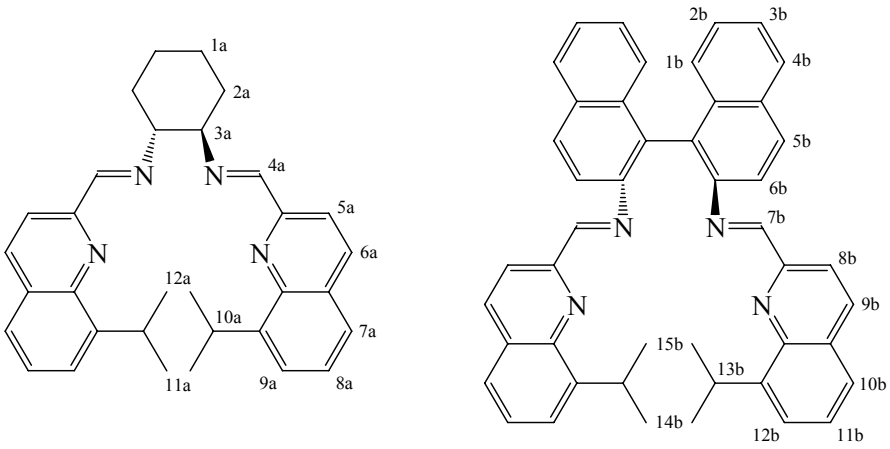
Table 3.1 Ligand and Zn(II) complex ^{1}H NMR chemical shifts[a]

	Chemical shifts, $\delta(^3J,^4J)$		
	Imine C–H	Aliphatic C–H	aromatic C–H
(*R,R*)-**35**	8.54	1.25(6.9), 1.36(6.9), 1.54-1.65, 1.80-2.04, 3.61-3.70, 4.29(6.9)	7.41-7.46, 7.50-7.58, 8.00-8.08
(*R*)-**36**	8.62	1.11(6.9), 1.27(6.9), 4.12(6.9)	7.28-7.34, 7.39-7.58, 7.62(8.5), 7.91-7.98, 8.03(8.7)
(*R,R*)-**62**	9.25	1.40(6.6), 1.49(6.6), 1.59-1.68, 1.96-2.09, 2.54-2.69, 4.58(6.6), 4.64-4.72	7.67-7.76, 7.88(8.2), 7.93(6.9,1.8), 8.51(8.2)
(*R*)-**63**	8.54	1.38(6.6), 1.43(6.6), 4.49(6.6)	7.41-7.57, 7.68-7.78, 7.89-7.98, 8.17(8.7), 8.40-8.45

[a]taken in $CDCl_3$.

their integrations was suggestive of C_2 symmetric species, this did not allow for differentiation between mono- and dimetallation (figure 3.3) as both exhibit C_2 symmetry. The spectra are depicted in figures 3.5 and 3.6.

For the free ligand (*R,R*)-**35** (figure 3.4) the imine proton appears in the aromatic region at 8.54 ppm. The remaining aryl-type signals are attributable to the quinoline rings, with the H_{5a}



(*R,R*)-**35** (*R*)-**36**

Figure 3.4 Atom numbering

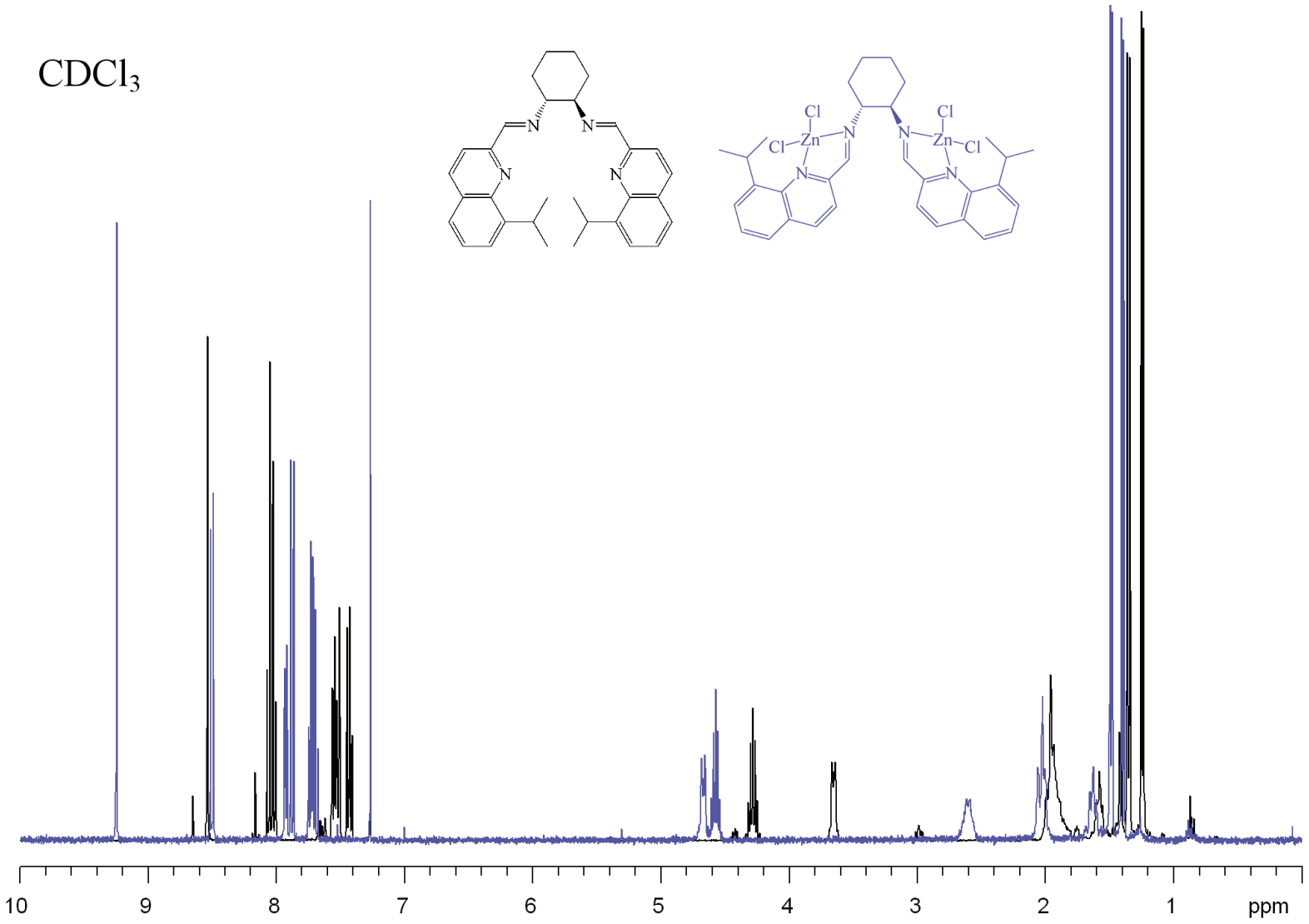


Figure 3.5 Overlaid ^{1}H NMR spectra of (*R,R*)-**35** (black) and (*R,R*)-**62** (blue)

and H_{6a} protons giving rise to the 8.00-8.08 ppm multiplet. At 4.29 ppm, and at 1.25 and 1.36 ppm, there are three bands that correspond to the isopropyl methine, and the two sets of methyl protons (H_{10a} and H_{11a}/H_{12a} respectively). Interestingly, the methyl signal is diastereotopically split, despite the intervening distance to the chiral center. The H_{11a} and H_{12a} nuclei are non-equivalent in the zinc complex (*R,R*)-**62** also, although the chemical shift difference between the doublets is slightly smaller. The remaining unassigned signals of (*R,R*)-**35** can be attributed to the cyclohexyl moiety, with the farthest downfield at 3.61-3.70 ppm, arising from H_{3a}.

Upon metallation to (*R,R*)-**62** the ligand electron density decreases, inducing a general downfield shift. The largest difference occurs for H_{3a}, which is now seen at ~4.7 ppm as compared to ~3.7 ppm in the free ligand. Given that the downfield movement of H_{4a} is less, (~0.7 ppm) this is suggestive of primarily inductive electron withdrawal, counterbalanced to a degree by back-bonding. The zinc d_{π}-orbitals are fully occupied, and it would seem, donate into the antibonding π-orbitals of the imine moiety. The aromatic signals are, on average, shifted to a lesser extent, though we could not precisely measure the positional changes owing to overlap of the bands. The nuclei that are non-conjugated and are spatially isolated from the metal, such as H_{1a}, H_{11a}, and H_{12a}, were observed to be affected the least by zinc coordination.

The ^{1}H NMR spectrum of the ligand, (*R*)-**36**, is of high complexity in the 7-9 ppm region, due to the multiple aromatic signals of the binaphthyl and quinoline groups. Accordingly, we could not with certainty assign the (*R*)-**36** aryl bands, nor those of the complex, (*R*)-**63**, with the exception of the readily identifiable H_{7b} imine signal. This, in analogy to its counterpart in the binap-Zn(salen) complex, (*R*)-**55**, was slightly shielded (-0.08 ppm) by metallation. A result which is counterintuitive considering the ability of Zn(II) to attract electrons, and its close proximity to the metal. The opposite, a deshielding effect, was by contrast observed for the

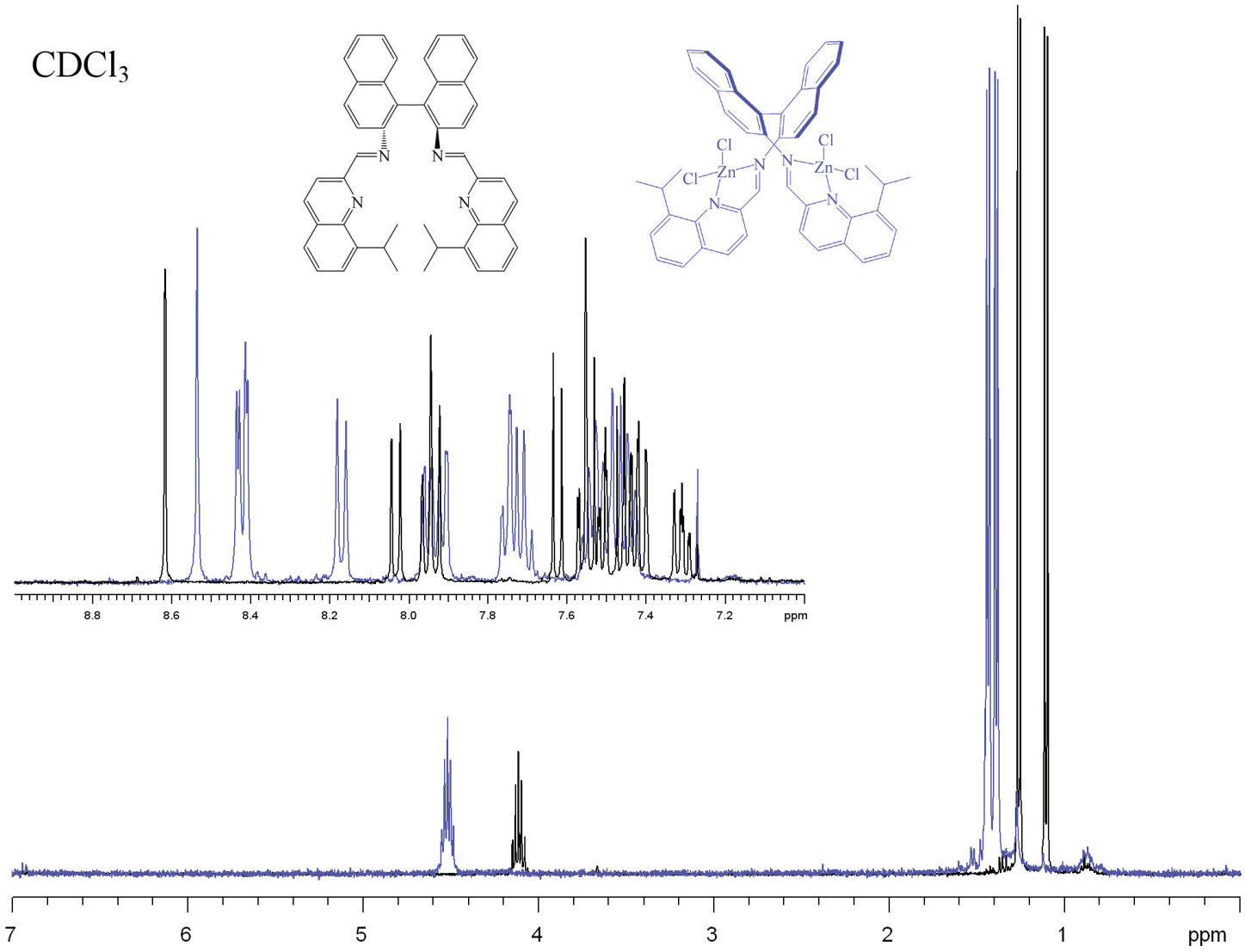


Figure 3.6 Overlaid ^{1}H NMR spectra of (*R*)-**36** (black) and (*R*)-**63** (blue)

imine H_{4a} proton of (*R,R*)-**62**. It is therefore unlikely that the innate electronic characteristics of zinc increase the electron shielding magnitude, but rather that other factors are the cause. The loss of coplanarity and resonance occurring between the naphthyl and quinolyl groups is one such possibility. Regarding the remaining signals both aliphatic and aromatic, the general trend is for a downfield shift. The proton H_{13b}, for example, is shifted by +0.3 ppm, and H_{14b}/H_{15b} are on average moved by +0.22 ppm. This is indicative of an inductive electron withdrawing effect operating on the ligand, due to the charged zinc ion.

3.3 Structural Studies

The zinc complexes were structurally characterized via X-ray crystallographic analysis. Suitable quality crystals of (*R,R*)-**62** and (*R*)-**63**, were respectively grown from CH_2Cl_2/Et_2O by slow diffusion, and from hot toluene by slow cooling. In figure 3.7 are shown the two crystal structures. (*R*)-**36** could not be obtained in crystalline form, affording instead a fine powder. The occurrence of (*R,R*)-**35** as an oil, precluded the growth of crystals.

In this work where phenoxides have constituted the side-arm donor groups, helical complexes have resulted. We had also hoped monohelimeric structures would form from ligands with pyridyl-like side-arms, despite their tendency to form helicates.[46] Unfortunately, as the crystal structures of (*R,R*)-**62** and (*R*)-**63** show, this is not the case. Each ligand coordinates to two $ZnCl_2$ groups, yielding complexes that are dimetallated and of the helicate class. A large quinolinyl separation is apparent in both, and no isopropyl-isopropyl overlap occurs between the side-arm fragments. Thus, given that the substances were intended to act as monoheliomeric

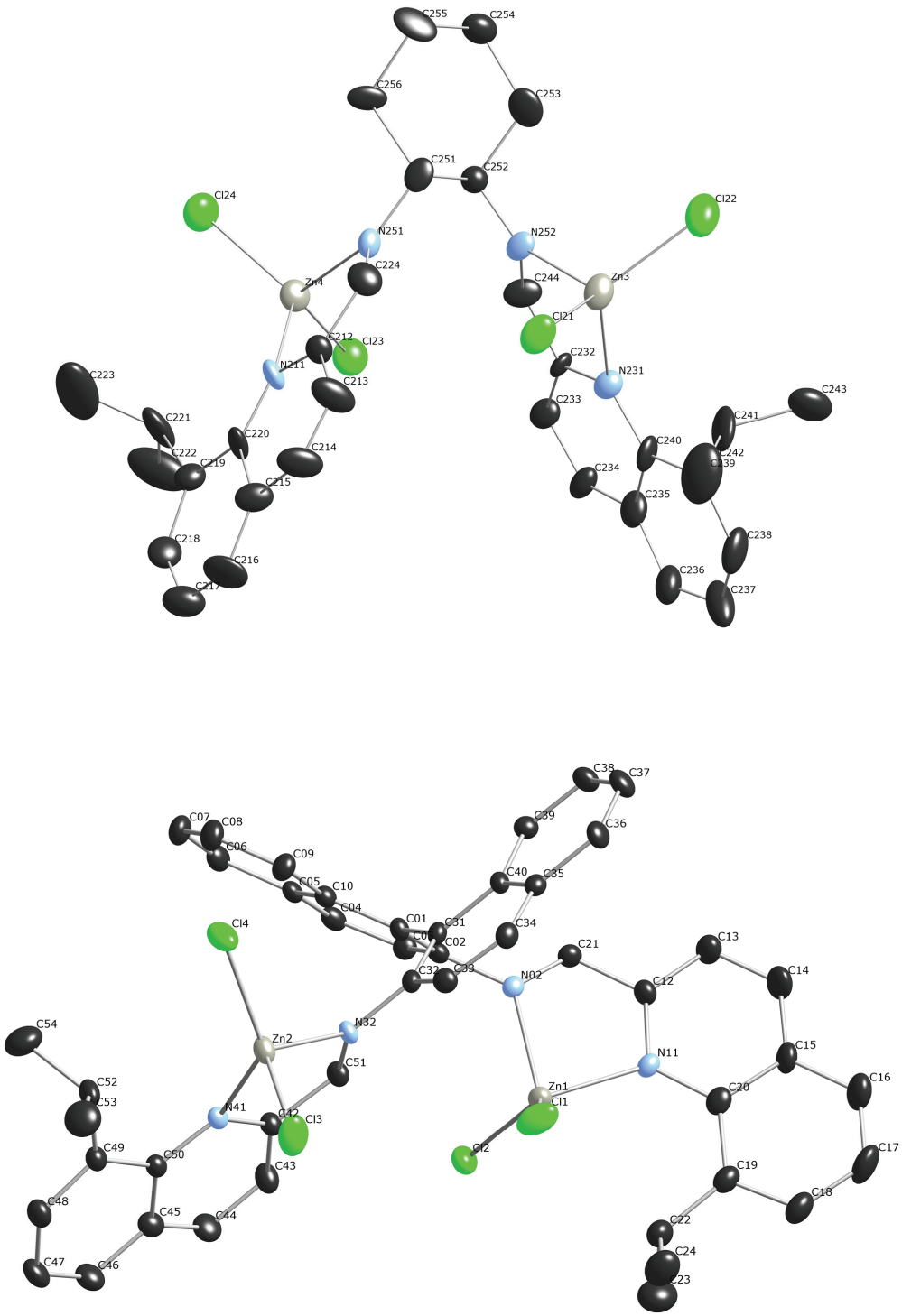


Figure 3.7 Thermal ellipsoid plots (50% probability) of the Zn(II) complexes (*R,R*)-**62** and (*R*)-**63** (top and bottom respectively)

catalysts, the structural modes encountered are undesirable. We attribute the preference for these geometries relative to monohelices, to the coordination numbers of the dinuclear species vs that of the unformed helimers, and to the binding ability of the ligating groups. Since, to accommodate two chloride ions in addition to four imine donors will very likely overcrowd the coordination sphere, and the only other possibility, chloride dissociation, will likely be energetically unfavorable. Spacefilling models of (*R,R*)-**62** (figure 3.8), for instance, indicate

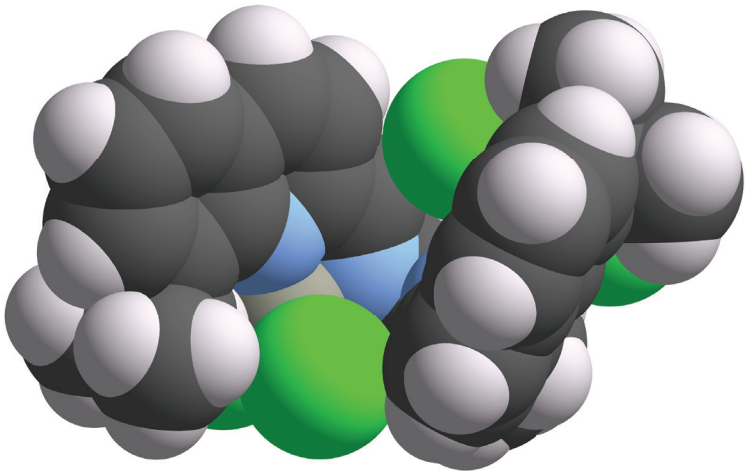


Figure 3.8 A side-on spacefilling plot of (*R,R*)-**62**

that there is little free space available around the zinc ions. In comparison, the phenoxide donor complexes in chapter 2 were five-coordinate at most, and where two complexes were otherwise analogous (see figures 2.18 and 2.20), the coordination of a fifth (solvent) group engendered reorientation of the bulk ligand, and of the remaining donors. For (*R,R*)-**62** there does however appear to be a helical twist (side-on view figure 3.8), which may allow the complex to act as a helimeric catalyst, though not in the manner we anticipated.

CHAPTER 4

Synthesis, Characterization, and Study of Benz[a]anthryl Derived Complexes

4.1 Introduction

With the phenanthryl derived salen complexes in chapter 2, the solid state structures were found to simultaneously incorporate *M* and *P* helices. Also, for these, the extent of ligand arm overlap was moderate at best. It was hypothesized that these two factors were related, and that an increase in the amount of side-arm arm overlap might well result in exclusive adoption of the *M* geometry. Moreover, a secondary benefit was thought possible, in that a larger 'step' to the M(salen) and binap-M(salen) structures, would increase the variation in topology between the different regions of each chiral face – an outcome beneficial for enantioselective catalysis. The work that is included in this chapter originates from these conjectures, namely, the synthesis and study of complexes of **43**, the benz[a]anthryl group.

4.2 Synthesis

Our initial methodology for preparing **43** utilized anthracene as the starting point (figure 4.1). Its reactivity towards acylation,[93] however, was such that predominately the 9-substituted product formed, in preference to the 2-isomer. Upon purification we, at most, were able to isolate **65** in 11% yield, which due to the number of steps involved was insufficient for the

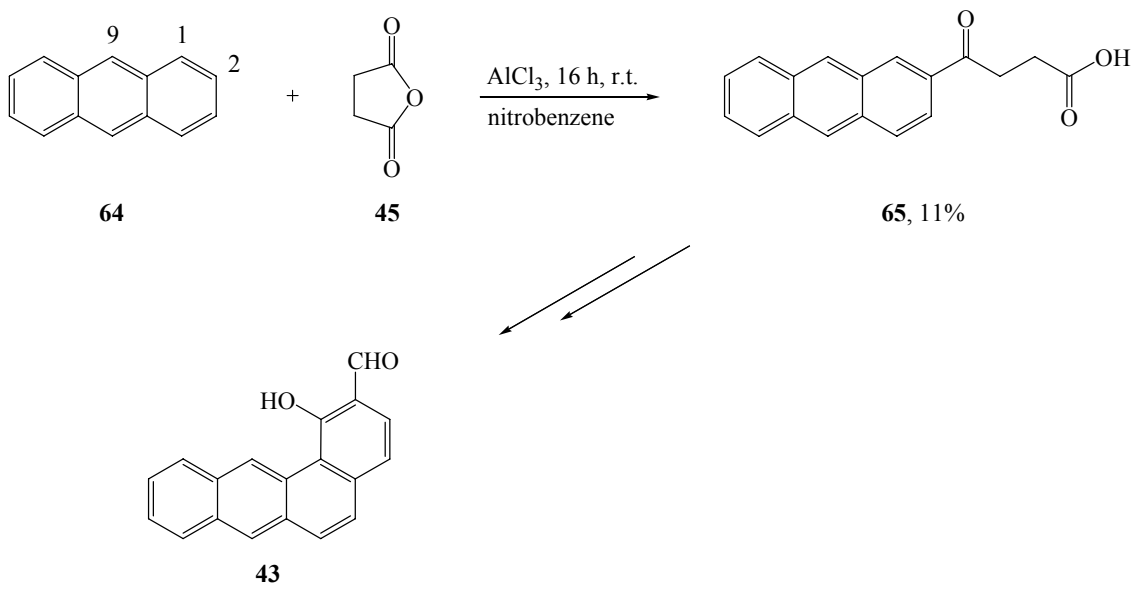


Figure 4.1 Attempted/planned route for the synthesis of **43**

synthesis of **43** in multi-gram quantities. Our attention therefore turned to a modified preparative route utilizing 9,10-dihydro-anthracene (figure 4.2). Formation of the 9/10-substituted regiomer of **66** did not occur, as the aforementioned positions are inert to electrophilic aromatic substitution. Rather, carboxylic acid **67** was the major product, and after purification was isolated in 61% yield. Analysis of **67** showed it to contain a small quantity (3-5%) of an analogue in which the central ring was fully aromatized, and whose removal we did not attempt, since via our methodology this is ultimately converted to **43**. Derivatives corresponding to this oxidized form were also present in the end products of the succeeding two steps, constituting approximately 10% of the isolated material. In the next step, standard Wolf-Kishner[94] conditions were employed to reduce the ketone group to a methylene unit, affording **68**. Due to unfavorable regioselectivity[95] all attempts to cyclize at this point gave primarily the linear ketone (figure 4.3), necessitating that **68** be aromatized prior to cyclization (figure 4.2). The compound was methylated to prevent substrate derived catalyst inactivation, and subsequently dehydrogenated

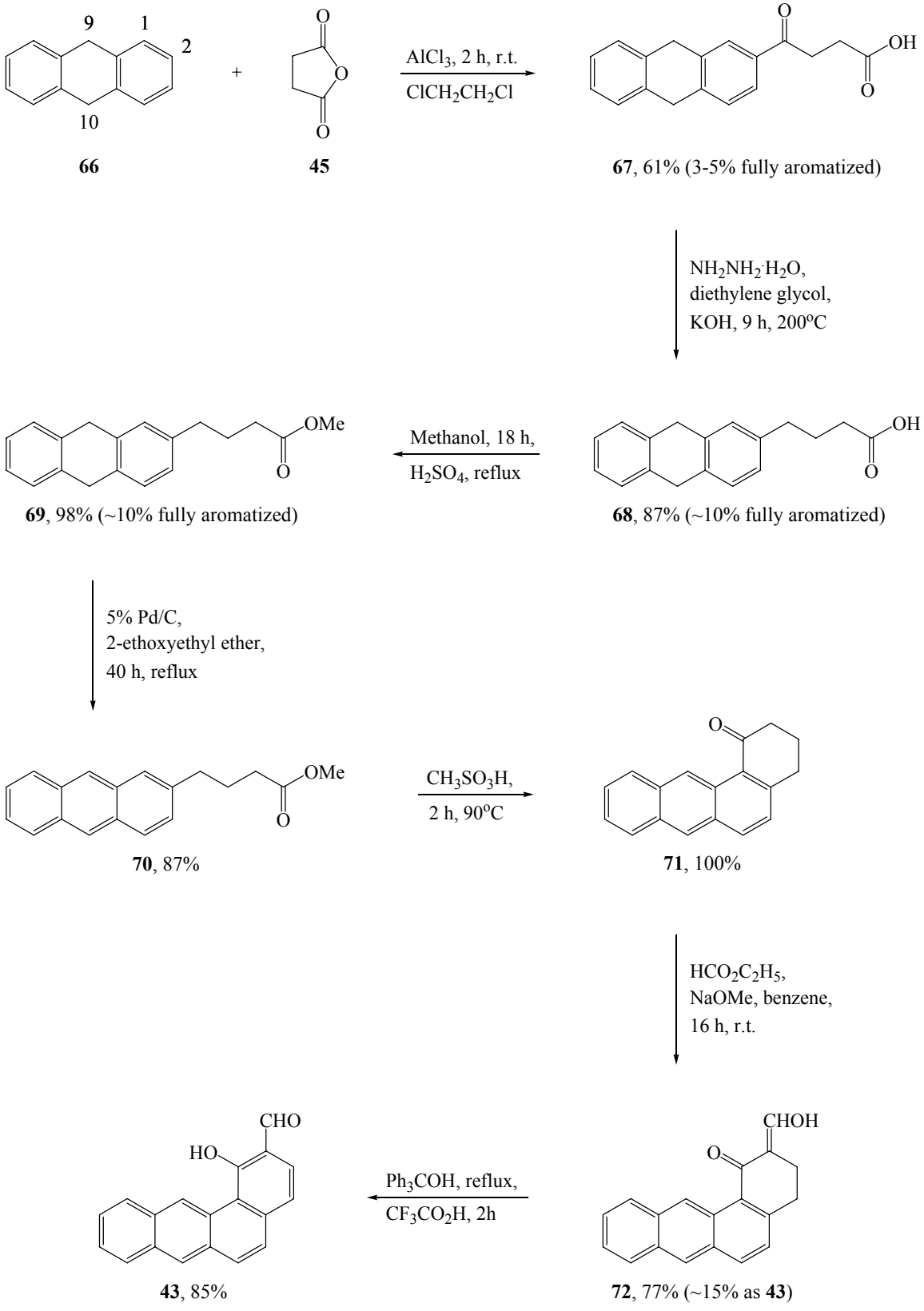


Figure 4.2 Preparation of **43**

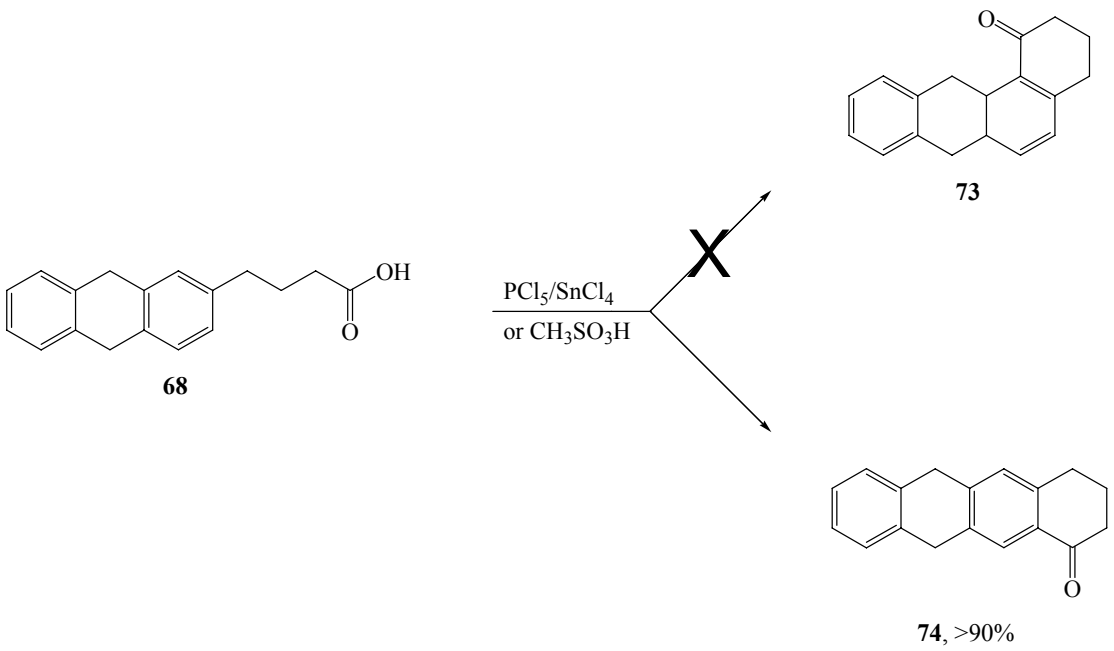


Figure 4.3 Attempted cyclization of **68** to **73**

(aromatized) to **70** using Pd/C in high boiling ether solvent.[96] The product ester **70** was then treated with methanesulfonic acid,[69] proceeding via a Friedel-Crafts[97] type reaction, to give heterocycle **71** in quantitative yield. ^{1}H NMR analysis indicated it to be contaminated by the analogous linear ketone in trace quantities only. Employing basic conditions this was condensed with ethyl formate, which resulted in formation of **72**. With regards to the material isolated after workup, approximately 15% of the 77% was in fact found to be **43**, the desired end product. Conjugation across the entire molecule evidently furnishes a system that is favored thermodynamically, in comparison to its partially conjugated precursor. In the final step, triphenylmethanol in TFA[72] was utilized to oxidize the predominately **72** mixture to **43**. The yield over the 7 steps was 30%, a modest improvement over the synthesis of the 3-ring phenanthryl analogue, **41** (23%), despite the larger number of steps required.

Our next goal was to prepare ligands from aldehyde **43**, and thereafter metallate. Using our previously determined standard Schiff-base formative conditions, the aldehyde and stoichometric quantities of (*R,R*)-**39** and (*R*)-**40**, were condensed in refluxing ethanol. (*R,R*)-**37**

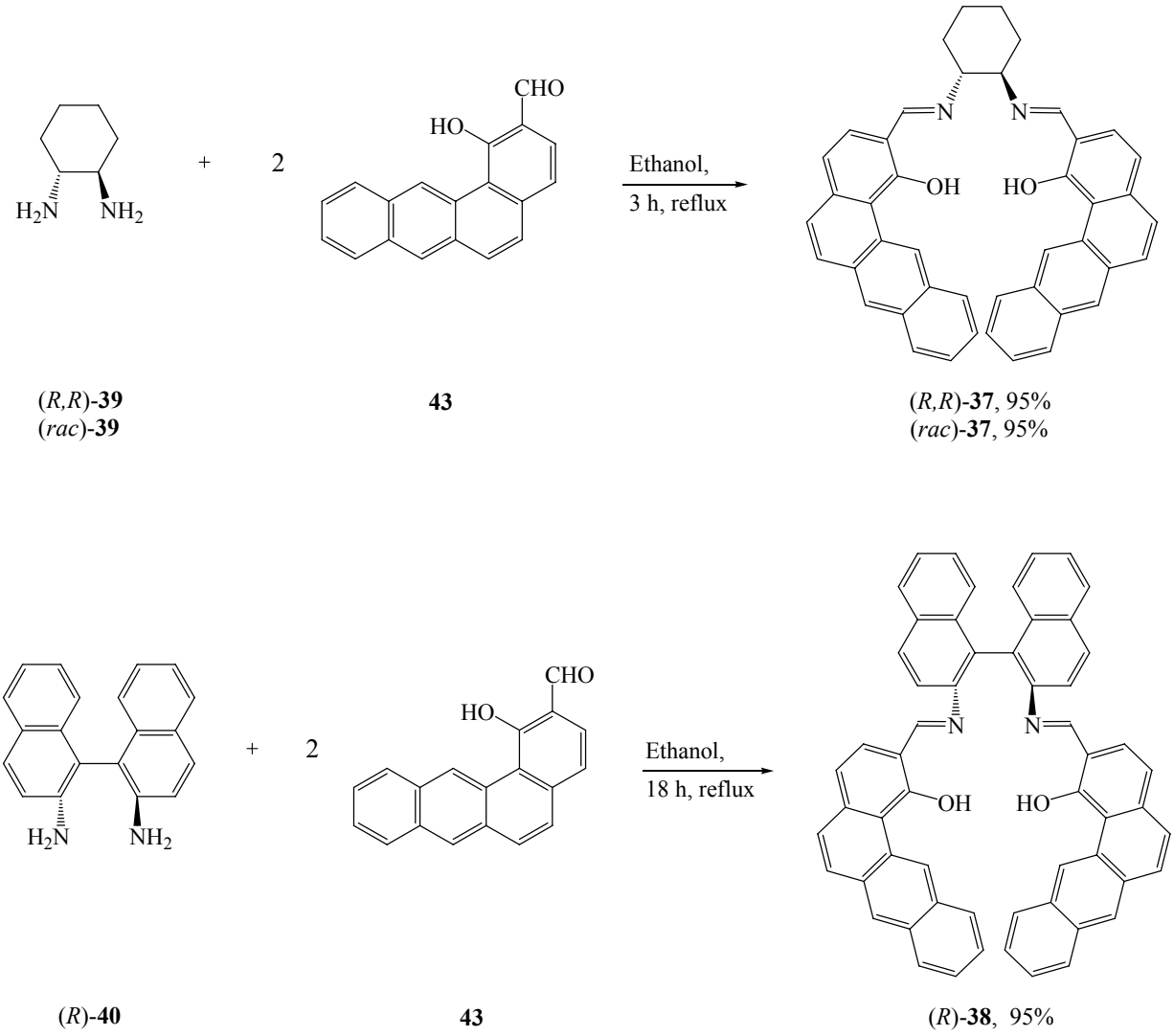


Figure 4.4 Preparation of (*R,R*)-**37**, (*rac*)-**37** and (*R*)-**38**

and (*R*)-**38** were generated as the respective products (figures 4.4). The binaphthyl ligand formed considerably more slowly than the corresponding cyclohexyl ligand, and required longer

reaction times to reach completion. We additionally synthesized (*rac*)-**37** (racemic, trans **37**) from (*rac*)-1,2-cyclohexanediamine, via conditions identical to that for the pure *R,R*-enantiomer. The ligands (*R,R*)-**37**, (*rac*)-**37**, and (*R*)-**38**, were isolated in close to quantitative yields (95%).

Subsequently, the ligands were metallated with $FeCl_2$ and $ZnCl_2$, employing sodium methoxide as the requisite base (figure 4.5). For the solvent system a mixture of either methylene chloride and ethanol, or benzene and ethanol was chosen. The use of a combination

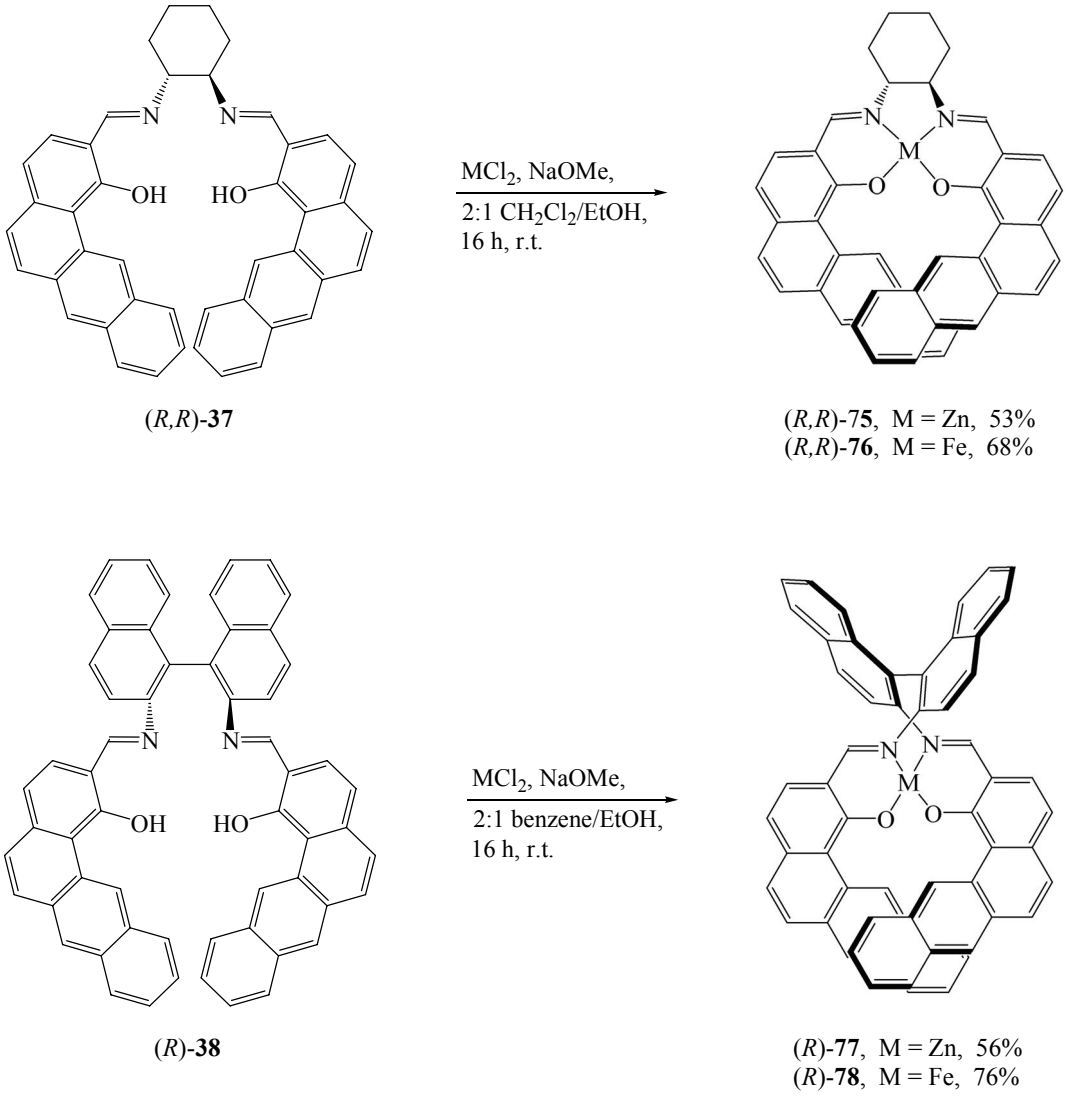


Figure 4.5 Inclusion of Zn(II) and Fe(II)

of polar and non-polar solvents was necessary, given that the sodium salts of (*R,R*)-**37** and (*R*)-**38** were otherwise insoluble. Poor yields resulted if either of the two solvents were used uncombined. The complexes incorporating iron(II) were found to be highly sensitive to air and water, which was also the case for the phenanthryl analogues discussed in chapter 2. Upon exposure, minimal traces engendered a rapid change in color, concurrent with the formation of uncharacterized oxidation products. The zinc(II) complexes were, by contrast, air stable as solids, though they exhibited some slight sensitivity to water via hydrolysis, when in non-anhydrous solvents.

4.3 NMR Spectroscopy of the Ligands & Diamagnetic Zinc Complexes

To characterize, the ^{1}H and ^{13}C NMR spectra of the Schiff bases and zinc complexes were recorded. In Table 4.1 are listed the respective ^{1}H NMR chemical shifts. The spectra were consistent with C_2 symmetric molecular species, generally exhibiting well resolved bands. Signals equating to both helimeric types were not seen for (*R,R*)-**75** and (*R*)-**77** (-90ºC to +90ºC), suggesting the existence of one form only in solution. For (*R,R*)-**75**, the possibility of interconversion faster than the NMR timescale could not be ruled out, but is unlikely due to the occurrence of extensive ligand arm overlap (figure 4.7). Presumably, this will slow the movement of the ligand arms past one another, and consequently inhibit the interconversion process.

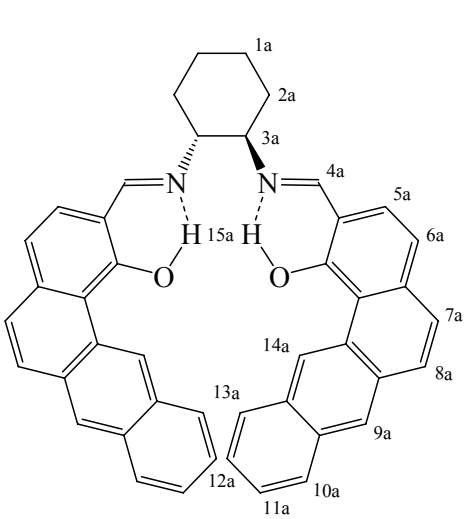
The spectrum of the ligand, (*R,R*)-**37**, incorporates several readily identifiable low-field signals. The intramolecularly H-bonded proton H_{15a} (figure 4.6), is visible at 16.28 ppm, and at

Table 4.1 Ligand and Zn(II) complex ^{1}H NMR chemical shifts[a]

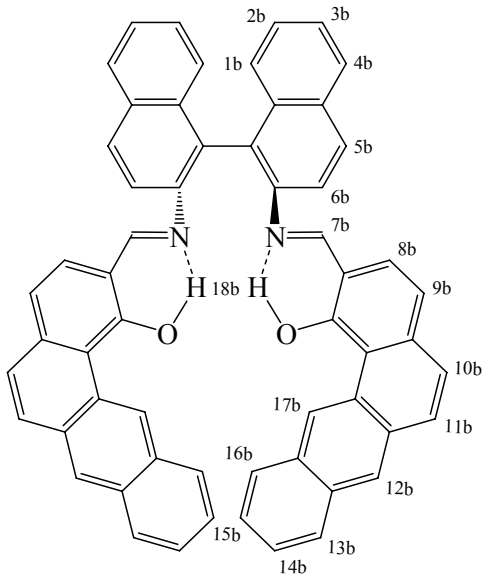
	Chemical shifts, $\delta(^{3}J,^{4}J)$			
	Imine C–H	O··H··N	Aliphatic C–H	Aromatic C–H
(*R,R*)-**37**[b]	8.63	16.28	1.34-1.49, 1.62-1.82, 1.99-2.08, 3.44-3.55	7.11(8.1), 7.37(8.1), 7.51(8.8), 7.56-7.63, 7.91(8.8), 8.09-8.16, 8.27-8.34, 8.46, 11.21
(*R*)-**38**[c]	8.93	15.17		7.17(8.0), 7.34(8.0), 7.42-7.50, 7.57-7.67, 7.71(7.4), 7.80(8.7), 7.95(8.7), 8.04(8.2), 8.21-8.27, 8.30, 8.38(8.7), 9.96
(*R,R*)-**75**[b]	8.68		1.25-1.40, 1.76-1.87, 2.29-2.40, 3.27-3.36	6.45(7.4), 7.12(7.4), 7.29(8.0), 7.48(8.3), 7.68(8.0), 7.76(8.8), 7.91(8.3), 8.05(8.8), 8.47, 12.15
(*R*)-**77**[c]	8.58			6.70(7.5), 6.99(8.6), 7.09(8.2), 7.19(7.5), 7.23-7.29, 7.44(7.6), 7.48(8.5), 7.51-7.55, 7.84(8.3), 7.91(8.2), 7.95(8.8), 8.02(8.6), 8.32, 11.30

[a]For (*rac*)-**37** see the relevant (*R*, *R*)-enantiomer chemical shifts. [b]Taken in pyridine-d_5. [c]Taken in $CDCl_3$.

8.63, 8.46, and 11.21 ppm, are singlets that respectively correspond to the H_{5a}, H_{9a}, and H_{14a} protons. The individual H-bonded tautomers were not discernable on the NMR time scale, and



(*R,R*)-**37**



(*R*)-**38**

Figure 4.6 Atom numbering

only the average structures were seen. We also, based upon literature values, assign the multiplet at 7.6 ppm to the overlapped resonances of H_{11a} and H_{12a}, and those at 8.1 and 8.3 ppm to H_{10a} and H_{13a}.[98] The signals of the cyclohexyl moiety appear in the 0-4 ppm region, H_{3a} affording the most downfield at 3.5 ppm.

Metallation to prepare (*R,R*)-**75**, results in a number of significant chemical shift differences relative to the free ligand. The terminal aryl rings are closely overlapped in the complex (figure 4.7), wherein each induces in the other an opposing diamagnetic ring-current.[99] The protons H_{10a}, H_{11a}, H_{12a}, and H_{13a}, are therefore shielded and moved upfield, with, for

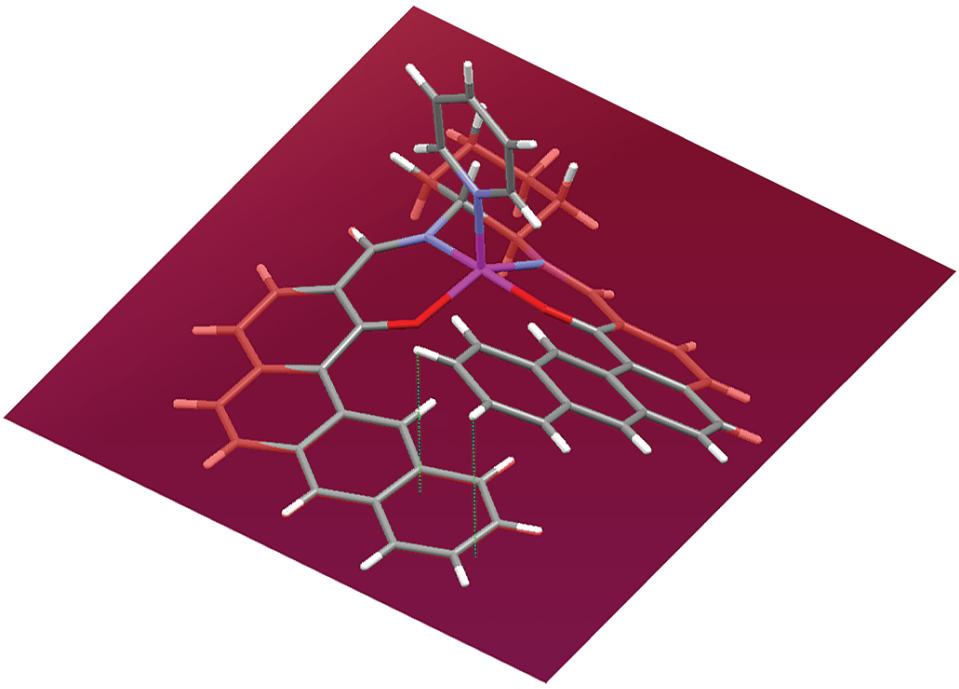


Figure 4.7 Position of H_{12a} and H_{13a} in the (*R,R*)-**75**·py crystal structure

example, H_{11a} shifted by -0.5 ppm to 7.1 ppm. The upfield movement of H_{12a} is notably the largest of the four (-1.1 ppm), which can be attributed to its relative spatial position. The proton being situated approximately above the centre of the underlying ring, and in the region of

greatest induced shielding. A contribution from the diamagnetic anisotropy of the π-electrons is moreover expected, that will likely factor into the upfield (shielding) shift.[99a] The complexity of the spectrum did not allow for exact assignment of H_{5a}-H_{8a}, although, for these, a general downfield signal movement was apparent. H_{5a}, H_{9a}, and H_{14a}, were similarly deshielded via inductive electron withdrawal, as a result of the electropositive zinc.

For (*R*)-**38**, the majority of signals could not be assigned with sufficient certainty, due to the sheer number of contiguous and overlapping aryl bands. Only those at 8.93, 8.30, 9.96, and 15.17 ppm were identified, and respectively ascribed to the protons H_{7b}, H_{12b}, H_{17b}, and H_{18b}. For the same reasons, difficulties were encountered in our attempts to assign the spectrum of the zinc complex, (*R*)-**77**. Here, solely the 8.58, 8.32, 6.70, and 11.30 ppm signals, which correlate to the H_{7b}, H_{12b}, H_{15b}, and H_{17b} protons, were denoted. From the chemical shift of the H_{15b} signal, it is evident that the same inductive diamagnetic ring-current mechanism, as evinced in (*R*)-**75** is in operation. The higher shift value vs H_{12a} (6.70 vs 6.45 ppm) may be explained by less ring overlap, which gives rise to a smaller shielding effect. A general upfield shift also manifests for most of the remaining signals. This, we attribute to the structural reorientation and consequent loss of resonance, occurring upon formation of the zinc complex.

4.4 NMR Spectroscopy of the Paramagnetic Iron Complexes

The ^{1}H NMR spectra of the iron complexes (*R,R*)-**76** and (*R*)-**78** were collected, and are depicted in figure 4.8. Table 4.2 lists their respective chemical shifts. Spectral bands were visible outside of the normal diamagnetic range, and broadened to linewidths of between

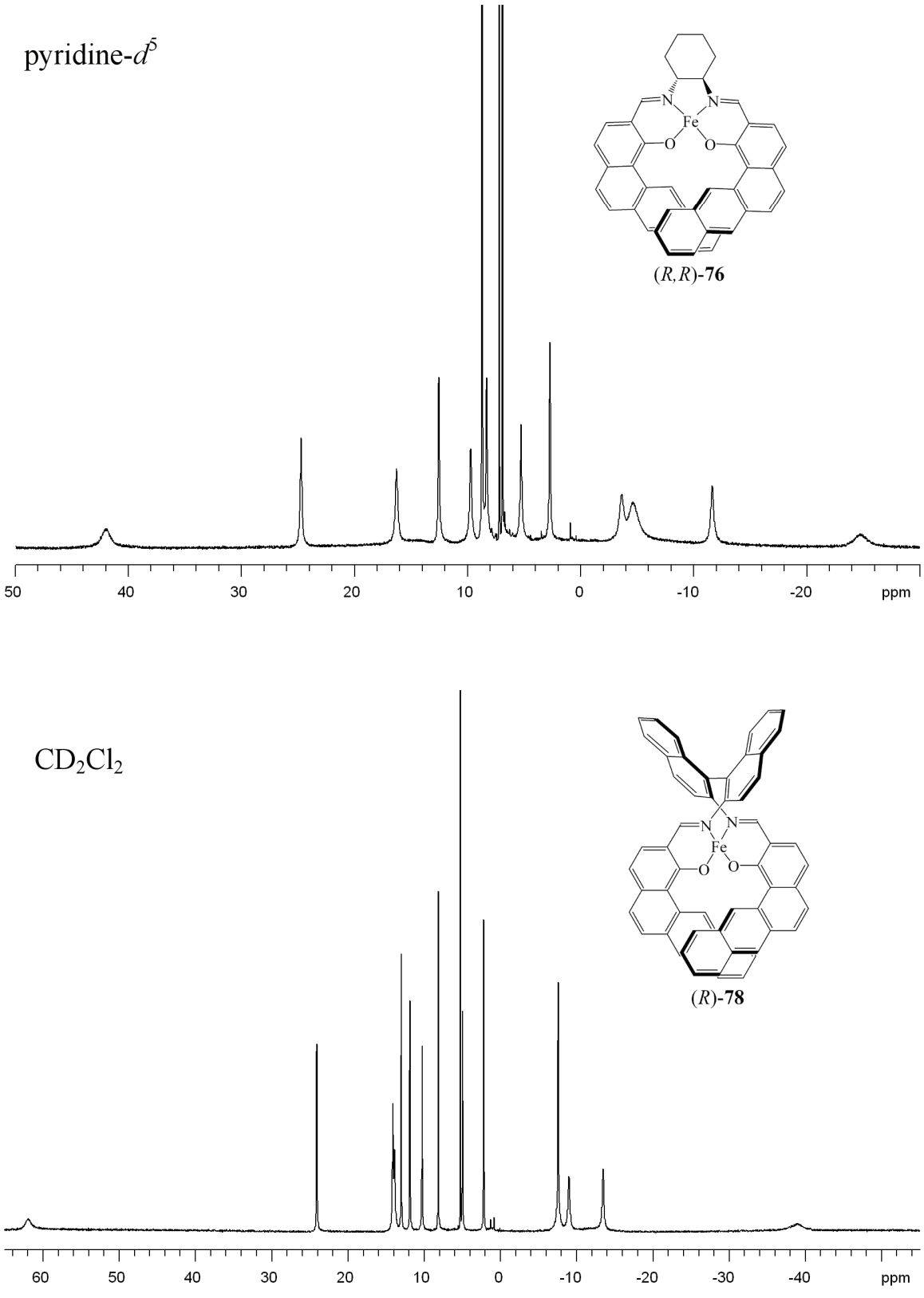


Figure 4.8 400MHz ^{1}H NMR spectra of (*R,R*)-**76** and (*R*)-**78**

Table 4.2 Fe(II) complex ^{1}H NMR chemical shifts

	Chemical shifts, δ
(*R,R*)-**76**[a]	⁻24.70, ⁻11.61, ⁻4.60, ⁻3.63, 2.74, 5.29, 8.34, 9.75, 12.57, 16.31, 24.76, 41.96
(*R*)-**78**[b]	⁻38.90, ⁻13.43, ⁻8.94, ⁻7.52, 2.25, 5.02, 8.18, 10.33, 11.90, 13.05, 13.92, 14.16, 24.12, 61.97

[a]Taken in pyridine-d_5. [b]Taken in CD_2Cl_2.

100 to 2500 Hz. The major basis of this effect, dipolar relaxation, attenuates rapidly on distance, having an inverse r^6 dependence on the metal-nuclei separation.[74] As such, signals that arise from protons in close proximity to the high-spin paramagnetic Fe(II) ion, will exhibit the most line broadening. The through-bond (contact) relaxation mechanisms in operation are substantially weaker in effect, and contribute to linewidths to a lesser extent. Thus, the ⁻24.70, ⁻4.60, and 41.96 ppm signals of (*R,R*)-**76**, likely derive from H_{3a}, H_{4a}, and H_{14a}. In analogy, those at ⁻38.90 and 61.97 ppm for (*R*)-**76**, we denote to H_{7b} and H_{17b}. With regards to the chemical shifts, the pattern of alternate upfield and downfield shifted signals is indicative of a spin polarization pathway.[75] The unpaired spin density in the Fe(II) *d*-orbitals is delocalized across the π system, and contact shift interactions dominate both (*R,R*)-**76** and (*R*)-**78**.

4.5 Structural Studies of the M(salen) Ligands and Complexes

Crystals suitable for X-ray analysis were grown of the M(salen) complexes (*R,R*)-**75** and (*R,R*)-**76**. Table 4.3 lists for each the conditions employed, where A is the solvent into which the substance was first dissolved, and over which B was subsequently overlaid. Our attempts to

Table 4.3 Crystal growth conditions

	Method	Solvent A	Solvent B
(*R,R*)-**75**	Diffusion	Pyridine	Diethyl ether
(*R,R*)-**76**	Diffusion	Pyridine	Ethanol

prepare crystals of (*R,R*)-**37** via the same and also other alternate methods, were unsuccessful, yielding in all cases an oily residue. The use of a racemic mixture, an approach which at times we have found effective, gave for (*rac*)-**37** material that was again unsuitable and only partly crystalline in character.

The crystal structure of (*R,R*)-**75** was found to incorporate exclusively *M*-helicies. As shown in figure 4.9, the benz[a]anthryl arms are extensively overlapped, with the final 2/3 of the

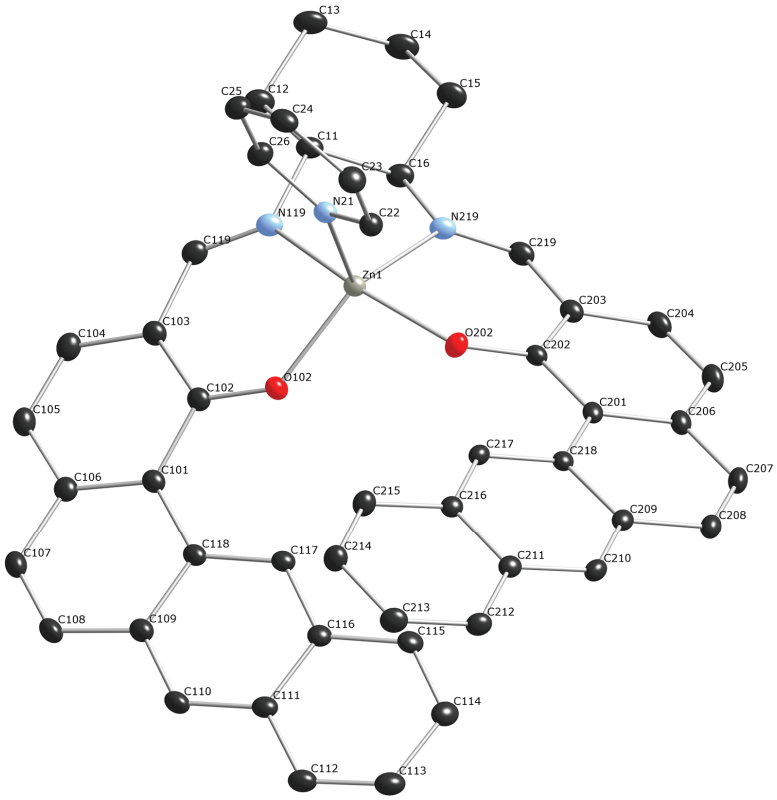


Figure 4.9 A thermal ellipsoid plot (50% probability) of (*R,R*)-**75**·py

terminal aryl rings approximately overlying. Interconversion to the *P*-helimer is as a result likely to be slow, and engender considerable strain in the transitory process. This contrasts with the solid-state structure of (*R,R*)-**76** in which we, surprisingly, observed both of the helimeric forms (figure 4.10). The sole difference chemically is a change from Zn(II) to Fe(II), that in some way must direct the structural preference. Notably, no such structural divergence occurred between the phenanthryl analogues, (*R,R*)-**53** and (*R,R*)-**54**. This suggests that while the differences in energies are small, the *M*-helimer as we have previously alluded, is favored. To examine the energy/structure relationship we therefore calculated the B3LYP energies,[100] of DFT minimized *P* and *M* (*R,R*)-**76**·py, and of (*R,R*)-**75**·py (see appendix IV). As no *P* (*R,R*)-**75**·py structure crystallographically occurs, the Fe(II) ion of *P* (*R,R*)-**76**·py was substituted with Zn(II), to generate this initial geometry. Our results from these computations were insightful, showing that for the iron(II) complex the *M*-helimer was favored by less than 1.0 kcal/mol, and that for the zinc analogues the difference was substantially larger at ~3.5 kcal/mol. As such, this trend clarifies why in the first case a pseudo-racemic mixture is seen, and in the second only *M*-helices.

The molecular structure of (*R,R*)-**75**·py generally resembles the *M*-helimer of (*R,R*)-**53**·py, albeit with some differences. The ligand arms which are inclined toward the zinc ion in a pyramidal fashion in (*R,R*)-**53**·py (figure 2.12), are less so orientated in the benz[a]anthryl complex (figure 4.11). This is expressed in the N=C–C=C torsion angles, which for N119–C102 and N219–C202 of (*R,R*)-**75**·py, are -9.7(3)^{o} and 6.3(3)^{o} respectively. By comparison the N12–C202 and N11–C102 torsions of *M* (*R,R*)-**53**·py, their equivalents, are -3.5(8)^{o} and -0.4(9)^{o}. Upon transmission and amplification along the side-arms this equates to a lessening of the pyramidalization effect. As to the overall cause, its origin appears to lie in the sizes of the

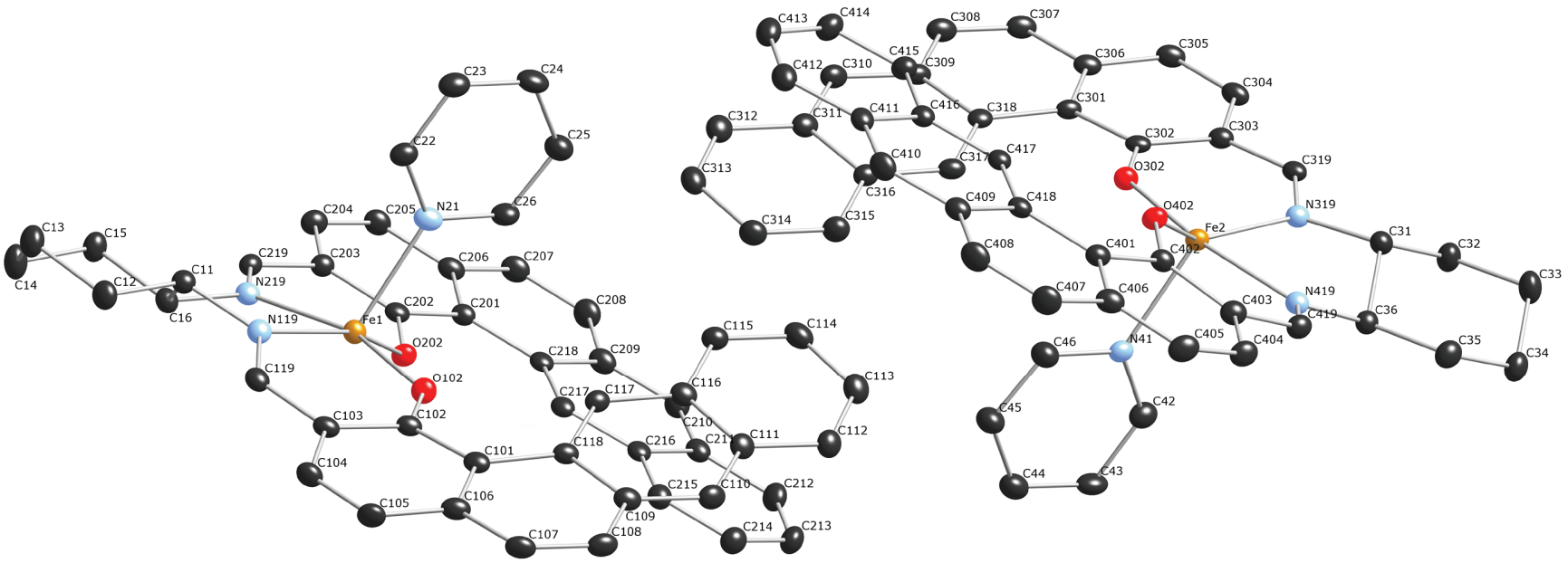


Figure 4.10 Thermal ellipsoid plots (50% probability) of *P* and *M* (*R*,*R*)-**76**·py (*P* left, *M* right)

phenanthryl and benz[a]anthryl groups; a greater degree of tilt is not readily possible, without generating increasingly unfavorable edge to face steric interactions.

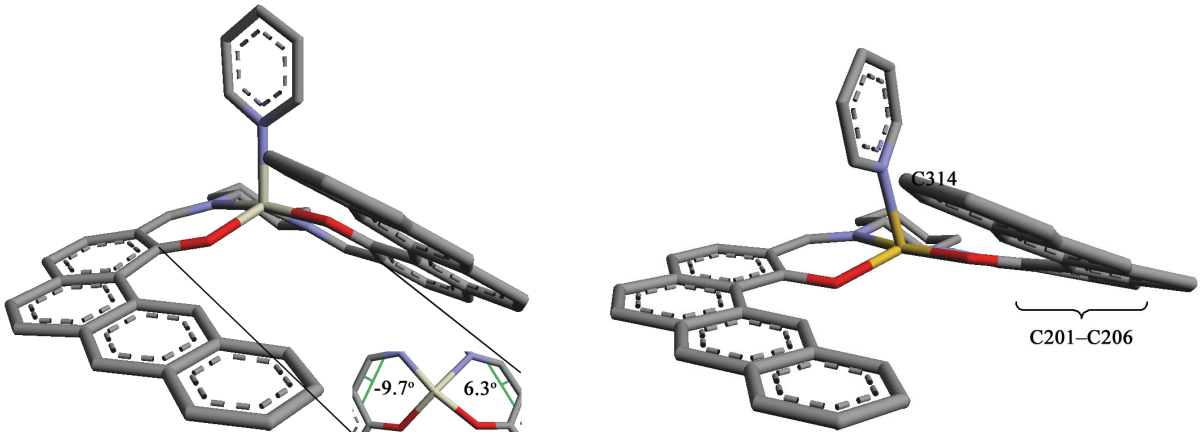


Figure 4.11 Side-by-side comparisons of (*R,R*)-**75**·py (left) and *M* (*R,R*)-**76**·py (right)

For the *P* and *M* helimers of (*R,R*)-**76**·py (figure 4.11, only *M*-helimer shown), though of greater magnitude, a pyramidalization decrease which parallels that of the zinc complex is seen. The underlying side-arms are slightly downward tilted, and the slant of the upper arms appears to result more from curvature of the benz[a]anthryl groups, than from the N=C–C=C torsion angles. C314 of the upper terminal ring of *M* (*R,R*)-**76**·py, for example, is situated 0.66 Å above the plane defined by the atoms C201 to C206, which constitute the first, and metal-adjacent aryl ring (figures 4.10 & 4.11). Consistent with this molecular arrangement, is a relatively small deformation of the Fe(II) ion from the mean N,N,O,O donor planes (table 4.4). The displacement for (*R,R*)-**76**·py is on average 0.290 Å, while that of (*R,R*)-**75**·py is significantly larger at 0.472 Å. A smaller displacement allows for less drawn-in and upward tilted ligand arms, which appears to facilitate π-π interactions. The terminal aryl rings are half offset, a

necessary occurrence for σ-π electron association, and the carbon to centroid distances are within the 3.4-3.6 Å range expected for attractive π-π stacking.[101]

In both complexes the metal geometry is five-coordinate and slightly distorted from square-pyramidal. The axial sites are occupied by pyridine, with each ligating molecule approximately perpendicular to the adjoining N,N,O,O donor plane. The coordinate bond lengths, listed in table 4.4, for the most part reflect the variation in the ionic radii where Zn(II) is

Table 4.4 Selected bond lengths, their averages, and metal atom displacements from the mean N,N,O,O donor planes for (*R,R*)-**75**·py and (*R,R*)-**76**·py

		Bond lengths, Å						Displace-Ments, Å
(*R,R*)-**75**·py	(*M*)	Zn_1–N_{119}	2.063(2)	Zn_1–O_{102}	1.978(1)	Zn_1–N_{21}	2.123(2)	0.472
		Zn_1–N_{219}	2.105(2)	Zn_1–O_{202}	1.984(1)			
	Av.		2.084		1.981			
(*R,R*)-**76**·py	(*P*)	Fe_1–N_{119}	2.105(2)	Fe_1–O_{102}	1.970(2)	Fe_1–N_{21}	2.147(2)	0.288
		Fe_1–N_{219}	2.113(2)	Fe_1–O_{202}	1.982(2)			
	(*M*)	Fe_2–N_{319}	2.095(2)	Fe_2–O_{302}	1.993(2)	Fe_2–N_{41}	2.154(2)	0.292
		Fe_2–N_{419}	2.108(2)	Fe_2–O_{402}	1.964(2)			
	Av.		2.105		1.977		2.151	0.290

marginally smaller (~0.03 Å). The M–O distances deviate from this trend, but the radii difference is of a size that may easily be offset by other forces. One such are repulsive edge to face contacts that lead to a maximized benz[a]anthryl-benz[a]anthryl separation, thereby affecting the bridging M–O bonds. In comparison to their phenanthryl counterparts, the coordinate bond average lengths for (*R,R*)-**75**·py and (*R,R*)-**76**·py, are between 0-0.04 Å greater. The increases appear more substantial for the iron(II) complex, which may relate to the necessity of half offset aryl rings for attractive π-π stacking.[101]

4.6 Structural Studies of the binap-M(salen) Ligands and Complexes

Single crystals suitable for X-ray analysis were grown of (*R*)-**38**, (*R*)-**77**, and (*R*)-**78** via slow diffusion. Table 4.5 lists the conditions employed, where A is the primary solvent into which the substance was dissolved, prior to layering with solvent B.

Table 4.5 Crystal growth conditions

	Method	Solvent A	Solvent B
(*R*)-**38**	Diffusion	Methylene chloride	Hexanes
(*R*)-**77**	Diffusion	Methylene chloride	Diethyl ether
(*R*)-**78**	Diffusion	Methylene chloride	Diethyl ether

The structure of (*R*)-**38** consists of a single, approximately C_2 symmetric ligand molecule (figure 4.12). The naphthyl and benz[a]anthryl groups which comprise each half of the structure are extensively π-delocalized, and show near co-planarity, as indicated by the inter-plane angles of 7.0° and 7.6°. Further stabilizing this arrangement are H-bonding contacts, which occur between the hydroxyl moieties and imine nitrogen atoms. The contact distances for H102–N119 and H202–N219, are 1.75 and 1.77 Å respectively. The dihedral angle arising between the naphthyl planes is 108.1°, and unambiguously within the ~60-130° limits, that define the walls of the steep-sided torsional energy well.[32] The energy minima of the naphthyl dihedral of 1,1-binaphthyl, by comparison, is situated at ~90°.

For (*R*)-**77**, each asymmetric unit of the crystal incorporates two slightly varying molecules. Figure 4.13 depicts thermal ellipsoid and space filling plots of one of the two (henceforth termed (*R*)-**77A**). The ligand side-arms overlap to a moderate degree, although less than in (*R,R*)-**75**, the analogous cyclohexyl complex. Both forms are organized in a distorted

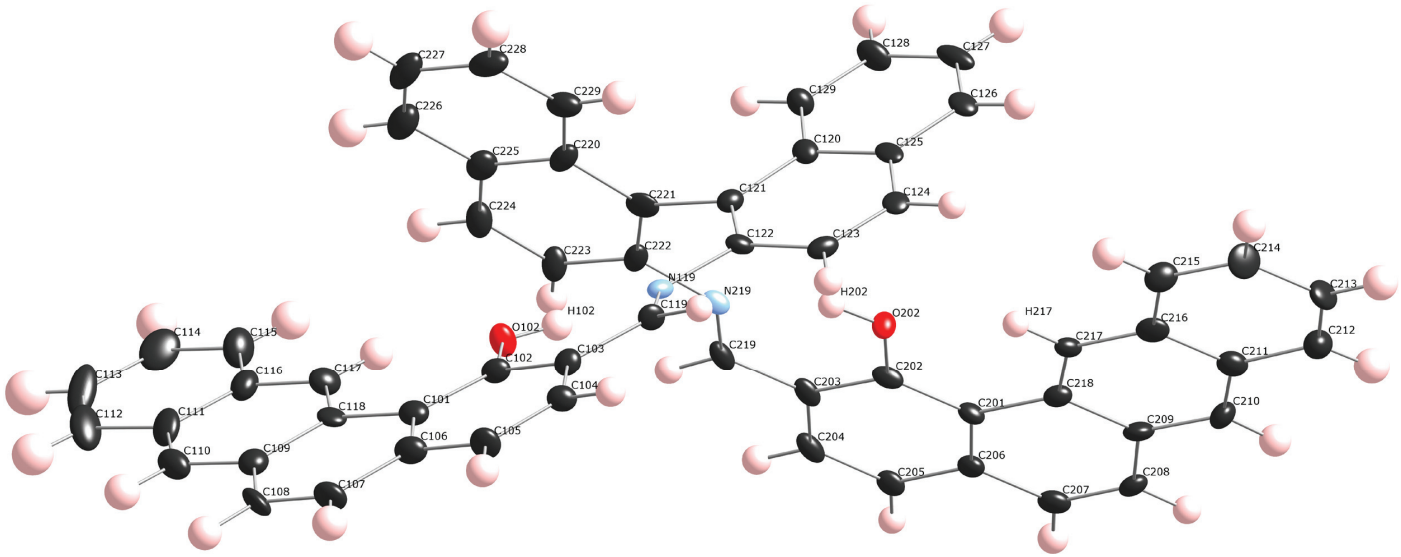


Figure 4.12 A thermal ellipsoid plot (50% probability) of the binaphthyl-benz[a]anthryl ligand, (*R*)-**38**

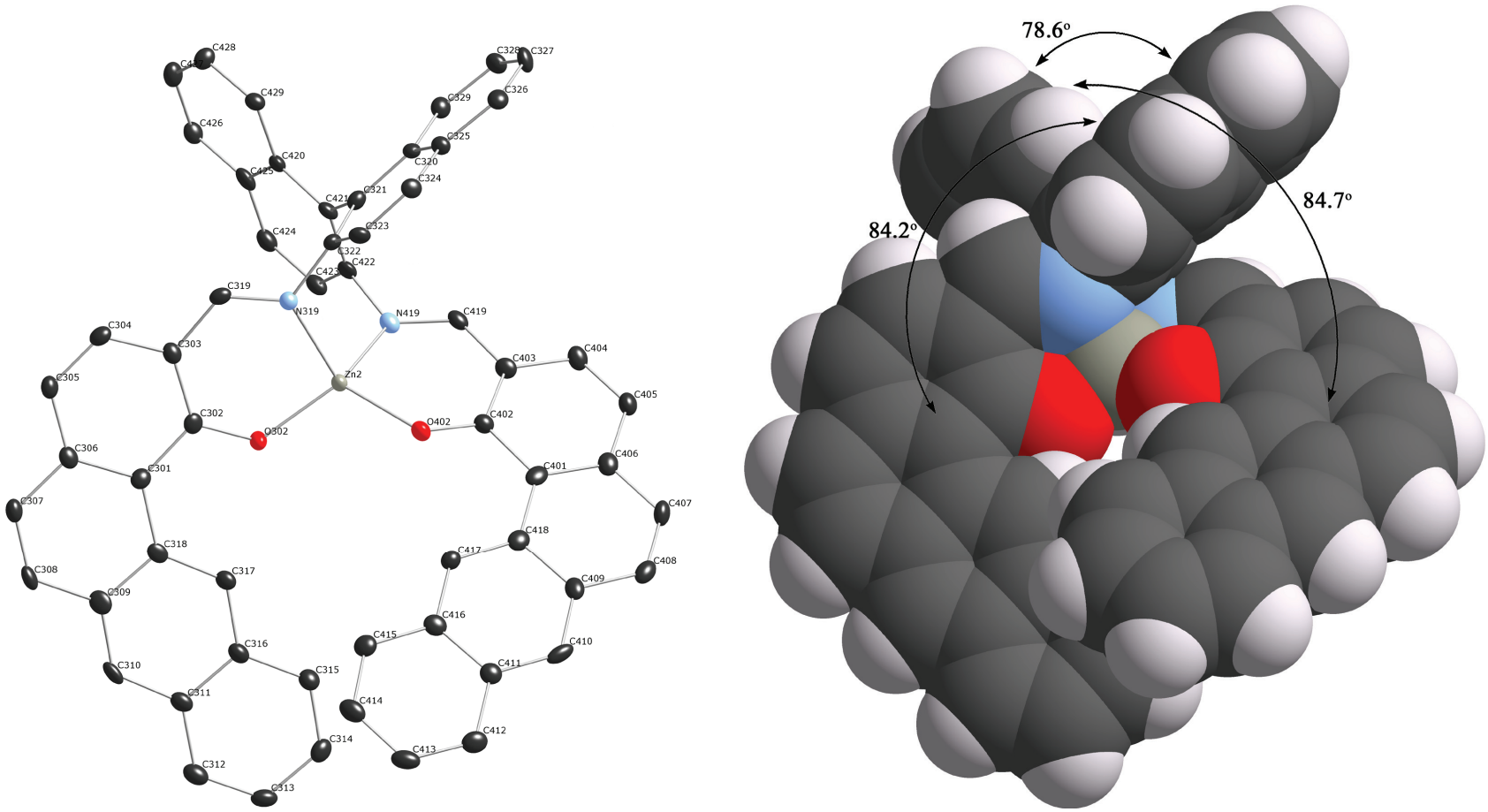


Figure 4.13 Thermal ellipsoid (50% probability) and space filling plots of (*R*)-**77A**

tetrahedral arrangement around the four-coordinate zinc, and are of the expected *M*-helicity. Importantly, the interconversion of these to *P*-helimers is not possible without isomerization of the backbone chirality, from *R* to *S*, due to *P* geometry spatial requirements. Given that the energy barrier to this is high,[102] it is not surprising that only *M*-helimers are crystallographically observed.

The molecular structures comprising (*R*)-**77** differ substantially from that of the free ligand. The dihedral angle between the naphthyl fragments decreases from 108.1°, to 78.6° and 78.4° for (*R*)-**77A** and **B** respectively (see figure 4.13 for **A** helimer angles). The naphthyl-benz[a]anthryl moieties are also no longer coplanar, and lie approximately at right-angles, with inter-plane torsions in the range of 84.2° to 99.7°. Similar, non-conjugated and perpendicular relationships, have been observed for other binaphthyl salen-type complexes.[28] In contrast to the analogous Zn(II) system with phenanthryl side-arms, neither of the *M* forms is ligated by solvent. The angles and coordinate bond lengths of (*R*)-**77**, as a consequence diverge significantly from those of (*R*)-**55**·MeOH. The naphthyl-naphthyl and two naphthyl-phenanthryl torsion angles are respectively 69.7°, 63.9°, and 76.1°, in five-coordinate (*R*)-**55**·MeOH, and are between 9.0° and 36.0° less than their counterparts in (*R*)-**77**. The M–O and M–N bonds as expected are elongated by penta-, as compared to tetra- coordination, and in the case of (*R*)-**55**·MeOH average 0.07 Å longer.

For the iron(II) complex (*R*)-**78**, a single *M* geometry is found in the solid state that structurally resembles (*R*)-**77A**, and slightly less so, (*R*)-**77B** (figure 4.14). The angles accordingly approximate those of the **A** molecule, and are within 5° for the naphthyl-naphthyl and naphthyl-benz[a]anthryl torsions. The inter-plane angle differences relative to the **B** molecule appear moderately larger, occurring in the range of 4° to 12°. The high uniformity

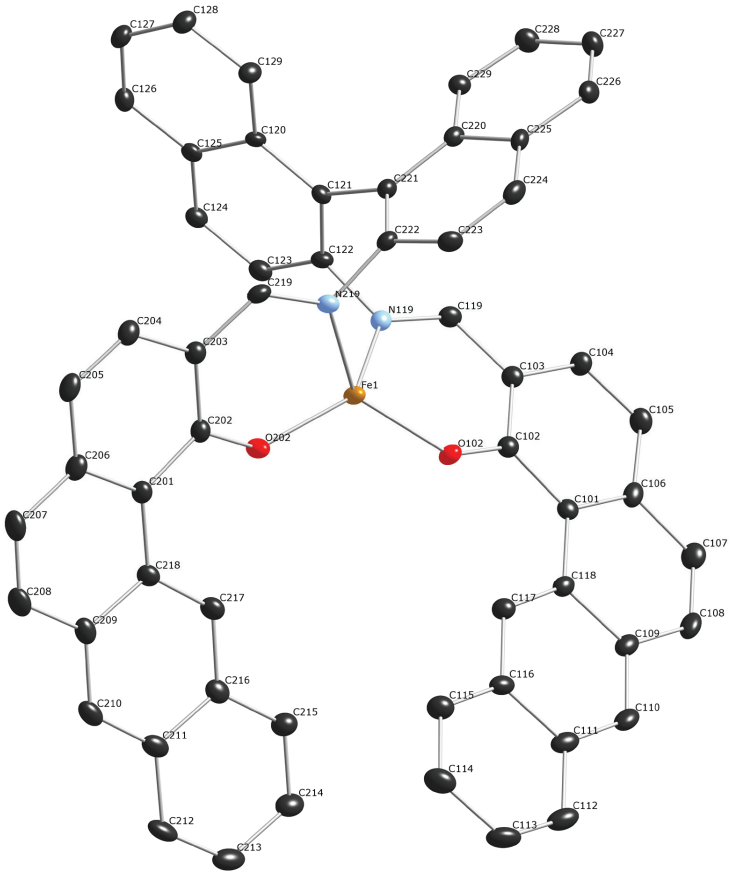


Figure 4.14 A thermal ellipsoid (50% probability) plot of (*R*)-**78**

which exists between these two complexes, (*R*)-**77** and(*R*)-**78**, is suggestive of helimer conformations that are predominantly controlled by the ligand, rather than by the metal. This is not unexpected given the limited flexibility of the binaphthyl moiety, and the constraints thereby placed on which geometries are accessible. There is also, in either case, little evidence of π-π stacking. The carbon-centroid distances lie outside of the favored 3.4-3.6 Å range, and the angles between the benz[a]anthryl planes (34-36^{o}), are overly large for such interactions.

4.7 Solid State vs Solution Structures

To investigate the solution conformations of the cyclohexyl-benz[a]anthryl complexes, a series of theoretical and spectral CD analyses were undertaken on (*R,R*)-**75**. The uncoordinated and THF coordinated *M* structures for the computations, were derived from (*R,R*)-**75**·py. Since *P*-helimers do not exist in this crystal structure, the initial *P* geometry was created by replacement of the Fe(II) ion, of *P* (*R,R*)-**76**·py with Zn(II). The methodology used to generate the energetically minimized geometries, and subsequently the spectra, thereafter parallels that in section 2.6 (see appendix IV also). A solution ECD spectrum for the complex was acquired in THF. From the results it was apparent that the simulated spectra for *M* and *P* (*R,R*)-**75**, exhibited

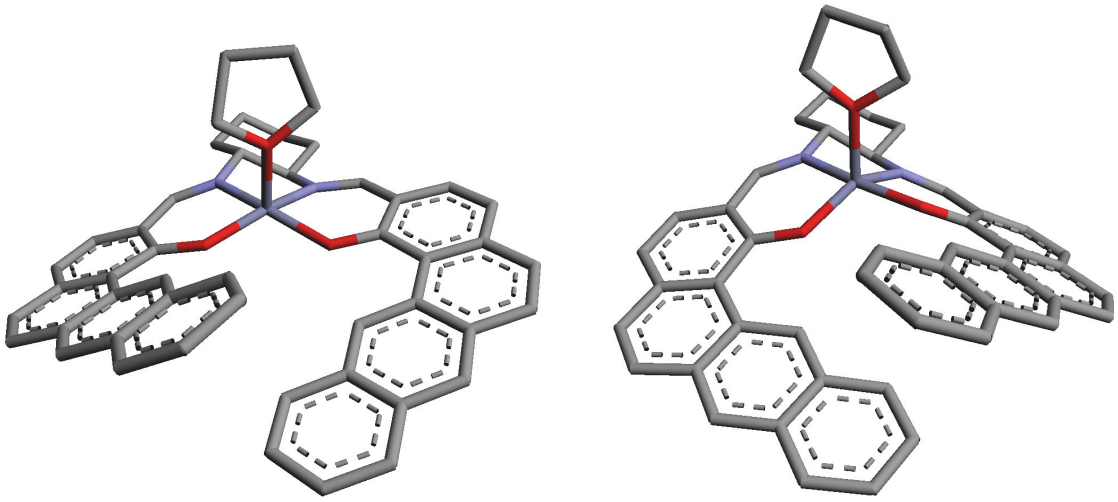


Figure 4.15 Minimized structures for *P* and *M* (*R,R*)-**75**·THF (left & right respectively)

less accuracy to the experimental spectrum than the solvated helimers. Accordingly, although comparisons to these are made (figure 4.17), they will not be discussed. The structures of the closer agreeing (*R,R*)-**75**·THF helimers, are depicted in figure 4.15. These differ from

unsolvated (*R,R*)-**75** chiefly in the degree of zinc atom pyramidalization, and have atomic displacements from the N,N,O,O donor planes, that are 0.08-0.09 Å larger.

In figure 4.16a are shown the (*R,R*)-**75**·THF experimental, simulated *P*, and simulated 1 : 1 *P* + *M* spectra. Evidently, across most wavelength regions, there is poor correlation between the theoretical and experimental results. This appears particularly true for the *P*-helimer spectrum, where the majority of bands are of opposite sign to that expected. This includes, for example, the 250, 281, 323, and 455 nm maxima. The sheer extent and magnitude of these inconsistencies, make it unlikely that they are attributable to errors in the computational model. Rather, it is probable that the *P* geometry does not accurately mimic the solution structures. The sign inversion between many of the theoretical/experimental bands, moreover, is evidence for predominately *M*-helimers – the phenanthryl arm positions are pseudo-enantiomeric from *M* to *P*, and the incorrect helimer type should therefore afford an approximately inverted spectrum.

In comparison, for the 1 : 1 *P* + *M* simulation the differences are somewhat less. The computed 246 and 450 nm maxima, approximate those signals visible at 236 and 456 nm. Also, no band lies diametrically opposite that observed by experiment at 325 nm, as was the case for the pure *P* spectrum. Major discrepancies, nonetheless, occur across most spectral regions, with for instance the 261, 278, and 395 nm signals, all poorly or not all reproduced. These differences indicate that a 1 : 1 mixture of helimers, or similar ratio, is unlikely to exist in solution.

The simulated spectrum afforded for the *M*-helimer is shown in figure 4.16b. As is evident, the maxima between 275 and 375 nm, are for the most part duplicated in terms of sign, intensity, and energy. Outside of this region the correlation between the spectra is less, although still greater than for the *P* and *P* + *M* simulations. It is interesting to note that while the 432 nm band is incorrectly duplicated by *M*·THF, the analogous unsolvated structure accurately predicts

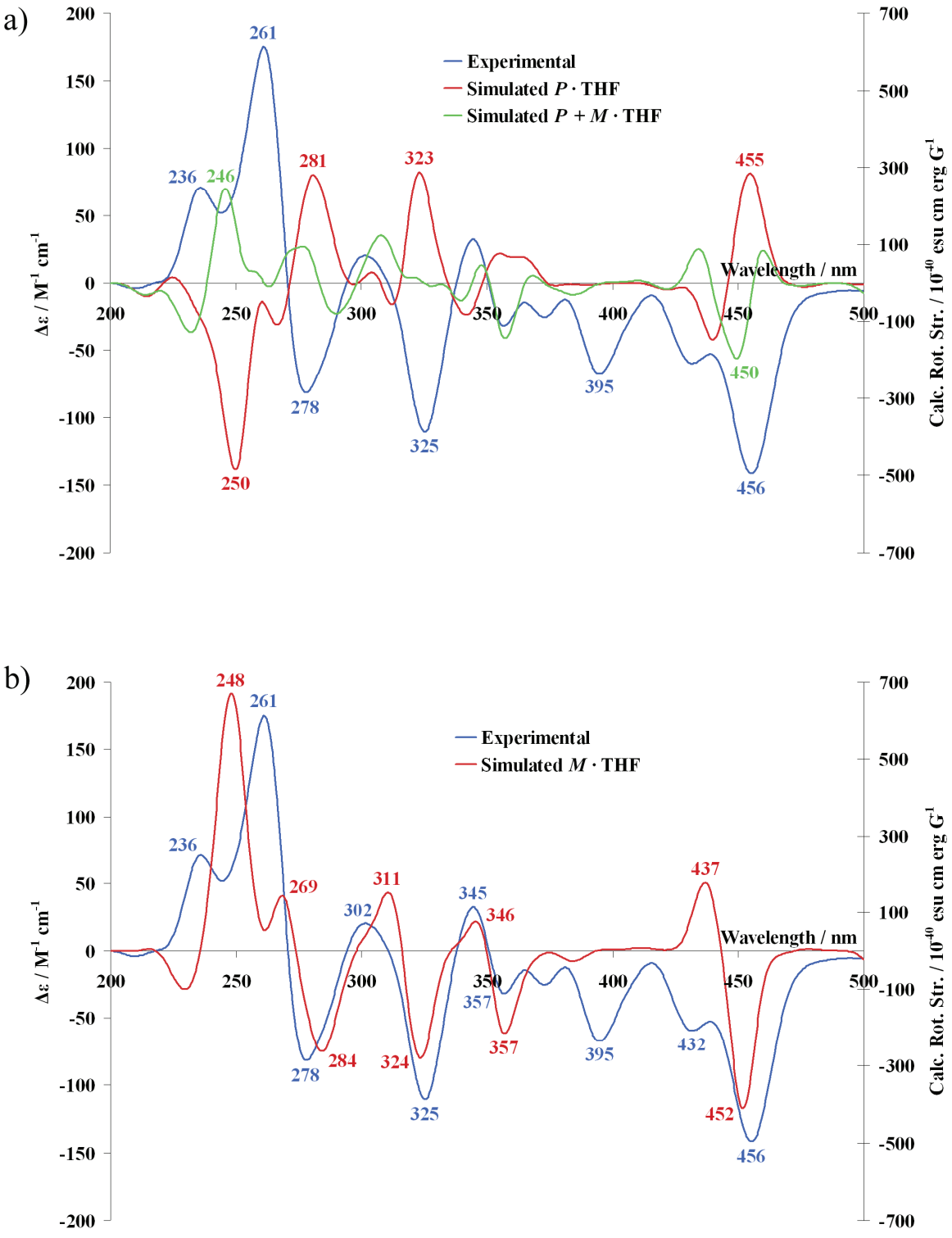


Figure 4.16 a) Simulated *P*, *P* + *M*, and experimental ECD spectra for (*R*,*R*)-**75**·THF. b) Simulated *M* and experimental ECD spectra for (*R*,*R*)-**75**·THF.

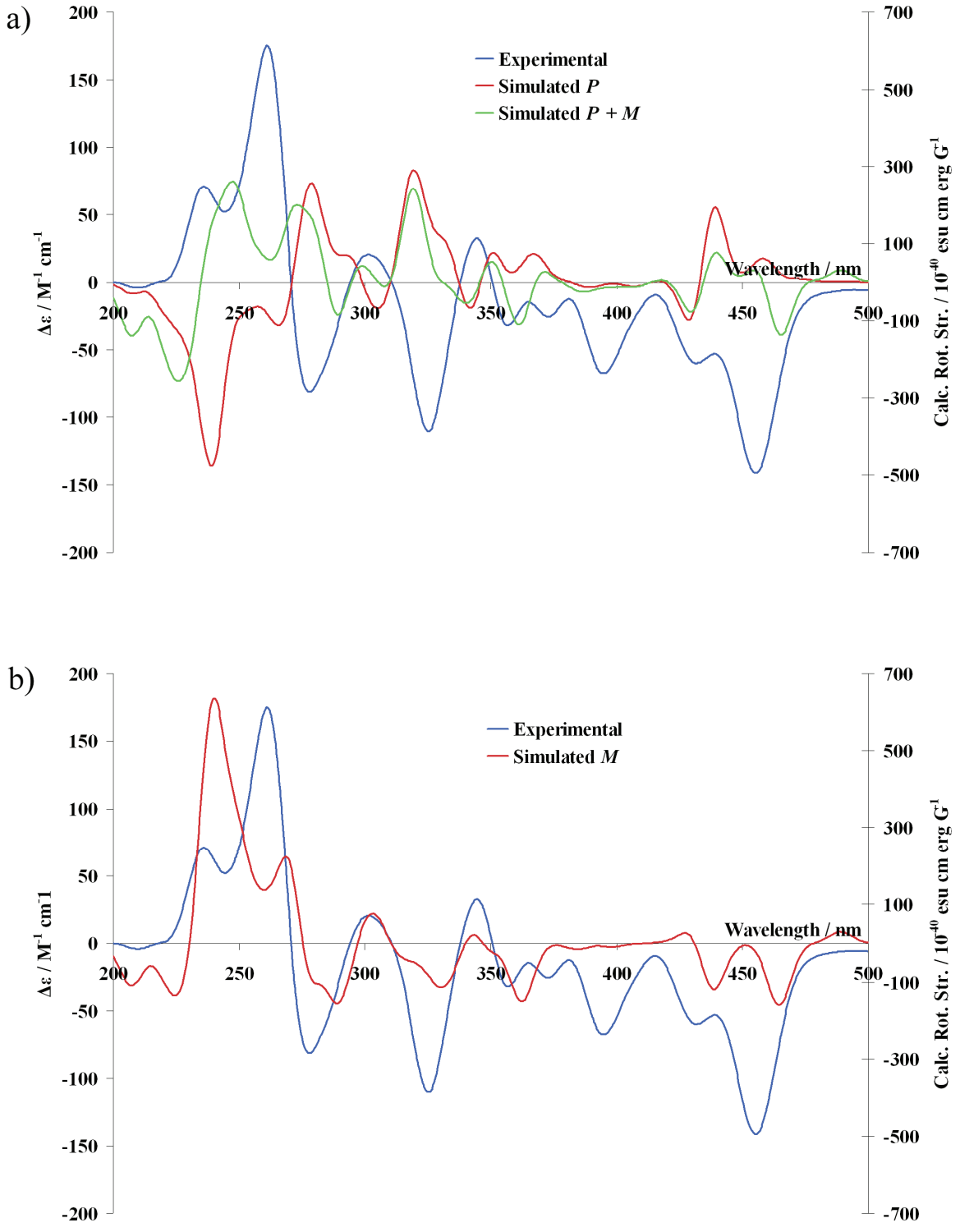


Figure 4.17 a) Simulated *P*, *P* + *M*, and experimental ECD spectra for (*R*,*R*)-**75**. b) Simulated *M* and experimental ECD spectra for (*R*,*R*)-**75**.

the signal (figure 4.17b). This discrepancy results from differences in the estimated orbitals and charge displacements, though unfortunately, it is not possible to relate these to differences in helimer structure. The bands at 248 and 269 nm also diverge significantly in intensity and position, but are of the correct rotational sign, unlike the mirroring signals in the simulated *P* spectrum. Notwithstanding these inconsistencies between theory and experiment, the data supports the notion that the *M* form is the dominant helimer. There is manifestly less disagreement, than with the other alternate simulations.

Conclusions

In the text of this thesis, we have prepared, characterized, and studied, a series of zinc and iron containing complexes, that, by nature, were intended to be monohelical. Our efforts were moderately successful in this regard, affording structures that did indeed, incorporate a helical motif. To our surprise, it was found that while the M(binap-salen)s were exclusively *M*-helimeric in the solid state, the M(salen)s with the exception of (*R,R*)-**75**, existed as 1 : 1 mixtures of *P* and *M* helimers. A result that we attribute to a relatively small *P*–*M* energy difference, enabling crystal packing forces to control and drive the molecular structure. The π-π stacking interactions evident in (*R,R*)-**76** presumably do not bear much geometric influence, since the contacts appear more or less identical for the two conformers. Our spectral and computational studies on the other hand, have indicated that in THF solution the *M* configuration predominates. Clearly, therefore, we have a rare case[103] of chiral switching in which the *P* : *M* ratio varies depending upon the surrounding environment, though such a process might not be thought possible for (*R,R*)-**75** and (*R,R*)-**76**, given the extensive side-arm overlap seen in the crystal structures. Interchange, for these, likely requires either temporary cleavage of one or more of the coordinate bonds, or considerable tilting of one side-arm group, enabling the other to rotate past. The mechanism in operation is liable to involve high energy states, though the data shows that the energy barriers are not insurmountable.

We have also examined the M(pyridyl-imine) complexes (*R,R*)-**62** and (*R*)-**63**. In contrast to the salen-type systems, these afforded dinuclear helicates. The coordination spheres appeared congested in both, which we believe to be the chief reason for non-formation of hexa-coordinate helimers. The M(pyridyl-imine) complexes, nonetheless, still exhibit chirality and

may act as catalysts, although not in the manner we first envisioned. Moreover, the use of weakly binding counterions such as PF_6^- and ^-OTf may provide a route to avoiding dinucleation, and to generating the desired complexes. Since, counterions of this type are much less likely to occupy the coordination sphere. The use of ^-OTf was briefly examined in this work, and our research group is currently investigating this modified approach.

Future Work

The overriding goal is, of course, to utilize these complexes as asymmetric catalysts. Several intermediate objectives, however, still remain whose attainment is desirable. One such is to ascertain, if possible, the mechanism of interconversion, as this may yield clues on how/if the process can be blocked. Another, is to precisely measure the solution *M* : *P* ratio's of the M(salen)s, and to determine the relationship this bears to the metal ion and solvent. Other metals such as chromium, cobalt, and manganese, have been shown to have advantageous catalytic properties, and it is desirable that these also be investigated. Their product complexes would need to be characterized, and in each instance the binding modes and solid and solution state geometries examined.

Experimental Section

General Methods

All reactions were run under inert atmospheres unless otherwise noted. Solvents used in metallation reactions were stored over sodium benzophenone ketyl or calcium hydride, and degassed prior to transfer via high-vacuum line techniques. Inert gases were purified by passage though 4Å molecular sieves and a Engelhard Q5 catalyst bed. Preparation and workup of Fe(II) and Fe(III) compounds was completed under rigorously inert conditions to prevent decomposition.

Elemental analyses were carried out by Desert Analytics of Tucson, Arizona. UV-vis spectra were obtained on a Varian Cary 500 spectrometer, and CD spectra on a JASCO 720 spectropolarimeter. Solution samples for these two techniques were prepared using dried spectroscopic grade THF, at concentrations that ranged between 1.5 and 2.5 $\times$ 10^{-5} M. A 1 cm pathlength quartz cell was employed for the analysis. ^{1}H and ^{13}C NMR spectra were obtained on a Varian Unity 400 MHz spectrometer employing residual solvent protons as an internal standard. Crystallographic data was collected using either a Bruker SMART 1000 CCD or a Bruker-AXS SMART APEX CCD. Full structural information is included in appendix III.

Magnetic susceptibilities were measured at 296 K using a Magway Mk1 mangnetic susceptibility balance that was calibrated with $Hg[Co(NCS)_4]$ standard. The iron complex magnetic susceptibilities were corrected for metal core electrons and the diamagnetism of the free ligands. Effective magnetic moments were calculated from the corrected susceptibilities as $\mu_{eff} = (8\chi_M T)^{½}$.

3,3'-[(1*R*,2*R*)-1,2-Cyclohexanediylbis(nitrilomethylidyne)]bis-4-phenanthrenol ((*R*,*R*)-33). A mixture of **41** (1.505 g, 6.8 mmol) and (1*R*,2*R*)-1,2-cyclohexanediamine (0.387 g, 3.4 mmol) in ethanol (80 ml) was refluxed for 2 h. The resulting suspension was hot filtered, and the collected yellow precipitate washed with boiling ethanol (40 ml) to give (*R*,*R*)-**33** (1.662 g, 94% yield). ^{1}H NMR (pyridine-d_5, 400 MHz): δ 1.34–1.50 (m, 2 H, CH), 1.66–1.82 (m, 4 H, CH), 2.02–2.13 (m, 2 H, CH), 3.53–3.65 (m, 2 H, CH), 7.11 (d, 2 H, *J* = 8.3 Hz, CH), 7.32 (d, 2 H, *J* = 8.3 Hz, CH), 7.60–7.66 (m, 4 H, CH), 7.77–7.83 (m, 2 H, CH), 7.86 (d, 2 H, *J* = 8.7 Hz, CH), 7.96 (dd, 2 H, *J* = 1.3, 7.9, CH), 8.61 (d, 2 H, *J* = 4.3 Hz, CH), 10.61 (d, 2 H, *J* = 8.7 Hz, CH), 15.97 (s, 2 H, OH). ^{13}C NMR (pyridine- d_5, 100 MHz): δ 24.78, 33.11, 69.74, 114.91, 118.25, 121.91, 126.64, 127.92, 127.92, 129.20, 129.36, 130.32, 131.33, 132.75, 133.29, 138.07, 165.94, 169.64. Anal. Calcd for $C_{36}H_{30}N_2O_2$: C 82.73, H 5.79, N 5.36. Found: C 82.62, H 6.01, N 5.36.

3,3'-[*Trans*-1,2-cyclohexanediylbis(nitrilomethylidyne)]bis-4-phenanthrenol ((*rac*)-33). The procedure for (*R*,*R*)-**33** was followed using *trans*-1,2-cyclohexanediamine in place of the *R*,*R*-enantiomer to give (*rac*)-**33** (0.339 g, 96% yield). ^{1}H and ^{13}C NMR spectra were identical to that of compound (*R*,*R*)-**33**. Anal. Calcd for $C_{36}H_{30}N_2O_2$: C 82.73, H 5.79, N 5.36. Found: C 82.41, H 5.82, N 5.37. Single crystals suitable for X-ray analysis were grown by slow diffusion of hexanes into a solution of (*rac*)-**33** in methylene chloride.

3,3'-[(1*R*)-[1,1'-Binaphthalene]-2,2'-diylbis(nitrilomethylidyne)]bis-4-phenanthrenol ((*R*)-34). A mixture of **41** (2.077 g, 9.3 mmol) and (*R*)-[1,1'-binaphthalene]-2,2'-diamine (1.329 g, 4.7

mmol) in ethanol (100 ml) was brought to reflux. After 16 h the resultant suspension was hot filtered, and the precipitate washed with boiling ethanol (40 ml) to give (*R*)-**34** (2.958 g, 91% yield) as a bright red solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.16 (d, 2 H, *J* = 8.2 Hz, CH), 7.25 (d, 2 H, *J* = 8.2 Hz, CH), 7.38–7.43 (m, 2 H, CH), 7.50–7.60 (m, 8 H, CH), 7.64–7.69 (m, 2 H, CH), 7.75 (d, 2 H, *J* = 8.6 Hz, CH), 7.81–7.85 (m, 4 H, CH), 8.12 (d, 2 H, *J* = 8.2 Hz, CH), 8.24 (d, 2 H, *J* = 8.8 Hz, CH), 8.80 (s, 2 H, CH), 9.44 (d, 2 H, *J* = 8.6 Hz, CH), 15.19 (s, 2 H, OH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 115.23, 116.89, 118.58, 120.37, 125.95, 126.27, 126.78, 126.91, 127.11, 117.55, 128.35, 128.54, 128.77, 129.16, 130.43, 130.78, 131.58, 132.55, 133.13, 133.78, 137.01, 142.44, 160.38, 165.71 (one signal not observed). Anal. Calcd for $C_{50}H_{32}N_2O_2$: C 86.68, H 4.66, N 4.04. Found: C 86.93, H 4.85, N 4.25. Single crystals suitable for X-ray analysis were grown by slow diffusion of hexanes into a solution of (*R*)-**34** in methylene chloride.

3,3'-[(1*S*)-[1,1'-Binaphthalene]-2,2'-diylbis(nitrilomethylidyne)]bis-4-phenanthrenol ((*S*)-34). The procedure for (*R*)-**34** was followed using (*S*)-[1,1'-binaphthalene]-2,2'-diamine in place of the *R*-enantiomer to give (*S*)-**34** (1.487 g, 90% yield). ^{1}H and ^{13}C NMR spectra were identical to that of compound (*R*)-**34**. Anal. Calcd for $C_{50}H_{32}N_2O_2$: C 86.68, H 4.66, N 4.04. Found: C 86.66, H 4.88, N 4.12.

(1*R*,2*R*)-N,N'-Bis[(8-isopropyl-2-quinolinyl)methylene]-1,2-cyclohexanediamine ((*R*,*R*)-35). (1*R*,2*R*)-1,2-Cyclohexanediamine (0.288 g, 2.5 mmol) and **42** (1.006 g, 5.0 mmol) were stirred in pet ether (20 ml) in the presence of 4 Å molecular sieves for 2 h. The reaction mixture was filtered and the collected solids extracted with pet ether (5 ml). The extract/filtrate were

combined and concentrated to give the crude product (*R*,*R*)-**35** (1.089 g) that was used without further purification. ^{1}H NMR ((product peaks only) $CDCl_3$, 400 MHz): δ 1.25 (d, 6 H, *J* = 6.9 Hz, CH_3), 1.36 (d, 6 H, *J* = 6.9 Hz, CH_3), 1.54–1.65 (m, 2 H, CH), 1.80–2.04 (m, 6 H, CH), 3.61–3.70 (m, 2 H, CH), 4.29 (sept, 2 H, *J* = 6.9 Hz, CH), 7.41–7.46 (m, 2 H, CH), 7.50–7.58 (m, 4 H, CH), 8.00–8.08 (m, 4 H, CH), 8.54 (s, 2 H, CH).

(1*R*)-N,N'-Bis[(8-isopropyl-2-quinolinyl)methylene]-[1,1'-binaphthalene]-2,2'-diamine ((*R*)-36). (*R*)-[1,1'-Binaphthalene]-2,2'-diamine (1.429 g, 5.0 mmol) and **42** (2.003 g, 10.1 mmol) were refluxed in ethanol (30 ml) in the presence of 3 Å molecular sieves for 40 h. The reaction mixture was filtered and the collected solid washed with hot ethanol (5 ml). Remaining solvent was removed in vacuo. The resulting sieves/product mixture was stirred into methylene chloride (20 ml), filtered, and the insoluble material washed with a further portion of methylene chloride (5 ml). The filtrates were combined and diluted with pet ether (125 ml). Upon concentration to ⅓ volume a white precipitate formed that was collected to afford (*R*)-**36** (1.772 g, 55%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.11 (d, 6 H, *J* = 6.9 Hz, CH_3), 1.27 (d, 6 H, *J* = 6.9 Hz, CH_3), 4.12 (sept, 2 H, *J* = 6.9 Hz, CH), 7.28–7.34 (m, 2 H, CH), 7.39–7.58 (m, 12 H, CH), 7.62 (d, 2 H, *J* = 8.5 Hz, CH), 7.91–7.98 (m, 4 H, CH), 8.03 (d, 2 H, *J* = 8.7 Hz, CH), 8.62 (s, 2 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.47, 23.51, 27.39, 118.10, 118.77, 125.33, 125.41, 125.45, 126.72, 127.30, 127.58, 128.13, 128.19, 128.97, 129.44, 132.32, 133.81, 136.69, 145.78, 147.90, 148.07, 153.86, 162.14.

2,2'-[(1*R*,2*R*)-1,2-Cyclohexanediylbis(nitrilomethylidyne)]bisbenz[a]anthracen-1-ol (*R*,*R*)-37). A mixture of **43** (2.006 g, 7.4 mmol) and (1*R*,2*R*)-1,2-cyclohexanediamine (0.421 g, 3.7 mmol) in ethanol (150 ml) was refluxed for 3 h. The resulting suspension was hot filtered, and the collected yellow precipitate washed with boiling ethanol (50 ml) to give (*R*,*R*)-**37** (2.177 g, 95% yield). ^{1}H NMR (pyridine- d_5, 400 MHz): δ 1.34–1.49 (m, 2 H, CH), 1.62–1.82 (m, 4 H, CH), 1.99–2.08 (m, 2 H, CH), 3.44–3.55 (m, 2 H, CH), 7.11 (d, 2 H, J = 8.1 Hz, CH), 7.37 (d, 2 H, J = 8.1 Hz, CH), 7.51 (d, 2 H, J = 8.8 Hz, CH), 7.56–7.63 (m, 4 H, CH), 7.91 (d, 2 H, J = 8.8 Hz, CH), 8.09–8.16 (m, 2 H, CH), 8.27–8.34 (m, 2 H, CH), 8.46 (s, 2 H, CH), 8.63 (s, 2 H, CH), 11.21 (s, 2 H, CH), 16.28 (s, 2 H, OH). ^{13}C NMR (pyridine- d_5, 100 MHz): δ 24.87, 33.16, 70.57, 116.30, 118.89, 121.00, 126.50, 126.72, 127.44, 128.21, 128.41, 128.99, 130.08, 130.41, 131.00, 131.51, 132.17, 133.67, 138.03, 166.30, 167.49 (one signal not observed). Anal. Calcd for $C_{44}H_{34}N_2O_2$: C 84.86, H 5.50, N 4.50. Found: C 84.52, H 5.67, N 4.48.

3,3'-[*Trans*-1,2-cyclohexanediylbis(nitrilomethylidyne)]bisbenz[a]anthracen-1-ol ((*rac*)-37). The procedure for (*R*,*R*)-**37** was followed using trans-1,2-cyclohexanediamine in place of the *R*-enantiomer to give (*rac*)-**37** (0.361 g, 95% yield). ^{1}H and ^{13}C NMR spectra were identical to that of compound (*R*,*R*)-**37**. Anal. Calcd for $C_{44}H_{34}N_2O_2$: C 84.86, H 5.50, N 4.50. Found: C 84.49, H 5.57, N 4.49.

2,2'-[(1*R*)-[1,1'-Binaphthalene]-2,2'-diylbis(nitrilomethylidyne)]bisbenz[a]anthracen-1-ol ((*R*)-38). A mixture of **43** (3.009 g, 11.1 mmol) and (*R*)-[1,1'-Binaphthalene]-2,2'-diamine

(1.571 g, 5.5 mmol) in ethanol (150 ml) was brought to reflux. After 18 h the resultant suspension was hot filtered, and the precipitate washed with boiling ethanol (100 ml) to give (*R*)-**38** (4.149 g, 95% yield) as a bright red solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.17 (d, 2 H, *J* = 8.0 Hz, CH), 7.34 (d, 2 H, *J* = 8.0 Hz, CH), 7.42–7.50 (m, 4 H, CH), 7.57–7.67 (m, 6 H, CH), 7.71 (t, 2 H, *J* = 7.4 Hz, CH), 7.80 (d, 2 H, *J* = 8.7 Hz, CH), 7.95 (d, 2 H, *J* = 8.7 Hz, CH), 8.04 (d, 2 H, *J* = 8.2 Hz, CH), 8.21-8.27 (m, 4 H, CH), 8.30 (s, 2 H, CH), 8.38 (d, 2 H, *J* = 8.7 Hz, CH), 8.93 (s, 2 H, CH), 9.96 (s, 2 H, CH), 15.17 (s, 2 H, OH). ^{13}C NMR (TFA-*d*, 100 MHz): δ 115.68, 117.13, 122.26, 125.97, 126.10, 126.32, 127.27, 127.32, 127.56, 129.57, 129.89, 129.95, 130.05, 131.40, 131.59, 131.83, 132.47, 132.74, 134.50, 134.73, 135.37, 135.51, 136.09, 136.64, 138.48, 146.25, 161.43, 163.26 (one signal not observed). Anal. Calcd for $C_{58}H_{36}N_2O_2$: C 87.86, H 4.58, N 3.53. Found: C 87.84, H 4.62, N 3.56. Single crystals suitable for X-ray analysis were grown by slow diffusion of hexanes into a solution of (*R*)-**38** in methylene chloride.

4-Hydroxy-3-phenanthrenecarboxaldehyde (41). (Method A) To a solution of **50** (18.61 g, 83 mmol) in dioxane (200 ml) was added DDQ (18.84 g, 83 mmol) and acetic acid (13 ml). After stirring at room temperature for 1.5 h, the solution was filtered to remove DDQ byproduct, and the dioxane solution concentrated to a brown oil. The oil was dissolved into diethyl ether (400 ml), and consecutively washed with 1 M $NaHCO_3$ (3 X 100 ml), and with 1 M HCl (1 X 100 ml). The organic layer was dried over $MgSO_4$, filtered, and concentrated to give **41** (7.77 g, 42% yield) as a light brown solid. (Method B) A mixture of **50** (22.82 g, 102 mmol) and triphenylmethanol (52.98 g, 204 mmol) in trifluoroacetic acid (400 ml) was refluxed for 2 h. After allowing to cool, the solution was diluted with H_2O (800 ml). The resulting precipitate was

collected and suspended into 1 M NaOH (400 ml), and after stirring for 15 minutes, filtered to remove insoluble solids. The filtrate was adjusted to pH 1 with 5 M HCl to yield a yellow precipitate that was collected, washed with H_2O (200 ml), and recrystallized from boiling ethanol to give **41** (5.68 g, 82% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.50 (d, 1 H, *J* = 8.3 Hz, CH), 7.64–7.80 (m, 4 H, CH), 7.93–7.96 (m, 2 H, CH), 9.83 (d, 1 H, *J* = 8.2 Hz, CH), 10.05 (s, 1 H, CH), 13.56 (s, 1 H, OH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 117.10, 119.85, 120.52, 126.68, 126.83, 127.99, 128.72, 128.84, 129.39, 131.21, 132.65, 139.44, 164.16, 196.78 (one signal not observed). Anal. Calcd for $C_{15}H_{10}O_2$: C 81.07, H 4.54. Found: C 81.24, H 4.75.

8-Isopropyl-2-quinolinecarboxaldehyde (42). A solution of **59** (23.07 g, 125 mmol) in dioxane (25 ml) was added to a solution of selenium dioxide (13.82 g, 125 mmol) in dioxane (120 ml) and H_2O (7 ml). The reaction mixture was refluxed for 3 h, and after cooling, filtered to remove precipitated selenium. The solution was concentrated to an oil that was redissolved into diethyl ether (150 ml), and consecutively washed with 1 M HCl (4 X 50 ml), 1 M NaOH (3 X 50 ml), and H_2O (1 X 50 ml). The ether phase was dried over $MgSO_4$, filtered, and concentrated to give **42** (20.89 g, 84% yield) as a brown oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.44 (d, 6 H, *J* = 7.0 Hz, CH_3), 4.49 (sept, 1 H, *J* = 7.0 Hz, CH), 7.62–7.75 (m, 3 H, CH), 8.01 (d, 1 H, *J* = 8.4 Hz, CH), 8.27 (d, 1 H, *J* = 8.4 Hz, CH), 10.25 (s, 1 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.70, 27.60, 116.98, 125.67, 126.38, 129.44, 130.42, 137.77, 146.03, 149.23, 151.71, 194.54.

1-Hydroxybenz[a]anthracene-2-carboxaldehyde (43). A mixture of **72** (33.08 g, 121 mmol) and triphenylmethanol (62.78 g, 241 mmol) in trifluoroacetic acid (500 ml) was refluxed for 2 h. After allowing to cool, the solution was diluted with H_2O (1 L). The precipitate was collected, washed with H_2O (200 ml), and suspended into 2:1 1 M NaOH/ethanol (600 ml). The mixture was stirred for 15 minutes, filtered, and the insoluble material washed with a further portion of 2:1 1 M NaOH/ethanol (100 ml). The filtrates were combined, acidified to pH 1 with 5 M HCl, and extracted with methylene chloride (1 X 700 ml, 2 X 200 ml). The organic extracts were combined, dried over $MgSO_4$, filtered, and concentrated. The resulting solid was recrystallized from ethyl acetate/ethanol to afford **43** (27.85 g, 85% yield) as a yellow-green powder. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.38 (d, 1 H, *J* = 8.1 Hz, CH), 7.51 (d, 1 H, *J* = 8.9 Hz, CH), 7.57–7.63 (m, 3 H, CH), 7.92 (d, 1 H, *J* = 8.9 Hz, CH), 8.00–8.06 (m, 1 H, CH), 8.15–8.21 (m, 1 H, CH), 8.33 (s, 1 H, CH), 9.98 (s, 1 H, CH), 10.28 (s, 1 H, CH), 13.44 (s, 1 H, OH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 117.86, 119.52, 120.54, 126.16, 126.51, 126.64, 127.25, 127.60, 128.38, 128.68, 129.66, 130.57, 130.99, 131.58, 132.97, 133.13, 139.97, 163.50, 196.74. Anal. Calcd for $C_{19}H_{12}O_2$: C 83.81, H 4.44. Found: C 83.52, H 4.53.

3-(2-Naphthoyl)propionic acid (47). To a 0^{o}C solution of $AlCl_3$ (100.16 g, 751 mmol) in nitrobenzene (285 ml), was added naphthalene (72.17 g, 563 mmol) and succinic anhydride (37.59 g, 362 mmol). The mixture was stirred for 10 minutes, allowed to warm to room temperature, and subsequently stirred for a further 16 h. Thereafter, the reaction mixture was poured into crushed ice (300 g) and acidified with 5 M HCl (200 ml), yielding a brown precipitate upon vigorous agitation. This was collected via vacuum filtration, and washed with

H_2O (150 ml) and hexanes (150 ml). The solid was suspended into benzene (300 ml) at 60°C for 15 minutes, allowed to cool, and filtered to give **47** (31.81 g, 37% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.90 (d, 2 H, *J* = 6.6 Hz, CH_2), 3.49 (d, 2 H, *J* = 6.6 Hz, CH_2), 7.55–7.65 (m, 2 H, CH), 7.88–7.94 (m, 2 H, CH), 7.99 (d, 1 H, *J* = 8.1 Hz, CH), 8.06 (dd, 1 H, *J* = 1.5, 8.6 CH), 8.53 (s, 1 H, CH) (OH proton not observed). ^{13}C NMR (DMSO-d6, 100 MHz): δ 27.98, 33.16, 123.44, 126.88, 127.62, 128.25, 128.57, 129.59, 129.73, 132.20, 133.75, 135.04, 173.82, 198.41.

4-(2-Naphthyl)butanoic acid (48). To a solution of **47** (31.81 g, 139 mmol) in diethylene glycol (250 ml) at 100°C was added hydrazine monohydrate (20.5 ml, 418 mmol). The reaction mixture was stirred for 1 h, then potassium hydroxide added (22.68 g, 404 mmol) and the temperature raised to 200°C. After 5 h the mixture was allowed to cool, and diluted with H_2O (750 ml). The solution was acidified to pH 1 with 5 M HCl and the resulting precipitate collected and washed with H_2O (200 ml), to yield **48** (27.15 g, 91% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.08 (quin, 2 H, *J* = 7.5 Hz, CH_2), 2.43 (t, 2 H, *J* = 7.4 Hz, CH_2), 2.86 (t, 2 H, *J* = 7.6 Hz, CH_2), 7.34 (dd, 1 H, *J* = 1.6, 8.4 Hz, CH), 7.40–7.49 (m, 2 H, CH), 7.63 (s, 1 H, CH), 7.77–7.84 (m, 3 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 26.27, 33.51, 35.35, 125.48, 126.19, 126.85, 127.40, 127.67, 127.83, 128.27, 132.35, 133.83, 138.89, 139.87.

2,3-Dihydro-4-(*1H*)-phenanthrenone (49). A solution of **48** (27.15 g, 126 mmol) in methanesulfonic acid (150 ml) was heated to 90°C and stirred for 1 h. The reaction mixture was allowed to cool and subsequently poured into ice water (400 ml). The resulting aqueous mixture was

extracted with diethyl ether (3 X 200 ml), and the extracts combined and washed consecutively with 1 M $NaHCO_3$ (150 ml) and H_2O (150 ml). The organic solution was dried over $MgSO_4$, filtered, and concentrated to afford **49** (23.55 g, 91% yield) as a yellow-brown solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.21 (quin, 2 H, *J* = 6.3 Hz, CH_2), 2.80 (t, 2 H, *J* = 6.6 Hz, CH_2), 3.14 (t, 2 H, *J* = 6.1 Hz, CH_2), 7.34 (d, 1 H, *J* = 8.4 Hz, CH), 7.47–7.53 (m, 1 H, CH), 7.61–7.67 (m, 1 H, CH), 7.82 (d, 1 H, *J* = 8.1 Hz, CH), 7.93 (d, 1 H, *J* = 8.4 Hz, CH), 9.42 (d, 1 H, *J* = 8.8 Hz, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.20, 31.78, 41.28, 126.00, 126.89, 127.14, 127.52, 128.50, 128.99, 131.60, 133.00, 134.37, 146.90, 200.58.

2,3-Dihydro-3-(hydroxymethylene)-4-(*1H*)-phenanthrenone (50). To a solution of **49** (23.53 g, 120 mmol) in benzene (350 ml) was added ethyl formate (8.88 g, 120 mmol), and sodium methoxide (12.95 g, 240 mmol). The reaction mixture was stirred for 12 h at room temperature and the resulting precipitate collected and washed with benzene (2 X 50 ml). The solid was then dissolved into 1 M NaOH (500 ml), and the aqueous solution washed with hexanes (3 X 100 ml). Acidification to pH 1 with 5 M HCl gave a precipitate that was extracted into diethyl ether (3 X 150 ml), and the extracts were combined, dried over $MgSO_4$, filtered, and concentrated to give **50** (23.12 g, 86% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.56 (t, 2 H, *J* = 7.1 Hz, CH_2), 3.05 (t, 2 H, *J* = 7.1 Hz, CH_2), 7.36 (d, 1 H, *J* = 8.2 Hz, CH), 7.50–7.54 (m, 1 H, CH), 7.61–7.66 (m, 1 H, CH), 7.82–7.87 (m, 2 H, CH), 7.94 (d, 1 H, *J* = 8.2 Hz, CH), 9.26 (d, 1 H, *J* = 8.7 Hz, CH), 15.06 (d, 1 H, *J* = 8.8 Hz, OH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.77, 31.30, 110.90, 126.09, 126.63, 126.72, 127.65 128.52, 128.70, 131.39, 133.43, 134.18, 144.58, 169.32, 189.98. Anal. Calcd for $C_{15}H_{12}O_2$: C 80.34, H 5.39. Found: C 80.07, H 5.47.

Zn(II)-(*R*,*R*)-33 complex ((*R*,*R*)-53). Zinc chloride (0.079 g, 0.58 mmol), sodium methoxide (0.093 g, 1.73 mmol) and (*R*,*R*)-**33** (0.301 g, 0.58 mmol) were suspended into a 2:1 mixture of methylene chloride/ethanol (15 ml). After stirring overnight the reaction mixture was concentrated to a yellow solid that was dissolved into THF (20 ml). The solution was carefully filtered to remove fine insoluble solids, and the clear filtrate diluted with ethanol (40 ml). Stirring for 3 h resulted in the gradual formation of a yellow precipitate. The precipitate was collected and consecutively washed with methylene chloride (5 ml) and ethanol (5 ml) to afford (*R*,*R*)-**53** (0.200 g, 59% yield). ^{1}H NMR (pyridine- d_5, 400 MHz): δ 1.20–1.34 (m, 4 H, CH), 1.79 (br, s, 2 H, CH), 2.31 (br, s, 2 H, CH), 3.22 (br, s, 2 H, CH), 7.30 (d, 2 H, J = 8.2 Hz, CH), 7.57–7.66 (m, 4 H, CH), 7.80–7.87 (m, 4 H, CH), 7.96 (d, 2 H, J = 8.6 Hz, CH), 8.01 (d, 2 H, J = 7.9 Hz, CH), 8.63 (s, 2 H, CH), 11.79 (d, 2 H, J = 8.5 Hz, CH). ^{13}C NMR (pyridine- d_5, 100 MHz): δ 25.08, 28.79, 66.31, 114.43, 117.48, 125.31, 125.69, 128.36, 128.55, 128.95, 130.04, 130.84, 133.31, 134.26, 134.98, 138.71, 166.27, 174.70. Anal. Calcd for $C_{36}H_{28}N_2O_2Zn$: C 73.79, H 4.82, N 4.78. Found: C 73.60, H 5.01, N 4.68. Single crystals of (*R*,*R*)-**53** suitable for X-ray analysis were grown via slow cooling from boiling pyridine.

Fe(II)-(*R*,*R*)-33 complex (*R*,*R*)-54). Iron (II) chloride (0.073 g, 0.58 mmol), sodium methoxide (0.093 g, 1.73 mmol) and (*R*,*R*)-**33** (0.301 g, 0.58 mmol) were suspended into a 2:1 mixture of methylene chloride/ethanol (15 ml). After stirring overnight the reaction mixture was concentrated to a green-brown solid. Co-ordinated solvent was removed in vacuo, and the solid dissolved into THF (15 ml). The solution was filtered to remove fine insoluble solids, and the clear filtrate diluted with ethanol (45 ml). This was stirred for 30 minutes to give a purple

precipitate that was collected and suspended into methylene chloride (10 ml). After stirring for 15 minutes the solid was recollected to afford (*R*,*R*)-**54** (0.211 g, 64% yield). ^{1}H NMR (pyridine- d_5, 400 MHz): δ −25.11 (br, s, 2 H, CH), −11.69 (s, 2 H, CH), −4.80 (br, s, 2 H, CH), −3.28 (s, 2 H, CH), 1.66 (s, 2 H, CH), 5.26 (s, 2 H, CH), 10.13 (s, 2 H, CH), 10.90 (s, 2 H, CH), 17.14 (s, 2 H, CH), 24.61 (s, 2 H, CH), 40.42 (br, s, 2 H, CH). Anal. Calcd for $C_{36}H_{28}N_2O_2Fe$: C 75.01, H 4.90, N 4.86. Found: C 74.94, H 5.00, N 4.71. Single crystals suitable for X-ray analysis were grown by slow diffusion of methanol into a solution of (*R*,*R*)-**54** in pyridine.

Zn(II)-(*R*)-34 complex ((*R*)-55). Zinc chloride (0.065 g, 0.48 mmol), sodium methoxide (0.070 g, 1.30 mmol) and (*R*)-**34** (0.300 g, 0.43 mmol) were suspended into a 2:1 mixture of benzene/ethanol (15 ml). After stirring overnight the reaction mixture was concentrated to a yellow solid that was dissolved into methylene chloride (15 ml). The solution was carefully filtered to remove fine insoluble solids, and the clear filtrate diluted with ethanol (45 ml). Upon stirring for 3 h a yellow precipitate formed that was collected to afford (*R*)-**55** (0.213 g, 65%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.95 (d, 2 H, J = 8.5 Hz, CH), 7.08 (d, 2 H, J = 8.3 Hz, CH), 7.21–7.26 (m, 4 H, CH), 7.40–7.52 (m, 8 H, CH), 7.60 (d, 2 H, J = 8.7 Hz, CH), 7.83–7.88 (m, 4 H, CH), 7.90 (d, 2 H, J = 8.2 Hz, CH), 8.03 (d, 2 H, J = 8.6 Hz, CH), 8.57 (s, 2 H, CH), 10.50–10.56 (m, 2 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 115.40, 116.06, 122.17, 124.34, 125.67, 125.82, 126.53, 126.81, 126.87, 127.27, 127.74, 128.30, 128.57, 128.87, 131.01, 131.70, 132.32, 132.60, 132.92, 132.98, 134.25, 139.14, 145.53, 170.26, 174.26. Anal. Calcd for $C_{50}H_{30}N_2O_2Zn$: C 79.42, H 4.00, N 3.70. Found: C 79.06, H 3.86, N 3.77. Single crystals suitable for X-ray

analysis were grown by slow diffusion of methanol into a solution of (*R*)-**55** in methylene chloride.

Fe(II)-(*R*)-34 complex ((*R*)-56). The procedure for (*R*)-**55** was followed using iron (II) chloride, and with THF in place of methylene chloride during work-up. It was also necessary to concentrate the THF/ethanol solution to ¾ volume for precipitation of the product to occur. The product, (*R*)-**56**, was afforded as a red-brown powder (0.156 g, 48% yield). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ −39.04 (br, s, 2 H, CH), −15.27 (s, 2 H, CH), −9.23 (s, 2 H, CH), −7.60 (s, 2 H, CH), 0.56 (s, 2 H, CH), 1.28 (s, 2 H, CH), 10.68 (s, 2 H, CH), 11.68 (s, 2 H, CH), 12.08 (s, 2 H, CH), 13.71 (s, 2 H, CH), 15.29 (s, 2 H, CH), 24.52 (s, 2 H, CH), 60.63 (br, s, 2 H, CH). Anal. Calcd for $C_{50}H_{30}N_2O_2Fe$: C 80.43, H 4.05, N 3.75. Found: C 80.46, H 3.84, N 3.90.

Fe(II)-(*R*)-34/(*S*)-34 complex ((*rac*)-56). The procedure for (*R*)-**55** was followed using iron (II) chloride, with a 1:1 mixture of (*R*)-**34** and (*S*)-**34** in place of pure (*R*)-**34**, and THF in place of methylene chloride during work-up. The racemic product, (*rac*)-**56**, was afforded as a red-brown powder (0.206 g, 64% yield). ^{1}H NMR spectra were identical to that of compound (*R*)-**56**. Anal. Calcd for $C_{50}H_{30}N_2O_2Fe$: C 80.43, H 4.05, N 3.75. Found: C 80.73, H 3.80, N 3.57. Single crystals suitable for X-ray analysis were grown by slow diffusion of methanol into a solution of (*rac*)-**56** in methylene chloride.

Fe(III)-(*R*,*R*)-33 complex ((*R*,*R*)-57). Iron (III) chloride (0.093 g, 0.56 mmol), sodium methoxide (0.093 g, 1.67 mmol) and (*R*,*R*)-**33** (0.291 g, 0.56 mmol) were suspended into a 2:1 mixture of THF/ethanol (15 ml) and stirred overnight. The reaction mixture was concentrated to a solid and fresh THF (80 ml) added. After stirring for 15 minutes, insoluble material was removed by filtration and the red/black solution diluted with ethanol (80 ml). Upon concentration to ½ volume a black precipitate formed that was collected to afford (*R*,*R*)-**57** (0.082 g, 24%). Multiple broad overlapping bands that cannot be readily quoted were observed in the ^{1}H NMR spectrum, see appendix I. Anal. Calcd for $C_{36}H_{28}N_2O_2FeCl$: C 70.66, H 4.61, N 4.58. Found: C 70.40, H 4.34, N 4.52. Single crystals suitable for X-ray analysis were grown by slow diffusion of diethyl ether into a solution of (*R*,*R*)-**57** in methylene chloride.

2-Methyl-8-isopropylquinoline (59). To a mixture of 2-isopropylaniline (30.00 g, 222 mmol) and sodium m-nitrobenzenesulfonate (60.00 g, 266 mmol) in 3:1 H_2SO_4/H_2O (180 ml), was added crotonaldehyde (74 ml, 906 mmol) dropwise over 2 h at 100^{o}C. The reaction mixture was stirred at 100^{o}C for a further 2 h, and after cooling, diluted with H_2O (800 ml). This was neutralized by the gradual addition of sodium hydroxide pellets, and allowed to sit until complete precipitation of by-product occurred. The black tarry solid was removed via vacuum filtration and the aqueous filtrate extracted with diethyl ether (3 X 300 ml). The black tarry solid was also extracted with diethyl ether (3 X 300 ml). The extracts were combined, dried over $MgSO_4$, filtered, and concentrated to give an oil that was redissolved into methylene chloride (100 ml). Benzoyl chloride (5 ml, 43 mmol) was added, and after stirring for 1h, the methylene chloride solution extracted with 2 M HCl (5 X 100 ml). The extracts were combined and made basic by

the addition of 5 M NaOH. The aqueous mixture was then extracted with diethyl ether (3 X 300 ml), and the ether extracts combined, dried over $MgSO_4$, filtered, and concentrated to afford **59** (23.80 g, 58% yield) as a light brown oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.39 (d, 6 H, *J* = 6.9 Hz, CH_3), 2.75 (s, 3 H, CH_3), 4.40 (sept, 1 H, *J* = 6.9 Hz, CH), 7.26 (d, 1 H, *J* = 8.3 Hz, CH), 7.44 (t, 1 H, *J* = 7.6 Hz, CH), 7.56–7.62 (m, 2 H, CH), 8.01 (d, 1 H, *J* = 8.3 Hz, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.80, 25.90, 27.20, 121.63, 125.17, 125.38, 125.64 126.65, 136.47, 145.96, 147.10, 157.69.

Zn(II)Cl_2-(*R*,*R*)-35 complex ((*R*,*R*)-62). A solution of (*R*,*R*)-**35** (0.203 g) and zinc chloride (0.058 g, 0.43 mmol) in ethanol was stirred at 50^{o}C for 2 h. After cooling, the reaction mixture was filtered and the collected solid extracted with ethanol (2 ml). The extract/filtrate were combined and concentrated to an oily residue. This was redissolved into methylene chloride (5 ml) and filtered to remove trace solids. The clear solution was diluted with pet ether (25 ml), and the resulting white precipitate collected and washed with pet ether (5 ml) to afford (*R*,*R*)-**62** (0.065g, 25%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.40 (d, 6 H, *J* = 6.6 Hz, CH_3), 1.49 (d, 6 H, *J* = 6.6 Hz, CH_3), 1.59–1.68 (m, 2 H, CH), 1.96–2.09 (m, 4 H, CH), 2.54–2.69 (m, 2 H, CH), 4.58 (sept, 2 H, *J* = 6.6 Hz, CH), 4.64–4.72 (m, 2 H, CH), 7.67–7.76 (m, 4 H, CH), 7.88 (d, 2 H, *J* = 8.2 Hz, CH), 7.93 (dd, 2 H, *J* = 1.8, 6.9, CH), 8.51 (d, 2 H, *J* = 8.2 Hz, CH), 9.25 (s, 2 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.99, 24.67, 26.11, 28.64, 33.45, 72.87, 124.22, 127.09, 129.94, 131.65, 132.31, 143.43, 143.84, 147.14, 147.99, 166.96.

Zn(II)Cl_2-(*R*)-36 complex ((*R*)-63). Zinc chloride (0.057 g, 0.42 mmol) and (*R*)-**36** (0.271 g, 0.42 mmol) were refluxed in toluene (15 ml) for 16 h. After cooling, the resultant yellow precipitate was collected and consecutively washed with toluene (1 ml) and pet ether (5 ml) to afford (*R*)-**63** (0.104 g, 32%). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.38 (d, 6 H, *J* = 6.6 Hz, CH_3), 1.43 (d, 6 H, *J* = 6.6 Hz, CH_3), 4.49 (sept, 2 H, *J* = 6.6 Hz, CH), 7.41–7.57 (m, 8 H, CH), 7.68–7.78 (m, 4 H, CH), 7.89–7.98 (m, 4 H, CH), 8.17 (d, 2 H, *J* = 8.7 Hz, CH), 8.40–8.45 (m, 4 H, CH), 8.54 (s, 2 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 24.78, 25.70, 28.92, 123.83, 124.47, 124.73, 127.24, 127.40, 127.88, 128.86, 129.19, 130.16, 131.49, 131.65, 132.39, 133.02, 133.26, 142.79, 143.40, 143.90, 146.86, 147.74, 163.43.

3-(9,10-Dihydro-2-anthroyl)propionic acid (67). To a solution of 9,10-dihydroanthracene (74.23 g, 412 mmol) in 1,2-dichloroethane (325 ml) at 0^{o}C was added a mixture of succinic anhydride (37.50 g, 374 mmol) and aluminium chloride (99.83 g, 749 mmol) in small portions over 1 h and 20 minutes. The reaction mixture was allowed to warm to room temperature and stirred for a further 2 h. It was then quenched via the addition of H_2O (1.25 L), and diluted with hexanes (1.5 L). The resulting precipitate was collected, washed with H_2O (500 ml), and suspended into 5 M NaOH (1 L). After stirring for 30 minutes the precipitate was recollected, washed with 5 M NaOH (3 X 300 ml), and dissolved into 4:1 H_2O/ethanol (1L). The solution was filtered to remove trace insoluble solids, and acidified to pH 1 with 5 M HCl. The resulting light yellow solid was collected and washed with H_2O (500 ml) to afford **67** (63.61 g, 61% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.83 (t, 2 H, *J* = 6.5 Hz, CH_2), 3.33 (t, 2 H, *J* = 6.5 Hz, CH_2), 4.01 (s, 4 H, CH_2), 7.20–7.26 (m, 2 H, CH), 7.29–7.35 (m, 2 H, CH), 7.40 (d, 1 H, *J* = 7.8

Hz, CH), 7.83 (dd, 1 H, *J* = 1.8, 7.8 CH), 7.93 (d, 1 H, *J* = 1.8 Hz, CH), 10.65 (br, s, 1 H, OH). ^{1}H NMR analysis indicated the presence of 3-5% of the fully aromatized analogue of the product. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 28.33, 33.35, 36.26, 36.51, 126.29, 126.59, 126.63, 127.29, 127.62, 127.65, 127.87, 134.84, 135.74, 136.16, 137.44, 142.92, 178.98, 197.83. Anal. Calcd for $C_{18}H_{16}O_3$: C 77.12, H 5.75. Found: C 76.87, H 5.50.

4-(9,10-Dihydro-2-anthryl)butanoic acid (68). To a solution of **67** (63.07 g, 225 mmol) in diethylene glycol (600 ml) at 100°C was added hydrazine monohydrate (33 ml, 679 mmol). The reaction mixture was stirred for 1 h, then potassium hydroxide added (37.89 g, 675 mmol) and the temperature raised to 200°C. After 8 h the reaction mixture was allowed to cool, and diluted with H_2O (2.4 L). The solution was filtered twice through a celite plug to remove insoluble solids, and the clear filtrate acidified to pH 1 with 5 M HCl. The resulting precipitate was collected, washed with H_2O (750 ml), and dissolved into methylene chloride (700 ml). The aqueous layer was separated and discarded, and the organic solution dried over $MgSO_4$, filtered, and concentrated to give **68** (52.02 g, 87% yield) as a light tan solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.99 (quin, 2 H, *J* = 7.5 Hz, CH_2), 2.40 (t, 2 H, *J* = 7.5 Hz, CH_2), 2.69 (t, 2 H, *J* = 7.5 Hz, CH_2), 3.95 (s, 4 H, CH_2), 7.05 (dd, 1 H, *J* = 1.8, 7.6 Hz, CH), 7.15 (d, 1 H, *J* = 1.8 Hz, CH), 7.19–7.26 (m, 3 H, CH), 7.29–7.35 (m, 2 H, CH), 11.54 (br, s, 1 H, OH). ^{1}H NMR analysis indicated the presence of approximately 10% of the fully aromatized analogue of the product. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 26.56, 33.52, 34.87, 35.97, 36.37, 126.27, 126.27, 126.45, 127.60, 127.62, 127.64, 127.73, 134.61, 136.89, 136.96, 137.02, 139.22, 179.93. Anal. Calcd for $C_{18}H_{18}O_2$: C 81.17, H 6.81. Found: C 80.63, H 6.71.

Methyl 4-(9,10-dihydro-2-anthryl)butanoate (69). A mixture of **68** (51.79 g, 194 mmol) and sulfuric acid (5.2 ml) in methanol (520 ml) was refluxed for 18 h. After cooling, the reaction mixture was diluted with diethyl ether (800 ml) and consecutively washed with 1 M $NaHCO_3$ (800 ml) and H_2O (500 ml). The organic solution was dried over $MgSO_4$, filtered, and concentrated to afford **69** (53.37 g, 98% yield) as a red-brown oil. ^1H NMR ($CDCl_3$, 400 MHz): δ 1.97 (quin, 2 H, J = 7.5 Hz, CH_2), 2.35 (t, 2 H, J = 7.5 Hz, CH_2), 2.65 (t, 2 H, J = 7.5 Hz, CH_2), 3.68 (s, 3 H, CH_3), 3.93 (s, 4 H, CH_2), 7.03 (dd, 1 H, J = 1.4, 7.6 Hz, CH), 7.14 (d, 1 H, J = 1.4 Hz, CH), 7.18–7.25 (m, 3 H, CH), 7.28–7.34 (m, 2 H, CH). ^1H NMR analysis indicated the presence of approximately 10% of the fully aromatized analogue of the product. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 26.85, 33.62, 35.00, 35.98, 36.39, 51.67, 126.26, 126.26, 126.45, 127.59, 127.59, 127.59, 127.73, 134.54, 136.91, 136.91, 137.05, 139.41, 174.17. Anal. Calcd for $C_{19}H_{20}O_2$: C 81.40, H 7.19. Found: C 81.60, H 7.02.

Methyl 4-(2-anthryl)butanoate (70). A solution of **69** (53.18 g, 190 mmol) in 2-ethoxyethyl ether (200 ml) was refluxed in the presence of 5% Pd/C catalyst (5.32 g) for 40 h. After cooling, the reaction mixture was poured into acetone (300 ml), and the solution filtered to remove palladium catalyst. Dilution of the filtrate with H_2O (750 ml) gave a precipitate that was collected, and washed with a further portion of H_2O (200 ml). The precipitate was dissolved into methylene chloride (250 ml), and the aqueous layer separated and discarded. The organic solution was dried over $MgSO_4$, filtered, and diluted with hexanes (1.25 L). Upon concentration to ½ volume a cream colored precipitate formed, and this was collected and washed with hexanes (200 ml) to yield **70** (45.90 g, 87% yield). ^1H NMR ($CDCl_3$, 400 MHz): δ 2.12 (quin, 2

H, J = 7.5 Hz, CH_2), 2.42 (t, 2 H, J = 7.5 Hz, CH_2), 2.87 (t, 2 H, J = 7.6 Hz, CH_2), 3.68 (s, 3 H, CH_3), 7.33 (dd, 1 H, J = 1.5, 8.7 Hz, CH), 7.42–7.49 (m, 2 H, CH), 7.77 (s, 1 H, CH), 7.93–8.02 (m, 3 H, CH), 8.35 (s, 1 H, CH), 8.40 (s, 1 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 26.18, 33.64, 35.65, 51.70, 125.25, 125.51, 125.70, 126.17, 126.40, 127.43, 128.28, 128.38, 128.52, 130.84, 131.61, 132.10, 132.10, 138.44, 174.11. Anal. Calcd for $C_{19}H_{18}O_2$: C 81.99, H 6.52. Found: C 81.51, H 6.76.

3,4-Dihydrobenz[a]anthracen-1(*2H*)-one (71). A solution of **70** (45.70 g, 164 mmol) in methanesulfonic acid (450 ml) was heated to 90°C and stirred for 2 h. The reaction mixture was poured into H_2O (900 ml) and allowed to cool. The resulting aqueous mixture was extracted with methylene chloride (1 X 300 ml, 4 X 100 ml), and the extracts combined and washed consecutively with 1 M $NaHCO_3$ (300 ml) and H_2O (300 ml). The organic solution was dried over $MgSO_4$, filtered, and concentrated to afford **71** (40.31 g, 100% yield) as a yellow-brown solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.23 (quin, 2 H, J = 6.4 Hz, CH_2), 2.84 (t, 2 H, J = 6.6 Hz, CH_2), 3.13 (t, 2 H, J = 6.1 Hz, CH_2), 7.25 (d, 1 H, J = 8.6, Hz, CH), 7.47–7.55 (m, 2 H, CH), 7.95–8.00 (m, 1 H, CH), 8.06 (d, 1 H, J = 8.6, Hz, CH), 8.11–8.16 (m, 1 H, CH), 8.34 (s, 1 H, CH), 10.11 (s, 1 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.13, 32.09, 41.24, 126.11, 126.16, 126.61, 126.95, 127.01, 127.87, 128.63, 129.69, 131.27, 131.27, 133.89, 135.11, 148.01, 200.38 (one signal not observed). Anal. Calcd for $C_{18}H_{14}O$: C 87.78, H 5.73. Found: C 87.75, H 5.72.

3,4-Dihydro-2-(hydroxymethylene)benz[a]anthracen-1(*2H*)-one (72). To a solution of ethyl formate (23.49 g, 317 mmol) in benzene (500 ml) was added sodium methoxide (12.85 g, 238 mmol). To this was added with vigorous stirring a solution of **71** (39.05 g, 158 mmol) in benzene (500 ml) and the reaction mixture then stirred for 16 h. This was diluted with hexanes (1 L), filtered, and the collected solid washed with a further portion of hexanes (500 ml). The solid was redissolved into methanol (300 ml), acidified with 2.5 M HCl (700 ml), and the precipitate extracted into methylene chloride (3 X 300 ml). The extracts were combined, dried over $MgSO_4$, filtered, and concentrated. Purification of the crude residue via filtration through a silica gel plug (1:1 hexanes/methylene chloride) gave **72** (33.35 g, 77% yield) as a bright orange solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 2.57 (t, 2 H, *J* = 6.8 Hz, CH_2), 3.04 (t, 2 H, *J* = 6.8 Hz, CH_2), 7.27 (d, 1 H, *J* = 8.6 Hz, CH), 7.48–7.56 (m, 2 H, CH), 7.79 (d, 1 H, *J* = 8.4, Hz, CH), 7.96–8.01 (m, 1 H, CH), 8.06 (d, 1 H, *J* = 8.6 Hz, CH), 8.09–8.14 (m, 1 H, CH), 8.38 (s, 1 H, CH), 9.91 (s, 1 H, CH), 15.11 (d, 1 H, *J* = 8.8 Hz, OH). ^{1}H NMR analysis indicated the presence of approximately 15% of the fully aromatized analogue of the product. ^{13}C NMR ($CDCl_3$, 100 MHz): δ 23.43, 31.44, 110.75, 126.17, 126.23, 126.29, 126.50, 127.28, 127.32, 127.93, 128.33, 129.54, 131.36, 131.55, 133.47, 134.94, 145.66, 168.04, 190.45. Anal. Calcd for $C_{19}H_{14}O_2$: C 83.19, H 5.14. Found: C 82.97, H 4.76.

***Zn*(II)-(*R*,*R*)-37 complex ((*R*,*R*)-75).** Zinc chloride (0.066 g, 0.48 mmol), sodium methoxide (0.078 g, 1.45 mmol) and (*R*,*R*)-**37** (0.301 g, 0.48 mmol) were suspended into a 2:1 mixture of methylene chloride/ethanol (15 ml) and stirred overnight. The reaction mixture was concentrated to a yellow solid that was dissolved into THF (20 ml), and filtered to remove fine

insoluble solids. The clear filtrate was stirred for 2 h, resulting in gradual formation of a yellow precipitate. The precipitate was collected and washed consecutively with THF (5 ml) and ethanol (5 ml) to afford (*R*,*R*)-**75** (0.177 g, 53% yield). ^{1}H NMR (pyridine- d_5, 400 MHz): δ 1.25–1.40 (m, 4 H, CH), 1.76–1.87 (m, 2 H, CH), 2.29–2.40 (m, 2 H, CH), 3.27–3.36 (m, 2 H, CH), 6.45 (t, 2 H, *J* = 7.4 Hz, CH), 7.12 (t, 2 H, *J* = 7.4 Hz, CH), 7.29 (d, 2 H, *J* = 8.0 Hz, CH), 7.48 (d, 2 H, *J* = 8.3 Hz, CH), 7.68 (d, 2 H, *J* = 8.0 Hz, CH), 7.76 (d, 2 H, *J* = 8.8 Hz, CH), 7.91 (d, 2 H, *J* = 8.3 Hz, CH), 8.05 (d, 2 H, *J* = 8.8 Hz, CH), 8.47 (s, 2 H, CH), 8.68 (s, 2 H, CH), 12.15 (s, 2 H, CH). ^{13}C NMR (pyridine- d_5, 100 MHz): δ 25.11, 29.04, 66.51, 114.74, 118.77, 124.50, 124.76, 125.75, 126.79, 127.38, 128.77, 129.27, 130.60, 131.22, 131.58, 132.30, 132.42, 133.89, 134.85, 138.69, 166.57, 174.40. Anal. Calcd for $C_{44}H_{32}N_2O_2Zn$: C 77.02, H 4.70, N 4.08. Found: C 77.19, H 4.65, N 4.21. Single crystals suitable for X-ray analysis were grown by slow diffusion of diethyl ether into a solution of (*R*,*R*)-**75** in pyridine.

Fe(II)-(*R*,*R*)-37 complex ((*R*,*R*)-76). Iron (II) chloride (0.061 g, 0.48 mmol), sodium methoxide (0.078 g, 1.45 mmol) and (*R*,*R*)-**37** (0.300 g, 0.48 mmol) were suspended into a 2:1 mixture of methylene chloride/ethanol (15 ml). After stirring overnight the reaction mixture was concentrated to a solid that was dissolved into THF (15 ml). The solution was filtered to remove fine insoluble solids, and the clear filtrate diluted with ethanol (15 ml). Upon stirring for 30 minutes a black precipitate formed, and this was collected to afford (*R*,*R*)-**76** (0.223 g, 68% yield). ^{1}H NMR (pyridine- d_5, 400 MHz): δ −24.14 (br, s, 2 H, CH), −11.24 (s, 2 H, CH), −5.60–−2.40 (m, 6 H, CH), 2.99 (s, 2 H, CH), 5.50 (s, 2 H, CH), 8.53 (s, 2 H, CH), 9.91 (s, 2 H, CH), 12.72 (s, 2 H, CH), 16.29 (s, 2 H, CH), 24.69 (s, 2 H, CH), 41.69 (br, s, 2 H, CH). Anal.

Calcd for $C_{44}H_{32}N_2O_2Fe$: C 78.11, H 4.77, N 4.14. Found: C 78.12, H 5.02, N 3.90. Single crystals suitable for X-ray analysis were grown by slow diffusion of ethanol into a solution of (*R*,*R*)-**76** in pyridine.

Zn(II)-(*R*)-38 complex ((*R*)-77). Zinc chloride (0.048 g, 0.35 mmol), sodium methoxide (0.052 g, 0.96 mmol) and (*R*)-**38** (0.252 g, 0.32 mmol) were suspended into a 2:1 mixture of benzene/ethanol (15 ml) and stirred overnight. The reaction mixture was concentrated to a yellow solid that was dissolved into THF (10 ml), and filtered to remove fine insoluble solids. The clear filtrate was diluted with ethanol (20 ml), and concentrated to 2/3 volume resulting in formation of a yellow precipitate. The precipitate was collected to afford (*R*)-**77** (0.153 g, 56% yield). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.70 (t, 2 H, *J* = 7.5 Hz, CH), 6.99 (d, 2 H, *J* = 8.6 Hz, CH), 7.09 (d, 2 H, *J* = 8.2 Hz, CH), 7.19 (t, 2 H, *J* = 7.5 Hz, CH), 7.23–7.29 (m, 4 H, CH), 7.44 (t, 2 H, *J* = 7.6 Hz, CH), 7.48 (d, 2 H, *J* = 8.5 Hz, CH), 7.51–7.55 (m, 4 H, CH), 7.84 (d, 2 H, *J* = 8.3 Hz, CH), 7.91 (d, 2 H, *J* = 8.2 Hz, CH), 7.95 (d, 2 H, *J* = 8.8 Hz, CH), 8.02 (d, 2 H, *J* = 8.6 Hz, CH), 8.32 (s, 2 H, CH), 8.58 (s, 2 H, CH), 11.30 (s, 2 H, CH). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 116.30, 116.47, 122.37, 123.79, 124.94, 125.54, 125.89, 126.48, 126.59, 126.87, 126.87, 127.10, 127.31, 128.36, 128.61, 129.76, 130.32, 131.02, 131.07, 131.40, 132.31, 132.35, 133.13, 133.99, 134.20, 139.55, 145.53, 170.59, 173.65. Anal. Calcd for $C_{58}H_{34}N_2O_2Zn$: C 81.35, H 4.00, N 3.27. Found: C 80.53, H 4.35, N 3.05. Single crystals suitable for X-ray analysis were grown by slow diffusion of diethyl ether into a solution of (*R*)-**77** in methylene chloride.

Fe(II)-(*R*)-38 complex ((*R*)-78). Iron (II) chloride (0.053 g, 0.42 mmol), sodium methoxide (0.061 g, 1.14 mmol) and (*R*)-**38** (0.300 g, 0.38 mmol) were suspended into a 2:1 mixture of benzene/ethanol (15 ml) and stirred overnight. The reaction mixture was concentrated to a brown-black residue that was dissolved into THF (15 ml), and filtered to remove fine insoluble solids. The clear filtrate was diluted with ethanol (45 ml), and stirred for 30 minutes. A brown precipitate gradually formed that was collected to afford (*R*)-**78** (0.244 g, 76% yield). ^{1}H NMR (CD_2Cl_2, 400 MHz): δ $^{-}$38.86 (br, s, 2 H, CH), $^{-}$13.43 (s, 2 H, CH), $^{-}$8.90 (s, 2 H, CH), $^{-}$7.52 (s, 4 H, CH), 2.25 (s, 2 H, CH), 5.02 (s, 2 H, CH), 8.18 (s, 2 H, CH), 10.33 (s, 2 H, CH), 11.90 (s, 2 H, CH), 13.05 (s, 2 H, CH), 13.60–14.40 (m, 4 H, CH), 24.12 (s, 2 H, CH), 62.02 (br, s, 2 H, CH). Anal. Calcd for $C_{58}H_{34}N_2O_2Fe$: C 82.27, H 4.05, N 3.31. Found: C 82.38, H 4.29, N 3.22. Single crystals suitable for X-ray analysis were grown by slow diffusion of diethyl ether into a solution of (*R*)-**78** in methylene chloride.

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Appendix I

^{1}H NMR spectra

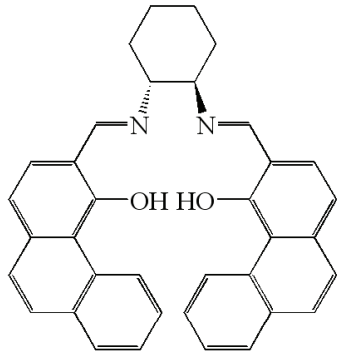
(Numerical order)

STANDARD 1H OBSERVE

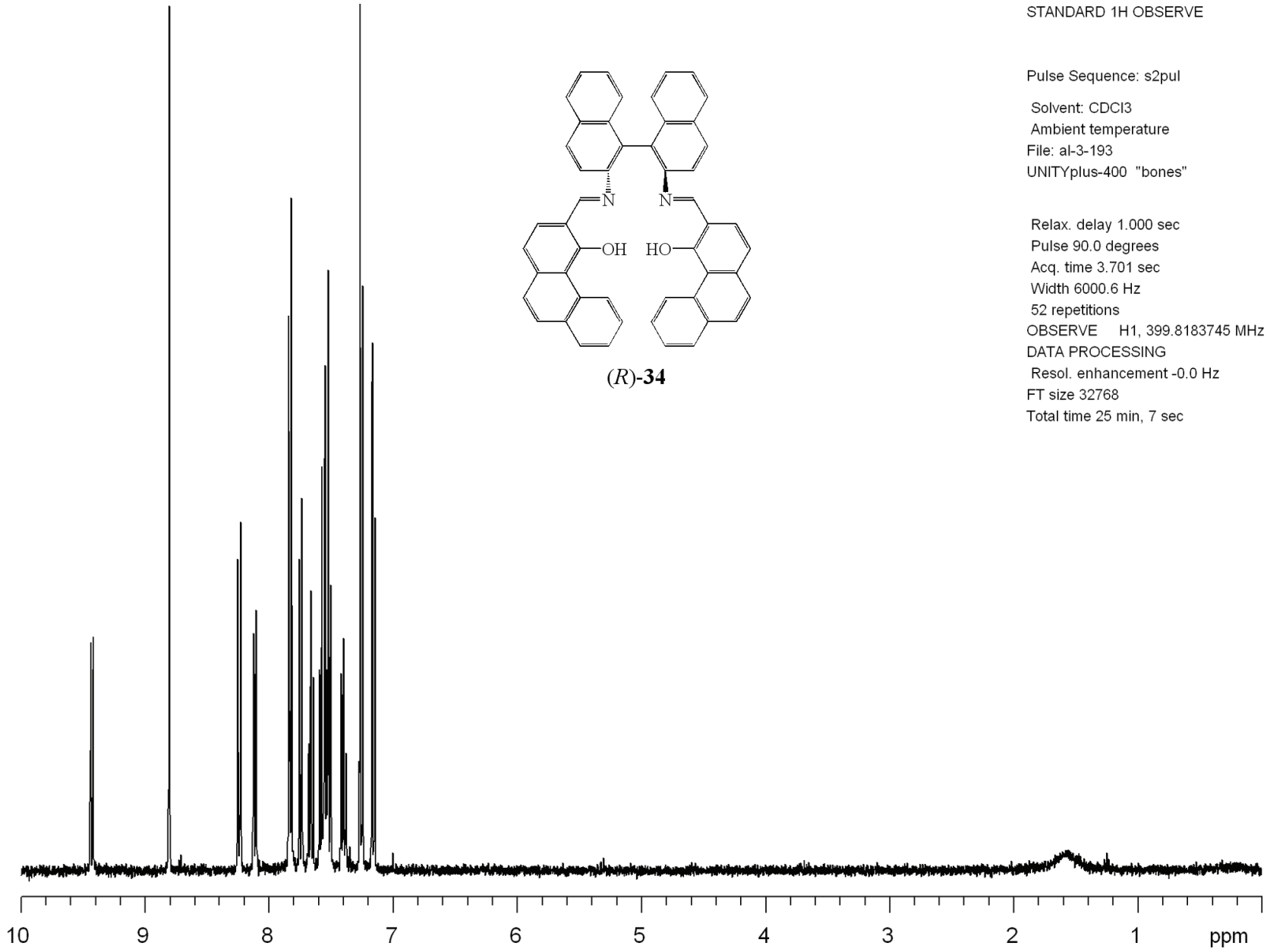
Pulse Sequence: s2pul

Solvent: pyridine
Ambient temperature
File: al-4-130_pyridine_d5
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 10000.0 Hz
176 repetitions
OBSERVE H1, 399.7923289 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



(*R,R*)-**33**


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-193
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
52 repetitions
OBSERVE H1, 399.8183745 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
OH
HO
N
N
10
9
8
7
6
5
4
3
2
1
ppm

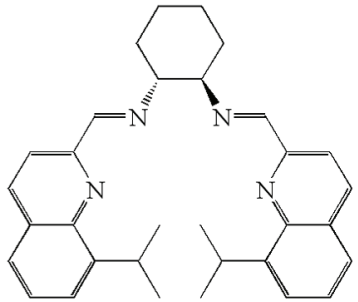
(*R*)-**34**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-188
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
40 repetitions
OBSERVE H1, 399.7988363 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



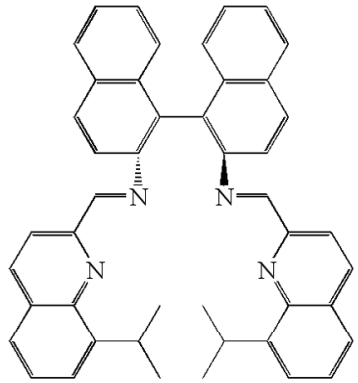
(*R*,*R*)-**35**

STANDARD 1H OBSERVE

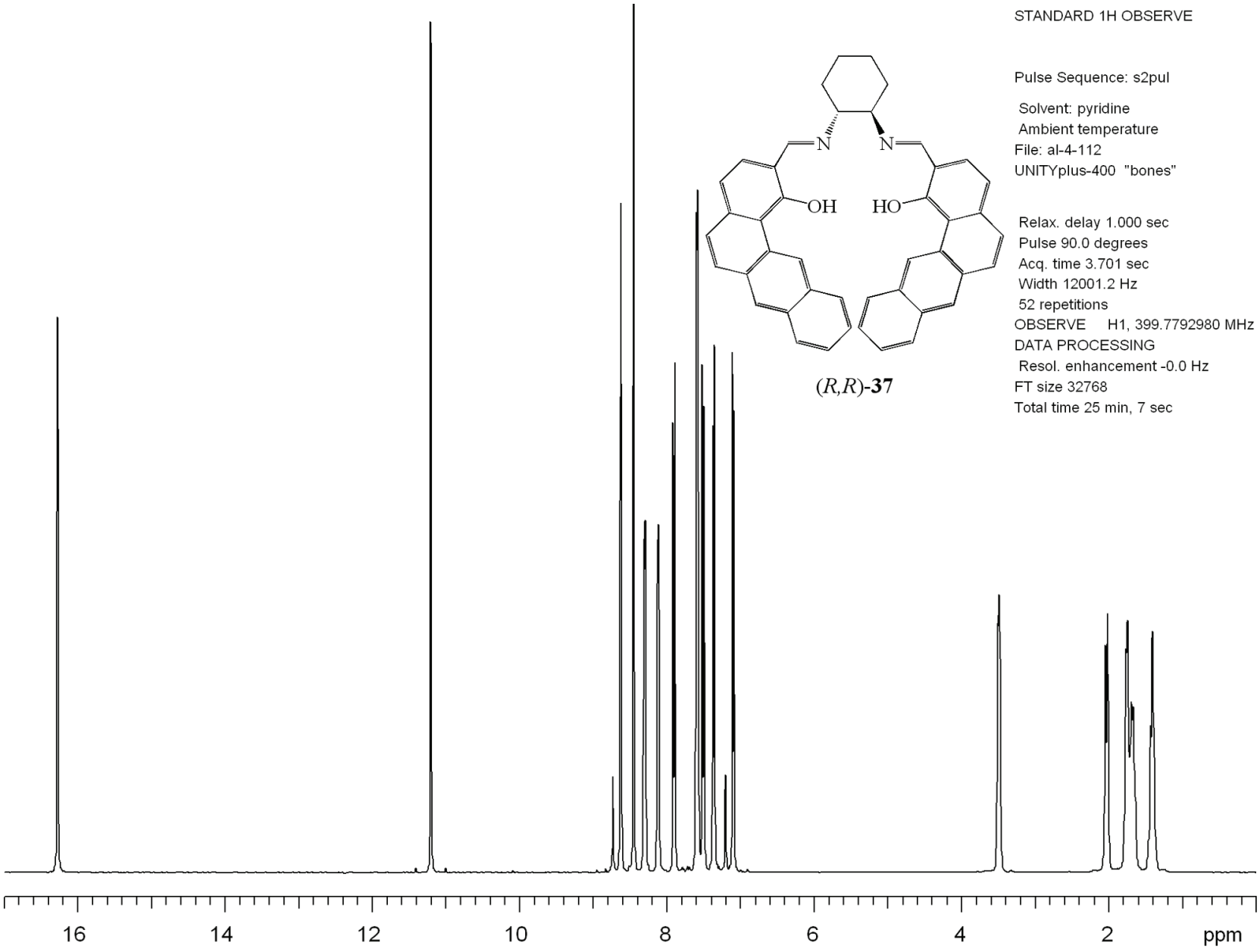
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-178
UNITYplus-400 "bones"

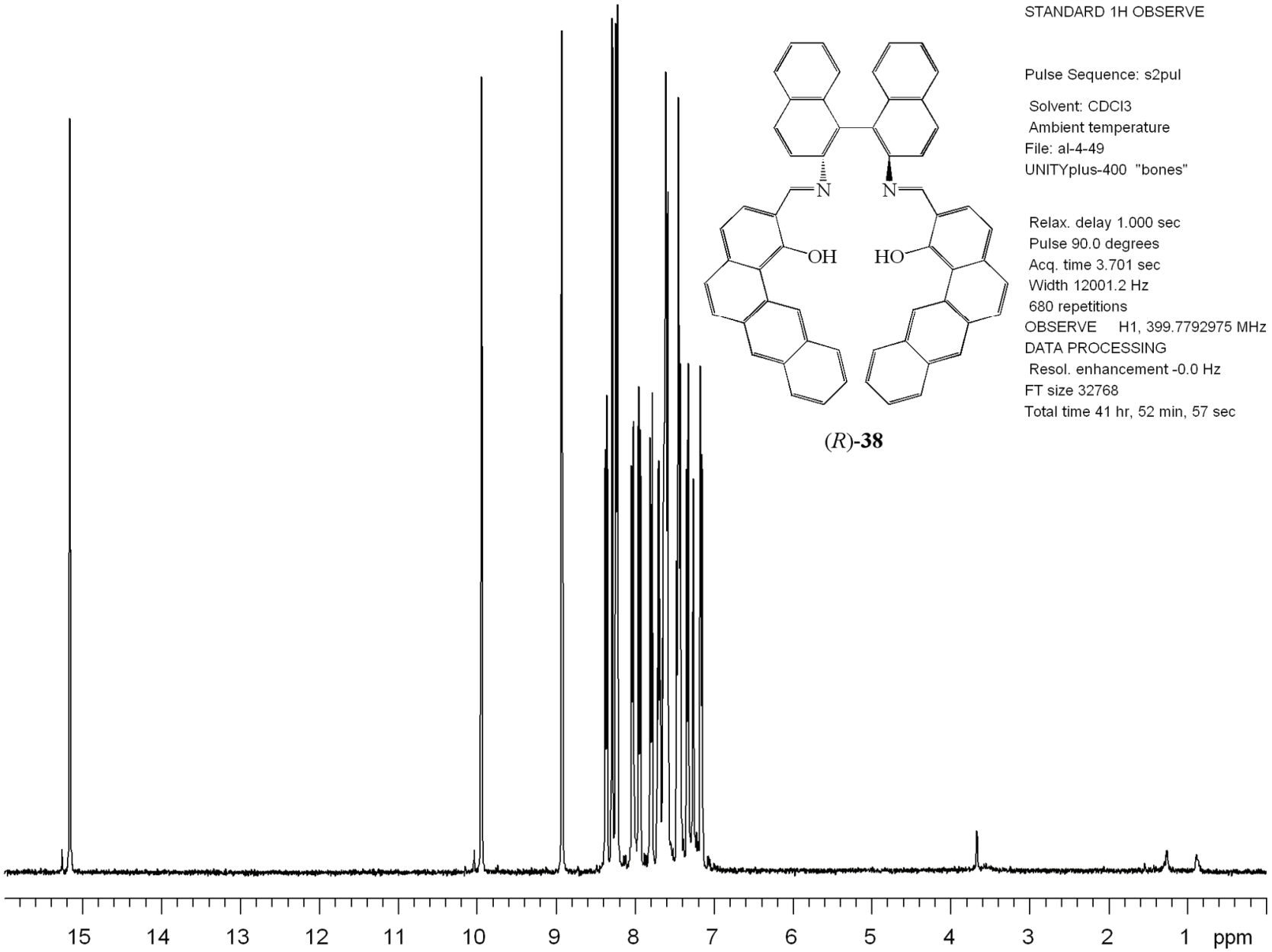
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
56 repetitions
OBSERVE H1, 399.8183757 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



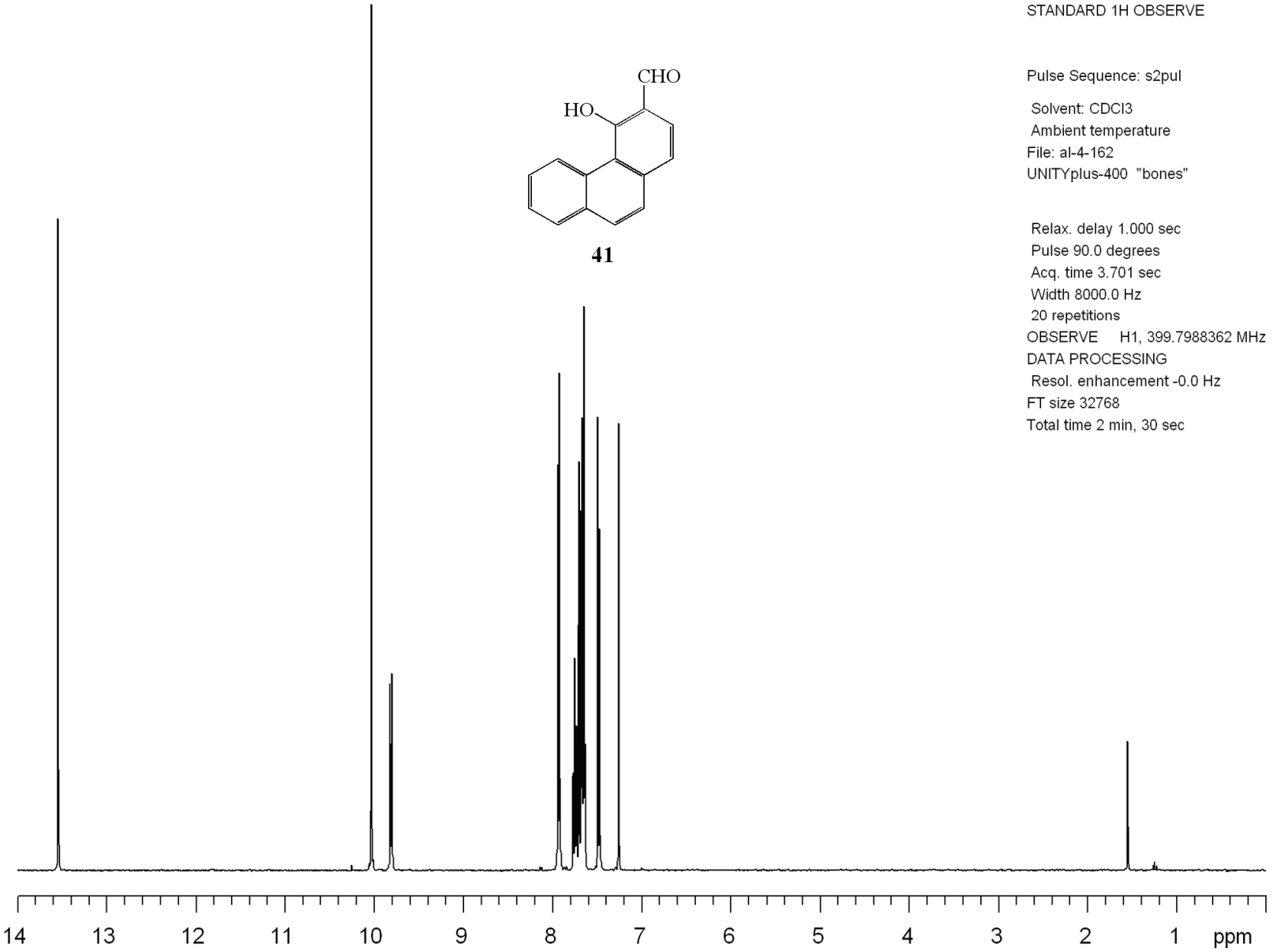
(*R*)-**36**


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-112
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 12001.2 Hz
52 repetitions
OBSERVE H1, 399.7792980 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
N
N
OH
HO
16
14
12
10
8
6
4
2
ppm

(*R*,*R*)-**37**


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-49
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 12001.2 Hz
680 repetitions
OBSERVE H1, 399.7792975 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 41 hr, 52 min, 57 sec
N
N
OH
HO
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

(*R*)-**38**

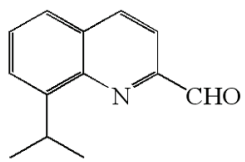

CHO
HO
41
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-162
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 8000.0 Hz
20 repetitions
OBSERVE H1, 399.7988362 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 2 min, 30 sec
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

STANDARD 1H OBSERVE

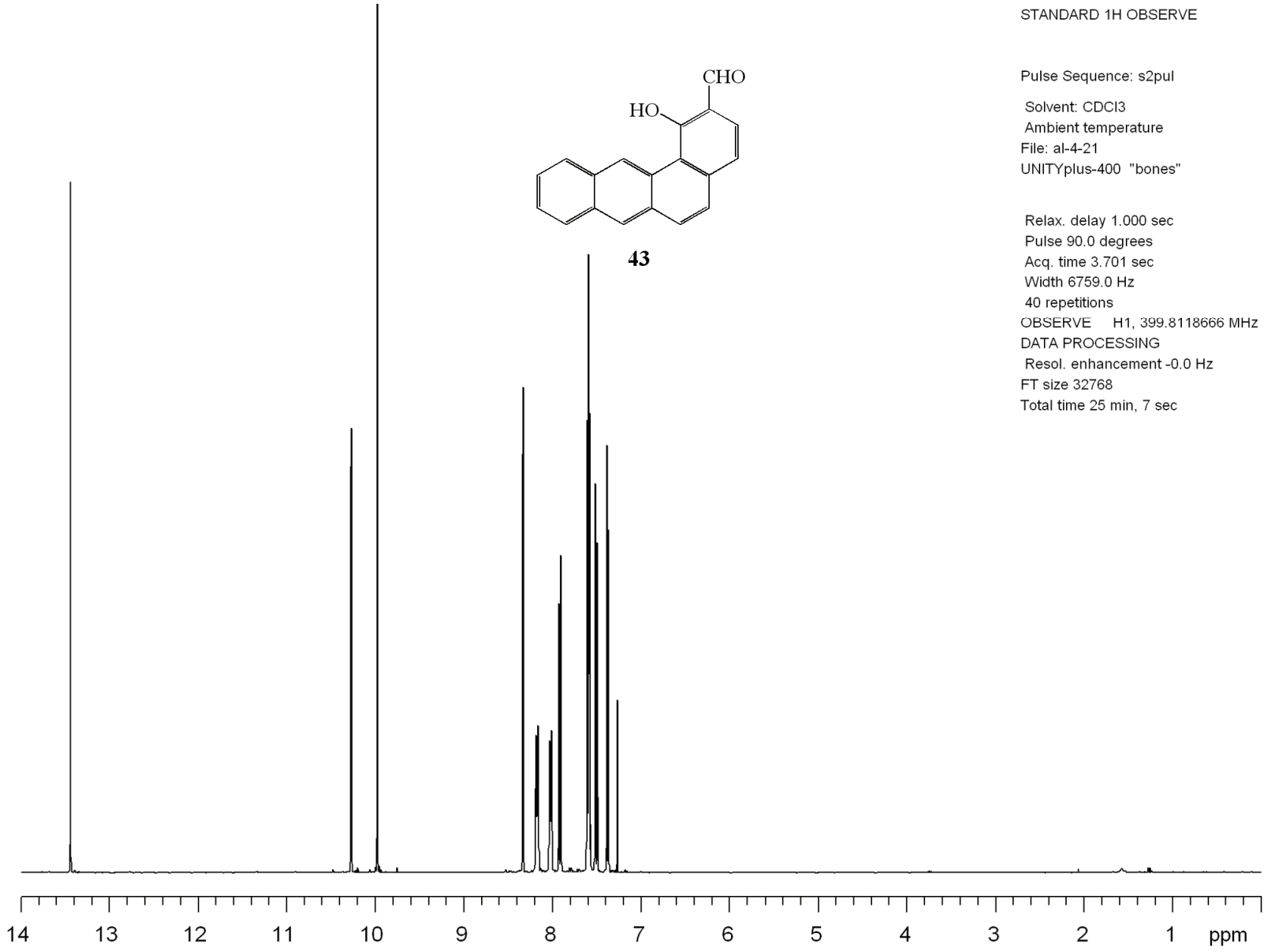
Pulse Sequence: s2pul

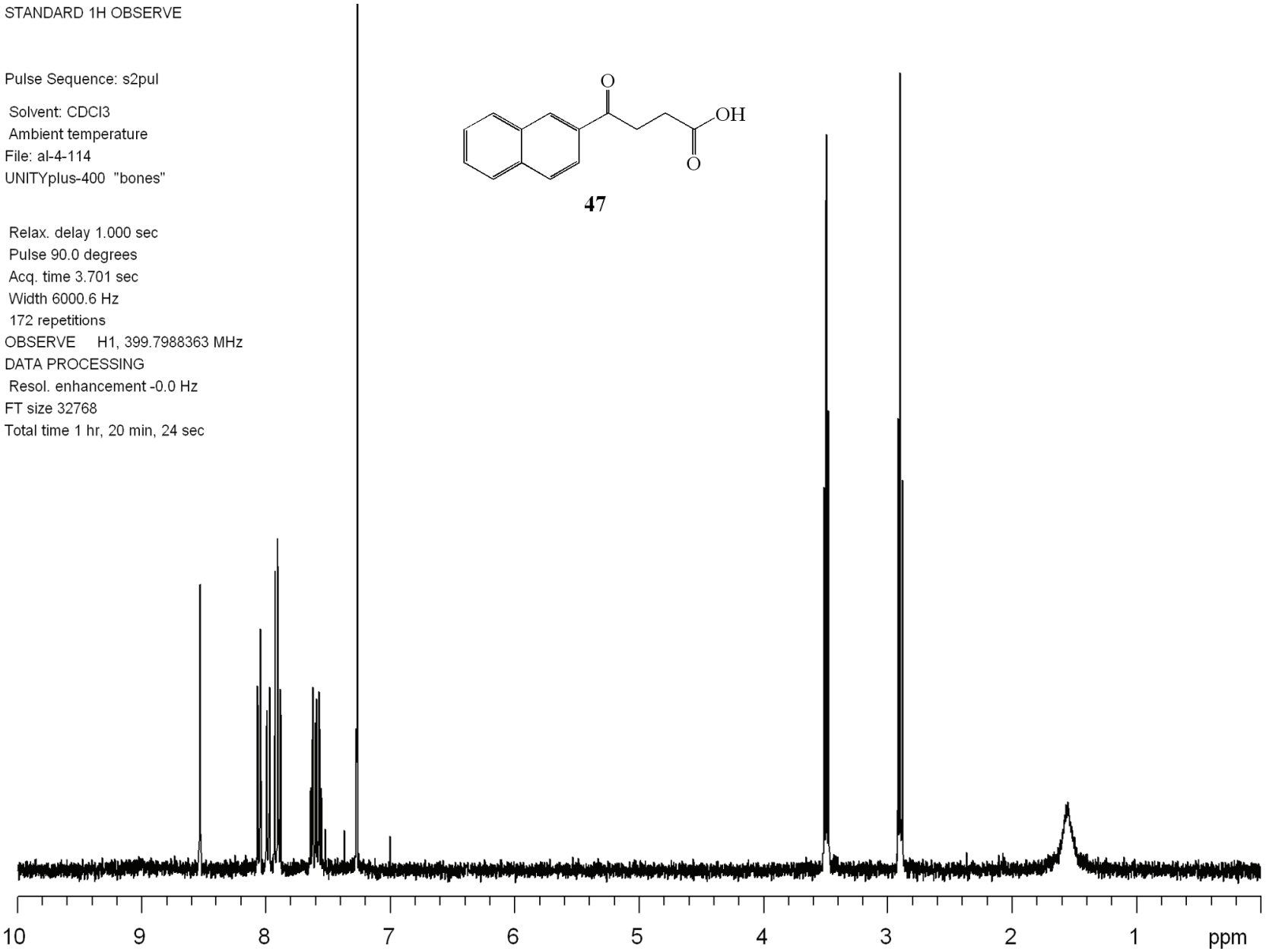
Solvent: CDCl3
Ambient temperature
File: al-3-75
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 5000.0 Hz
32 repetitions
OBSERVE H1, 399.7988360 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 23 min, 33 sec

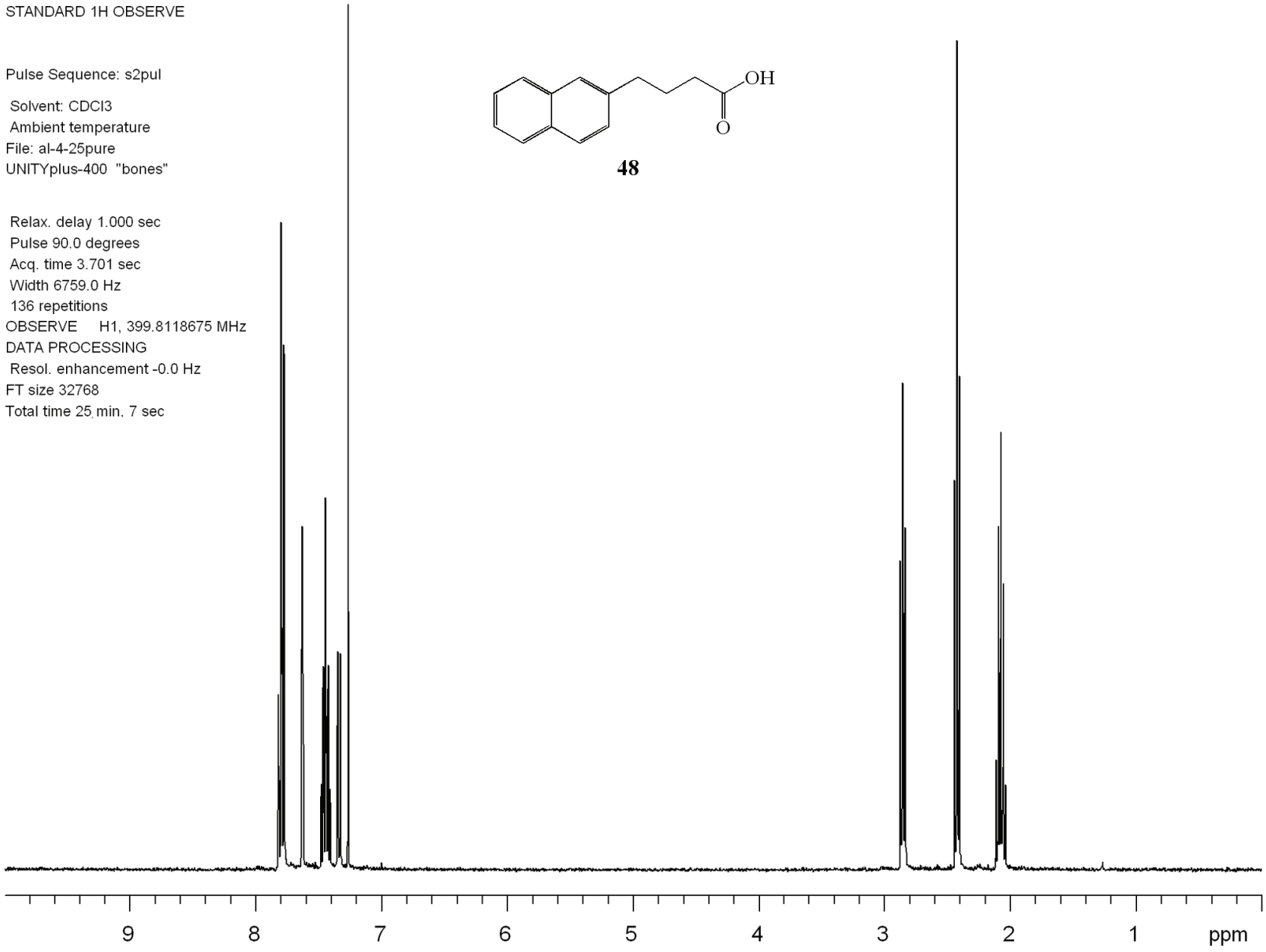


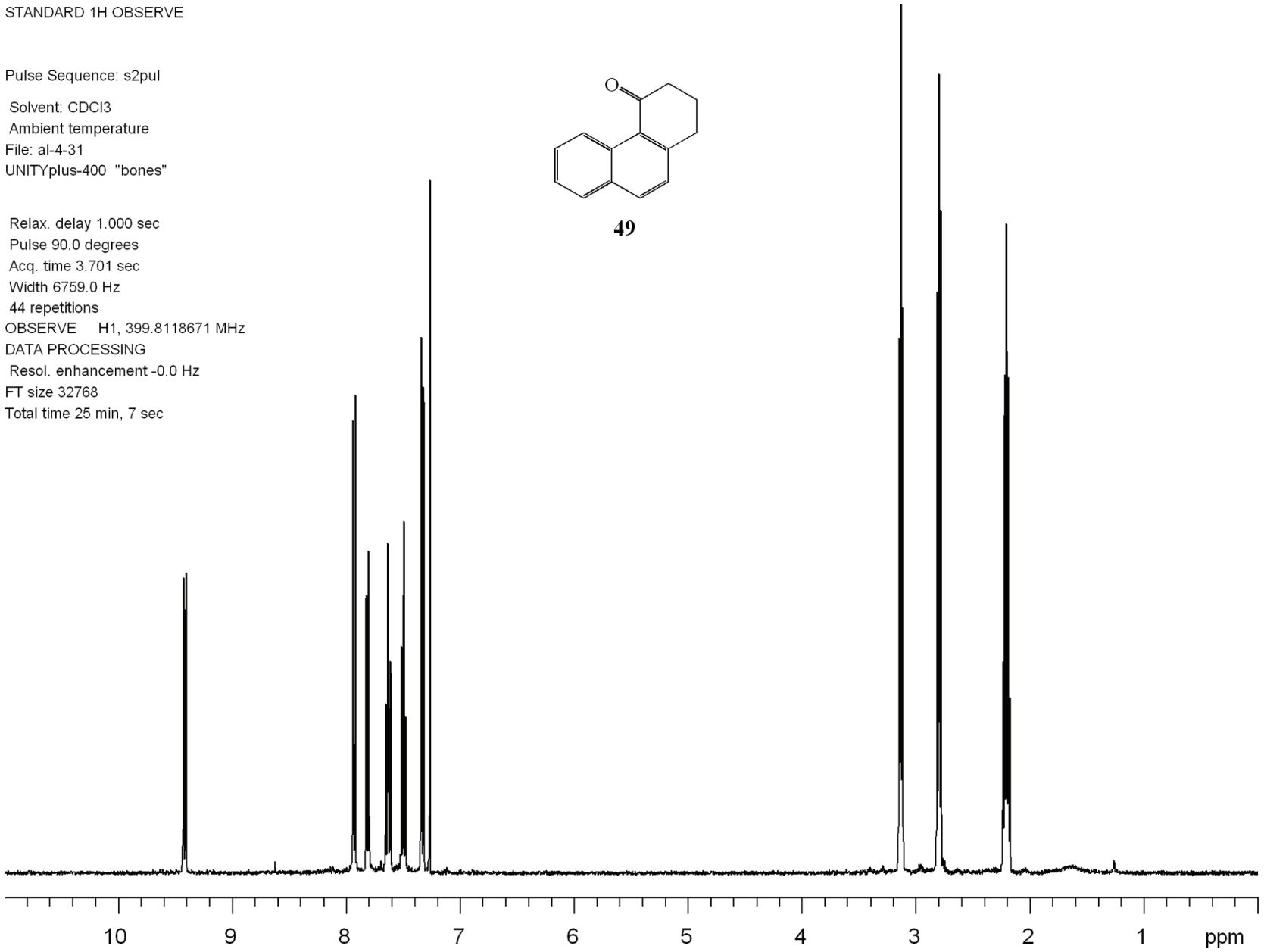
42


CHO
HO
43
STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-21
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6759.0 Hz
40 repetitions
OBSERVE H1, 399.8118666 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-114
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
172 repetitions
OBSERVE H1, 399.7988363 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 1 hr, 20 min, 24 sec
O
OH
O
10
9
8
7
6
5
4
3
2
1
ppm

47


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-25pure
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6759.0 Hz
136 repetitions
OBSERVE H1, 399.8118675 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
OH
O
48
9
8
7
6
5
4
3
2
1
ppm

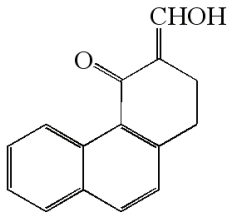

STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-31
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6759.0 Hz
44 repetitions
OBSERVE H1, 399.8118671 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
O
49
10
9
8
7
6
5
4
3
2
1
ppm

STANDARD 1H OBSERVE

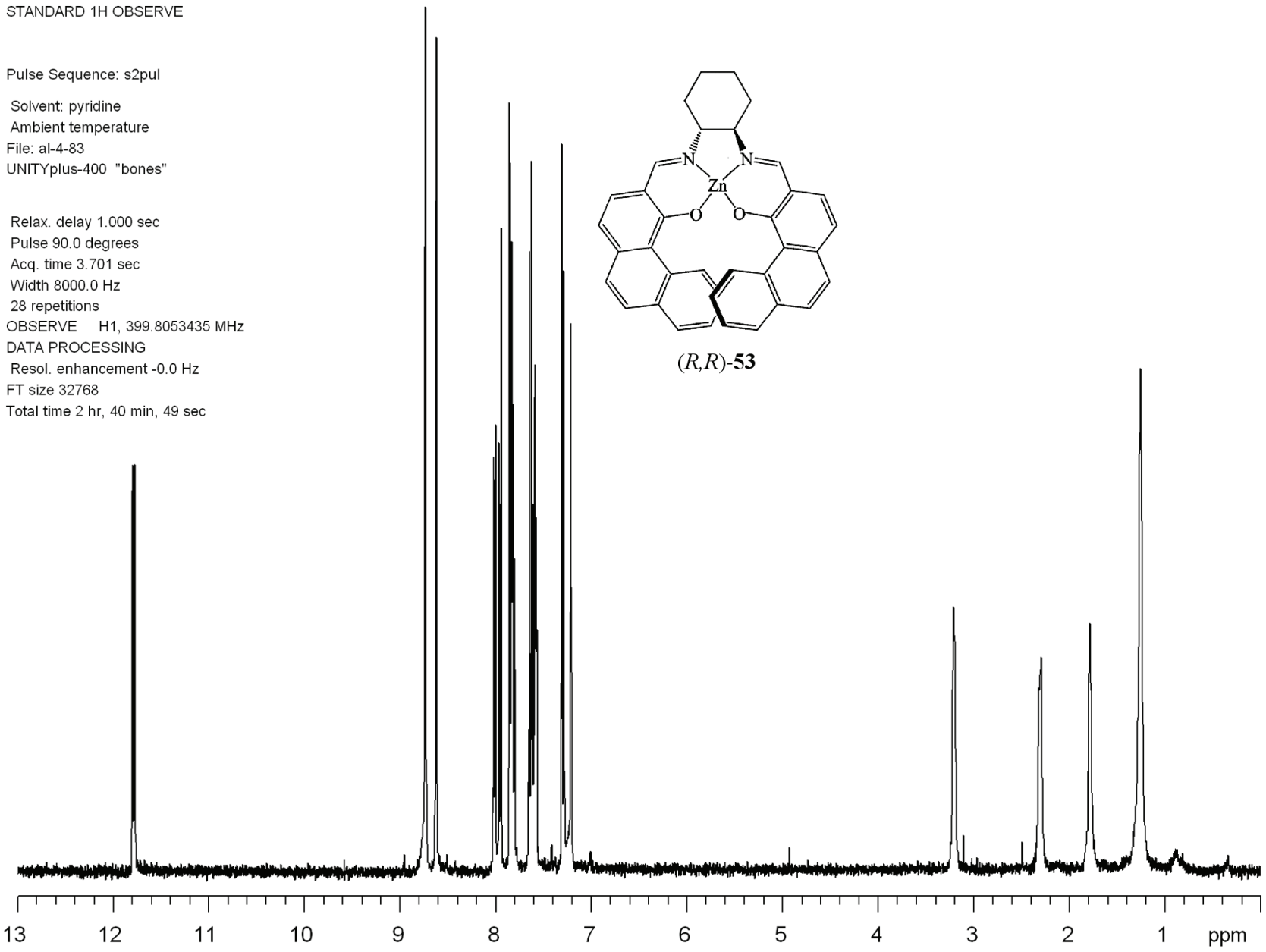
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-209
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 9000.9 Hz
92 repetitions
OBSERVE H1, 399.8183741 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



50


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-83
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 8000.0 Hz
28 repetitions
OBSERVE H1, 399.8053435 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 2 hr, 40 min, 49 sec
N
N
Zn
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

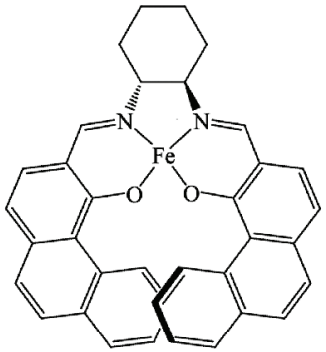
(*R*,*R*)-**53**

STANDARD 1H OBSERVE

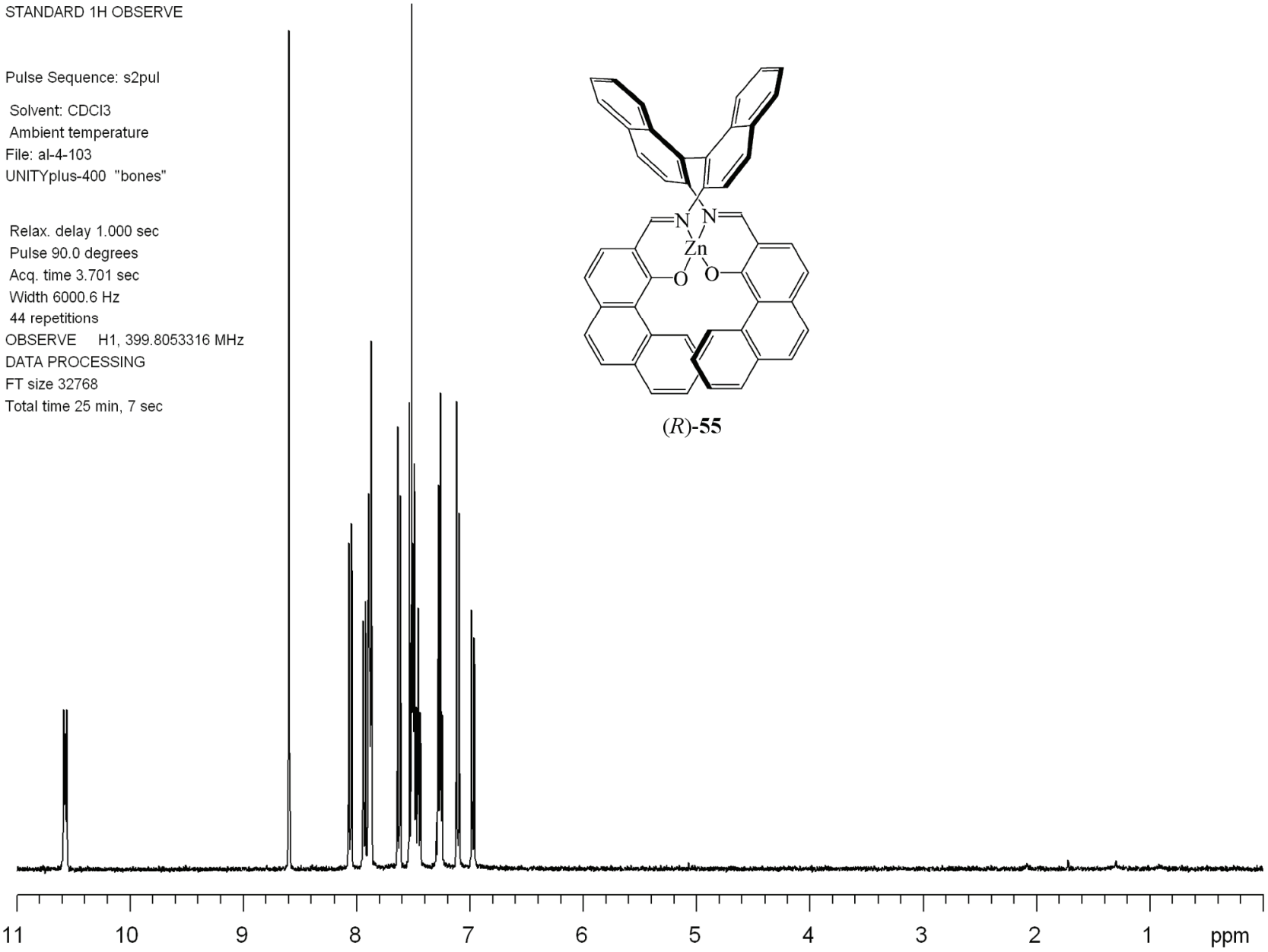
Pulse Sequence: s2pul

Solvent: pyridine
Ambient temperature
File: al-4-139
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.000 sec
Width 48019.2 Hz
112 repetitions
OBSERVE H1, 399.7989516 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 10 min, 43 sec



(*R*,*R*)-**54**


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-103
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
44 repetitions
OBSERVE H1, 399.8053316 MHz
DATA PROCESSING
FT size 32768
Total time 25 min, 7 sec
N
N
Zn
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm

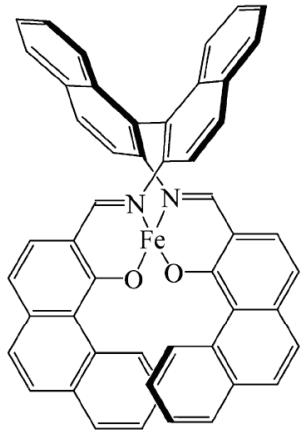
(*R*)-**55**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CD2Cl2
Ambient temperature
File: al-4-157
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 1.000 sec
Width 48019.2 Hz
2964 repetitions
OBSERVE H1, 399.7996161 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 17 hr, 52 min, 26 sec



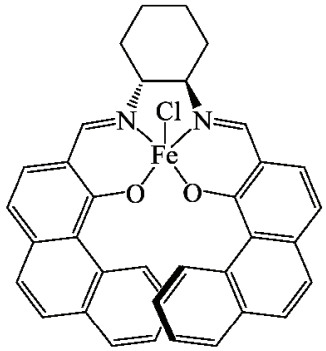
(*R*)-**56**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: DMSO
Ambient temperature
File: al-4-137
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 0.500 sec
Width 48019.2 Hz
468 repetitions
OBSERVE H1, 399.8007259 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 51 min, 34 sec



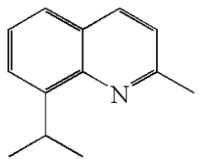
(*R*,*R*)-**57**

STANDARD 1H OBSERVE

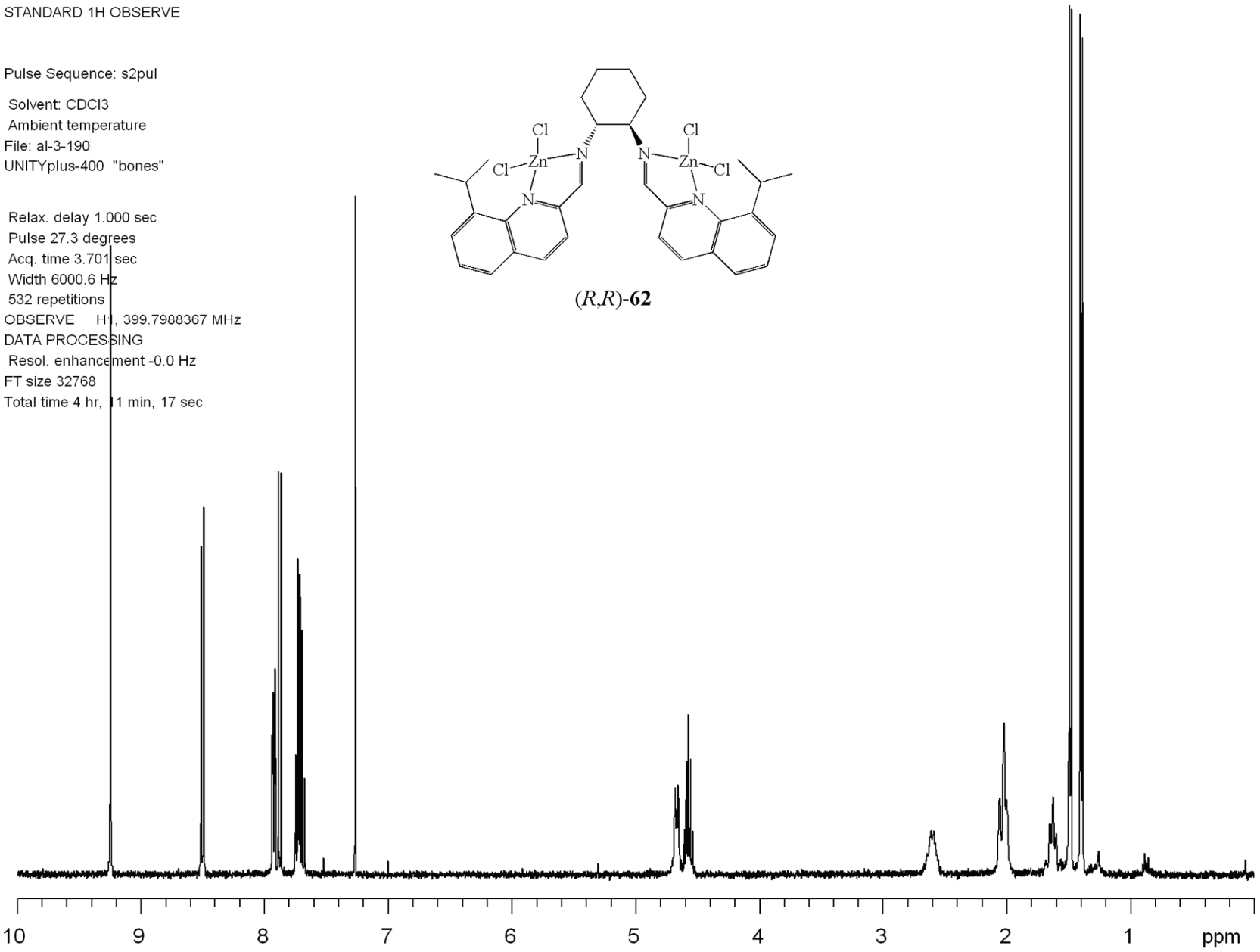
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-64
UNITYplus-400 "bones"

Relax. delay 2.000 sec
Pulse 9.5 degrees
Acq. time 3.700 sec
Width 8000.0 Hz
32 repetitions
OBSERVE H1, 399.8248986 MHz
DATA PROCESSING
Line broadening 0.3 Hz
FT size 32768
Total time 3 min, 2 sec



59


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-190
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
532 repetitions
OBSERVE H1, 399.7988367 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 4 hr, 11 min, 17 sec
Cl
Zn
N
Cl
Cl
Zn
N
Cl
N
N
10
9
8
7
6
5
4
3
2
1
ppm

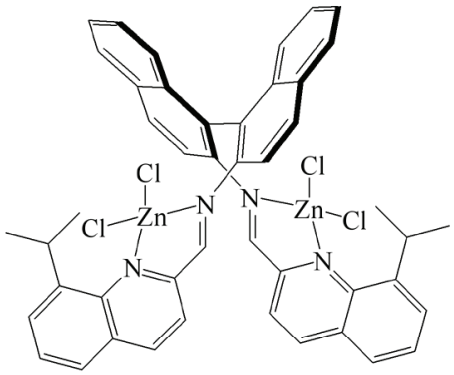
(*R*,*R*)-**62**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-163
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
224 repetitions
OBSERVE H1, 399.7988363 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 4 hr, 11 min, 17 sec



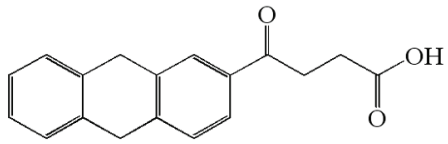
(*R*)-**63**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-282
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
60 repetitions
OBSERVE H1, 399.8118668 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



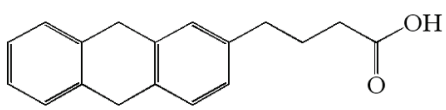
67

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-284
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
32 repetitions
OBSERVE H1, 399.8118668 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



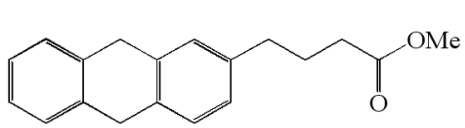
68

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-286
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
60 repetitions
OBSERVE H1, 399.8118660 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



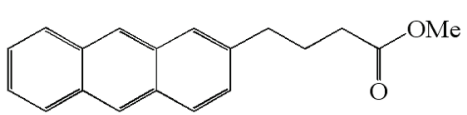
69

STANDARD 1H OBSERVE

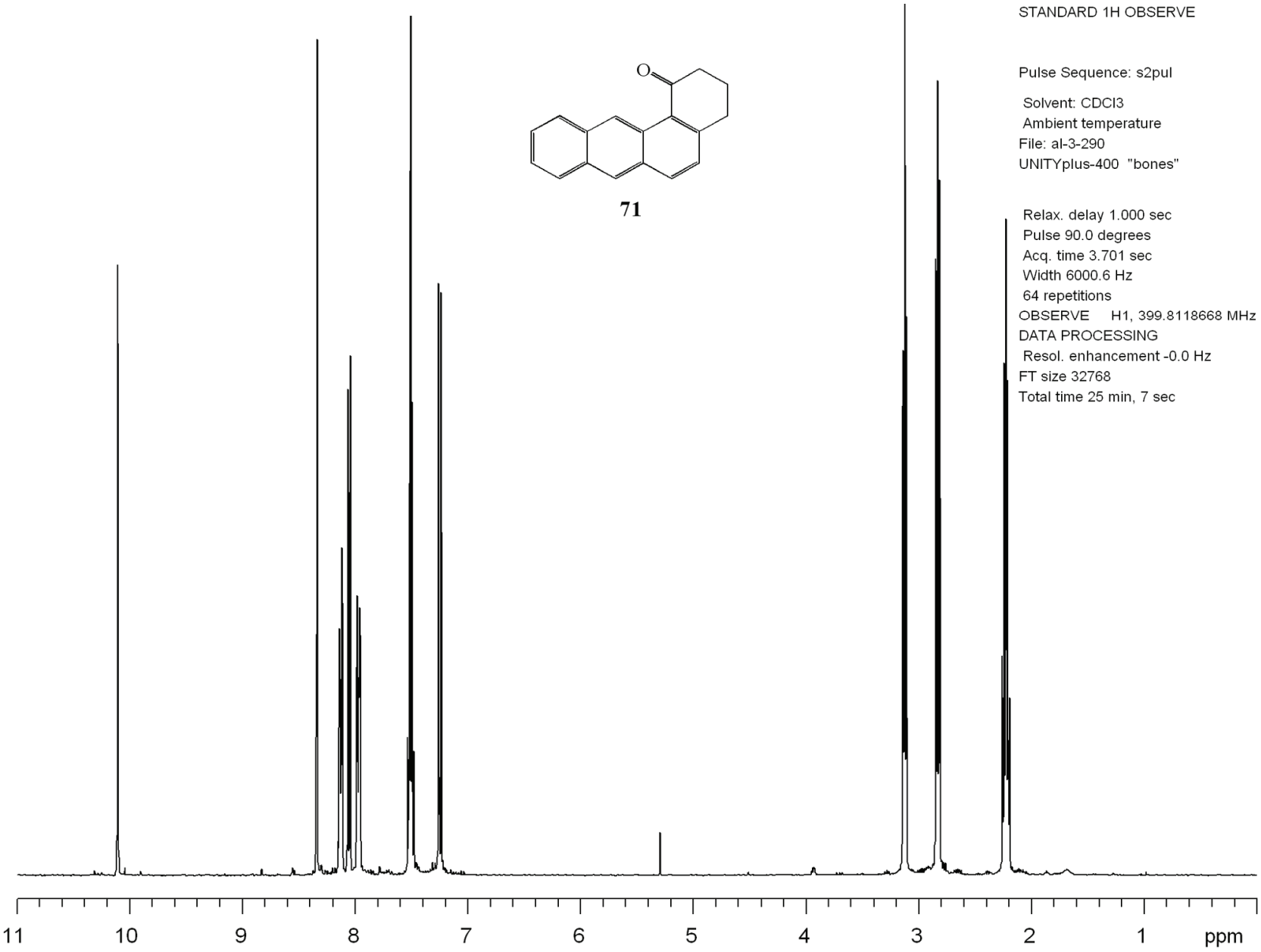
Pulse Sequence: s2pul

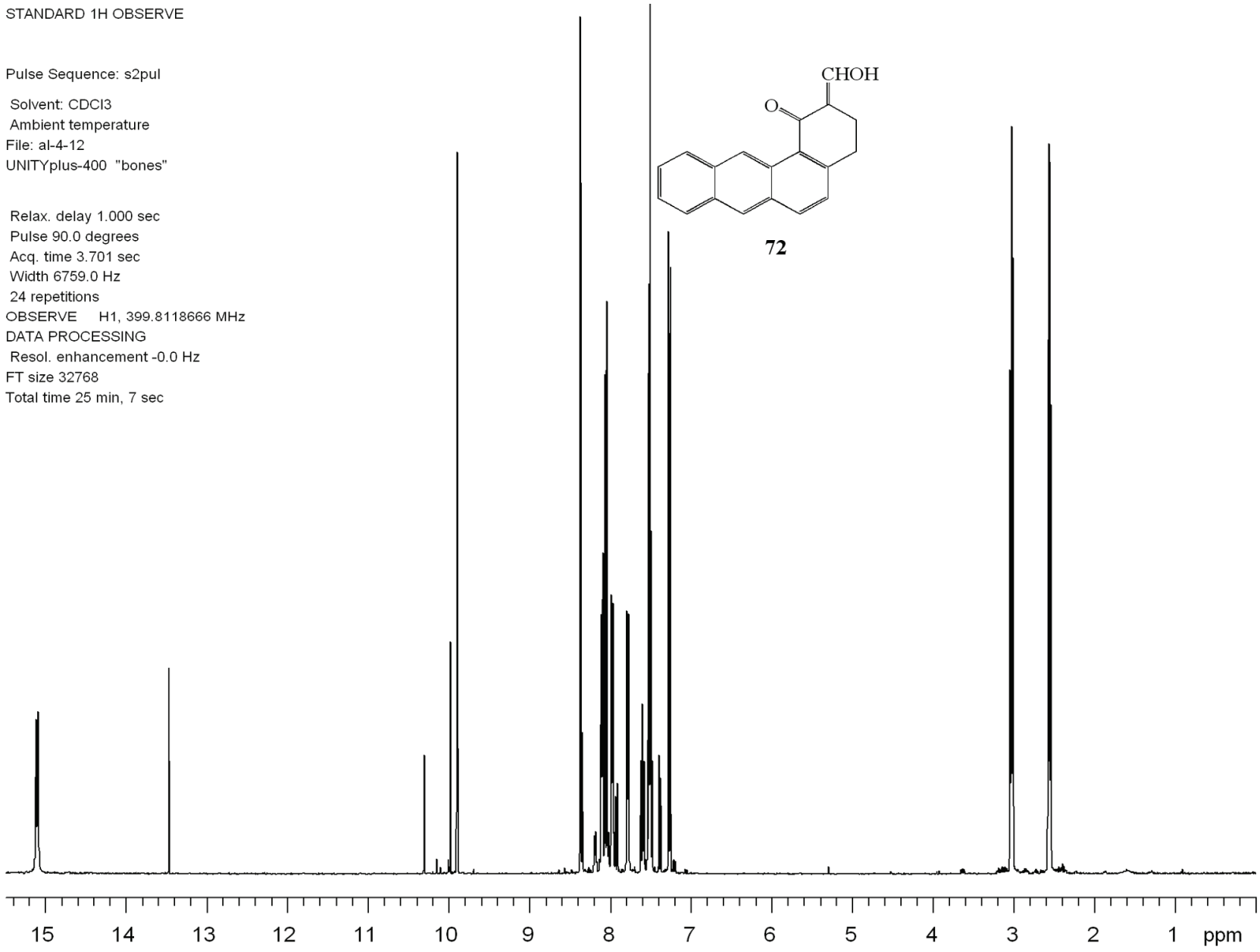
Solvent: CDCl3
Ambient temperature
File: al-3-288
UNITYplus-400 "bones"

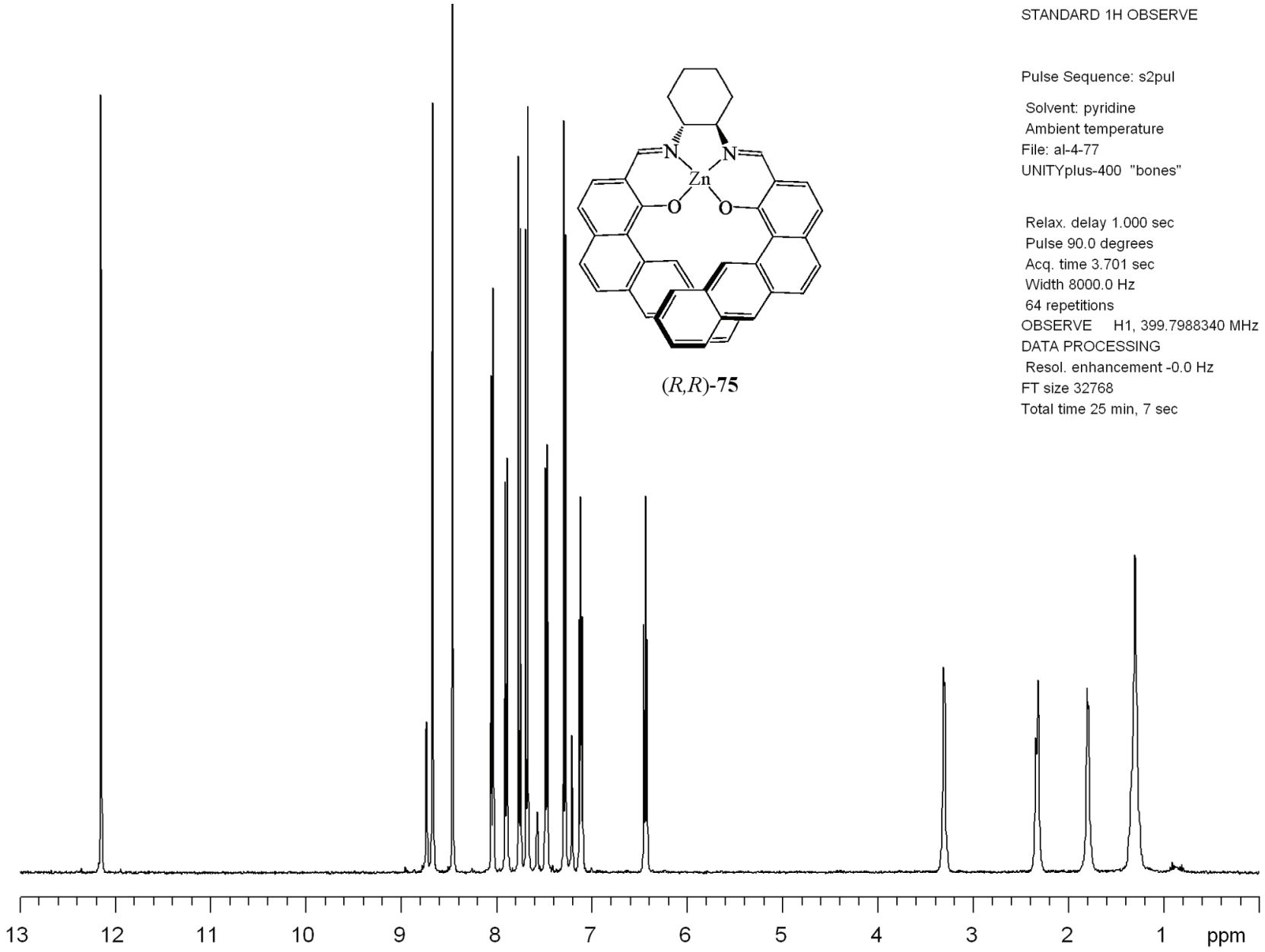
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
28 repetitions
OBSERVE H1, 399.8118664 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec



70


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-290
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6000.6 Hz
64 repetitions
OBSERVE H1, 399.8118668 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
O
71
11
10
9
8
7
6
5
4
3
2
1
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-12
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6759.0 Hz
24 repetitions
OBSERVE H1, 399.8118666 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
CHOH
O
72
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-77
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 8000.0 Hz
64 repetitions
OBSERVE H1, 399.7988340 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
N
N
Zn
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm

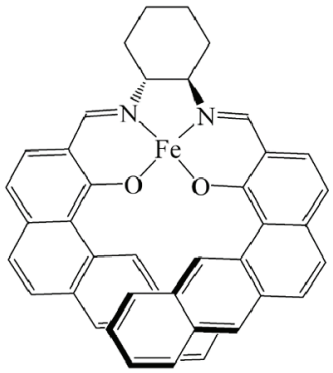
(*R*,*R*)-**75**

STANDARD 1H OBSERVE

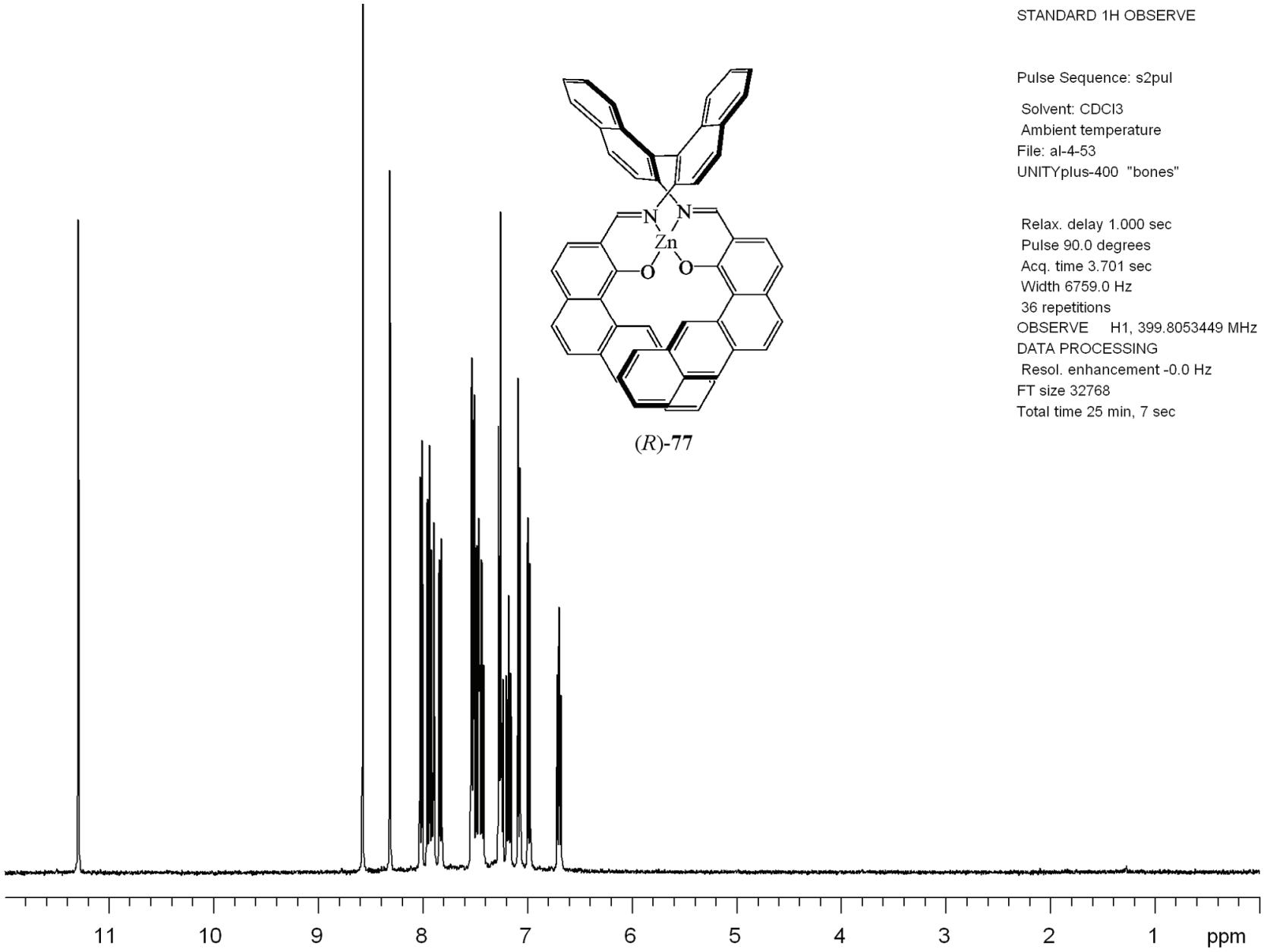
Pulse Sequence: s2pul

Solvent: pyridine
Ambient temperature
File: al-4-143
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 27.3 degrees
Acq. time 1.000 sec
Width 48019.2 Hz
712 repetitions
OBSERVE H1, 399.7989399 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 1 hr, 47 min, 14 sec



(*R,R*)-**76**


STANDARD 1H OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-53
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 6759.0 Hz
36 repetitions
OBSERVE H1, 399.8053449 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec
N
N
Zn
O
O
11
10
9
8
7
6
5
4
3
2
1
ppm

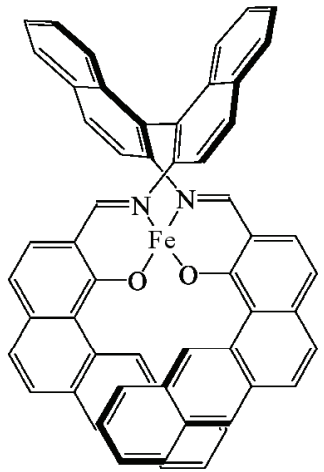
(*R*)-**77**

STANDARD 1H OBSERVE

Pulse Sequence: s2pul

Solvent: pyridine
Ambient temperature
File: al-4-110
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 3.701 sec
Width 12001.2 Hz
52 repetitions
OBSERVE H1, 399.7792980 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 32768
Total time 25 min, 7 sec

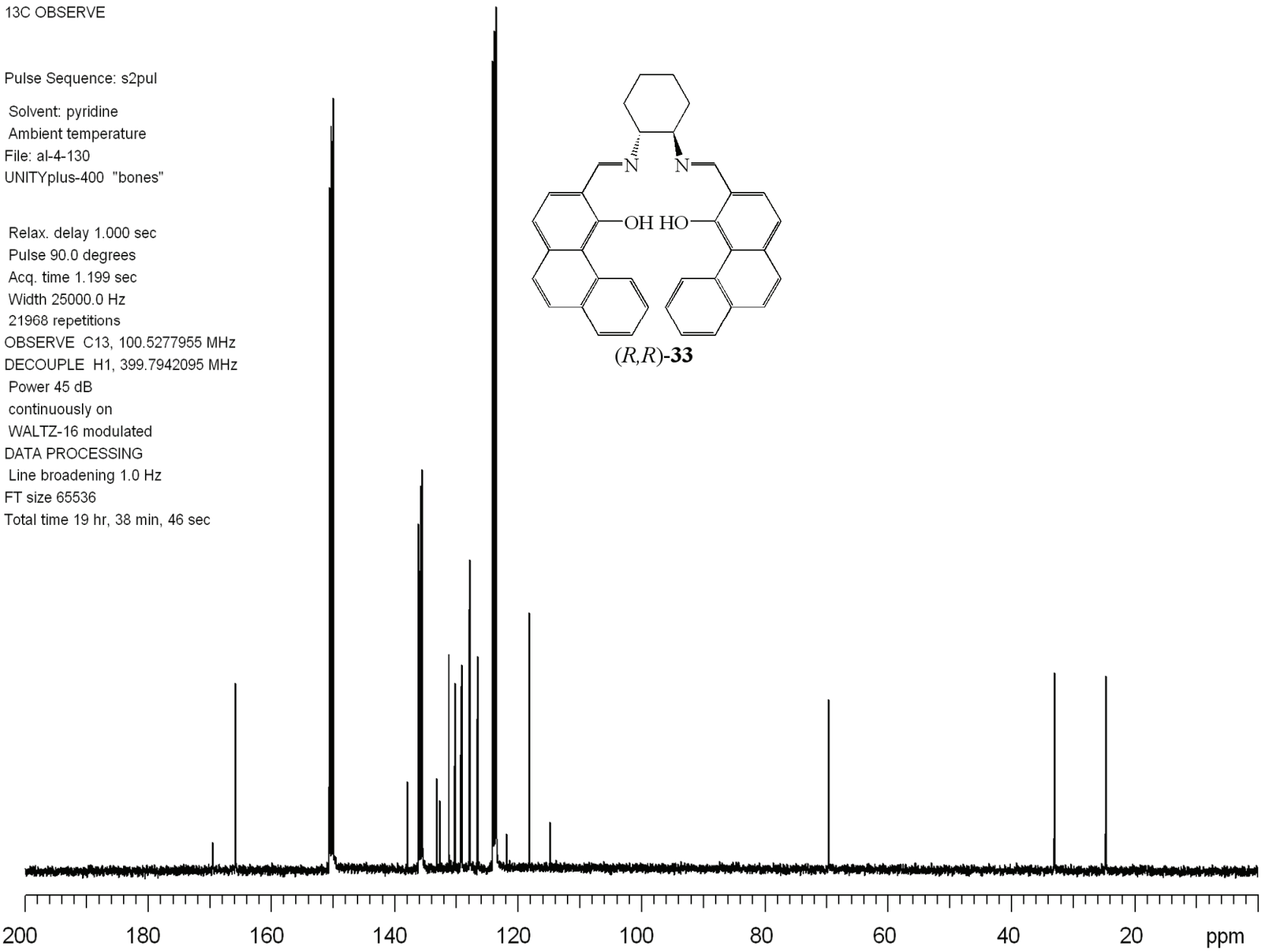


(*R*)-**78**

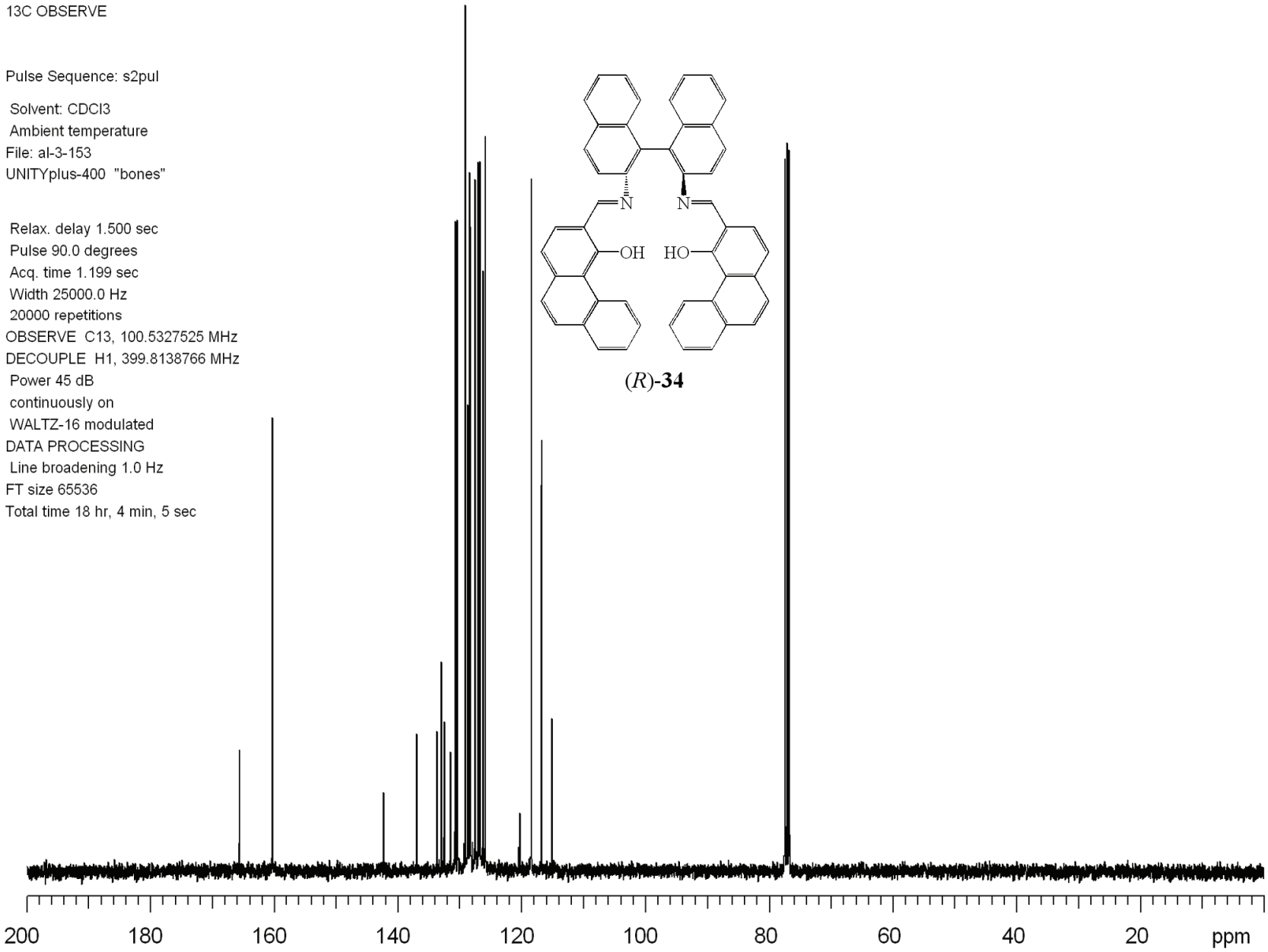
Appendix II

^{13}C NMR spectra

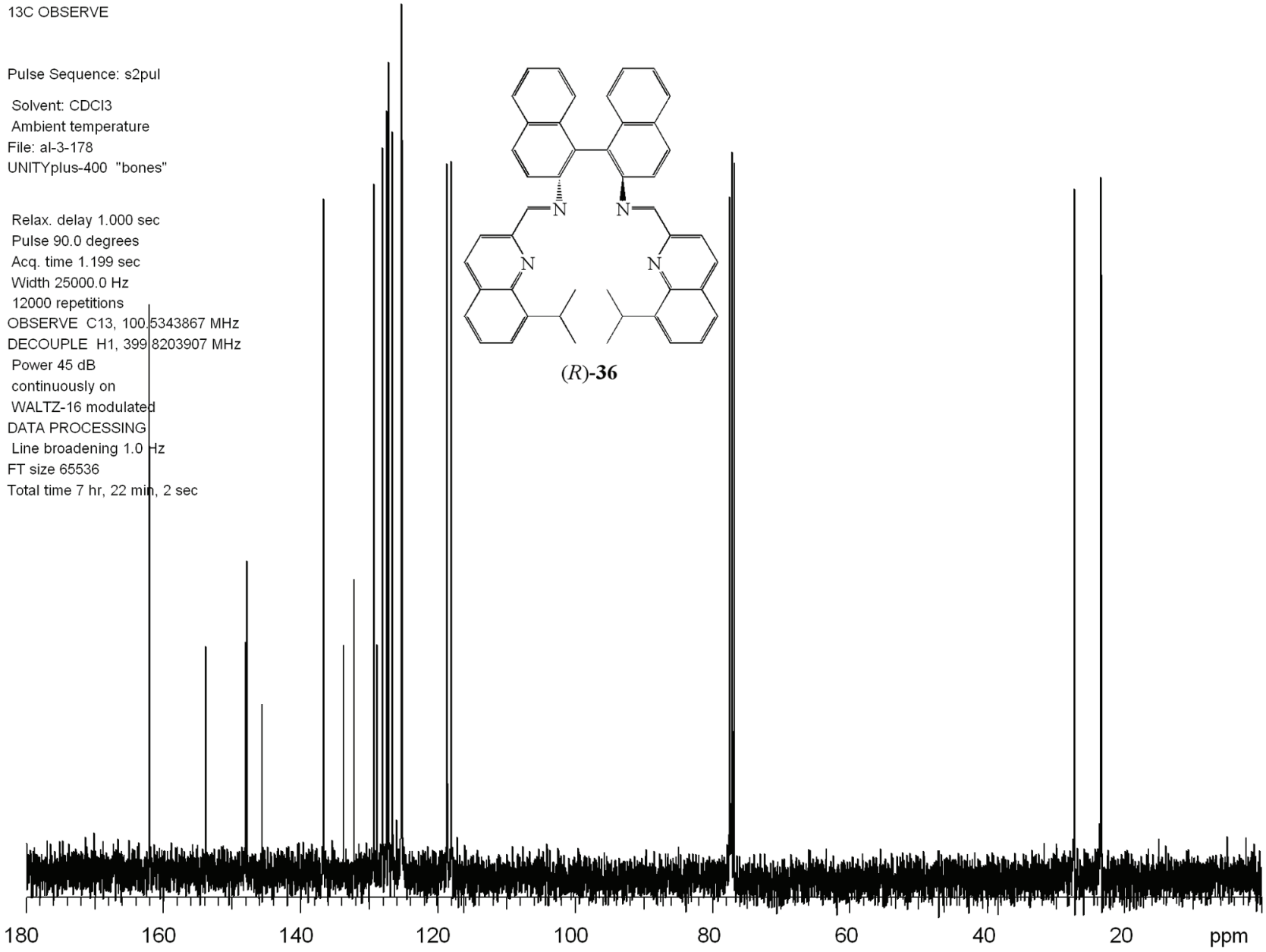
(Numerical order)


13C OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-130
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
21968 repetitions
OBSERVE C13, 100.5277955 MHz
DECOUPLE H1, 399.7942095 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 19 hr, 38 min, 46 sec
N
N
OH HO
200
180
160
140
120
100
80
60
40
20
ppm

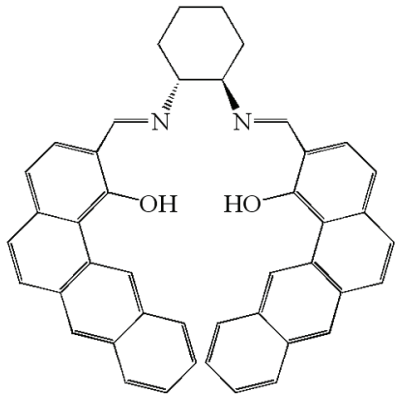
(*R*,*R*)-**33**


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-153
UNITYplus-400 "bones"
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
20000 repetitions
OBSERVE C13, 100.5327525 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 18 hr, 4 min, 5 sec
N
N
OH
HO
200
180
160
140
120
100
80
60
40
20
ppm

(*R*)-**34**


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-178
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
12000 repetitions
OBSERVE C13, 100.5343867 MHz
DECOUPLE H1, 399.8203907 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 7 hr, 22 min, 2 sec
N
N
N
N
180
160
140
120
100
80
60
40
20
ppm

(*R*)-**36**



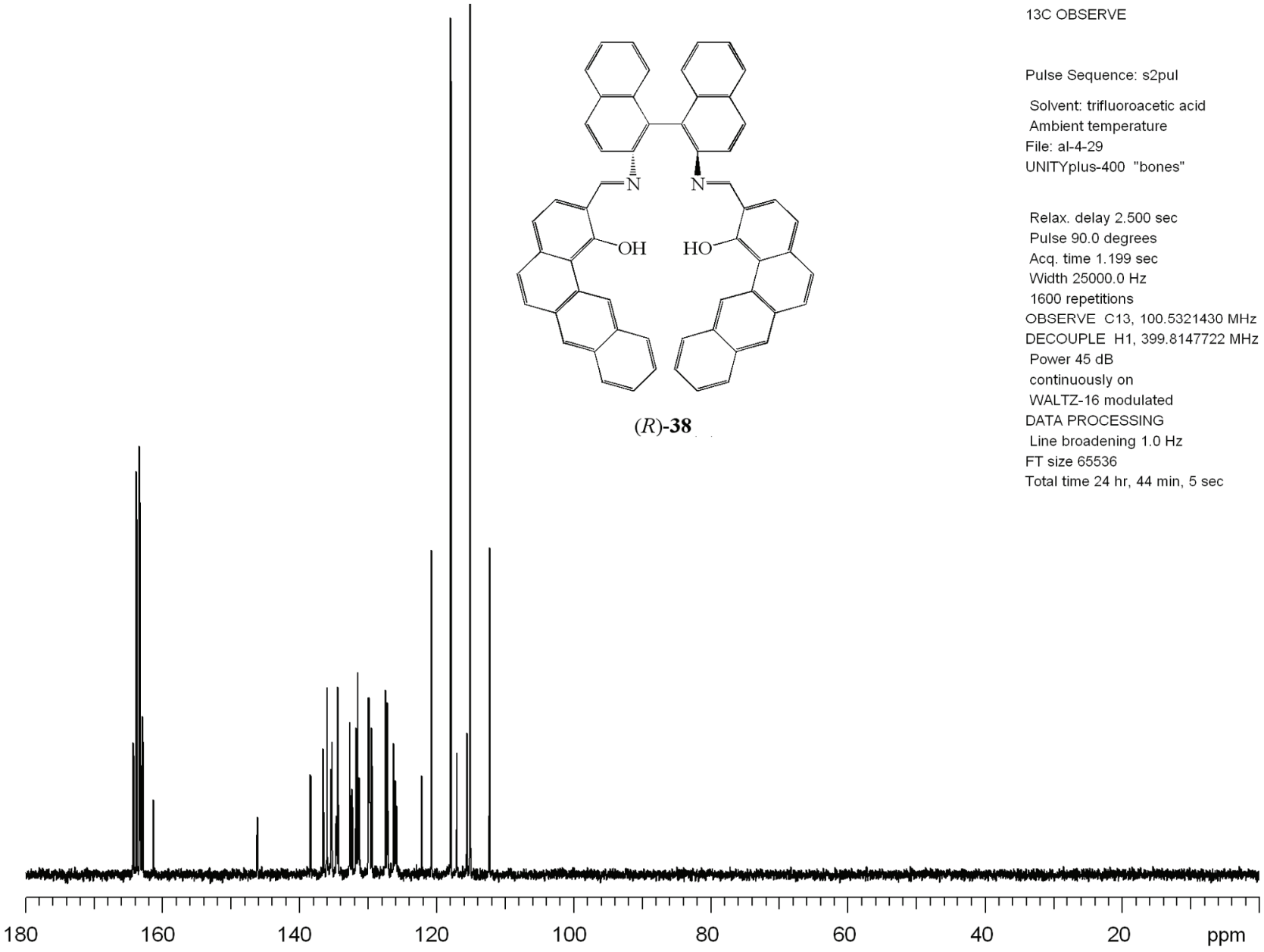
(*R*,*R*)-**37**

13C OBSERVE

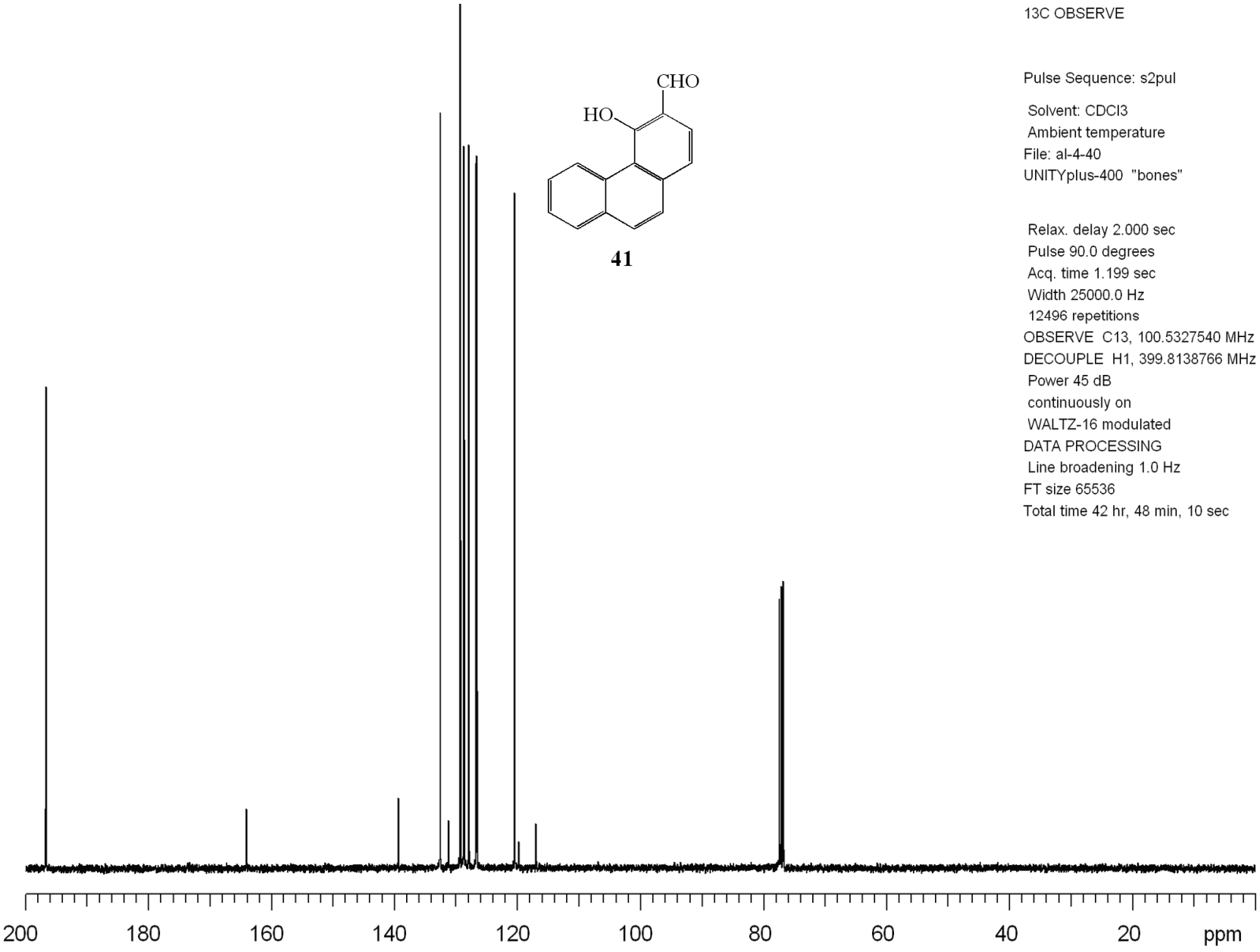
Pulse Sequence: s2pul

Solvent: pyridine
Ambient temperature
File: al-4-112
UNITYplus-400 "bones"

Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
23712 repetitions
OBSERVE C13, 100.5245165 MHz
DECOUPLE H1, 399.7811808 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 14 hr, 44 min, 5 sec


13C OBSERVE
Pulse Sequence: s2pul
Solvent: trifluoroacetic acid
Ambient temperature
File: al-4-29
UNITYplus-400 "bones"
Relax. delay 2.500 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1600 repetitions
OBSERVE C13, 100.5321430 MHz
DECOUPLE H1, 399.8147722 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 24 hr, 44 min, 5 sec
N
N
OH
HO
180
160
140
120
100
80
60
40
20
ppm

(*R*)-**38**

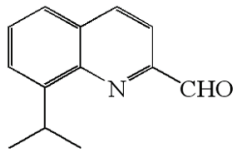

CHO
HO
41
13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-40
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
12496 repetitions
OBSERVE C13, 100.5327540 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
200
180
160
140
120
100
80
60
40
20
ppm

13C OBSERVE

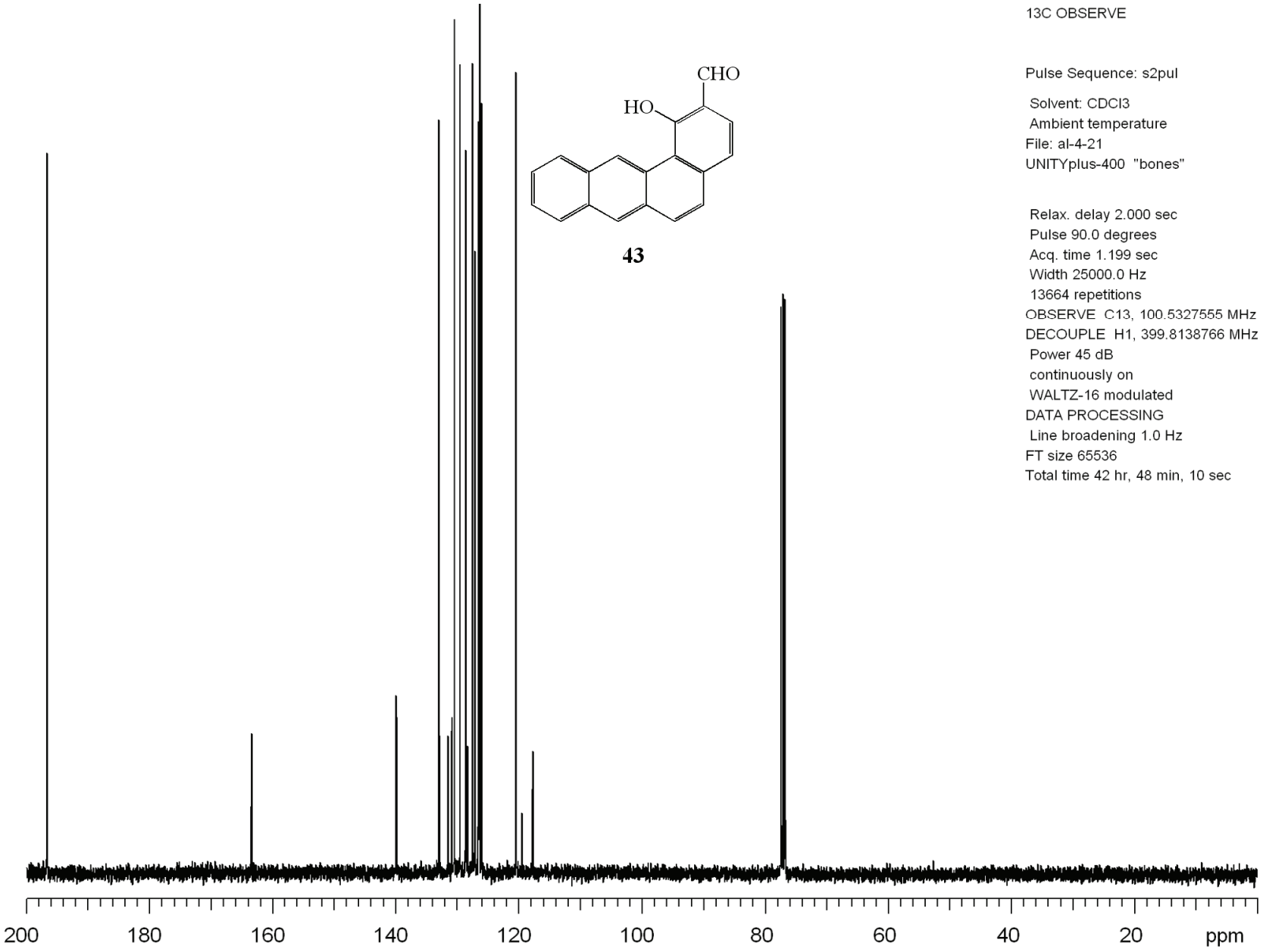
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-75
UNITYplus-400 "bones"

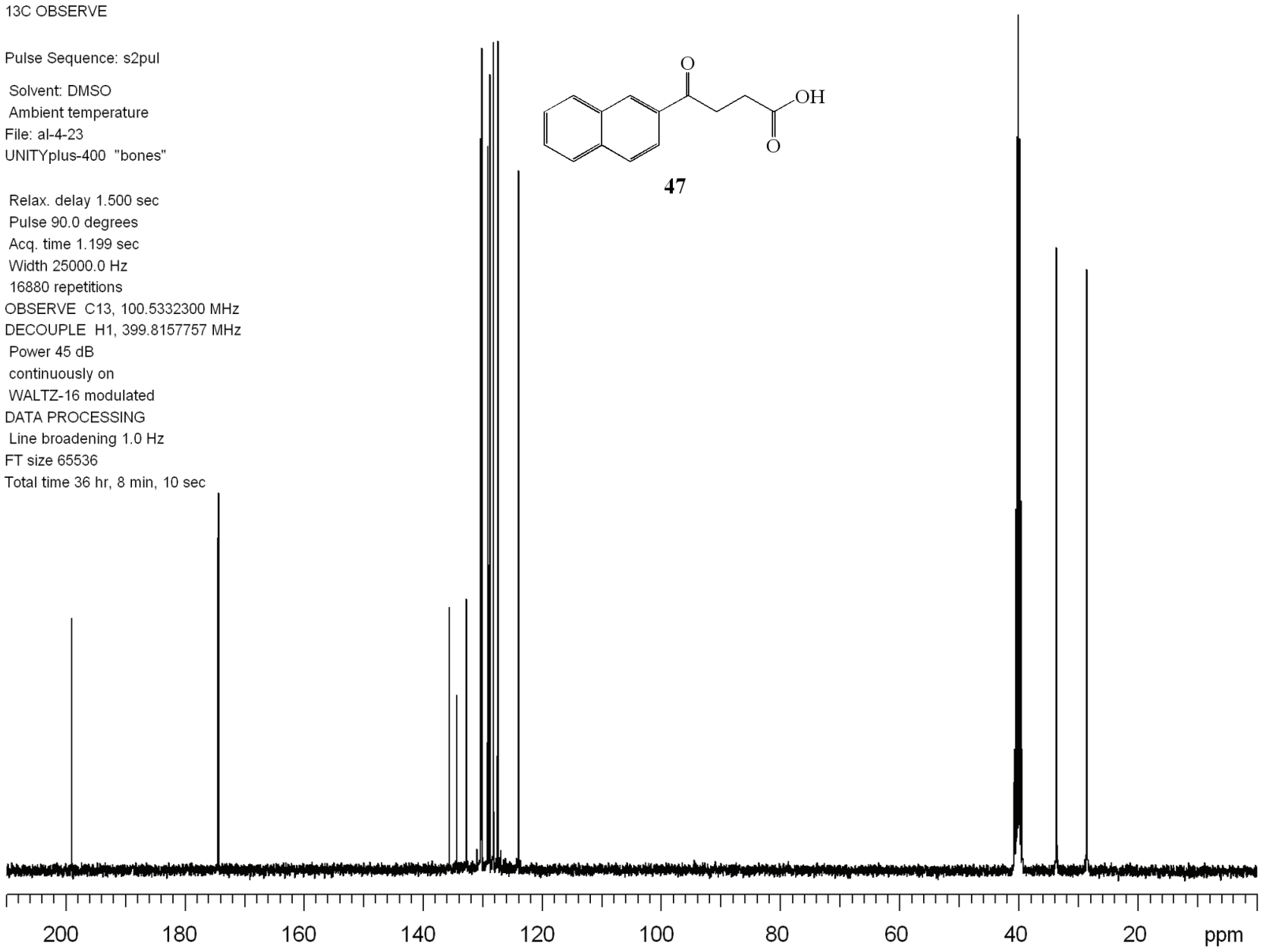
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
13008 repetitions
OBSERVE C13, 100.5294764 MHz
DECOUPLE H1, 399.8008479 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 28 hr, 32 min, 6 sec

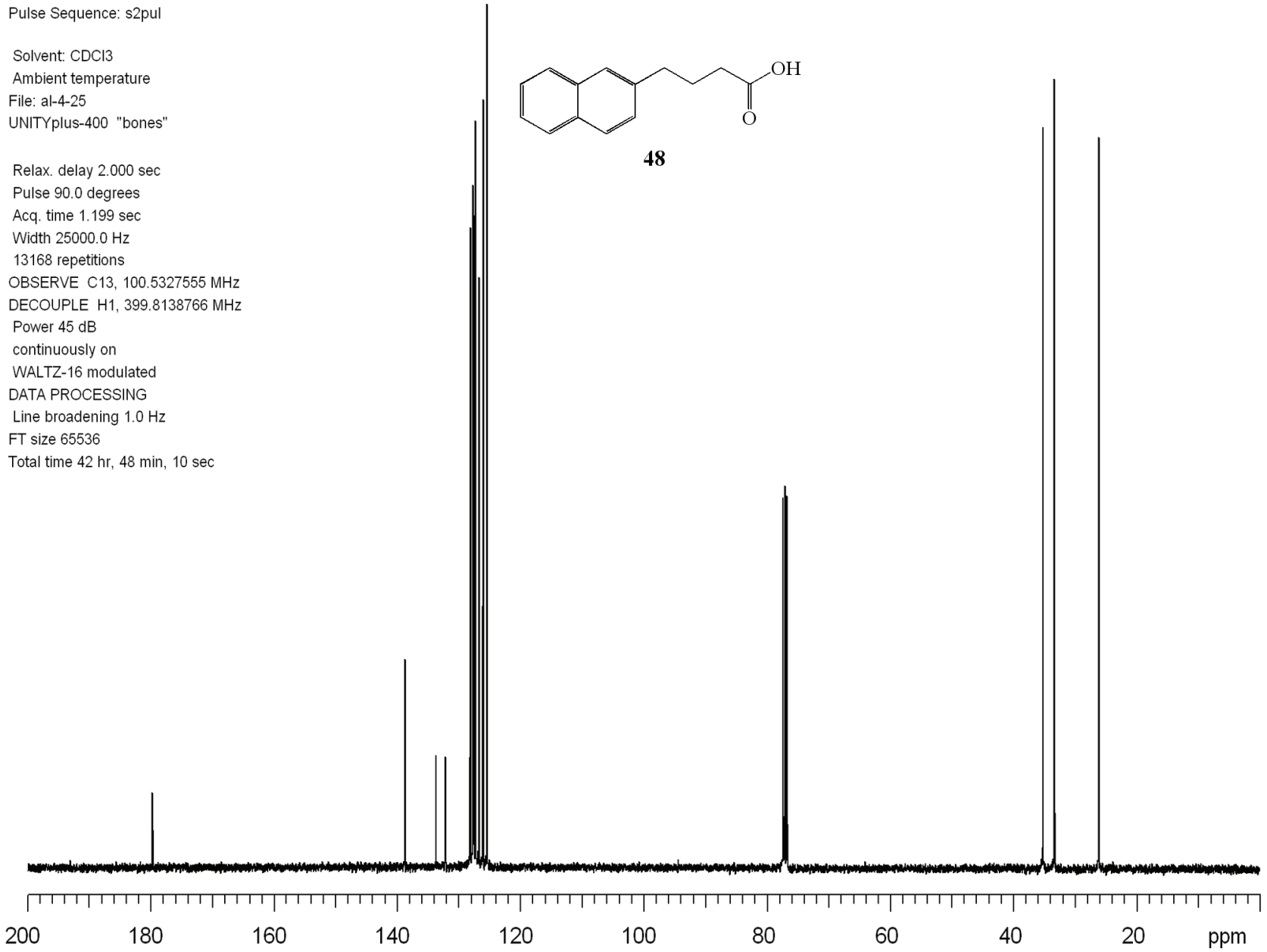


42


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-21
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
13664 repetitions
OBSERVE C13, 100.5327555 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
CHO
HO
200
180
160
140
120
100
80
60
40
20
ppm

43


13C OBSERVE
Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: al-4-23
UNITYplus-400 "bones"
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
16880 repetitions
OBSERVE C13, 100.5332300 MHz
DECOUPLE H1, 399.8157757 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 36 hr, 8 min, 10 sec
O
OH
O
47
200
180
160
140
120
100
80
60
40
20
ppm

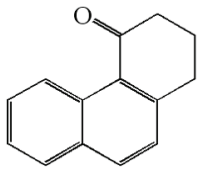

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-25
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
13168 repetitions
OBSERVE C13, 100.5327555 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
OH
O
48
200
180
160
140
120
100
80
60
40
20
ppm

13C OBSERVE

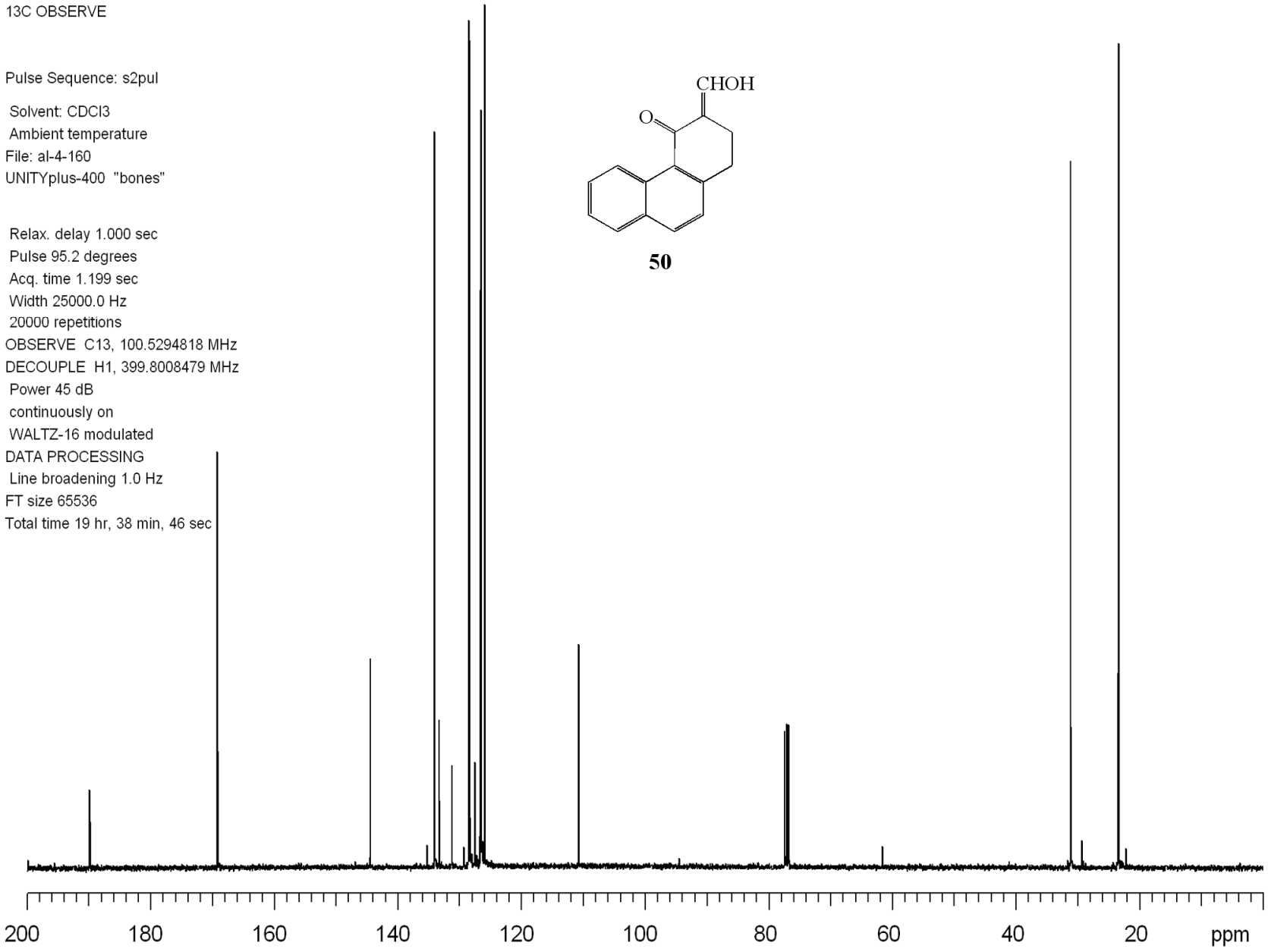
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-4-31
UNITYplus-400 "bones"

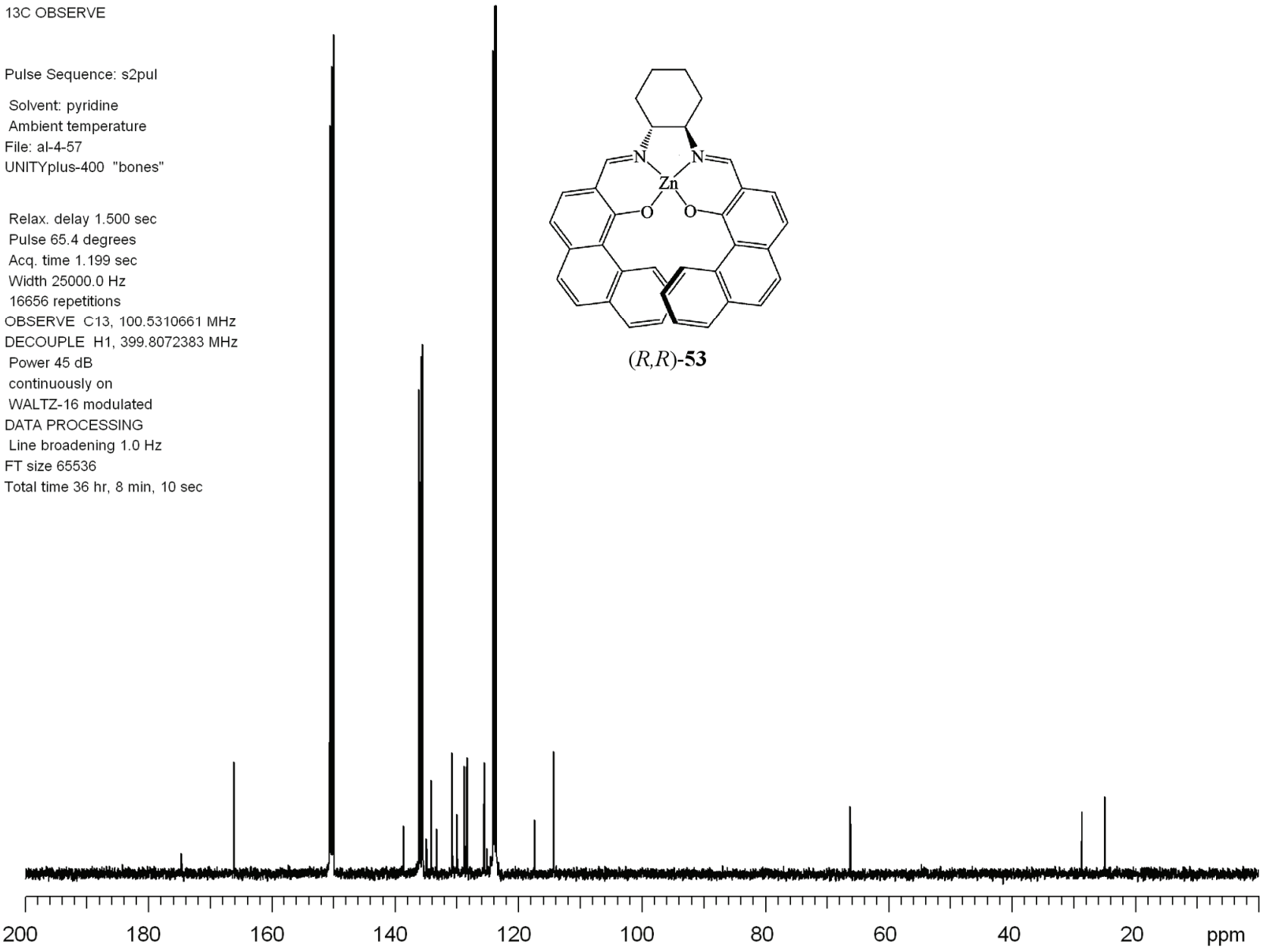
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
15408 repetitions
OBSERVE C13, 100.5327548 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec



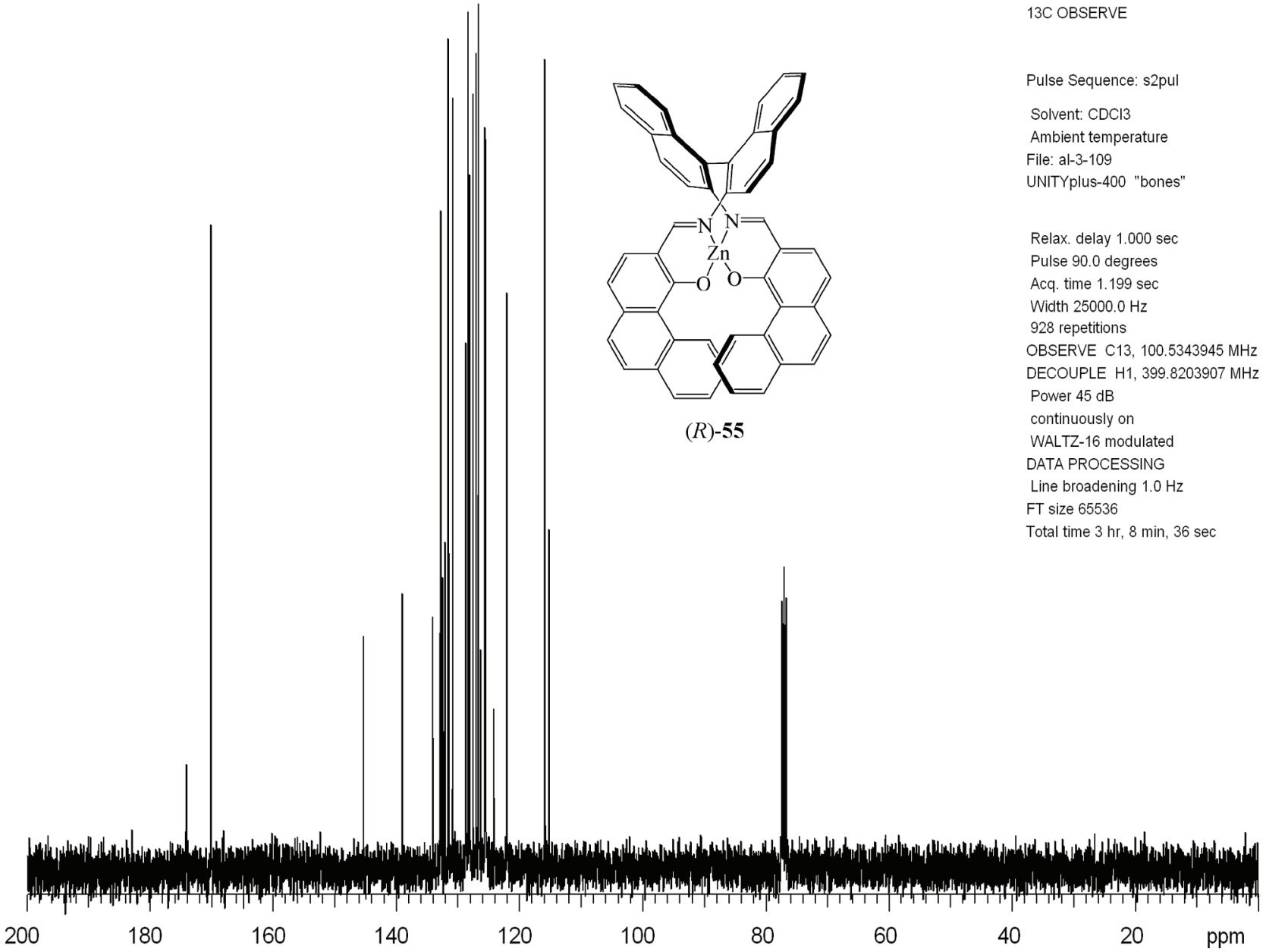
49


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-160
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 95.2 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
20000 repetitions
OBSERVE C13, 100.5294818 MHz
DECOUPLE H1, 399.8008479 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 19 hr, 38 min, 46 sec
CHOH
O
200
180
160
140
120
100
80
60
40
20
ppm

50


13C OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-57
UNITYplus-400 "bones"
Relax. delay 1.500 sec
Pulse 65.4 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
16656 repetitions
OBSERVE C13, 100.5310661 MHz
DECOUPLE H1, 399.8072383 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 36 hr, 8 min, 10 sec
N
N
Zn
O
O
200
180
160
140
120
100
80
60
40
20
ppm

(*R*,*R*)-**53**


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-109
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
928 repetitions
OBSERVE C13, 100.5343945 MHz
DECOUPLE H1, 399.8203907 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 3 hr, 8 min, 36 sec
N
N
Zn
O
O
200
180
160
140
120
100
80
60
40
20
ppm

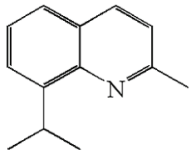
(*R*)-**55**

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-64
UNITYplus-400 "bones"

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
14208 repetitions
OBSERVE C13, 100.5294741 MHz
DECOUPLE H1, 399.8008479 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 28 hr, 32 min, 6 sec



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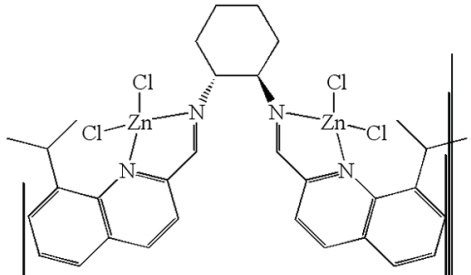
13C OBSERVE

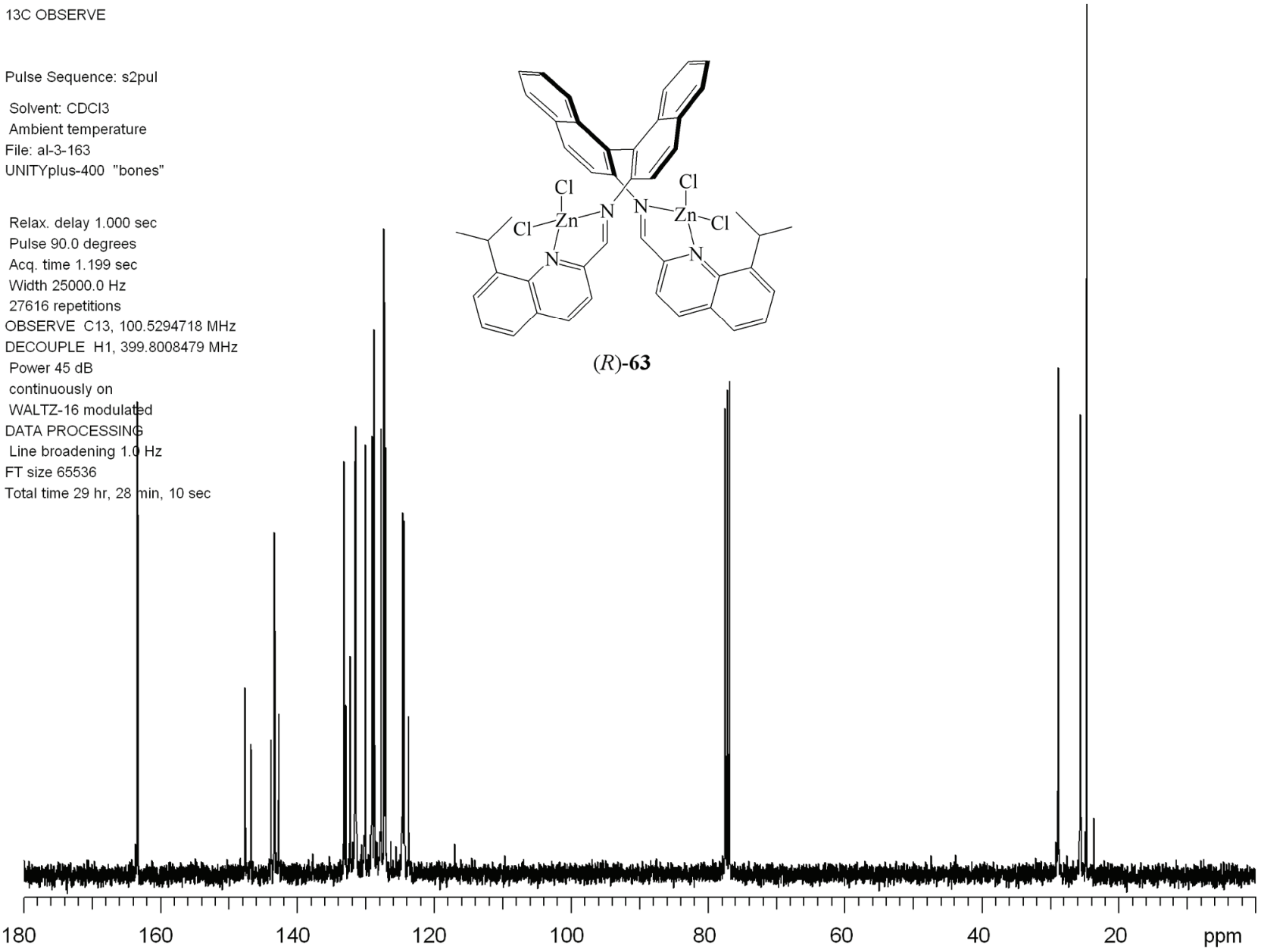
Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-190
UNITYplus-400 "bones"

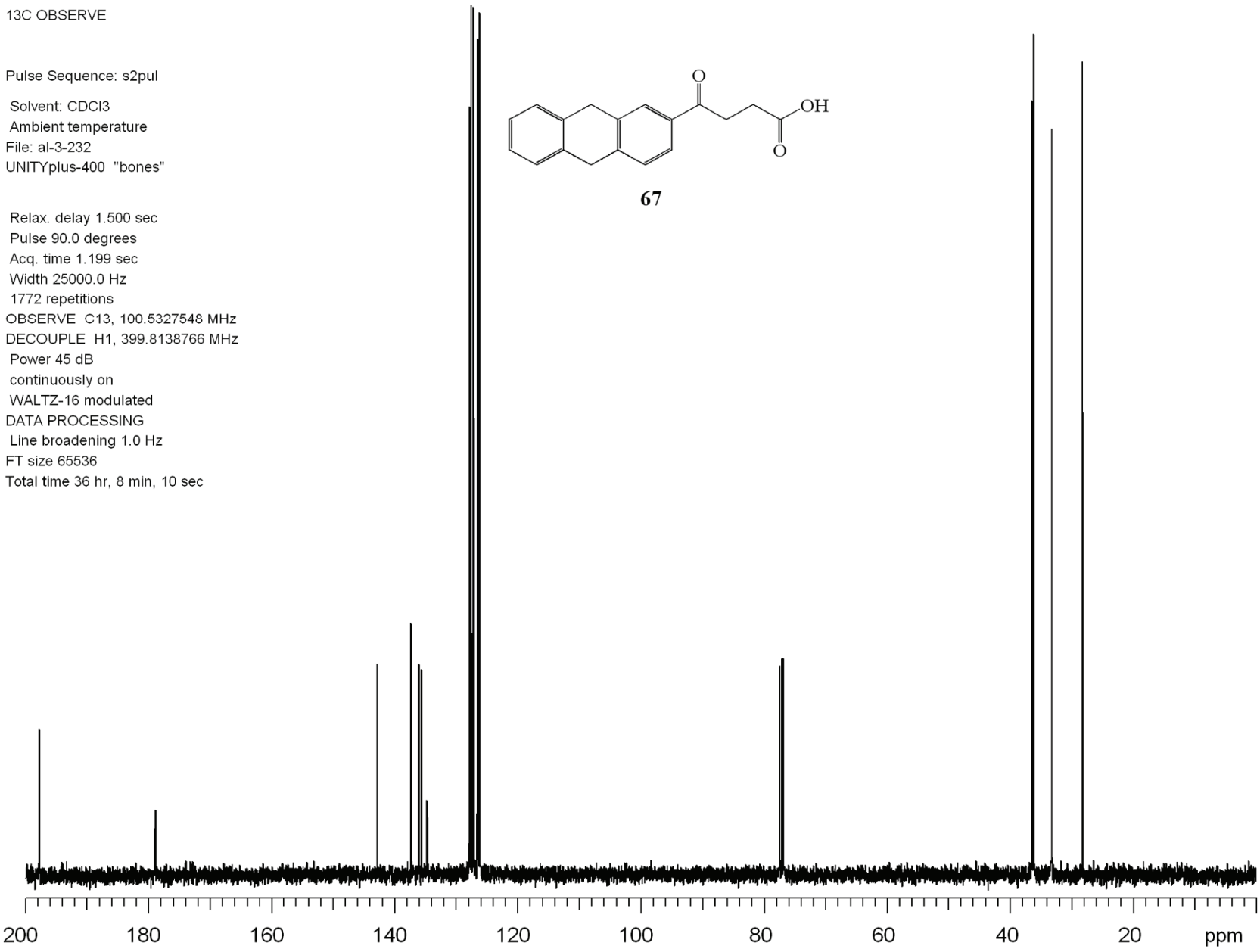
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
30096 repetitions
OBSERVE C13, 100.5343844 MHz
DECOUPLE H1, 399.8203910 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 21 hr, 30 min, 53 sec



(*R*,*R*)-**62**


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-163
UNITYplus-400 "bones"
Relax. delay 1.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
27616 repetitions
OBSERVE C13, 100.5294718 MHz
DECOUPLE H1, 399.8008479 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 29 hr, 28 min, 10 sec
Cl
Zn
N
Cl
Zn
Cl
N
N
Cl
Zn
Cl
N
180
160
140
120
100
80
60
40
20
ppm

(*R*)-**63**


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-232
UNITYplus-400 "bones"
Relax. delay 1.500 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
1772 repetitions
OBSERVE C13, 100.5327548 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 36 hr, 8 min, 10 sec
O
OH
O
200
180
160
140
120
100
80
60
40
20
ppm

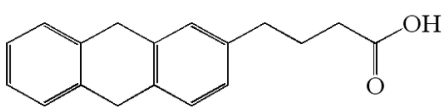
67

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-284
UNITYplus-400 "bones"

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
13728 repetitions
OBSERVE C13, 100.5327540 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec



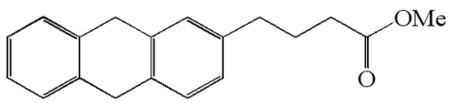
68

13C OBSERVE

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: al-3-286
UNITYplus-400 "bones"

Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
13344 repetitions
OBSERVE C13, 100.5327525 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec



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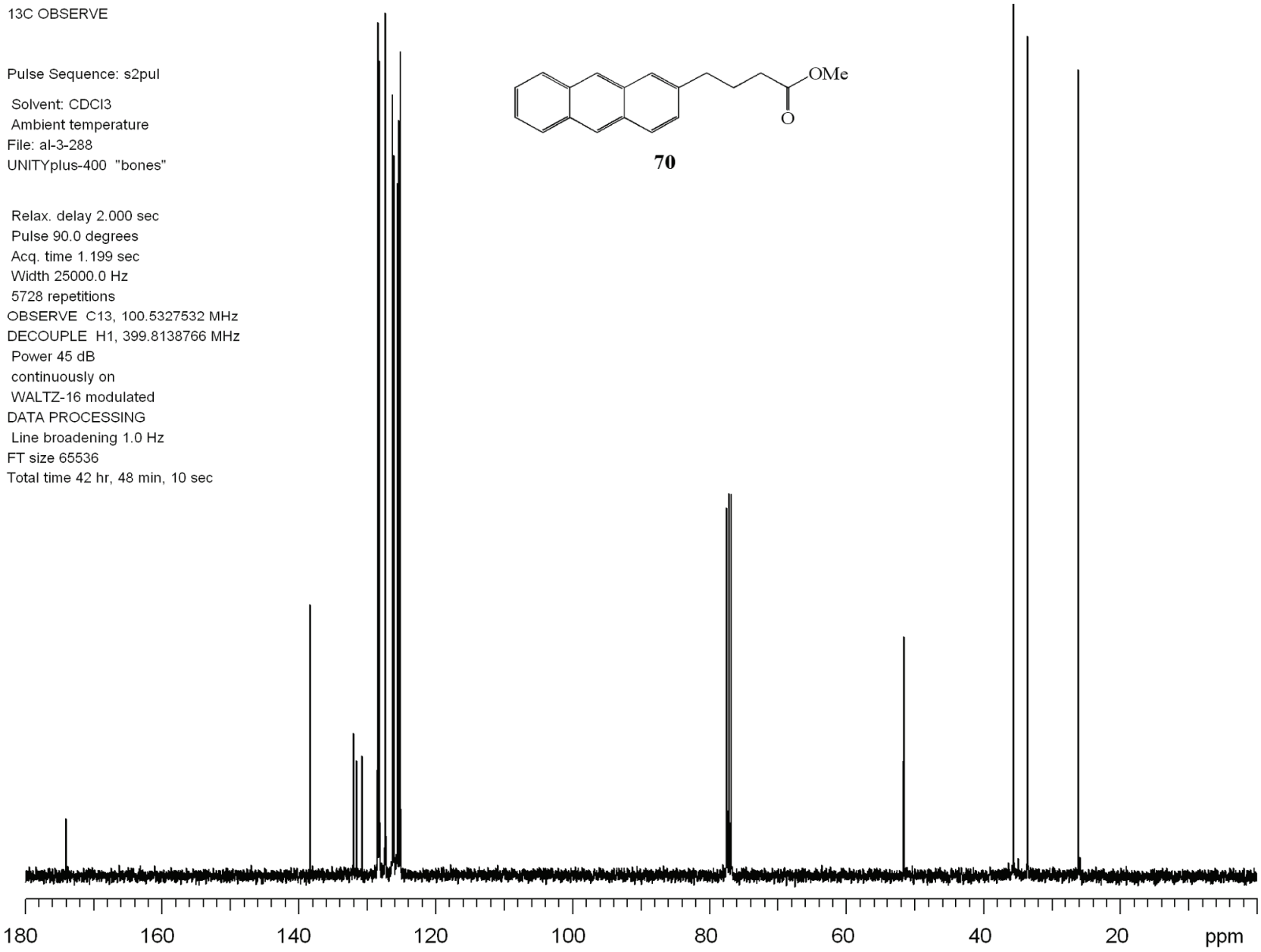
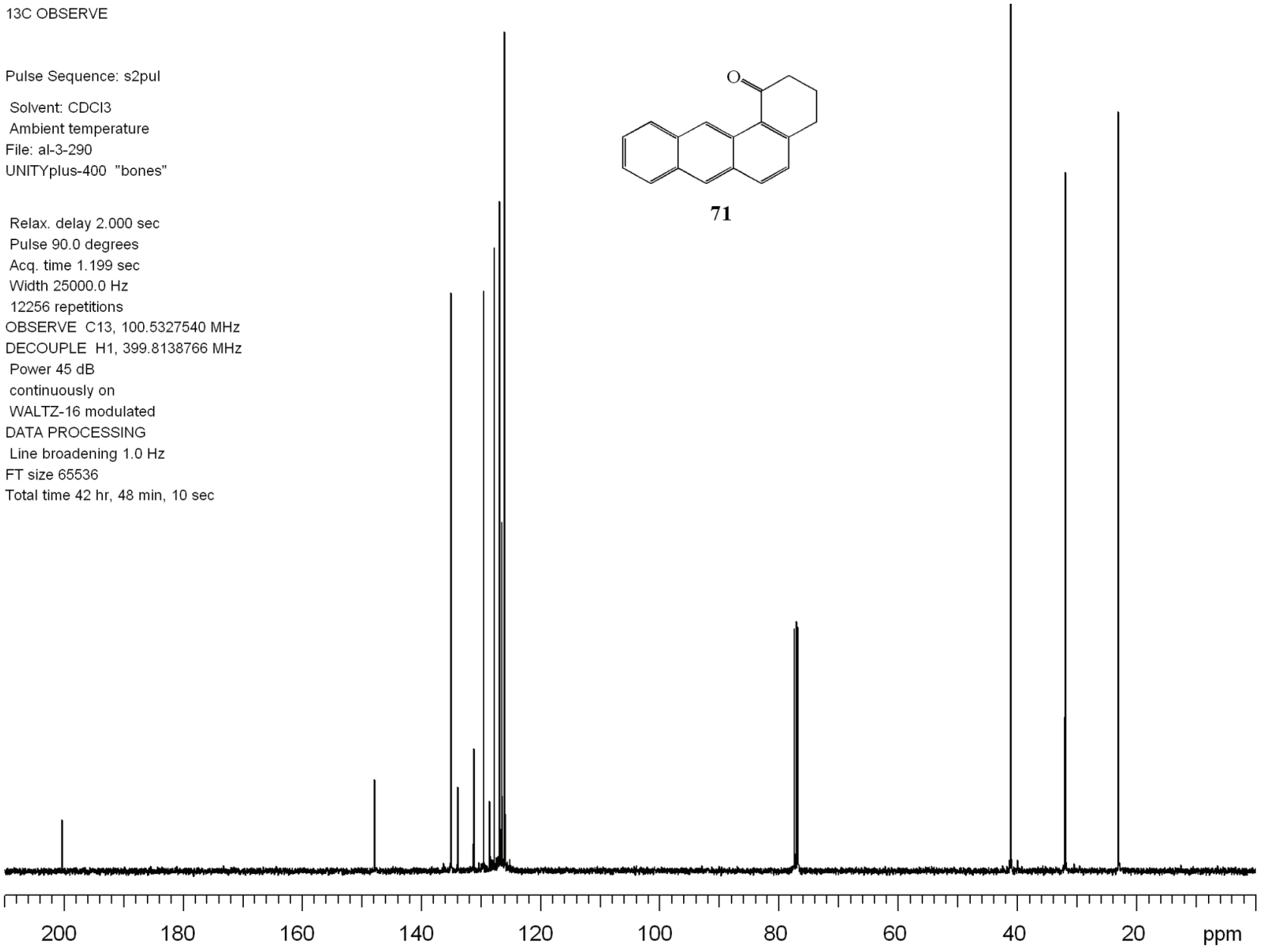
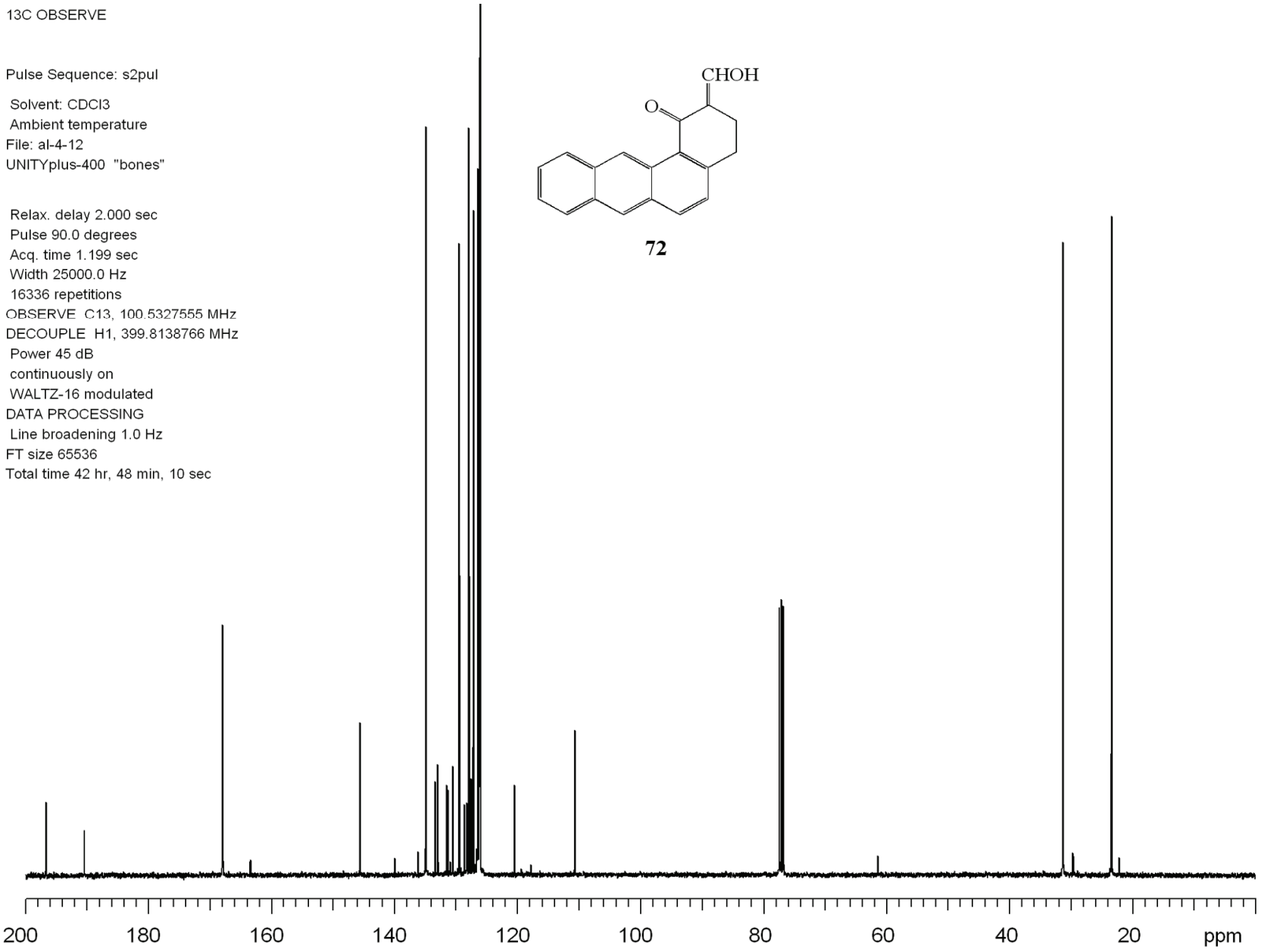
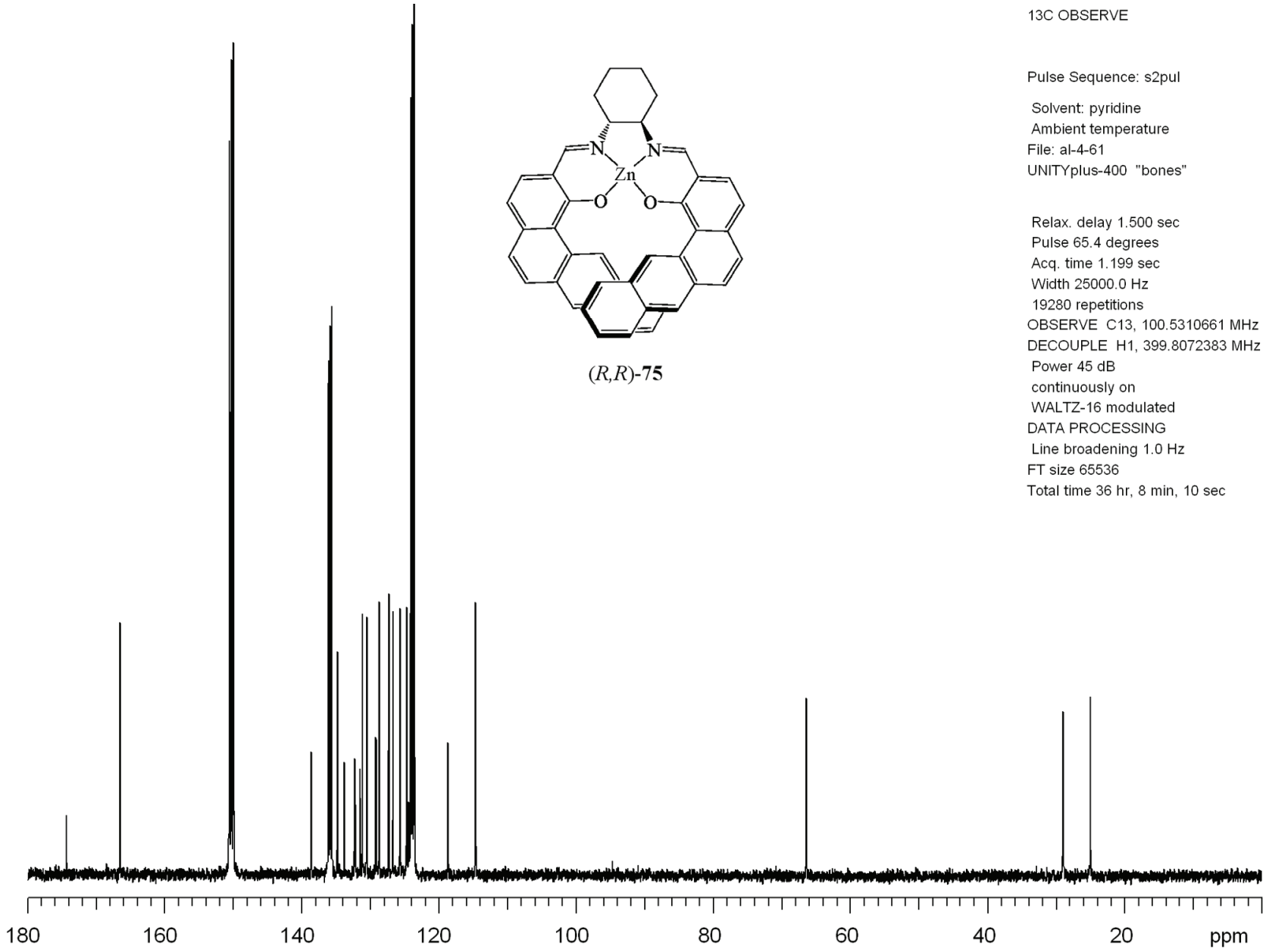

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-288
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
5728 repetitions
OBSERVE C13, 100.5327532 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
OMe
O
70
180
160
140
120
100
80
60
40
20
ppm

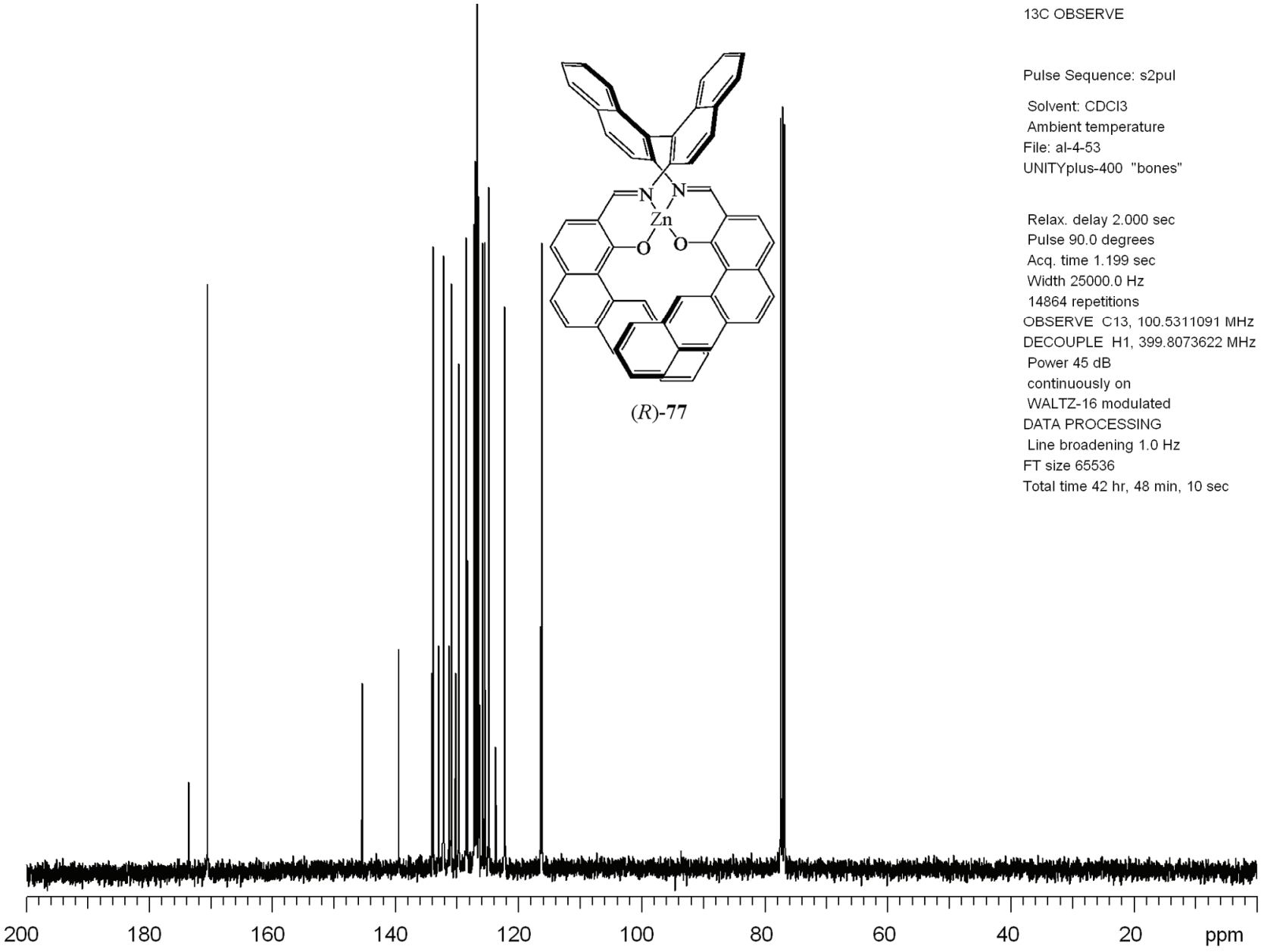

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-3-290
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
12256 repetitions
OBSERVE C13, 100.5327540 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
O
71
200
180
160
140
120
100
80
60
40
20
ppm


13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-12
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
16336 repetitions
OBSERVE C13, 100.5327555 MHz
DECOUPLE H1, 399.8138766 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
CHOH
O
200
180
160
140
120
100
80
60
40
20
ppm

72


13C OBSERVE
Pulse Sequence: s2pul
Solvent: pyridine
Ambient temperature
File: al-4-61
UNITYplus-400 "bones"
Relax. delay 1.500 sec
Pulse 65.4 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
19280 repetitions
OBSERVE C13, 100.5310661 MHz
DECOUPLE H1, 399.8072383 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 36 hr, 8 min, 10 sec
N
Zn
N
O
O
180
160
140
120
100
80
60
40
20
ppm

(*R*,*R*)-**75**

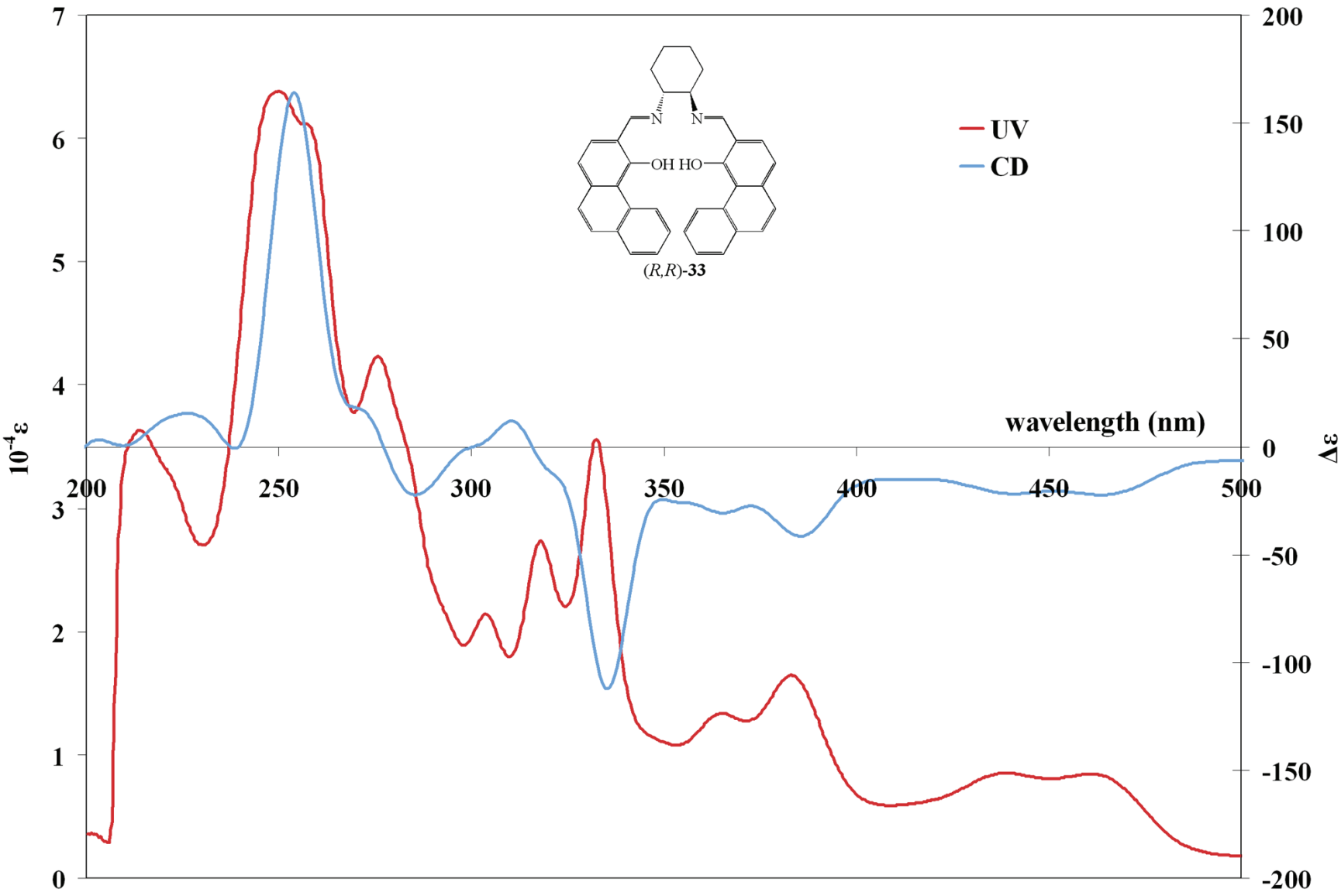

13C OBSERVE
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: al-4-53
UNITYplus-400 "bones"
Relax. delay 2.000 sec
Pulse 90.0 degrees
Acq. time 1.199 sec
Width 25000.0 Hz
14864 repetitions
OBSERVE C13, 100.5311091 MHz
DECOUPLE H1, 399.8073622 MHz
Power 45 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 42 hr, 48 min, 10 sec
N
N
Zn
O
O
200
180
160
140
120
100
80
60
40
20
ppm

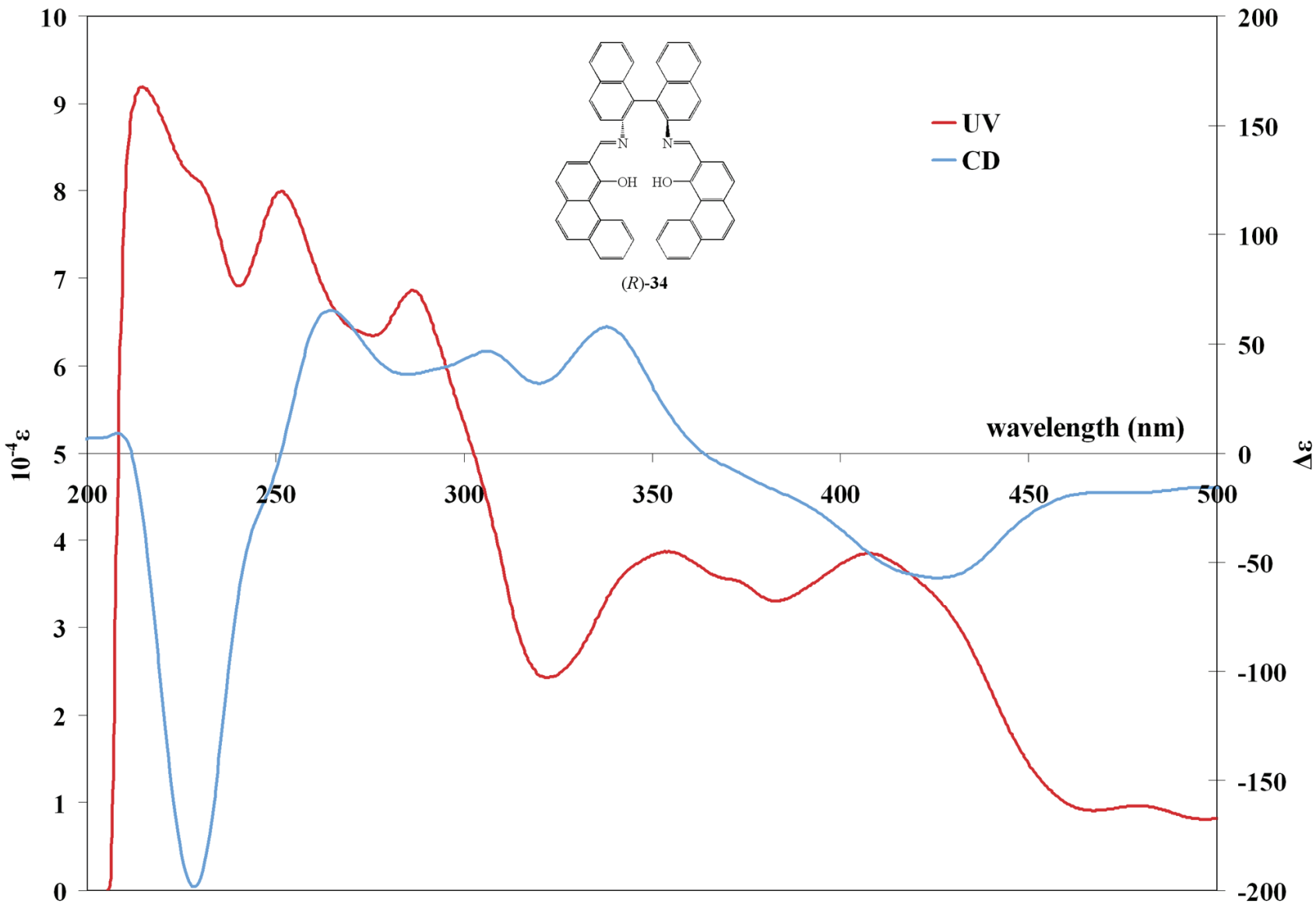
(*R*)-**77**

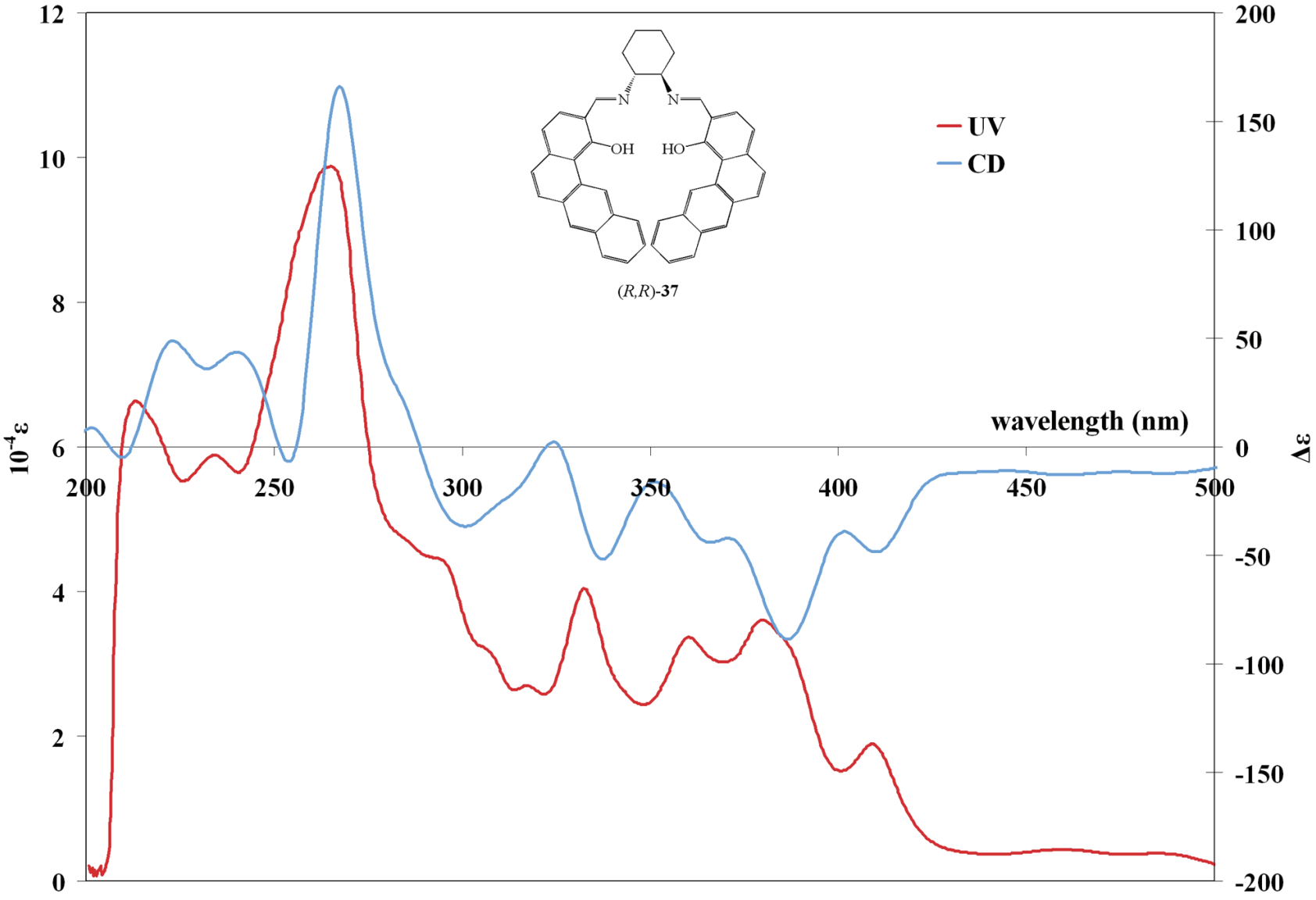
Appendix III

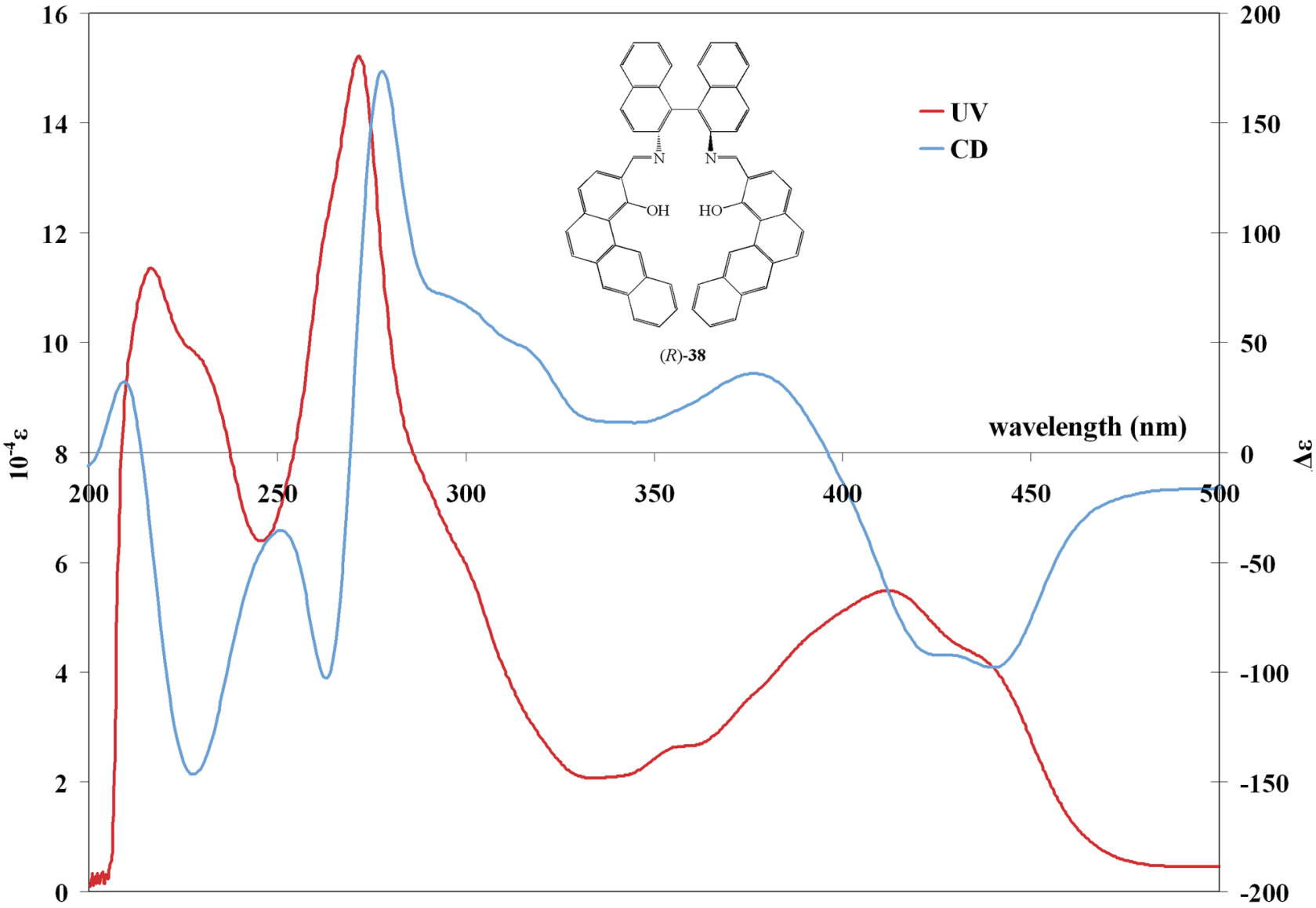
UV & ECD Spectra

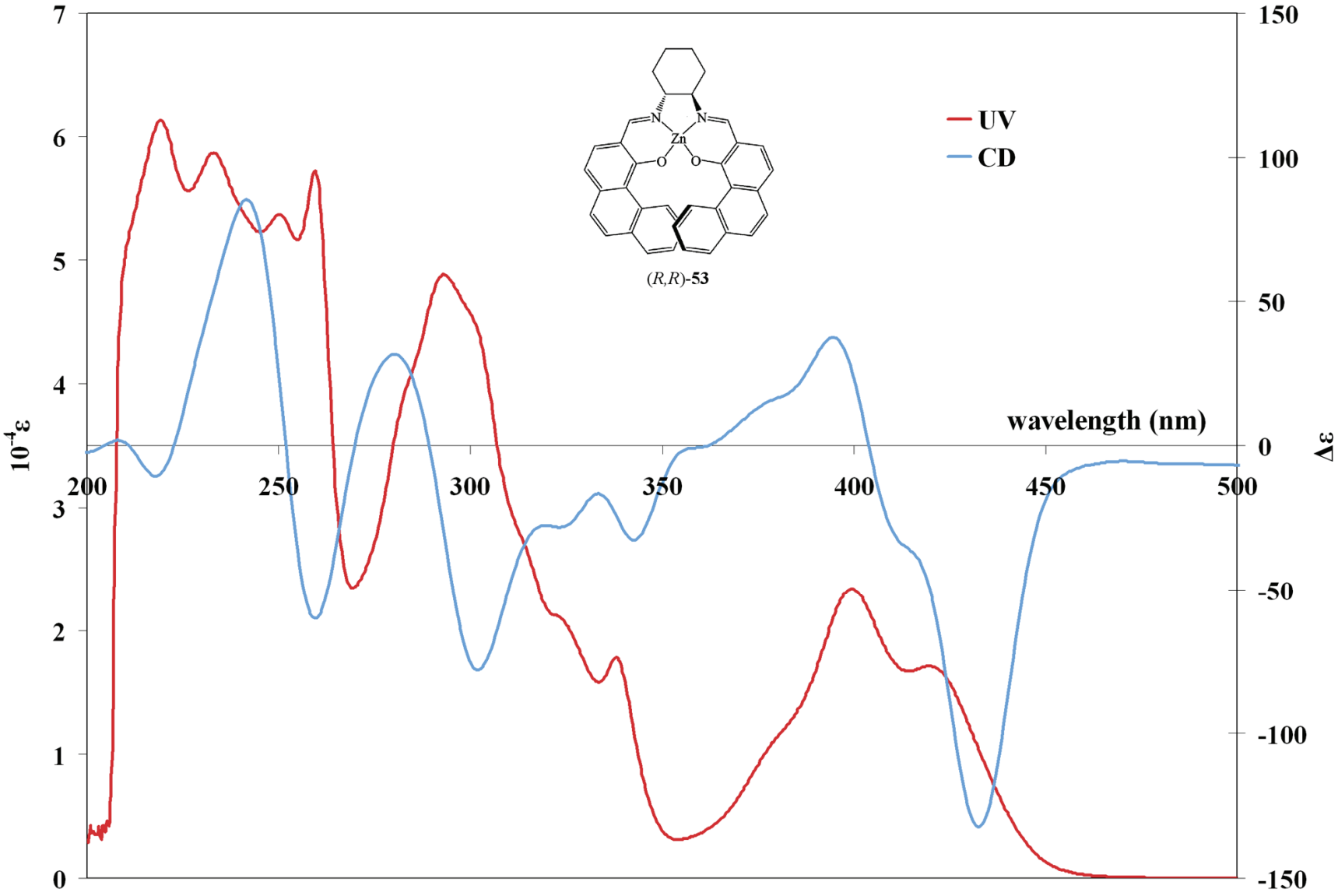
(Numerical order)


7
6
5
4
3
2
1
0
$10^{-4}\varepsilon$
200
150
100
50
0
-50
-100
-150
-200
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
OH HO
(R,R)-33

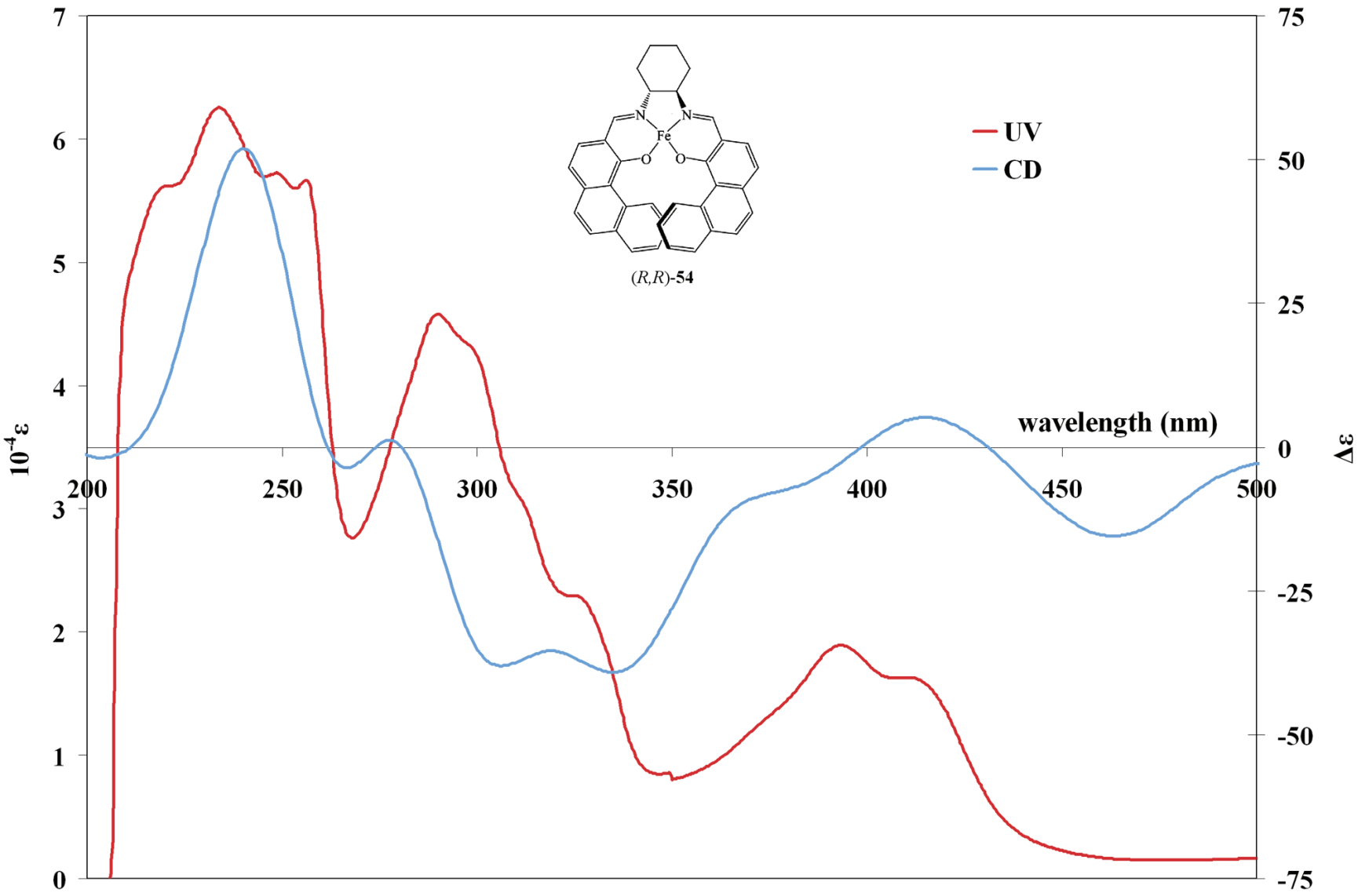

10
9
8
7
6
5
4
3
2
1
0
$10^{-4}\varepsilon$
200
150
100
50
0
-50
-100
-150
-200
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
OH
HO
(R)-34


12
10
8
6
4
2
0
$10^{-4}\varepsilon$
200
150
100
50
0
-50
-100
-150
-200
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
OH
HO
(R,R)-37

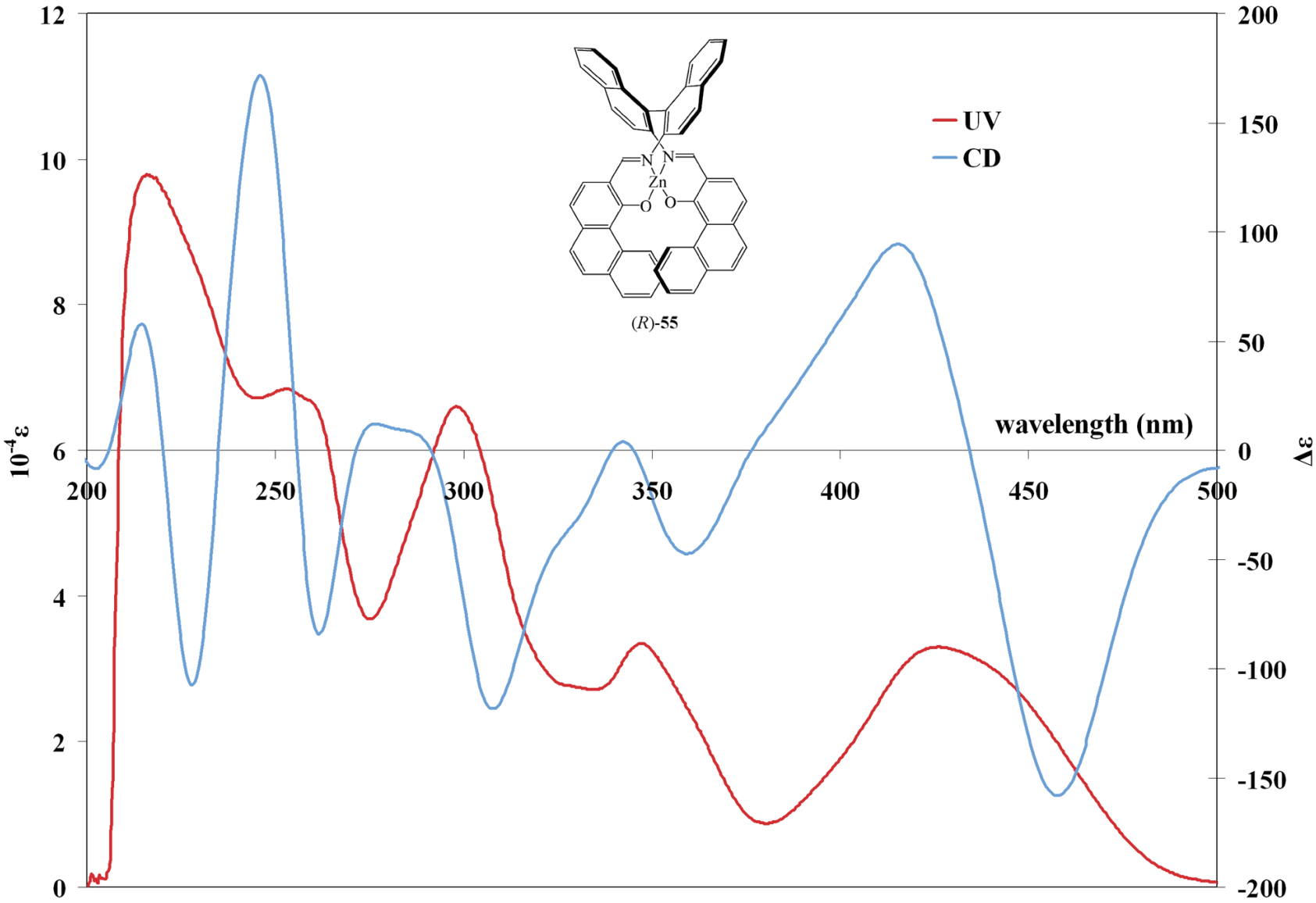

16
14
12
10
8
6
4
2
0
200
150
100
50
0
-50
-100
-150
-200
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
10-4ε
Δε
OH
HO
N
N
(R)-38

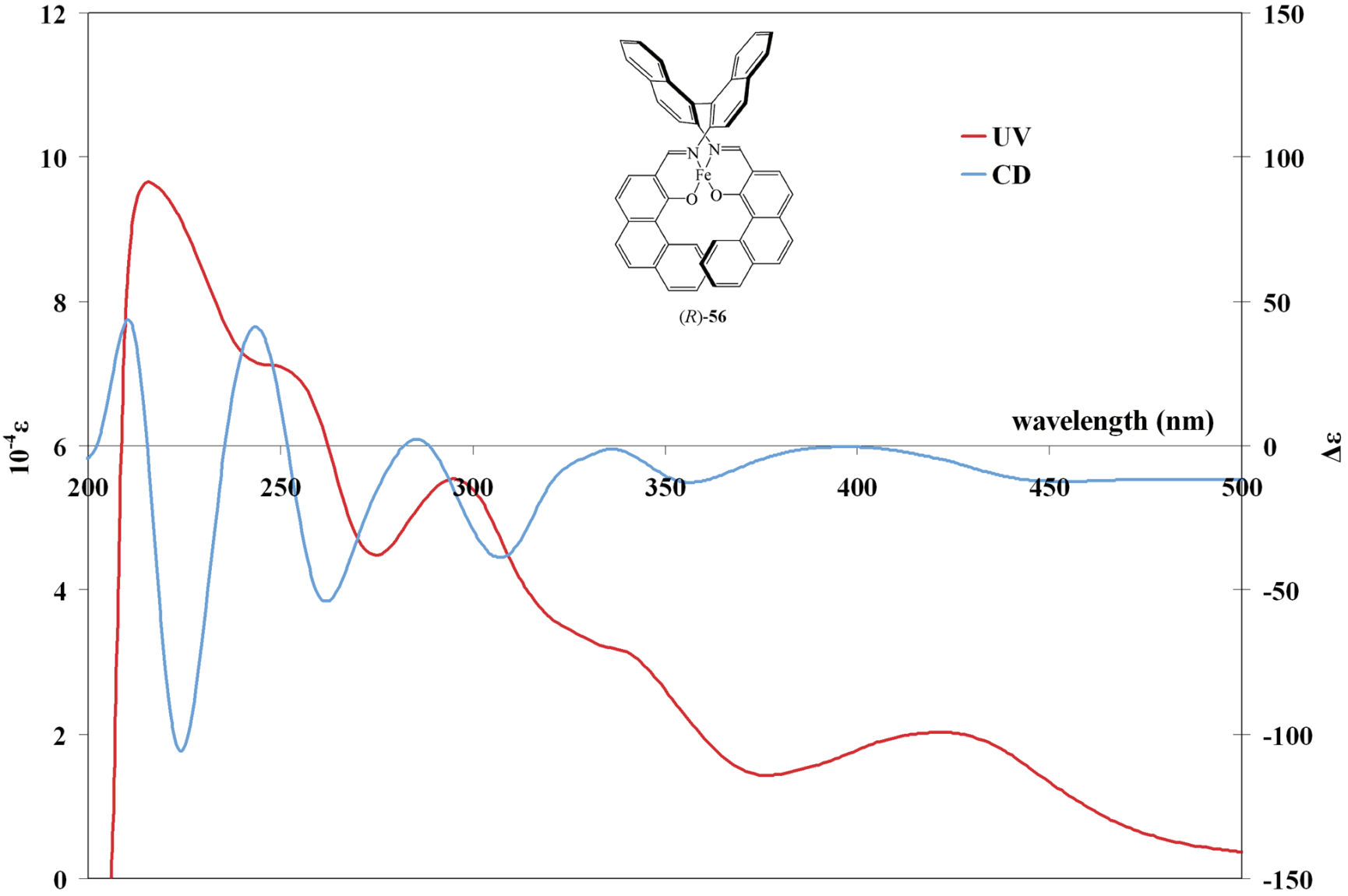

7
6
5
4
3
2
1
0
$10^{-4}\varepsilon$
150
100
50
0
-50
-100
-150
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
Zn
O
O

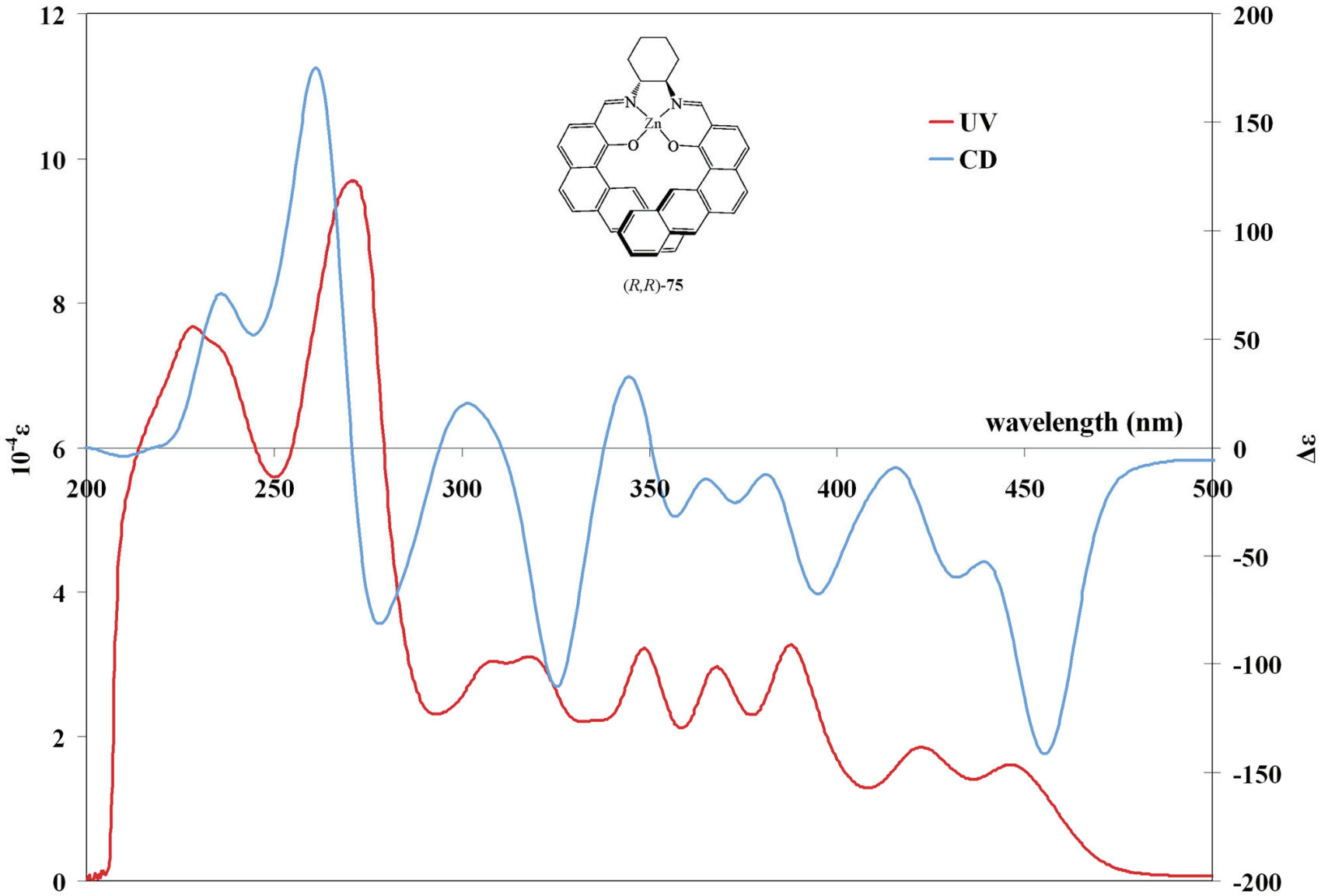
(*R*,*R*)-**53**

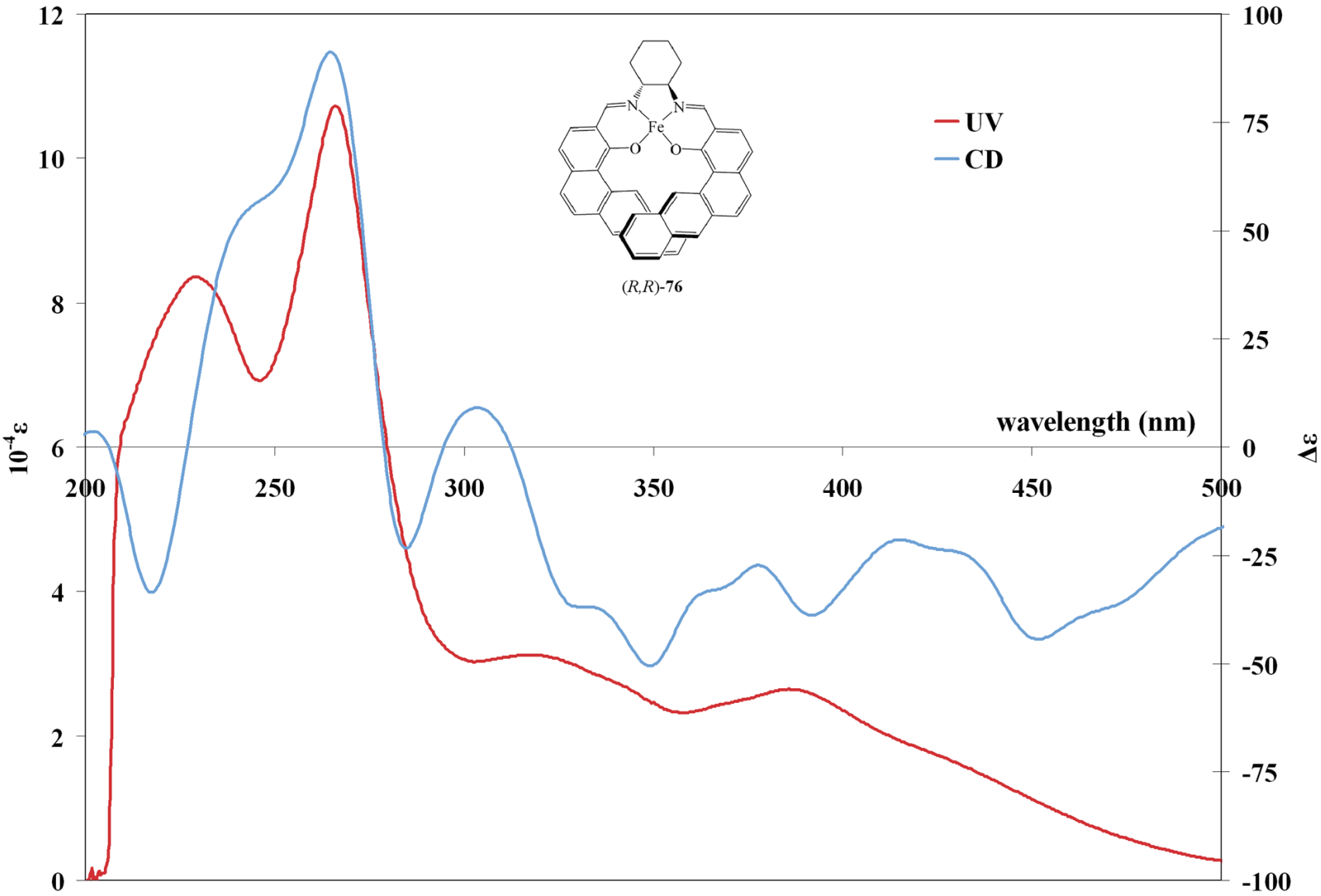

7
6
5
4
3
2
1
0
$10^{-4}\varepsilon$
75
50
25
0
-25
-50
-75
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
Fe
O
O

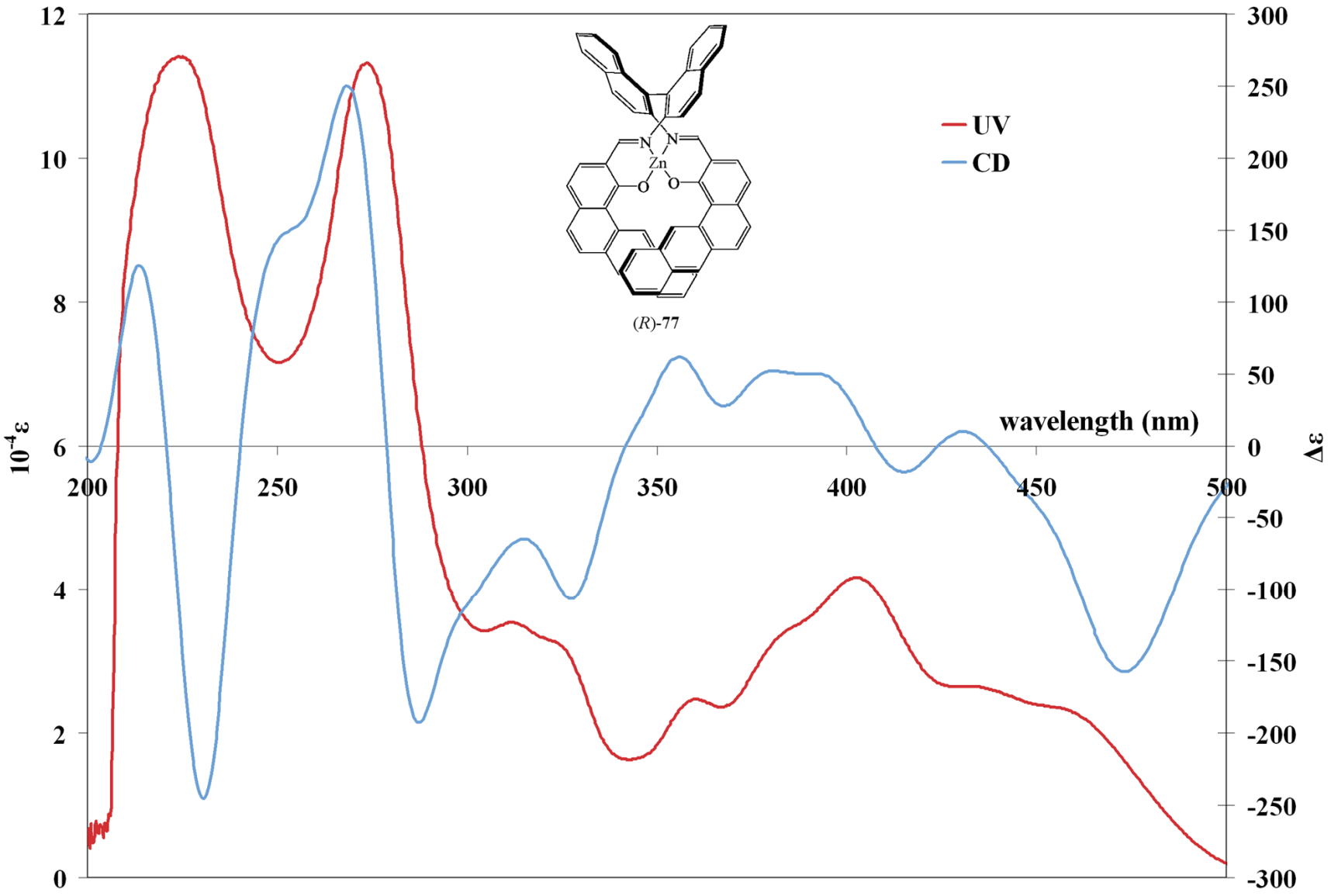
(*R*,*R*)-**54**

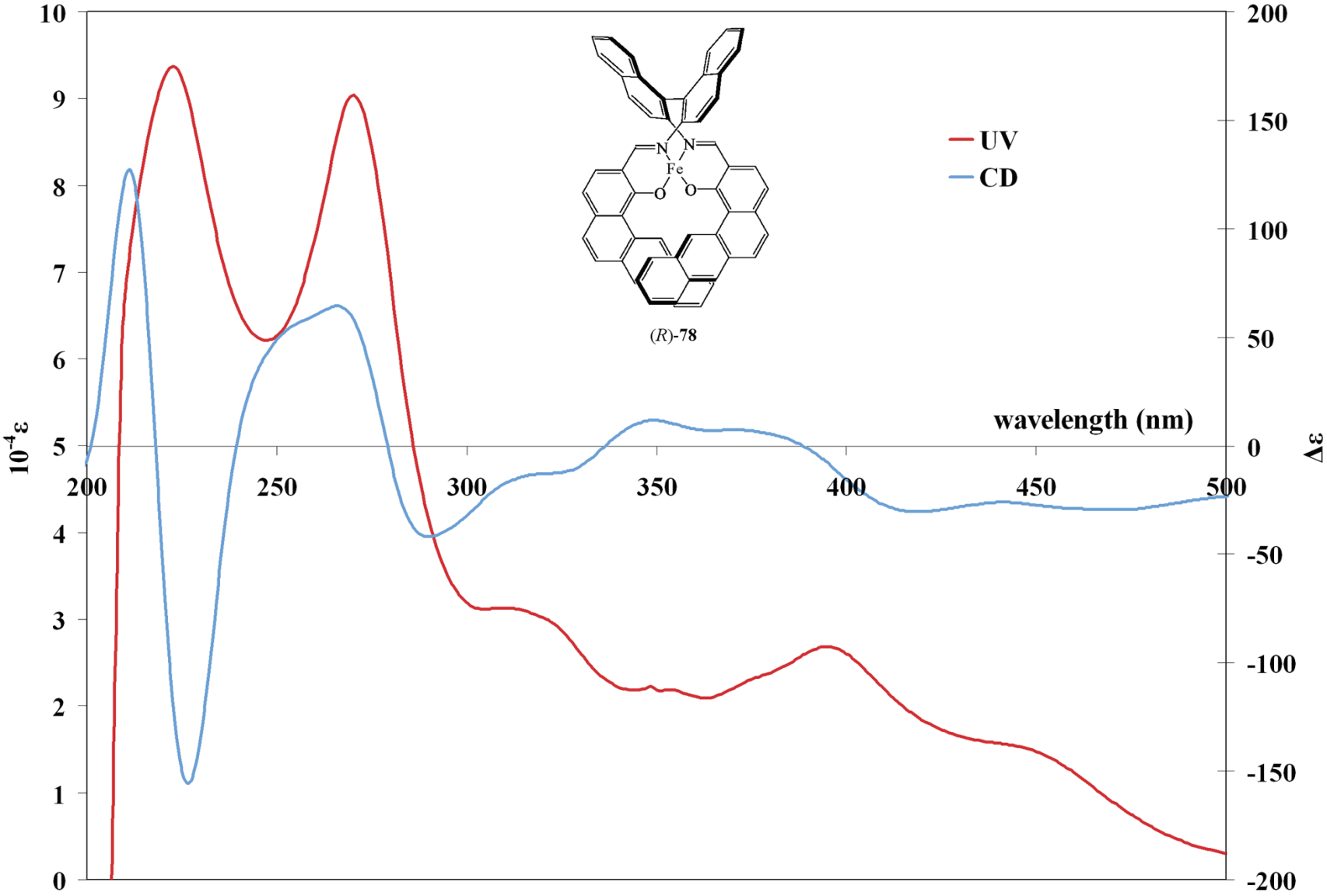

12
10
8
6
4
2
0
200
150
100
50
0
-50
-100
-150
-200
$10^{-4}\varepsilon$
$\Delta\varepsilon$
UV
CD
wavelength (nm)
200
250
300
350
400
450
500
N
N
Zn
O
O
(R)-55


12
10
8
6
4
2
0
150
100
50
0
-50
-100
-150
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
$10^{-4}\varepsilon$
$\Delta\varepsilon$
N
N
Fe
O
O
(R)-56


12
10
8
6
4
2
0
$10^{-4}\varepsilon$
200
150
100
50
0
-50
-100
-150
-200
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
Zn
O
O
(R,R)-75


12
10
8
6
4
2
0
$10^{-4}\varepsilon$
100
75
50
25
0
-25
-50
-75
-100
Δε
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
(R,R)-76


12
10
8
6
4
2
0
$10^{-4}\varepsilon$
300
250
200
150
100
50
0
-50
-100
-150
-200
-250
-300
$\Delta\varepsilon$
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
N
N
Zn
O
O
(R)-77


10
9
8
7
6
5
4
3
2
1
0
200
150
100
50
0
-50
-100
-150
-200
200
250
300
350
400
450
500
wavelength (nm)
UV
CD
10-4ε
Δε
N
N
Fe
O
O

(*R*)-**78**

Appendix IV

Crystal Data

(Numerical order)

Table 1. Crystal data and structure refinement for (*rac*)-**33**.

Identification code	(*rac*)-**33**	
Empirical formula	C36 H30 N2 O2	
Formula weight	522.62	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9861(9) Å	α = 87.046(5)°.
	b = 14.1047(11) Å	β = 84.757(5)°.
	c = 18.9046(15) Å	γ = 86.979(5)°.
Volume	2645.0(4) $Å^3$	
Z	4	
Density (calculated)	1.312 g/cm^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1104	
Crystal size	0.35 x 0.25 x 0.15 mm^3	
Theta range for data collection	1.45 to 27.47°.	
Index ranges	-12<=h<=12, -17<=k<=18, -24<=l<=22	
Reflections collected	19156	
Independent reflections	11481 [R(int) = 0.1082]	
Completeness to theta = 27.47°	95.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11481 / 0 / 734	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0740, wR2 = 0.1826	
R indices (all data)	R1 = 0.1151, wR2 = 0.2034	
Extinction coefficient	0.0159(16)	
Largest diff. peak and hole	0.399 and -0.380 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*rac*)-**33**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(11)	2635(3)	3429(2)	6669(1)	33(1)
N(11)	2164(2)	4197(2)	6193(1)	32(1)
C(12)	4126(3)	3225(2)	6451(1)	32(1)
N(12)	4265(2)	2963(1)	5712(1)	32(1)
C(13)	4710(3)	2419(2)	6918(2)	45(1)
C(14)	4390(3)	2580(2)	7705(2)	50(1)
C(15)	2900(3)	2761(2)	7892(2)	50(1)
C(16)	2364(3)	3612(2)	7452(1)	42(1)
C(21)	1557(2)	8677(2)	6619(1)	30(1)
N(21)	1288(2)	7938(1)	7175(1)	29(1)
C(22)	2528(3)	9364(2)	6855(1)	31(1)
N(22)	1945(2)	9838(1)	7486(1)	36(1)
C(23)	2878(3)	10103(2)	6258(2)	45(1)
C(24)	3448(3)	9646(2)	5583(2)	43(1)

C(25)	2493(3)	8956(2)	5348(1)	44(1)
C(26)	2133(3)	8220(2)	5943(1)	36(1)
C(101)	1014(2)	6323(2)	4639(1)	28(1)
C(102)	1471(2)	5601(2)	5147(1)	30(1)
O(112)	2495(2)	5016(1)	4977(1)	35(1)
C(103)	795(2)	5534(2)	5838(1)	31(1)
C(104)	-288(2)	6172(2)	6035(1)	33(1)
C(105)	-667(3)	6886(2)	5578(1)	36(1)
C(106)	-20(2)	6977(2)	4889(1)	32(1)
C(107)	-418(3)	7755(2)	4425(2)	38(1)
C(108)	97(3)	7837(2)	3748(2)	39(1)
C(109)	1034(3)	7139(2)	3451(1)	34(1)
C(110)	1421(3)	7182(2)	2722(2)	40(1)
C(111)	2282(3)	6508(2)	2422(2)	47(1)
C(112)	2793(3)	5764(2)	2850(2)	42(1)
C(113)	2434(3)	5703(2)	3569(1)	35(1)
C(114)	1531(2)	6385(2)	3896(1)	30(1)
C(115)	1189(3)	4814(2)	6341(1)	33(1)
C(201)	4154(2)	2243(2)	3548(1)	28(1)
C(202)	4165(2)	2444(2)	4283(1)	28(1)
O(212)	3601(2)	1893(1)	4788(1)	32(1)
C(203)	4814(2)	3254(2)	4471(1)	28(1)
C(204)	5435(2)	3856(2)	3938(1)	32(1)
C(205)	5439(3)	3681(2)	3243(1)	34(1)
C(206)	4824(2)	2870(2)	3037(1)	31(1)
C(207)	4909(3)	2667(2)	2302(1)	35(1)
C(208)	4379(3)	1895(2)	2077(1)	37(1)
C(209)	3682(2)	1250(2)	2560(1)	33(1)
C(210)	3119(3)	451(2)	2309(2)	43(1)
C(211)	2439(3)	-171(2)	2762(2)	50(1)
C(212)	2269(3)	-6(2)	3481(2)	47(1)
C(213)	2803(3)	768(2)	3743(2)	38(1)
C(214)	3540(2)	1422(2)	3297(1)	29(1)
C(215)	4835(2)	3474(2)	5196(1)	33(1)
C(301)	684(3)	5518(2)	8614(1)	39(1)
C(302)	942(3)	6334(2)	8141(1)	32(1)
O(312)	2149(2)	6631(1)	7999(1)	38(1)
C(303)	-141(3)	6838(2)	7830(1)	33(1)
C(304)	-1458(3)	6529(2)	7971(2)	43(1)
C(305)	-1703(3)	5755(2)	8405(2)	52(1)
C(306)	-649(3)	5239(2)	8727(2)	46(1)
C(307)	-952(4)	4422(2)	9181(2)	64(1)
C(308)	9(5)	3915(2)	9502(2)	69(1)
C(309)	1368(4)	4177(2)	9419(2)	57(1)
C(310)	2365(6)	3658(2)	9786(2)	78(1)
C(311)	3660(6)	3916(3)	9728(2)	84(1)
C(312)	4017(4)	4682(3)	9284(2)	73(1)
C(313)	3079(3)	5209(2)	8922(2)	55(1)
C(314)	1728(3)	4978(2)	8970(1)	45(1)
C(315)	108(3)	7630(2)	7346(1)	32(1)
C(401)	338(2)	11059(2)	9433(1)	29(1)
C(402)	850(3)	10702(2)	8770(1)	30(1)
O(412)	29(2)	10646(1)	8252(1)	38(1)
C(403)	2202(3)	10390(2)	8640(1)	33(1)

C(404)	3083(3)	10469(2)	9166(2)	39(1)
C(405)	2633(3)	10818(2)	9804(2)	38(1)
C(406)	1274(3)	11102(2)	9953(1)	34(1)
C(407)	814(3)	11407(2)	10642(1)	38(1)
C(408)	-475(3)	11665(2)	10816(1)	39(1)
C(409)	-1449(3)	11652(2)	10313(1)	35(1)
C(410)	-2791(3)	11933(2)	10515(2)	43(1)
C(411)	-3753(3)	11923(2)	10050(2)	50(1)
C(412)	-3390(3)	11645(2)	9363(2)	50(1)
C(413)	-2086(3)	11366(2)	9149(1)	41(1)
C(414)	-1056(3)	11356(2)	9617(1)	31(1)
C(415)	2686(3)	9948(2)	7990(1)	35(1)

Table 3. Bond lengths [Å] and angles [°] for (*rac*)-**33**.

C(11)-N(11)	1.459(3)	C(23)-H(23B)	0.9900
C(11)-C(16)	1.512(4)	C(24)-C(25)	1.508(4)
C(11)-C(12)	1.525(4)	C(24)-H(24A)	0.9900
C(11)-H(11A)	1.0000	C(24)-H(24B)	0.9900
N(11)-C(115)	1.293(3)	C(25)-C(26)	1.522(4)
N(11)-H(11)	1.04(3)	C(25)-H(25A)	0.9900
C(12)-N(12)	1.455(3)	C(25)-H(25B)	0.9900
C(12)-C(13)	1.528(3)	C(26)-H(26A)	0.9900
C(12)-H(12A)	1.0000	C(26)-H(26B)	0.9900
N(12)-C(215)	1.289(3)	C(101)-C(106)	1.412(3)
N(12)-H(12)	1.10(3)	C(101)-C(102)	1.449(3)
C(13)-C(14)	1.519(4)	C(101)-C(114)	1.451(3)
C(13)-H(13A)	0.9900	C(102)-O(112)	1.307(3)
C(13)-H(13B)	0.9900	C(102)-C(103)	1.414(4)
C(14)-C(15)	1.508(4)	C(103)-C(104)	1.406(3)
C(14)-H(14A)	0.9900	C(103)-C(115)	1.421(3)
C(14)-H(14B)	0.9900	C(104)-C(105)	1.355(3)
C(15)-C(16)	1.526(4)	C(104)-H(104)	0.9500
C(15)-H(15A)	0.9900	C(105)-C(106)	1.402(4)
C(15)-H(15B)	0.9900	C(105)-H(105)	0.9500
C(16)-H(16A)	0.9900	C(106)-C(107)	1.432(3)
C(16)-H(16B)	0.9900	C(107)-C(108)	1.337(4)
C(21)-N(21)	1.459(3)	C(107)-H(107)	0.9500
C(21)-C(26)	1.513(4)	C(108)-C(109)	1.422(4)
C(21)-C(22)	1.518(4)	C(108)-H(108)	0.9500
C(21)-H(21A)	1.0000	C(109)-C(110)	1.397(4)
N(21)-C(315)	1.285(3)	C(109)-C(114)	1.419(3)
N(21)-H(21)	1.13(2)	C(110)-C(111)	1.358(4)
C(22)-N(22)	1.457(3)	C(110)-H(110)	0.9500
C(22)-C(23)	1.526(4)	C(111)-C(112)	1.395(4)
C(22)-H(22A)	1.0000	C(111)-H(111)	0.9500
N(22)-C(415)	1.279(3)	C(112)-C(113)	1.373(4)
C(23)-C(24)	1.509(4)	C(112)-H(112)	0.9500
C(23)-H(23A)	0.9900	C(113)-C(114)	1.411(3)

C(113)-H(113)	0.9500	C(313)-H(313)	0.9500
C(115)-H(115)	0.9500	C(315)-H(315)	0.9500
C(201)-C(206)	1.421(3)	C(401)-C(402)	1.418(3)
C(201)-C(202)	1.433(3)	C(401)-C(406)	1.422(3)
C(201)-C(214)	1.458(3)	C(401)-C(414)	1.449(3)
C(202)-O(212)	1.305(3)	C(402)-O(412)	1.341(3)
C(202)-C(203)	1.419(3)	C(402)-C(403)	1.402(3)
C(203)-C(204)	1.407(3)	O(412)-H(22)	0.86(3)
C(203)-C(215)	1.423(3)	C(403)-C(404)	1.400(4)
C(204)-C(205)	1.347(4)	C(403)-C(415)	1.439(4)
C(204)-H(204)	0.9500	C(404)-C(405)	1.354(4)
C(205)-C(206)	1.416(4)	C(404)-H(404)	0.9500
C(205)-H(205)	0.9500	C(405)-C(406)	1.402(4)
C(206)-C(207)	1.426(3)	C(405)-H(405)	0.9500
C(207)-C(208)	1.340(4)	C(406)-C(407)	1.420(4)
C(207)-H(207)	0.9500	C(407)-C(408)	1.335(4)
C(208)-C(209)	1.419(4)	C(407)-H(407)	0.9500
C(208)-H(208)	0.9500	C(408)-C(409)	1.423(4)
C(209)-C(210)	1.408(4)	C(408)-H(408)	0.9500
C(209)-C(214)	1.419(3)	C(409)-C(410)	1.402(4)
C(210)-C(211)	1.358(4)	C(409)-C(414)	1.416(4)
C(210)-H(210)	0.9500	C(410)-C(411)	1.361(4)
C(211)-C(212)	1.386(4)	C(410)-H(410)	0.9500
C(211)-H(211)	0.9500	C(411)-C(412)	1.387(4)
C(212)-C(213)	1.373(4)	C(411)-H(411)	0.9500
C(212)-H(212)	0.9500	C(412)-C(413)	1.371(4)
C(213)-C(214)	1.409(4)	C(412)-H(412)	0.9500
C(213)-H(213)	0.9500	C(413)-C(414)	1.416(4)
C(215)-H(215)	0.9500	C(413)-H(413)	0.9500
C(301)-C(306)	1.403(4)	C(415)-H(415)	0.9500
C(301)-C(302)	1.441(3)		
C(301)-C(314)	1.453(4)	N(11)-C(11)-C(16)	114.6(2)
C(302)-O(312)	1.297(3)	N(11)-C(11)-C(12)	107.3(2)
C(302)-C(303)	1.419(3)	C(16)-C(11)-C(12)	112.4(2)
C(303)-C(304)	1.406(4)	N(11)-C(11)-H(11A)	107.4
C(303)-C(315)	1.424(4)	C(16)-C(11)-H(11A)	107.4
C(304)-C(305)	1.350(4)	C(12)-C(11)-H(11A)	107.4
C(304)-H(304)	0.9500	C(115)-N(11)-C(11)	126.2(2)
C(305)-C(306)	1.415(4)	C(115)-N(11)-H(11)	104.1(14)
C(305)-H(305)	0.9500	C(11)-N(11)-H(11)	129.7(14)
C(306)-C(307)	1.429(4)	N(12)-C(12)-C(11)	108.18(19)
C(307)-C(308)	1.338(5)	N(12)-C(12)-C(13)	109.8(2)
C(307)-H(307)	0.9500	C(11)-C(12)-C(13)	111.2(2)
C(308)-C(309)	1.419(5)	N(12)-C(12)-H(12A)	109.2
C(308)-H(308)	0.9500	C(11)-C(12)-H(12A)	109.2
C(309)-C(310)	1.416(5)	C(13)-C(12)-H(12A)	109.2
C(309)-C(314)	1.419(4)	C(215)-N(12)-C(12)	124.1(2)
C(310)-C(311)	1.355(6)	C(215)-N(12)-H(12)	103.8(14)
C(310)-H(310)	0.9500	C(12)-N(12)-H(12)	131.6(14)
C(311)-C(312)	1.375(6)	C(14)-C(13)-C(12)	112.1(2)
C(311)-H(311)	0.9500	C(14)-C(13)-H(13A)	109.2
C(312)-C(313)	1.375(4)	C(12)-C(13)-H(13A)	109.2
C(312)-H(312)	0.9500	C(14)-C(13)-H(13B)	109.2
C(313)-C(314)	1.398(5)	C(12)-C(13)-H(13B)	109.2

H(13A)-C(13)-H(13B)	107.9	C(21)-C(26)-H(26A)	109.2
C(15)-C(14)-C(13)	111.7(2)	C(25)-C(26)-H(26A)	109.2
C(15)-C(14)-H(14A)	109.3	C(21)-C(26)-H(26B)	109.2
C(13)-C(14)-H(14A)	109.3	C(25)-C(26)-H(26B)	109.2
C(15)-C(14)-H(14B)	109.3	H(26A)-C(26)-H(26B)	107.9
C(13)-C(14)-H(14B)	109.3	C(106)-C(101)-C(102)	117.0(2)
H(14A)-C(14)-H(14B)	107.9	C(106)-C(101)-C(114)	119.4(2)
C(14)-C(15)-C(16)	110.8(2)	C(102)-C(101)-C(114)	123.6(2)
C(14)-C(15)-H(15A)	109.5	O(112)-C(102)-C(103)	119.9(2)
C(16)-C(15)-H(15A)	109.5	O(112)-C(102)-C(101)	121.0(2)
C(14)-C(15)-H(15B)	109.5	C(103)-C(102)-C(101)	119.1(2)
C(16)-C(15)-H(15B)	109.5	C(104)-C(103)-C(102)	120.6(2)
H(15A)-C(15)-H(15B)	108.1	C(104)-C(103)-C(115)	118.9(2)
C(11)-C(16)-C(15)	109.6(2)	C(102)-C(103)-C(115)	120.5(2)
C(11)-C(16)-H(16A)	109.8	C(105)-C(104)-C(103)	120.6(2)
C(15)-C(16)-H(16A)	109.8	C(105)-C(104)-H(104)	119.7
C(11)-C(16)-H(16B)	109.8	C(103)-C(104)-H(104)	119.7
C(15)-C(16)-H(16B)	109.8	C(104)-C(105)-C(106)	120.4(2)
H(16A)-C(16)-H(16B)	108.2	C(104)-C(105)-H(105)	119.8
N(21)-C(21)-C(26)	109.24(19)	C(106)-C(105)-H(105)	119.8
N(21)-C(21)-C(22)	110.01(19)	C(105)-C(106)-C(101)	121.9(2)
C(26)-C(21)-C(22)	110.7(2)	C(105)-C(106)-C(107)	119.1(2)
N(21)-C(21)-H(21A)	108.9	C(101)-C(106)-C(107)	119.0(2)
C(26)-C(21)-H(21A)	108.9	C(108)-C(107)-C(106)	121.5(2)
C(22)-C(21)-H(21A)	108.9	C(108)-C(107)-H(107)	119.2
C(315)-N(21)-C(21)	123.0(2)	C(106)-C(107)-H(107)	119.2
C(315)-N(21)-H(21)	104.2(13)	C(107)-C(108)-C(109)	121.4(2)
C(21)-N(21)-H(21)	131.7(14)	C(107)-C(108)-H(108)	119.3
N(22)-C(22)-C(21)	110.6(2)	C(109)-C(108)-H(108)	119.3
N(22)-C(22)-C(23)	109.7(2)	C(110)-C(109)-C(114)	120.5(2)
C(21)-C(22)-C(23)	110.1(2)	C(110)-C(109)-C(108)	119.9(2)
N(22)-C(22)-H(22A)	108.8	C(114)-C(109)-C(108)	119.5(2)
C(21)-C(22)-H(22A)	108.8	C(111)-C(110)-C(109)	121.0(2)
C(23)-C(22)-H(22A)	108.8	C(111)-C(110)-H(110)	119.5
C(415)-N(22)-C(22)	119.0(2)	C(109)-C(110)-H(110)	119.5
C(24)-C(23)-C(22)	111.8(2)	C(110)-C(111)-C(112)	119.5(3)
C(24)-C(23)-H(23A)	109.2	C(110)-C(111)-H(111)	120.2
C(22)-C(23)-H(23A)	109.2	C(112)-C(111)-H(111)	120.2
C(24)-C(23)-H(23B)	109.2	C(113)-C(112)-C(111)	120.9(3)
C(22)-C(23)-H(23B)	109.2	C(113)-C(112)-H(112)	119.5
H(23A)-C(23)-H(23B)	107.9	C(111)-C(112)-H(112)	119.5
C(25)-C(24)-C(23)	111.2(2)	C(112)-C(113)-C(114)	121.1(2)
C(25)-C(24)-H(24A)	109.4	C(112)-C(113)-H(113)	119.5
C(23)-C(24)-H(24A)	109.4	C(114)-C(113)-H(113)	119.5
C(25)-C(24)-H(24B)	109.4	C(113)-C(114)-C(109)	116.9(2)
C(23)-C(24)-H(24B)	109.4	C(113)-C(114)-C(101)	124.2(2)
H(24A)-C(24)-H(24B)	108.0	C(109)-C(114)-C(101)	118.7(2)
C(24)-C(25)-C(26)	110.6(2)	N(11)-C(115)-C(103)	122.1(2)
C(24)-C(25)-H(25A)	109.5	N(11)-C(115)-H(115)	118.9
C(26)-C(25)-H(25A)	109.5	C(103)-C(115)-H(115)	118.9
C(24)-C(25)-H(25B)	109.5	C(206)-C(201)-C(202)	117.6(2)
C(26)-C(25)-H(25B)	109.5	C(206)-C(201)-C(214)	118.3(2)
H(25A)-C(25)-H(25B)	108.1	C(202)-C(201)-C(214)	124.1(2)
C(21)-C(26)-C(25)	112.0(2)	O(212)-C(202)-C(203)	118.8(2)

O(212)-C(202)-C(201)	121.6(2)	C(304)-C(305)-H(305)	119.4
C(203)-C(202)-C(201)	119.6(2)	C(306)-C(305)-H(305)	119.4
C(204)-C(203)-C(202)	119.9(2)	C(301)-C(306)-C(305)	121.2(3)
C(204)-C(203)-C(215)	119.2(2)	C(301)-C(306)-C(307)	119.5(3)
C(202)-C(203)-C(215)	120.9(2)	C(305)-C(306)-C(307)	119.3(3)
C(205)-C(204)-C(203)	121.5(2)	C(308)-C(307)-C(306)	121.5(4)
C(205)-C(204)-H(204)	119.3	C(308)-C(307)-H(307)	119.2
C(203)-C(204)-H(204)	119.3	C(306)-C(307)-H(307)	119.2
C(204)-C(205)-C(206)	120.1(2)	C(307)-C(308)-C(309)	121.4(3)
C(204)-C(205)-H(205)	119.9	C(307)-C(308)-H(308)	119.3
C(206)-C(205)-H(205)	119.9	C(309)-C(308)-H(308)	119.3
C(205)-C(206)-C(201)	121.2(2)	C(310)-C(309)-C(308)	120.8(3)
C(205)-C(206)-C(207)	119.2(2)	C(310)-C(309)-C(314)	119.7(4)
C(201)-C(206)-C(207)	119.6(2)	C(308)-C(309)-C(314)	119.5(3)
C(208)-C(207)-C(206)	121.9(3)	C(311)-C(310)-C(309)	121.5(3)
C(208)-C(207)-H(207)	119.1	C(311)-C(310)-H(310)	119.2
C(206)-C(207)-H(207)	119.1	C(309)-C(310)-H(310)	119.2
C(207)-C(208)-C(209)	121.2(3)	C(310)-C(311)-C(312)	119.0(4)
C(207)-C(208)-H(208)	119.4	C(310)-C(311)-H(311)	120.5
C(209)-C(208)-H(208)	119.4	C(312)-C(311)-H(311)	120.5
C(210)-C(209)-C(208)	120.1(2)	C(313)-C(312)-C(311)	121.3(4)
C(210)-C(209)-C(214)	120.2(3)	C(313)-C(312)-H(312)	119.3
C(208)-C(209)-C(214)	119.6(2)	C(311)-C(312)-H(312)	119.3
C(211)-C(210)-C(209)	121.2(3)	C(312)-C(313)-C(314)	121.9(3)
C(211)-C(210)-H(210)	119.4	C(312)-C(313)-H(313)	119.1
C(209)-C(210)-H(210)	119.4	C(314)-C(313)-H(313)	119.1
C(210)-C(211)-C(212)	119.4(3)	C(313)-C(314)-C(309)	116.6(3)
C(210)-C(211)-H(211)	120.3	C(313)-C(314)-C(301)	124.5(3)
C(212)-C(211)-H(211)	120.3	C(309)-C(314)-C(301)	118.9(3)
C(213)-C(212)-C(211)	120.9(3)	N(21)-C(315)-C(303)	123.3(2)
C(213)-C(212)-H(212)	119.6	N(21)-C(315)-H(315)	118.3
C(211)-C(212)-H(212)	119.6	C(303)-C(315)-H(315)	118.3
C(212)-C(213)-C(214)	121.8(3)	C(402)-C(401)-C(406)	116.5(2)
C(212)-C(213)-H(213)	119.1	C(402)-C(401)-C(414)	124.7(2)
C(214)-C(213)-H(213)	119.1	C(406)-C(401)-C(414)	118.8(2)
C(213)-C(214)-C(209)	116.5(2)	O(412)-C(402)-C(403)	118.5(2)
C(213)-C(214)-C(201)	124.1(2)	O(412)-C(402)-C(401)	119.9(2)
C(209)-C(214)-C(201)	119.4(2)	C(403)-C(402)-C(401)	121.6(2)
N(12)-C(215)-C(203)	122.5(2)	C(402)-O(412)-H(22)	106.7(19)
N(12)-C(215)-H(215)	118.7	C(404)-C(403)-C(402)	119.4(2)
C(203)-C(215)-H(215)	118.7	C(404)-C(403)-C(415)	119.3(2)
C(306)-C(301)-C(302)	117.4(3)	C(402)-C(403)-C(415)	121.3(2)
C(306)-C(301)-C(314)	119.3(3)	C(405)-C(404)-C(403)	120.6(3)
C(302)-C(301)-C(314)	123.4(3)	C(405)-C(404)-H(404)	119.7
O(312)-C(302)-C(303)	118.8(2)	C(403)-C(404)-H(404)	119.7
O(312)-C(302)-C(301)	121.3(2)	C(404)-C(405)-C(406)	120.9(2)
C(303)-C(302)-C(301)	119.8(2)	C(404)-C(405)-H(405)	119.6
C(304)-C(303)-C(302)	120.1(2)	C(406)-C(405)-H(405)	119.6
C(304)-C(303)-C(315)	119.6(2)	C(405)-C(406)-C(407)	119.6(2)
C(302)-C(303)-C(315)	120.2(2)	C(405)-C(406)-C(401)	121.0(2)
C(305)-C(304)-C(303)	120.3(3)	C(407)-C(406)-C(401)	119.4(2)
C(305)-C(304)-H(304)	119.8	C(408)-C(407)-C(406)	121.9(2)
C(303)-C(304)-H(304)	119.8	C(408)-C(407)-H(407)	119.0
C(304)-C(305)-C(306)	121.1(3)	C(406)-C(407)-H(407)	119.0

C(407)-C(408)-C(409)	121.1(3)	N(22)-C(415)-H(415)	118.3
C(407)-C(408)-H(408)	119.5	N(22)-C(415)-C(403)	123.3(2)
C(409)-C(408)-H(408)	119.5	C(403)-C(415)-H(415)	118.3
C(410)-C(409)-C(414)	120.9(2)	C(413)-C(412)-C(411)	121.1(3)
C(410)-C(409)-C(408)	119.3(3)	C(413)-C(412)-H(412)	119.5
C(414)-C(409)-C(408)	119.8(2)	C(411)-C(412)-H(412)	119.5
C(411)-C(410)-C(409)	120.9(3)	C(412)-C(413)-C(414)	121.5(3)
C(411)-C(410)-H(410)	119.5	C(412)-C(413)-H(413)	119.2
C(409)-C(410)-H(410)	119.5	C(414)-C(413)-H(413)	119.2
C(410)-C(411)-C(412)	119.3(3)	C(409)-C(414)-C(413)	116.3(2)
C(410)-C(411)-H(411)	120.3	C(409)-C(414)-C(401)	119.0(2)
C(412)-C(411)-H(411)	120.3	C(413)-C(414)-C(401)	124.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*rac*)-**33**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(11)	42(2)	30(1)	29(1)	1(1)	-6(1)	-5(1)
N(11)	37(1)	33(1)	28(1)	1(1)	-4(1)	-4(1)
C(12)	40(2)	27(1)	31(1)	-4(1)	-8(1)	-6(1)
N(12)	36(1)	28(1)	33(1)	-3(1)	-5(1)	-2(1)
C(13)	54(2)	37(2)	45(2)	2(1)	-17(1)	2(1)
C(14)	62(2)	50(2)	39(2)	10(1)	-19(2)	-4(2)
C(15)	67(2)	55(2)	29(2)	7(1)	-7(1)	-9(2)
C(16)	55(2)	42(2)	29(1)	1(1)	-3(1)	-3(1)
C(21)	27(1)	34(1)	27(1)	6(1)	-2(1)	3(1)
N(21)	29(1)	32(1)	27(1)	3(1)	1(1)	0(1)
C(22)	32(1)	28(1)	33(1)	0(1)	0(1)	0(1)
N(22)	40(1)	30(1)	36(1)	-3(1)	-3(1)	1(1)
C(23)	56(2)	30(1)	48(2)	3(1)	8(1)	-3(1)
C(24)	47(2)	36(2)	43(2)	13(1)	7(1)	1(1)
C(25)	45(2)	56(2)	30(2)	6(1)	1(1)	5(1)
C(26)	36(2)	39(1)	33(1)	-1(1)	-4(1)	-4(1)
C(101)	26(1)	27(1)	33(1)	-3(1)	-7(1)	-5(1)
C(102)	29(1)	29(1)	32(1)	-5(1)	-6(1)	-3(1)
O(112)	36(1)	36(1)	32(1)	0(1)	-1(1)	6(1)
C(103)	31(1)	29(1)	35(1)	-3(1)	-6(1)	-7(1)
C(104)	31(1)	36(1)	31(1)	-9(1)	-1(1)	-7(1)
C(105)	28(1)	37(1)	43(2)	-6(1)	-4(1)	2(1)
C(106)	26(1)	32(1)	39(2)	-3(1)	-10(1)	-5(1)
C(107)	32(1)	33(1)	50(2)	-3(1)	-10(1)	1(1)
C(108)	34(1)	34(1)	48(2)	8(1)	-11(1)	-3(1)
C(109)	34(1)	34(1)	35(2)	3(1)	-10(1)	-11(1)
C(110)	44(2)	40(2)	40(2)	4(1)	-14(1)	-10(1)
C(111)	54(2)	54(2)	33(2)	1(1)	-6(1)	-11(2)
C(112)	48(2)	45(2)	34(2)	-6(1)	-4(1)	-4(1)
C(113)	38(2)	35(1)	32(1)	-1(1)	-5(1)	-5(1)

C(114)	26(1)	35(1)	31(1)	-3(1)	-7(1)	-8(1)
C(115)	35(1)	35(1)	29(1)	-3(1)	-3(1)	-7(1)
C(201)	23(1)	31(1)	30(1)	-1(1)	-3(1)	3(1)
C(202)	23(1)	29(1)	31(1)	-1(1)	-2(1)	3(1)
O(212)	35(1)	30(1)	30(1)	0(1)	-1(1)	-6(1)
C(203)	26(1)	25(1)	32(1)	-2(1)	0(1)	1(1)
C(204)	32(1)	25(1)	38(2)	-5(1)	1(1)	-2(1)
C(205)	32(1)	32(1)	35(2)	2(1)	3(1)	0(1)
C(206)	25(1)	33(1)	33(1)	0(1)	2(1)	5(1)
C(207)	31(1)	45(2)	29(1)	2(1)	2(1)	0(1)
C(208)	34(1)	48(2)	29(1)	-2(1)	-1(1)	-1(1)
C(209)	28(1)	42(1)	31(1)	-5(1)	-5(1)	1(1)
C(210)	50(2)	50(2)	31(2)	-8(1)	-12(1)	-4(1)
C(211)	63(2)	44(2)	47(2)	-6(1)	-17(2)	-15(1)
C(212)	57(2)	47(2)	39(2)	4(1)	-13(1)	-17(1)
C(213)	41(2)	39(2)	33(1)	1(1)	-9(1)	-6(1)
C(214)	23(1)	35(1)	30(1)	-1(1)	-4(1)	2(1)
C(215)	32(1)	28(1)	38(2)	-5(1)	-4(1)	0(1)
C(301)	59(2)	31(1)	26(1)	-5(1)	6(1)	-10(1)
C(302)	35(1)	34(1)	24(1)	-3(1)	6(1)	-5(1)
O(312)	31(1)	41(1)	40(1)	12(1)	1(1)	-3(1)
C(303)	34(1)	40(1)	25(1)	-7(1)	2(1)	-6(1)
C(304)	35(2)	59(2)	37(2)	-9(1)	3(1)	-14(1)
C(305)	48(2)	65(2)	46(2)	-14(2)	10(2)	-31(2)
C(306)	64(2)	43(2)	31(2)	-7(1)	7(1)	-24(1)
C(307)	93(3)	55(2)	45(2)	-13(2)	17(2)	-39(2)
C(308)	132(4)	37(2)	38(2)	0(1)	7(2)	-28(2)
C(309)	108(3)	26(1)	36(2)	-3(1)	6(2)	-12(2)
C(310)	162(5)	27(2)	44(2)	8(1)	-12(3)	7(2)
C(311)	131(4)	51(2)	70(3)	10(2)	-25(3)	22(3)
C(312)	84(3)	65(2)	68(2)	14(2)	-17(2)	20(2)
C(313)	68(2)	48(2)	46(2)	8(2)	-7(2)	6(2)
C(314)	77(2)	29(1)	27(1)	-3(1)	3(1)	-1(1)
C(315)	30(1)	41(1)	26(1)	-6(1)	-1(1)	1(1)
C(401)	38(1)	22(1)	26(1)	2(1)	-3(1)	-4(1)
C(402)	39(1)	24(1)	28(1)	2(1)	-8(1)	-2(1)
O(412)	40(1)	46(1)	29(1)	-8(1)	-9(1)	7(1)
C(403)	38(1)	28(1)	35(1)	1(1)	-6(1)	-2(1)
C(404)	35(2)	34(1)	49(2)	2(1)	-6(1)	-4(1)
C(405)	39(2)	40(2)	39(2)	-2(1)	-16(1)	-7(1)
C(406)	43(2)	26(1)	32(1)	3(1)	-5(1)	-8(1)
C(407)	49(2)	35(1)	33(2)	-1(1)	-10(1)	-12(1)
C(408)	52(2)	35(1)	29(1)	-5(1)	1(1)	-11(1)
C(409)	49(2)	25(1)	31(1)	0(1)	-1(1)	-3(1)
C(410)	52(2)	38(2)	39(2)	-3(1)	4(1)	3(1)
C(411)	45(2)	51(2)	50(2)	8(2)	3(2)	14(1)
C(412)	43(2)	62(2)	44(2)	5(2)	-9(1)	14(1)
C(413)	47(2)	47(2)	27(1)	0(1)	-4(1)	10(1)
C(414)	40(1)	24(1)	29(1)	3(1)	-4(1)	-1(1)
C(415)	35(1)	27(1)	41(2)	2(1)	0(1)	-3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*rac*)-**33**.

	x	y	z	U(eq)
H(11A)	2151	2850	6579	40
H(11)	2530(30)	4394(19)	5678(15)	39
H(12A)	4626	3811	6495	38
H(12)	3840(30)	2390(19)	5445(14)	38
H(13A)	4339	1812	6806	54
H(13B)	5699	2364	6809	54
H(14A)	4708	2014	7986	60
H(14B)	4877	3130	7834	60
H(15A)	2732	2885	8404	60
H(15B)	2417	2190	7801	60
H(16A)	1383	3714	7574	51
H(16B)	2810	4191	7560	51
H(21A)	693	9033	6528	36
H(21)	1980(30)	7417(18)	7455(13)	35
H(22A)	3372	9000	6972	38
H(22)	500(30)	10380(20)	7904(16)	43
H(23A)	2057	10496	6162	54
H(23B)	3543	10528	6411	54
H(24A)	3618	10145	5203	52
H(24B)	4317	9307	5665	52
H(25A)	2918	8632	4926	53
H(25B)	1663	9306	5212	53
H(26A)	1466	7798	5787	43
H(26B)	2949	7823	6041	43
H(104)	-759	6101	6493	39
H(105)	-1375	7329	5725	43
H(107)	-1062	8223	4602	45
H(108)	-168	8373	3459	46
H(110)	1078	7690	2431	48
H(111)	2534	6542	1925	56
H(112)	3399	5294	2641	50
H(113)	2799	5193	3850	42
H(115)	722	4786	6802	39
H(204)	5861	4399	4069	38
H(205)	5856	4102	2892	40
H(207)	5355	3091	1963	42
H(208)	4472	1778	1584	44
H(210)	3217	346	1814	52
H(211)	2082	-716	2586	60
H(212)	1778	-434	3798	56
H(213)	2670	864	4239	45
H(215)	5286	4017	5305	39
H(304)	-2180	6867	7759	52
H(305)	-2598	5555	8495	63
H(307)	-1855	4234	9256	77
H(308)	-224	3368	9792	83
H(310)	2121	3116	10079	94
H(311)	4311	3573	9989	101

H(312)	4930	4851	9227	88
H(313)	3356	5745	8630	66
H(315)	-635	7946	7140	39
H(404)	4006	10275	9076	47
H(405)	3246	10872	10153	46
H(407)	1442	11429	10988	46
H(408)	-746	11860	11283	47
H(410)	-3032	12134	10984	52
H(411)	-4662	12104	10195	60
H(412)	-4057	11647	9035	60
H(413)	-1868	11176	8676	49
H(415)	3602	9725	7933	42

Table 6. Torsion angles [°] for (*rac*)-**33**.

C(16)-C(11)-N(11)-C(115)	-25.9(4)	O(112)-C(102)-C(103)-C(104)	178.5(2)
C(12)-C(11)-N(11)-C(115)	-151.5(2)	C(101)-C(102)-C(103)-C(104)	-1.4(4)
N(11)-C(11)-C(12)-N(12)	-58.9(2)	O(112)-C(102)-C(103)-C(115)	-2.2(4)
C(16)-C(11)-C(12)-N(12)	174.2(2)	C(101)-C(102)-C(103)-C(115)	178.0(2)
N(11)-C(11)-C(12)-C(13)	-179.5(2)	C(102)-C(103)-C(104)-C(105)	-2.8(4)
C(16)-C(11)-C(12)-C(13)	53.6(3)	C(115)-C(103)-C(104)-C(105)	177.9(2)
C(11)-C(12)-N(12)-C(215)	112.5(3)	C(103)-C(104)-C(105)-C(106)	2.7(4)
C(13)-C(12)-N(12)-C(215)	-126.0(3)	C(104)-C(105)-C(106)-C(101)	1.7(4)
N(12)-C(12)-C(13)-C(14)	-170.6(2)	C(104)-C(105)-C(106)-C(107)	-178.3(2)
C(11)-C(12)-C(13)-C(14)	-50.9(3)	C(102)-C(101)-C(106)-C(105)	-5.6(4)
C(12)-C(13)-C(14)-C(15)	53.5(3)	C(114)-C(101)-C(106)-C(105)	172.4(2)
C(13)-C(14)-C(15)-C(16)	-57.2(3)	C(102)-C(101)-C(106)-C(107)	174.3(2)
N(11)-C(11)-C(16)-C(15)	180.0(2)	C(114)-C(101)-C(106)-C(107)	-7.6(3)
C(12)-C(11)-C(16)-C(15)	-57.1(3)	C(105)-C(106)-C(107)-C(108)	-175.2(3)
C(14)-C(15)-C(16)-C(11)	58.5(3)	C(101)-C(106)-C(107)-C(108)	4.9(4)
C(26)-C(21)-N(21)-C(315)	-99.9(3)	C(106)-C(107)-C(108)-C(109)	2.0(4)
C(22)-C(21)-N(21)-C(315)	138.4(2)	C(107)-C(108)-C(109)-C(110)	171.9(3)
N(21)-C(21)-C(22)-N(22)	-62.0(2)	C(107)-C(108)-C(109)-C(114)	-5.9(4)
C(26)-C(21)-C(22)-N(22)	177.19(18)	C(114)-C(109)-C(110)-C(111)	-0.2(4)
N(21)-C(21)-C(22)-C(23)	176.60(19)	C(108)-C(109)-C(110)-C(111)	-178.0(3)
C(26)-C(21)-C(22)-C(23)	55.8(3)	C(109)-C(110)-C(111)-C(112)	-0.4(4)
C(21)-C(22)-N(22)-C(415)	137.6(2)	C(110)-C(111)-C(112)-C(113)	0.3(4)
C(23)-C(22)-N(22)-C(415)	-100.7(3)	C(111)-C(112)-C(113)-C(114)	0.4(4)
N(22)-C(22)-C(23)-C(24)	-178.3(2)	C(112)-C(113)-C(114)-C(109)	-1.0(4)
C(21)-C(22)-C(23)-C(24)	-56.3(3)	C(112)-C(113)-C(114)-C(101)	174.4(2)
C(22)-C(23)-C(24)-C(25)	56.2(3)	C(110)-C(109)-C(114)-C(113)	0.9(4)
C(23)-C(24)-C(25)-C(26)	-55.0(3)	C(108)-C(109)-C(114)-C(113)	178.6(2)
N(21)-C(21)-C(26)-C(25)	-177.6(2)	C(110)-C(109)-C(114)-C(101)	-174.8(2)
C(22)-C(21)-C(26)-C(25)	-56.3(3)	C(108)-C(109)-C(114)-C(101)	3.0(4)
C(24)-C(25)-C(26)-C(21)	55.6(3)	C(106)-C(101)-C(114)-C(113)	-171.6(2)
C(106)-C(101)-C(102)-O(112)	-174.5(2)	C(102)-C(101)-C(114)-C(113)	6.3(4)
C(114)-C(101)-C(102)-O(112)	7.6(4)	C(106)-C(101)-C(114)-C(109)	3.7(3)
C(106)-C(101)-C(102)-C(103)	5.4(3)	C(102)-C(101)-C(114)-C(109)	-178.3(2)
C(114)-C(101)-C(102)-C(103)	-172.6(2)	C(11)-N(11)-C(115)-C(103)	-179.4(2)

C(104)-C(103)-C(115)-N(11)	179.1(2)	C(314)-C(301)-C(306)-C(305)	178.5(3)
C(102)-C(103)-C(115)-N(11)	-0.3(4)	C(302)-C(301)-C(306)-C(307)	178.7(3)
C(206)-C(201)-C(202)-O(212)	-178.4(2)	C(314)-C(301)-C(306)-C(307)	-1.0(4)
C(214)-C(201)-C(202)-O(212)	-0.6(3)	C(304)-C(305)-C(306)-C(301)	0.7(4)
C(206)-C(201)-C(202)-C(203)	0.9(3)	C(304)-C(305)-C(306)-C(307)	-179.8(3)
C(214)-C(201)-C(202)-C(203)	178.8(2)	C(301)-C(306)-C(307)-C(308)	0.1(5)
O(212)-C(202)-C(203)-C(204)	179.7(2)	C(305)-C(306)-C(307)-C(308)	-179.4(3)
C(201)-C(202)-C(203)-C(204)	0.3(3)	C(306)-C(307)-C(308)-C(309)	1.3(5)
O(212)-C(202)-C(203)-C(215)	-1.0(3)	C(307)-C(308)-C(309)-C(310)	177.3(3)
C(201)-C(202)-C(203)-C(215)	179.65(19)	C(307)-C(308)-C(309)-C(314)	-1.7(5)
C(202)-C(203)-C(204)-C(205)	-0.5(3)	C(308)-C(309)-C(310)-C(311)	-178.1(4)
C(215)-C(203)-C(204)-C(205)	-179.8(2)	C(314)-C(309)-C(310)-C(311)	1.0(5)
C(203)-C(204)-C(205)-C(206)	-0.7(3)	C(309)-C(310)-C(311)-C(312)	-2.1(6)
C(204)-C(205)-C(206)-C(201)	2.1(3)	C(310)-C(311)-C(312)-C(313)	2.5(6)
C(204)-C(205)-C(206)-C(207)	-176.3(2)	C(311)-C(312)-C(313)-C(314)	-1.8(6)
C(202)-C(201)-C(206)-C(205)	-2.1(3)	C(312)-C(313)-C(314)-C(309)	0.6(5)
C(214)-C(201)-C(206)-C(205)	179.90(19)	C(312)-C(313)-C(314)-C(301)	178.5(3)
C(202)-C(201)-C(206)-C(207)	176.24(19)	C(310)-C(309)-C(314)-C(313)	-0.3(4)
C(214)-C(201)-C(206)-C(207)	-1.7(3)	C(308)-C(309)-C(314)-C(313)	178.8(3)
C(205)-C(206)-C(207)-C(208)	178.1(2)	C(310)-C(309)-C(314)-C(301)	-178.3(3)
C(201)-C(206)-C(207)-C(208)	-0.3(3)	C(308)-C(309)-C(314)-C(301)	0.8(4)
C(206)-C(207)-C(208)-C(209)	1.2(4)	C(306)-C(301)-C(314)-C(313)	-177.3(3)
C(207)-C(208)-C(209)-C(210)	179.2(2)	C(302)-C(301)-C(314)-C(313)	3.0(4)
C(207)-C(208)-C(209)-C(214)	0.0(4)	C(306)-C(301)-C(314)-C(309)	0.5(4)
C(208)-C(209)-C(210)-C(211)	-179.5(3)	C(302)-C(301)-C(314)-C(309)	-179.2(2)
C(214)-C(209)-C(210)-C(211)	-0.4(4)	C(21)-N(21)-C(315)-C(303)	172.7(2)
C(209)-C(210)-C(211)-C(212)	1.5(4)	C(304)-C(303)-C(315)-N(21)	-177.9(3)
C(210)-C(211)-C(212)-C(213)	-1.3(4)	C(302)-C(303)-C(315)-N(21)	-1.2(4)
C(211)-C(212)-C(213)-C(214)	0.0(4)	C(406)-C(401)-C(402)-O(412)	-179.6(2)
C(212)-C(213)-C(214)-C(209)	1.1(4)	C(414)-C(401)-C(402)-O(412)	1.9(4)
C(212)-C(213)-C(214)-C(201)	-178.6(2)	C(406)-C(401)-C(402)-C(403)	1.2(3)
C(210)-C(209)-C(214)-C(213)	-0.9(3)	C(414)-C(401)-C(402)-C(403)	-177.3(2)
C(208)-C(209)-C(214)-C(213)	178.2(2)	O(412)-C(402)-C(403)-C(404)	178.2(2)
C(210)-C(209)-C(214)-C(201)	178.8(2)	C(401)-C(402)-C(403)-C(404)	-2.7(4)
C(208)-C(209)-C(214)-C(201)	-2.1(3)	O(412)-C(402)-C(403)-C(415)	-5.0(3)
C(206)-C(201)-C(214)-C(213)	-177.4(2)	C(401)-C(402)-C(403)-C(415)	174.1(2)
C(202)-C(201)-C(214)-C(213)	4.8(3)	C(402)-C(403)-C(404)-C(405)	1.8(4)
C(206)-C(201)-C(214)-C(209)	2.9(3)	C(415)-C(403)-C(404)-C(405)	-175.1(2)
C(202)-C(201)-C(214)-C(209)	-174.9(2)	C(403)-C(404)-C(405)-C(406)	0.5(4)
C(12)-N(12)-C(215)-C(203)	-172.4(2)	C(404)-C(405)-C(406)-C(407)	176.0(2)
C(204)-C(203)-C(215)-N(12)	178.7(2)	C(404)-C(405)-C(406)-C(401)	-2.0(4)
C(202)-C(203)-C(215)-N(12)	-0.6(3)	C(402)-C(401)-C(406)-C(405)	1.1(3)
C(306)-C(301)-C(302)-O(312)	-179.0(2)	C(414)-C(401)-C(406)-C(405)	179.7(2)
C(314)-C(301)-C(302)-O(312)	0.7(4)	C(402)-C(401)-C(406)-C(407)	-176.9(2)
C(306)-C(301)-C(302)-C(303)	2.1(4)	C(414)-C(401)-C(406)-C(407)	1.7(3)
C(314)-C(301)-C(302)-C(303)	-178.2(2)	C(405)-C(406)-C(407)-C(408)	-178.6(2)
O(312)-C(302)-C(303)-C(304)	179.6(2)	C(401)-C(406)-C(407)-C(408)	-0.5(4)
C(301)-C(302)-C(303)-C(304)	-1.5(4)	C(406)-C(407)-C(408)-C(409)	-0.6(4)
O(312)-C(302)-C(303)-C(315)	2.9(4)	C(407)-C(408)-C(409)-C(410)	-179.6(2)
C(301)-C(302)-C(303)-C(315)	-178.2(2)	C(407)-C(408)-C(409)-C(414)	0.4(4)
C(302)-C(303)-C(304)-C(305)	0.4(4)	C(414)-C(409)-C(410)-C(411)	0.5(4)
C(315)-C(303)-C(304)-C(305)	177.2(3)	C(408)-C(409)-C(410)-C(411)	-179.5(3)
C(303)-C(304)-C(305)-C(306)	0.0(4)	C(409)-C(410)-C(411)-C(412)	-1.1(4)
C(302)-C(301)-C(306)-C(305)	-1.7(4)	C(410)-C(411)-C(412)-C(413)	1.0(5)

C(411)-C(412)-C(413)-C(414)	-0.4(5)	C(402)-C(401)-C(414)-C(409)	176.6(2)
C(410)-C(409)-C(414)-C(413)	0.2(4)	C(406)-C(401)-C(414)-C(409)	-1.9(3)
C(408)-C(409)-C(414)-C(413)	-179.8(2)	C(402)-C(401)-C(414)-C(413)	-2.6(4)
C(410)-C(409)-C(414)-C(401)	-179.1(2)	C(406)-C(401)-C(414)-C(413)	178.9(2)
C(408)-C(409)-C(414)-C(401)	0.8(3)	C(22)-N(22)-C(415)-C(403)	-178.9(2)
C(412)-C(413)-C(414)-C(409)	-0.2(4)	C(404)-C(403)-C(415)-N(22)	179.2(2)
C(412)-C(413)-C(414)-C(401)	179.0(3)	C(402)-C(403)-C(415)-N(22)	2.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for (*rac*)-**33** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(11)-H(11)...O(112)	1.04(3)	1.55(3)	2.521(3)	153(2)
N(12)-H(12)...O(212)	1.10(3)	1.50(3)	2.521(3)	152(2)
N(21)-H(21)...O(312)	1.13(2)	1.49(2)	2.519(2)	149(2)
O(412)-H(22)...N(22)	0.86(3)	1.74(3)	2.547(3)	155(3)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**34**.

Identification code	(*R*)-**34**	
Empirical formula	C50 H32 N2 O2	
Formula weight	692.78	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 11.0977(6) Å	α = 90°.
	b = 16.4934(10) Å	β = 90°.
	c = 18.7071(11) Å	γ = 90°.
Volume	3424.1(3) $Å^3$	
Z	4	
Density (calculated)	1.344 g/cm^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	1448	
Crystal size	0.35 x 0.30 x 0.25 mm^3	
Theta range for data collection	2.13 to 28.28°.	
Index ranges	-14<=h<=14, -21<=k<=21, -24<=l<=24	
Reflections collected	24779	
Independent reflections	4512 [R(int) = 0.0886]	
Completeness to theta = 28.28°	95.6 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4512 / 0 / 494	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0488, wR2 = 0.1102	
R indices (all data)	R1 = 0.0646, wR2 = 0.1182	
Absolute structure parameter	3.0(16)	
Extinction coefficient	0.0085(10)	
Largest diff. peak and hole	0.357 and -0.326 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**34**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(01)	3058(2)	4449(1)	4767(1)	27(1)
C(02)	1888(2)	4292(1)	4550(1)	30(1)
N(02)	1295(2)	4895(1)	4147(1)	33(1)
C(03)	1316(2)	3568(1)	4756(1)	36(1)
C(04)	1876(2)	3030(1)	5183(1)	37(1)
C(05)	3030(2)	3182(1)	5457(1)	32(1)
C(06)	3592(3)	2664(1)	5956(1)	41(1)
C(07)	4705(3)	2831(2)	6212(1)	45(1)
C(08)	5336(3)	3510(2)	5968(1)	44(1)
C(09)	4822(2)	4030(1)	5493(1)	36(1)
C(10)	3642(2)	3894(1)	5235(1)	29(1)
C(11)	3706(2)	5178(1)	4498(1)	28(1)
C(12)	4563(2)	5092(1)	3972(1)	31(1)

N(12)	4781(2)	4297(1)	3729(1)	33(1)
C(13)	5193(2)	5776(1)	3706(1)	40(1)
C(14)	4921(3)	6527(1)	3951(1)	41(1)
C(15)	4040(2)	6646(1)	4482(1)	35(1)
C(16)	3734(3)	7429(1)	4731(1)	43(1)
C(17)	2895(3)	7528(2)	5246(2)	46(1)
C(18)	2340(3)	6855(2)	5553(1)	42(1)
C(19)	2600(2)	6087(1)	5325(1)	36(1)
C(20)	3449(2)	5965(1)	4773(1)	30(1)
C(21)	9(2)	6202(1)	3505(1)	32(1)
O(21)	1005(2)	6385(1)	3861(1)	43(1)
C(22)	-347(2)	5384(1)	3454(1)	33(1)
C(23)	-1367(2)	5183(2)	3046(1)	40(1)
C(24)	-1999(2)	5758(2)	2695(1)	39(1)
C(25)	-1671(2)	6585(2)	2755(1)	35(1)
C(26)	-2364(2)	7174(2)	2379(1)	42(1)
C(27)	-2080(3)	7964(2)	2408(1)	45(1)
C(28)	-1118(3)	8247(2)	2839(1)	39(1)
C(29)	-877(3)	9078(2)	2889(1)	48(1)
C(30)	-5(3)	9366(2)	3318(2)	53(1)
C(31)	672(3)	8834(2)	3727(2)	53(1)
C(32)	487(3)	8015(2)	3687(1)	43(1)
C(33)	-409(2)	7687(1)	3236(1)	35(1)
C(34)	-676(2)	6826(1)	3172(1)	31(1)
C(35)	314(2)	4755(1)	3804(1)	34(1)
C(41)	5158(2)	2641(1)	3418(1)	31(1)
O(41)	4345(2)	2823(1)	3905(1)	38(1)
C(42)	5757(2)	3270(1)	3054(1)	33(1)
C(43)	6627(2)	3076(2)	2531(1)	40(1)
C(44)	6919(3)	2292(2)	2398(1)	43(1)
C(45)	6355(2)	1660(2)	2771(1)	39(1)
C(46)	6731(3)	840(2)	2642(2)	49(1)
C(47)	6216(3)	216(2)	2981(2)	52(1)
C(48)	5271(3)	335(2)	3481(2)	45(1)
C(49)	4744(3)	-334(2)	3825(2)	56(1)
C(50)	3852(3)	-240(2)	4318(2)	61(1)
C(51)	3446(3)	539(2)	4475(2)	53(1)
C(52)	3932(2)	1202(2)	4144(1)	42(1)
C(53)	4867(2)	1130(1)	3641(1)	35(1)
C(54)	5444(2)	1809(1)	3276(1)	33(1)
C(55)	5533(2)	4100(1)	3231(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**34**.

C(01)-C(02)	1.384(3)	N(02)-C(35)	1.285(3)
C(01)-C(10)	1.423(3)	C(03)-C(04)	1.346(3)
C(01)-C(11)	1.488(3)	C(03)-H(03)	0.9400
C(02)-C(03)	1.407(3)	C(04)-C(05)	1.403(4)
C(02)-N(02)	1.411(3)	C(04)-H(04)	0.9400

C(05)-C(06)	1.411(3)	C(32)-H(32)	0.9400
C(05)-C(10)	1.418(3)	C(33)-C(34)	1.456(3)
C(06)-C(07)	1.353(4)	C(35)-H(35)	0.9400
C(06)-H(06)	0.9400	C(41)-O(41)	1.318(3)
C(07)-C(08)	1.397(4)	C(41)-C(42)	1.408(3)
C(07)-H(07)	0.9400	C(41)-C(54)	1.434(3)
C(08)-C(09)	1.361(3)	O(41)-H(41)	1.03(3)
C(08)-H(08)	0.9400	C(42)-C(43)	1.412(3)
C(09)-C(10)	1.414(3)	C(42)-C(55)	1.429(3)
C(09)-H(09)	0.9400	C(43)-C(44)	1.355(4)
C(11)-C(12)	1.375(3)	C(43)-H(43)	0.9400
C(11)-C(20)	1.426(3)	C(44)-C(45)	1.403(4)
C(12)-N(12)	1.408(3)	C(44)-H(44)	0.9400
C(12)-C(13)	1.419(3)	C(45)-C(54)	1.405(3)
N(12)-C(55)	1.293(3)	C(45)-C(46)	1.435(4)
C(13)-C(14)	1.354(3)	C(46)-C(47)	1.338(4)
C(13)-H(13)	0.9400	C(46)-H(46)	0.9400
C(14)-C(15)	1.407(4)	C(47)-C(48)	1.419(4)
C(14)-H(14)	0.9400	C(47)-H(47)	0.9400
C(15)-C(20)	1.410(3)	C(48)-C(49)	1.405(4)
C(15)-C(16)	1.414(3)	C(48)-C(53)	1.418(3)
C(16)-C(17)	1.350(4)	C(49)-C(50)	1.361(5)
C(16)-H(16)	0.9400	C(49)-H(49)	0.9400
C(17)-C(18)	1.393(4)	C(50)-C(51)	1.393(4)
C(17)-H(17)	0.9400	C(50)-H(50)	0.9400
C(18)-C(19)	1.367(3)	C(51)-C(52)	1.367(4)
C(18)-H(18)	0.9400	C(51)-H(51)	0.9400
C(19)-C(20)	1.412(3)	C(52)-C(53)	1.406(4)
C(19)-H(19)	0.9400	C(52)-H(52)	0.9400
C(21)-O(21)	1.325(3)	C(53)-C(54)	1.458(3)
C(21)-C(22)	1.409(3)	C(55)-H(55)	0.9400
C(21)-C(34)	1.424(3)		
O(21)-H(21)	0.99(3)	C(02)-C(01)-C(10)	119.2(2)
C(22)-C(23)	1.404(3)	C(02)-C(01)-C(11)	120.4(2)
C(22)-C(35)	1.429(3)	C(10)-C(01)-C(11)	120.4(2)
C(23)-C(24)	1.349(4)	C(01)-C(02)-C(03)	120.1(2)
C(23)-H(23)	0.9400	C(01)-C(02)-N(02)	117.5(2)
C(24)-C(25)	1.415(4)	C(03)-C(02)-N(02)	122.3(2)
C(24)-H(24)	0.9400	C(35)-N(02)-C(02)	122.4(2)
C(25)-C(34)	1.409(3)	C(04)-C(03)-C(02)	120.9(2)
C(25)-C(26)	1.424(3)	C(04)-C(03)-H(03)	119.5
C(26)-C(27)	1.343(4)	C(02)-C(03)-H(03)	119.5
C(26)-H(26)	0.9400	C(03)-C(04)-C(05)	121.4(2)
C(27)-C(28)	1.417(4)	C(03)-C(04)-H(04)	119.3
C(27)-H(27)	0.9400	C(05)-C(04)-H(04)	119.3
C(28)-C(29)	1.398(4)	C(04)-C(05)-C(06)	122.5(2)
C(28)-C(33)	1.422(3)	C(04)-C(05)-C(10)	118.6(2)
C(29)-C(30)	1.345(4)	C(06)-C(05)-C(10)	119.0(2)
C(29)-H(29)	0.9400	C(07)-C(06)-C(05)	121.0(2)
C(30)-C(31)	1.386(4)	C(07)-C(06)-H(06)	119.5
C(30)-H(30)	0.9400	C(05)-C(06)-H(06)	119.5
C(31)-C(32)	1.369(4)	C(06)-C(07)-C(08)	120.3(2)
C(31)-H(31)	0.9400	C(06)-C(07)-H(07)	119.9
C(32)-C(33)	1.412(4)	C(08)-C(07)-H(07)	119.9

C(09)-C(08)-C(07)	120.6(3)	C(34)-C(25)-C(26)	120.3(2)
C(09)-C(08)-H(08)	119.7	C(24)-C(25)-C(26)	118.6(2)
C(07)-C(08)-H(08)	119.7	C(27)-C(26)-C(25)	121.0(3)
C(08)-C(09)-C(10)	120.7(2)	C(27)-C(26)-H(26)	119.5
C(08)-C(09)-H(09)	119.6	C(25)-C(26)-H(26)	119.5
C(10)-C(09)-H(09)	119.6	C(26)-C(27)-C(28)	121.3(2)
C(09)-C(10)-C(05)	118.4(2)	C(26)-C(27)-H(27)	119.3
C(09)-C(10)-C(01)	122.0(2)	C(28)-C(27)-H(27)	119.3
C(05)-C(10)-C(01)	119.7(2)	C(29)-C(28)-C(27)	120.3(3)
C(12)-C(11)-C(20)	119.3(2)	C(29)-C(28)-C(33)	119.8(3)
C(12)-C(11)-C(01)	119.49(19)	C(27)-C(28)-C(33)	120.0(2)
C(20)-C(11)-C(01)	121.2(2)	C(30)-C(29)-C(28)	121.5(3)
C(11)-C(12)-N(12)	116.5(2)	C(30)-C(29)-H(29)	119.2
C(11)-C(12)-C(13)	120.7(2)	C(28)-C(29)-H(29)	119.2
N(12)-C(12)-C(13)	122.8(2)	C(29)-C(30)-C(31)	119.8(3)
C(55)-N(12)-C(12)	125.4(2)	C(29)-C(30)-H(30)	120.1
C(14)-C(13)-C(12)	119.9(2)	C(31)-C(30)-H(30)	120.1
C(14)-C(13)-H(13)	120.0	C(32)-C(31)-C(30)	120.9(3)
C(12)-C(13)-H(13)	120.0	C(32)-C(31)-H(31)	119.6
C(13)-C(14)-C(15)	121.4(2)	C(30)-C(31)-H(31)	119.6
C(13)-C(14)-H(14)	119.3	C(31)-C(32)-C(33)	121.1(3)
C(15)-C(14)-H(14)	119.3	C(31)-C(32)-H(32)	119.4
C(14)-C(15)-C(20)	119.0(2)	C(33)-C(32)-H(32)	119.4
C(14)-C(15)-C(16)	121.8(2)	C(32)-C(33)-C(28)	116.9(2)
C(20)-C(15)-C(16)	119.2(2)	C(32)-C(33)-C(34)	124.5(2)
C(17)-C(16)-C(15)	120.8(2)	C(28)-C(33)-C(34)	118.6(2)
C(17)-C(16)-H(16)	119.6	C(25)-C(34)-C(21)	117.2(2)
C(15)-C(16)-H(16)	119.6	C(25)-C(34)-C(33)	118.7(2)
C(16)-C(17)-C(18)	120.1(2)	C(21)-C(34)-C(33)	124.1(2)
C(16)-C(17)-H(17)	120.0	N(02)-C(35)-C(22)	122.3(2)
C(18)-C(17)-H(17)	120.0	N(02)-C(35)-H(35)	118.9
C(19)-C(18)-C(17)	121.2(3)	C(22)-C(35)-H(35)	118.9
C(19)-C(18)-H(18)	119.4	O(41)-C(41)-C(42)	119.29(19)
C(17)-C(18)-H(18)	119.4	O(41)-C(41)-C(54)	119.9(2)
C(18)-C(19)-C(20)	120.0(2)	C(42)-C(41)-C(54)	120.8(2)
C(18)-C(19)-H(19)	120.0	C(41)-O(41)-H(41)	106.7(15)
C(20)-C(19)-H(19)	120.0	C(41)-C(42)-C(43)	119.4(2)
C(15)-C(20)-C(19)	118.6(2)	C(41)-C(42)-C(55)	120.8(2)
C(15)-C(20)-C(11)	119.6(2)	C(43)-C(42)-C(55)	119.8(2)
C(19)-C(20)-C(11)	121.8(2)	C(44)-C(43)-C(42)	120.5(2)
O(21)-C(21)-C(22)	119.2(2)	C(44)-C(43)-H(43)	119.8
O(21)-C(21)-C(34)	120.0(2)	C(42)-C(43)-H(43)	119.8
C(22)-C(21)-C(34)	120.8(2)	C(43)-C(44)-C(45)	120.8(2)
C(21)-O(21)-H(21)	107.3(15)	C(43)-C(44)-H(44)	119.6
C(23)-C(22)-C(21)	119.3(2)	C(45)-C(44)-H(44)	119.6
C(23)-C(22)-C(35)	119.5(2)	C(44)-C(45)-C(54)	121.7(2)
C(21)-C(22)-C(35)	121.3(2)	C(44)-C(45)-C(46)	119.1(2)
C(24)-C(23)-C(22)	121.2(2)	C(54)-C(45)-C(46)	119.2(3)
C(24)-C(23)-H(23)	119.4	C(47)-C(46)-C(45)	121.3(3)
C(22)-C(23)-H(23)	119.4	C(47)-C(46)-H(46)	119.3
C(23)-C(24)-C(25)	120.3(2)	C(45)-C(46)-H(46)	119.3
C(23)-C(24)-H(24)	119.8	C(46)-C(47)-C(48)	121.5(2)
C(25)-C(24)-H(24)	119.8	C(46)-C(47)-H(47)	119.3
C(34)-C(25)-C(24)	121.1(2)	C(48)-C(47)-H(47)	119.3

C(49)-C(48)-C(53)	119.9(3)	C(51)-C(52)-C(53)	121.8(2)
C(49)-C(48)-C(47)	120.1(3)	C(51)-C(52)-H(52)	119.1
C(53)-C(48)-C(47)	120.0(3)	C(53)-C(52)-H(52)	119.1
C(50)-C(49)-C(48)	121.6(3)	C(52)-C(53)-C(48)	116.9(2)
C(50)-C(49)-H(49)	119.2	C(52)-C(53)-C(54)	124.9(2)
C(48)-C(49)-H(49)	119.2	C(48)-C(53)-C(54)	118.2(2)
C(49)-C(50)-C(51)	118.9(3)	C(45)-C(54)-C(41)	116.8(2)
C(49)-C(50)-H(50)	120.6	C(45)-C(54)-C(53)	119.7(2)
C(51)-C(50)-H(50)	120.6	C(41)-C(54)-C(53)	123.4(2)
C(52)-C(51)-C(50)	121.0(3)	N(12)-C(55)-C(42)	121.4(2)
C(52)-C(51)-H(51)	119.5	N(12)-C(55)-H(55)	119.3
C(50)-C(51)-H(51)	119.5	C(42)-C(55)-H(55)	119.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**34**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(01)	29(1)	24(1)	28(1)	-3(1)	3(1)	1(1)
C(02)	31(1)	29(1)	30(1)	0(1)	4(1)	1(1)
N(02)	26(1)	36(1)	36(1)	2(1)	0(1)	-1(1)
C(03)	30(1)	41(1)	37(1)	-1(1)	1(1)	-6(1)
C(04)	41(1)	32(1)	39(1)	2(1)	7(1)	-8(1)
C(05)	37(1)	31(1)	30(1)	-1(1)	6(1)	3(1)
C(06)	55(2)	30(1)	38(1)	7(1)	6(1)	5(1)
C(07)	57(2)	39(1)	39(1)	7(1)	-4(1)	13(1)
C(08)	42(2)	46(1)	44(1)	0(1)	-10(1)	6(1)
C(09)	37(1)	33(1)	38(1)	-1(1)	-5(1)	1(1)
C(10)	33(1)	26(1)	28(1)	-3(1)	2(1)	3(1)
C(11)	26(1)	25(1)	32(1)	1(1)	-3(1)	0(1)
C(12)	31(1)	26(1)	37(1)	-3(1)	-2(1)	-1(1)
N(12)	32(1)	28(1)	37(1)	-3(1)	2(1)	-1(1)
C(13)	39(1)	35(1)	47(1)	-1(1)	7(1)	-8(1)
C(14)	43(2)	27(1)	52(1)	2(1)	2(1)	-10(1)
C(15)	38(1)	27(1)	41(1)	-1(1)	-7(1)	0(1)
C(16)	51(2)	25(1)	52(2)	-4(1)	-7(1)	0(1)
C(17)	58(2)	28(1)	52(2)	-8(1)	-6(2)	7(1)
C(18)	43(2)	40(1)	43(1)	-10(1)	-4(1)	9(1)
C(19)	38(1)	33(1)	38(1)	-3(1)	-2(1)	2(1)
C(20)	29(1)	28(1)	33(1)	-1(1)	-6(1)	2(1)
C(21)	27(1)	40(1)	31(1)	-2(1)	-1(1)	-2(1)
O(21)	33(1)	40(1)	56(1)	6(1)	-17(1)	-5(1)
C(22)	27(1)	37(1)	36(1)	-1(1)	-1(1)	-1(1)
C(23)	32(1)	41(1)	46(1)	-4(1)	-4(1)	-8(1)
C(24)	28(1)	46(1)	41(1)	-4(1)	-5(1)	-3(1)
C(25)	27(1)	45(1)	34(1)	-1(1)	2(1)	3(1)
C(26)	31(1)	54(2)	41(1)	0(1)	-2(1)	10(1)
C(27)	41(2)	52(2)	43(1)	1(1)	-1(1)	18(1)

C(28)	42(2)	41(1)	34(1)	1(1)	8(1)	8(1)
C(29)	61(2)	41(1)	43(1)	3(1)	15(1)	10(1)
C(30)	71(2)	37(1)	51(2)	-4(1)	18(2)	-1(2)
C(31)	60(2)	49(2)	50(2)	-10(1)	2(2)	-9(2)
C(32)	44(2)	42(1)	41(1)	-3(1)	1(1)	-3(1)
C(33)	34(1)	37(1)	33(1)	-2(1)	6(1)	1(1)
C(34)	26(1)	36(1)	31(1)	-2(1)	3(1)	2(1)
C(35)	30(1)	33(1)	39(1)	-2(1)	0(1)	0(1)
C(41)	27(1)	33(1)	33(1)	-5(1)	-3(1)	1(1)
O(41)	38(1)	30(1)	46(1)	-5(1)	12(1)	0(1)
C(42)	31(1)	34(1)	34(1)	-5(1)	1(1)	2(1)
C(43)	38(1)	45(2)	37(1)	-4(1)	6(1)	0(1)
C(44)	40(2)	50(2)	39(1)	-8(1)	5(1)	6(1)
C(45)	38(2)	41(1)	39(1)	-11(1)	-7(1)	6(1)
C(46)	49(2)	45(2)	53(2)	-15(1)	-3(1)	15(1)
C(47)	53(2)	37(1)	65(2)	-12(1)	-9(2)	14(1)
C(48)	44(2)	34(1)	58(2)	-6(1)	-17(1)	5(1)
C(49)	50(2)	29(1)	89(2)	4(1)	-13(2)	2(1)
C(50)	49(2)	37(2)	97(2)	13(2)	-7(2)	-5(1)
C(51)	45(2)	42(2)	71(2)	10(1)	-2(2)	-3(1)
C(52)	39(2)	30(1)	57(2)	2(1)	-4(1)	-1(1)
C(53)	31(1)	29(1)	46(1)	-3(1)	-10(1)	0(1)
C(54)	32(1)	33(1)	34(1)	-6(1)	-7(1)	5(1)
C(55)	30(1)	35(1)	36(1)	2(1)	0(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**34**.

	x	y	z	U(eq)
H(03)	531	3458	4592	43
H(04)	1485	2542	5300	45
H(06)	3187	2196	6113	49
H(07)	5056	2488	6556	54
H(08)	6122	3608	6134	53
H(09)	5256	4485	5334	43
H(13)	5799	5709	3360	48
H(14)	5329	6978	3762	49
H(16)	4119	7885	4536	51
H(17)	2684	8053	5398	55
H(18)	1778	6930	5922	51
H(19)	2213	5640	5536	44
H(21)	1360(30)	5869(16)	4032(14)	43
H(23)	-1613	4639	3016	48
H(24)	-2660	5609	2410	46
H(26)	-3030	7006	2106	50
H(27)	-2530	8338	2138	54
H(29)	-1336	9443	2615	58
H(30)	144	9926	3342	63

H(31)	1268	9038	4036	63
H(32)	964	7665	3964	51
H(35)	21	4221	3783	41
H(41)	4360(30)	3447(17)	3960(13)	45
H(43)	7008	3493	2273	48
H(44)	7505	2171	2052	52
H(46)	7351	740	2311	59
H(47)	6487	-313	2887	62
H(49)	5014	-859	3713	67
H(50)	3515	-693	4547	73
H(51)	2829	610	4813	63
H(52)	3633	1720	4256	51
H(55)	5941	4510	2980	40

Table 6. Torsion angles [°] for (*R*)-**34**.

C(10)-C(01)-C(02)-C(03)	-3.9(3)	C(01)-C(11)-C(12)-C(13)	179.9(2)
C(11)-C(01)-C(02)-C(03)	174.54(19)	C(11)-C(12)-N(12)-C(55)	178.7(2)
C(10)-C(01)-C(02)-N(02)	173.57(18)	C(13)-C(12)-N(12)-C(55)	-2.2(4)
C(11)-C(01)-C(02)-N(02)	-7.9(3)	C(11)-C(12)-C(13)-C(14)	-2.5(4)
C(01)-C(02)-N(02)-C(35)	166.1(2)	N(12)-C(12)-C(13)-C(14)	178.5(2)
C(03)-C(02)-N(02)-C(35)	-16.4(3)	C(12)-C(13)-C(14)-C(15)	1.6(4)
C(01)-C(02)-C(03)-C(04)	2.2(3)	C(13)-C(14)-C(15)-C(20)	1.3(4)
N(02)-C(02)-C(03)-C(04)	-175.2(2)	C(13)-C(14)-C(15)-C(16)	-178.8(3)
C(02)-C(03)-C(04)-C(05)	2.1(4)	C(14)-C(15)-C(16)-C(17)	-179.3(2)
C(03)-C(04)-C(05)-C(06)	174.2(2)	C(20)-C(15)-C(16)-C(17)	0.6(4)
C(03)-C(04)-C(05)-C(10)	-4.4(3)	C(15)-C(16)-C(17)-C(18)	1.7(4)
C(04)-C(05)-C(06)-C(07)	-179.7(2)	C(16)-C(17)-C(18)-C(19)	-2.2(4)
C(10)-C(05)-C(06)-C(07)	-1.2(3)	C(17)-C(18)-C(19)-C(20)	0.4(4)
C(05)-C(06)-C(07)-C(08)	-2.0(4)	C(14)-C(15)-C(20)-C(19)	177.6(2)
C(06)-C(07)-C(08)-C(09)	2.7(4)	C(16)-C(15)-C(20)-C(19)	-2.3(3)
C(07)-C(08)-C(09)-C(10)	-0.2(4)	C(14)-C(15)-C(20)-C(11)	-3.4(3)
C(08)-C(09)-C(10)-C(05)	-3.0(3)	C(16)-C(15)-C(20)-C(11)	176.7(2)
C(08)-C(09)-C(10)-C(01)	176.7(2)	C(18)-C(19)-C(20)-C(15)	1.8(4)
C(04)-C(05)-C(10)-C(09)	-177.8(2)	C(18)-C(19)-C(20)-C(11)	-177.2(2)
C(06)-C(05)-C(10)-C(09)	3.6(3)	C(12)-C(11)-C(20)-C(15)	2.5(3)
C(04)-C(05)-C(10)-C(01)	2.5(3)	C(01)-C(11)-C(20)-C(15)	-176.9(2)
C(06)-C(05)-C(10)-C(01)	-176.1(2)	C(12)-C(11)-C(20)-C(19)	-178.4(2)
C(02)-C(01)-C(10)-C(09)	-178.1(2)	C(01)-C(11)-C(20)-C(19)	2.1(3)
C(11)-C(01)-C(10)-C(09)	3.4(3)	O(21)-C(21)-C(22)-C(23)	-176.7(2)
C(02)-C(01)-C(10)-C(05)	1.6(3)	C(34)-C(21)-C(22)-C(23)	2.3(3)
C(11)-C(01)-C(10)-C(05)	-176.92(19)	O(21)-C(21)-C(22)-C(35)	2.9(3)
C(02)-C(01)-C(11)-C(12)	-103.1(3)	C(34)-C(21)-C(22)-C(35)	-178.1(2)
C(10)-C(01)-C(11)-C(12)	75.3(3)	C(21)-C(22)-C(23)-C(24)	0.9(4)
C(02)-C(01)-C(11)-C(20)	76.3(3)	C(35)-C(22)-C(23)-C(24)	-178.6(2)
C(10)-C(01)-C(11)-C(20)	-105.2(2)	C(22)-C(23)-C(24)-C(25)	-2.5(4)
C(20)-C(11)-C(12)-N(12)	179.5(2)	C(23)-C(24)-C(25)-C(34)	0.8(4)
C(01)-C(11)-C(12)-N(12)	-1.0(3)	C(23)-C(24)-C(25)-C(26)	-179.8(2)
C(20)-C(11)-C(12)-C(13)	0.4(3)	C(34)-C(25)-C(26)-C(27)	0.5(4)

C(24)-C(25)-C(26)-C(27)	-178.9(3)	C(55)-C(42)-C(43)-C(44)	174.7(2)
C(25)-C(26)-C(27)-C(28)	-2.9(4)	C(42)-C(43)-C(44)-C(45)	0.6(4)
C(26)-C(27)-C(28)-C(29)	-176.8(3)	C(43)-C(44)-C(45)-C(54)	2.2(4)
C(26)-C(27)-C(28)-C(33)	1.8(4)	C(43)-C(44)-C(45)-C(46)	-176.9(3)
C(27)-C(28)-C(29)-C(30)	176.9(2)	C(44)-C(45)-C(46)-C(47)	-179.6(3)
C(33)-C(28)-C(29)-C(30)	-1.7(4)	C(54)-C(45)-C(46)-C(47)	1.3(4)
C(28)-C(29)-C(30)-C(31)	-0.3(4)	C(45)-C(46)-C(47)-C(48)	0.4(4)
C(29)-C(30)-C(31)-C(32)	1.6(4)	C(46)-C(47)-C(48)-C(49)	179.6(3)
C(30)-C(31)-C(32)-C(33)	-0.8(4)	C(46)-C(47)-C(48)-C(53)	-1.2(4)
C(31)-C(32)-C(33)-C(28)	-1.2(4)	C(53)-C(48)-C(49)-C(50)	-0.5(4)
C(31)-C(32)-C(33)-C(34)	-178.9(3)	C(47)-C(48)-C(49)-C(50)	178.7(3)
C(29)-C(28)-C(33)-C(32)	2.4(3)	C(48)-C(49)-C(50)-C(51)	0.8(5)
C(27)-C(28)-C(33)-C(32)	-176.2(2)	C(49)-C(50)-C(51)-C(52)	-0.1(5)
C(29)-C(28)-C(33)-C(34)	-179.7(2)	C(50)-C(51)-C(52)-C(53)	-0.8(4)
C(27)-C(28)-C(33)-C(34)	1.7(3)	C(51)-C(52)-C(53)-C(48)	1.1(4)
C(24)-C(25)-C(34)-C(21)	2.4(3)	C(51)-C(52)-C(53)-C(54)	-178.9(3)
C(26)-C(25)-C(34)-C(21)	-177.1(2)	C(49)-C(48)-C(53)-C(52)	-0.5(4)
C(24)-C(25)-C(34)-C(33)	-177.7(2)	C(47)-C(48)-C(53)-C(52)	-179.7(2)
C(26)-C(25)-C(34)-C(33)	2.9(3)	C(49)-C(48)-C(53)-C(54)	179.5(2)
O(21)-C(21)-C(34)-C(25)	175.1(2)	C(47)-C(48)-C(53)-C(54)	0.3(4)
C(22)-C(21)-C(34)-C(25)	-3.9(3)	C(44)-C(45)-C(54)-C(41)	-3.0(3)
O(21)-C(21)-C(34)-C(33)	-4.9(3)	C(46)-C(45)-C(54)-C(41)	176.1(2)
C(22)-C(21)-C(34)-C(33)	176.2(2)	C(44)-C(45)-C(54)-C(53)	178.8(2)
C(32)-C(33)-C(34)-C(25)	173.8(2)	C(46)-C(45)-C(54)-C(53)	-2.1(3)
C(28)-C(33)-C(34)-C(25)	-3.9(3)	O(41)-C(41)-C(54)-C(45)	-177.5(2)
C(32)-C(33)-C(34)-C(21)	-6.2(4)	C(42)-C(41)-C(54)-C(45)	1.1(3)
C(28)-C(33)-C(34)-C(21)	176.1(2)	O(41)-C(41)-C(54)-C(53)	0.7(3)
C(02)-N(02)-C(35)-C(22)	173.8(2)	C(42)-C(41)-C(54)-C(53)	179.2(2)
C(23)-C(22)-C(35)-N(02)	175.5(2)	C(52)-C(53)-C(54)-C(45)	-178.7(2)
C(21)-C(22)-C(35)-N(02)	-4.0(4)	C(48)-C(53)-C(54)-C(45)	1.3(3)
O(41)-C(41)-C(42)-C(43)	-179.9(2)	C(52)-C(53)-C(54)-C(41)	3.2(4)
C(54)-C(41)-C(42)-C(43)	1.5(3)	C(48)-C(53)-C(54)-C(41)	-176.7(2)
O(41)-C(41)-C(42)-C(55)	3.0(3)	C(12)-N(12)-C(55)-C(42)	175.5(2)
C(54)-C(41)-C(42)-C(55)	-175.6(2)	C(41)-C(42)-C(55)-N(12)	0.2(4)
C(41)-C(42)-C(43)-C(44)	-2.4(4)	C(43)-C(42)-C(55)-N(12)	-176.9(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for (*R*)-**34** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(21)-H(21)...N(02)	0.99(3)	1.62(3)	2.536(2)	151(2)
O(41)-H(41)...N(12)	1.03(3)	1.54(3)	2.501(2)	152(2)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**38**.

Identification code	(*R*)-**38**	
Empirical formula	C59 H38 Cl2 N2 O2	
Formula weight	877.81	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.8321(14) Å	α= 90°.
	b = 11.5748(18) Å	β= 90°.
	c = 42.316(7) Å	γ = 90°.
Volume	4325.9(12) $Å^3$	
Z	4	
Density (calculated)	1.348 g/cm^3	
Absorption coefficient	0.200 mm^{-1}	
F(000)	1824	
Crystal size	0.05 x 0.15 x 0.22 mm^3	
Theta range for data collection	2.28 to 25.71°.	
Index ranges	-10<=h<=10, -13<=k<=14, -50<=l<=47	
Reflections collected	24399	
Independent reflections	7579 [R(int) = 0.0467]	
Completeness to theta = 25.71°	94.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7579 / 3 / 608	
Goodness-of-fit on F^2	1.353	
Final R indices [I>2sigma(I)]	R1 = 0.0928, wR2 = 0.1882	
R indices (all data)	R1 = 0.0957, wR2 = 0.1896	
Absolute structure parameter	0.04(17)	
Largest diff. peak and hole	0.299 and -0.332 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**38**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	6930(30)	1477(14)	5849(4)	58(5)
Cl(1A)	8058(4)	2717(3)	5926(1)	54(1)
Cl(2A)	6246(11)	914(7)	6199(2)	71(2)
C(1B)	6450(40)	1093(15)	5876(4)	58(5)
Cl(1B)	6885(13)	2344(4)	5663(2)	159(5)
Cl(2B)	6536(11)	1256(9)	6272(2)	77(3)
C(101)	9939(6)	7925(4)	4249(1)	29(1)
C(102)	9001(6)	7483(4)	4002(1)	24(1)
O(102)	8607(4)	6385(3)	4006(1)	28(1)
C(103)	8506(6)	8227(4)	3761(1)	24(1)
C(104)	8982(6)	9389(4)	3750(1)	26(1)
C(105)	9939(7)	9788(4)	3976(1)	32(1)
C(106)	10410(6)	9091(4)	4228(1)	32(1)
C(107)	11393(7)	9565(5)	4467(1)	36(1)
C(108)	11831(6)	8952(5)	4716(1)	33(1)

C(109)	11338(6)	7789(5)	4761(1)	32(1)
C(110)	11733(7)	7195(5)	5031(1)	38(1)
C(111)	11302(7)	6050(5)	5089(1)	39(1)
C(112)	11681(8)	5441(6)	5367(2)	51(2)
C(113)	11228(9)	4329(6)	5409(1)	58(2)
C(114)	10340(8)	3772(5)	5178(2)	48(2)
C(115)	9945(8)	4340(5)	4909(1)	43(2)
C(116)	10401(7)	5507(5)	4856(1)	34(1)
C(117)	9973(6)	6090(5)	4583(1)	32(1)
C(118)	10393(5)	7230(4)	4528(1)	25(1)
C(119)	7519(5)	7781(4)	3511(1)	21(1)
N(119)	7166(4)	6701(3)	3505(1)	19(1)
C(120)	4663(6)	4573(4)	3120(1)	23(1)
C(121)	5672(5)	5117(4)	3338(1)	21(1)
C(122)	6211(5)	6195(4)	3269(1)	21(1)
C(123)	5897(6)	6739(4)	2982(1)	23(1)
C(124)	4968(5)	6231(4)	2767(1)	21(1)
C(125)	4313(5)	5140(4)	2831(1)	25(1)
C(126)	3319(5)	4595(4)	2616(1)	28(1)
C(127)	2714(6)	3543(4)	2681(2)	35(1)
C(128)	3046(6)	2979(4)	2963(1)	32(1)
C(129)	4011(6)	3476(4)	3177(1)	26(1)
C(201)	8660(5)	2292(4)	2367(1)	19(1)
C(202)	8320(5)	2640(4)	2678(1)	21(1)
O(202)	7358(4)	3520(3)	2727(1)	21(1)
C(203)	8930(6)	2091(4)	2943(1)	21(1)
C(204)	9946(6)	1145(4)	2894(1)	25(1)
C(205)	10283(5)	788(4)	2596(1)	21(1)
C(206)	9648(5)	1334(4)	2332(1)	24(1)
C(207)	9988(6)	894(4)	2023(1)	28(1)
C(208)	9375(5)	1350(4)	1764(1)	24(1)
C(209)	8349(6)	2312(5)	1782(1)	29(1)
C(210)	7725(6)	2758(5)	1506(1)	30(1)
C(211)	6719(6)	3693(4)	1509(1)	29(1)
C(212)	6029(6)	4145(5)	1230(1)	38(1)
C(213)	5085(7)	5054(5)	1246(1)	36(1)
C(214)	4749(6)	5571(4)	1539(1)	32(1)
C(215)	5362(6)	5177(4)	1811(1)	31(1)
C(216)	6381(6)	4201(4)	1804(1)	26(1)
C(217)	7026(5)	3760(4)	2081(1)	20(1)
C(218)	7995(5)	2825(4)	2083(1)	21(1)
C(219)	8581(6)	2434(4)	3260(1)	23(1)
N(219)	7624(4)	3252(3)	3318(1)	18(1)
C(220)	5597(6)	4891(4)	3938(1)	28(1)
C(221)	6135(6)	4506(4)	3636(1)	25(1)
C(222)	7140(6)	3589(4)	3622(1)	23(1)
C(223)	7606(7)	3012(4)	3898(1)	27(1)
C(224)	7105(7)	3384(4)	4186(1)	33(1)
C(225)	6085(7)	4325(5)	4214(1)	33(1)
C(226)	5605(7)	4727(5)	4513(1)	44(2)
C(227)	4647(7)	5642(6)	4538(1)	44(2)
C(228)	4160(7)	6200(5)	4260(1)	41(2)
C(229)	4606(6)	5835(5)	3973(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**38**.

C(1A)-Cl(2A)	1.727(13)	C(123)-C(124)	1.358(7)
C(1A)-Cl(1A)	1.777(16)	C(123)-H(123)	0.9500
C(1A)-H(1A)	0.9900	C(124)-C(125)	1.415(7)
C(1A)-H(1B)	0.9900	C(124)-H(124)	0.9500
C(1B)-Cl(2B)	1.689(14)	C(125)-C(126)	1.412(7)
C(1B)-Cl(1B)	1.749(15)	C(126)-C(127)	1.357(8)
C(1B)-H(1C)	0.9900	C(126)-H(126)	0.9500
C(1B)-H(1D)	0.9900	C(127)-C(128)	1.391(8)
C(101)-C(106)	1.415(7)	C(127)-H(127)	0.9500
C(101)-C(102)	1.429(7)	C(128)-C(129)	1.371(7)
C(101)-C(118)	1.485(7)	C(128)-H(128)	0.9500
C(102)-O(102)	1.318(5)	C(129)-H(129)	0.9500
C(102)-C(103)	1.404(7)	C(201)-C(202)	1.408(7)
O(102)-H(102)	0.8400	C(201)-C(206)	1.419(7)
C(103)-C(104)	1.409(7)	C(201)-C(218)	1.472(7)
C(103)-C(119)	1.465(7)	C(202)-O(202)	1.343(5)
C(104)-C(105)	1.357(7)	C(202)-C(203)	1.399(7)
C(104)-H(104)	0.9500	O(202)-H(202)	0.8400
C(105)-C(106)	1.400(8)	C(203)-C(204)	1.431(7)
C(105)-H(105)	0.9500	C(203)-C(219)	1.434(7)
C(106)-C(107)	1.442(7)	C(204)-C(205)	1.361(7)
C(107)-C(108)	1.329(8)	C(204)-H(204)	0.9500
C(107)-H(107)	0.9500	C(205)-C(206)	1.399(7)
C(108)-C(109)	1.427(8)	C(205)-H(205)	0.9500
C(108)-H(108)	0.9500	C(206)-C(207)	1.435(7)
C(109)-C(110)	1.381(8)	C(207)-C(208)	1.331(7)
C(109)-C(118)	1.443(7)	C(207)-H(207)	0.9500
C(110)-C(111)	1.400(9)	C(208)-C(209)	1.438(7)
C(110)-H(110)	0.9500	C(208)-H(208)	0.9500
C(111)-C(112)	1.410(8)	C(209)-C(210)	1.390(7)
C(111)-C(116)	1.414(8)	C(209)-C(218)	1.438(7)
C(112)-C(113)	1.360(10)	C(210)-C(211)	1.400(7)
C(112)-H(112)	0.9500	C(210)-H(210)	0.9500
C(113)-C(114)	1.409(10)	C(211)-C(216)	1.413(7)
C(113)-H(113)	0.9500	C(211)-C(212)	1.428(8)
C(114)-C(115)	1.362(8)	C(212)-C(213)	1.344(8)
C(114)-H(114)	0.9500	C(212)-H(212)	0.9500
C(115)-C(116)	1.426(8)	C(213)-C(214)	1.408(8)
C(115)-H(115)	0.9500	C(213)-H(213)	0.9500
C(116)-C(117)	1.391(7)	C(214)-C(215)	1.353(7)
C(117)-C(118)	1.389(7)	C(214)-H(214)	0.9500
C(117)-H(117)	0.9500	C(215)-C(216)	1.445(7)
C(119)-N(119)	1.289(6)	C(215)-H(215)	0.9500
C(119)-H(119)	0.9500	C(216)-C(217)	1.399(7)
N(119)-C(122)	1.432(6)	C(217)-C(218)	1.380(7)
C(120)-C(129)	1.416(7)	C(217)-H(217)	0.9500
C(120)-C(125)	1.423(7)	C(219)-N(219)	1.292(6)
C(120)-C(121)	1.428(7)	C(219)-H(219)	0.9500
C(121)-C(122)	1.367(7)	N(219)-C(222)	1.412(6)
C(121)-C(221)	1.504(7)	C(220)-C(225)	1.406(8)
C(122)-C(123)	1.398(7)	C(220)-C(229)	1.408(7)

C(220)-C(221)	1.433(7)	C(110)-C(109)-C(118)	119.2(5)
C(221)-C(222)	1.384(7)	C(108)-C(109)-C(118)	120.6(5)
C(222)-C(223)	1.407(7)	C(109)-C(110)-C(111)	123.2(5)
C(223)-C(224)	1.367(7)	C(109)-C(110)-H(110)	118.4
C(223)-H(223)	0.9500	C(111)-C(110)-H(110)	118.4
C(224)-C(225)	1.418(8)	C(110)-C(111)-C(112)	123.6(6)
C(224)-H(224)	0.9500	C(110)-C(111)-C(116)	116.9(5)
C(225)-C(226)	1.415(8)	C(112)-C(111)-C(116)	119.5(6)
C(226)-C(227)	1.360(9)	C(113)-C(112)-C(111)	120.9(6)
C(226)-H(226)	0.9500	C(113)-C(112)-H(112)	119.6
C(227)-C(228)	1.410(9)	C(111)-C(112)-H(112)	119.6
C(227)-H(227)	0.9500	C(112)-C(113)-C(114)	120.4(6)
C(228)-C(229)	1.346(7)	C(112)-C(113)-H(113)	119.8
C(228)-H(228)	0.9500	C(114)-C(113)-H(113)	119.8
C(229)-H(230)	0.9500	C(115)-C(114)-C(113)	120.1(6)
		C(115)-C(114)-H(114)	119.9
Cl(2A)-C(1A)-Cl(1A)	110.2(9)	C(113)-C(114)-H(114)	119.9
Cl(2A)-C(1A)-H(1A)	109.6	C(114)-C(115)-C(116)	121.0(6)
Cl(1A)-C(1A)-H(1A)	109.6	C(114)-C(115)-H(115)	119.5
Cl(2A)-C(1A)-H(1B)	109.6	C(116)-C(115)-H(115)	119.5
Cl(1A)-C(1A)-H(1B)	109.6	C(117)-C(116)-C(111)	121.1(6)
H(1A)-C(1A)-H(1B)	108.1	C(117)-C(116)-C(115)	120.8(6)
Cl(2B)-C(1B)-Cl(1B)	114.1(10)	C(111)-C(116)-C(115)	118.1(5)
Cl(2B)-C(1B)-H(1C)	108.7	C(118)-C(117)-C(116)	121.7(5)
Cl(1B)-C(1B)-H(1C)	108.7	C(118)-C(117)-H(117)	119.1
Cl(2B)-C(1B)-H(1D)	108.7	C(116)-C(117)-H(117)	119.1
Cl(1B)-C(1B)-H(1D)	108.7	C(117)-C(118)-C(109)	117.8(5)
H(1C)-C(1B)-H(1D)	107.6	C(117)-C(118)-C(101)	125.1(5)
C(106)-C(101)-C(102)	117.7(5)	C(109)-C(118)-C(101)	117.1(5)
C(106)-C(101)-C(118)	119.3(5)	N(119)-C(119)-C(103)	120.0(4)
C(102)-C(101)-C(118)	123.0(5)	N(119)-C(119)-H(119)	120.0
O(102)-C(102)-C(103)	121.2(4)	C(103)-C(119)-H(119)	120.0
O(102)-C(102)-C(101)	119.4(4)	C(119)-N(119)-C(122)	123.5(4)
C(103)-C(102)-C(101)	119.5(4)	C(129)-C(120)-C(125)	118.2(5)
C(102)-O(102)-H(102)	109.5	C(129)-C(120)-C(121)	122.6(5)
C(102)-C(103)-C(104)	121.1(5)	C(125)-C(120)-C(121)	119.2(4)
C(102)-C(103)-C(119)	119.5(4)	C(122)-C(121)-C(120)	118.9(4)
C(104)-C(103)-C(119)	119.3(5)	C(122)-C(121)-C(221)	120.8(4)
C(105)-C(104)-C(103)	119.1(5)	C(120)-C(121)-C(221)	120.3(4)
C(105)-C(104)-H(104)	120.4	C(121)-C(122)-C(123)	121.8(5)
C(103)-C(104)-H(104)	120.4	C(121)-C(122)-N(119)	115.5(4)
C(104)-C(105)-C(106)	121.7(5)	C(123)-C(122)-N(119)	122.7(4)
C(104)-C(105)-H(105)	119.2	C(124)-C(123)-C(122)	120.5(4)
C(106)-C(105)-H(105)	119.2	C(124)-C(123)-H(123)	119.7
C(105)-C(106)-C(101)	120.7(5)	C(122)-C(123)-H(123)	119.7
C(105)-C(106)-C(107)	119.6(5)	C(123)-C(124)-C(125)	120.4(5)
C(101)-C(106)-C(107)	119.6(5)	C(123)-C(124)-H(124)	119.8
C(108)-C(107)-C(106)	122.0(5)	C(125)-C(124)-H(124)	119.8
C(108)-C(107)-H(107)	119.0	C(126)-C(125)-C(124)	122.1(5)
C(106)-C(107)-H(107)	119.0	C(126)-C(125)-C(120)	118.9(5)
C(107)-C(108)-C(109)	121.3(5)	C(124)-C(125)-C(120)	119.1(4)
C(107)-C(108)-H(108)	119.3	C(127)-C(126)-C(125)	121.0(5)
C(109)-C(108)-H(108)	119.3	C(127)-C(126)-H(126)	119.5
C(110)-C(109)-C(108)	120.1(5)	C(125)-C(126)-H(126)	119.5

C(126)-C(127)-C(128)	120.8(5)	C(215)-C(214)-C(213)	121.5(5)
C(126)-C(127)-H(127)	119.6	C(215)-C(214)-H(214)	119.3
C(128)-C(127)-H(127)	119.6	C(213)-C(214)-H(214)	119.3
C(129)-C(128)-C(127)	120.1(5)	C(214)-C(215)-C(216)	119.7(5)
C(129)-C(128)-H(128)	120.0	C(214)-C(215)-H(215)	120.1
C(127)-C(128)-H(128)	120.0	C(216)-C(215)-H(215)	120.1
C(128)-C(129)-C(120)	121.1(5)	C(217)-C(216)-C(211)	120.1(5)
C(128)-C(129)-H(129)	119.5	C(217)-C(216)-C(215)	121.5(5)
C(120)-C(129)-H(129)	119.5	C(211)-C(216)-C(215)	118.3(5)
C(202)-C(201)-C(206)	116.8(4)	C(218)-C(217)-C(216)	123.0(5)
C(202)-C(201)-C(218)	123.9(4)	C(218)-C(217)-H(217)	118.5
C(206)-C(201)-C(218)	119.2(4)	C(216)-C(217)-H(217)	118.5
O(202)-C(202)-C(203)	117.7(4)	C(217)-C(218)-C(209)	116.9(5)
O(202)-C(202)-C(201)	119.8(4)	C(217)-C(218)-C(201)	125.5(4)
C(203)-C(202)-C(201)	122.5(4)	C(209)-C(218)-C(201)	117.5(4)
C(202)-O(202)-H(202)	109.5	N(219)-C(219)-C(203)	121.3(4)
C(202)-C(203)-C(204)	118.2(4)	N(219)-C(219)-H(219)	119.4
C(202)-C(203)-C(219)	122.9(4)	C(203)-C(219)-H(219)	119.4
C(204)-C(203)-C(219)	118.9(4)	C(219)-N(219)-C(222)	124.9(4)
C(205)-C(204)-C(203)	120.3(4)	C(225)-C(220)-C(229)	117.7(5)
C(205)-C(204)-H(204)	119.9	C(225)-C(220)-C(221)	119.5(5)
C(203)-C(204)-H(204)	119.9	C(229)-C(220)-C(221)	122.7(5)
C(204)-C(205)-C(206)	120.9(4)	C(222)-C(221)-C(220)	119.3(5)
C(204)-C(205)-H(205)	119.5	C(222)-C(221)-C(121)	119.9(5)
C(206)-C(205)-H(205)	119.5	C(220)-C(221)-C(121)	120.7(4)
C(205)-C(206)-C(201)	121.1(4)	C(221)-C(222)-C(223)	121.1(5)
C(205)-C(206)-C(207)	118.8(5)	C(221)-C(222)-N(219)	116.4(4)
C(201)-C(206)-C(207)	120.1(5)	C(223)-C(222)-N(219)	122.5(5)
C(208)-C(207)-C(206)	121.5(5)	C(224)-C(223)-C(222)	119.7(5)
C(208)-C(207)-H(207)	119.2	C(224)-C(223)-H(223)	120.1
C(206)-C(207)-H(207)	119.2	C(222)-C(223)-H(223)	120.1
C(207)-C(208)-C(209)	121.4(5)	C(223)-C(224)-C(225)	121.4(5)
C(207)-C(208)-H(208)	119.3	C(223)-C(224)-H(224)	119.3
C(209)-C(208)-H(208)	119.3	C(225)-C(224)-H(224)	119.3
C(210)-C(209)-C(208)	119.6(5)	C(220)-C(225)-C(226)	119.9(5)
C(210)-C(209)-C(218)	120.2(5)	C(220)-C(225)-C(224)	119.0(5)
C(208)-C(209)-C(218)	120.2(5)	C(226)-C(225)-C(224)	121.1(6)
C(209)-C(210)-C(211)	122.1(5)	C(227)-C(226)-C(225)	120.8(6)
C(209)-C(210)-H(210)	118.9	C(227)-C(226)-H(226)	119.6
C(211)-C(210)-H(210)	118.9	C(225)-C(226)-H(226)	119.6
C(210)-C(211)-C(216)	117.6(5)	C(226)-C(227)-C(228)	118.8(5)
C(210)-C(211)-C(212)	123.2(5)	C(226)-C(227)-H(227)	120.6
C(216)-C(211)-C(212)	119.2(5)	C(228)-C(227)-H(227)	120.6
C(213)-C(212)-C(211)	120.7(6)	C(229)-C(228)-C(227)	121.4(6)
C(213)-C(212)-H(212)	119.7	C(229)-C(228)-H(228)	119.3
C(211)-C(212)-H(212)	119.7	C(227)-C(228)-H(228)	119.3
C(212)-C(213)-C(214)	120.5(5)	C(228)-C(229)-C(220)	121.3(6)
C(212)-C(213)-H(213)	119.7	C(228)-C(229)-H(230)	119.3
C(214)-C(213)-H(213)	119.7	C(220)-C(229)-H(230)	119.3

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**38**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	97(17)	20(11)	56(5)	16(6)	-21(7)	14(8)
Cl(1A)	62(2)	28(2)	73(3)	19(2)	13(2)	13(1)
Cl(2A)	47(3)	66(3)	102(7)	18(4)	20(4)	-6(2)
C(1B)	97(17)	20(11)	56(5)	16(6)	-21(7)	14(8)
Cl(1B)	328(13)	49(3)	99(5)	7(3)	59(7)	-6(5)
Cl(2B)	57(5)	132(8)	42(2)	-9(4)	-15(3)	45(5)
C(101)	26(3)	28(3)	32(3)	-11(2)	3(2)	3(2)
C(102)	27(3)	15(2)	29(3)	-5(2)	4(2)	-3(2)
O(102)	38(2)	17(2)	28(2)	2(2)	-8(2)	-6(2)
C(103)	28(3)	20(2)	24(3)	-5(2)	3(2)	-2(2)
C(104)	25(3)	21(2)	32(3)	-2(2)	1(2)	-2(2)
C(105)	36(3)	25(3)	35(3)	-2(2)	-3(3)	-16(2)
C(106)	32(3)	25(3)	38(3)	-9(2)	3(3)	-4(2)
C(107)	31(3)	34(3)	42(3)	-10(3)	-4(3)	-14(3)
C(108)	24(3)	39(3)	36(3)	-15(3)	-13(2)	-6(2)
C(109)	26(3)	38(3)	31(3)	-4(2)	4(2)	6(3)
C(110)	31(3)	41(3)	41(3)	-19(3)	-4(3)	3(3)
C(111)	43(4)	48(4)	24(3)	-14(3)	0(3)	17(3)
C(112)	64(5)	49(4)	40(4)	-5(3)	-16(3)	35(4)
C(113)	98(6)	49(4)	27(3)	-3(3)	0(4)	51(4)
C(114)	65(5)	25(3)	54(4)	3(3)	11(4)	24(3)
C(115)	55(4)	40(3)	35(3)	5(3)	-5(3)	14(3)
C(116)	37(3)	41(3)	25(3)	0(2)	5(3)	11(3)
C(117)	27(3)	32(3)	37(3)	4(2)	-2(3)	5(2)
C(118)	12(2)	31(3)	32(3)	-7(2)	1(2)	8(2)
C(119)	20(3)	19(2)	25(3)	9(2)	2(2)	-6(2)
N(119)	14(2)	20(2)	23(2)	6(2)	3(2)	0(2)
C(120)	23(3)	23(2)	25(3)	-8(2)	0(2)	6(2)
C(121)	19(3)	21(2)	24(3)	2(2)	4(2)	3(2)
C(122)	13(2)	20(2)	30(3)	1(2)	-1(2)	0(2)
C(123)	22(3)	16(2)	31(3)	4(2)	9(2)	3(2)
C(124)	17(2)	21(2)	26(3)	-5(2)	2(2)	11(2)
C(125)	17(3)	27(3)	30(3)	-17(2)	0(2)	11(2)
C(126)	17(3)	32(3)	34(3)	-11(2)	-3(2)	12(2)
C(127)	18(3)	29(3)	57(4)	-26(3)	-6(3)	6(2)
C(128)	28(3)	23(3)	46(3)	-8(2)	-9(3)	-6(2)
C(129)	27(3)	22(2)	28(3)	0(2)	-4(2)	-3(2)
C(201)	14(2)	15(2)	27(3)	1(2)	-4(2)	2(2)
C(202)	17(2)	9(2)	37(3)	-1(2)	-4(2)	0(2)
O(202)	24(2)	18(2)	20(2)	0(1)	-1(1)	9(1)
C(203)	24(3)	11(2)	29(3)	3(2)	-11(2)	-6(2)
C(204)	27(3)	14(2)	34(3)	6(2)	-14(2)	-5(2)
C(205)	20(3)	13(2)	31(3)	-2(2)	-5(2)	-6(2)
C(206)	18(3)	25(3)	27(3)	-5(2)	0(2)	-6(2)
C(207)	19(3)	24(3)	40(3)	0(2)	1(2)	-6(2)
C(208)	20(3)	26(3)	25(3)	-1(2)	10(2)	-3(2)
C(209)	15(3)	38(3)	33(3)	1(2)	7(2)	-1(2)
C(210)	30(3)	40(3)	20(3)	0(2)	7(2)	-4(2)

C(211)	26(3)	26(3)	35(3)	4(2)	0(2)	-6(2)
C(212)	31(3)	53(4)	29(3)	3(3)	1(3)	-1(3)
C(213)	34(3)	45(3)	30(3)	20(3)	-8(3)	10(3)
C(214)	37(3)	22(2)	37(3)	17(2)	-4(3)	11(2)
C(215)	34(3)	21(2)	37(3)	4(2)	6(3)	-1(2)
C(216)	23(3)	14(2)	39(3)	0(2)	4(2)	-9(2)
C(217)	15(2)	20(2)	26(3)	7(2)	1(2)	-2(2)
C(218)	18(2)	18(2)	28(3)	-1(2)	5(2)	-3(2)
C(219)	26(3)	16(2)	27(3)	7(2)	-12(2)	-7(2)
N(219)	18(2)	8(2)	29(2)	2(2)	-4(2)	2(2)
C(220)	34(3)	24(3)	25(3)	-4(2)	9(2)	-15(2)
C(221)	22(3)	11(2)	41(3)	-4(2)	-1(2)	-9(2)
C(222)	30(3)	20(2)	19(2)	2(2)	2(2)	-14(2)
C(223)	45(3)	14(2)	23(3)	0(2)	-4(3)	-7(2)
C(224)	48(4)	26(3)	26(3)	2(2)	-6(3)	-13(3)
C(225)	36(3)	29(3)	33(3)	0(2)	4(3)	-14(3)
C(226)	53(4)	46(4)	32(3)	-9(3)	9(3)	-18(3)
C(227)	48(4)	54(4)	31(3)	-14(3)	18(3)	-24(3)
C(228)	31(3)	40(3)	52(4)	-23(3)	15(3)	-11(3)
C(229)	25(3)	30(3)	45(3)	-13(2)	4(3)	-5(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**38**.

	x	y	z	U(eq)
H(1A)	6073	1689	5710	70
H(1B)	7545	886	5739	70
H(1C)	5410	842	5819	70
H(1D)	7153	471	5813	70
H(102)	8190	6214	3833	33
H(104)	8636	9886	3587	31
H(105)	10299	10560	3963	38
H(107)	11738	10338	4446	43
H(108)	12485	9294	4868	40
H(110)	12327	7581	5186	45
H(112)	12261	5813	5526	61
H(113)	11511	3926	5596	70
H(114)	10015	2999	5211	58
H(115)	9358	3954	4753	52
H(117)	9378	5699	4429	38
H(119)	7140	8287	3353	25
H(123)	6336	7469	2936	28
H(124)	4756	6611	2573	26
H(126)	3069	4970	2423	33
H(127)	2057	3188	2532	42
H(128)	2602	2249	3007	39
H(129)	4247	3077	3367	31
H(202)	7203	3595	2921	25

H(204)	10387	764	3070	30
H(205)	10959	159	2566	26
H(207)	10667	261	2003	33
H(208)	9620	1033	1564	28
H(210)	7990	2418	1310	36
H(212)	6238	3799	1031	45
H(213)	4642	5350	1058	43
H(214)	4077	6211	1545	38
H(215)	5123	5541	2006	37
H(217)	6787	4120	2276	24
H(219)	9062	2052	3432	28
H(223)	8267	2367	3884	33
H(224)	7446	3004	4372	40
H(226)	5956	4353	4699	52
H(227)	4312	5901	4739	53
H(228)	3503	6848	4276	49
H(230)	4244	6223	3790	40

Table 6. Torsion angles [°] for (*R*)-**38**.

C(106)-C(101)-C(102)-O(102)	176.4(5)	C(112)-C(113)-C(114)-C(115)	0.9(10)
C(118)-C(101)-C(102)-O(102)	-5.5(8)	C(113)-C(114)-C(115)-C(116)	-0.9(10)
C(106)-C(101)-C(102)-C(103)	-4.0(7)	C(110)-C(111)-C(116)-C(117)	0.2(8)
C(118)-C(101)-C(102)-C(103)	174.1(5)	C(112)-C(111)-C(116)-C(117)	178.4(6)
O(102)-C(102)-C(103)-C(104)	-177.2(5)	C(110)-C(111)-C(116)-C(115)	179.9(5)
C(101)-C(102)-C(103)-C(104)	3.3(7)	C(112)-C(111)-C(116)-C(115)	-1.8(8)
O(102)-C(102)-C(103)-C(119)	0.7(7)	C(114)-C(115)-C(116)-C(117)	-178.9(6)
C(101)-C(102)-C(103)-C(119)	-178.8(5)	C(114)-C(115)-C(116)-C(111)	1.3(9)
C(102)-C(103)-C(104)-C(105)	0.3(8)	C(111)-C(116)-C(117)-C(118)	-0.8(8)
C(119)-C(103)-C(104)-C(105)	-177.6(5)	C(115)-C(116)-C(117)-C(118)	179.4(5)
C(103)-C(104)-C(105)-C(106)	-3.1(8)	C(116)-C(117)-C(118)-C(109)	2.0(8)
C(104)-C(105)-C(106)-C(101)	2.2(9)	C(116)-C(117)-C(118)-C(101)	-177.7(5)
C(104)-C(105)-C(106)-C(107)	-178.2(5)	C(110)-C(109)-C(118)-C(117)	-2.7(7)
C(102)-C(101)-C(106)-C(105)	1.4(8)	C(108)-C(109)-C(118)-C(117)	178.9(5)
C(118)-C(101)-C(106)-C(105)	-176.8(5)	C(110)-C(109)-C(118)-C(101)	177.1(5)
C(102)-C(101)-C(106)-C(107)	-178.2(5)	C(108)-C(109)-C(118)-C(101)	-1.3(7)
C(118)-C(101)-C(106)-C(107)	3.6(8)	C(106)-C(101)-C(118)-C(117)	178.1(5)
C(105)-C(106)-C(107)-C(108)	177.7(6)	C(102)-C(101)-C(118)-C(117)	0.0(8)
C(101)-C(106)-C(107)-C(108)	-2.7(9)	C(106)-C(101)-C(118)-C(109)	-1.7(7)
C(106)-C(107)-C(108)-C(109)	-0.4(9)	C(102)-C(101)-C(118)-C(109)	-179.7(5)
C(107)-C(108)-C(109)-C(110)	-176.0(6)	C(102)-C(103)-C(119)-N(119)	-3.1(7)
C(107)-C(108)-C(109)-C(118)	2.4(8)	C(104)-C(103)-C(119)-N(119)	174.9(5)
C(108)-C(109)-C(110)-C(111)	-179.4(5)	C(103)-C(119)-N(119)-C(122)	-179.9(4)
C(118)-C(109)-C(110)-C(111)	2.2(8)	C(129)-C(120)-C(121)-C(122)	-177.8(5)
C(109)-C(110)-C(111)-C(112)	-179.1(6)	C(125)-C(120)-C(121)-C(122)	3.4(7)
C(109)-C(110)-C(111)-C(116)	-0.9(8)	C(129)-C(120)-C(121)-C(221)	2.6(7)
C(110)-C(111)-C(112)-C(113)	-180.0(6)	C(125)-C(120)-C(121)-C(221)	-176.3(4)
C(116)-C(111)-C(112)-C(113)	1.9(9)	C(120)-C(121)-C(122)-C(123)	-5.0(7)
C(111)-C(112)-C(113)-C(114)	-1.4(10)	C(221)-C(121)-C(122)-C(123)	174.6(4)

C(120)-C(121)-C(122)-N(119)	177.5(4)	C(210)-C(211)-C(216)-C(217)	-0.9(7)
C(221)-C(121)-C(122)-N(119)	-2.8(7)	C(212)-C(211)-C(216)-C(217)	179.0(5)
C(119)-N(119)-C(122)-C(121)	-165.5(5)	C(210)-C(211)-C(216)-C(215)	179.1(4)
C(119)-N(119)-C(122)-C(123)	17.1(7)	C(212)-C(211)-C(216)-C(215)	-1.0(7)
C(121)-C(122)-C(123)-C(124)	3.7(7)	C(214)-C(215)-C(216)-C(217)	-179.3(5)
N(119)-C(122)-C(123)-C(124)	-179.1(4)	C(214)-C(215)-C(216)-C(211)	0.7(7)
C(122)-C(123)-C(124)-C(125)	-0.5(7)	C(211)-C(216)-C(217)-C(218)	-0.4(7)
C(123)-C(124)-C(125)-C(126)	178.8(4)	C(215)-C(216)-C(217)-C(218)	179.6(5)
C(123)-C(124)-C(125)-C(120)	-1.1(7)	C(216)-C(217)-C(218)-C(209)	0.9(7)
C(129)-C(120)-C(125)-C(126)	0.9(7)	C(216)-C(217)-C(218)-C(201)	-177.3(5)
C(121)-C(120)-C(125)-C(126)	179.8(4)	C(210)-C(209)-C(218)-C(217)	0.0(7)
C(129)-C(120)-C(125)-C(124)	-179.2(4)	C(208)-C(209)-C(218)-C(217)	178.7(4)
C(121)-C(120)-C(125)-C(124)	-0.3(7)	C(210)-C(209)-C(218)-C(201)	178.4(5)
C(124)-C(125)-C(126)-C(127)	179.5(4)	C(208)-C(209)-C(218)-C(201)	-2.9(7)
C(120)-C(125)-C(126)-C(127)	-0.7(7)	C(202)-C(201)-C(218)-C(217)	3.5(8)
C(125)-C(126)-C(127)-C(128)	0.7(8)	C(206)-C(201)-C(218)-C(217)	-179.7(4)
C(126)-C(127)-C(128)-C(129)	-1.0(8)	C(202)-C(201)-C(218)-C(209)	-174.7(4)
C(127)-C(128)-C(129)-C(120)	1.3(8)	C(206)-C(201)-C(218)-C(209)	2.1(7)
C(125)-C(120)-C(129)-C(128)	-1.2(7)	C(202)-C(203)-C(219)-N(219)	2.7(7)
C(121)-C(120)-C(129)-C(128)	179.9(5)	C(204)-C(203)-C(219)-N(219)	-177.2(4)
C(206)-C(201)-C(202)-O(202)	-178.1(4)	C(203)-C(219)-N(219)-C(222)	175.5(4)
C(218)-C(201)-C(202)-O(202)	-1.2(7)	C(225)-C(220)-C(221)-C(222)	-0.7(7)
C(206)-C(201)-C(202)-C(203)	0.8(7)	C(229)-C(220)-C(221)-C(222)	178.3(5)
C(218)-C(201)-C(202)-C(203)	177.8(4)	C(225)-C(220)-C(221)-C(121)	-178.1(5)
O(202)-C(202)-C(203)-C(204)	179.4(4)	C(229)-C(220)-C(221)-C(121)	0.9(7)
C(201)-C(202)-C(203)-C(204)	0.5(7)	C(122)-C(121)-C(221)-C(222)	-106.5(5)
O(202)-C(202)-C(203)-C(219)	-0.5(7)	C(120)-C(121)-C(221)-C(222)	73.1(6)
C(201)-C(202)-C(203)-C(219)	-179.5(4)	C(122)-C(121)-C(221)-C(220)	70.9(6)
C(202)-C(203)-C(204)-C(205)	-0.9(7)	C(120)-C(121)-C(221)-C(220)	-109.5(5)
C(219)-C(203)-C(204)-C(205)	179.0(4)	C(220)-C(221)-C(222)-C(223)	1.8(7)
C(203)-C(204)-C(205)-C(206)	0.0(7)	C(121)-C(221)-C(222)-C(223)	179.2(4)
C(204)-C(205)-C(206)-C(201)	1.4(7)	C(220)-C(221)-C(222)-N(219)	179.9(4)
C(204)-C(205)-C(206)-C(207)	-177.4(5)	C(121)-C(221)-C(222)-N(219)	-2.6(6)
C(202)-C(201)-C(206)-C(205)	-1.8(7)	C(219)-N(219)-C(222)-C(221)	178.4(4)
C(218)-C(201)-C(206)-C(205)	-178.9(4)	C(219)-N(219)-C(222)-C(223)	-3.4(7)
C(202)-C(201)-C(206)-C(207)	177.0(4)	C(221)-C(222)-C(223)-C(224)	-2.3(7)
C(218)-C(201)-C(206)-C(207)	-0.1(7)	N(219)-C(222)-C(223)-C(224)	179.6(5)
C(205)-C(206)-C(207)-C(208)	177.5(5)	C(222)-C(223)-C(224)-C(225)	1.7(8)
C(201)-C(206)-C(207)-C(208)	-1.2(7)	C(229)-C(220)-C(225)-C(226)	-1.4(7)
C(206)-C(207)-C(208)-C(209)	0.4(7)	C(221)-C(220)-C(225)-C(226)	177.6(5)
C(207)-C(208)-C(209)-C(210)	-179.6(5)	C(229)-C(220)-C(225)-C(224)	-178.9(5)
C(207)-C(208)-C(209)-C(218)	1.7(7)	C(221)-C(220)-C(225)-C(224)	0.1(7)
C(208)-C(209)-C(210)-C(211)	179.9(5)	C(223)-C(224)-C(225)-C(220)	-0.6(8)
C(218)-C(209)-C(210)-C(211)	-1.3(8)	C(223)-C(224)-C(225)-C(226)	-178.1(5)
C(209)-C(210)-C(211)-C(216)	1.7(8)	C(220)-C(225)-C(226)-C(227)	1.4(8)
C(209)-C(210)-C(211)-C(212)	-178.1(5)	C(224)-C(225)-C(226)-C(227)	178.9(5)
C(210)-C(211)-C(212)-C(213)	-179.1(5)	C(225)-C(226)-C(227)-C(228)	-1.2(9)
C(216)-C(211)-C(212)-C(213)	1.0(8)	C(226)-C(227)-C(228)-C(229)	1.0(9)
C(211)-C(212)-C(213)-C(214)	-0.6(9)	C(227)-C(228)-C(229)-C(220)	-1.0(8)
C(212)-C(213)-C(214)-C(215)	0.2(9)	C(225)-C(220)-C(229)-C(228)	1.2(8)
C(213)-C(214)-C(215)-C(216)	-0.3(8)	C(221)-C(220)-C(229)-C(228)	-177.8(5)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for (*R*)-**38** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(102)-H(102)...N(119)	0.84	1.75	2.497(5)	147.0
O(102)-H(102)...N(119)	0.84	1.75	2.497(5)	147.0

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*,*R*)-**53**·py.

Identification code	(*R*,*R*)-**53**·py	
Empirical formula	C41 H33 N3 O2 Zn	
Formula weight	665.07	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.4421(4) Å	α = 90°.
	b = 20.4458(10) Å	β = 95.085(3)°.
	c = 17.8670(8) Å	γ = 90°.
Volume	3071.8(3) Å^3	
Z	4	
Density (calculated)	1.438 Mg/m^3	
Absorption coefficient	0.843 mm^{-1}	
F(000)	1384	
Crystal size	0.30 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.14 to 28.33°.	
Index ranges	-10<=h<=9, -26<=k<=27, -23<=l<=23	
Reflections collected	27171	
Independent reflections	13665 [R(int) = 0.0424]	
Completeness to theta = 28.33°	93.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13665 / 1 / 847	
Goodness-of-fit on F^2	0.874	
Final R indices [I>2sigma(I)]	R1 = 0.0377, wR2 = 0.0768	
R indices (all data)	R1 = 0.0724, wR2 = 0.0860	
Absolute structure parameter	-0.020(13)	
Largest diff. peak and hole	0.258 and -0.558 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for (*R*,*R*)-**53**·py. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	4960(1)	3107(1)	5236(1)	23(1)
C(11)	5416(4)	3109(2)	6922(2)	28(1)
N(11)	4946(5)	3537(2)	6279(2)	27(1)
C(12)	6333(5)	2523(2)	6634(2)	28(1)
N(12)	5451(5)	2310(2)	5929(2)	26(1)
C(13)	6630(6)	2028(3)	7254(3)	34(2)
C(14)	7633(5)	2327(2)	7920(2)	37(1)
C(15)	6815(6)	2932(3)	8202(2)	43(1)
C(16)	6413(7)	3425(3)	7586(3)	42(2)
N(31)	7242(4)	3233(3)	4893(2)	26(1)
C(32)	7685(6)	3830(3)	4672(3)	27(1)
C(33)	9218(6)	3952(3)	4485(3)	35(2)
C(34)	10300(6)	3451(3)	4517(3)	34(2)
C(35)	9841(6)	2839(3)	4737(3)	32(2)

C(36)	8307(6)	2748(3)	4925(3)	28(1)
C(101)	2571(6)	4917(3)	4607(3)	26(1)
C(102)	3410(6)	4438(3)	5077(3)	26(1)
O(102)	4075(4)	3940(2)	4792(2)	25(1)
C(103)	3446(6)	4522(3)	5874(3)	29(1)
C(104)	2646(7)	5057(3)	6172(4)	40(2)
C(105)	1774(7)	5467(3)	5730(4)	42(2)
C(106)	1732(6)	5418(3)	4948(4)	33(2)
C(107)	773(7)	5860(3)	4486(4)	44(2)
C(108)	699(7)	5843(3)	3736(4)	41(2)
C(109)	1606(6)	5384(3)	3371(4)	36(2)
C(110)	1588(7)	5386(4)	2581(4)	39(2)
C(111)	2443(7)	4964(3)	2200(4)	38(2)
C(112)	3390(6)	4511(4)	2607(3)	38(2)
C(113)	3439(6)	4482(3)	3375(3)	32(2)
C(114)	2571(6)	4906(3)	3795(4)	28(1)
C(115)	4215(5)	4065(3)	6414(3)	28(1)
C(201)	2789(6)	1563(3)	3856(3)	26(1)
C(202)	3565(5)	1882(3)	4521(3)	25(1)
O(202)	3730(4)	2512(2)	4532(2)	28(1)
C(203)	4122(6)	1476(3)	5144(3)	28(1)
C(204)	3871(6)	808(3)	5119(4)	36(2)
C(205)	3152(7)	512(4)	4503(3)	36(2)
C(206)	2608(7)	881(4)	3861(4)	36(2)
C(207)	1924(6)	541(4)	3215(4)	41(2)
C(208)	1427(7)	856(4)	2593(4)	42(2)
C(209)	1587(6)	1549(3)	2537(3)	31(2)
C(210)	1078(6)	1867(4)	1866(3)	38(2)
C(211)	1126(6)	2536(4)	1799(4)	41(2)
C(212)	1697(6)	2902(3)	2434(3)	34(2)
C(213)	2227(6)	2601(3)	3091(3)	28(1)
C(214)	2202(5)	1924(4)	3172(3)	27(2)
C(215)	4996(5)	1724(3)	5813(3)	26(1)
Zn(2)	5015(1)	6897(1)	-228(1)	24(1)
C(21)	3727(4)	6792(2)	-1802(2)	30(1)
N(21)	4681(5)	6388(2)	-1246(2)	28(1)
C(22)	4478(5)	7467(2)	-1779(2)	28(1)
N(22)	4886(5)	7662(2)	-989(2)	25(1)
C(23)	3384(7)	7949(3)	-2237(3)	35(2)
C(24)	3128(5)	7701(2)	-3045(2)	39(1)
C(25)	2477(5)	7016(3)	-3091(2)	39(1)
C(26)	3497(7)	6535(3)	-2594(3)	36(2)
N(41)	2724(4)	6805(3)	107(2)	23(1)
C(42)	2242(6)	6229(3)	326(3)	34(2)
C(43)	713(7)	6100(3)	491(4)	39(2)
C(44)	-365(6)	6606(4)	441(3)	37(2)
C(45)	124(6)	7210(4)	238(3)	34(2)
C(46)	1674(6)	7292(3)	67(3)	29(1)
C(301)	7285(6)	5074(3)	383(3)	28(1)
C(302)	6466(6)	5566(3)	-98(3)	27(1)
O(302)	5910(4)	6079(2)	215(2)	29(1)
C(303)	6280(6)	5452(3)	-880(3)	29(1)
C(304)	7047(7)	4930(3)	-1180(4)	41(2)
C(305)	7972(7)	4501(3)	-753(4)	43(2)

C(306)	8112(7)	4579(3)	34(4)	36(2)
C(307)	9096(7)	4124(3)	483(4)	43(2)
C(308)	9162(7)	4146(3)	1223(4)	47(2)
C(309)	8236(6)	4605(3)	1618(4)	35(2)
C(310)	8264(7)	4565(4)	2395(4)	44(2)
C(311)	7366(7)	4985(4)	2777(4)	44(2)
C(312)	6457(6)	5454(4)	2380(3)	39(2)
C(313)	6428(6)	5505(3)	1619(3)	32(2)
C(314)	7340(6)	5073(3)	1208(4)	30(2)
C(315)	5349(5)	5851(3)	-1398(3)	32(1)
C(401)	7324(6)	8414(3)	1156(3)	26(1)
C(402)	6496(5)	8099(3)	500(3)	24(1)
O(402)	6211(4)	7482(2)	504(2)	28(1)
C(403)	6056(6)	8496(3)	-132(3)	27(1)
C(404)	6375(7)	9180(3)	-115(3)	37(2)
C(405)	7122(7)	9469(4)	495(4)	41(2)
C(406)	7594(6)	9098(3)	1127(3)	31(2)
C(407)	8412(6)	9416(4)	1764(4)	40(2)
C(408)	8874(7)	9093(4)	2405(4)	39(2)
C(409)	8616(6)	8415(3)	2466(3)	31(1)
C(410)	9022(6)	8098(4)	3153(3)	38(2)
C(411)	8760(7)	7454(4)	3231(4)	37(2)
C(412)	8093(6)	7090(4)	2635(3)	35(2)
C(413)	7643(6)	7387(3)	1959(3)	29(1)
C(414)	7842(6)	8068(4)	1842(3)	28(2)
C(415)	5396(5)	8241(3)	-843(3)	31(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*,*R*)-**53**·py.

Zn(1)-O(202)	1.978(4)	C(15)-C(16)	1.510(8)
Zn(1)-O(102)	1.995(4)	C(15)-H(15A)	0.9900
Zn(1)-N(11)	2.061(4)	C(15)-H(15B)	0.9900
Zn(1)-N(12)	2.066(5)	C(16)-H(16A)	0.9900
Zn(1)-N(31)	2.089(4)	C(16)-H(16B)	0.9900
C(11)-N(11)	1.470(6)	N(31)-C(36)	1.337(7)
C(11)-C(16)	1.535(7)	N(31)-C(32)	1.345(7)
C(11)-C(12)	1.540(5)	C(32)-C(33)	1.388(7)
C(11)-H(11)	1.0000	C(32)-H(32)	0.9500
N(11)-C(115)	1.278(7)	C(33)-C(34)	1.371(9)
C(12)-N(12)	1.470(6)	C(33)-H(33)	0.9500
C(12)-C(13)	1.505(7)	C(34)-C(35)	1.377(8)
C(12)-H(12)	1.0000	C(34)-H(34)	0.9500
N(12)-C(215)	1.270(7)	C(35)-C(36)	1.379(7)
C(13)-C(14)	1.526(7)	C(35)-H(35)	0.9500
C(13)-H(13A)	0.9900	C(36)-H(36)	0.9500
C(13)-H(13B)	0.9900	C(101)-C(106)	1.414(8)
C(14)-C(15)	1.524(6)	C(101)-C(102)	1.437(8)
C(14)-H(14A)	0.9900	C(101)-C(114)	1.450(9)
C(14)-H(14B)	0.9900	C(102)-O(102)	1.289(7)

C(102)-C(103)	1.432(8)	Zn(2)-N(21)	2.093(5)
C(103)-C(104)	1.413(8)	C(21)-N(21)	1.475(6)
C(103)-C(115)	1.453(8)	C(21)-C(26)	1.505(7)
C(104)-C(105)	1.328(9)	C(21)-C(22)	1.518(6)
C(104)-H(104)	0.9500	C(21)-H(21)	1.0000
C(105)-C(106)	1.398(9)	N(21)-C(315)	1.274(7)
C(105)-H(105)	0.9500	C(22)-N(22)	1.477(6)
C(106)-C(107)	1.426(9)	C(22)-C(23)	1.536(7)
C(107)-C(108)	1.337(9)	C(22)-H(22)	1.0000
C(107)-H(107)	0.9500	N(22)-C(415)	1.278(7)
C(108)-C(109)	1.408(8)	C(23)-C(24)	1.528(7)
C(108)-H(108)	0.9500	C(23)-H(23A)	0.9900
C(109)-C(110)	1.410(10)	C(23)-H(23B)	0.9900
C(109)-C(114)	1.445(9)	C(24)-C(25)	1.503(7)
C(110)-C(111)	1.346(9)	C(24)-H(24A)	0.9900
C(110)-H(110)	0.9500	C(24)-H(24B)	0.9900
C(111)-C(112)	1.388(9)	C(25)-C(26)	1.537(8)
C(111)-H(111)	0.9500	C(25)-H(25A)	0.9900
C(112)-C(113)	1.369(8)	C(25)-H(25B)	0.9900
C(112)-H(112)	0.9500	C(26)-H(26A)	0.9900
C(113)-C(114)	1.397(8)	C(26)-H(26B)	0.9900
C(113)-H(113)	0.9500	N(41)-C(42)	1.317(8)
C(115)-H(115)	0.9500	N(41)-C(46)	1.330(7)
C(201)-C(206)	1.404(9)	C(42)-C(43)	1.375(7)
C(201)-C(202)	1.459(8)	C(42)-H(42)	0.9500
C(201)-C(214)	1.474(8)	C(43)-C(44)	1.375(9)
C(202)-O(202)	1.295(7)	C(43)-H(43)	0.9500
C(202)-C(203)	1.435(8)	C(44)-C(45)	1.361(9)
C(203)-C(204)	1.383(8)	C(44)-H(44)	0.9500
C(203)-C(215)	1.439(8)	C(45)-C(46)	1.380(7)
C(204)-C(205)	1.351(9)	C(45)-H(45)	0.9500
C(204)-H(204)	0.9500	C(46)-H(46)	0.9500
C(205)-C(206)	1.415(9)	C(301)-C(306)	1.406(8)
C(205)-H(205)	0.9500	C(301)-C(302)	1.457(8)
C(206)-C(207)	1.425(9)	C(301)-C(314)	1.470(9)
C(207)-C(208)	1.320(9)	C(302)-O(302)	1.297(7)
C(207)-H(207)	0.9500	C(302)-C(303)	1.411(8)
C(208)-C(209)	1.427(9)	C(303)-C(304)	1.380(8)
C(208)-H(208)	0.9500	C(303)-C(315)	1.417(8)
C(209)-C(210)	1.398(9)	C(304)-C(305)	1.363(9)
C(209)-C(214)	1.430(8)	C(304)-H(304)	0.9500
C(210)-C(211)	1.374(10)	C(305)-C(306)	1.410(9)
C(210)-H(210)	0.9500	C(305)-H(305)	0.9500
C(211)-C(212)	1.408(9)	C(306)-C(307)	1.442(9)
C(211)-H(211)	0.9500	C(307)-C(308)	1.320(9)
C(212)-C(213)	1.365(9)	C(307)-H(307)	0.9500
C(212)-H(212)	0.9500	C(308)-C(309)	1.444(9)
C(213)-C(214)	1.392(9)	C(308)-H(308)	0.9500
C(213)-H(213)	0.9500	C(309)-C(314)	1.388(9)
C(215)-H(215)	0.9500	C(309)-C(310)	1.390(10)
Zn(2)-O(302)	1.973(4)	C(310)-C(311)	1.366(9)
Zn(2)-O(402)	1.982(4)	C(310)-H(310)	0.9500
Zn(2)-N(22)	2.069(5)	C(311)-C(312)	1.384(9)
Zn(2)-N(41)	2.083(4)	C(311)-H(311)	0.9500

C(312)-C(313)	1.362(8)	C(13)-C(12)-C(11)	109.4(3)
C(312)-H(312)	0.9500	N(12)-C(12)-H(12)	107.5
C(313)-C(314)	1.419(8)	C(13)-C(12)-H(12)	107.5
C(313)-H(313)	0.9500	C(11)-C(12)-H(12)	107.5
C(315)-H(315)	0.9500	C(215)-N(12)-C(12)	122.8(5)
C(401)-C(406)	1.419(8)	C(215)-N(12)-Zn(1)	127.2(4)
C(401)-C(414)	1.448(9)	C(12)-N(12)-Zn(1)	109.8(3)
C(401)-C(402)	1.461(8)	C(12)-C(13)-C(14)	110.5(5)
C(402)-O(402)	1.284(7)	C(12)-C(13)-H(13A)	109.6
C(402)-C(403)	1.412(8)	C(14)-C(13)-H(13A)	109.6
C(403)-C(404)	1.423(8)	C(12)-C(13)-H(13B)	109.6
C(403)-C(415)	1.439(8)	C(14)-C(13)-H(13B)	109.6
C(404)-C(405)	1.345(9)	H(13A)-C(13)-H(13B)	108.1
C(404)-H(404)	0.9500	C(15)-C(14)-C(13)	110.3(4)
C(405)-C(406)	1.388(9)	C(15)-C(14)-H(14A)	109.6
C(405)-H(405)	0.9500	C(13)-C(14)-H(14A)	109.6
C(406)-C(407)	1.434(9)	C(15)-C(14)-H(14B)	109.6
C(407)-C(408)	1.349(9)	C(13)-C(14)-H(14B)	109.6
C(407)-H(407)	0.9500	H(14A)-C(14)-H(14B)	108.1
C(408)-C(409)	1.409(9)	C(16)-C(15)-C(14)	112.3(4)
C(408)-H(408)	0.9500	C(16)-C(15)-H(15A)	109.1
C(409)-C(410)	1.403(9)	C(14)-C(15)-H(15A)	109.1
C(409)-C(414)	1.430(8)	C(16)-C(15)-H(15B)	109.1
C(410)-C(411)	1.344(10)	C(14)-C(15)-H(15B)	109.1
C(410)-H(410)	0.9500	H(15A)-C(15)-H(15B)	107.9
C(411)-C(412)	1.379(9)	C(15)-C(16)-C(11)	110.8(5)
C(411)-H(411)	0.9500	C(15)-C(16)-H(16A)	109.5
C(412)-C(413)	1.375(8)	C(11)-C(16)-H(16A)	109.5
C(412)-H(412)	0.9500	C(15)-C(16)-H(16B)	109.5
C(413)-C(414)	1.419(9)	C(11)-C(16)-H(16B)	109.5
C(413)-H(413)	0.9500	H(16A)-C(16)-H(16B)	108.1
C(415)-H(415)	0.9500	C(36)-N(31)-C(32)	118.8(5)
		C(36)-N(31)-Zn(1)	122.0(4)
O(202)-Zn(1)-O(102)	96.57(17)	C(32)-N(31)-Zn(1)	119.0(4)
O(202)-Zn(1)-N(11)	142.43(15)	N(31)-C(32)-C(33)	121.6(6)
O(102)-Zn(1)-N(11)	87.98(17)	N(31)-C(32)-H(32)	119.2
O(202)-Zn(1)-N(12)	87.80(18)	C(33)-C(32)-H(32)	119.2
O(102)-Zn(1)-N(12)	163.64(14)	C(34)-C(33)-C(32)	119.2(6)
N(11)-Zn(1)-N(12)	79.13(19)	C(34)-C(33)-H(33)	120.4
O(202)-Zn(1)-N(31)	109.56(17)	C(32)-C(33)-H(33)	120.4
O(102)-Zn(1)-N(31)	95.79(17)	C(33)-C(34)-C(35)	119.2(5)
N(11)-Zn(1)-N(31)	107.01(17)	C(33)-C(34)-H(34)	120.4
N(12)-Zn(1)-N(31)	97.58(18)	C(35)-C(34)-H(34)	120.4
N(11)-C(11)-C(16)	116.4(4)	C(34)-C(35)-C(36)	119.2(6)
N(11)-C(11)-C(12)	108.1(3)	C(34)-C(35)-H(35)	120.4
C(16)-C(11)-C(12)	109.2(4)	C(36)-C(35)-H(35)	120.4
N(11)-C(11)-H(11)	107.6	N(31)-C(36)-C(35)	122.1(6)
C(16)-C(11)-H(11)	107.6	N(31)-C(36)-H(36)	119.0
C(12)-C(11)-H(11)	107.6	C(35)-C(36)-H(36)	119.0
C(115)-N(11)-C(11)	117.2(4)	C(106)-C(101)-C(102)	118.8(6)
C(115)-N(11)-Zn(1)	124.9(4)	C(106)-C(101)-C(114)	119.1(6)
C(11)-N(11)-Zn(1)	115.5(3)	C(102)-C(101)-C(114)	122.0(5)
N(12)-C(12)-C(13)	118.0(4)	O(102)-C(102)-C(103)	121.1(6)
N(12)-C(12)-C(11)	106.6(3)	O(102)-C(102)-C(101)	121.1(5)

C(103)-C(102)-C(101)	117.8(5)	C(204)-C(205)-C(206)	120.8(7)
C(102)-O(102)-Zn(1)	132.6(4)	C(204)-C(205)-H(205)	119.6
C(104)-C(103)-C(102)	119.9(6)	C(206)-C(205)-H(205)	119.6
C(104)-C(103)-C(115)	116.6(5)	C(201)-C(206)-C(205)	120.5(6)
C(102)-C(103)-C(115)	123.5(6)	C(201)-C(206)-C(207)	121.0(7)
C(105)-C(104)-C(103)	121.5(6)	C(205)-C(206)-C(207)	118.5(7)
C(105)-C(104)-H(104)	119.2	C(208)-C(207)-C(206)	121.4(7)
C(103)-C(104)-H(104)	119.2	C(208)-C(207)-H(207)	119.3
C(104)-C(105)-C(106)	120.8(6)	C(206)-C(207)-H(207)	119.3
C(104)-C(105)-H(105)	119.6	C(207)-C(208)-C(209)	121.2(7)
C(106)-C(105)-H(105)	119.6	C(207)-C(208)-H(208)	119.4
C(105)-C(106)-C(101)	120.9(6)	C(209)-C(208)-H(208)	119.4
C(105)-C(106)-C(107)	119.7(6)	C(210)-C(209)-C(208)	119.9(6)
C(101)-C(106)-C(107)	119.3(6)	C(210)-C(209)-C(214)	119.6(7)
C(108)-C(107)-C(106)	122.5(6)	C(208)-C(209)-C(214)	120.5(6)
C(108)-C(107)-H(107)	118.7	C(211)-C(210)-C(209)	121.9(6)
C(106)-C(107)-H(107)	118.7	C(211)-C(210)-H(210)	119.1
C(107)-C(108)-C(109)	120.2(6)	C(209)-C(210)-H(210)	119.1
C(107)-C(108)-H(108)	119.9	C(210)-C(211)-C(212)	118.1(6)
C(109)-C(108)-H(108)	119.9	C(210)-C(211)-H(211)	121.0
C(108)-C(109)-C(110)	120.3(6)	C(212)-C(211)-H(211)	121.0
C(108)-C(109)-C(114)	120.8(6)	C(213)-C(212)-C(211)	121.0(7)
C(110)-C(109)-C(114)	118.9(6)	C(213)-C(212)-H(212)	119.5
C(111)-C(110)-C(109)	123.0(6)	C(211)-C(212)-H(212)	119.5
C(111)-C(110)-H(110)	118.5	C(212)-C(213)-C(214)	122.1(6)
C(109)-C(110)-H(110)	118.5	C(212)-C(213)-H(213)	118.9
C(110)-C(111)-C(112)	118.2(6)	C(214)-C(213)-H(213)	118.9
C(110)-C(111)-H(111)	120.9	C(213)-C(214)-C(209)	117.3(6)
C(112)-C(111)-H(111)	120.9	C(213)-C(214)-C(201)	125.2(6)
C(113)-C(112)-C(111)	121.3(6)	C(209)-C(214)-C(201)	117.4(7)
C(113)-C(112)-H(112)	119.3	N(12)-C(215)-C(203)	126.4(6)
C(111)-C(112)-H(112)	119.3	N(12)-C(215)-H(215)	116.8
C(112)-C(113)-C(114)	122.7(6)	C(203)-C(215)-H(215)	116.8
C(112)-C(113)-H(113)	118.6	O(302)-Zn(2)-O(402)	95.27(17)
C(114)-C(113)-H(113)	118.6	O(302)-Zn(2)-N(22)	154.31(15)
C(113)-C(114)-C(109)	115.8(6)	O(402)-Zn(2)-N(22)	88.36(18)
C(113)-C(114)-C(101)	126.5(6)	O(302)-Zn(2)-N(41)	98.04(17)
C(109)-C(114)-C(101)	117.7(5)	O(402)-Zn(2)-N(41)	107.26(16)
N(11)-C(115)-C(103)	127.8(5)	N(22)-Zn(2)-N(41)	105.15(18)
N(11)-C(115)-H(115)	116.1	O(302)-Zn(2)-N(21)	86.83(17)
C(103)-C(115)-H(115)	116.1	O(402)-Zn(2)-N(21)	153.54(15)
C(206)-C(201)-C(202)	118.7(6)	N(22)-Zn(2)-N(21)	79.04(19)
C(206)-C(201)-C(214)	118.3(6)	N(41)-Zn(2)-N(21)	98.51(16)
C(202)-C(201)-C(214)	123.0(6)	N(21)-C(21)-C(26)	117.1(4)
O(202)-C(202)-C(203)	122.4(6)	N(21)-C(21)-C(22)	106.8(3)
O(202)-C(202)-C(201)	119.8(6)	C(26)-C(21)-C(22)	111.3(4)
C(203)-C(202)-C(201)	117.8(6)	N(21)-C(21)-H(21)	107.1
C(202)-O(202)-Zn(1)	132.2(4)	C(26)-C(21)-H(21)	107.1
C(204)-C(203)-C(202)	120.5(6)	C(22)-C(21)-H(21)	107.1
C(204)-C(203)-C(215)	116.2(6)	C(315)-N(21)-C(21)	124.4(5)
C(202)-C(203)-C(215)	123.3(6)	C(315)-N(21)-Zn(2)	125.8(4)
C(205)-C(204)-C(203)	121.6(6)	C(21)-N(21)-Zn(2)	109.3(3)
C(205)-C(204)-H(204)	119.2	N(22)-C(22)-C(21)	109.5(3)
C(203)-C(204)-H(204)	119.2	N(22)-C(22)-C(23)	114.5(4)

C(21)-C(22)-C(23)	109.8(4)	C(303)-C(302)-C(301)	118.4(6)
N(22)-C(22)-H(22)	107.6	C(302)-O(302)-Zn(2)	130.8(4)
C(21)-C(22)-H(22)	107.6	C(304)-C(303)-C(302)	119.8(6)
C(23)-C(22)-H(22)	107.6	C(304)-C(303)-C(315)	116.3(6)
C(415)-N(22)-C(22)	119.5(5)	C(302)-C(303)-C(315)	123.9(6)
C(415)-N(22)-Zn(2)	124.6(4)	C(305)-C(304)-C(303)	123.1(6)
C(22)-N(22)-Zn(2)	114.7(3)	C(305)-C(304)-H(304)	118.5
C(24)-C(23)-C(22)	108.6(5)	C(303)-C(304)-H(304)	118.5
C(24)-C(23)-H(23A)	110.0	C(304)-C(305)-C(306)	118.6(6)
C(22)-C(23)-H(23A)	110.0	C(304)-C(305)-H(305)	120.7
C(24)-C(23)-H(23B)	110.0	C(306)-C(305)-H(305)	120.7
C(22)-C(23)-H(23B)	110.0	C(301)-C(306)-C(305)	121.6(6)
H(23A)-C(23)-H(23B)	108.3	C(301)-C(306)-C(307)	120.1(6)
C(25)-C(24)-C(23)	112.4(4)	C(305)-C(306)-C(307)	118.3(6)
C(25)-C(24)-H(24A)	109.1	C(308)-C(307)-C(306)	120.4(6)
C(23)-C(24)-H(24A)	109.1	C(308)-C(307)-H(307)	119.8
C(25)-C(24)-H(24B)	109.1	C(306)-C(307)-H(307)	119.8
C(23)-C(24)-H(24B)	109.1	C(307)-C(308)-C(309)	122.3(6)
H(24A)-C(24)-H(24B)	107.9	C(307)-C(308)-H(308)	118.8
C(24)-C(25)-C(26)	112.4(4)	C(309)-C(308)-H(308)	118.8
C(24)-C(25)-H(25A)	109.1	C(314)-C(309)-C(310)	121.8(6)
C(26)-C(25)-H(25A)	109.1	C(314)-C(309)-C(308)	118.9(6)
C(24)-C(25)-H(25B)	109.1	C(310)-C(309)-C(308)	119.3(7)
C(26)-C(25)-H(25B)	109.1	C(311)-C(310)-C(309)	120.1(7)
H(25A)-C(25)-H(25B)	107.9	C(311)-C(310)-H(310)	119.9
C(21)-C(26)-C(25)	109.8(5)	C(309)-C(310)-H(310)	119.9
C(21)-C(26)-H(26A)	109.7	C(310)-C(311)-C(312)	119.1(6)
C(25)-C(26)-H(26A)	109.7	C(310)-C(311)-H(311)	120.4
C(21)-C(26)-H(26B)	109.7	C(312)-C(311)-H(311)	120.4
C(25)-C(26)-H(26B)	109.7	C(313)-C(312)-C(311)	121.6(6)
H(26A)-C(26)-H(26B)	108.2	C(313)-C(312)-H(312)	119.2
C(42)-N(41)-C(46)	117.6(5)	C(311)-C(312)-H(312)	119.2
C(42)-N(41)-Zn(2)	119.1(4)	C(312)-C(313)-C(314)	120.4(6)
C(46)-N(41)-Zn(2)	123.2(4)	C(312)-C(313)-H(313)	119.8
N(41)-C(42)-C(43)	123.8(6)	C(314)-C(313)-H(313)	119.8
N(41)-C(42)-H(42)	118.1	C(309)-C(314)-C(313)	116.9(6)
C(43)-C(42)-H(42)	118.1	C(309)-C(314)-C(301)	119.8(6)
C(42)-C(43)-C(44)	118.0(6)	C(313)-C(314)-C(301)	123.2(6)
C(42)-C(43)-H(43)	121.0	N(21)-C(315)-C(303)	126.0(5)
C(44)-C(43)-H(43)	121.0	N(21)-C(315)-H(315)	117.0
C(45)-C(44)-C(43)	119.0(5)	C(303)-C(315)-H(315)	117.0
C(45)-C(44)-H(44)	120.5	C(406)-C(401)-C(414)	118.4(6)
C(43)-C(44)-H(44)	120.5	C(406)-C(401)-C(402)	118.1(6)
C(44)-C(45)-C(46)	119.0(6)	C(414)-C(401)-C(402)	123.4(6)
C(44)-C(45)-H(45)	120.5	O(402)-C(402)-C(403)	122.2(5)
C(46)-C(45)-H(45)	120.5	O(402)-C(402)-C(401)	120.3(5)
N(41)-C(46)-C(45)	122.5(6)	C(403)-C(402)-C(401)	117.5(6)
N(41)-C(46)-H(46)	118.8	C(402)-O(402)-Zn(2)	132.3(4)
C(45)-C(46)-H(46)	118.8	C(402)-C(403)-C(404)	120.8(6)
C(306)-C(301)-C(302)	117.6(6)	C(402)-C(403)-C(415)	123.4(6)
C(306)-C(301)-C(314)	118.1(6)	C(404)-C(403)-C(415)	115.6(6)
C(302)-C(301)-C(314)	124.3(5)	C(405)-C(404)-C(403)	121.5(6)
O(302)-C(302)-C(303)	123.2(6)	C(405)-C(404)-H(404)	119.3
O(302)-C(302)-C(301)	118.3(5)	C(403)-C(404)-H(404)	119.3

C(404)-C(405)-C(406)	119.9(7)	C(409)-C(410)-H(410)	119.5
C(404)-C(405)-H(405)	120.0	C(410)-C(411)-C(412)	120.5(6)
C(406)-C(405)-H(405)	120.0	C(410)-C(411)-H(411)	119.8
C(405)-C(406)-C(401)	122.2(6)	C(412)-C(411)-H(411)	119.8
C(405)-C(406)-C(407)	118.8(6)	C(413)-C(412)-C(411)	120.2(7)
C(401)-C(406)-C(407)	119.0(6)	C(413)-C(412)-H(412)	119.9
C(408)-C(407)-C(406)	122.3(7)	C(411)-C(412)-H(412)	119.9
C(408)-C(407)-H(407)	118.8	C(412)-C(413)-C(414)	122.4(6)
C(406)-C(407)-H(407)	118.8	C(412)-C(413)-H(413)	118.8
C(407)-C(408)-C(409)	120.8(6)	C(414)-C(413)-H(413)	118.8
C(407)-C(408)-H(408)	119.6	C(413)-C(414)-C(409)	115.0(6)
C(409)-C(408)-H(408)	119.6	C(413)-C(414)-C(401)	125.0(6)
C(410)-C(409)-C(408)	119.7(6)	C(409)-C(414)-C(401)	120.0(7)
C(410)-C(409)-C(414)	120.8(7)	N(22)-C(415)-C(403)	127.9(6)
C(408)-C(409)-C(414)	119.4(6)	N(22)-C(415)-H(415)	116.1
C(411)-C(410)-C(409)	121.0(6)	C(403)-C(415)-H(415)	116.1
C(411)-C(410)-H(410)	119.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*,*R*)-**53**·py. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	19(1)	27(1)	22(1)	0(1)	0(1)	1(1)
C(11)	27(2)	33(2)	25(2)	0(2)	0(2)	-1(2)
N(11)	29(2)	28(2)	24(2)	-3(2)	-4(2)	-2(2)
C(12)	26(2)	35(3)	22(2)	0(2)	-2(2)	0(2)
N(12)	23(2)	31(3)	23(2)	1(2)	0(2)	1(2)
C(13)	34(3)	42(5)	24(3)	0(3)	-4(3)	7(3)
C(14)	33(2)	55(3)	21(2)	6(2)	-4(2)	1(2)
C(15)	48(3)	51(4)	27(2)	-1(2)	-9(2)	-6(3)
C(16)	48(4)	44(5)	31(4)	-7(3)	-10(3)	-10(3)
N(31)	18(2)	34(3)	24(2)	-3(2)	1(2)	0(2)
C(32)	25(3)	21(3)	34(3)	-3(3)	2(2)	-7(2)
C(33)	28(3)	37(4)	40(3)	-2(3)	5(3)	-8(3)
C(34)	21(3)	49(5)	33(3)	-7(3)	2(2)	-9(3)
C(35)	21(3)	46(5)	29(3)	-6(3)	-5(2)	7(2)
C(36)	30(3)	31(4)	24(3)	0(3)	2(2)	3(3)
C(101)	18(2)	19(4)	40(3)	-1(3)	-1(2)	-6(2)
C(102)	22(2)	27(4)	28(3)	-5(3)	4(2)	-5(2)
O(102)	23(2)	26(3)	27(2)	-1(2)	2(2)	5(2)
C(103)	29(2)	23(3)	35(3)	-3(2)	1(2)	-5(2)
C(104)	55(3)	25(4)	42(3)	-7(3)	16(3)	8(3)
C(105)	47(3)	29(4)	52(4)	-7(3)	17(3)	8(3)
C(106)	26(3)	26(4)	47(4)	-2(3)	1(2)	-1(2)
C(107)	39(3)	20(4)	75(5)	4(4)	9(3)	14(3)
C(108)	39(3)	38(5)	46(4)	4(3)	-5(3)	10(3)
C(109)	26(3)	31(4)	48(4)	6(3)	-6(3)	-6(2)

C(110)	39(3)	34(4)	43(4)	11(3)	-9(3)	2(3)
C(111)	38(3)	40(4)	32(3)	9(3)	-6(2)	-6(3)
C(112)	37(3)	39(4)	37(4)	0(3)	6(3)	1(3)
C(113)	28(3)	32(4)	37(4)	9(3)	2(2)	0(3)
C(114)	22(3)	20(4)	40(4)	11(3)	0(2)	-3(2)
C(115)	35(2)	28(3)	23(2)	-5(2)	7(2)	-10(2)
C(201)	16(2)	32(4)	28(3)	1(3)	0(2)	-1(2)
C(202)	20(2)	21(4)	36(3)	-8(3)	7(2)	-5(2)
O(202)	28(2)	27(3)	27(2)	-2(2)	-5(2)	0(2)
C(203)	24(2)	36(4)	23(3)	0(3)	3(2)	-2(2)
C(204)	34(3)	32(4)	40(4)	7(3)	-2(2)	-1(2)
C(205)	43(3)	25(4)	40(3)	3(3)	1(2)	-3(2)
C(206)	33(3)	39(4)	37(3)	-6(3)	7(2)	-4(3)
C(207)	44(3)	33(4)	44(4)	-8(3)	2(3)	-6(3)
C(208)	42(3)	44(4)	37(3)	-12(3)	-4(2)	-10(3)
C(209)	21(2)	39(4)	32(3)	-7(3)	0(2)	2(2)
C(210)	33(3)	48(5)	33(3)	-16(4)	-1(3)	-3(3)
C(211)	31(3)	60(6)	31(3)	-8(4)	-12(2)	16(3)
C(212)	35(3)	33(4)	34(3)	-1(3)	-1(2)	5(2)
C(213)	22(2)	40(4)	21(3)	-6(3)	-1(2)	7(2)
C(214)	14(2)	38(4)	28(3)	-3(3)	2(2)	2(3)
C(215)	24(2)	32(3)	23(2)	3(2)	4(2)	2(2)
Zn(2)	20(1)	28(1)	23(1)	0(1)	0(1)	0(1)
C(21)	26(2)	41(3)	23(2)	3(2)	-5(2)	-3(2)
N(21)	28(2)	29(3)	26(2)	1(2)	-1(2)	-3(2)
C(22)	28(2)	36(3)	20(2)	0(2)	-2(2)	-1(2)
N(22)	23(2)	30(3)	21(2)	0(2)	-1(1)	3(2)
C(23)	37(3)	37(5)	31(3)	6(3)	-5(3)	-1(3)
C(24)	34(2)	54(3)	26(2)	7(2)	-7(2)	1(2)
C(25)	36(2)	55(3)	23(2)	-2(2)	-8(2)	-4(2)
C(26)	42(3)	39(4)	26(3)	-1(3)	-1(3)	-3(3)
N(41)	20(2)	27(3)	21(2)	-2(2)	0(2)	-3(2)
C(42)	23(3)	37(4)	41(4)	-8(3)	3(2)	6(2)
C(43)	34(3)	34(4)	49(4)	-6(3)	7(3)	-14(3)
C(44)	15(2)	60(5)	36(3)	-7(3)	3(2)	-1(3)
C(45)	22(3)	50(5)	31(3)	-3(3)	3(2)	13(3)
C(46)	23(3)	38(4)	24(3)	0(3)	-2(2)	6(3)
C(301)	21(2)	23(4)	39(3)	0(3)	2(2)	-1(2)
C(302)	16(2)	19(4)	45(4)	2(3)	2(2)	-3(2)
O(302)	31(2)	29(3)	27(2)	-2(2)	-1(2)	7(2)
C(303)	30(2)	25(3)	34(3)	-3(2)	8(2)	-3(2)
C(304)	51(3)	37(4)	36(3)	-3(3)	7(2)	-3(3)
C(305)	53(3)	27(4)	50(4)	-6(3)	13(3)	1(3)
C(306)	31(3)	21(4)	56(4)	4(3)	7(3)	-2(2)
C(307)	39(3)	30(4)	57(5)	-6(4)	-1(3)	2(3)
C(308)	37(3)	26(4)	73(5)	13(4)	-12(3)	6(3)
C(309)	31(3)	26(4)	47(4)	4(3)	-5(3)	1(3)
C(310)	44(3)	36(4)	50(4)	13(4)	-12(3)	-6(3)
C(311)	41(3)	51(5)	37(3)	6(3)	-5(3)	-7(3)
C(312)	37(3)	41(4)	38(4)	8(3)	-3(3)	-3(3)
C(313)	28(3)	34(4)	33(3)	2(3)	-3(2)	0(3)
C(314)	24(3)	28(4)	36(4)	-1(3)	-3(2)	-10(2)
C(315)	35(3)	26(3)	35(3)	-5(2)	6(2)	-9(2)
C(401)	21(2)	28(4)	30(3)	-6(3)	7(2)	-1(2)

C(402)	16(2)	35(4)	21(3)	1(3)	4(2)	6(3)
O(402)	30(2)	25(3)	27(2)	1(2)	-7(2)	-1(2)
C(403)	26(2)	25(4)	28(3)	0(3)	-2(2)	-2(2)
C(404)	46(3)	33(4)	31(3)	3(3)	4(2)	0(3)
C(405)	49(3)	26(4)	47(4)	-2(3)	7(3)	-12(3)
C(406)	33(3)	26(4)	35(3)	-3(3)	6(2)	-6(2)
C(407)	39(3)	33(4)	48(4)	-11(3)	7(3)	-16(2)
C(408)	35(3)	44(4)	37(3)	-11(3)	-3(2)	-2(2)
C(409)	22(2)	35(4)	35(3)	-11(3)	2(2)	-1(2)
C(410)	32(3)	54(5)	26(3)	-8(4)	-11(2)	14(3)
C(411)	43(3)	38(5)	29(3)	5(3)	-6(3)	9(3)
C(412)	31(3)	44(4)	29(3)	-2(3)	-7(2)	11(2)
C(413)	24(3)	33(4)	31(3)	-4(3)	-4(2)	-2(2)
C(414)	23(3)	34(4)	28(3)	-10(3)	4(2)	-1(3)
C(415)	30(2)	32(3)	32(3)	10(2)	3(2)	3(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**53**·py.

	x	y	z	U(eq)
H(11)	4421	2936	7115	34
H(12)	7392	2688	6506	33
H(13A)	7190	1644	7065	41
H(13B)	5602	1876	7417	41
H(14A)	7788	2001	8330	44
H(14B)	8692	2448	7766	44
H(15A)	5826	2798	8419	51
H(15B)	7521	3139	8606	51
H(16A)	7407	3603	7411	50
H(16B)	5812	3792	7785	50
H(32)	6930	4175	4642	32
H(33)	9515	4378	4337	42
H(34)	11354	3524	4388	41
H(35)	10571	2485	4759	39
H(36)	7998	2326	5082	34
H(104)	2735	5124	6700	48
H(105)	1171	5797	5948	50
H(107)	163	6178	4721	53
H(108)	34	6143	3449	49
H(110)	942	5699	2304	47
H(111)	2399	4977	1667	45
H(112)	4016	4215	2349	45
H(113)	4091	4159	3632	39
H(115)	4169	4173	6929	34
H(204)	4213	550	5546	43
H(205)	3011	51	4501	44
H(207)	1825	79	3232	49
H(208)	953	617	2175	50

H(210)	688	1613	1443	46
H(211)	783	2745	1339	50
H(212)	1715	3366	2405	41
H(213)	2625	2862	3506	34
H(215)	5259	1419	6206	32
H(21)	2647	6839	-1620	36
H(22)	5492	7437	-2026	34
H(23A)	2350	7981	-2017	42
H(23B)	3876	8388	-2227	42
H(24A)	2381	7997	-3339	47
H(24B)	4153	7712	-3274	47
H(25A)	2423	6866	-3619	46
H(25B)	1382	7018	-2934	46
H(26A)	2965	6103	-2597	43
H(26B)	4543	6478	-2795	43
H(42)	2995	5883	373	40
H(43)	409	5674	635	47
H(44)	-1435	6535	547	45
H(45)	-591	7569	215	41
H(46)	2004	7712	-86	35
H(304)	6924	4868	-1709	49
H(305)	8511	4156	-981	51
H(307)	9700	3807	244	51
H(308)	9843	3850	1506	56
H(310)	8909	4247	2662	53
H(311)	7365	4954	3307	52
H(312)	5839	5748	2646	47
H(313)	5793	5832	1362	38
H(315)	5210	5704	-1904	39
H(404)	6053	9438	-543	44
H(405)	7327	9925	493	49
H(407)	8636	9870	1734	48
H(408)	9380	9326	2820	47
H(410)	9490	8341	3568	46
H(411)	9035	7248	3702	45
H(412)	7945	6632	2690	42
H(413)	7182	7128	1556	35
H(415)	5333	8538	-1253	37

Table 6. Torsion angles [°] for (*R*,*R*)-**53**·py.

C(16)-C(11)-N(11)-C(115)	-54.4(6)	O(202)-Zn(1)-N(11)-C(11)	77.4(4)
C(12)-C(11)-N(11)-C(115)	-177.6(4)	O(102)-Zn(1)-N(11)-C(11)	175.6(3)
C(16)-C(11)-N(11)-Zn(1)	142.3(3)	N(12)-Zn(1)-N(11)-C(11)	5.7(3)
C(12)-C(11)-N(11)-Zn(1)	19.1(4)	N(31)-Zn(1)-N(11)-C(11)	-89.0(3)
O(202)-Zn(1)-N(11)-C(115)	-84.4(5)	N(11)-C(11)-C(12)-N(12)	-43.4(4)
O(102)-Zn(1)-N(11)-C(115)	13.7(4)	C(16)-C(11)-C(12)-N(12)	-170.8(4)
N(12)-Zn(1)-N(11)-C(115)	-156.2(4)	N(11)-C(11)-C(12)-C(13)	-172.0(4)
N(31)-Zn(1)-N(11)-C(115)	109.2(4)	C(16)-C(11)-C(12)-C(13)	60.5(5)

C(13)-C(12)-N(12)-C(215)	-3.2(6)	C(102)-C(101)-C(106)-C(105)	3.0(9)
C(11)-C(12)-N(12)-C(215)	-126.6(4)	C(114)-C(101)-C(106)-C(105)	-176.5(5)
C(13)-C(12)-N(12)-Zn(1)	172.6(3)	C(102)-C(101)-C(106)-C(107)	-174.1(5)
C(11)-C(12)-N(12)-Zn(1)	49.2(4)	C(114)-C(101)-C(106)-C(107)	6.4(9)
O(202)-Zn(1)-N(12)-C(215)	0.1(4)	C(105)-C(106)-C(107)-C(108)	179.1(6)
O(102)-Zn(1)-N(12)-C(215)	106.1(7)	C(101)-C(106)-C(107)-C(108)	-3.8(10)
N(11)-Zn(1)-N(12)-C(215)	144.7(4)	C(106)-C(107)-C(108)-C(109)	-0.9(11)
N(31)-Zn(1)-N(12)-C(215)	-109.4(4)	C(107)-C(108)-C(109)-C(110)	-177.0(6)
O(202)-Zn(1)-N(12)-C(12)	-175.5(3)	C(107)-C(108)-C(109)-C(114)	2.8(10)
O(102)-Zn(1)-N(12)-C(12)	-69.4(7)	C(108)-C(109)-C(110)-C(111)	179.2(6)
N(11)-Zn(1)-N(12)-C(12)	-30.9(3)	C(114)-C(109)-C(110)-C(111)	-0.6(10)
N(31)-Zn(1)-N(12)-C(12)	75.1(3)	C(109)-C(110)-C(111)-C(112)	-0.3(10)
N(12)-C(12)-C(13)-C(14)	177.0(4)	C(110)-C(111)-C(112)-C(113)	1.1(10)
C(11)-C(12)-C(13)-C(14)	-61.0(5)	C(111)-C(112)-C(113)-C(114)	-0.9(10)
C(12)-C(13)-C(14)-C(15)	57.3(5)	C(112)-C(113)-C(114)-C(109)	-0.1(9)
C(13)-C(14)-C(15)-C(16)	-54.3(6)	C(112)-C(113)-C(114)-C(101)	-178.9(6)
C(14)-C(15)-C(16)-C(11)	54.8(6)	C(108)-C(109)-C(114)-C(113)	-179.0(6)
N(11)-C(11)-C(16)-C(15)	-179.8(4)	C(110)-C(109)-C(114)-C(113)	0.8(9)
C(12)-C(11)-C(16)-C(15)	-57.1(5)	C(108)-C(109)-C(114)-C(101)	0.0(9)
O(202)-Zn(1)-N(31)-C(36)	-68.4(5)	C(110)-C(109)-C(114)-C(101)	179.8(5)
O(102)-Zn(1)-N(31)-C(36)	-167.5(4)	C(106)-C(101)-C(114)-C(113)	174.3(6)
N(11)-Zn(1)-N(31)-C(36)	102.8(5)	C(102)-C(101)-C(114)-C(113)	-5.1(9)
N(12)-Zn(1)-N(31)-C(36)	21.9(5)	C(106)-C(101)-C(114)-C(109)	-4.5(8)
O(202)-Zn(1)-N(31)-C(32)	115.3(4)	C(102)-C(101)-C(114)-C(109)	176.0(5)
O(102)-Zn(1)-N(31)-C(32)	16.2(4)	C(11)-N(11)-C(115)-C(103)	-171.0(4)
N(11)-Zn(1)-N(31)-C(32)	-73.4(4)	Zn(1)-N(11)-C(115)-C(103)	-9.5(7)
N(12)-Zn(1)-N(31)-C(32)	-154.3(4)	C(104)-C(103)-C(115)-N(11)	176.9(5)
C(36)-N(31)-C(32)-C(33)	-0.7(8)	C(102)-C(103)-C(115)-N(11)	-0.4(9)
Zn(1)-N(31)-C(32)-C(33)	175.7(4)	C(206)-C(201)-C(202)-O(202)	-179.3(4)
N(31)-C(32)-C(33)-C(34)	1.0(9)	C(214)-C(201)-C(202)-O(202)	1.5(7)
C(32)-C(33)-C(34)-C(35)	-0.4(9)	C(206)-C(201)-C(202)-C(203)	0.8(7)
C(33)-C(34)-C(35)-C(36)	-0.4(9)	C(214)-C(201)-C(202)-C(203)	-178.4(4)
C(32)-N(31)-C(36)-C(35)	-0.2(8)	C(203)-C(202)-O(202)-Zn(1)	10.5(7)
Zn(1)-N(31)-C(36)-C(35)	-176.4(4)	C(201)-C(202)-O(202)-Zn(1)	-169.4(3)
C(34)-C(35)-C(36)-N(31)	0.7(9)	O(102)-Zn(1)-O(202)-C(202)	-171.9(4)
C(106)-C(101)-C(102)-O(102)	173.8(5)	N(11)-Zn(1)-O(202)-C(202)	-76.7(5)
C(114)-C(101)-C(102)-O(102)	-6.7(9)	N(12)-Zn(1)-O(202)-C(202)	-7.7(4)
C(106)-C(101)-C(102)-C(103)	-4.4(8)	N(31)-Zn(1)-O(202)-C(202)	89.5(4)
C(114)-C(101)-C(102)-C(103)	175.0(5)	O(202)-C(202)-C(203)-C(204)	177.7(4)
C(103)-C(102)-O(102)-Zn(1)	11.6(8)	C(201)-C(202)-C(203)-C(204)	-2.4(7)
C(101)-C(102)-O(102)-Zn(1)	-166.7(4)	O(202)-C(202)-C(203)-C(215)	-4.1(7)
O(202)-Zn(1)-O(102)-C(102)	126.8(5)	C(201)-C(202)-C(203)-C(215)	175.8(4)
N(11)-Zn(1)-O(102)-C(102)	-15.8(5)	C(202)-C(203)-C(204)-C(205)	2.4(8)
N(12)-Zn(1)-O(102)-C(102)	22.0(9)	C(215)-C(203)-C(204)-C(205)	-175.9(5)
N(31)-Zn(1)-O(102)-C(102)	-122.7(5)	C(203)-C(204)-C(205)-C(206)	-0.9(9)
O(102)-C(102)-C(103)-C(104)	-177.2(5)	C(202)-C(201)-C(206)-C(205)	0.7(7)
C(101)-C(102)-C(103)-C(104)	1.1(8)	C(214)-C(201)-C(206)-C(205)	179.9(5)
O(102)-C(102)-C(103)-C(115)	0.1(8)	C(202)-C(201)-C(206)-C(207)	-177.1(5)
C(101)-C(102)-C(103)-C(115)	178.4(5)	C(214)-C(201)-C(206)-C(207)	2.1(7)
C(102)-C(103)-C(104)-C(105)	4.1(10)	C(204)-C(205)-C(206)-C(201)	-0.7(8)
C(115)-C(103)-C(104)-C(105)	-173.3(6)	C(204)-C(205)-C(206)-C(207)	177.1(5)
C(103)-C(104)-C(105)-C(106)	-5.8(11)	C(201)-C(206)-C(207)-C(208)	-0.6(9)
C(104)-C(105)-C(106)-C(101)	2.3(10)	C(205)-C(206)-C(207)-C(208)	-178.5(5)
C(104)-C(105)-C(106)-C(107)	179.3(6)	C(206)-C(207)-C(208)-C(209)	1.5(9)

C(207)-C(208)-C(209)-C(210)	178.7(5)	C(22)-C(21)-C(26)-C(25)	-57.0(5)
C(207)-C(208)-C(209)-C(214)	-4.0(8)	C(24)-C(25)-C(26)-C(21)	53.2(5)
C(208)-C(209)-C(210)-C(211)	176.2(5)	O(302)-Zn(2)-N(41)-C(42)	-16.8(4)
C(214)-C(209)-C(210)-C(211)	-1.1(8)	O(402)-Zn(2)-N(41)-C(42)	-115.0(4)
C(209)-C(210)-C(211)-C(212)	-0.4(8)	N(22)-Zn(2)-N(41)-C(42)	152.0(4)
C(210)-C(211)-C(212)-C(213)	1.6(8)	N(21)-Zn(2)-N(41)-C(42)	71.1(4)
C(211)-C(212)-C(213)-C(214)	-1.3(8)	O(302)-Zn(2)-N(41)-C(46)	167.6(4)
C(212)-C(213)-C(214)-C(209)	-0.3(7)	O(402)-Zn(2)-N(41)-C(46)	69.5(5)
C(212)-C(213)-C(214)-C(201)	178.4(5)	N(22)-Zn(2)-N(41)-C(46)	-23.6(5)
C(210)-C(209)-C(214)-C(213)	1.4(7)	N(21)-Zn(2)-N(41)-C(46)	-104.4(5)
C(208)-C(209)-C(214)-C(213)	-175.9(5)	C(46)-N(41)-C(42)-C(43)	2.1(9)
C(210)-C(209)-C(214)-C(201)	-177.4(4)	Zn(2)-N(41)-C(42)-C(43)	-173.7(5)
C(208)-C(209)-C(214)-C(201)	5.4(7)	N(41)-C(42)-C(43)-C(44)	-1.6(10)
C(206)-C(201)-C(214)-C(213)	176.9(5)	C(42)-C(43)-C(44)-C(45)	-0.5(10)
C(202)-C(201)-C(214)-C(213)	-3.9(7)	C(43)-C(44)-C(45)-C(46)	1.9(9)
C(206)-C(201)-C(214)-C(209)	-4.4(7)	C(42)-N(41)-C(46)-C(45)	-0.6(8)
C(202)-C(201)-C(214)-C(209)	174.8(4)	Zn(2)-N(41)-C(46)-C(45)	175.1(4)
C(12)-N(12)-C(215)-C(203)	179.6(4)	C(44)-C(45)-C(46)-N(41)	-1.4(9)
Zn(1)-N(12)-C(215)-C(203)	4.6(7)	C(306)-C(301)-C(302)-O(302)	-169.4(5)
C(204)-C(203)-C(215)-N(12)	174.8(5)	C(314)-C(301)-C(302)-O(302)	8.7(8)
C(202)-C(203)-C(215)-N(12)	-3.5(8)	C(306)-C(301)-C(302)-C(303)	12.2(8)
C(26)-C(21)-N(21)-C(315)	2.0(6)	C(314)-C(301)-C(302)-C(303)	-169.7(5)
C(22)-C(21)-N(21)-C(315)	-123.4(5)	C(303)-C(302)-O(302)-Zn(2)	-11.3(8)
C(26)-C(21)-N(21)-Zn(2)	174.2(3)	C(301)-C(302)-O(302)-Zn(2)	170.4(4)
C(22)-C(21)-N(21)-Zn(2)	48.8(4)	O(402)-Zn(2)-O(302)-C(302)	-134.7(5)
O(302)-Zn(2)-N(21)-C(315)	-17.1(4)	N(22)-Zn(2)-O(302)-C(302)	-37.5(7)
O(402)-Zn(2)-N(21)-C(315)	78.4(6)	N(41)-Zn(2)-O(302)-C(302)	117.0(5)
N(22)-Zn(2)-N(21)-C(315)	141.4(4)	N(21)-Zn(2)-O(302)-C(302)	18.8(5)
N(41)-Zn(2)-N(21)-C(315)	-114.7(4)	O(302)-C(302)-C(303)-C(304)	173.2(5)
O(302)-Zn(2)-N(21)-C(21)	170.9(3)	C(301)-C(302)-C(303)-C(304)	-8.5(8)
O(402)-Zn(2)-N(21)-C(21)	-93.7(4)	O(302)-C(302)-C(303)-C(315)	-6.1(9)
N(22)-Zn(2)-N(21)-C(21)	-30.7(3)	C(301)-C(302)-C(303)-C(315)	172.2(5)
N(41)-Zn(2)-N(21)-C(21)	73.2(3)	C(302)-C(303)-C(304)-C(305)	1.3(10)
N(21)-C(21)-C(22)-N(22)	-43.4(4)	C(315)-C(303)-C(304)-C(305)	-179.4(5)
C(26)-C(21)-C(22)-N(22)	-172.3(4)	C(303)-C(304)-C(305)-C(306)	2.2(10)
N(21)-C(21)-C(22)-C(23)	-169.9(3)	C(302)-C(301)-C(306)-C(305)	-9.1(9)
C(26)-C(21)-C(22)-C(23)	61.3(5)	C(314)-C(301)-C(306)-C(305)	172.7(5)
C(21)-C(22)-N(22)-C(415)	-173.5(4)	C(302)-C(301)-C(306)-C(307)	172.8(5)
C(23)-C(22)-N(22)-C(415)	-49.8(5)	C(314)-C(301)-C(306)-C(307)	-5.5(9)
C(21)-C(22)-N(22)-Zn(2)	18.8(4)	C(304)-C(305)-C(306)-C(301)	2.0(10)
C(23)-C(22)-N(22)-Zn(2)	142.5(3)	C(304)-C(305)-C(306)-C(307)	-179.9(6)
O(302)-Zn(2)-N(22)-C(415)	-103.0(5)	C(301)-C(306)-C(307)-C(308)	3.6(10)
O(402)-Zn(2)-N(22)-C(415)	-4.2(4)	C(305)-C(306)-C(307)-C(308)	-174.6(6)
N(41)-Zn(2)-N(22)-C(415)	103.2(4)	C(306)-C(307)-C(308)-C(309)	1.8(10)
N(21)-Zn(2)-N(22)-C(415)	-160.8(4)	C(307)-C(308)-C(309)-C(314)	-5.2(10)
O(302)-Zn(2)-N(22)-C(22)	64.0(5)	C(307)-C(308)-C(309)-C(310)	174.7(7)
O(402)-Zn(2)-N(22)-C(22)	162.7(3)	C(314)-C(309)-C(310)-C(311)	1.5(11)
N(41)-Zn(2)-N(22)-C(22)	-89.8(3)	C(308)-C(309)-C(310)-C(311)	-178.4(6)
N(21)-Zn(2)-N(22)-C(22)	6.1(3)	C(309)-C(310)-C(311)-C(312)	-1.2(11)
N(22)-C(22)-C(23)-C(24)	177.4(4)	C(310)-C(311)-C(312)-C(313)	0.5(11)
C(21)-C(22)-C(23)-C(24)	-59.0(5)	C(311)-C(312)-C(313)-C(314)	0.0(10)
C(22)-C(23)-C(24)-C(25)	56.0(5)	C(310)-C(309)-C(314)-C(313)	-1.0(10)
C(23)-C(24)-C(25)-C(26)	-53.9(5)	C(308)-C(309)-C(314)-C(313)	178.9(6)
N(21)-C(21)-C(26)-C(25)	179.9(4)	C(310)-C(309)-C(314)-C(301)	-176.9(6)

C(308)-C(309)-C(314)-C(301)	3.0(9)	C(404)-C(405)-C(406)-C(407)	179.0(5)
C(312)-C(313)-C(314)-C(309)	0.3(9)	C(414)-C(401)-C(406)-C(405)	-179.4(5)
C(312)-C(313)-C(314)-C(301)	176.0(6)	C(402)-C(401)-C(406)-C(405)	-1.1(8)
C(306)-C(301)-C(314)-C(309)	2.1(9)	C(414)-C(401)-C(406)-C(407)	2.0(7)
C(302)-C(301)-C(314)-C(309)	-176.0(5)	C(402)-C(401)-C(406)-C(407)	-179.7(5)
C(306)-C(301)-C(314)-C(313)	-173.5(6)	C(405)-C(406)-C(407)-C(408)	178.4(5)
C(302)-C(301)-C(314)-C(313)	8.4(9)	C(401)-C(406)-C(407)-C(408)	-3.0(8)
C(21)-N(21)-C(315)-C(303)	179.6(4)	C(406)-C(407)-C(408)-C(409)	2.2(9)
Zn(2)-N(21)-C(315)-C(303)	8.7(7)	C(407)-C(408)-C(409)-C(410)	-176.2(5)
C(304)-C(303)-C(315)-N(21)	-172.6(5)	C(407)-C(408)-C(409)-C(414)	-0.5(8)
C(302)-C(303)-C(315)-N(21)	6.7(8)	C(408)-C(409)-C(410)-C(411)	178.6(5)
C(406)-C(401)-C(402)-O(402)	-179.3(4)	C(414)-C(409)-C(410)-C(411)	3.0(8)
C(414)-C(401)-C(402)-O(402)	-1.0(7)	C(409)-C(410)-C(411)-C(412)	0.5(8)
C(406)-C(401)-C(402)-C(403)	1.7(7)	C(410)-C(411)-C(412)-C(413)	-2.1(8)
C(414)-C(401)-C(402)-C(403)	179.9(4)	C(411)-C(412)-C(413)-C(414)	0.3(8)
C(403)-C(402)-O(402)-Zn(2)	-5.9(7)	C(412)-C(413)-C(414)-C(409)	2.9(7)
C(401)-C(402)-O(402)-Zn(2)	175.1(3)	C(412)-C(413)-C(414)-C(401)	-176.9(5)
O(302)-Zn(2)-O(402)-C(402)	164.2(4)	C(410)-C(409)-C(414)-C(413)	-4.5(7)
N(22)-Zn(2)-O(402)-C(402)	9.6(4)	C(408)-C(409)-C(414)-C(413)	179.8(5)
N(41)-Zn(2)-O(402)-C(402)	-95.7(4)	C(410)-C(409)-C(414)-C(401)	175.3(5)
N(21)-Zn(2)-O(402)-C(402)	70.7(6)	C(408)-C(409)-C(414)-C(401)	-0.3(7)
O(402)-C(402)-C(403)-C(404)	179.3(4)	C(406)-C(401)-C(414)-C(413)	179.4(4)
C(401)-C(402)-C(403)-C(404)	-1.6(7)	C(402)-C(401)-C(414)-C(413)	1.2(8)
O(402)-C(402)-C(403)-C(415)	-6.2(7)	C(406)-C(401)-C(414)-C(409)	-0.5(7)
C(401)-C(402)-C(403)-C(415)	172.9(4)	C(402)-C(401)-C(414)-C(409)	-178.7(4)
C(402)-C(403)-C(404)-C(405)	0.9(8)	C(22)-N(22)-C(415)-C(403)	-170.8(4)
C(415)-C(403)-C(404)-C(405)	-174.0(5)	Zn(2)-N(22)-C(415)-C(403)	-4.4(7)
C(403)-C(404)-C(405)-C(406)	-0.3(9)	C(402)-C(403)-C(415)-N(22)	11.6(8)
C(404)-C(405)-C(406)-C(401)	0.4(9)	C(404)-C(403)-C(415)-N(22)	-173.6(5)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*,*R*)-**54**·py.

Identification code	(*R*,*R*)-**54**·py	
Empirical formula	C41 H33 Fe N3 O2	
Formula weight	655.55	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 8.386(3) Å	α = 90°.
	b = 20.709(7) Å	β = 94.86(2)°.
	c = 17.704(6) Å	γ = 90°.
Volume	3063.3(17) $Å^3$	
Z	4	
Density (calculated)	1.421 g/cm^3	
Absorption coefficient	0.536 mm^{-1}	
F(000)	1368	
Crystal size	0.40 x 0.40 x 0.15 mm^3	
Theta range for data collection	1.15 to 28.32°.	
Index ranges	-11<=h<=11, -26<=k<=25, -22<=l<=21	
Reflections collected	35237	
Independent reflections	11319 [R(int) = 0.0487]	
Completeness to theta = 28.32°	92.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11319 / 1 / 847	
Goodness-of-fit on F^2	0.955	
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0784	
R indices (all data)	R1 = 0.0562, wR2 = 0.0852	
Absolute structure parameter	-0.031(15)	
Largest diff. peak and hole	0.229 and -0.606 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**54**·py. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4878(1)	3105(1)	5193(1)	23(1)
C(01)	2557(5)	888(3)	3828(3)	37(1)
C(02)	3061(5)	522(3)	4468(3)	39(1)
C(03)	3787(5)	812(2)	5087(3)	37(1)
C(04)	4104(5)	1477(2)	5109(2)	29(1)
C(05)	3593(4)	1870(2)	4472(2)	25(1)
O(05)	3855(3)	2489(2)	4479(2)	28(1)
C(06)	2781(5)	1563(2)	3814(3)	27(1)
C(07)	2227(4)	1911(3)	3127(2)	28(1)
C(08)	2248(4)	2591(2)	3052(2)	29(1)
C(09)	1702(5)	2889(2)	2378(2)	35(1)
C(10)	1148(5)	2536(3)	1750(3)	40(1)
C(11)	1103(5)	1881(3)	1806(2)	38(1)
C(12)	1594(5)	1559(2)	2482(2)	31(1)

C(13)	1418(5)	869(2)	2533(3)	40(1)
C(14)	1873(5)	559(3)	3165(3)	42(1)
C(15)	4985(4)	1722(2)	5778(2)	30(1)
N(15)	5395(4)	2313(2)	5892(2)	26(1)
C(16)	6323(4)	2512(2)	6591(2)	27(1)
C(17)	6619(5)	2014(2)	7217(2)	33(1)
C(18)	7681(4)	2302(2)	7869(2)	37(1)
C(21)	1825(5)	5425(2)	4976(3)	34(1)
C(22)	1941(5)	5482(3)	5770(3)	44(1)
C(23)	2822(5)	5066(2)	6206(3)	39(1)
C(24)	3577(5)	4532(2)	5894(2)	30(1)
C(25)	3478(4)	4445(2)	5094(2)	25(1)
O(25)	4092(3)	3944(1)	4800(2)	27(1)
C(26)	2635(5)	4923(2)	4625(3)	29(1)
C(27)	2578(5)	4922(2)	3796(3)	27(1)
C(28)	3426(5)	4486(2)	3369(3)	35(1)
C(29)	3366(5)	4520(3)	2605(3)	41(1)
C(30)	2415(5)	4971(3)	2199(3)	41(1)
C(31)	1570(5)	5392(3)	2589(3)	43(1)
C(32)	1617(5)	5390(2)	3384(3)	35(1)
C(33)	750(5)	5845(3)	3773(3)	43(1)
C(34)	875(5)	5875(2)	4525(3)	43(1)
C(35)	4331(4)	4068(2)	6416(2)	29(1)
N(35)	5016(4)	3538(2)	6257(2)	26(1)
C(36)	5496(4)	3100(2)	6893(2)	27(1)
C(37)	6587(6)	3402(2)	7534(3)	44(1)
C(38)	6982(5)	2912(2)	8160(2)	44(1)
N(41)	7256(4)	3232(2)	4888(2)	27(1)
C(42)	8301(5)	2752(2)	4881(2)	29(1)
C(43)	9832(5)	2841(3)	4688(3)	37(1)
C(44)	10323(5)	3447(3)	4511(3)	39(1)
C(45)	9253(5)	3946(3)	4511(3)	41(1)
C(46)	7734(5)	3826(2)	4699(3)	30(1)
Fe(2)	5083(1)	6896(1)	-180(1)	24(1)
C(51)	7645(5)	9082(2)	1178(3)	31(1)
C(52)	7208(5)	9448(2)	527(3)	40(1)
C(53)	6444(5)	9171(2)	-82(3)	38(1)
C(54)	6081(5)	8498(2)	-89(2)	28(1)
C(55)	6482(4)	8116(2)	553(2)	25(1)
O(55)	6112(3)	7505(2)	559(2)	27(1)
C(56)	7332(5)	8404(2)	1213(2)	26(1)
C(57)	7826(4)	8056(2)	1900(2)	26(1)
C(58)	7604(5)	7390(2)	2013(2)	30(1)
C(59)	8018(5)	7087(3)	2685(2)	35(1)
C(60)	8678(5)	7450(3)	3303(3)	38(1)
C(61)	8960(5)	8090(3)	3220(2)	39(1)
C(62)	8579(5)	8403(2)	2531(3)	33(1)
C(63)	8886(5)	9066(3)	2467(3)	41(1)
C(64)	8459(5)	9393(3)	1820(3)	41(1)
C(65)	5383(4)	8246(2)	-797(2)	29(1)
N(65)	4898(4)	7661(2)	-941(2)	25(1)
C(66)	4465(4)	7480(2)	-1737(2)	28(1)
C(67)	3379(5)	7955(2)	-2187(2)	37(1)
C(68)	3094(4)	7727(2)	-3007(2)	40(1)

C(71)	8006(5)	4562(2)	2(3)	34(1)
C(72)	7831(5)	4494(2)	-790(3)	42(1)
C(73)	6892(5)	4917(2)	-1214(3)	41(1)
C(74)	6176(5)	5447(2)	-885(2)	31(1)
C(75)	6396(4)	5542(2)	-98(3)	27(1)
O(75)	5865(3)	6063(1)	217(2)	29(1)
C(76)	7234(4)	5060(2)	370(3)	28(1)
C(77)	7300(5)	5067(2)	1191(3)	31(1)
C(78)	6436(5)	5489(2)	1628(2)	33(1)
C(79)	6478(5)	5438(3)	2405(3)	40(1)
C(80)	7420(5)	4968(3)	2790(3)	43(1)
C(81)	8292(6)	4557(3)	2394(3)	45(1)
C(82)	8225(5)	4592(2)	1602(3)	37(1)
C(83)	9116(5)	4135(3)	1193(3)	47(1)
C(84)	9016(5)	4119(3)	436(3)	45(1)
C(85)	5244(4)	5861(2)	-1390(2)	30(1)
N(85)	4646(4)	6406(2)	-1210(2)	26(1)
C(86)	3694(4)	6812(2)	-1758(2)	29(1)
C(87)	3432(5)	6566(2)	-2564(2)	36(1)
C(88)	2399(5)	7046(2)	-3048(2)	40(1)
N(91)	2705(3)	6793(2)	119(2)	25(1)
C(92)	1657(5)	7279(2)	103(2)	31(1)
C(93)	109(5)	7197(3)	280(2)	36(1)
C(94)	-404(5)	6592(3)	470(3)	42(1)
C(95)	643(5)	6089(3)	477(3)	46(1)
C(96)	2183(5)	6215(3)	309(3)	40(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*,*R*)-**54**·py.

Fe(1)-O(05)	1.943(3)	C(11)-C(12)	1.401(6)
Fe(1)-O(25)	1.966(3)	C(12)-C(13)	1.440(6)
Fe(1)-N(15)	2.077(4)	C(13)-C(14)	1.318(7)
Fe(1)-N(35)	2.081(3)	C(15)-N(15)	1.282(5)
Fe(1)-N(41)	2.126(3)	N(15)-C(16)	1.465(4)
C(01)-C(02)	1.399(7)	C(16)-C(17)	1.520(5)
C(01)-C(06)	1.411(6)	C(16)-C(36)	1.520(4)
C(01)-C(14)	1.434(6)	C(17)-C(18)	1.519(5)
C(02)-C(03)	1.349(6)	C(18)-C(38)	1.503(5)
C(03)-C(04)	1.402(6)	C(21)-C(22)	1.406(7)
C(04)-C(05)	1.426(6)	C(21)-C(26)	1.413(6)
C(04)-C(15)	1.435(6)	C(21)-C(34)	1.427(6)
C(05)-O(05)	1.301(5)	C(22)-C(23)	1.337(6)
C(05)-C(06)	1.445(6)	C(23)-C(24)	1.409(6)
C(06)-C(07)	1.455(6)	C(24)-C(25)	1.422(6)
C(07)-C(08)	1.414(7)	C(24)-C(35)	1.443(6)
C(07)-C(12)	1.419(6)	C(25)-O(25)	1.288(5)
C(08)-C(09)	1.386(6)	C(25)-C(26)	1.439(6)
C(09)-C(10)	1.378(6)	C(26)-C(27)	1.466(6)
C(10)-C(11)	1.361(7)	C(27)-C(28)	1.408(6)

C(27)-C(32)	1.421(6)	C(75)-C(76)	1.441(6)
C(28)-C(29)	1.351(6)	C(76)-C(77)	1.451(7)
C(29)-C(30)	1.389(7)	C(77)-C(78)	1.408(6)
C(30)-C(31)	1.349(7)	C(77)-C(82)	1.416(6)
C(31)-C(32)	1.405(7)	C(78)-C(79)	1.376(6)
C(32)-C(33)	1.406(6)	C(79)-C(80)	1.395(7)
C(33)-C(34)	1.327(7)	C(80)-C(81)	1.355(7)
C(35)-N(35)	1.282(5)	C(81)-C(82)	1.401(7)
N(35)-C(36)	1.474(4)	C(82)-C(83)	1.438(7)
C(36)-C(37)	1.529(5)	C(83)-C(84)	1.337(7)
C(37)-C(38)	1.517(6)	C(85)-N(85)	1.285(5)
N(41)-C(42)	1.326(5)	N(85)-C(86)	1.468(4)
N(41)-C(46)	1.346(5)	C(86)-C(87)	1.514(5)
C(42)-C(43)	1.368(6)	C(87)-C(88)	1.531(6)
C(43)-C(44)	1.366(6)	N(91)-C(96)	1.328(6)
C(44)-C(45)	1.367(7)	N(91)-C(92)	1.335(5)
C(45)-C(46)	1.366(5)	C(92)-C(93)	1.371(5)
Fe(2)-O(75)	1.953(3)	C(93)-C(94)	1.374(7)
Fe(2)-O(55)	1.965(3)	C(94)-C(95)	1.362(7)
Fe(2)-N(65)	2.078(4)	C(95)-C(96)	1.374(6)
Fe(2)-N(85)	2.092(3)		
Fe(2)-N(91)	2.116(3)	O(05)-Fe(1)-O(25)	103.49(13)
C(51)-C(52)	1.402(7)	O(05)-Fe(1)-N(15)	85.86(14)
C(51)-C(64)	1.429(6)	O(25)-Fe(1)-N(15)	162.89(12)
C(51)-C(56)	1.432(6)	O(05)-Fe(1)-N(35)	149.23(12)
C(52)-C(53)	1.337(6)	O(25)-Fe(1)-N(35)	86.05(13)
C(53)-C(54)	1.426(6)	N(15)-Fe(1)-N(35)	78.93(14)
C(54)-C(55)	1.402(6)	O(05)-Fe(1)-N(41)	106.75(13)
C(54)-C(65)	1.436(6)	O(25)-Fe(1)-N(41)	95.41(13)
C(55)-O(55)	1.302(5)	N(15)-Fe(1)-N(41)	95.51(13)
C(55)-C(56)	1.444(6)	N(35)-Fe(1)-N(41)	101.26(12)
C(56)-C(57)	1.444(6)	C(02)-C(01)-C(06)	121.3(5)
C(57)-C(58)	1.409(7)	C(02)-C(01)-C(14)	118.6(5)
C(57)-C(62)	1.430(6)	C(06)-C(01)-C(14)	120.1(5)
C(58)-C(59)	1.362(6)	C(03)-C(02)-C(01)	120.1(5)
C(59)-C(60)	1.402(6)	C(02)-C(03)-C(04)	122.1(5)
C(60)-C(61)	1.357(7)	C(03)-C(04)-C(05)	119.7(4)
C(61)-C(62)	1.394(7)	C(03)-C(04)-C(15)	117.0(4)
C(62)-C(63)	1.402(7)	C(05)-C(04)-C(15)	123.4(4)
C(63)-C(64)	1.353(7)	O(05)-C(05)-C(04)	121.0(4)
C(65)-N(65)	1.296(5)	O(05)-C(05)-C(06)	120.6(4)
N(65)-C(66)	1.473(4)	C(04)-C(05)-C(06)	118.4(4)
C(66)-C(67)	1.520(5)	C(05)-O(05)-Fe(1)	135.9(3)
C(66)-C(86)	1.524(4)	C(01)-C(06)-C(05)	118.4(4)
C(67)-C(68)	1.527(5)	C(01)-C(06)-C(07)	118.1(4)
C(68)-C(88)	1.526(5)	C(05)-C(06)-C(07)	123.4(4)
C(71)-C(72)	1.403(7)	C(08)-C(07)-C(12)	116.2(4)
C(71)-C(76)	1.407(6)	C(08)-C(07)-C(06)	124.5(4)
C(71)-C(84)	1.427(7)	C(12)-C(07)-C(06)	119.3(5)
C(72)-C(73)	1.360(6)	C(09)-C(08)-C(07)	121.2(4)
C(73)-C(74)	1.402(6)	C(10)-C(09)-C(08)	121.5(5)
C(74)-C(75)	1.403(6)	C(11)-C(10)-C(09)	118.6(5)
C(74)-C(85)	1.424(6)	C(10)-C(11)-C(12)	121.9(5)
C(75)-O(75)	1.311(5)	C(11)-C(12)-C(07)	120.4(5)

C(11)-C(12)-C(13)	120.1(5)	C(43)-C(44)-C(45)	118.9(4)
C(07)-C(12)-C(13)	119.5(4)	C(46)-C(45)-C(44)	119.3(5)
C(14)-C(13)-C(12)	120.8(5)	N(41)-C(46)-C(45)	122.0(4)
C(13)-C(14)-C(01)	122.0(5)	O(75)-Fe(2)-O(55)	102.24(13)
N(15)-C(15)-C(04)	125.5(4)	O(75)-Fe(2)-N(65)	155.61(12)
C(15)-N(15)-C(16)	121.2(4)	O(55)-Fe(2)-N(65)	86.90(13)
C(15)-N(15)-Fe(1)	128.3(3)	O(75)-Fe(2)-N(85)	85.12(13)
C(16)-N(15)-Fe(1)	110.5(2)	O(55)-Fe(2)-N(85)	157.94(12)
N(15)-C(16)-C(17)	117.8(3)	N(65)-Fe(2)-N(85)	78.84(14)
N(15)-C(16)-C(36)	107.3(3)	O(75)-Fe(2)-N(91)	96.69(13)
C(17)-C(16)-C(36)	109.8(3)	O(55)-Fe(2)-N(91)	105.57(12)
C(18)-C(17)-C(16)	109.6(4)	N(65)-Fe(2)-N(91)	102.61(13)
C(38)-C(18)-C(17)	111.7(3)	N(85)-Fe(2)-N(91)	94.00(12)
C(22)-C(21)-C(26)	120.4(4)	C(52)-C(51)-C(64)	119.0(5)
C(22)-C(21)-C(34)	119.6(5)	C(52)-C(51)-C(56)	122.0(4)
C(26)-C(21)-C(34)	120.0(4)	C(64)-C(51)-C(56)	119.0(5)
C(23)-C(22)-C(21)	120.7(5)	C(53)-C(52)-C(51)	120.4(5)
C(22)-C(23)-C(24)	121.6(5)	C(52)-C(53)-C(54)	120.9(5)
C(23)-C(24)-C(25)	120.0(4)	C(55)-C(54)-C(53)	120.6(4)
C(23)-C(24)-C(35)	117.3(4)	C(55)-C(54)-C(65)	123.6(4)
C(25)-C(24)-C(35)	122.6(4)	C(53)-C(54)-C(65)	115.7(4)
O(25)-C(25)-C(24)	120.9(4)	O(55)-C(55)-C(54)	120.9(4)
O(25)-C(25)-C(26)	121.0(4)	O(55)-C(55)-C(56)	119.7(4)
C(24)-C(25)-C(26)	118.1(4)	C(54)-C(55)-C(56)	119.4(4)
C(25)-O(25)-Fe(1)	134.6(3)	C(55)-O(55)-Fe(2)	135.2(3)
C(21)-C(26)-C(25)	118.9(4)	C(51)-C(56)-C(57)	119.0(4)
C(21)-C(26)-C(27)	117.8(4)	C(51)-C(56)-C(55)	116.7(4)
C(25)-C(26)-C(27)	123.3(4)	C(57)-C(56)-C(55)	124.2(4)
C(28)-C(27)-C(32)	116.9(4)	C(58)-C(57)-C(62)	115.8(4)
C(28)-C(27)-C(26)	124.3(4)	C(58)-C(57)-C(56)	125.2(4)
C(32)-C(27)-C(26)	118.8(4)	C(62)-C(57)-C(56)	118.9(5)
C(29)-C(28)-C(27)	121.7(5)	C(59)-C(58)-C(57)	123.2(4)
C(28)-C(29)-C(30)	121.6(5)	C(58)-C(59)-C(60)	119.2(5)
C(31)-C(30)-C(29)	118.2(5)	C(61)-C(60)-C(59)	120.1(5)
C(30)-C(31)-C(32)	122.6(5)	C(60)-C(61)-C(62)	121.2(5)
C(33)-C(32)-C(31)	121.2(5)	C(61)-C(62)-C(63)	119.7(5)
C(33)-C(32)-C(27)	120.0(5)	C(61)-C(62)-C(57)	120.2(5)
C(31)-C(32)-C(27)	118.8(5)	C(63)-C(62)-C(57)	120.1(5)
C(34)-C(33)-C(32)	121.5(5)	C(64)-C(63)-C(62)	121.4(5)
C(33)-C(34)-C(21)	121.6(5)	C(63)-C(64)-C(51)	121.5(5)
N(35)-C(35)-C(24)	127.6(4)	N(65)-C(65)-C(54)	127.6(4)
C(35)-N(35)-C(36)	117.2(3)	C(65)-N(65)-C(66)	118.3(4)
C(35)-N(35)-Fe(1)	125.2(3)	C(65)-N(65)-Fe(2)	125.5(3)
C(36)-N(35)-Fe(1)	114.7(2)	C(66)-N(65)-Fe(2)	115.1(3)
N(35)-C(36)-C(16)	109.1(2)	N(65)-C(66)-C(67)	115.1(3)
N(35)-C(36)-C(37)	115.1(3)	N(65)-C(66)-C(86)	109.0(3)
C(16)-C(36)-C(37)	109.0(3)	C(67)-C(66)-C(86)	109.9(3)
C(38)-C(37)-C(36)	110.4(4)	C(66)-C(67)-C(68)	109.7(4)
C(18)-C(38)-C(37)	112.3(3)	C(88)-C(68)-C(67)	111.1(3)
C(42)-N(41)-C(46)	118.2(4)	C(72)-C(71)-C(76)	121.5(4)
C(42)-N(41)-Fe(1)	123.0(3)	C(72)-C(71)-C(84)	118.7(5)
C(46)-N(41)-Fe(1)	118.8(3)	C(76)-C(71)-C(84)	119.8(5)
N(41)-C(42)-C(43)	122.4(5)	C(73)-C(72)-C(71)	119.6(5)
C(44)-C(43)-C(42)	119.3(4)	C(72)-C(73)-C(74)	121.5(5)

C(73)-C(74)-C(75)	119.9(4)	C(84)-C(83)-C(82)	122.0(5)
C(73)-C(74)-C(85)	116.3(4)	C(83)-C(84)-C(71)	120.5(5)
C(75)-C(74)-C(85)	123.9(4)	N(85)-C(85)-C(74)	125.4(4)
O(75)-C(75)-C(74)	121.2(4)	C(85)-N(85)-C(86)	122.8(3)
O(75)-C(75)-C(76)	119.5(4)	C(85)-N(85)-Fe(2)	126.7(3)
C(74)-C(75)-C(76)	119.3(4)	C(86)-N(85)-Fe(2)	110.1(2)
C(75)-O(75)-Fe(2)	133.6(3)	N(85)-C(86)-C(87)	117.2(3)
C(71)-C(76)-C(75)	117.6(4)	N(85)-C(86)-C(66)	107.3(3)
C(71)-C(76)-C(77)	119.4(4)	C(87)-C(86)-C(66)	110.9(3)
C(75)-C(76)-C(77)	123.0(4)	C(86)-C(87)-C(88)	109.8(3)
C(78)-C(77)-C(82)	115.8(4)	C(68)-C(88)-C(87)	112.1(3)
C(78)-C(77)-C(76)	125.4(4)	C(96)-N(91)-C(92)	117.0(4)
C(82)-C(77)-C(76)	118.7(4)	C(96)-N(91)-Fe(2)	119.5(3)
C(79)-C(78)-C(77)	122.1(5)	C(92)-N(91)-Fe(2)	123.5(3)
C(78)-C(79)-C(80)	120.5(5)	N(91)-C(92)-C(93)	122.4(5)
C(81)-C(80)-C(79)	119.6(5)	C(92)-C(93)-C(94)	119.4(4)
C(80)-C(81)-C(82)	120.5(5)	C(95)-C(94)-C(93)	118.9(4)
C(81)-C(82)-C(77)	121.6(5)	C(94)-C(95)-C(96)	118.0(5)
C(81)-C(82)-C(83)	119.5(5)	N(91)-C(96)-C(95)	124.2(5)
C(77)-C(82)-C(83)	119.0(5)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*,*R*)-**54**·py. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	22(1)	25(1)	22(1)	-1(1)	-1(1)	1(1)
C(01)	35(2)	37(3)	39(3)	-5(2)	6(2)	-1(2)
C(02)	46(2)	30(3)	41(3)	1(2)	0(2)	-3(2)
C(03)	40(2)	36(3)	35(3)	6(2)	3(2)	5(2)
C(04)	28(2)	28(3)	30(2)	4(2)	1(2)	2(2)
C(05)	21(2)	29(3)	26(2)	-10(2)	3(2)	-1(2)
O(05)	33(2)	25(2)	25(2)	-1(2)	-5(1)	-1(1)
C(06)	21(2)	32(3)	29(2)	-4(2)	3(2)	4(2)
C(07)	18(2)	32(3)	35(2)	-4(2)	5(2)	-1(2)
C(08)	23(2)	39(3)	25(2)	-7(2)	-2(2)	5(2)
C(09)	36(2)	35(3)	34(2)	-1(2)	-1(2)	3(2)
C(10)	32(2)	57(4)	29(2)	-4(2)	-9(2)	12(2)
C(11)	38(2)	51(4)	25(2)	-14(3)	-6(2)	-2(2)
C(12)	22(2)	40(3)	29(2)	-6(2)	-1(2)	1(2)
C(13)	43(2)	37(3)	38(3)	-14(2)	-5(2)	-7(2)
C(14)	48(2)	30(3)	46(3)	-8(2)	-3(2)	-4(2)
C(15)	30(2)	36(3)	23(2)	3(2)	1(1)	4(2)
N(15)	25(2)	31(2)	21(2)	-2(1)	-2(1)	4(1)
C(16)	25(2)	34(2)	20(2)	-2(1)	-1(1)	1(2)
C(17)	35(2)	38(3)	26(2)	4(2)	2(2)	9(2)
C(18)	33(2)	51(2)	26(2)	9(2)	-4(2)	2(2)
C(21)	30(2)	25(3)	44(3)	-1(2)	2(2)	1(2)

C(22)	55(3)	31(3)	46(3)	-5(2)	10(2)	7(2)
C(23)	56(3)	24(3)	38(3)	-5(2)	9(2)	4(2)
C(24)	31(2)	30(3)	29(2)	-1(2)	3(2)	-3(2)
C(25)	22(2)	23(3)	29(2)	0(2)	1(2)	-7(2)
O(25)	27(2)	27(2)	26(2)	0(2)	-1(1)	3(1)
C(26)	25(2)	26(3)	34(2)	4(2)	-1(2)	-5(2)
C(27)	25(2)	24(3)	32(2)	1(2)	-2(2)	-5(2)
C(28)	33(2)	35(3)	37(3)	7(2)	-3(2)	1(2)
C(29)	45(2)	42(3)	35(3)	4(2)	1(2)	2(2)
C(30)	44(3)	42(3)	36(3)	7(2)	-5(2)	-9(2)
C(31)	41(3)	39(3)	45(3)	21(3)	-12(2)	-3(2)
C(32)	29(2)	27(3)	47(3)	7(2)	-8(2)	-4(2)
C(33)	37(2)	33(3)	56(3)	1(3)	-8(2)	10(2)
C(34)	44(3)	21(3)	64(4)	5(3)	4(2)	7(2)
C(35)	34(2)	29(2)	25(2)	-4(2)	5(2)	-5(2)
N(35)	25(2)	26(2)	24(2)	4(1)	0(1)	-1(1)
C(36)	27(2)	33(2)	21(1)	2(1)	-1(1)	-3(2)
C(37)	56(3)	41(3)	32(3)	-2(2)	-15(2)	-5(2)
C(38)	60(3)	44(2)	25(2)	0(2)	-15(2)	-4(2)
N(41)	23(2)	34(2)	24(2)	-6(2)	2(1)	1(2)
C(42)	29(2)	38(3)	21(2)	3(2)	-1(2)	3(2)
C(43)	30(2)	49(3)	31(3)	-4(2)	0(2)	12(2)
C(44)	25(2)	55(4)	37(3)	-8(2)	3(2)	-5(2)
C(45)	34(2)	39(3)	49(3)	-2(2)	5(2)	-5(2)
C(46)	28(2)	24(3)	38(3)	0(2)	2(2)	-3(2)
Fe(2)	22(1)	26(1)	22(1)	0(1)	-1(1)	1(1)
C(51)	34(2)	27(3)	33(2)	-4(2)	3(2)	-7(2)
C(52)	49(2)	25(3)	47(3)	-3(2)	8(2)	-12(2)
C(53)	52(2)	26(3)	36(3)	6(2)	1(2)	-3(2)
C(54)	27(2)	29(3)	26(2)	-3(2)	0(2)	-3(2)
C(55)	22(2)	25(3)	28(2)	6(2)	6(2)	2(2)
O(55)	29(2)	27(2)	25(2)	3(2)	-4(1)	-2(1)
C(56)	23(2)	28(3)	29(2)	-2(2)	6(2)	-3(2)
C(57)	20(2)	35(3)	22(2)	-6(2)	0(2)	2(2)
C(58)	28(2)	33(3)	27(2)	0(2)	-1(2)	-1(2)
C(59)	30(2)	43(3)	31(2)	2(2)	-9(2)	8(2)
C(60)	41(2)	44(3)	28(2)	1(2)	-4(2)	4(2)
C(61)	30(2)	55(4)	31(2)	-10(3)	-9(2)	7(2)
C(62)	24(2)	39(3)	35(3)	-12(2)	2(2)	-2(2)
C(63)	36(2)	47(3)	38(3)	-15(2)	-3(2)	-4(2)
C(64)	42(2)	34(3)	48(3)	-14(2)	11(2)	-14(2)
C(65)	32(2)	27(2)	28(2)	9(2)	0(2)	0(2)
N(65)	23(1)	32(2)	21(2)	2(1)	1(1)	2(1)
C(66)	28(2)	34(2)	23(2)	2(1)	0(1)	-1(2)
C(67)	37(2)	44(4)	28(2)	6(2)	-8(2)	-2(2)
C(68)	37(2)	53(2)	27(2)	8(2)	-6(2)	-3(2)
C(71)	34(2)	20(3)	47(3)	3(2)	3(2)	-2(2)
C(72)	53(3)	24(3)	52(3)	-7(2)	10(2)	5(2)
C(73)	53(3)	36(3)	34(2)	-7(2)	5(2)	4(2)
C(74)	33(2)	24(2)	35(2)	-3(2)	4(2)	-2(2)
C(75)	19(2)	26(3)	37(3)	-3(2)	3(2)	0(2)
O(75)	28(2)	31(2)	27(2)	-1(2)	-2(1)	8(1)
C(76)	22(2)	21(3)	40(3)	-2(2)	1(2)	-2(2)
C(77)	22(2)	27(3)	44(3)	9(2)	-4(2)	-8(2)

C(78)	34(2)	31(3)	33(3)	4(2)	0(2)	1(2)
C(79)	43(3)	40(3)	36(3)	6(2)	3(2)	-5(2)
C(80)	48(3)	45(3)	34(3)	10(2)	-5(2)	-9(2)
C(81)	46(3)	36(3)	49(3)	5(3)	-13(2)	-7(2)
C(82)	35(2)	29(3)	45(3)	6(2)	-5(2)	-6(2)
C(83)	46(3)	30(3)	62(4)	12(3)	-9(2)	4(2)
C(84)	43(3)	35(3)	58(3)	-6(3)	-2(2)	7(2)
C(85)	34(2)	32(2)	24(2)	-3(2)	2(1)	-7(2)
N(85)	26(2)	28(2)	24(2)	0(1)	-1(1)	-3(1)
C(86)	26(2)	37(2)	24(2)	1(1)	-2(1)	0(2)
C(87)	42(3)	42(3)	24(2)	-4(2)	-1(2)	1(2)
C(88)	42(2)	49(3)	28(2)	0(2)	-8(2)	-2(2)
N(91)	22(2)	32(2)	21(2)	0(2)	-1(1)	-2(2)
C(92)	31(2)	36(3)	27(2)	-4(2)	2(2)	8(2)
C(93)	25(2)	52(4)	29(2)	-6(2)	0(2)	10(2)
C(94)	17(2)	73(4)	38(3)	-12(3)	2(2)	-5(2)
C(95)	33(2)	51(4)	54(3)	-11(3)	8(2)	-23(2)
C(96)	29(2)	43(3)	47(3)	-12(2)	6(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**54**·py.

	x	y	z	U(eq)
H(02)	2893	73	4467	47
H(03)	4090	560	5517	44
H(08)	2639	2845	3467	35
H(09)	1710	3342	2349	42
H(10)	807	2743	1292	48
H(11)	733	1637	1379	46
H(13)	973	637	2110	48
H(14)	1746	108	3181	50
H(15)	5287	1425	6165	36
H(16)	7383	2656	6449	32
H(17A)	5597	1878	7397	40
H(17B)	7138	1632	7019	40
H(18A)	7820	1986	8282	45
H(18B)	8739	2395	7698	45
H(22)	1394	5817	5998	53
H(23)	2941	5130	6733	47
H(28)	4050	4163	3623	42
H(29)	3984	4231	2342	49
H(30)	2360	4982	1667	49
H(31)	925	5699	2318	51
H(33)	65	6134	3495	51
H(34)	326	6202	4765	52
H(35)	4318	4166	6934	35
H(36)	4511	2950	7110	33
H(37A)	7578	3552	7335	53

H(37B)	6052	3775	7740	53
H(38A)	7746	3104	8546	53
H(38B)	6005	2807	8402	53
H(42)	7979	2335	5012	35
H(43)	10538	2489	4678	45
H(44)	11378	3521	4391	47
H(45)	9560	4366	4384	49
H(46)	7000	4170	4695	36
H(52)	7454	9891	519	48
H(53)	6141	9423	-512	46
H(58)	7149	7142	1606	36
H(59)	7863	6640	2733	42
H(60)	8925	7250	3774	46
H(61)	9420	8328	3636	47
H(63)	9401	9287	2883	49
H(64)	8703	9835	1793	49
H(65)	5264	8539	-1203	35
H(66)	5469	7447	-1990	34
H(67A)	3878	8384	-2173	44
H(67B)	2355	7989	-1961	44
H(68A)	2354	8023	-3290	47
H(68B)	4109	7732	-3244	47
H(72)	8360	4159	-1025	51
H(73)	6720	4852	-1740	49
H(78)	5812	5816	1382	39
H(79)	5867	5723	2678	48
H(80)	7450	4937	3320	52
H(81)	8946	4246	2654	54
H(83)	9788	3838	1467	56
H(84)	9617	3815	187	55
H(85)	5049	5725	-1896	36
H(86)	2624	6862	-1568	35
H(87A)	2900	6145	-2568	43
H(87B)	4466	6512	-2776	43
H(88A)	2308	6900	-3576	48
H(88B)	1320	7054	-2874	48
H(92)	1992	7693	-35	38
H(93)	-594	7550	272	43
H(94)	-1461	6527	593	51
H(95)	322	5668	593	55
H(96)	2913	5870	330	47

Table 6. Torsion angles [°] for (*R*,*R*)-**54**·py.

C(06)-C(01)-C(02)-C(03)	-0.5(6)	C(03)-C(04)-C(05)-O(05)	179.3(3)
C(14)-C(01)-C(02)-C(03)	176.4(4)	C(15)-C(04)-C(05)-O(05)	-2.7(6)
C(01)-C(02)-C(03)-C(04)	-1.8(6)	C(03)-C(04)-C(05)-C(06)	-1.1(5)
C(02)-C(03)-C(04)-C(05)	2.6(6)	C(15)-C(04)-C(05)-C(06)	177.0(3)
C(02)-C(03)-C(04)-C(15)	-175.6(4)	C(04)-C(05)-O(05)-Fe(1)	0.5(6)

C(06)-C(05)-O(05)-Fe(1)	-179.2(3)	C(21)-C(22)-C(23)-C(24)	-4.2(8)
O(25)-Fe(1)-O(05)-C(05)	-163.6(3)	C(22)-C(23)-C(24)-C(25)	3.2(7)
N(15)-Fe(1)-O(05)-C(05)	1.9(3)	C(22)-C(23)-C(24)-C(35)	-172.4(4)
N(35)-Fe(1)-O(05)-C(05)	-58.3(5)	C(23)-C(24)-C(25)-O(25)	-176.5(4)
N(41)-Fe(1)-O(05)-C(05)	96.4(4)	C(35)-C(24)-C(25)-O(25)	-1.2(6)
C(02)-C(01)-C(06)-C(05)	1.9(6)	C(23)-C(24)-C(25)-C(26)	1.8(6)
C(14)-C(01)-C(06)-C(05)	-175.0(4)	C(35)-C(24)-C(25)-C(26)	177.1(4)
C(02)-C(01)-C(06)-C(07)	179.9(4)	C(24)-C(25)-O(25)-Fe(1)	14.7(6)
C(14)-C(01)-C(06)-C(07)	3.0(6)	C(26)-C(25)-O(25)-Fe(1)	-163.6(3)
O(05)-C(05)-C(06)-C(01)	178.6(3)	O(05)-Fe(1)-O(25)-C(25)	131.5(4)
C(04)-C(05)-C(06)-C(01)	-1.1(5)	N(15)-Fe(1)-O(25)-C(25)	9.7(7)
O(05)-C(05)-C(06)-C(07)	0.7(5)	N(35)-Fe(1)-O(25)-C(25)	-18.9(4)
C(04)-C(05)-C(06)-C(07)	-179.0(3)	N(41)-Fe(1)-O(25)-C(25)	-119.8(4)
C(01)-C(06)-C(07)-C(08)	174.5(4)	C(22)-C(21)-C(26)-C(25)	4.7(7)
C(05)-C(06)-C(07)-C(08)	-7.6(6)	C(34)-C(21)-C(26)-C(25)	-175.0(4)
C(01)-C(06)-C(07)-C(12)	-4.5(5)	C(22)-C(21)-C(26)-C(27)	-174.9(4)
C(05)-C(06)-C(07)-C(12)	173.4(3)	C(34)-C(21)-C(26)-C(27)	5.4(6)
C(12)-C(07)-C(08)-C(09)	-1.1(5)	O(25)-C(25)-C(26)-C(21)	172.8(4)
C(06)-C(07)-C(08)-C(09)	179.9(4)	C(24)-C(25)-C(26)-C(21)	-5.5(6)
C(07)-C(08)-C(09)-C(10)	-1.3(6)	O(25)-C(25)-C(26)-C(27)	-7.7(6)
C(08)-C(09)-C(10)-C(11)	1.7(6)	C(24)-C(25)-C(26)-C(27)	174.0(4)
C(09)-C(10)-C(11)-C(12)	0.4(6)	C(21)-C(26)-C(27)-C(28)	174.8(4)
C(10)-C(11)-C(12)-C(07)	-2.8(6)	C(25)-C(26)-C(27)-C(28)	-4.7(7)
C(10)-C(11)-C(12)-C(13)	175.4(4)	C(21)-C(26)-C(27)-C(32)	-4.9(6)
C(08)-C(07)-C(12)-C(11)	3.1(5)	C(25)-C(26)-C(27)-C(32)	175.6(4)
C(06)-C(07)-C(12)-C(11)	-177.8(4)	C(32)-C(27)-C(28)-C(29)	1.7(7)
C(08)-C(07)-C(12)-C(13)	-175.2(3)	C(26)-C(27)-C(28)-C(29)	-178.0(4)
C(06)-C(07)-C(12)-C(13)	3.9(5)	C(27)-C(28)-C(29)-C(30)	-2.6(7)
C(11)-C(12)-C(13)-C(14)	-180.0(4)	C(28)-C(29)-C(30)-C(31)	1.7(8)
C(07)-C(12)-C(13)-C(14)	-1.7(6)	C(29)-C(30)-C(31)-C(32)	-0.1(8)
C(12)-C(13)-C(14)-C(01)	0.1(7)	C(30)-C(31)-C(32)-C(33)	178.6(5)
C(02)-C(01)-C(14)-C(13)	-177.8(4)	C(30)-C(31)-C(32)-C(27)	-0.7(7)
C(06)-C(01)-C(14)-C(13)	-0.9(7)	C(28)-C(27)-C(32)-C(33)	-179.4(4)
C(03)-C(04)-C(15)-N(15)	179.2(4)	C(26)-C(27)-C(32)-C(33)	0.3(6)
C(05)-C(04)-C(15)-N(15)	1.1(6)	C(28)-C(27)-C(32)-C(31)	-0.1(6)
C(04)-C(15)-N(15)-C(16)	-178.8(3)	C(26)-C(27)-C(32)-C(31)	179.6(4)
C(04)-C(15)-N(15)-Fe(1)	2.5(6)	C(31)-C(32)-C(33)-C(34)	-175.2(5)
O(05)-Fe(1)-N(15)-C(15)	-3.3(3)	C(27)-C(32)-C(33)-C(34)	4.1(7)
O(25)-Fe(1)-N(15)-C(15)	120.8(5)	C(32)-C(33)-C(34)-C(21)	-3.7(8)
N(35)-Fe(1)-N(15)-C(15)	149.8(3)	C(22)-C(21)-C(34)-C(33)	179.0(5)
N(41)-Fe(1)-N(15)-C(15)	-109.7(3)	C(26)-C(21)-C(34)-C(33)	-1.2(7)
O(05)-Fe(1)-N(15)-C(16)	177.9(2)	C(23)-C(24)-C(35)-N(35)	176.6(4)
O(25)-Fe(1)-N(15)-C(16)	-58.0(5)	C(25)-C(24)-C(35)-N(35)	1.1(6)
N(35)-Fe(1)-N(15)-C(16)	-29.0(2)	C(24)-C(35)-N(35)-C(36)	-171.5(4)
N(41)-Fe(1)-N(15)-C(16)	71.5(2)	C(24)-C(35)-N(35)-Fe(1)	-12.0(6)
C(15)-N(15)-C(16)-C(17)	-7.0(5)	O(05)-Fe(1)-N(35)-C(35)	-93.9(4)
Fe(1)-N(15)-C(16)-C(17)	171.9(2)	O(25)-Fe(1)-N(35)-C(35)	16.1(3)
C(15)-N(15)-C(16)-C(36)	-131.5(3)	N(15)-Fe(1)-N(35)-C(35)	-155.7(3)
Fe(1)-N(15)-C(16)-C(36)	47.4(3)	N(41)-Fe(1)-N(35)-C(35)	110.8(3)
N(15)-C(16)-C(17)-C(18)	176.6(3)	O(05)-Fe(1)-N(35)-C(36)	66.2(3)
C(36)-C(16)-C(17)-C(18)	-60.2(4)	O(25)-Fe(1)-N(35)-C(36)	176.1(2)
C(16)-C(17)-C(18)-C(38)	55.9(4)	N(15)-Fe(1)-N(35)-C(36)	4.3(2)
C(26)-C(21)-C(22)-C(23)	0.2(7)	N(41)-Fe(1)-N(35)-C(36)	-89.2(2)
C(34)-C(21)-C(22)-C(23)	179.9(5)	C(35)-N(35)-C(36)-C(16)	-178.4(3)

Fe(1)-N(35)-C(36)-C(16)	19.9(3)	C(62)-C(57)-C(58)-C(59)	2.3(5)
C(35)-N(35)-C(36)-C(37)	-55.6(4)	C(56)-C(57)-C(58)-C(59)	-176.6(4)
Fe(1)-N(35)-C(36)-C(37)	142.7(3)	C(57)-C(58)-C(59)-C(60)	0.9(6)
N(15)-C(16)-C(36)-N(35)	-42.9(3)	C(58)-C(59)-C(60)-C(61)	-2.7(6)
C(17)-C(16)-C(36)-N(35)	-172.1(3)	C(59)-C(60)-C(61)-C(62)	1.1(6)
N(15)-C(16)-C(36)-C(37)	-169.3(3)	C(60)-C(61)-C(62)-C(63)	180.0(4)
C(17)-C(16)-C(36)-C(37)	61.5(4)	C(60)-C(61)-C(62)-C(57)	2.2(6)
N(35)-C(36)-C(37)-C(38)	179.2(3)	C(58)-C(57)-C(62)-C(61)	-3.9(5)
C(16)-C(36)-C(37)-C(38)	-58.0(4)	C(56)-C(57)-C(62)-C(61)	175.1(4)
C(17)-C(18)-C(38)-C(37)	-53.6(5)	C(58)-C(57)-C(62)-C(63)	178.4(4)
C(36)-C(37)-C(38)-C(18)	54.5(5)	C(56)-C(57)-C(62)-C(63)	-2.6(5)
O(05)-Fe(1)-N(41)-C(42)	-60.2(3)	C(61)-C(62)-C(63)-C(64)	-176.5(4)
O(25)-Fe(1)-N(41)-C(42)	-166.0(3)	C(57)-C(62)-C(63)-C(64)	1.2(6)
N(15)-Fe(1)-N(41)-C(42)	27.2(3)	C(62)-C(63)-C(64)-C(51)	1.3(7)
N(35)-Fe(1)-N(41)-C(42)	106.9(3)	C(52)-C(51)-C(64)-C(63)	179.0(4)
O(05)-Fe(1)-N(41)-C(46)	120.3(3)	C(56)-C(51)-C(64)-C(63)	-2.4(6)
O(25)-Fe(1)-N(41)-C(46)	14.5(3)	C(55)-C(54)-C(65)-N(65)	6.2(6)
N(15)-Fe(1)-N(41)-C(46)	-152.4(3)	C(53)-C(54)-C(65)-N(65)	-177.4(4)
N(35)-Fe(1)-N(41)-C(46)	-72.6(3)	C(54)-C(65)-N(65)-C(66)	-170.1(3)
C(46)-N(41)-C(42)-C(43)	0.0(6)	C(54)-C(65)-N(65)-Fe(2)	-2.7(6)
Fe(1)-N(41)-C(42)-C(43)	-179.6(3)	O(75)-Fe(2)-N(65)-C(65)	-113.6(4)
N(41)-C(42)-C(43)-C(44)	1.3(6)	O(55)-Fe(2)-N(65)-C(65)	-0.4(3)
C(42)-C(43)-C(44)-C(45)	-1.8(7)	N(85)-Fe(2)-N(65)-C(65)	-163.4(3)
C(43)-C(44)-C(45)-C(46)	0.9(7)	N(91)-Fe(2)-N(65)-C(65)	104.9(3)
C(42)-N(41)-C(46)-C(45)	-0.8(6)	O(75)-Fe(2)-N(65)-C(66)	54.2(4)
Fe(1)-N(41)-C(46)-C(45)	178.7(3)	O(55)-Fe(2)-N(65)-C(66)	167.4(2)
C(44)-C(45)-C(46)-N(41)	0.4(7)	N(85)-Fe(2)-N(65)-C(66)	4.3(2)
C(64)-C(51)-C(52)-C(53)	-179.9(4)	N(91)-Fe(2)-N(65)-C(66)	-87.3(2)
C(56)-C(51)-C(52)-C(53)	1.5(7)	C(65)-N(65)-C(66)-C(67)	-47.4(4)
C(51)-C(52)-C(53)-C(54)	-1.1(6)	Fe(2)-N(65)-C(66)-C(67)	143.9(3)
C(52)-C(53)-C(54)-C(55)	1.7(6)	C(65)-N(65)-C(66)-C(86)	-171.4(3)
C(52)-C(53)-C(54)-C(65)	-174.8(4)	Fe(2)-N(65)-C(66)-C(86)	20.0(3)
C(53)-C(54)-C(55)-O(55)	177.9(3)	N(65)-C(66)-C(67)-C(68)	177.2(3)
C(65)-C(54)-C(55)-O(55)	-5.9(6)	C(86)-C(66)-C(67)-C(68)	-59.3(4)
C(53)-C(54)-C(55)-C(56)	-2.7(5)	C(66)-C(67)-C(68)-C(88)	56.4(4)
C(65)-C(54)-C(55)-C(56)	173.5(3)	C(76)-C(71)-C(72)-C(73)	-0.2(7)
C(54)-C(55)-O(55)-Fe(2)	2.5(5)	C(84)-C(71)-C(72)-C(73)	-179.0(5)
C(56)-C(55)-O(55)-Fe(2)	-176.9(2)	C(71)-C(72)-C(73)-C(74)	4.3(7)
O(75)-Fe(2)-O(55)-C(55)	157.5(3)	C(72)-C(73)-C(74)-C(75)	-1.3(7)
N(65)-Fe(2)-O(55)-C(55)	0.4(3)	C(72)-C(73)-C(74)-C(85)	178.9(4)
N(85)-Fe(2)-O(55)-C(55)	49.9(5)	C(73)-C(74)-C(75)-O(75)	173.7(4)
N(91)-Fe(2)-O(55)-C(55)	-101.8(3)	C(85)-C(74)-C(75)-O(75)	-6.5(6)
C(52)-C(51)-C(56)-C(57)	179.5(4)	C(73)-C(74)-C(75)-C(76)	-5.7(6)
C(64)-C(51)-C(56)-C(57)	0.9(6)	C(85)-C(74)-C(75)-C(76)	174.0(4)
C(52)-C(51)-C(56)-C(55)	-2.4(6)	C(74)-C(75)-O(75)-Fe(2)	-13.8(6)
C(64)-C(51)-C(56)-C(55)	179.0(4)	C(76)-C(75)-O(75)-Fe(2)	165.6(3)
O(55)-C(55)-C(56)-C(51)	-177.6(3)	O(55)-Fe(2)-O(75)-C(75)	-137.4(4)
C(54)-C(55)-C(56)-C(51)	3.0(5)	N(65)-Fe(2)-O(75)-C(75)	-27.2(6)
O(55)-C(55)-C(56)-C(57)	0.3(6)	N(85)-Fe(2)-O(75)-C(75)	21.6(4)
C(54)-C(55)-C(56)-C(57)	-179.1(3)	N(91)-Fe(2)-O(75)-C(75)	115.1(4)
C(51)-C(56)-C(57)-C(58)	-179.6(3)	C(72)-C(71)-C(76)-C(75)	-6.6(6)
C(55)-C(56)-C(57)-C(58)	2.5(6)	C(84)-C(71)-C(76)-C(75)	172.2(4)
C(51)-C(56)-C(57)-C(62)	1.5(5)	C(72)-C(71)-C(76)-C(77)	172.9(4)
C(55)-C(56)-C(57)-C(62)	-176.4(3)	C(84)-C(71)-C(76)-C(77)	-8.3(7)

O(75)-C(75)-C(76)-C(71)	-170.0(4)	O(75)-Fe(2)-N(85)-C(86)	169.5(2)
C(74)-C(75)-C(76)-C(71)	9.4(6)	O(55)-Fe(2)-N(85)-C(86)	-79.7(4)
O(75)-C(75)-C(76)-C(77)	10.5(6)	N(65)-Fe(2)-N(85)-C(86)	-29.0(2)
C(74)-C(75)-C(76)-C(77)	-170.0(4)	N(91)-Fe(2)-N(85)-C(86)	73.1(2)
C(71)-C(76)-C(77)-C(78)	-172.2(4)	C(85)-N(85)-C(86)-C(87)	-0.2(5)
C(75)-C(76)-C(77)-C(78)	7.3(7)	Fe(2)-N(85)-C(86)-C(87)	172.9(3)
C(71)-C(76)-C(77)-C(82)	3.8(6)	C(85)-N(85)-C(86)-C(66)	-125.6(4)
C(75)-C(76)-C(77)-C(82)	-176.7(4)	Fe(2)-N(85)-C(86)-C(66)	47.5(3)
C(82)-C(77)-C(78)-C(79)	-0.6(7)	N(65)-C(66)-C(86)-N(85)	-43.2(4)
C(76)-C(77)-C(78)-C(79)	175.5(4)	C(67)-C(66)-C(86)-N(85)	-170.2(3)
C(77)-C(78)-C(79)-C(80)	1.4(7)	N(65)-C(66)-C(86)-C(87)	-172.3(3)
C(78)-C(79)-C(80)-C(81)	-0.4(8)	C(67)-C(66)-C(86)-C(87)	60.7(4)
C(79)-C(80)-C(81)-C(82)	-1.4(8)	N(85)-C(86)-C(87)-C(88)	179.1(3)
C(80)-C(81)-C(82)-C(77)	2.3(8)	C(66)-C(86)-C(87)-C(88)	-57.2(4)
C(80)-C(81)-C(82)-C(83)	-177.7(5)	C(67)-C(68)-C(88)-C(87)	-54.5(4)
C(78)-C(77)-C(82)-C(81)	-1.2(7)	C(86)-C(87)-C(88)-C(68)	54.3(4)
C(76)-C(77)-C(82)-C(81)	-177.6(4)	O(75)-Fe(2)-N(91)-C(96)	-14.9(3)
C(78)-C(77)-C(82)-C(83)	178.8(4)	O(55)-Fe(2)-N(91)-C(96)	-119.6(3)
C(76)-C(77)-C(82)-C(83)	2.4(6)	N(65)-Fe(2)-N(91)-C(96)	150.1(3)
C(81)-C(82)-C(83)-C(84)	175.7(5)	N(85)-Fe(2)-N(91)-C(96)	70.7(3)
C(77)-C(82)-C(83)-C(84)	-4.3(7)	O(75)-Fe(2)-N(91)-C(92)	167.5(3)
C(82)-C(83)-C(84)-C(71)	-0.1(8)	O(55)-Fe(2)-N(91)-C(92)	62.8(3)
C(72)-C(71)-C(84)-C(83)	-174.7(5)	N(65)-Fe(2)-N(91)-C(92)	-27.5(3)
C(76)-C(71)-C(84)-C(83)	6.5(7)	N(85)-Fe(2)-N(91)-C(92)	-106.9(3)
C(73)-C(74)-C(85)-N(85)	-171.8(4)	C(96)-N(91)-C(92)-C(93)	0.6(6)
C(75)-C(74)-C(85)-N(85)	8.4(6)	Fe(2)-N(91)-C(92)-C(93)	178.3(3)
C(74)-C(85)-N(85)-C(86)	179.9(3)	N(91)-C(92)-C(93)-C(94)	-1.1(6)
C(74)-C(85)-N(85)-Fe(2)	8.0(6)	C(92)-C(93)-C(94)-C(95)	0.0(7)
O(75)-Fe(2)-N(85)-C(85)	-17.8(3)	C(93)-C(94)-C(95)-C(96)	1.5(7)
O(55)-Fe(2)-N(85)-C(85)	93.1(5)	C(92)-N(91)-C(96)-C(95)	1.0(7)
N(65)-Fe(2)-N(85)-C(85)	143.8(3)	Fe(2)-N(91)-C(96)-C(95)	-176.8(4)
N(91)-Fe(2)-N(85)-C(85)	-114.2(3)	C(94)-C(95)-C(96)-N(91)	-2.1(7)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**55**·MeOH.

Identification code	(*R*)-**55**·MeOH	
Empirical formula	C52 H36.75 Cl0.50 N2 O3.75 Zn	
Formula weight	832.68	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.3373(4) Å	α = 90°.
	b = 13.3410(5) Å	β = 90°.
	c = 23.6254(8) Å	γ = 90°.
Volume	3888.6(2) $Å^3$	
Z	4	
Density (calculated)	1.422 g/cm^3	
Absorption coefficient	0.718 mm^{-1}	
F(000)	1725	
Crystal size	0.40 x 0.40 x 0.35 mm^3	
Theta range for data collection	1.72 to 28.32°.	
Index ranges	-16<=h<=16, -17<=k<=15, -31<=l<=31	
Reflections collected	41396	
Independent reflections	9192 [R(int) = 0.0421]	
Completeness to theta = 28.32°	95.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9192 / 3 / 555	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0348, wR2 = 0.0808	
R indices (all data)	R1 = 0.0492, wR2 = 0.0874	
Absolute structure parameter	-0.021(8)	
Largest diff. peak and hole	0.315 and -0.604 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**55**·MeOH. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1S)	6813(3)	3111(2)	2313(1)	58(1)
C(1S)	7590(4)	3602(4)	2643(2)	70(1)
C(2S)	8198(15)	3574(10)	2827(6)	101(6)
Cl(1)	8584(3)	4620(2)	2422(2)	70(1)
Cl(2)	7347(3)	2747(3)	2443(2)	72(1)
Zn(1)	3822(1)	5005(1)	2051(1)	27(1)
C(01)	4355(2)	6417(2)	784(1)	24(1)
C(02)	3342(2)	6284(2)	1021(1)	26(1)
N(02)	3032(1)	5387(1)	1308(1)	26(1)
C(03)	2580(2)	7075(2)	1021(1)	35(1)
C(04)	2832(2)	7988(2)	806(1)	37(1)
C(05)	3878(2)	8184(2)	599(1)	30(1)
C(06)	4189(2)	9154(2)	420(1)	40(1)
C(07)	5212(2)	9339(2)	235(1)	39(1)

C(08)	5976(2)	8566(2)	222(1)	38(1)
C(09)	5699(2)	7623(2)	392(1)	31(1)
C(10)	4651(2)	7397(2)	588(1)	26(1)
C(11)	5159(2)	5591(1)	720(1)	24(1)
C(12)	5664(2)	5179(2)	1185(1)	27(1)
N(12)	5316(2)	5481(1)	1737(1)	27(1)
C(13)	6508(2)	4487(2)	1131(1)	33(1)
C(14)	6856(2)	4202(2)	607(1)	34(1)
C(15)	6361(2)	4577(2)	117(1)	30(1)
C(16)	6691(2)	4278(2)	-431(1)	36(1)
C(17)	6230(2)	4656(2)	-904(1)	38(1)
C(18)	5407(2)	5370(2)	-854(1)	34(1)
C(19)	5049(2)	5667(2)	-333(1)	29(1)
C(20)	5503(2)	5284(2)	168(1)	26(1)
C(21)	1711(2)	3915(2)	2002(1)	27(1)
O(21)	2494(1)	4283(1)	2291(1)	34(1)
C(22)	1511(2)	4218(2)	1436(1)	27(1)
C(23)	641(2)	3800(2)	1124(1)	35(1)
C(24)	39(2)	3046(2)	1336(1)	43(1)
C(25)	230(2)	2691(2)	1889(1)	40(1)
C(26)	-365(3)	1852(2)	2089(1)	58(1)
C(27)	-230(3)	1477(2)	2607(1)	58(1)
C(28)	503(2)	1944(2)	2994(1)	42(1)
C(29)	626(3)	1558(2)	3547(1)	52(1)
C(30)	1273(3)	2016(2)	3930(1)	49(1)
C(31)	1822(2)	2893(2)	3776(1)	43(1)
C(32)	1736(2)	3274(2)	3239(1)	35(1)
C(33)	1096(2)	2799(2)	2826(1)	31(1)
C(34)	999(2)	3153(2)	2245(1)	28(1)
C(35)	2116(2)	4988(2)	1155(1)	27(1)
C(41)	4860(2)	6217(2)	2919(1)	27(1)
O(41)	3964(1)	5974(1)	2667(1)	37(1)
C(42)	5870(2)	6216(2)	2635(1)	29(1)
C(43)	6804(2)	6601(2)	2906(1)	33(1)
C(44)	6756(2)	6987(2)	3435(1)	32(1)
C(45)	5778(2)	6957(2)	3740(1)	28(1)
C(46)	5748(2)	7358(2)	4302(1)	32(1)
C(47)	4866(2)	7290(2)	4626(1)	32(1)
C(48)	3924(2)	6789(2)	4427(1)	28(1)
C(49)	3039(2)	6634(2)	4794(1)	34(1)
C(50)	2151(2)	6104(2)	4629(1)	37(1)
C(51)	2118(2)	5718(2)	4081(1)	39(1)
C(52)	2954(2)	5871(2)	3708(1)	34(1)
C(53)	3888(2)	6412(1)	3866(1)	25(1)
C(54)	4833(2)	6527(2)	3507(1)	25(1)
C(55)	6022(2)	5886(2)	2064(1)	28(1)
C(61)	4656(3)	3557(2)	3013(2)	61(1)
O(61)	4717(2)	3790(1)	2428(1)	50(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**55**·MeOH.

O(1S)-C(1S)	1.400(6)	C(19)-H(19)	0.9400
C(1S)-H(1SA)	0.9700	C(21)-O(21)	1.281(3)
C(1S)-H(1SB)	0.9700	C(21)-C(22)	1.417(3)
C(1S)-H(1SC)	0.9700	C(21)-C(34)	1.461(3)
C(2S)-Cl(1)	1.758(10)	C(22)-C(23)	1.417(3)
C(2S)-Cl(2)	1.772(10)	C(22)-C(35)	1.432(3)
C(2S)-H(2SA)	0.9800	C(23)-C(24)	1.347(3)
C(2S)-H(2SB)	0.9800	C(23)-H(23)	0.9400
Zn(1)-O(41)	1.9553(16)	C(24)-C(25)	1.408(4)
Zn(1)-O(21)	1.9828(15)	C(24)-H(24)	0.9400
Zn(1)-N(02)	2.0708(18)	C(25)-C(34)	1.410(3)
Zn(1)-N(12)	2.0861(18)	C(25)-C(26)	1.420(3)
Zn(1)-O(61)	2.1542(18)	C(26)-C(27)	1.333(4)
C(01)-C(02)	1.381(3)	C(26)-H(26)	0.9400
C(01)-C(10)	1.435(3)	C(27)-C(28)	1.428(4)
C(01)-C(11)	1.490(3)	C(27)-H(27)	0.9400
C(02)-C(03)	1.413(3)	C(28)-C(29)	1.412(4)
C(02)-N(02)	1.427(3)	C(28)-C(33)	1.413(3)
N(02)-C(35)	1.301(3)	C(29)-C(30)	1.353(4)
C(03)-C(04)	1.356(3)	C(29)-H(29)	0.9400
C(03)-H(03)	0.9400	C(30)-C(31)	1.400(4)
C(04)-C(05)	1.404(4)	C(30)-H(30)	0.9400
C(04)-H(04)	0.9400	C(31)-C(32)	1.372(3)
C(05)-C(06)	1.415(3)	C(31)-H(31)	0.9400
C(05)-C(10)	1.418(3)	C(32)-C(33)	1.407(3)
C(06)-C(07)	1.359(4)	C(32)-H(32)	0.9400
C(06)-H(06)	0.9400	C(33)-C(34)	1.455(3)
C(07)-C(08)	1.397(4)	C(35)-H(35)	0.9400
C(07)-H(07)	0.9400	C(41)-O(41)	1.297(3)
C(08)-C(09)	1.364(3)	C(41)-C(42)	1.415(3)
C(08)-H(08)	0.9400	C(41)-C(54)	1.450(3)
C(09)-C(10)	1.407(3)	C(42)-C(43)	1.414(3)
C(09)-H(09)	0.9400	C(42)-C(55)	1.433(3)
C(11)-C(12)	1.377(3)	C(43)-C(44)	1.354(3)
C(11)-C(20)	1.431(3)	C(43)-H(43)	0.9400
C(12)-C(13)	1.398(3)	C(44)-C(45)	1.406(3)
C(12)-N(12)	1.430(3)	C(44)-H(44)	0.9400
N(12)-C(55)	1.284(3)	C(45)-C(54)	1.411(3)
C(13)-C(14)	1.364(3)	C(45)-C(46)	1.431(3)
C(13)-H(13)	0.9400	C(46)-C(47)	1.334(3)
C(14)-C(15)	1.401(3)	C(46)-H(46)	0.9400
C(14)-H(14)	0.9400	C(47)-C(48)	1.421(3)
C(15)-C(16)	1.413(3)	C(47)-H(47)	0.9400
C(15)-C(20)	1.423(3)	C(48)-C(49)	1.410(3)
C(16)-C(17)	1.353(4)	C(48)-C(53)	1.417(3)
C(16)-H(16)	0.9400	C(49)-C(50)	1.360(3)
C(17)-C(18)	1.397(3)	C(49)-H(49)	0.9400
C(17)-H(17)	0.9400	C(50)-C(51)	1.393(4)
C(18)-C(19)	1.367(3)	C(50)-H(50)	0.9400
C(18)-H(18)	0.9400	C(51)-C(52)	1.372(3)
C(19)-C(20)	1.405(3)	C(51)-H(51)	0.9400

C(52)-C(53)	1.409(3)	C(06)-C(07)-H(07)	120.0
C(52)-H(52)	0.9400	C(08)-C(07)-H(07)	120.0
C(53)-C(54)	1.450(3)	C(09)-C(08)-C(07)	120.3(2)
C(55)-H(55)	0.9400	C(09)-C(08)-H(08)	119.8
C(61)-O(61)	1.420(4)	C(07)-C(08)-H(08)	119.8
C(61)-H(61A)	0.9700	C(08)-C(09)-C(10)	121.7(2)
C(61)-H(61B)	0.9700	C(08)-C(09)-H(09)	119.2
C(61)-H(61C)	0.9700	C(10)-C(09)-H(09)	119.2
O(61)-H(61)	0.9881	C(09)-C(10)-C(05)	117.7(2)
		C(09)-C(10)-C(01)	122.4(2)
O(1S)-C(1S)-H(1SA)	109.5	C(05)-C(10)-C(01)	119.8(2)
O(1S)-C(1S)-H(1SB)	109.5	C(12)-C(11)-C(20)	118.58(19)
H(1SA)-C(1S)-H(1SB)	109.5	C(12)-C(11)-C(01)	121.02(19)
O(1S)-C(1S)-H(1SC)	109.5	C(20)-C(11)-C(01)	120.09(18)
H(1SA)-C(1S)-H(1SC)	109.5	C(11)-C(12)-C(13)	121.8(2)
H(1SB)-C(1S)-H(1SC)	109.5	C(11)-C(12)-N(12)	118.64(18)
Cl(1)-C(2S)-Cl(2)	112.0(7)	C(13)-C(12)-N(12)	119.52(19)
Cl(1)-C(2S)-H(2SA)	109.2	C(55)-N(12)-C(12)	117.62(19)
Cl(2)-C(2S)-H(2SA)	109.2	C(55)-N(12)-Zn(1)	120.94(15)
Cl(1)-C(2S)-H(2SB)	109.2	C(12)-N(12)-Zn(1)	120.23(14)
Cl(2)-C(2S)-H(2SB)	109.2	C(14)-C(13)-C(12)	120.1(2)
H(2SA)-C(2S)-H(2SB)	107.9	C(14)-C(13)-H(13)	119.9
O(41)-Zn(1)-O(21)	100.52(7)	C(12)-C(13)-H(13)	119.9
O(41)-Zn(1)-N(02)	120.71(7)	C(13)-C(14)-C(15)	120.8(2)
O(21)-Zn(1)-N(02)	88.49(7)	C(13)-C(14)-H(14)	119.6
O(41)-Zn(1)-N(12)	89.07(7)	C(15)-C(14)-H(14)	119.6
O(21)-Zn(1)-N(12)	168.37(7)	C(14)-C(15)-C(16)	121.9(2)
N(02)-Zn(1)-N(12)	92.26(7)	C(14)-C(15)-C(20)	119.4(2)
O(41)-Zn(1)-O(61)	98.26(8)	C(16)-C(15)-C(20)	118.7(2)
O(21)-Zn(1)-O(61)	86.53(7)	C(17)-C(16)-C(15)	122.0(2)
N(02)-Zn(1)-O(61)	140.95(8)	C(17)-C(16)-H(16)	119.0
N(12)-Zn(1)-O(61)	85.58(7)	C(15)-C(16)-H(16)	119.0
C(02)-C(01)-C(10)	118.6(2)	C(16)-C(17)-C(18)	119.3(2)
C(02)-C(01)-C(11)	123.30(18)	C(16)-C(17)-H(17)	120.4
C(10)-C(01)-C(11)	118.14(19)	C(18)-C(17)-H(17)	120.4
C(01)-C(02)-C(03)	120.40(19)	C(19)-C(18)-C(17)	120.7(2)
C(01)-C(02)-N(02)	122.81(19)	C(19)-C(18)-H(18)	119.7
C(03)-C(02)-N(02)	116.66(19)	C(17)-C(18)-H(18)	119.7
C(35)-N(02)-C(02)	116.37(19)	C(18)-C(19)-C(20)	121.6(2)
C(35)-N(02)-Zn(1)	122.89(15)	C(18)-C(19)-H(19)	119.2
C(02)-N(02)-Zn(1)	118.85(14)	C(20)-C(19)-H(19)	119.2
C(04)-C(03)-C(02)	121.3(2)	C(19)-C(20)-C(15)	117.8(2)
C(04)-C(03)-H(03)	119.4	C(19)-C(20)-C(11)	123.00(19)
C(02)-C(03)-H(03)	119.4	C(15)-C(20)-C(11)	119.20(19)
C(03)-C(04)-C(05)	120.5(2)	O(21)-C(21)-C(22)	121.61(19)
C(03)-C(04)-H(04)	119.8	O(21)-C(21)-C(34)	120.6(2)
C(05)-C(04)-H(04)	119.8	C(22)-C(21)-C(34)	117.76(19)
C(04)-C(05)-C(06)	121.5(2)	C(21)-O(21)-Zn(1)	131.04(15)
C(04)-C(05)-C(10)	119.1(2)	C(23)-C(22)-C(21)	120.7(2)
C(06)-C(05)-C(10)	119.3(2)	C(23)-C(22)-C(35)	115.8(2)
C(07)-C(06)-C(05)	121.0(2)	C(21)-C(22)-C(35)	123.45(19)
C(07)-C(06)-H(06)	119.5	C(24)-C(23)-C(22)	121.2(2)
C(05)-C(06)-H(06)	119.5	C(24)-C(23)-H(23)	119.4
C(06)-C(07)-C(08)	120.0(2)	C(22)-C(23)-H(23)	119.4

C(23)-C(24)-C(25)	120.2(2)	C(43)-C(44)-C(45)	120.0(2)
C(23)-C(24)-H(24)	119.9	C(43)-C(44)-H(44)	120.0
C(25)-C(24)-H(24)	119.9	C(45)-C(44)-H(44)	120.0
C(24)-C(25)-C(34)	121.3(2)	C(44)-C(45)-C(54)	121.4(2)
C(24)-C(25)-C(26)	119.1(2)	C(44)-C(45)-C(46)	119.1(2)
C(34)-C(25)-C(26)	119.6(2)	C(54)-C(45)-C(46)	119.5(2)
C(27)-C(26)-C(25)	122.4(3)	C(47)-C(46)-C(45)	121.9(2)
C(27)-C(26)-H(26)	118.8	C(47)-C(46)-H(46)	119.1
C(25)-C(26)-H(26)	118.8	C(45)-C(46)-H(46)	119.1
C(26)-C(27)-C(28)	120.3(2)	C(46)-C(47)-C(48)	120.6(2)
C(26)-C(27)-H(27)	119.9	C(46)-C(47)-H(47)	119.7
C(28)-C(27)-H(27)	119.9	C(48)-C(47)-H(47)	119.7
C(29)-C(28)-C(33)	120.0(2)	C(49)-C(48)-C(53)	119.9(2)
C(29)-C(28)-C(27)	120.1(2)	C(49)-C(48)-C(47)	119.9(2)
C(33)-C(28)-C(27)	119.9(2)	C(53)-C(48)-C(47)	120.1(2)
C(30)-C(29)-C(28)	121.2(2)	C(50)-C(49)-C(48)	121.6(2)
C(30)-C(29)-H(29)	119.4	C(50)-C(49)-H(49)	119.2
C(28)-C(29)-H(29)	119.4	C(48)-C(49)-H(49)	119.2
C(29)-C(30)-C(31)	119.2(3)	C(49)-C(50)-C(51)	118.8(2)
C(29)-C(30)-H(30)	120.4	C(49)-C(50)-H(50)	120.6
C(31)-C(30)-H(30)	120.4	C(51)-C(50)-H(50)	120.6
C(32)-C(31)-C(30)	120.9(3)	C(52)-C(51)-C(50)	121.3(2)
C(32)-C(31)-H(31)	119.5	C(52)-C(51)-H(51)	119.4
C(30)-C(31)-H(31)	119.5	C(50)-C(51)-H(51)	119.4
C(31)-C(32)-C(33)	121.2(2)	C(51)-C(52)-C(53)	121.4(2)
C(31)-C(32)-H(32)	119.4	C(51)-C(52)-H(52)	119.3
C(33)-C(32)-H(32)	119.4	C(53)-C(52)-H(52)	119.3
C(32)-C(33)-C(28)	117.3(2)	C(52)-C(53)-C(48)	117.0(2)
C(32)-C(33)-C(34)	123.6(2)	C(52)-C(53)-C(54)	123.85(19)
C(28)-C(33)-C(34)	119.1(2)	C(48)-C(53)-C(54)	118.92(19)
C(25)-C(34)-C(33)	118.4(2)	C(45)-C(54)-C(53)	118.67(19)
C(25)-C(34)-C(21)	118.2(2)	C(45)-C(54)-C(41)	118.1(2)
C(33)-C(34)-C(21)	123.2(2)	C(53)-C(54)-C(41)	123.27(19)
N(02)-C(35)-C(22)	128.1(2)	N(12)-C(55)-C(42)	127.4(2)
N(02)-C(35)-H(35)	115.9	N(12)-C(55)-H(55)	116.3
C(22)-C(35)-H(35)	115.9	C(42)-C(55)-H(55)	116.3
O(41)-C(41)-C(42)	122.1(2)	O(61)-C(61)-H(61A)	109.5
O(41)-C(41)-C(54)	119.5(2)	O(61)-C(61)-H(61B)	109.5
C(42)-C(41)-C(54)	118.36(19)	H(61A)-C(61)-H(61B)	109.5
C(41)-O(41)-Zn(1)	125.79(15)	O(61)-C(61)-H(61C)	109.5
C(43)-C(42)-C(41)	120.2(2)	H(61A)-C(61)-H(61C)	109.5
C(43)-C(42)-C(55)	115.5(2)	H(61B)-C(61)-H(61C)	109.5
C(41)-C(42)-C(55)	124.3(2)	C(61)-O(61)-Zn(1)	122.72(18)
C(44)-C(43)-C(42)	121.3(2)	C(61)-O(61)-H(61)	101.9
C(44)-C(43)-H(43)	119.3	Zn(1)-O(61)-H(61)	119.9
C(42)-C(43)-H(43)	119.3		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**55**·MeOH. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1S)	49(2)	59(2)	67(2)	6(2)	0(2)	5(2)
C(1S)	67(3)	80(3)	62(3)	18(3)	-3(3)	9(3)
Cl(1)	64(2)	54(2)	92(3)	6(2)	5(2)	3(2)
Cl(2)	55(2)	61(2)	101(3)	-12(2)	-24(2)	3(2)
Zn(1)	27(1)	36(1)	20(1)	0(1)	-2(1)	-8(1)
C(01)	28(1)	28(1)	18(1)	-2(1)	-1(1)	1(1)
C(02)	29(1)	28(1)	22(1)	1(1)	-1(1)	-1(1)
N(02)	26(1)	30(1)	22(1)	1(1)	3(1)	-2(1)
C(03)	28(1)	40(1)	36(1)	-1(1)	2(1)	2(1)
C(04)	35(1)	32(1)	43(2)	-1(1)	-3(1)	8(1)
C(05)	38(1)	27(1)	26(1)	-1(1)	0(1)	2(1)
C(06)	55(2)	27(1)	37(1)	2(1)	-2(1)	-1(1)
C(07)	58(2)	27(1)	33(1)	4(1)	-1(1)	-10(1)
C(08)	42(2)	42(1)	30(1)	5(1)	2(1)	-14(1)
C(09)	34(1)	35(1)	26(1)	2(1)	-2(1)	-3(1)
C(10)	33(1)	28(1)	18(1)	1(1)	-1(1)	-3(1)
C(11)	25(1)	24(1)	22(1)	-2(1)	1(1)	-3(1)
C(12)	30(1)	30(1)	21(1)	-1(1)	1(1)	-2(1)
N(12)	28(1)	33(1)	19(1)	3(1)	0(1)	-1(1)
C(13)	36(1)	32(1)	30(1)	3(1)	-7(1)	5(1)
C(14)	35(1)	28(1)	39(1)	-3(1)	2(1)	6(1)
C(15)	32(1)	28(1)	30(1)	-4(1)	2(1)	-2(1)
C(16)	35(1)	33(1)	39(1)	-7(1)	8(1)	-1(1)
C(17)	41(1)	45(1)	28(1)	-13(1)	9(1)	-10(1)
C(18)	31(1)	47(1)	25(1)	-2(1)	-1(1)	-10(1)
C(19)	26(1)	37(1)	26(1)	-1(1)	-2(1)	-5(1)
C(20)	26(1)	29(1)	24(1)	-2(1)	2(1)	-5(1)
C(21)	23(1)	32(1)	25(1)	-4(1)	3(1)	-3(1)
O(21)	31(1)	47(1)	23(1)	2(1)	-2(1)	-15(1)
C(22)	26(1)	30(1)	25(1)	-4(1)	1(1)	-2(1)
C(23)	33(1)	46(1)	25(1)	-2(1)	-4(1)	-10(1)
C(24)	43(2)	56(2)	30(1)	-6(1)	-6(1)	-22(1)
C(25)	42(1)	45(1)	33(1)	-4(1)	4(1)	-15(1)
C(26)	63(2)	68(2)	44(2)	-3(2)	0(2)	-40(2)
C(27)	72(2)	56(2)	47(2)	6(2)	5(2)	-35(2)
C(28)	49(2)	42(1)	34(1)	4(1)	10(1)	-12(1)
C(29)	63(2)	50(2)	43(2)	9(1)	13(2)	-15(1)
C(30)	57(2)	58(2)	33(1)	15(1)	6(1)	1(1)
C(31)	46(2)	57(2)	27(1)	5(1)	-2(1)	-4(1)
C(32)	34(1)	42(1)	29(1)	4(1)	4(1)	-3(1)
C(33)	29(1)	34(1)	30(1)	0(1)	7(1)	1(1)
C(34)	27(1)	32(1)	25(1)	-2(1)	4(1)	-5(1)
C(35)	28(1)	33(1)	20(1)	1(1)	1(1)	1(1)
C(41)	27(1)	28(1)	25(1)	0(1)	-5(1)	-4(1)
O(41)	26(1)	59(1)	27(1)	-14(1)	-1(1)	-9(1)
C(42)	31(1)	33(1)	23(1)	3(1)	-2(1)	-6(1)
C(43)	25(1)	42(1)	32(1)	2(1)	1(1)	-8(1)
C(44)	27(1)	40(1)	30(1)	-3(1)	-6(1)	-9(1)

C(45)	28(1)	29(1)	26(1)	1(1)	-5(1)	-1(1)
C(46)	30(1)	35(1)	33(1)	-8(1)	-8(1)	-3(1)
C(47)	34(1)	36(1)	26(1)	-9(1)	-5(1)	2(1)
C(48)	30(1)	26(1)	27(1)	-4(1)	0(1)	4(1)
C(49)	36(1)	36(1)	28(1)	-5(1)	4(1)	5(1)
C(50)	32(1)	44(1)	33(1)	-1(1)	11(1)	0(1)
C(51)	31(1)	48(1)	36(1)	-4(1)	5(1)	-10(1)
C(52)	31(1)	43(1)	27(1)	-3(1)	1(1)	-7(1)
C(53)	28(1)	26(1)	22(1)	1(1)	-4(1)	1(1)
C(54)	27(1)	27(1)	23(1)	0(1)	-3(1)	-2(1)
C(55)	27(1)	32(1)	25(1)	2(1)	2(1)	-4(1)
C(61)	65(2)	61(2)	58(2)	17(2)	-8(2)	9(2)
O(61)	44(1)	55(1)	52(1)	21(1)	6(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**55**·MeOH.

	x	y	z	U(eq)
H(1SA)	8174	3141	2733	105
H(1SB)	7258	3836	2991	105
H(1SC)	7878	4169	2435	105
H(2SA)	7816	3803	3167	122
H(2SB)	8849	3212	2949	122
H(03)	1886	6966	1173	42
H(04)	2302	8495	796	44
H(06)	3679	9678	428	48
H(07)	5407	9987	116	47
H(08)	6684	8697	95	45
H(09)	6222	7112	377	38
H(13)	6836	4217	1456	39
H(14)	7436	3749	574	41
H(16)	7248	3801	-467	43
H(17)	6461	4441	-1263	46
H(18)	5097	5648	-1181	41
H(19)	4486	6140	-309	35
H(23)	480	4054	762	42
H(24)	-511	2756	1115	52
H(26)	-873	1549	1847	70
H(27)	-618	904	2719	70
H(29)	251	973	3651	62
H(30)	1355	1747	4296	59
H(31)	2254	3225	4045	52
H(32)	2112	3864	3145	42
H(35)	1812	5236	818	33
H(43)	7471	6588	2714	39
H(44)	7377	7276	3598	39
H(46)	6367	7678	4446	39
H(47)	4867	7576	4989	39

H(49)	3062	6903	5161	40
H(50)	1571	6000	4880	44
H(51)	1512	5345	3965	46
H(52)	2903	5610	3340	40
H(55)	6718	5978	1911	33
H(61A)	5073	2955	3089	92
H(61B)	3906	3446	3119	92
H(61C)	4948	4109	3232	92
H(61)	5501	3720	2352	60

Table 6. Torsion angles [°] for (*R*)-**55**·MeOH.

C(10)-C(01)-C(02)-C(03)	5.9(3)	C(10)-C(01)-C(11)-C(12)	110.4(2)
C(11)-C(01)-C(02)-C(03)	-174.0(2)	C(02)-C(01)-C(11)-C(20)	116.8(2)
C(10)-C(01)-C(02)-N(02)	-169.9(2)	C(10)-C(01)-C(11)-C(20)	-63.1(3)
C(11)-C(01)-C(02)-N(02)	10.2(3)	C(20)-C(11)-C(12)-C(13)	1.1(3)
C(01)-C(02)-N(02)-C(35)	-130.2(2)	C(01)-C(11)-C(12)-C(13)	-172.54(19)
C(03)-C(02)-N(02)-C(35)	53.8(3)	C(20)-C(11)-C(12)-N(12)	-179.59(18)
C(01)-C(02)-N(02)-Zn(1)	65.0(2)	C(01)-C(11)-C(12)-N(12)	6.8(3)
C(03)-C(02)-N(02)-Zn(1)	-111.0(2)	C(11)-C(12)-N(12)-C(55)	-120.6(2)
O(41)-Zn(1)-N(02)-C(35)	-112.62(17)	C(13)-C(12)-N(12)-C(55)	58.7(3)
O(21)-Zn(1)-N(02)-C(35)	-11.27(18)	C(11)-C(12)-N(12)-Zn(1)	71.9(2)
N(12)-Zn(1)-N(02)-C(35)	157.12(18)	C(13)-C(12)-N(12)-Zn(1)	-108.8(2)
O(61)-Zn(1)-N(02)-C(35)	71.3(2)	O(41)-Zn(1)-N(12)-C(55)	24.63(17)
O(41)-Zn(1)-N(02)-C(02)	51.16(17)	O(21)-Zn(1)-N(12)-C(55)	-121.2(3)
O(21)-Zn(1)-N(02)-C(02)	152.51(15)	N(02)-Zn(1)-N(12)-C(55)	145.33(17)
N(12)-Zn(1)-N(02)-C(02)	-39.11(15)	O(61)-Zn(1)-N(12)-C(55)	-73.73(17)
O(61)-Zn(1)-N(02)-C(02)	-124.88(15)	O(41)-Zn(1)-N(12)-C(12)	-168.29(16)
C(01)-C(02)-C(03)-C(04)	-2.1(4)	O(21)-Zn(1)-N(12)-C(12)	45.9(4)
N(02)-C(02)-C(03)-C(04)	173.9(2)	N(02)-Zn(1)-N(12)-C(12)	-47.59(16)
C(02)-C(03)-C(04)-C(05)	-2.7(4)	O(61)-Zn(1)-N(12)-C(12)	93.35(16)
C(03)-C(04)-C(05)-C(06)	-174.3(2)	C(11)-C(12)-C(13)-C(14)	0.1(3)
C(03)-C(04)-C(05)-C(10)	3.5(4)	N(12)-C(12)-C(13)-C(14)	-179.2(2)
C(04)-C(05)-C(06)-C(07)	178.1(2)	C(12)-C(13)-C(14)-C(15)	-1.5(4)
C(10)-C(05)-C(06)-C(07)	0.3(4)	C(13)-C(14)-C(15)-C(16)	-178.6(2)
C(05)-C(06)-C(07)-C(08)	-0.2(4)	C(13)-C(14)-C(15)-C(20)	1.7(3)
C(06)-C(07)-C(08)-C(09)	0.2(4)	C(14)-C(15)-C(16)-C(17)	-178.5(2)
C(07)-C(08)-C(09)-C(10)	-0.5(4)	C(20)-C(15)-C(16)-C(17)	1.2(3)
C(08)-C(09)-C(10)-C(05)	0.6(3)	C(15)-C(16)-C(17)-C(18)	0.5(3)
C(08)-C(09)-C(10)-C(01)	-178.1(2)	C(16)-C(17)-C(18)-C(19)	-1.6(3)
C(04)-C(05)-C(10)-C(09)	-178.4(2)	C(17)-C(18)-C(19)-C(20)	1.1(3)
C(06)-C(05)-C(10)-C(09)	-0.5(3)	C(18)-C(19)-C(20)-C(15)	0.6(3)
C(04)-C(05)-C(10)-C(01)	0.4(3)	C(18)-C(19)-C(20)-C(11)	179.0(2)
C(06)-C(05)-C(10)-C(01)	178.2(2)	C(14)-C(15)-C(20)-C(19)	178.0(2)
C(02)-C(01)-C(10)-C(09)	173.6(2)	C(16)-C(15)-C(20)-C(19)	-1.7(3)
C(11)-C(01)-C(10)-C(09)	-6.4(3)	C(14)-C(15)-C(20)-C(11)	-0.4(3)
C(02)-C(01)-C(10)-C(05)	-5.0(3)	C(16)-C(15)-C(20)-C(11)	179.86(19)
C(11)-C(01)-C(10)-C(05)	174.92(19)	C(12)-C(11)-C(20)-C(19)	-179.2(2)
C(02)-C(01)-C(11)-C(12)	-69.7(3)	C(01)-C(11)-C(20)-C(19)	-5.6(3)

C(12)-C(11)-C(20)-C(15)	-0.9(3)	C(54)-C(41)-O(41)-Zn(1)	-150.12(16)
C(01)-C(11)-C(20)-C(15)	172.78(18)	O(21)-Zn(1)-O(41)-C(41)	137.37(18)
C(22)-C(21)-O(21)-Zn(1)	-18.6(3)	N(02)-Zn(1)-O(41)-C(41)	-128.08(18)
C(34)-C(21)-O(21)-Zn(1)	160.66(16)	N(12)-Zn(1)-O(41)-C(41)	-36.00(19)
O(41)-Zn(1)-O(21)-C(21)	143.81(19)	O(61)-Zn(1)-O(41)-C(41)	49.39(19)
N(02)-Zn(1)-O(21)-C(21)	22.8(2)	O(41)-C(41)-C(42)-C(43)	172.3(2)
N(12)-Zn(1)-O(21)-C(21)	-71.1(4)	C(54)-C(41)-C(42)-C(43)	-6.0(3)
O(61)-Zn(1)-O(21)-C(21)	-118.4(2)	O(41)-C(41)-C(42)-C(55)	-4.5(3)
O(21)-C(21)-C(22)-C(23)	179.9(2)	C(54)-C(41)-C(42)-C(55)	177.2(2)
C(34)-C(21)-C(22)-C(23)	0.7(3)	C(41)-C(42)-C(43)-C(44)	-0.7(3)
O(21)-C(21)-C(22)-C(35)	-3.6(3)	C(55)-C(42)-C(43)-C(44)	176.4(2)
C(34)-C(21)-C(22)-C(35)	177.1(2)	C(42)-C(43)-C(44)-C(45)	3.8(4)
C(21)-C(22)-C(23)-C(24)	-5.7(4)	C(43)-C(44)-C(45)-C(54)	0.1(3)
C(35)-C(22)-C(23)-C(24)	177.6(2)	C(43)-C(44)-C(45)-C(46)	179.2(2)
C(22)-C(23)-C(24)-C(25)	3.3(4)	C(44)-C(45)-C(46)-C(47)	-175.4(2)
C(23)-C(24)-C(25)-C(34)	4.2(4)	C(54)-C(45)-C(46)-C(47)	3.7(3)
C(23)-C(24)-C(25)-C(26)	-175.8(3)	C(45)-C(46)-C(47)-C(48)	1.6(4)
C(24)-C(25)-C(26)-C(27)	-179.8(3)	C(46)-C(47)-C(48)-C(49)	173.5(2)
C(34)-C(25)-C(26)-C(27)	0.2(5)	C(46)-C(47)-C(48)-C(53)	-4.1(3)
C(25)-C(26)-C(27)-C(28)	2.6(5)	C(53)-C(48)-C(49)-C(50)	1.8(3)
C(26)-C(27)-C(28)-C(29)	178.6(3)	C(47)-C(48)-C(49)-C(50)	-175.9(2)
C(26)-C(27)-C(28)-C(33)	-0.7(5)	C(48)-C(49)-C(50)-C(51)	-0.8(4)
C(33)-C(28)-C(29)-C(30)	2.6(4)	C(49)-C(50)-C(51)-C(52)	-0.6(4)
C(27)-C(28)-C(29)-C(30)	-176.7(3)	C(50)-C(51)-C(52)-C(53)	1.0(4)
C(28)-C(29)-C(30)-C(31)	0.7(5)	C(51)-C(52)-C(53)-C(48)	0.0(3)
C(29)-C(30)-C(31)-C(32)	-2.0(4)	C(51)-C(52)-C(53)-C(54)	174.7(2)
C(30)-C(31)-C(32)-C(33)	0.1(4)	C(49)-C(48)-C(53)-C(52)	-1.3(3)
C(31)-C(32)-C(33)-C(28)	3.1(4)	C(47)-C(48)-C(53)-C(52)	176.3(2)
C(31)-C(32)-C(33)-C(34)	-178.2(2)	C(49)-C(48)-C(53)-C(54)	-176.3(2)
C(29)-C(28)-C(33)-C(32)	-4.4(4)	C(47)-C(48)-C(53)-C(54)	1.3(3)
C(27)-C(28)-C(33)-C(32)	174.9(3)	C(44)-C(45)-C(54)-C(53)	172.8(2)
C(29)-C(28)-C(33)-C(34)	176.9(2)	C(46)-C(45)-C(54)-C(53)	-6.3(3)
C(27)-C(28)-C(33)-C(34)	-3.8(4)	C(44)-C(45)-C(54)-C(41)	-6.8(3)
C(24)-C(25)-C(34)-C(33)	175.2(2)	C(46)-C(45)-C(54)-C(41)	174.08(19)
C(26)-C(25)-C(34)-C(33)	-4.7(4)	C(52)-C(53)-C(54)-C(45)	-170.8(2)
C(24)-C(25)-C(34)-C(21)	-9.0(4)	C(48)-C(53)-C(54)-C(45)	3.9(3)
C(26)-C(25)-C(34)-C(21)	171.0(2)	C(52)-C(53)-C(54)-C(41)	8.8(3)
C(32)-C(33)-C(34)-C(25)	-172.2(2)	C(48)-C(53)-C(54)-C(41)	-176.57(19)
C(28)-C(33)-C(34)-C(25)	6.5(3)	O(41)-C(41)-C(54)-C(45)	-168.8(2)
C(32)-C(33)-C(34)-C(21)	12.4(4)	C(42)-C(41)-C(54)-C(45)	9.6(3)
C(28)-C(33)-C(34)-C(21)	-169.0(2)	O(41)-C(41)-C(54)-C(53)	11.6(3)
O(21)-C(21)-C(34)-C(25)	-172.8(2)	C(42)-C(41)-C(54)-C(53)	-169.98(19)
C(22)-C(21)-C(34)-C(25)	6.5(3)	C(12)-N(12)-C(55)-C(42)	-177.9(2)
O(21)-C(21)-C(34)-C(33)	2.7(3)	Zn(1)-N(12)-C(55)-C(42)	-10.5(3)
C(22)-C(21)-C(34)-C(33)	-178.1(2)	C(43)-C(42)-C(55)-N(12)	177.5(2)
C(02)-N(02)-C(35)-C(22)	-166.8(2)	C(41)-C(42)-C(55)-N(12)	-5.6(4)
Zn(1)-N(02)-C(35)-C(22)	-2.7(3)	O(41)-Zn(1)-O(61)-C(61)	38.3(2)
C(23)-C(22)-C(35)-N(02)	-169.0(2)	O(21)-Zn(1)-O(61)-C(61)	-61.9(2)
C(21)-C(22)-C(35)-N(02)	14.4(4)	N(02)-Zn(1)-O(61)-C(61)	-145.2(2)
C(42)-C(41)-O(41)-Zn(1)	31.5(3)	N(12)-Zn(1)-O(61)-C(61)	126.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*rac*)-**56**.

Identification code	(*rac*)-**56**	
Empirical formula	C51 H32 Cl2 Fe N2 O2	
Formula weight	831.54	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.1443(12) Å	α = 99.736(6)°.
	b = 16.4557(15) Å	β = 104.006(6)°.
	c = 18.9601(17) Å	γ = 94.156(4)°.
Volume	3894.1(6) $Å^3$	
Z	4	
Density (calculated)	1.418 g/cm^3	
Absorption coefficient	0.571 mm^{-1}	
F(000)	1712	
Crystal size	0.35 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.26 to 28.39°.	
Index ranges	-17<=h<=17, -21<=k<=20, -25<=l<=25	
Reflections collected	49344	
Independent reflections	17792 [R(int) = 0.1024]	
Completeness to theta = 28.39°	91.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17792 / 0 / 1045	
Goodness-of-fit on F^2	0.905	
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1255	
R indices (all data)	R1 = 0.1632, wR2 = 0.1642	
Largest diff. peak and hole	0.515 and -0.771 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*rac*)-**56**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6428(4)	6001(3)	2743(3)	67(1)
Cl(1)	7695(1)	6369(1)	3312(1)	80(1)
Cl(2)	6165(1)	6433(1)	1950(1)	82(1)
C(2)	8771(4)	9139(3)	2326(3)	64(1)
Cl(3)	7452(1)	8826(1)	1849(1)	79(1)
Cl(4)	9146(1)	8718(1)	3122(1)	78(1)
Fe(1)	4648(1)	1856(1)	2986(1)	35(1)
Fe(2)	624(1)	3264(1)	2023(1)	35(1)
C(101)	4166(3)	2809(2)	4634(2)	28(1)
C(102)	3445(3)	2634(2)	3950(2)	31(1)
N(102)	3423(2)	1879(2)	3447(2)	33(1)
C(103)	2795(3)	3225(2)	3699(2)	39(1)
C(104)	2843(3)	3973(2)	4142(2)	39(1)
C(105)	3575(3)	4190(2)	4838(2)	34(1)
C(106)	3671(3)	4980(2)	5285(2)	42(1)

C(107)	4429(3)	5206(2)	5926(2)	42(1)
C(108)	5137(3)	4648(2)	6163(2)	37(1)
C(109)	5041(3)	3867(2)	5756(2)	32(1)
C(110)	4264(3)	3607(2)	5081(2)	31(1)
C(111)	4803(3)	2148(2)	4900(2)	27(1)
C(112)	5566(3)	1873(2)	4574(2)	30(1)
N(112)	5759(2)	2199(2)	3960(2)	31(1)
C(113)	6133(3)	1216(2)	4796(2)	38(1)
C(114)	5943(3)	866(2)	5348(2)	38(1)
C(115)	5196(3)	1148(2)	5727(2)	35(1)
C(116)	5033(3)	818(2)	6337(2)	44(1)
C(117)	4336(4)	1109(3)	6710(2)	50(1)
C(118)	3736(3)	1725(3)	6475(2)	46(1)
C(119)	3863(3)	2054(2)	5885(2)	36(1)
C(120)	4611(3)	1792(2)	5500(2)	29(1)
C(121)	3324(3)	245(2)	2458(2)	37(1)
O(121)	4107(2)	770(2)	2450(1)	38(1)
C(122)	2658(3)	451(2)	2922(2)	35(1)
C(123)	1873(3)	-156(3)	2976(2)	49(1)
C(124)	1751(3)	-932(3)	2571(3)	56(1)
C(125)	2384(3)	-1155(3)	2072(3)	51(1)
C(126)	2216(4)	-1985(3)	1651(3)	66(2)
C(127)	2817(4)	-2210(3)	1189(3)	69(2)
C(128)	3589(4)	-1656(3)	1071(3)	59(1)
C(129)	4171(4)	-1916(3)	567(3)	72(2)
C(130)	4898(4)	-1389(4)	420(3)	81(2)
C(131)	5075(4)	-575(3)	796(2)	65(1)
C(132)	4535(3)	-295(3)	1298(2)	54(1)
C(133)	3766(3)	-820(2)	1463(2)	45(1)
C(134)	3158(3)	-571(2)	1996(2)	40(1)
C(135)	2744(3)	1247(2)	3393(2)	35(1)
C(141)	6294(3)	3043(2)	2796(2)	37(1)
O(141)	5330(2)	2636(2)	2572(1)	41(1)
C(142)	6940(3)	3042(2)	3500(2)	36(1)
C(143)	7972(3)	3479(2)	3722(2)	47(1)
C(144)	8334(4)	3912(3)	3273(3)	53(1)
C(145)	7687(4)	3946(2)	2581(3)	47(1)
C(146)	8074(4)	4452(3)	2145(3)	61(1)
C(147)	7475(5)	4561(3)	1500(3)	66(2)
C(148)	6460(4)	4130(3)	1195(3)	57(1)
C(149)	5848(5)	4227(3)	506(3)	76(2)
C(150)	4879(5)	3803(3)	179(3)	68(2)
C(151)	4477(4)	3233(3)	546(3)	61(1)
C(152)	5037(4)	3133(3)	1226(2)	52(1)
C(153)	6033(4)	3578(2)	1584(2)	46(1)
C(154)	6652(3)	3518(2)	2310(2)	41(1)
C(155)	6640(3)	2647(2)	4036(2)	35(1)
C(201)	983(3)	2198(2)	376(2)	30(1)
C(202)	1759(3)	2419(2)	1035(2)	30(1)
N(202)	1803(2)	3190(2)	1518(2)	32(1)
C(203)	2480(3)	1861(2)	1261(2)	43(1)
C(204)	2418(3)	1102(2)	843(2)	46(1)
C(205)	1618(3)	838(2)	183(2)	36(1)
C(206)	1504(4)	28(2)	-248(2)	49(1)

C(207)	684(4)	-233(3)	-844(2)	52(1)
C(208)	-75(3)	295(2)	-1058(2)	45(1)
C(209)	21(3)	1081(2)	-676(2)	36(1)
C(210)	871(3)	1386(2)	-47(2)	31(1)
C(211)	312(3)	2832(2)	98(2)	29(1)
C(212)	-416(3)	3146(2)	438(2)	33(1)
N(212)	-554(2)	2875(2)	1088(2)	34(1)
C(213)	-1020(3)	3772(2)	185(2)	43(1)
C(214)	-883(3)	4063(2)	-416(2)	44(1)
C(215)	-165(3)	3749(2)	-803(2)	39(1)
C(216)	-56(3)	4008(3)	-1452(2)	49(1)
C(217)	617(4)	3673(3)	-1830(3)	59(1)
C(218)	1242(4)	3090(3)	-1563(2)	53(1)
C(219)	1179(3)	2831(2)	-934(2)	40(1)
C(220)	452(3)	3132(2)	-538(2)	34(1)
C(221)	1976(3)	4878(2)	2439(2)	36(1)
O(221)	1212(2)	4367(2)	2513(1)	39(1)
C(222)	2595(3)	4620(2)	1954(2)	38(1)
C(223)	3362(3)	5206(3)	1843(2)	48(1)
C(224)	3504(4)	6001(3)	2181(3)	54(1)
C(225)	2914(3)	6268(3)	2683(3)	52(1)
C(226)	3076(4)	7124(3)	3027(3)	65(1)
C(227)	2495(4)	7420(3)	3482(3)	65(2)
C(228)	1744(4)	6906(3)	3671(2)	58(1)
C(229)	1162(4)	7228(3)	4146(3)	75(2)
C(230)	468(4)	6751(3)	4376(3)	72(2)
C(231)	318(4)	5882(3)	4108(3)	66(2)
C(232)	867(3)	5542(3)	3621(2)	51(1)
C(233)	1585(3)	6026(2)	3370(2)	46(1)
C(234)	2161(3)	5719(2)	2846(2)	42(1)
C(235)	2472(3)	3803(2)	1526(2)	35(1)
C(241)	-945(3)	2128(2)	2339(2)	40(1)
O(241)	-5(2)	2542(2)	2507(1)	41(1)
C(242)	-1664(3)	2097(2)	1648(2)	40(1)
C(243)	-2685(3)	1647(3)	1480(3)	57(1)
C(244)	-2954(4)	1227(3)	1982(3)	68(2)
C(245)	-2253(4)	1221(3)	2654(3)	60(1)
C(246)	-2542(5)	715(3)	3134(4)	87(2)
C(247)	-1871(6)	651(3)	3764(4)	90(2)
C(248)	-851(5)	1112(3)	4020(4)	73(2)
C(249)	-149(6)	1052(4)	4708(4)	88(2)
C(250)	785(6)	1499(4)	4962(4)	94(2)
C(251)	1083(4)	2073(3)	4566(3)	70(2)
C(252)	443(4)	2142(3)	3893(3)	56(1)
C(253)	-531(4)	1656(3)	3590(3)	53(1)
C(254)	-1231(3)	1678(2)	2868(3)	48(1)
C(255)	-1428(3)	2450(2)	1069(2)	39(1)

Table 3. Bond lengths [Å] and angles [°] for (*rac*)-**56**.

C(1)-Cl(2)	1.741(5)	C(118)-C(119)	1.363(5)
C(1)-Cl(1)	1.750(5)	C(118)-H(118)	0.9500
C(1)-H(1A)	0.9900	C(119)-C(120)	1.410(5)
C(1)-H(1B)	0.9900	C(119)-H(119)	0.9500
C(2)-Cl(3)	1.743(5)	C(121)-O(121)	1.299(4)
C(2)-Cl(4)	1.744(5)	C(121)-C(122)	1.405(5)
C(2)-H(2A)	0.9900	C(121)-C(134)	1.443(5)
C(2)-H(2B)	0.9900	C(122)-C(123)	1.417(5)
Fe(1)-O(121)	1.893(2)	C(122)-C(135)	1.434(5)
Fe(1)-O(141)	1.894(3)	C(123)-C(124)	1.351(6)
Fe(1)-N(102)	2.008(3)	C(123)-H(123)	0.9500
Fe(1)-N(112)	2.021(3)	C(124)-C(125)	1.424(6)
Fe(2)-O(241)	1.879(3)	C(124)-H(124)	0.9500
Fe(2)-O(221)	1.907(2)	C(125)-C(134)	1.398(6)
Fe(2)-N(202)	2.010(3)	C(125)-C(126)	1.433(6)
Fe(2)-N(212)	2.022(3)	C(126)-C(127)	1.341(7)
C(101)-C(102)	1.379(5)	C(126)-H(126)	0.9500
C(101)-C(110)	1.417(5)	C(127)-C(128)	1.398(7)
C(101)-C(111)	1.501(5)	C(127)-H(127)	0.9500
C(102)-C(103)	1.408(5)	C(128)-C(129)	1.395(7)
C(102)-N(102)	1.426(4)	C(128)-C(133)	1.422(5)
N(102)-C(135)	1.294(4)	C(129)-C(130)	1.354(7)
C(103)-C(104)	1.355(5)	C(129)-H(129)	0.9500
C(103)-H(103)	0.9500	C(130)-C(131)	1.382(6)
C(104)-C(105)	1.404(5)	C(130)-H(130)	0.9500
C(104)-H(104)	0.9500	C(131)-C(132)	1.360(6)
C(105)-C(106)	1.406(5)	C(131)-H(131)	0.9500
C(105)-C(110)	1.424(5)	C(132)-C(133)	1.409(6)
C(106)-C(107)	1.348(5)	C(132)-H(132)	0.9500
C(106)-H(106)	0.9500	C(133)-C(134)	1.460(6)
C(107)-C(108)	1.405(5)	C(135)-H(135)	0.9500
C(107)-H(107)	0.9500	C(141)-O(141)	1.326(4)
C(108)-C(109)	1.363(5)	C(141)-C(142)	1.398(5)
C(108)-H(108)	0.9500	C(141)-C(154)	1.443(5)
C(109)-C(110)	1.408(5)	C(142)-C(155)	1.411(5)
C(109)-H(109)	0.9500	C(142)-C(143)	1.419(5)
C(111)-C(112)	1.365(5)	C(143)-C(144)	1.345(6)
C(111)-C(120)	1.429(5)	C(143)-H(143)	0.9500
C(112)-C(113)	1.421(5)	C(144)-C(145)	1.393(6)
C(112)-N(112)	1.430(4)	C(144)-H(144)	0.9500
N(112)-C(155)	1.290(4)	C(145)-C(146)	1.417(6)
C(113)-C(114)	1.342(5)	C(145)-C(154)	1.418(6)
C(113)-H(113)	0.9500	C(146)-C(147)	1.333(6)
C(114)-C(115)	1.411(5)	C(146)-H(146)	0.9500
C(114)-H(114)	0.9500	C(147)-C(148)	1.403(7)
C(115)-C(116)	1.411(5)	C(147)-H(147)	0.9500
C(115)-C(120)	1.419(5)	C(148)-C(149)	1.399(7)
C(116)-C(117)	1.353(6)	C(148)-C(153)	1.427(6)
C(116)-H(116)	0.9500	C(149)-C(150)	1.356(7)
C(117)-C(118)	1.395(6)	C(149)-H(149)	0.9500
C(117)-H(117)	0.9500	C(150)-C(151)	1.404(7)

C(150)-H(150)	0.9500	C(224)-H(224)	0.9500
C(151)-C(152)	1.365(6)	C(225)-C(234)	1.416(6)
C(151)-H(151)	0.9500	C(225)-C(226)	1.425(6)
C(152)-C(153)	1.405(6)	C(226)-C(227)	1.340(7)
C(152)-H(152)	0.9500	C(226)-H(226)	0.9500
C(153)-C(154)	1.443(6)	C(227)-C(228)	1.405(7)
C(155)-H(155)	0.9500	C(227)-H(227)	0.9500
C(201)-C(202)	1.382(5)	C(228)-C(229)	1.381(7)
C(201)-C(210)	1.414(5)	C(228)-C(233)	1.444(6)
C(201)-C(211)	1.497(5)	C(229)-C(230)	1.357(7)
C(202)-C(203)	1.409(5)	C(229)-H(229)	0.9500
C(202)-N(202)	1.422(4)	C(230)-C(231)	1.416(6)
N(202)-C(235)	1.285(4)	C(230)-H(230)	0.9500
C(203)-C(204)	1.347(5)	C(231)-C(232)	1.376(6)
C(203)-H(203)	0.9500	C(231)-H(231)	0.9500
C(204)-C(205)	1.405(5)	C(232)-C(233)	1.409(6)
C(204)-H(204)	0.9500	C(232)-H(232)	0.9500
C(205)-C(206)	1.417(5)	C(233)-C(234)	1.437(6)
C(205)-C(210)	1.423(5)	C(235)-H(235)	0.9500
C(206)-C(207)	1.343(6)	C(241)-O(241)	1.306(4)
C(206)-H(206)	0.9500	C(241)-C(242)	1.409(6)
C(207)-C(208)	1.402(6)	C(241)-C(254)	1.445(6)
C(207)-H(207)	0.9500	C(242)-C(255)	1.412(6)
C(208)-C(209)	1.353(5)	C(242)-C(243)	1.422(5)
C(208)-H(208)	0.9500	C(243)-C(244)	1.364(7)
C(209)-C(210)	1.411(5)	C(243)-H(243)	0.9500
C(209)-H(209)	0.9500	C(244)-C(245)	1.381(7)
C(211)-C(212)	1.362(5)	C(244)-H(244)	0.9500
C(211)-C(220)	1.423(5)	C(245)-C(254)	1.421(6)
C(212)-C(213)	1.421(5)	C(245)-C(246)	1.430(7)
C(212)-N(212)	1.426(5)	C(246)-C(247)	1.328(8)
N(212)-C(255)	1.290(5)	C(246)-H(246)	0.9500
C(213)-C(214)	1.353(6)	C(247)-C(248)	1.422(8)
C(213)-H(213)	0.9500	C(247)-H(247)	0.9500
C(214)-C(215)	1.405(6)	C(248)-C(253)	1.415(6)
C(214)-H(214)	0.9500	C(248)-C(249)	1.426(8)
C(215)-C(216)	1.402(6)	C(249)-C(250)	1.320(8)
C(215)-C(220)	1.427(5)	C(249)-H(249)	0.9500
C(216)-C(217)	1.359(6)	C(250)-C(251)	1.391(7)
C(216)-H(216)	0.9500	C(250)-H(250)	0.9500
C(217)-C(218)	1.390(6)	C(251)-C(252)	1.376(6)
C(217)-H(217)	0.9500	C(251)-H(251)	0.9500
C(218)-C(219)	1.351(5)	C(252)-C(253)	1.397(6)
C(218)-H(218)	0.9500	C(252)-H(252)	0.9500
C(219)-C(220)	1.419(5)	C(253)-C(254)	1.461(6)
C(219)-H(219)	0.9500	C(255)-H(255)	0.9500
C(221)-O(221)	1.311(4)		
C(221)-C(222)	1.403(5)	Cl(2)-C(1)-Cl(1)	111.5(3)
C(221)-C(234)	1.438(5)	Cl(2)-C(1)-H(1A)	109.3
C(222)-C(223)	1.422(5)	Cl(1)-C(1)-H(1A)	109.3
C(222)-C(235)	1.424(5)	Cl(2)-C(1)-H(1B)	109.3
C(223)-C(224)	1.334(6)	Cl(1)-C(1)-H(1B)	109.3
C(223)-H(223)	0.9500	H(1A)-C(1)-H(1B)	108.0
C(224)-C(225)	1.401(6)	Cl(3)-C(2)-Cl(4)	112.5(3)

Cl(3)-C(2)-H(2A)	109.1	C(111)-C(112)-N(112)	120.4(3)
Cl(4)-C(2)-H(2A)	109.1	C(113)-C(112)-N(112)	118.1(3)
Cl(3)-C(2)-H(2B)	109.1	C(155)-N(112)-C(112)	119.6(3)
Cl(4)-C(2)-H(2B)	109.1	C(155)-N(112)-Fe(1)	123.5(3)
H(2A)-C(2)-H(2B)	107.8	C(112)-N(112)-Fe(1)	116.8(2)
O(121)-Fe(1)-O(141)	121.68(11)	C(114)-C(113)-C(112)	120.2(4)
O(121)-Fe(1)-N(102)	89.95(11)	C(114)-C(113)-H(113)	119.9
O(141)-Fe(1)-N(102)	133.38(12)	C(112)-C(113)-H(113)	119.9
O(121)-Fe(1)-N(112)	128.37(12)	C(113)-C(114)-C(115)	121.1(4)
O(141)-Fe(1)-N(112)	90.52(12)	C(113)-C(114)-H(114)	119.4
N(102)-Fe(1)-N(112)	94.80(12)	C(115)-C(114)-H(114)	119.4
O(241)-Fe(2)-O(221)	121.06(11)	C(116)-C(115)-C(114)	121.7(4)
O(241)-Fe(2)-N(202)	133.44(12)	C(116)-C(115)-C(120)	119.2(4)
O(221)-Fe(2)-N(202)	89.48(11)	C(114)-C(115)-C(120)	119.1(4)
O(241)-Fe(2)-N(212)	90.39(12)	C(117)-C(116)-C(115)	121.3(4)
O(221)-Fe(2)-N(212)	129.28(12)	C(117)-C(116)-H(116)	119.4
N(202)-Fe(2)-N(212)	95.70(12)	C(115)-C(116)-H(116)	119.4
C(102)-C(101)-C(110)	118.8(3)	C(116)-C(117)-C(118)	119.7(4)
C(102)-C(101)-C(111)	119.8(3)	C(116)-C(117)-H(117)	120.1
C(110)-C(101)-C(111)	121.4(3)	C(118)-C(117)-H(117)	120.1
C(101)-C(102)-C(103)	121.3(3)	C(119)-C(118)-C(117)	120.8(4)
C(101)-C(102)-N(102)	120.1(3)	C(119)-C(118)-H(118)	119.6
C(103)-C(102)-N(102)	118.3(3)	C(117)-C(118)-H(118)	119.6
C(135)-N(102)-C(102)	120.6(3)	C(118)-C(119)-C(120)	121.2(4)
C(135)-N(102)-Fe(1)	125.0(3)	C(118)-C(119)-H(119)	119.4
C(102)-N(102)-Fe(1)	113.8(2)	C(120)-C(119)-H(119)	119.4
C(104)-C(103)-C(102)	120.1(3)	C(119)-C(120)-C(115)	117.7(3)
C(104)-C(103)-H(103)	120.0	C(119)-C(120)-C(111)	122.9(3)
C(102)-C(103)-H(103)	120.0	C(115)-C(120)-C(111)	119.3(3)
C(103)-C(104)-C(105)	121.1(4)	O(121)-C(121)-C(122)	121.1(3)
C(103)-C(104)-H(104)	119.5	O(121)-C(121)-C(134)	119.2(4)
C(105)-C(104)-H(104)	119.5	C(122)-C(121)-C(134)	119.7(4)
C(104)-C(105)-C(106)	121.5(4)	C(121)-O(121)-Fe(1)	133.3(2)
C(104)-C(105)-C(110)	119.0(3)	C(121)-C(122)-C(123)	120.1(4)
C(106)-C(105)-C(110)	119.4(3)	C(121)-C(122)-C(135)	124.1(3)
C(107)-C(106)-C(105)	121.2(4)	C(123)-C(122)-C(135)	115.7(4)
C(107)-C(106)-H(106)	119.4	C(124)-C(123)-C(122)	120.1(4)
C(105)-C(106)-H(106)	119.4	C(124)-C(123)-H(123)	119.9
C(106)-C(107)-C(108)	120.2(4)	C(122)-C(123)-H(123)	119.9
C(106)-C(107)-H(107)	119.9	C(123)-C(124)-C(125)	121.3(4)
C(108)-C(107)-H(107)	119.9	C(123)-C(124)-H(124)	119.4
C(109)-C(108)-C(107)	120.1(4)	C(125)-C(124)-H(124)	119.4
C(109)-C(108)-H(108)	119.9	C(134)-C(125)-C(124)	120.3(4)
C(107)-C(108)-H(108)	119.9	C(134)-C(125)-C(126)	120.7(5)
C(108)-C(109)-C(110)	121.5(3)	C(124)-C(125)-C(126)	119.0(4)
C(108)-C(109)-H(109)	119.3	C(127)-C(126)-C(125)	119.8(5)
C(110)-C(109)-H(109)	119.3	C(127)-C(126)-H(126)	120.1
C(109)-C(110)-C(101)	122.8(3)	C(125)-C(126)-H(126)	120.1
C(109)-C(110)-C(105)	117.5(3)	C(126)-C(127)-C(128)	122.7(5)
C(101)-C(110)-C(105)	119.6(3)	C(126)-C(127)-H(127)	118.6
C(112)-C(111)-C(120)	119.0(3)	C(128)-C(127)-H(127)	118.6
C(112)-C(111)-C(101)	121.0(3)	C(129)-C(128)-C(127)	120.4(5)
C(120)-C(111)-C(101)	120.1(3)	C(129)-C(128)-C(133)	120.2(5)
C(111)-C(112)-C(113)	121.3(4)	C(127)-C(128)-C(133)	119.4(5)

C(130)-C(129)-C(128)	122.0(5)	C(150)-C(151)-H(151)	119.8
C(130)-C(129)-H(129)	119.0	C(151)-C(152)-C(153)	122.3(5)
C(128)-C(129)-H(129)	119.0	C(151)-C(152)-H(152)	118.8
C(129)-C(130)-C(131)	118.4(5)	C(153)-C(152)-H(152)	118.8
C(129)-C(130)-H(130)	120.8	C(152)-C(153)-C(148)	117.0(4)
C(131)-C(130)-H(130)	120.8	C(152)-C(153)-C(154)	125.1(4)
C(132)-C(131)-C(130)	121.8(5)	C(148)-C(153)-C(154)	117.9(4)
C(132)-C(131)-H(131)	119.1	C(145)-C(154)-C(141)	116.2(4)
C(130)-C(131)-H(131)	119.1	C(145)-C(154)-C(153)	119.4(4)
C(131)-C(132)-C(133)	121.7(4)	C(141)-C(154)-C(153)	124.5(4)
C(131)-C(132)-H(132)	119.2	N(112)-C(155)-C(142)	126.9(4)
C(133)-C(132)-H(132)	119.2	N(112)-C(155)-H(155)	116.5
C(132)-C(133)-C(128)	116.0(4)	C(142)-C(155)-H(155)	116.5
C(132)-C(133)-C(134)	125.1(4)	C(202)-C(201)-C(210)	119.4(3)
C(128)-C(133)-C(134)	118.9(4)	C(202)-C(201)-C(211)	119.7(3)
C(125)-C(134)-C(121)	118.3(4)	C(210)-C(201)-C(211)	120.8(3)
C(125)-C(134)-C(133)	118.4(4)	C(201)-C(202)-C(203)	120.4(3)
C(121)-C(134)-C(133)	123.4(4)	C(201)-C(202)-N(202)	120.6(3)
N(102)-C(135)-C(122)	125.8(4)	C(203)-C(202)-N(202)	118.8(3)
N(102)-C(135)-H(135)	117.1	C(235)-N(202)-C(202)	119.7(3)
C(122)-C(135)-H(135)	117.1	C(235)-N(202)-Fe(2)	125.0(3)
O(141)-C(141)-C(142)	120.9(4)	C(202)-N(202)-Fe(2)	114.6(2)
O(141)-C(141)-C(154)	118.6(4)	C(204)-C(203)-C(202)	120.7(4)
C(142)-C(141)-C(154)	120.4(4)	C(204)-C(203)-H(203)	119.7
C(141)-O(141)-Fe(1)	131.0(3)	C(202)-C(203)-H(203)	119.7
C(141)-C(142)-C(155)	125.0(4)	C(203)-C(204)-C(205)	120.9(4)
C(141)-C(142)-C(143)	119.5(4)	C(203)-C(204)-H(204)	119.5
C(155)-C(142)-C(143)	115.5(4)	C(205)-C(204)-H(204)	119.5
C(144)-C(143)-C(142)	121.3(4)	C(204)-C(205)-C(206)	122.0(4)
C(144)-C(143)-H(143)	119.4	C(204)-C(205)-C(210)	119.2(3)
C(142)-C(143)-H(143)	119.4	C(206)-C(205)-C(210)	118.7(4)
C(143)-C(144)-C(145)	119.9(4)	C(207)-C(206)-C(205)	121.0(4)
C(143)-C(144)-H(144)	120.0	C(207)-C(206)-H(206)	119.5
C(145)-C(144)-H(144)	120.0	C(205)-C(206)-H(206)	119.5
C(144)-C(145)-C(146)	118.1(4)	C(206)-C(207)-C(208)	120.5(4)
C(144)-C(145)-C(154)	122.6(4)	C(206)-C(207)-H(207)	119.8
C(146)-C(145)-C(154)	119.2(5)	C(208)-C(207)-H(207)	119.8
C(147)-C(146)-C(145)	121.6(5)	C(209)-C(208)-C(207)	120.4(4)
C(147)-C(146)-H(146)	119.2	C(209)-C(208)-H(208)	119.8
C(145)-C(146)-H(146)	119.2	C(207)-C(208)-H(208)	119.8
C(146)-C(147)-C(148)	121.4(5)	C(208)-C(209)-C(210)	121.3(4)
C(146)-C(147)-H(147)	119.3	C(208)-C(209)-H(209)	119.4
C(148)-C(147)-H(147)	119.3	C(210)-C(209)-H(209)	119.4
C(149)-C(148)-C(147)	121.1(5)	C(209)-C(210)-C(201)	122.8(3)
C(149)-C(148)-C(153)	118.6(5)	C(209)-C(210)-C(205)	118.0(3)
C(147)-C(148)-C(153)	120.2(5)	C(201)-C(210)-C(205)	119.1(3)
C(150)-C(149)-C(148)	123.2(5)	C(212)-C(211)-C(220)	118.6(3)
C(150)-C(149)-H(149)	118.4	C(212)-C(211)-C(201)	122.5(3)
C(148)-C(149)-H(149)	118.4	C(220)-C(211)-C(201)	118.8(3)
C(149)-C(150)-C(151)	118.3(5)	C(211)-C(212)-C(213)	121.9(4)
C(149)-C(150)-H(150)	120.9	C(211)-C(212)-N(212)	119.9(3)
C(151)-C(150)-H(150)	120.9	C(213)-C(212)-N(212)	118.1(3)
C(152)-C(151)-C(150)	120.4(5)	C(255)-N(212)-C(212)	119.8(3)
C(152)-C(151)-H(151)	119.8	C(255)-N(212)-Fe(2)	123.5(3)

C(212)-N(212)-Fe(2)	116.6(2)	C(229)-C(230)-H(230)	120.7
C(214)-C(213)-C(212)	119.6(4)	C(231)-C(230)-H(230)	120.7
C(214)-C(213)-H(213)	120.2	C(232)-C(231)-C(230)	119.8(5)
C(212)-C(213)-H(213)	120.2	C(232)-C(231)-H(231)	120.1
C(213)-C(214)-C(215)	121.2(4)	C(230)-C(231)-H(231)	120.1
C(213)-C(214)-H(214)	119.4	C(231)-C(232)-C(233)	122.6(4)
C(215)-C(214)-H(214)	119.4	C(231)-C(232)-H(232)	118.7
C(216)-C(215)-C(214)	122.1(4)	C(233)-C(232)-H(232)	118.7
C(216)-C(215)-C(220)	119.1(4)	C(232)-C(233)-C(234)	125.8(4)
C(214)-C(215)-C(220)	118.8(4)	C(232)-C(233)-C(228)	116.2(4)
C(217)-C(216)-C(215)	120.9(4)	C(234)-C(233)-C(228)	118.0(4)
C(217)-C(216)-H(216)	119.6	C(225)-C(234)-C(233)	119.7(4)
C(215)-C(216)-H(216)	119.6	C(225)-C(234)-C(221)	117.0(4)
C(216)-C(217)-C(218)	120.3(4)	C(233)-C(234)-C(221)	123.2(4)
C(216)-C(217)-H(217)	119.9	N(202)-C(235)-C(222)	126.8(4)
C(218)-C(217)-H(217)	119.9	N(202)-C(235)-H(235)	116.6
C(219)-C(218)-C(217)	121.0(4)	C(222)-C(235)-H(235)	116.6
C(219)-C(218)-H(218)	119.5	O(241)-C(241)-C(242)	121.0(4)
C(217)-C(218)-H(218)	119.5	O(241)-C(241)-C(254)	118.9(4)
C(218)-C(219)-C(220)	120.9(4)	C(242)-C(241)-C(254)	120.0(4)
C(218)-C(219)-H(219)	119.6	C(241)-O(241)-Fe(2)	132.1(3)
C(220)-C(219)-H(219)	119.6	C(241)-C(242)-C(255)	124.4(4)
C(219)-C(220)-C(211)	122.5(3)	C(241)-C(242)-C(243)	120.0(4)
C(219)-C(220)-C(215)	117.8(4)	C(255)-C(242)-C(243)	115.4(4)
C(211)-C(220)-C(215)	119.8(4)	C(244)-C(243)-C(242)	119.7(5)
O(221)-C(221)-C(222)	120.7(3)	C(244)-C(243)-H(243)	120.2
O(221)-C(221)-C(234)	119.5(4)	C(242)-C(243)-H(243)	120.2
C(222)-C(221)-C(234)	119.8(4)	C(243)-C(244)-C(245)	121.6(5)
C(221)-O(221)-Fe(2)	133.0(2)	C(243)-C(244)-H(244)	119.2
C(221)-C(222)-C(223)	119.3(4)	C(245)-C(244)-H(244)	119.2
C(221)-C(222)-C(235)	124.0(4)	C(244)-C(245)-C(254)	121.8(5)
C(223)-C(222)-C(235)	116.5(4)	C(244)-C(245)-C(246)	119.4(5)
C(224)-C(223)-C(222)	121.9(4)	C(254)-C(245)-C(246)	118.8(6)
C(224)-C(223)-H(223)	119.1	C(247)-C(246)-C(245)	121.5(6)
C(222)-C(223)-H(223)	119.1	C(247)-C(246)-H(246)	119.2
C(223)-C(224)-C(225)	119.7(4)	C(245)-C(246)-H(246)	119.2
C(223)-C(224)-H(224)	120.2	C(246)-C(247)-C(248)	122.2(6)
C(225)-C(224)-H(224)	120.2	C(246)-C(247)-H(247)	118.9
C(224)-C(225)-C(234)	122.1(4)	C(248)-C(247)-H(247)	118.9
C(224)-C(225)-C(226)	118.2(5)	C(253)-C(248)-C(247)	119.3(6)
C(234)-C(225)-C(226)	119.7(5)	C(253)-C(248)-C(249)	119.1(6)
C(227)-C(226)-C(225)	120.7(5)	C(247)-C(248)-C(249)	121.6(6)
C(227)-C(226)-H(226)	119.6	C(250)-C(249)-C(248)	122.0(6)
C(225)-C(226)-H(226)	119.6	C(250)-C(249)-H(249)	119.0
C(226)-C(227)-C(228)	122.2(5)	C(248)-C(249)-H(249)	119.0
C(226)-C(227)-H(227)	118.9	C(249)-C(250)-C(251)	119.4(7)
C(228)-C(227)-H(227)	118.9	C(249)-C(250)-H(250)	120.3
C(229)-C(228)-C(227)	121.0(5)	C(251)-C(250)-H(250)	120.3
C(229)-C(228)-C(233)	119.6(5)	C(252)-C(251)-C(250)	120.7(6)
C(227)-C(228)-C(233)	119.5(5)	C(252)-C(251)-H(251)	119.7
C(230)-C(229)-C(228)	123.2(5)	C(250)-C(251)-H(251)	119.7
C(230)-C(229)-H(229)	118.4	C(251)-C(252)-C(253)	121.6(5)
C(228)-C(229)-H(229)	118.4	C(251)-C(252)-H(252)	119.2
C(229)-C(230)-C(231)	118.6(5)	C(253)-C(252)-H(252)	119.2

C(252)-C(253)-C(248)	117.0(5)	C(241)-C(254)-C(253)	124.0(4)
C(252)-C(253)-C(254)	124.4(4)	N(212)-C(255)-C(242)	126.6(4)
C(248)-C(253)-C(254)	118.6(5)	N(212)-C(255)-H(255)	116.7
C(245)-C(254)-C(241)	116.8(5)	C(242)-C(255)-H(255)	116.7
C(245)-C(254)-C(253)	119.2(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*rac*)-**56**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	68(3)	75(4)	66(3)	10(3)	34(3)	13(3)
Cl(1)	73(1)	89(1)	78(1)	9(1)	20(1)	29(1)
Cl(2)	78(1)	116(1)	61(1)	20(1)	31(1)	15(1)
C(2)	70(3)	76(4)	62(3)	23(3)	38(3)	23(3)
Cl(3)	74(1)	88(1)	83(1)	20(1)	24(1)	33(1)
Cl(4)	88(1)	101(1)	60(1)	30(1)	34(1)	26(1)
Fe(1)	38(1)	33(1)	32(1)	2(1)	9(1)	2(1)
Fe(2)	36(1)	33(1)	34(1)	3(1)	8(1)	2(1)
C(101)	30(2)	28(2)	30(2)	9(2)	12(2)	7(2)
C(102)	33(2)	28(2)	37(2)	10(2)	13(2)	7(2)
N(102)	34(2)	27(2)	33(2)	3(1)	3(1)	3(2)
C(103)	34(2)	44(3)	37(2)	10(2)	2(2)	11(2)
C(104)	41(2)	37(2)	44(2)	14(2)	9(2)	19(2)
C(105)	40(2)	28(2)	39(2)	10(2)	16(2)	11(2)
C(106)	48(3)	33(2)	50(3)	10(2)	17(2)	21(2)
C(107)	58(3)	27(2)	47(3)	4(2)	21(2)	14(2)
C(108)	45(2)	31(2)	35(2)	5(2)	9(2)	5(2)
C(109)	44(2)	27(2)	28(2)	9(2)	11(2)	11(2)
C(110)	37(2)	27(2)	32(2)	10(2)	12(2)	9(2)
C(111)	33(2)	21(2)	27(2)	3(2)	5(2)	7(2)
C(112)	37(2)	25(2)	26(2)	2(2)	5(2)	6(2)
N(112)	37(2)	27(2)	30(2)	2(1)	12(1)	7(2)
C(113)	37(2)	29(2)	44(2)	2(2)	5(2)	9(2)
C(114)	43(2)	22(2)	46(2)	9(2)	4(2)	12(2)
C(115)	38(2)	24(2)	38(2)	7(2)	-1(2)	-1(2)
C(116)	52(3)	30(2)	46(3)	17(2)	-2(2)	2(2)
C(117)	60(3)	45(3)	49(3)	24(2)	11(2)	-6(2)
C(118)	53(3)	49(3)	42(2)	13(2)	17(2)	6(2)
C(119)	43(2)	32(2)	35(2)	8(2)	12(2)	6(2)
C(120)	34(2)	22(2)	27(2)	5(2)	2(2)	2(2)
C(121)	36(2)	32(2)	36(2)	7(2)	-4(2)	9(2)
O(121)	39(2)	30(2)	43(2)	1(1)	9(1)	3(1)
C(122)	31(2)	30(2)	41(2)	10(2)	0(2)	3(2)
C(123)	38(2)	43(3)	62(3)	15(2)	1(2)	5(2)
C(124)	35(2)	35(3)	85(4)	20(2)	-10(2)	-6(2)
C(125)	41(3)	35(3)	62(3)	7(2)	-12(2)	7(2)
C(126)	55(3)	39(3)	79(4)	11(3)	-25(3)	-6(2)

C(127)	68(4)	41(3)	74(4)	-14(3)	-14(3)	14(3)
C(128)	53(3)	40(3)	63(3)	-11(2)	-13(2)	14(2)
C(129)	74(4)	50(3)	70(4)	-24(3)	-4(3)	25(3)
C(130)	76(4)	78(4)	69(4)	-25(3)	3(3)	30(3)
C(131)	61(3)	68(3)	56(3)	-13(3)	9(2)	28(3)
C(132)	48(3)	46(3)	52(3)	-8(2)	-6(2)	14(2)
C(133)	43(2)	32(2)	44(2)	-8(2)	-14(2)	19(2)
C(134)	35(2)	26(2)	46(2)	3(2)	-12(2)	7(2)
C(135)	27(2)	43(2)	37(2)	14(2)	6(2)	10(2)
C(141)	41(2)	26(2)	50(3)	5(2)	24(2)	11(2)
O(141)	46(2)	41(2)	39(2)	10(1)	16(1)	7(1)
C(142)	39(2)	28(2)	43(2)	5(2)	16(2)	10(2)
C(143)	37(2)	42(3)	61(3)	4(2)	16(2)	7(2)
C(144)	45(3)	43(3)	74(3)	5(2)	28(3)	3(2)
C(145)	56(3)	31(2)	65(3)	9(2)	38(3)	10(2)
C(146)	75(4)	43(3)	78(4)	8(3)	47(3)	6(3)
C(147)	92(4)	45(3)	79(4)	10(3)	58(3)	12(3)
C(148)	92(4)	44(3)	55(3)	14(2)	49(3)	30(3)
C(149)	138(6)	45(3)	64(4)	13(3)	55(4)	27(4)
C(150)	125(5)	57(3)	39(3)	18(3)	33(3)	48(3)
C(151)	82(4)	64(3)	49(3)	11(3)	29(3)	41(3)
C(152)	75(3)	53(3)	41(2)	17(2)	30(2)	32(3)
C(153)	63(3)	35(2)	53(3)	12(2)	33(2)	22(2)
C(154)	59(3)	30(2)	49(3)	9(2)	36(2)	20(2)
C(155)	34(2)	29(2)	41(2)	0(2)	9(2)	8(2)
C(201)	32(2)	28(2)	32(2)	11(2)	10(2)	8(2)
C(202)	31(2)	27(2)	35(2)	11(2)	10(2)	7(2)
N(202)	31(2)	33(2)	32(2)	6(1)	4(1)	9(2)
C(203)	41(2)	43(3)	43(2)	14(2)	2(2)	15(2)
C(204)	51(3)	36(3)	59(3)	21(2)	14(2)	22(2)
C(205)	49(2)	28(2)	40(2)	13(2)	21(2)	15(2)
C(206)	71(3)	32(2)	55(3)	18(2)	29(3)	25(2)
C(207)	83(4)	27(2)	53(3)	4(2)	32(3)	13(2)
C(208)	58(3)	35(2)	40(2)	2(2)	16(2)	5(2)
C(209)	41(2)	32(2)	37(2)	6(2)	12(2)	7(2)
C(210)	43(2)	26(2)	30(2)	12(2)	15(2)	8(2)
C(211)	31(2)	23(2)	28(2)	3(2)	2(2)	7(2)
C(212)	34(2)	26(2)	34(2)	3(2)	3(2)	2(2)
N(212)	31(2)	29(2)	40(2)	2(1)	9(2)	9(2)
C(213)	37(2)	30(2)	52(3)	-2(2)	1(2)	11(2)
C(214)	41(2)	29(2)	55(3)	11(2)	-6(2)	9(2)
C(215)	37(2)	26(2)	47(2)	12(2)	-5(2)	2(2)
C(216)	51(3)	37(3)	54(3)	25(2)	-4(2)	4(2)
C(217)	69(3)	56(3)	54(3)	30(2)	9(3)	-3(3)
C(218)	62(3)	51(3)	55(3)	25(2)	21(2)	12(2)
C(219)	45(2)	40(2)	40(2)	17(2)	12(2)	9(2)
C(220)	39(2)	23(2)	34(2)	8(2)	-1(2)	1(2)
C(221)	32(2)	25(2)	42(2)	9(2)	-8(2)	5(2)
O(221)	38(2)	35(2)	39(2)	2(1)	7(1)	9(1)
C(222)	33(2)	35(2)	42(2)	11(2)	-1(2)	7(2)
C(223)	39(2)	46(3)	55(3)	15(2)	1(2)	0(2)
C(224)	50(3)	41(3)	64(3)	14(2)	-1(2)	-1(2)
C(225)	45(3)	30(2)	63(3)	13(2)	-20(2)	0(2)
C(226)	59(3)	43(3)	74(4)	14(3)	-15(3)	-4(2)

C(227)	68(3)	38(3)	68(3)	5(3)	-15(3)	4(3)
C(228)	54(3)	51(3)	51(3)	-7(2)	-10(2)	21(3)
C(229)	76(4)	56(4)	70(4)	-13(3)	-9(3)	29(3)
C(230)	67(4)	74(4)	55(3)	-25(3)	-5(3)	36(3)
C(231)	56(3)	71(4)	61(3)	-8(3)	7(2)	30(3)
C(232)	48(3)	52(3)	43(3)	-9(2)	-2(2)	26(2)
C(233)	39(2)	33(2)	50(3)	-3(2)	-12(2)	11(2)
C(234)	41(2)	36(2)	39(2)	3(2)	-8(2)	14(2)
C(235)	32(2)	35(2)	39(2)	12(2)	7(2)	7(2)
C(241)	50(3)	27(2)	55(3)	5(2)	34(2)	14(2)
O(241)	38(2)	45(2)	43(2)	14(1)	15(1)	3(1)
C(242)	33(2)	28(2)	60(3)	-1(2)	19(2)	6(2)
C(243)	44(3)	48(3)	78(3)	-8(3)	27(3)	1(2)
C(244)	51(3)	43(3)	112(5)	-13(3)	46(3)	-7(2)
C(245)	75(4)	37(3)	89(4)	5(3)	63(3)	10(3)
C(246)	112(5)	45(3)	133(6)	3(4)	100(5)	4(3)
C(247)	149(7)	39(3)	130(6)	27(4)	119(5)	25(4)
C(248)	120(5)	43(3)	102(5)	33(3)	93(4)	41(3)
C(249)	160(7)	72(4)	94(5)	54(4)	105(5)	74(5)
C(250)	143(6)	105(5)	86(5)	58(4)	82(5)	85(5)
C(251)	83(4)	94(4)	61(3)	37(3)	45(3)	53(3)
C(252)	68(3)	66(3)	60(3)	31(3)	43(3)	35(3)
C(253)	81(4)	40(3)	67(3)	23(2)	58(3)	34(3)
C(254)	57(3)	32(2)	70(3)	9(2)	45(3)	14(2)
C(255)	34(2)	33(2)	46(2)	0(2)	9(2)	13(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*rac*)-**56**.

	x	y	z	U(eq)
H(1A)	6366	5389	2598	81
H(1B)	5899	6140	3024	81
H(2A)	8884	9752	2467	77
H(2B)	9225	8967	1994	77
H(103)	2322	3100	3219	47
H(104)	2374	4356	3979	47
H(106)	3193	5361	5133	50
H(107)	4485	5744	6219	51
H(108)	5683	4815	6608	45
H(109)	5510	3489	5931	38
H(113)	6647	1024	4552	46
H(114)	6319	421	5487	45
H(116)	5420	385	6489	53
H(117)	4255	894	7131	60
H(118)	3233	1917	6729	55
H(119)	3440	2468	5730	43
H(123)	1432	-17	3297	59
H(124)	1233	-1337	2620	67

H(126)	1679	-2375	1699	79
H(127)	2714	-2769	931	83
H(129)	4053	-2480	319	87
H(130)	5277	-1575	67	97
H(131)	5589	-201	701	78
H(132)	4679	270	1543	65
H(135)	2260	1315	3692	42
H(143)	8415	3467	4196	56
H(144)	9031	4194	3428	63
H(146)	8778	4719	2317	73
H(147)	7740	4939	1242	79
H(149)	6125	4609	257	91
H(150)	4483	3889	-288	82
H(151)	3810	2914	319	73
H(152)	4743	2749	1466	62
H(155)	7141	2719	4504	42
H(203)	3014	2022	1713	51
H(204)	2923	740	997	56
H(206)	2017	-335	-113	58
H(207)	617	-781	-1122	62
H(208)	-660	100	-1475	54
H(209)	-493	1435	-833	43
H(213)	-1516	3984	436	51
H(214)	-1279	4488	-578	53
H(216)	-459	4423	-1629	58
H(217)	660	3838	-2279	71
H(218)	1721	2869	-1827	63
H(219)	1627	2443	-754	48
H(223)	3784	5027	1518	58
H(224)	4003	6385	2083	65
H(226)	3600	7487	2933	78
H(227)	2595	7998	3684	78
H(229)	1253	7811	4321	89
H(230)	90	6995	4710	87
H(231)	-160	5536	4263	79
H(232)	758	4959	3446	61
H(235)	2932	3700	1212	42
H(243)	-3178	1638	1019	69
H(244)	-3641	932	1868	82
H(246)	-3230	419	3000	104
H(247)	-2080	284	4055	108
H(249)	-360	680	4992	106
H(250)	1249	1430	5411	112
H(251)	1734	2421	4763	84
H(252)	670	2530	3627	68
H(255)	-1968	2367	619	46

Table 6. Torsion angles [°] for (*rac*)-**56**.

C(110)-C(101)-C(102)-C(103)	-1.4(5)	N(102)-Fe(1)-N(112)-C(112)	37.3(3)
C(111)-C(101)-C(102)-C(103)	176.6(3)	C(111)-C(112)-C(113)-C(114)	-1.8(5)
C(110)-C(101)-C(102)-N(102)	171.8(3)	N(112)-C(112)-C(113)-C(114)	-177.1(3)
C(111)-C(101)-C(102)-N(102)	-10.2(5)	C(112)-C(113)-C(114)-C(115)	-1.0(5)
C(101)-C(102)-N(102)-C(135)	98.5(4)	C(113)-C(114)-C(115)-C(116)	-176.3(4)
C(103)-C(102)-N(102)-C(135)	-88.1(4)	C(113)-C(114)-C(115)-C(120)	2.2(5)
C(101)-C(102)-N(102)-Fe(1)	-72.6(4)	C(114)-C(115)-C(116)-C(117)	178.1(4)
C(103)-C(102)-N(102)-Fe(1)	100.8(3)	C(120)-C(115)-C(116)-C(117)	-0.4(5)
O(121)-Fe(1)-N(102)-C(135)	9.4(3)	C(115)-C(116)-C(117)-C(118)	2.3(6)
O(141)-Fe(1)-N(102)-C(135)	145.6(3)	C(116)-C(117)-C(118)-C(119)	-1.7(6)
N(112)-Fe(1)-N(102)-C(135)	-119.1(3)	C(117)-C(118)-C(119)-C(120)	-0.8(6)
O(121)-Fe(1)-N(102)-C(102)	180.0(2)	C(118)-C(119)-C(120)-C(115)	2.7(5)
O(141)-Fe(1)-N(102)-C(102)	-43.8(3)	C(118)-C(119)-C(120)-C(111)	-177.0(3)
N(112)-Fe(1)-N(102)-C(102)	51.5(2)	C(116)-C(115)-C(120)-C(119)	-2.0(5)
C(101)-C(102)-C(103)-C(104)	-2.3(6)	C(114)-C(115)-C(120)-C(119)	179.4(3)
N(102)-C(102)-C(103)-C(104)	-175.6(3)	C(116)-C(115)-C(120)-C(111)	177.6(3)
C(102)-C(103)-C(104)-C(105)	3.4(6)	C(114)-C(115)-C(120)-C(111)	-0.9(5)
C(103)-C(104)-C(105)-C(106)	176.5(4)	C(112)-C(111)-C(120)-C(119)	178.0(3)
C(103)-C(104)-C(105)-C(110)	-0.9(6)	C(101)-C(111)-C(120)-C(119)	-2.5(5)
C(104)-C(105)-C(106)-C(107)	-174.9(4)	C(112)-C(111)-C(120)-C(115)	-1.7(5)
C(110)-C(105)-C(106)-C(107)	2.6(6)	C(101)-C(111)-C(120)-C(115)	177.8(3)
C(105)-C(106)-C(107)-C(108)	-0.5(6)	C(122)-C(121)-O(121)-Fe(1)	1.9(5)
C(106)-C(107)-C(108)-C(109)	-1.8(6)	C(134)-C(121)-O(121)-Fe(1)	-176.4(2)
C(107)-C(108)-C(109)-C(110)	2.1(6)	O(141)-Fe(1)-O(121)-C(121)	-150.3(3)
C(108)-C(109)-C(110)-C(101)	177.9(4)	N(102)-Fe(1)-O(121)-C(121)	-6.5(3)
C(108)-C(109)-C(110)-C(105)	-0.1(5)	N(112)-Fe(1)-O(121)-C(121)	89.6(3)
C(102)-C(101)-C(110)-C(109)	-174.1(3)	O(121)-C(121)-C(122)-C(123)	-173.9(3)
C(111)-C(101)-C(110)-C(109)	7.9(5)	C(134)-C(121)-C(122)-C(123)	4.4(6)
C(102)-C(101)-C(110)-C(105)	3.9(5)	O(121)-C(121)-C(122)-C(135)	2.7(6)
C(111)-C(101)-C(110)-C(105)	-174.1(3)	C(134)-C(121)-C(122)-C(135)	-179.0(3)
C(104)-C(105)-C(110)-C(109)	175.3(3)	C(121)-C(122)-C(123)-C(124)	-1.1(6)
C(106)-C(105)-C(110)-C(109)	-2.2(5)	C(135)-C(122)-C(123)-C(124)	-178.0(4)
C(104)-C(105)-C(110)-C(101)	-2.8(5)	C(122)-C(123)-C(124)-C(125)	-1.4(6)
C(106)-C(105)-C(110)-C(101)	179.7(3)	C(123)-C(124)-C(125)-C(134)	0.6(6)
C(102)-C(101)-C(111)-C(112)	69.3(5)	C(123)-C(124)-C(125)-C(126)	-179.4(4)
C(110)-C(101)-C(111)-C(112)	-112.8(4)	C(134)-C(125)-C(126)-C(127)	1.2(7)
C(102)-C(101)-C(111)-C(120)	-110.3(4)	C(124)-C(125)-C(126)-C(127)	-178.8(4)
C(110)-C(101)-C(111)-C(120)	67.7(5)	C(125)-C(126)-C(127)-C(128)	-2.7(7)
C(120)-C(111)-C(112)-C(113)	3.0(5)	C(126)-C(127)-C(128)-C(129)	-178.0(5)
C(101)-C(111)-C(112)-C(113)	-176.5(3)	C(126)-C(127)-C(128)-C(133)	1.1(7)
C(120)-C(111)-C(112)-N(112)	178.3(3)	C(127)-C(128)-C(129)-C(130)	177.7(5)
C(101)-C(111)-C(112)-N(112)	-1.3(5)	C(133)-C(128)-C(129)-C(130)	-1.5(7)
C(111)-C(112)-N(112)-C(155)	112.6(4)	C(128)-C(129)-C(130)-C(131)	1.3(8)
C(113)-C(112)-N(112)-C(155)	-72.0(4)	C(129)-C(130)-C(131)-C(132)	-0.6(8)
C(111)-C(112)-N(112)-Fe(1)	-71.5(4)	C(130)-C(131)-C(132)-C(133)	0.2(7)
C(113)-C(112)-N(112)-Fe(1)	103.9(3)	C(131)-C(132)-C(133)-C(128)	-0.3(6)
O(121)-Fe(1)-N(112)-C(155)	119.4(3)	C(131)-C(132)-C(133)-C(134)	179.5(4)
O(141)-Fe(1)-N(112)-C(155)	-13.3(3)	C(129)-C(128)-C(133)-C(132)	1.0(6)
N(102)-Fe(1)-N(112)-C(155)	-146.9(3)	C(127)-C(128)-C(133)-C(132)	-178.2(4)
O(121)-Fe(1)-N(112)-C(112)	-56.4(3)	C(129)-C(128)-C(133)-C(134)	-178.9(4)
O(141)-Fe(1)-N(112)-C(112)	171.0(2)	C(127)-C(128)-C(133)-C(134)	1.9(6)

C(124)-C(125)-C(134)-C(121)	2.7(6)	C(152)-C(153)-C(154)-C(145)	174.4(4)
C(126)-C(125)-C(134)-C(121)	-177.3(4)	C(148)-C(153)-C(154)-C(145)	-5.4(5)
C(124)-C(125)-C(134)-C(133)	-178.2(4)	C(152)-C(153)-C(154)-C(141)	-5.6(6)
C(126)-C(125)-C(134)-C(133)	1.8(6)	C(148)-C(153)-C(154)-C(141)	174.6(4)
O(121)-C(121)-C(134)-C(125)	173.2(3)	C(112)-N(112)-C(155)-C(142)	-177.3(3)
C(122)-C(121)-C(134)-C(125)	-5.1(5)	Fe(1)-N(112)-C(155)-C(142)	7.0(5)
O(121)-C(121)-C(134)-C(133)	-5.8(5)	C(141)-C(142)-C(155)-N(112)	3.4(6)
C(122)-C(121)-C(134)-C(133)	175.8(3)	C(143)-C(142)-C(155)-N(112)	-178.2(3)
C(132)-C(133)-C(134)-C(125)	176.9(4)	C(210)-C(201)-C(202)-C(203)	4.3(5)
C(128)-C(133)-C(134)-C(125)	-3.3(5)	C(211)-C(201)-C(202)-C(203)	-172.4(3)
C(132)-C(133)-C(134)-C(121)	-4.1(6)	C(210)-C(201)-C(202)-N(202)	-171.8(3)
C(128)-C(133)-C(134)-C(121)	175.8(4)	C(211)-C(201)-C(202)-N(202)	11.6(5)
C(102)-N(102)-C(135)-C(122)	-178.6(3)	C(201)-C(202)-N(202)-C(235)	-100.9(4)
Fe(1)-N(102)-C(135)-C(122)	-8.6(5)	C(203)-C(202)-N(202)-C(235)	83.0(4)
C(121)-C(122)-C(135)-N(102)	1.2(6)	C(201)-C(202)-N(202)-Fe(2)	69.8(4)
C(123)-C(122)-C(135)-N(102)	178.0(3)	C(203)-C(202)-N(202)-Fe(2)	-106.3(3)
C(142)-C(141)-O(141)-Fe(1)	-11.1(5)	O(241)-Fe(2)-N(202)-C(235)	-144.5(3)
C(154)-C(141)-O(141)-Fe(1)	171.4(2)	O(221)-Fe(2)-N(202)-C(235)	-9.9(3)
O(121)-Fe(1)-O(141)-C(141)	-121.3(3)	N(212)-Fe(2)-N(202)-C(235)	119.5(3)
N(102)-Fe(1)-O(141)-C(141)	113.1(3)	O(241)-Fe(2)-N(202)-C(202)	45.3(3)
N(112)-Fe(1)-O(141)-C(141)	16.0(3)	O(221)-Fe(2)-N(202)-C(202)	179.9(2)
O(141)-C(141)-C(142)-C(155)	-2.1(6)	N(212)-Fe(2)-N(202)-C(202)	-50.7(2)
C(154)-C(141)-C(142)-C(155)	175.4(3)	C(201)-C(202)-C(203)-C(204)	-0.7(6)
O(141)-C(141)-C(142)-C(143)	179.6(3)	N(202)-C(202)-C(203)-C(204)	175.4(4)
C(154)-C(141)-C(142)-C(143)	-2.9(5)	C(202)-C(203)-C(204)-C(205)	-1.8(6)
C(141)-C(142)-C(143)-C(144)	1.4(6)	C(203)-C(204)-C(205)-C(206)	-176.9(4)
C(155)-C(142)-C(143)-C(144)	-177.0(4)	C(203)-C(204)-C(205)-C(210)	0.6(6)
C(142)-C(143)-C(144)-C(145)	1.0(6)	C(204)-C(205)-C(206)-C(207)	174.5(4)
C(143)-C(144)-C(145)-C(146)	176.0(4)	C(210)-C(205)-C(206)-C(207)	-3.0(6)
C(143)-C(144)-C(145)-C(154)	-2.0(6)	C(205)-C(206)-C(207)-C(208)	0.8(7)
C(144)-C(145)-C(146)-C(147)	-175.3(4)	C(206)-C(207)-C(208)-C(209)	1.3(7)
C(154)-C(145)-C(146)-C(147)	2.8(6)	C(207)-C(208)-C(209)-C(210)	-1.1(6)
C(145)-C(146)-C(147)-C(148)	-5.0(7)	C(208)-C(209)-C(210)-C(201)	-178.5(4)
C(146)-C(147)-C(148)-C(149)	-177.9(4)	C(208)-C(209)-C(210)-C(205)	-1.1(6)
C(146)-C(147)-C(148)-C(153)	1.9(7)	C(202)-C(201)-C(210)-C(209)	172.0(3)
C(147)-C(148)-C(149)-C(150)	177.7(4)	C(211)-C(201)-C(210)-C(209)	-11.4(5)
C(153)-C(148)-C(149)-C(150)	-2.1(7)	C(202)-C(201)-C(210)-C(205)	-5.4(5)
C(148)-C(149)-C(150)-C(151)	-0.6(7)	C(211)-C(201)-C(210)-C(205)	171.2(3)
C(149)-C(150)-C(151)-C(152)	2.1(7)	C(204)-C(205)-C(210)-C(209)	-174.5(4)
C(150)-C(151)-C(152)-C(153)	-0.9(6)	C(206)-C(205)-C(210)-C(209)	3.1(5)
C(151)-C(152)-C(153)-C(148)	-1.9(6)	C(204)-C(205)-C(210)-C(201)	3.0(5)
C(151)-C(152)-C(153)-C(154)	178.3(4)	C(206)-C(205)-C(210)-C(201)	-179.5(4)
C(149)-C(148)-C(153)-C(152)	3.3(6)	C(202)-C(201)-C(211)-C(212)	-69.3(5)
C(147)-C(148)-C(153)-C(152)	-176.5(4)	C(210)-C(201)-C(211)-C(212)	114.1(4)
C(149)-C(148)-C(153)-C(154)	-176.9(4)	C(202)-C(201)-C(211)-C(220)	109.5(4)
C(147)-C(148)-C(153)-C(154)	3.3(6)	C(210)-C(201)-C(211)-C(220)	-67.1(5)
C(144)-C(145)-C(154)-C(141)	0.5(6)	C(220)-C(211)-C(212)-C(213)	-1.2(5)
C(146)-C(145)-C(154)-C(141)	-177.4(3)	C(201)-C(211)-C(212)-C(213)	177.6(3)
C(144)-C(145)-C(154)-C(153)	-179.5(4)	C(220)-C(211)-C(212)-N(212)	-178.3(3)
C(146)-C(145)-C(154)-C(153)	2.5(6)	C(201)-C(211)-C(212)-N(212)	0.5(5)
O(141)-C(141)-C(154)-C(145)	179.5(3)	C(211)-C(212)-N(212)-C(255)	-113.3(4)
C(142)-C(141)-C(154)-C(145)	1.9(5)	C(213)-C(212)-N(212)-C(255)	69.5(4)
O(141)-C(141)-C(154)-C(153)	-0.5(5)	C(211)-C(212)-N(212)-Fe(2)	71.1(4)
C(142)-C(141)-C(154)-C(153)	-178.1(3)	C(213)-C(212)-N(212)-Fe(2)	-106.1(3)

O(241)-Fe(2)-N(212)-C(255)	13.8(3)	C(229)-C(228)-C(233)-C(234)	176.6(4)
O(221)-Fe(2)-N(212)-C(255)	-118.4(3)	C(227)-C(228)-C(233)-C(234)	-4.1(6)
N(202)-Fe(2)-N(212)-C(255)	147.6(3)	C(224)-C(225)-C(234)-C(233)	179.4(4)
O(241)-Fe(2)-N(212)-C(212)	-170.8(3)	C(226)-C(225)-C(234)-C(233)	-1.5(6)
O(221)-Fe(2)-N(212)-C(212)	57.0(3)	C(224)-C(225)-C(234)-C(221)	-3.6(6)
N(202)-Fe(2)-N(212)-C(212)	-37.0(3)	C(226)-C(225)-C(234)-C(221)	175.4(4)
C(211)-C(212)-C(213)-C(214)	0.7(5)	C(232)-C(233)-C(234)-C(225)	-175.6(4)
N(212)-C(212)-C(213)-C(214)	177.8(3)	C(228)-C(233)-C(234)-C(225)	4.7(5)
C(212)-C(213)-C(214)-C(215)	1.1(6)	C(232)-C(233)-C(234)-C(221)	7.7(6)
C(213)-C(214)-C(215)-C(216)	176.2(4)	C(228)-C(233)-C(234)-C(221)	-172.1(3)
C(213)-C(214)-C(215)-C(220)	-2.2(5)	O(221)-C(221)-C(234)-C(225)	-173.1(3)
C(214)-C(215)-C(216)-C(217)	-177.7(4)	C(222)-C(221)-C(234)-C(225)	5.2(5)
C(220)-C(215)-C(216)-C(217)	0.7(6)	O(221)-C(221)-C(234)-C(233)	3.8(5)
C(215)-C(216)-C(217)-C(218)	-2.6(7)	C(222)-C(221)-C(234)-C(233)	-178.0(4)
C(216)-C(217)-C(218)-C(219)	1.4(7)	C(202)-N(202)-C(235)-C(222)	177.7(3)
C(217)-C(218)-C(219)-C(220)	1.7(6)	Fe(2)-N(202)-C(235)-C(222)	8.0(5)
C(218)-C(219)-C(220)-C(211)	175.6(4)	C(221)-C(222)-C(235)-N(202)	-0.6(6)
C(218)-C(219)-C(220)-C(215)	-3.4(5)	C(223)-C(222)-C(235)-N(202)	-177.2(4)
C(212)-C(211)-C(220)-C(219)	-179.0(3)	C(242)-C(241)-O(241)-Fe(2)	7.7(5)
C(201)-C(211)-C(220)-C(219)	2.2(5)	C(254)-C(241)-O(241)-Fe(2)	-174.1(2)
C(212)-C(211)-C(220)-C(215)	0.0(5)	O(221)-Fe(2)-O(241)-C(241)	123.9(3)
C(201)-C(211)-C(220)-C(215)	-178.8(3)	N(202)-Fe(2)-O(241)-C(241)	-112.3(3)
C(216)-C(215)-C(220)-C(219)	2.2(5)	N(212)-Fe(2)-O(241)-C(241)	-14.1(3)
C(214)-C(215)-C(220)-C(219)	-179.3(3)	O(241)-C(241)-C(242)-C(255)	4.2(6)
C(216)-C(215)-C(220)-C(211)	-176.8(3)	C(254)-C(241)-C(242)-C(255)	-174.0(4)
C(214)-C(215)-C(220)-C(211)	1.7(5)	O(241)-C(241)-C(242)-C(243)	-179.6(3)
C(222)-C(221)-O(221)-Fe(2)	-5.1(5)	C(254)-C(241)-C(242)-C(243)	2.1(5)
C(234)-C(221)-O(221)-Fe(2)	173.1(2)	C(241)-C(242)-C(243)-C(244)	-1.7(6)
O(241)-Fe(2)-O(221)-C(221)	151.9(3)	C(255)-C(242)-C(243)-C(244)	174.8(4)
N(202)-Fe(2)-O(221)-C(221)	9.1(3)	C(242)-C(243)-C(244)-C(245)	-0.7(7)
N(212)-Fe(2)-O(221)-C(221)	-87.9(3)	C(243)-C(244)-C(245)-C(254)	2.6(7)
O(221)-C(221)-C(222)-C(223)	175.1(3)	C(243)-C(244)-C(245)-C(246)	-174.7(4)
C(234)-C(221)-C(222)-C(223)	-3.2(5)	C(244)-C(245)-C(246)-C(247)	176.0(5)
O(221)-C(221)-C(222)-C(235)	-1.5(6)	C(254)-C(245)-C(246)-C(247)	-1.5(7)
C(234)-C(221)-C(222)-C(235)	-179.7(3)	C(245)-C(246)-C(247)-C(248)	3.5(8)
C(221)-C(222)-C(223)-C(224)	-0.7(6)	C(246)-C(247)-C(248)-C(253)	-0.3(8)
C(235)-C(222)-C(223)-C(224)	176.1(4)	C(246)-C(247)-C(248)-C(249)	178.3(5)
C(222)-C(223)-C(224)-C(225)	2.4(6)	C(253)-C(248)-C(249)-C(250)	1.1(8)
C(223)-C(224)-C(225)-C(234)	-0.1(6)	C(247)-C(248)-C(249)-C(250)	-177.6(5)
C(223)-C(224)-C(225)-C(226)	-179.2(4)	C(248)-C(249)-C(250)-C(251)	2.8(9)
C(224)-C(225)-C(226)-C(227)	176.6(4)	C(249)-C(250)-C(251)-C(252)	-4.0(8)
C(234)-C(225)-C(226)-C(227)	-2.5(7)	C(250)-C(251)-C(252)-C(253)	1.4(7)
C(225)-C(226)-C(227)-C(228)	3.2(7)	C(251)-C(252)-C(253)-C(248)	2.4(6)
C(226)-C(227)-C(228)-C(229)	179.5(5)	C(251)-C(252)-C(253)-C(254)	-177.9(4)
C(226)-C(227)-C(228)-C(233)	0.2(7)	C(247)-C(248)-C(253)-C(252)	175.1(4)
C(227)-C(228)-C(229)-C(230)	-176.4(5)	C(249)-C(248)-C(253)-C(252)	-3.6(6)
C(233)-C(228)-C(229)-C(230)	2.9(7)	C(247)-C(248)-C(253)-C(254)	-4.6(6)
C(228)-C(229)-C(230)-C(231)	-1.0(8)	C(249)-C(248)-C(253)-C(254)	176.7(4)
C(229)-C(230)-C(231)-C(232)	-0.5(7)	C(244)-C(245)-C(254)-C(241)	-2.1(6)
C(230)-C(231)-C(232)-C(233)	-0.1(7)	C(246)-C(245)-C(254)-C(241)	175.3(4)
C(231)-C(232)-C(233)-C(234)	-177.9(4)	C(244)-C(245)-C(254)-C(253)	179.1(4)
C(231)-C(232)-C(233)-C(228)	1.8(6)	C(246)-C(245)-C(254)-C(253)	-3.5(6)
C(229)-C(228)-C(233)-C(232)	-3.2(6)	O(241)-C(241)-C(254)-C(245)	-178.5(3)
C(227)-C(228)-C(233)-C(232)	176.2(4)	C(242)-C(241)-C(254)-C(245)	-0.3(5)

O(241)-C(241)-C(254)-C(253)	0.2(6)	C(248)-C(253)-C(254)-C(241)	-172.2(4)
C(242)-C(241)-C(254)-C(253)	178.5(4)	C(212)-N(212)-C(255)-C(242)	176.0(3)
C(252)-C(253)-C(254)-C(245)	-173.2(4)	Fe(2)-N(212)-C(255)-C(242)	-8.7(5)
C(248)-C(253)-C(254)-C(245)	6.5(6)	C(241)-C(242)-C(255)-N(212)	-2.9(6)
C(252)-C(253)-C(254)-C(241)	8.1(6)	C(243)-C(242)-C(255)-N(212)	-179.2(4)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*,*R*)-**57**.

Identification code	(*R*,*R*)-**57**	
Empirical formula	C36 H28 Cl Fe N2 O2	
Formula weight	611.90	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.9436(6) Å	α = 90°.
	b = 20.7678(11) Å	β = 94.813(3)°.
	c = 12.3169(7) Å	γ = 90°.
Volume	2789.4(3) $Å^3$	
Z	4	
Density (calculated)	1.457 g/cm^3	
Absorption coefficient	0.674 mm^{-1}	
F(000)	1268	
Crystal size	0.45 x 0.30 x 0.15 mm^3	
Theta range for data collection	1.66 to 28.28°.	
Index ranges	-14<=h<=12, -27<=k<=27, -15<=l<=14	
Reflections collected	35811	
Independent reflections	11585 [R(int) = 0.0433]	
Completeness to theta = 28.28°	95.1 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11585 / 1 / 758	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0767	
R indices (all data)	R1 = 0.0372, wR2 = 0.0802	
Absolute structure parameter	-0.015(8)	
Extinction coefficient	0.0060(4)	
Largest diff. peak and hole	0.501 and -0.383 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**57**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	4731(1)	4438(1)	1387(1)	21(1)
Cl(1)	4025(1)	5204(1)	224(1)	35(1)
C(01)	8639(2)	5838(1)	2724(2)	28(1)
C(02)	8032(2)	6127(1)	3562(2)	33(1)
C(03)	6901(2)	5920(1)	3782(2)	30(1)
C(04)	6313(2)	5419(1)	3163(2)	26(1)
C(05)	6931(2)	5099(1)	2358(2)	24(1)
O(05)	6396(2)	4617(1)	1805(1)	28(1)
C(06)	8153(2)	5296(1)	2158(2)	25(1)
C(07)	8895(2)	4972(1)	1390(2)	26(1)
C(08)	8584(2)	4383(1)	870(2)	29(1)
C(09)	9373(2)	4080(1)	212(2)	32(1)
C(10)	10484(2)	4363(2)	14(2)	37(1)

C(11)	10790(2)	4940(2)	473(2)	38(1)
C(12)	10037(2)	5256(1)	1176(2)	32(1)
C(13)	10428(2)	5834(1)	1707(2)	37(1)
C(14)	9793(2)	6104(1)	2460(2)	37(1)
C(15)	5079(2)	5271(1)	3387(2)	26(1)
N(15)	4341(2)	4905(1)	2809(1)	24(1)
C(16)	3069(2)	4804(1)	3066(2)	24(1)
C(17)	2706(2)	5070(1)	4142(2)	31(1)
C(18)	1376(2)	4889(1)	4302(2)	36(1)
C(21)	4132(2)	2307(1)	-1118(2)	30(1)
C(22)	3035(3)	2150(1)	-669(2)	33(1)
C(23)	2617(2)	2527(1)	114(2)	31(1)
C(24)	3291(2)	3077(1)	505(2)	26(1)
C(25)	4366(2)	3255(1)	39(2)	23(1)
O(25)	5027(2)	3740(1)	447(1)	27(1)
C(26)	4779(2)	2883(1)	-842(2)	25(1)
C(27)	5831(2)	3046(1)	-1439(2)	28(1)
C(28)	6434(2)	3649(1)	-1370(2)	30(1)
C(29)	7389(2)	3776(1)	-1972(2)	35(1)
C(30)	7836(3)	3307(2)	-2669(2)	43(1)
C(31)	7266(3)	2729(2)	-2764(2)	42(1)
C(32)	6244(3)	2589(1)	-2175(2)	34(1)
C(33)	5617(3)	1992(1)	-2348(2)	40(1)
C(34)	4601(3)	1860(1)	-1871(2)	38(1)
C(35)	2879(2)	3375(1)	1455(2)	26(1)
N(35)	3350(2)	3875(1)	1952(1)	23(1)
C(36)	2872(2)	4077(1)	2983(2)	24(1)
C(37)	1532(2)	3910(1)	3129(2)	29(1)
C(38)	1184(2)	4172(1)	4216(2)	34(1)
Fe(2)	5221(1)	2345(1)	3517(1)	21(1)
Cl(2)	5865(1)	1522(1)	4574(1)	35(1)
C(51)	1431(2)	857(1)	2194(2)	27(1)
C(52)	2085(2)	593(1)	1370(2)	29(1)
C(53)	3184(2)	842(1)	1155(2)	29(1)
C(54)	3692(2)	1362(1)	1769(2)	23(1)
C(55)	3065(2)	1649(1)	2595(2)	22(1)
O(55)	3540(1)	2138(1)	3156(1)	25(1)
C(56)	1877(2)	1400(1)	2807(2)	24(1)
C(57)	1102(2)	1682(1)	3595(2)	24(1)
C(58)	1368(2)	2256(1)	4176(2)	27(1)
C(59)	562(2)	2514(1)	4848(2)	31(1)
C(60)	-539(2)	2206(1)	5010(2)	35(1)
C(61)	-813(2)	1639(1)	4498(2)	35(1)
C(62)	-24(2)	1371(1)	3768(2)	30(1)
C(63)	-400(2)	812(1)	3164(2)	36(1)
C(64)	283(2)	569(1)	2410(2)	33(1)
C(65)	4827(2)	1610(1)	1440(2)	25(1)
N(65)	5491(2)	2052(1)	1931(2)	24(1)
C(66)	6594(2)	2297(1)	1465(2)	24(1)
C(67)	7140(2)	1876(1)	611(2)	31(1)
C(68)	8301(2)	2197(1)	254(2)	35(1)
C(71)	5790(2)	4509(1)	5959(2)	32(1)
C(72)	6923(3)	4650(1)	5541(2)	36(1)
C(73)	7387(2)	4249(1)	4820(2)	34(1)

C(74)	6741(2)	3696(1)	4442(2)	28(1)
C(75)	5607(2)	3540(1)	4846(2)	26(1)
O(75)	4945(2)	3055(1)	4423(1)	27(1)
C(76)	5157(2)	3930(1)	5683(2)	27(1)
C(77)	4092(2)	3767(1)	6261(2)	29(1)
C(78)	3529(2)	3160(1)	6230(2)	31(1)
C(79)	2561(3)	3024(1)	6847(2)	37(1)
C(80)	2100(3)	3494(2)	7499(2)	43(1)
C(81)	2630(3)	4090(2)	7558(2)	44(1)
C(82)	3636(3)	4231(1)	6976(2)	34(1)
C(83)	4252(3)	4839(1)	7140(2)	43(1)
C(84)	5296(3)	4953(1)	6675(2)	40(1)
C(85)	7292(2)	3308(1)	3660(2)	27(1)
N(85)	6868(2)	2782(1)	3228(1)	23(1)
C(86)	7529(2)	2421(1)	2433(2)	24(1)
C(87)	8692(2)	2733(1)	2078(2)	30(1)
C(88)	9228(2)	2324(1)	1206(2)	36(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*,*R*)-**57**.

Fe(1)-O(05)	1.8880(16)	C(21)-C(22)	1.402(4)
Fe(1)-O(25)	1.9010(16)	C(21)-C(26)	1.418(3)
Fe(1)-N(15)	2.0772(18)	C(21)-C(34)	1.436(4)
Fe(1)-N(35)	2.078(2)	C(22)-C(23)	1.351(4)
Fe(1)-Cl(1)	2.2342(7)	C(23)-C(24)	1.422(3)
C(01)-C(06)	1.405(3)	C(24)-C(25)	1.402(3)
C(01)-C(02)	1.407(4)	C(24)-C(35)	1.428(3)
C(01)-C(14)	1.440(4)	C(25)-O(25)	1.314(3)
C(02)-C(03)	1.360(4)	C(25)-C(26)	1.434(3)
C(03)-C(04)	1.413(3)	C(26)-C(27)	1.458(4)
C(04)-C(05)	1.413(3)	C(27)-C(32)	1.411(3)
C(04)-C(15)	1.434(4)	C(27)-C(28)	1.415(4)
C(05)-O(05)	1.320(3)	C(28)-C(29)	1.357(4)
C(05)-C(06)	1.440(3)	C(29)-C(30)	1.413(4)
C(06)-C(07)	1.462(3)	C(30)-C(31)	1.352(4)
C(07)-C(08)	1.409(4)	C(31)-C(32)	1.413(4)
C(07)-C(12)	1.427(3)	C(32)-C(33)	1.426(4)
C(08)-C(09)	1.384(3)	C(33)-C(34)	1.329(4)
C(09)-C(10)	1.390(4)	C(35)-N(35)	1.290(3)
C(10)-C(11)	1.355(4)	N(35)-C(36)	1.475(3)
C(11)-C(12)	1.408(4)	C(36)-C(37)	1.532(3)
C(12)-C(13)	1.415(4)	C(37)-C(38)	1.523(3)
C(13)-C(14)	1.329(4)	Fe(2)-O(75)	1.8891(16)
C(15)-N(15)	1.280(3)	Fe(2)-O(55)	1.9055(16)
N(15)-C(16)	1.468(3)	Fe(2)-N(85)	2.0755(19)
C(16)-C(17)	1.519(3)	Fe(2)-N(65)	2.0910(18)
C(16)-C(36)	1.527(3)	Fe(2)-Cl(2)	2.2260(7)
C(17)-C(18)	1.532(3)	C(51)-C(52)	1.402(4)
C(18)-C(38)	1.507(3)	C(51)-C(56)	1.421(3)

C(51)-C(64)	1.436(3)	N(35)-Fe(1)-Cl(1)	113.16(5)
C(52)-C(53)	1.356(4)	C(06)-C(01)-C(02)	121.6(2)
C(53)-C(54)	1.405(3)	C(06)-C(01)-C(14)	119.8(2)
C(54)-C(55)	1.407(3)	C(02)-C(01)-C(14)	118.6(2)
C(54)-C(65)	1.435(3)	C(03)-C(02)-C(01)	120.3(2)
C(55)-O(55)	1.312(3)	C(02)-C(03)-C(04)	120.5(2)
C(55)-C(56)	1.442(3)	C(03)-C(04)-C(05)	120.1(2)
C(56)-C(57)	1.464(3)	C(03)-C(04)-C(15)	116.6(2)
C(57)-C(58)	1.409(3)	C(05)-C(04)-C(15)	123.3(2)
C(57)-C(62)	1.423(3)	O(05)-C(05)-C(04)	120.1(2)
C(58)-C(59)	1.368(3)	O(05)-C(05)-C(06)	120.4(2)
C(59)-C(60)	1.393(3)	C(04)-C(05)-C(06)	119.5(2)
C(60)-C(61)	1.359(4)	C(05)-O(05)-Fe(1)	131.74(15)
C(61)-C(62)	1.412(4)	C(01)-C(06)-C(05)	117.5(2)
C(62)-C(63)	1.421(4)	C(01)-C(06)-C(07)	118.9(2)
C(63)-C(64)	1.339(4)	C(05)-C(06)-C(07)	123.6(2)
C(65)-N(65)	1.290(3)	C(08)-C(07)-C(12)	117.2(2)
N(65)-C(66)	1.470(3)	C(08)-C(07)-C(06)	124.6(2)
C(66)-C(86)	1.526(3)	C(12)-C(07)-C(06)	118.1(2)
C(66)-C(67)	1.528(3)	C(09)-C(08)-C(07)	121.5(2)
C(67)-C(68)	1.532(3)	C(08)-C(09)-C(10)	120.5(3)
C(68)-C(88)	1.509(3)	C(11)-C(10)-C(09)	119.3(3)
C(71)-C(72)	1.413(4)	C(10)-C(11)-C(12)	122.2(2)
C(71)-C(84)	1.413(4)	C(11)-C(12)-C(13)	120.7(3)
C(71)-C(76)	1.415(3)	C(11)-C(12)-C(07)	119.2(2)
C(72)-C(73)	1.347(4)	C(13)-C(12)-C(07)	120.1(3)
C(73)-C(74)	1.407(3)	C(14)-C(13)-C(12)	121.7(3)
C(74)-C(75)	1.412(3)	C(13)-C(14)-C(01)	121.0(3)
C(74)-C(85)	1.427(3)	N(15)-C(15)-C(04)	125.5(2)
C(75)-O(75)	1.322(3)	C(15)-N(15)-C(16)	121.98(19)
C(75)-C(76)	1.430(3)	C(15)-N(15)-Fe(1)	125.54(17)
C(76)-C(77)	1.456(4)	C(16)-N(15)-Fe(1)	112.39(13)
C(77)-C(78)	1.402(4)	N(15)-C(16)-C(17)	117.25(18)
C(77)-C(82)	1.424(3)	N(15)-C(16)-C(36)	104.99(16)
C(78)-C(79)	1.384(4)	C(17)-C(16)-C(36)	111.90(18)
C(79)-C(80)	1.386(4)	C(16)-C(17)-C(18)	110.1(2)
C(80)-C(81)	1.367(4)	C(38)-C(18)-C(17)	111.2(2)
C(81)-C(82)	1.395(4)	C(22)-C(21)-C(26)	121.8(2)
C(82)-C(83)	1.437(4)	C(22)-C(21)-C(34)	118.0(2)
C(83)-C(84)	1.341(4)	C(26)-C(21)-C(34)	120.2(2)
C(85)-N(85)	1.284(3)	C(23)-C(22)-C(21)	120.0(2)
N(85)-C(86)	1.472(3)	C(22)-C(23)-C(24)	120.7(3)
C(86)-C(87)	1.524(3)	C(25)-C(24)-C(23)	120.1(2)
C(87)-C(88)	1.525(3)	C(25)-C(24)-C(35)	123.7(2)
		C(23)-C(24)-C(35)	115.8(2)
O(05)-Fe(1)-O(25)	96.10(7)	O(25)-C(25)-C(24)	119.9(2)
O(05)-Fe(1)-N(15)	86.59(7)	O(25)-C(25)-C(26)	120.2(2)
O(25)-Fe(1)-N(15)	158.00(7)	C(24)-C(25)-C(26)	119.8(2)
O(05)-Fe(1)-N(35)	137.04(7)	C(25)-O(25)-Fe(1)	134.53(16)
O(25)-Fe(1)-N(35)	86.56(7)	C(21)-C(26)-C(25)	117.0(2)
N(15)-Fe(1)-N(35)	76.89(7)	C(21)-C(26)-C(27)	118.3(2)
O(05)-Fe(1)-Cl(1)	108.01(6)	C(25)-C(26)-C(27)	124.7(2)
O(25)-Fe(1)-Cl(1)	102.73(5)	C(32)-C(27)-C(28)	117.4(2)
N(15)-Fe(1)-Cl(1)	97.12(5)	C(32)-C(27)-C(26)	118.5(2)

C(28)-C(27)-C(26)	124.0(2)	C(61)-C(62)-C(63)	119.3(2)
C(29)-C(28)-C(27)	121.0(2)	C(61)-C(62)-C(57)	120.0(2)
C(28)-C(29)-C(30)	121.3(3)	C(63)-C(62)-C(57)	120.6(2)
C(31)-C(30)-C(29)	119.0(3)	C(64)-C(63)-C(62)	121.1(2)
C(30)-C(31)-C(32)	121.1(3)	C(63)-C(64)-C(51)	121.4(2)
C(27)-C(32)-C(31)	120.1(3)	N(65)-C(65)-C(54)	126.2(2)
C(27)-C(32)-C(33)	120.3(3)	C(65)-N(65)-C(66)	120.80(18)
C(31)-C(32)-C(33)	119.6(3)	C(65)-N(65)-Fe(2)	121.80(16)
C(34)-C(33)-C(32)	121.5(3)	C(66)-N(65)-Fe(2)	116.69(13)
C(33)-C(34)-C(21)	120.6(3)	N(65)-C(66)-C(86)	105.79(15)
N(35)-C(35)-C(24)	126.6(2)	N(65)-C(66)-C(67)	116.83(19)
C(35)-N(35)-C(36)	118.8(2)	C(86)-C(66)-C(67)	111.06(17)
C(35)-N(35)-Fe(1)	124.51(17)	C(66)-C(67)-C(68)	109.3(2)
C(36)-N(35)-Fe(1)	116.68(14)	C(88)-C(68)-C(67)	111.89(19)
N(35)-C(36)-C(16)	106.29(17)	C(72)-C(71)-C(84)	119.1(3)
N(35)-C(36)-C(37)	116.66(18)	C(72)-C(71)-C(76)	121.0(2)
C(16)-C(36)-C(37)	110.30(18)	C(84)-C(71)-C(76)	119.9(3)
C(38)-C(37)-C(36)	109.55(19)	C(73)-C(72)-C(71)	120.2(2)
C(18)-C(38)-C(37)	111.7(2)	C(72)-C(73)-C(74)	121.1(3)
O(75)-Fe(2)-O(55)	96.58(7)	C(73)-C(74)-C(75)	120.1(2)
O(75)-Fe(2)-N(85)	86.78(8)	C(73)-C(74)-C(85)	117.0(2)
O(55)-Fe(2)-N(85)	153.35(7)	C(75)-C(74)-C(85)	122.8(2)
O(75)-Fe(2)-N(65)	145.19(7)	O(75)-C(75)-C(74)	120.3(2)
O(55)-Fe(2)-N(65)	85.72(7)	O(75)-C(75)-C(76)	120.3(2)
N(85)-Fe(2)-N(65)	76.94(7)	C(74)-C(75)-C(76)	119.3(2)
O(75)-Fe(2)-Cl(2)	108.22(5)	C(75)-O(75)-Fe(2)	135.88(16)
O(55)-Fe(2)-Cl(2)	102.47(5)	C(71)-C(76)-C(75)	117.6(2)
N(85)-Fe(2)-Cl(2)	101.51(5)	C(71)-C(76)-C(77)	118.4(2)
N(65)-Fe(2)-Cl(2)	105.10(5)	C(75)-C(76)-C(77)	124.0(2)
C(52)-C(51)-C(56)	121.5(2)	C(78)-C(77)-C(82)	116.7(2)
C(52)-C(51)-C(64)	118.6(2)	C(78)-C(77)-C(76)	124.3(2)
C(56)-C(51)-C(64)	119.9(2)	C(82)-C(77)-C(76)	118.8(2)
C(53)-C(52)-C(51)	120.4(2)	C(79)-C(78)-C(77)	121.6(2)
C(52)-C(53)-C(54)	120.4(2)	C(78)-C(79)-C(80)	120.4(3)
C(53)-C(54)-C(55)	121.3(2)	C(81)-C(80)-C(79)	119.7(3)
C(53)-C(54)-C(65)	115.9(2)	C(80)-C(81)-C(82)	120.8(3)
C(55)-C(54)-C(65)	122.6(2)	C(81)-C(82)-C(77)	120.6(3)
O(55)-C(55)-C(54)	120.9(2)	C(81)-C(82)-C(83)	119.6(3)
O(55)-C(55)-C(56)	120.4(2)	C(77)-C(82)-C(83)	119.8(3)
C(54)-C(55)-C(56)	118.7(2)	C(84)-C(83)-C(82)	120.1(3)
C(55)-O(55)-Fe(2)	129.05(15)	C(83)-C(84)-C(71)	122.4(3)
C(51)-C(56)-C(55)	117.5(2)	N(85)-C(85)-C(74)	126.9(2)
C(51)-C(56)-C(57)	118.5(2)	C(85)-N(85)-C(86)	121.9(2)
C(55)-C(56)-C(57)	123.9(2)	C(85)-N(85)-Fe(2)	126.13(17)
C(58)-C(57)-C(62)	117.0(2)	C(86)-N(85)-Fe(2)	111.92(14)
C(58)-C(57)-C(56)	124.7(2)	N(85)-C(86)-C(87)	116.29(19)
C(62)-C(57)-C(56)	118.3(2)	N(85)-C(86)-C(66)	105.74(16)
C(59)-C(58)-C(57)	121.5(2)	C(87)-C(86)-C(66)	111.67(17)
C(58)-C(59)-C(60)	121.1(2)	C(86)-C(87)-C(88)	110.2(2)
C(61)-C(60)-C(59)	119.5(2)	C(68)-C(88)-C(87)	111.81(19)
C(60)-C(61)-C(62)	120.9(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*,*R*)-**57**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	20(1)	22(1)	22(1)	-2(1)	4(1)	-1(1)
Cl(1)	32(1)	39(1)	36(1)	13(1)	8(1)	4(1)
C(01)	26(1)	28(1)	30(1)	7(1)	-5(1)	-2(1)
C(02)	35(2)	26(1)	35(1)	-4(1)	-7(1)	-3(1)
C(03)	35(1)	27(1)	27(1)	-3(1)	-2(1)	3(1)
C(04)	30(1)	23(1)	24(1)	1(1)	-1(1)	0(1)
C(05)	21(1)	26(1)	24(1)	3(1)	-1(1)	-1(1)
O(05)	23(1)	29(1)	33(1)	-10(1)	3(1)	-2(1)
C(06)	25(1)	24(1)	24(1)	6(1)	-3(1)	0(1)
C(07)	21(1)	33(1)	24(1)	9(1)	0(1)	1(1)
C(08)	25(1)	31(1)	31(1)	4(1)	3(1)	-1(1)
C(09)	30(1)	36(1)	32(1)	4(1)	8(1)	5(1)
C(10)	29(1)	55(2)	29(1)	5(1)	7(1)	8(1)
C(11)	24(1)	59(2)	32(1)	15(1)	4(1)	-2(1)
C(12)	25(1)	39(1)	30(1)	13(1)	-4(1)	-2(1)
C(13)	27(1)	43(2)	39(1)	14(1)	0(1)	-10(1)
C(14)	33(1)	31(1)	45(2)	5(1)	-8(1)	-8(1)
C(15)	29(1)	25(1)	25(1)	-2(1)	3(1)	5(1)
N(15)	24(1)	24(1)	24(1)	1(1)	5(1)	1(1)
C(16)	23(1)	26(1)	25(1)	1(1)	4(1)	2(1)
C(17)	33(1)	34(1)	27(1)	-4(1)	7(1)	2(1)
C(18)	33(1)	42(1)	34(1)	-1(1)	14(1)	6(1)
C(21)	36(1)	27(1)	25(1)	-1(1)	-5(1)	1(1)
C(22)	39(2)	28(1)	32(1)	-6(1)	-2(1)	-5(1)
C(23)	28(1)	27(1)	37(1)	-1(1)	-2(1)	-6(1)
C(24)	28(1)	24(1)	27(1)	-2(1)	-1(1)	2(1)
C(25)	23(1)	22(1)	25(1)	-1(1)	-1(1)	0(1)
O(25)	25(1)	27(1)	29(1)	-10(1)	6(1)	-2(1)
C(26)	28(1)	26(1)	21(1)	-3(1)	-3(1)	3(1)
C(27)	30(1)	34(1)	20(1)	-1(1)	-2(1)	4(1)
C(28)	32(1)	33(1)	23(1)	-2(1)	2(1)	4(1)
C(29)	38(2)	38(1)	30(1)	0(1)	6(1)	-1(1)
C(30)	42(2)	58(2)	32(1)	1(1)	14(1)	4(1)
C(31)	48(2)	51(2)	30(1)	-4(1)	15(1)	9(1)
C(32)	41(2)	40(1)	22(1)	-4(1)	2(1)	6(1)
C(33)	53(2)	36(2)	32(1)	-11(1)	6(1)	7(1)
C(34)	52(2)	32(1)	29(1)	-13(1)	-3(1)	-1(1)
C(35)	24(1)	24(1)	30(1)	3(1)	0(1)	-2(1)
N(35)	22(1)	24(1)	24(1)	2(1)	3(1)	3(1)
C(36)	23(1)	27(1)	21(1)	3(1)	3(1)	3(1)
C(37)	23(1)	35(1)	29(1)	3(1)	6(1)	-2(1)
C(38)	29(1)	44(1)	30(1)	3(1)	10(1)	2(1)
Fe(2)	19(1)	22(1)	21(1)	-1(1)	3(1)	-1(1)
Cl(2)	33(1)	33(1)	38(1)	14(1)	6(1)	3(1)
C(51)	26(1)	29(1)	26(1)	4(1)	-4(1)	-4(1)
C(52)	34(1)	25(1)	28(1)	-3(1)	-2(1)	-4(1)
C(53)	33(1)	26(1)	27(1)	-3(1)	2(1)	0(1)
C(54)	23(1)	23(1)	23(1)	0(1)	2(1)	1(1)

C(55)	22(1)	20(1)	23(1)	2(1)	-4(1)	1(1)
O(55)	19(1)	27(1)	29(1)	-6(1)	3(1)	-2(1)
C(56)	21(1)	27(1)	23(1)	4(1)	-1(1)	1(1)
C(57)	21(1)	28(1)	22(1)	6(1)	-1(1)	2(1)
C(58)	23(1)	31(1)	27(1)	5(1)	5(1)	3(1)
C(59)	32(1)	32(1)	29(1)	2(1)	2(1)	7(1)
C(60)	26(1)	51(2)	30(1)	9(1)	10(1)	10(1)
C(61)	22(1)	51(2)	32(1)	12(1)	4(1)	-2(1)
C(62)	22(1)	42(1)	27(1)	12(1)	2(1)	-3(1)
C(63)	28(1)	43(2)	35(1)	8(1)	-1(1)	-11(1)
C(64)	31(1)	35(1)	33(1)	2(1)	-2(1)	-12(1)
C(65)	25(1)	27(1)	22(1)	-1(1)	3(1)	2(1)
N(65)	20(1)	27(1)	25(1)	1(1)	4(1)	2(1)
C(66)	21(1)	28(1)	23(1)	3(1)	5(1)	2(1)
C(67)	28(1)	38(1)	28(1)	-1(1)	10(1)	2(1)
C(68)	30(1)	44(1)	32(1)	1(1)	13(1)	1(1)
C(71)	44(2)	23(1)	27(1)	-1(1)	-7(1)	1(1)
C(72)	47(2)	26(1)	32(1)	0(1)	-8(1)	-9(1)
C(73)	35(2)	33(1)	32(1)	2(1)	-2(1)	-8(1)
C(74)	28(1)	29(1)	26(1)	3(1)	-2(1)	-2(1)
C(75)	28(1)	22(1)	25(1)	1(1)	-6(1)	1(1)
O(75)	24(1)	29(1)	27(1)	-6(1)	1(1)	-1(1)
C(76)	30(1)	26(1)	24(1)	0(1)	-5(1)	4(1)
C(77)	36(1)	29(1)	20(1)	-3(1)	-5(1)	8(1)
C(78)	35(1)	33(1)	23(1)	-3(1)	-1(1)	4(1)
C(79)	41(2)	42(2)	26(1)	0(1)	2(1)	2(1)
C(80)	46(2)	52(2)	31(1)	-4(1)	10(1)	5(1)
C(81)	58(2)	43(2)	32(1)	-8(1)	9(1)	14(1)
C(82)	45(2)	30(1)	27(1)	-5(1)	-2(1)	8(1)
C(83)	68(2)	29(1)	32(1)	-10(1)	-2(1)	11(1)
C(84)	58(2)	28(1)	32(1)	-6(1)	-7(1)	-2(1)
C(85)	23(1)	32(1)	26(1)	3(1)	0(1)	-3(1)
N(85)	20(1)	29(1)	21(1)	2(1)	1(1)	0(1)
C(86)	20(1)	27(1)	24(1)	4(1)	4(1)	4(1)
C(87)	22(1)	37(1)	31(1)	5(1)	3(1)	-1(1)
C(88)	22(1)	49(2)	36(1)	10(1)	11(1)	7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**57**.

	x	y	z	U(eq)
H(02)	8415	6469	3975	39
H(03)	6503	6113	4356	36
H(08)	7816	4189	974	35
H(09)	9154	3675	-106	39
H(10)	11023	4154	-439	45
H(11)	11538	5137	314	46
H(13)	11163	6034	1521	44

H(14)	10105	6478	2830	44
H(15)	4784	5459	4018	31
H(16)	2524	5008	2472	29
H(17A)	2794	5545	4146	37
H(17B)	3256	4894	4748	37
H(18A)	1168	5039	5027	43
H(18B)	821	5108	3742	43
H(22)	2586	1779	-914	40
H(23)	1864	2424	405	38
H(28)	6166	3970	-894	35
H(29)	7765	4188	-1923	42
H(30)	8525	3395	-3064	52
H(31)	7558	2412	-3234	51
H(33)	5933	1680	-2815	48
H(34)	4181	1466	-2028	46
H(35)	2189	3186	1750	32
H(36)	3391	3871	3593	28
H(37A)	993	4101	2527	34
H(37B)	1420	3437	3107	34
H(38A)	312	4072	4299	41
H(38B)	1687	3956	4815	41
H(52)	1756	236	960	35
H(53)	3613	665	586	34
H(58)	2124	2469	4100	32
H(59)	756	2910	5209	37
H(60)	-1093	2392	5475	42
H(61)	-1547	1419	4633	42
H(63)	-1149	607	3298	43
H(64)	3	199	2010	40
H(65)	5118	1432	799	29
H(66)	6381	2722	1118	29
H(67A)	6535	1820	-26	37
H(67B)	7343	1445	921	37
H(68A)	8673	1915	-277	42
H(68B)	8077	2609	-115	42
H(72)	7360	5029	5768	43
H(73)	8163	4341	4563	40
H(78)	3819	2835	5774	37
H(79)	2211	2605	6823	44
H(80)	1418	3402	7902	51
H(81)	2308	4413	8002	53
H(83)	3919	5161	7577	52
H(84)	5719	5346	6832	48
H(85)	8053	3455	3435	32
H(86)	7763	1994	2765	28
H(87A)	9302	2777	2715	36
H(87B)	8501	3169	1786	36
H(88A)	9946	2548	945	43
H(88B)	9515	1908	1529	43

Table 6. Torsion angles [°] for (*R*,*R*)-**57**.

C(06)-C(01)-C(02)-C(03)	-5.6(4)	O(05)-Fe(1)-N(15)-C(16)	-167.90(14)
C(14)-C(01)-C(02)-C(03)	175.2(2)	O(25)-Fe(1)-N(15)-C(16)	-70.0(2)
C(01)-C(02)-C(03)-C(04)	-1.0(4)	N(35)-Fe(1)-N(15)-C(16)	-27.85(14)
C(02)-C(03)-C(04)-C(05)	4.4(4)	Cl(1)-Fe(1)-N(15)-C(16)	84.36(14)
C(02)-C(03)-C(04)-C(15)	-174.6(2)	C(15)-N(15)-C(16)-C(17)	-8.7(3)
C(03)-C(04)-C(05)-O(05)	177.8(2)	Fe(1)-N(15)-C(16)-C(17)	174.58(15)
C(15)-C(04)-C(05)-O(05)	-3.3(3)	C(15)-N(15)-C(16)-C(36)	-133.6(2)
C(03)-C(04)-C(05)-C(06)	-1.3(3)	Fe(1)-N(15)-C(16)-C(36)	49.68(18)
C(15)-C(04)-C(05)-C(06)	177.5(2)	N(15)-C(16)-C(17)-C(18)	-176.94(19)
C(04)-C(05)-O(05)-Fe(1)	30.2(3)	C(36)-C(16)-C(17)-C(18)	-55.6(2)
C(06)-C(05)-O(05)-Fe(1)	-150.71(17)	C(16)-C(17)-C(18)-C(38)	55.1(3)
O(25)-Fe(1)-O(05)-C(05)	170.5(2)	C(26)-C(21)-C(22)-C(23)	-5.3(4)
N(15)-Fe(1)-O(05)-C(05)	-31.4(2)	C(34)-C(21)-C(22)-C(23)	174.2(2)
N(35)-Fe(1)-O(05)-C(05)	-98.0(2)	C(21)-C(22)-C(23)-C(24)	-1.3(4)
Cl(1)-Fe(1)-O(05)-C(05)	65.0(2)	C(22)-C(23)-C(24)-C(25)	3.6(4)
C(02)-C(01)-C(06)-C(05)	8.4(3)	C(22)-C(23)-C(24)-C(35)	-169.6(2)
C(14)-C(01)-C(06)-C(05)	-172.5(2)	C(23)-C(24)-C(25)-O(25)	-175.8(2)
C(02)-C(01)-C(06)-C(07)	-172.6(2)	C(35)-C(24)-C(25)-O(25)	-3.3(3)
C(14)-C(01)-C(06)-C(07)	6.5(3)	C(23)-C(24)-C(25)-C(26)	0.6(3)
O(05)-C(05)-C(06)-C(01)	176.1(2)	C(35)-C(24)-C(25)-C(26)	173.2(2)
C(04)-C(05)-C(06)-C(01)	-4.8(3)	C(24)-C(25)-O(25)-Fe(1)	-17.2(3)
O(05)-C(05)-C(06)-C(07)	-2.9(3)	C(26)-C(25)-O(25)-Fe(1)	166.32(16)
C(04)-C(05)-C(06)-C(07)	176.2(2)	O(05)-Fe(1)-O(25)-C(25)	160.3(2)
C(01)-C(06)-C(07)-C(08)	172.0(2)	N(15)-Fe(1)-O(25)-C(25)	64.3(3)
C(05)-C(06)-C(07)-C(08)	-9.1(3)	N(35)-Fe(1)-O(25)-C(25)	23.3(2)
C(01)-C(06)-C(07)-C(12)	-5.7(3)	Cl(1)-Fe(1)-O(25)-C(25)	-89.7(2)
C(05)-C(06)-C(07)-C(12)	173.2(2)	C(22)-C(21)-C(26)-C(25)	9.1(3)
C(12)-C(07)-C(08)-C(09)	2.4(3)	C(34)-C(21)-C(26)-C(25)	-170.3(2)
C(06)-C(07)-C(08)-C(09)	-175.3(2)	C(22)-C(21)-C(26)-C(27)	-173.0(2)
C(07)-C(08)-C(09)-C(10)	-2.4(3)	C(34)-C(21)-C(26)-C(27)	7.6(3)
C(08)-C(09)-C(10)-C(11)	0.1(4)	O(25)-C(25)-C(26)-C(21)	169.75(19)
C(09)-C(10)-C(11)-C(12)	2.1(4)	C(24)-C(25)-C(26)-C(21)	-6.7(3)
C(10)-C(11)-C(12)-C(13)	175.1(2)	O(25)-C(25)-C(26)-C(27)	-8.0(3)
C(10)-C(11)-C(12)-C(07)	-2.0(3)	C(24)-C(25)-C(26)-C(27)	175.5(2)
C(08)-C(07)-C(12)-C(11)	-0.3(3)	C(21)-C(26)-C(27)-C(32)	-7.1(3)
C(06)-C(07)-C(12)-C(11)	177.6(2)	C(25)-C(26)-C(27)-C(32)	170.6(2)
C(08)-C(07)-C(12)-C(13)	-177.4(2)	C(21)-C(26)-C(27)-C(28)	169.6(2)
C(06)-C(07)-C(12)-C(13)	0.5(3)	C(25)-C(26)-C(27)-C(28)	-12.7(3)
C(11)-C(12)-C(13)-C(14)	-172.8(2)	C(32)-C(27)-C(28)-C(29)	-1.4(3)
C(07)-C(12)-C(13)-C(14)	4.3(4)	C(26)-C(27)-C(28)-C(29)	-178.1(2)
C(12)-C(13)-C(14)-C(01)	-3.6(4)	C(27)-C(28)-C(29)-C(30)	-1.5(4)
C(06)-C(01)-C(14)-C(13)	-2.0(4)	C(28)-C(29)-C(30)-C(31)	2.5(4)
C(02)-C(01)-C(14)-C(13)	177.2(2)	C(29)-C(30)-C(31)-C(32)	-0.4(4)
C(03)-C(04)-C(15)-N(15)	168.9(2)	C(28)-C(27)-C(32)-C(31)	3.5(3)
C(05)-C(04)-C(15)-N(15)	-10.0(4)	C(26)-C(27)-C(32)-C(31)	-179.6(2)
C(04)-C(15)-N(15)-C(16)	-176.9(2)	C(28)-C(27)-C(32)-C(33)	-175.1(2)
C(04)-C(15)-N(15)-Fe(1)	-0.7(3)	C(26)-C(27)-C(32)-C(33)	1.8(3)
O(05)-Fe(1)-N(15)-C(15)	15.56(19)	C(30)-C(31)-C(32)-C(27)	-2.6(4)
O(25)-Fe(1)-N(15)-C(15)	113.4(2)	C(30)-C(31)-C(32)-C(33)	176.0(3)
N(35)-Fe(1)-N(15)-C(15)	155.6(2)	C(27)-C(32)-C(33)-C(34)	3.4(4)
Cl(1)-Fe(1)-N(15)-C(15)	-92.18(19)	C(31)-C(32)-C(33)-C(34)	-175.2(3)

C(32)-C(33)-C(34)-C(21)	-3.0(4)	C(62)-C(57)-C(58)-C(59)	-2.1(3)
C(22)-C(21)-C(34)-C(33)	177.9(2)	C(56)-C(57)-C(58)-C(59)	175.6(2)
C(26)-C(21)-C(34)-C(33)	-2.6(4)	C(57)-C(58)-C(59)-C(60)	2.1(3)
C(25)-C(24)-C(35)-N(35)	6.9(4)	C(58)-C(59)-C(60)-C(61)	0.4(3)
C(23)-C(24)-C(35)-N(35)	179.7(2)	C(59)-C(60)-C(61)-C(62)	-2.8(3)
C(24)-C(35)-N(35)-C(36)	-174.2(2)	C(60)-C(61)-C(62)-C(63)	-173.6(2)
C(24)-C(35)-N(35)-Fe(1)	7.1(3)	C(60)-C(61)-C(62)-C(57)	2.7(3)
O(05)-Fe(1)-N(35)-C(35)	-111.99(18)	C(58)-C(57)-C(62)-C(61)	-0.3(3)
O(25)-Fe(1)-N(35)-C(35)	-16.74(18)	C(56)-C(57)-C(62)-C(61)	-178.1(2)
N(15)-Fe(1)-N(35)-C(35)	177.86(19)	C(58)-C(57)-C(62)-C(63)	176.0(2)
Cl(1)-Fe(1)-N(35)-C(35)	85.64(18)	C(56)-C(57)-C(62)-C(63)	-1.8(3)
O(05)-Fe(1)-N(35)-C(36)	69.30(18)	C(61)-C(62)-C(63)-C(64)	175.4(2)
O(25)-Fe(1)-N(35)-C(36)	164.55(15)	C(57)-C(62)-C(63)-C(64)	-1.0(4)
N(15)-Fe(1)-N(35)-C(36)	-0.85(14)	C(62)-C(63)-C(64)-C(51)	1.1(4)
Cl(1)-Fe(1)-N(35)-C(36)	-93.07(14)	C(52)-C(51)-C(64)-C(63)	-178.0(2)
C(35)-N(35)-C(36)-C(16)	-151.67(19)	C(56)-C(51)-C(64)-C(63)	1.7(4)
Fe(1)-N(35)-C(36)-C(16)	27.1(2)	C(53)-C(54)-C(65)-N(65)	-174.9(2)
C(35)-N(35)-C(36)-C(37)	-28.2(3)	C(55)-C(54)-C(65)-N(65)	10.2(4)
Fe(1)-N(35)-C(36)-C(37)	150.58(15)	C(54)-C(65)-N(65)-C(66)	-175.6(2)
N(15)-C(16)-C(36)-N(35)	-47.3(2)	C(54)-C(65)-N(65)-Fe(2)	14.3(3)
C(17)-C(16)-C(36)-N(35)	-175.49(18)	O(75)-Fe(2)-N(65)-C(65)	-126.48(18)
N(15)-C(16)-C(36)-C(37)	-174.63(16)	O(55)-Fe(2)-N(65)-C(65)	-31.10(18)
C(17)-C(16)-C(36)-C(37)	57.2(2)	N(85)-Fe(2)-N(65)-C(65)	169.28(19)
N(35)-C(36)-C(37)-C(38)	-178.25(18)	Cl(2)-Fe(2)-N(65)-C(65)	70.67(18)
C(16)-C(36)-C(37)-C(38)	-56.9(2)	O(75)-Fe(2)-N(65)-C(66)	63.0(2)
C(17)-C(18)-C(38)-C(37)	-57.1(3)	O(55)-Fe(2)-N(65)-C(66)	158.43(15)
C(36)-C(37)-C(38)-C(18)	57.7(3)	N(85)-Fe(2)-N(65)-C(66)	-1.19(14)
C(56)-C(51)-C(52)-C(53)	1.6(4)	Cl(2)-Fe(2)-N(65)-C(66)	-99.80(14)
C(64)-C(51)-C(52)-C(53)	-178.7(2)	C(65)-N(65)-C(66)-C(86)	-143.1(2)
C(51)-C(52)-C(53)-C(54)	1.2(4)	Fe(2)-N(65)-C(66)-C(86)	27.4(2)
C(52)-C(53)-C(54)-C(55)	-2.0(4)	C(65)-N(65)-C(66)-C(67)	-19.0(3)
C(52)-C(53)-C(54)-C(65)	-177.0(2)	Fe(2)-N(65)-C(66)-C(67)	151.59(15)
C(53)-C(54)-C(55)-O(55)	-179.2(2)	N(65)-C(66)-C(67)-C(68)	-178.01(18)
C(65)-C(54)-C(55)-O(55)	-4.5(3)	C(86)-C(66)-C(67)-C(68)	-56.6(2)
C(53)-C(54)-C(55)-C(56)	-0.1(3)	C(66)-C(67)-C(68)-C(88)	56.6(3)
C(65)-C(54)-C(55)-C(56)	174.6(2)	C(84)-C(71)-C(72)-C(73)	-177.1(2)
C(54)-C(55)-O(55)-Fe(2)	-29.7(3)	C(76)-C(71)-C(72)-C(73)	3.7(4)
C(56)-C(55)-O(55)-Fe(2)	151.13(16)	C(71)-C(72)-C(73)-C(74)	2.1(4)
O(75)-Fe(2)-O(55)-C(55)	-174.42(18)	C(72)-C(73)-C(74)-C(75)	-2.3(4)
N(85)-Fe(2)-O(55)-C(55)	89.6(2)	C(72)-C(73)-C(74)-C(85)	178.5(2)
N(65)-Fe(2)-O(55)-C(55)	40.47(18)	C(73)-C(74)-C(75)-O(75)	173.9(2)
Cl(2)-Fe(2)-O(55)-C(55)	-64.06(18)	C(85)-C(74)-C(75)-O(75)	-7.0(3)
C(52)-C(51)-C(56)-C(55)	-3.5(3)	C(73)-C(74)-C(75)-C(76)	-3.3(3)
C(64)-C(51)-C(56)-C(55)	176.8(2)	C(85)-C(74)-C(75)-C(76)	175.8(2)
C(52)-C(51)-C(56)-C(57)	175.3(2)	C(74)-C(75)-O(75)-Fe(2)	15.1(3)
C(64)-C(51)-C(56)-C(57)	-4.4(3)	C(76)-C(75)-O(75)-Fe(2)	-167.75(15)
O(55)-C(55)-C(56)-C(51)	-178.16(19)	O(55)-Fe(2)-O(75)-C(75)	-165.0(2)
C(54)-C(55)-C(56)-C(51)	2.7(3)	N(85)-Fe(2)-O(75)-C(75)	-11.6(2)
O(55)-C(55)-C(56)-C(57)	3.1(3)	N(65)-Fe(2)-O(75)-C(75)	-73.1(2)
C(54)-C(55)-C(56)-C(57)	-176.0(2)	Cl(2)-Fe(2)-O(75)-C(75)	89.5(2)
C(51)-C(56)-C(57)-C(58)	-173.2(2)	C(72)-C(71)-C(76)-C(75)	-9.0(3)
C(55)-C(56)-C(57)-C(58)	5.5(3)	C(84)-C(71)-C(76)-C(75)	171.8(2)
C(51)-C(56)-C(57)-C(62)	4.4(3)	C(72)-C(71)-C(76)-C(77)	171.0(2)
C(55)-C(56)-C(57)-C(62)	-176.9(2)	C(84)-C(71)-C(76)-C(77)	-8.2(3)

O(75)-C(75)-C(76)-C(71)	-168.47(19)	C(73)-C(74)-C(85)-N(85)	178.7(2)
C(74)-C(75)-C(76)-C(71)	8.7(3)	C(75)-C(74)-C(85)-N(85)	-0.4(4)
O(75)-C(75)-C(76)-C(77)	11.5(3)	C(74)-C(85)-N(85)-C(86)	-179.5(2)
C(74)-C(75)-C(76)-C(77)	-171.4(2)	C(74)-C(85)-N(85)-Fe(2)	1.4(3)
C(71)-C(76)-C(77)-C(78)	-166.9(2)	O(75)-Fe(2)-N(85)-C(85)	2.73(19)
C(75)-C(76)-C(77)-C(78)	13.2(3)	O(55)-Fe(2)-N(85)-C(85)	101.0(2)
C(71)-C(76)-C(77)-C(82)	8.0(3)	N(65)-Fe(2)-N(85)-C(85)	151.7(2)
C(75)-C(76)-C(77)-C(82)	-172.0(2)	Cl(2)-Fe(2)-N(85)-C(85)	-105.22(18)
C(82)-C(77)-C(78)-C(79)	1.3(3)	O(75)-Fe(2)-N(85)-C(86)	-176.44(13)
C(76)-C(77)-C(78)-C(79)	176.2(2)	O(55)-Fe(2)-N(85)-C(86)	-78.2(2)
C(77)-C(78)-C(79)-C(80)	1.6(4)	N(65)-Fe(2)-N(85)-C(86)	-27.43(13)
C(78)-C(79)-C(80)-C(81)	-2.1(4)	Cl(2)-Fe(2)-N(85)-C(86)	75.61(13)
C(79)-C(80)-C(81)-C(82)	-0.4(4)	C(85)-N(85)-C(86)-C(87)	-4.8(3)
C(80)-C(81)-C(82)-C(77)	3.4(4)	Fe(2)-N(85)-C(86)-C(87)	174.39(14)
C(80)-C(81)-C(82)-C(83)	-173.7(3)	C(85)-N(85)-C(86)-C(66)	-129.4(2)
C(78)-C(77)-C(82)-C(81)	-3.8(3)	Fe(2)-N(85)-C(86)-C(66)	49.84(18)
C(76)-C(77)-C(82)-C(81)	-179.0(2)	N(65)-C(66)-C(86)-N(85)	-47.8(2)
C(78)-C(77)-C(82)-C(83)	173.3(2)	C(67)-C(66)-C(86)-N(85)	-175.45(18)
C(76)-C(77)-C(82)-C(83)	-1.9(3)	N(65)-C(66)-C(86)-C(87)	-175.14(18)
C(81)-C(82)-C(83)-C(84)	172.9(3)	C(67)-C(66)-C(86)-C(87)	57.2(2)
C(77)-C(82)-C(83)-C(84)	-4.2(4)	N(85)-C(86)-C(87)-C(88)	-176.57(17)
C(82)-C(83)-C(84)-C(71)	4.2(4)	C(66)-C(86)-C(87)-C(88)	-55.1(2)
C(72)-C(71)-C(84)-C(83)	-177.1(2)	C(67)-C(68)-C(88)-C(87)	-56.5(3)
C(76)-C(71)-C(84)-C(83)	2.1(4)	C(86)-C(87)-C(88)-C(68)	54.7(3)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R,R*)-**62**.

Identification code	(*R,R*)-**62**	
Empirical formula	C33 H38 Cl6 N4 Zn2	
Formula weight	834.11	
Temperature	203(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P1	
Unit cell dimensions	a = 13.045(3) Å	α = 116.747(14)°.
	b = 13.450(3) Å	β = 91.053(12)°.
	c = 14.109(3) Å	γ = 115.182(15)°.
Volume	1931.8(8) $Å^3$	
Z	2	
Density (calculated)	1.434 g/cm^3	
Absorption coefficient	1.684 mm^{-1}	
F(000)	852	
Crystal size	0.25 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.94 to 28.44°.	
Index ranges	-17<=h<=17, -16<=k<=17, -17<=l<=18	
Reflections collected	20018	
Independent reflections	14246 [R(int) = 0.1111]	
Completeness to theta = 28.44°	84.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.521	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14246 / 92 / 776	
Goodness-of-fit on F^2	0.917	
Final R indices [I>2sigma(I)]	R1 = 0.0985, wR2 = 0.1988	
R indices (all data)	R1 = 0.3086, wR2 = 0.2738	
Absolute structure parameter	0.01(4)	
Largest diff. peak and hole	0.841 and -1.387 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-**62**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1S)	4660(60)	-500(40)	1190(60)	387(8)
Cl(5)	4580(30)	-2020(30)	730(20)	387(8)
Cl(6)	3820(30)	-280(30)	2170(20)	387(8)
C(2S)	5430(150)	450(90)	-750(100)	387(8)
Cl(7)	5390(60)	1920(70)	-150(50)	387(8)
Cl(8)	6000(60)	210(70)	-1920(50)	387(8)
C(3S)	6560(100)	3120(50)	-560(60)	387(8)
Cl(9)	5700(50)	1440(50)	-1170(40)	387(8)
Cl(10)	6350(40)	3870(40)	780(40)	387(8)
Zn11	10443(2)	7272(2)	7560(2)	46(1)
Cl11	9209(7)	5295(6)	6283(5)	60(2)
Cl21	12155(6)	7797(7)	8419(6)	67(2)
Zn21	8040(2)	7662(2)	4262(2)	40(1)

Cl31	7846(6)	8999(6)	5763(5)	50(2)
Cl41	8365(6)	8009(6)	2893(5)	51(2)
N111	6879(17)	5695(16)	3817(13)	34(4)
C121	7660(20)	5320(20)	3982(18)	42(5)
C131	7190(20)	4060(19)	3829(18)	49(6)
C141	6010(20)	3410(20)	3679(16)	48(5)
C151	5254(19)	3850(20)	3594(15)	37(4)
C161	4040(20)	3240(20)	3574(19)	55(5)
C171	3350(20)	3710(20)	3442(17)	51(5)
C181	3820(20)	4760(20)	3338(18)	56(5)
C191	4980(20)	5440(20)	3393(19)	49(5)
C201	5700(20)	5050(20)	3608(18)	42(5)
C211	5370(20)	6520(30)	3190(20)	64(7)
C221	4690(20)	7320(30)	3680(30)	122(12)
C231	5060(30)	5990(30)	1950(20)	91(9)
C241	8880(20)	6050(20)	4245(19)	38(6)
N311	9541(18)	8192(18)	8347(15)	43(4)
C321	9641(19)	8980(20)	7973(16)	34(5)
C331	9080(20)	9800(20)	8380(19)	46(6)
C341	8430(20)	9660(20)	9037(17)	38(5)
C351	8280(20)	8820(20)	9461(18)	37(5)
C361	7640(20)	8790(20)	10236(18)	46(5)
C371	7450(30)	7790(30)	10510(20)	62(7)
C381	8120(30)	7250(20)	10190(20)	61(7)
C391	8710(20)	7270(20)	9507(15)	40(5)
C401	8880(20)	8100(20)	9064(17)	39(5)
C411	9383(19)	6491(17)	9257(17)	35(6)
C421	8520(30)	5060(20)	8670(20)	69(10)
C431	10190(20)	6840(30)	10190(20)	63(9)
C441	10168(19)	8950(20)	7133(15)	34(5)
N511	9294(16)	7252(17)	4569(13)	33(4)
N521	10625(17)	8194(16)	6751(13)	42(5)
C511	10592(19)	8080(20)	4915(16)	48(6)
C521	11182(16)	8066(17)	5847(14)	32(4)
C531	12470(20)	9030(20)	6250(20)	55(7)
C541	13000(20)	8620(20)	5250(20)	62(7)
C551	12400(20)	8580(20)	4325(19)	49(6)
C561	11190(20)	7810(30)	3980(20)	64(9)
Zn32	-320(2)	2686(2)	2582(2)	43(1)
Cl12	917(6)	4718(5)	3806(5)	51(2)
Cl22	-2052(7)	2096(7)	1699(5)	64(2)
Zn42	1834(2)	2399(2)	5644(2)	39(1)
Cl32	1960(6)	1001(6)	4133(5)	51(2)
Cl42	1424(6)	1857(6)	6896(6)	59(2)
N112	3202(15)	4257(18)	6168(14)	38(4)
C122	2679(18)	4920(19)	6107(17)	32(5)
C132	3310(20)	6160(20)	6200(20)	60(7)
C142	4434(19)	6670(20)	6360(20)	59(7)
C152	5080(20)	6050(20)	6387(19)	44(5)
C162	6240(20)	6530(20)	6450(20)	58(7)
C172	6790(20)	5900(20)	6460(20)	61(6)
C182	6170(20)	4750(20)	6477(18)	46(5)
C192	5020(20)	4230(20)	6436(18)	40(5)
C202	4367(18)	4840(20)	6373(18)	38(5)

C212	4480(20)	3090(20)	6590(20)	67(9)
C222	4820(20)	2060(20)	5920(30)	108(12)
C232	4670(30)	3480(30)	7820(30)	144(18)
C242	1430(20)	4320(20)	5790(20)	47(7)
N312	583(17)	1801(17)	1583(15)	36(5)
C322	560(18)	963(19)	1854(15)	25(5)
C332	1153(19)	280(20)	1457(16)	37(6)
C342	1740(20)	500(20)	738(16)	38(6)
C352	1810(20)	1260(20)	364(18)	43(7)
C362	2520(20)	1620(20)	-293(19)	55(7)
C372	2470(30)	2230(30)	-700(20)	79(11)
C382	1850(30)	3000(20)	-230(20)	62(8)
C392	1180(20)	2800(20)	479(18)	37(6)
C402	1170(20)	2000(20)	850(17)	38(6)
C412	570(30)	3630(30)	857(19)	68(9)
C422	1480(30)	5090(30)	1420(30)	104(14)
C432	-400(20)	3190(30)	-90(20)	71(8)
C442	-49(19)	796(19)	2607(18)	40(6)
N512	793(16)	3125(16)	5462(13)	31(4)
N522	-484(15)	1525(15)	3202(13)	32(4)
C512	-451(19)	2600(17)	5123(14)	35(5)
C522	-974(16)	1354(18)	4003(14)	34(5)
C532	-2270(20)	860(20)	3680(20)	49(7)
C542	-2913(18)	640(20)	4535(17)	51(6)
C552	-2316(19)	1920(20)	5760(20)	54(7)
C562	-1038(19)	2340(20)	6010(20)	38(6)

Table 3. Bond lengths [Å] and angles [°] for (*R,R*)-**62**.

C(1S)-Cl(6)	1.78(2)	N111-C201	1.35(3)
C(1S)-Cl(5)	1.80(2)	N111-C121	1.37(2)
C(1S)-H(1A)	0.9800	C121-C241	1.40(3)
C(1S)-H(1B)	0.9800	C121-C131	1.44(3)
C(2S)-Cl(8)	1.77(2)	C131-C141	1.36(3)
C(2S)-Cl(7)	1.80(2)	C131-H131	0.9400
C(2S)-H(2A)	0.9800	C141-C151	1.38(3)
C(2S)-H(2B)	0.9800	C141-H141	0.9400
C(3S)-Cl(10)	1.78(2)	C151-C161	1.43(3)
C(3S)-Cl(9)	1.78(2)	C151-C201	1.46(3)
C(3S)-H(3A)	0.9800	C161-C171	1.36(3)
C(3S)-H(3B)	0.9800	C161-H161	0.9400
Zn11-N521	1.982(17)	C171-C181	1.36(3)
Zn11-N311	2.05(2)	C171-H171	0.9400
Zn11-Cl21	2.178(7)	C181-C191	1.37(3)
Zn11-Cl11	2.202(7)	C181-H181	0.9400
Zn21-N511	2.030(17)	C191-C201	1.33(3)
Zn21-N111	2.179(18)	C191-C211	1.48(3)
Zn21-Cl31	2.182(7)	C211-C231	1.54(4)
Zn21-Cl41	2.192(6)	C211-C221	1.62(4)

C211-H211	0.9900	C561-H56A1	0.9800
C221-H22A1	0.9700	C561-H56B1	0.9800
C221-H22B1	0.9700	Zn32-N522	2.049(16)
C221-H22C1	0.9700	Zn32-N312	2.130(18)
C231-H23A1	0.9700	Zn32-Cl22	2.184(7)
C231-H23B1	0.9700	Zn32-Cl12	2.225(7)
C231-H23C1	0.9700	Zn42-N512	2.050(15)
C241-N511	1.30(2)	Zn42-N112	2.11(2)
C241-H241	0.9400	Zn42-Cl32	2.185(7)
N311-C321	1.35(3)	Zn42-Cl42	2.192(7)
N311-C401	1.35(3)	N112-C202	1.33(3)
C321-C441	1.37(3)	N112-C122	1.36(2)
C321-C331	1.47(3)	C122-C242	1.42(3)
C331-C341	1.29(3)	C122-C132	1.45(3)
C331-H331	0.9400	C132-C142	1.29(3)
C341-C351	1.44(3)	C132-H132	0.9400
C341-H341	0.9400	C142-C152	1.42(3)
C351-C361	1.40(3)	C142-H142	0.9400
C351-C401	1.43(3)	C152-C162	1.35(3)
C361-C371	1.48(3)	C152-C202	1.49(3)
C361-H36A1	0.9800	C162-C172	1.32(3)
C361-H36B1	0.9800	C162-H162	0.9400
C371-C381	1.32(3)	C172-C182	1.42(3)
C371-H371	0.9400	C172-H172	0.9400
C381-C391	1.25(3)	C182-C192	1.35(3)
C381-H381	0.9400	C182-H182	0.9400
C391-C401	1.44(3)	C192-C202	1.43(3)
C391-C411	1.57(3)	C192-C212	1.52(3)
C411-C431	1.43(3)	C212-C232	1.54(4)
C411-C421	1.53(3)	C212-C222	1.54(3)
C411-H411	0.9900	C212-H212	0.9900
C421-H42A1	0.9700	C222-H22A2	0.9700
C421-H42B1	0.9700	C222-H22B2	0.9700
C421-H42C1	0.9700	C222-H22C2	0.9700
C431-H43A1	0.9700	C232-H23A2	0.9700
C431-H43B1	0.9700	C232-H23B2	0.9700
C431-H43C1	0.9700	C232-H23C2	0.9700
C441-N521	1.31(2)	C242-N512	1.29(3)
C441-H441	0.9400	C242-H242	0.9400
N511-C511	1.49(3)	N312-C322	1.33(2)
N521-C521	1.46(2)	N312-C402	1.36(3)
C511-C521	1.52(3)	C322-C442	1.38(3)
C511-C561	1.52(3)	C322-C332	1.39(3)
C511-H511	0.9900	C332-C342	1.34(3)
C521-C531	1.51(3)	C332-H332	0.9400
C521-H521	0.9900	C342-C352	1.32(3)
C531-C541	1.55(3)	C342-H342	0.9400
C531-H53A1	0.9800	C352-C362	1.42(3)
C531-H53B1	0.9800	C352-C402	1.51(3)
C541-C551	1.48(3)	C362-C372	1.22(3)
C541-H54A1	0.9800	C362-H362	0.9400
C541-H54B1	0.9800	C372-C382	1.51(3)
C551-C561	1.39(3)	C372-H372	0.9400
C551-H551	0.9400	C382-C392	1.38(3)

C382-H382	0.9400
C392-C402	1.38(3)
C392-C412	1.55(3)
C412-C432	1.52(3)
C412-C422	1.58(4)
C412-H412	0.9900
C422-H42A2	0.9700
C422-H42B2	0.9700
C422-H42C2	0.9700
C432-H43A2	0.9700
C432-H43B2	0.9700
C432-H43C2	0.9700
C442-N522	1.32(2)
C442-H442	0.9400
N512-C512	1.43(2)
N522-C522	1.37(2)
C512-C522	1.54(2)
C512-C562	1.58(3)
C512-H512	0.9900
C522-C532	1.51(3)
C522-H522	0.9900
C532-C542	1.54(3)
C532-H53A2	0.9800
C532-H53B2	0.9800
C542-C552	1.64(3)
C542-H54A2	0.9800
C542-H54B2	0.9800
C552-C562	1.49(3)
C552-H55A2	0.9800
C552-H55B2	0.9800
C562-H56A2	0.9800
C562-H56B2	0.9800
Cl(6)-C(1S)-Cl(5)	107.9(16)
Cl(6)-C(1S)-H(1A)	110.1
Cl(5)-C(1S)-H(1A)	110.1
Cl(6)-C(1S)-H(1B)	110.1
Cl(5)-C(1S)-H(1B)	110.1
H(1A)-C(1S)-H(1B)	108.4
Cl(8)-C(2S)-Cl(7)	110.6(17)
Cl(8)-C(2S)-H(2A)	109.5
Cl(7)-C(2S)-H(2A)	109.5
Cl(8)-C(2S)-H(2B)	109.5
Cl(7)-C(2S)-H(2B)	109.5
H(2A)-C(2S)-H(2B)	108.1
Cl(10)-C(3S)-Cl(9)	109.2(17)
Cl(10)-C(3S)-H(3A)	109.8
Cl(9)-C(3S)-H(3A)	109.8
Cl(10)-C(3S)-H(3B)	109.8
Cl(9)-C(3S)-H(3B)	109.8
H(3A)-C(3S)-H(3B)	108.3
N521-Zn11-N311	83.3(8)
N521-Zn11-Cl21	110.3(6)
N311-Zn11-Cl21	120.7(6)
N521-Zn11-Cl11	101.8(5)
N311-Zn11-Cl11	110.2(6)
Cl21-Zn11-Cl11	121.6(3)
N511-Zn21-N111	82.4(7)
N511-Zn21-Cl31	112.4(5)
N111-Zn21-Cl31	111.5(5)
N511-Zn21-Cl41	104.9(5)
N111-Zn21-Cl41	116.1(5)
Cl31-Zn21-Cl41	122.0(2)
C201-N111-C121	127.4(18)
C201-N111-Zn21	129.9(13)
C121-N111-Zn21	101.9(14)
N111-C121-C241	124.8(19)
N111-C121-C131	118(2)
C241-C121-C131	117.4(19)
C141-C131-C121	116.8(19)
C141-C131-H131	121.6
C121-C131-H131	121.6
C131-C141-C151	124(2)
C131-C141-H141	118.2
C151-C141-H141	118.2
C141-C151-C161	123(2)
C141-C151-C201	120(2)
C161-C151-C201	116(2)
C171-C161-C151	120(2)
C171-C161-H161	120.2
C151-C161-H161	120.2
C161-C171-C181	119(3)
C161-C171-H171	120.4
C181-C171-H171	120.4
C171-C181-C191	125(2)
C171-C181-H181	117.4
C191-C181-H181	117.4
C201-C191-C181	117(2)
C201-C191-C211	123(2)
C181-C191-C211	120(2)
C191-C201-N111	125(2)
C191-C201-C151	122(2)
N111-C201-C151	113.7(18)
C191-C211-C231	109(2)
C191-C211-C221	113(2)
C231-C211-C221	105(2)
C191-C211-H211	110.1
C231-C211-H211	110.1
C221-C211-H211	110.1
C211-C221-H22A1	109.5
C211-C221-H22B1	109.5
H22A1-C221-H22B1	109.5
C211-C221-H22C1	109.5
H22A1-C221-H22C1	109.5
H22B1-C221-H22C1	109.5
C211-C231-H23A1	109.5
C211-C231-H23B1	109.5
H23A1-C231-H23B1	109.5

C211-C231-H23C1	109.5	C411-C431-H43C1	109.5
H23A1-C231-H23C1	109.5	H43A1-C431-H43C1	109.5
H23B1-C231-H23C1	109.5	H43B1-C431-H43C1	109.5
N511-C241-C121	117(2)	N521-C441-C321	119(2)
N511-C241-H241	121.7	N521-C441-H441	120.4
C121-C241-H241	121.7	C321-C441-H441	120.4
C321-N311-C401	119.8(19)	C241-N511-C511	118.3(18)
C321-N311-Zn11	106.7(16)	C241-N511-Zn21	112.6(16)
C401-N311-Zn11	133.4(14)	C511-N511-Zn21	128.0(13)
N311-C321-C441	120(2)	C441-N521-C521	123.4(17)
N311-C321-C331	121(2)	C441-N521-Zn11	110.7(15)
C441-C321-C331	120(2)	C521-N521-Zn11	125.9(12)
C341-C331-C321	118(2)	N511-C511-C521	112.6(18)
C341-C331-H331	120.9	N511-C511-C561	114.2(18)
C321-C331-H331	120.9	C521-C511-C561	110.1(15)
C331-C341-C351	124(2)	N511-C511-H511	106.4
C331-C341-H341	118.0	C521-C511-H511	106.4
C351-C341-H341	118.0	C561-C511-H511	106.4
C361-C351-C401	124(2)	N521-C521-C531	111.9(16)
C361-C351-C341	121(2)	N521-C521-C511	115.7(15)
C401-C351-C341	115(2)	C531-C521-C511	110.0(17)
C351-C361-C371	116(2)	N521-C521-H521	106.2
C351-C361-H36A1	108.4	C531-C521-H521	106.2
C371-C361-H36A1	108.4	C511-C521-H521	106.2
C351-C361-H36B1	108.4	C521-C531-C541	106.4(19)
C371-C361-H36B1	108.4	C521-C531-H53A1	110.5
H36A1-C361-H36B1	107.4	C541-C531-H53A1	110.5
C381-C371-C361	116(3)	C521-C531-H53B1	110.5
C381-C371-H371	122.0	C541-C531-H53B1	110.5
C361-C371-H371	122.0	H53A1-C531-H53B1	108.6
C391-C381-C371	128(3)	C551-C541-C531	110.1(18)
C391-C381-H381	116.0	C551-C541-H54A1	109.6
C371-C381-H381	116.0	C531-C541-H54A1	109.6
C381-C391-C401	122(2)	C551-C541-H54B1	109.6
C381-C391-C411	117(2)	C531-C541-H54B1	109.6
C401-C391-C411	121(2)	H54A1-C541-H54B1	108.1
N311-C401-C351	122(2)	C561-C551-C541	115(2)
N311-C401-C391	124.4(19)	C561-C551-H551	122.3
C351-C401-C391	113(2)	C541-C551-H551	122.3
C431-C411-C421	109.8(18)	C551-C561-C511	113(2)
C431-C411-C391	115.1(18)	C551-C561-H56A1	108.9
C421-C411-C391	111(2)	C511-C561-H56A1	108.9
C431-C411-H411	106.8	C551-C561-H56B1	108.9
C421-C411-H411	106.8	C511-C561-H56B1	108.9
C391-C411-H411	106.8	H56A1-C561-H56B1	107.8
C411-C421-H42A1	109.5	N522-Zn32-N312	83.4(7)
C411-C421-H42B1	109.5	N522-Zn32-Cl22	109.2(5)
H42A1-C421-H42B1	109.5	N312-Zn32-Cl22	114.2(5)
C411-C421-H42C1	109.5	N522-Zn32-Cl12	111.4(5)
H42A1-C421-H42C1	109.5	N312-Zn32-Cl12	110.7(6)
H42B1-C421-H42C1	109.5	Cl22-Zn32-Cl12	121.4(3)
C411-C431-H43A1	109.5	N512-Zn42-N112	83.1(7)
C411-C431-H43B1	109.5	N512-Zn42-Cl32	116.5(5)
H43A1-C431-H43B1	109.5	N112-Zn42-Cl32	110.8(6)

N512-Zn42-Cl42	108.9(5)	C322-N312-C402	121.1(18)
N112-Zn42-Cl42	117.6(5)	C322-N312-Zn32	106.3(14)
Cl32-Zn42-Cl42	115.9(3)	C402-N312-Zn32	132.4(14)
C202-N112-C122	116.1(19)	N312-C322-C442	118.7(17)
C202-N112-Zn42	136.7(14)	N312-C322-C332	123.9(18)
C122-N112-Zn42	106.3(13)	C442-C322-C332	117.3(17)
N112-C122-C242	119.4(19)	C342-C332-C322	114.1(19)
N112-C122-C132	123.9(19)	C342-C332-H332	123.0
C242-C122-C132	116.1(18)	C322-C332-H332	123.0
C142-C132-C122	118.1(19)	C352-C342-C332	129(2)
C142-C132-H132	121.0	C352-C342-H342	115.6
C122-C132-H132	121.0	C332-C342-H342	115.6
C132-C142-C152	124(2)	C342-C352-C362	130(2)
C132-C142-H142	118.1	C342-C352-C402	115(2)
C152-C142-H142	118.1	C362-C352-C402	115(2)
C162-C152-C142	124(2)	C372-C362-C352	127(3)
C162-C152-C202	122.4(18)	C372-C362-H362	116.5
C142-C152-C202	113.5(19)	C352-C362-H362	116.5
C172-C162-C152	121(2)	C362-C372-C382	117(3)
C172-C162-H162	119.6	C362-C372-H372	121.4
C152-C162-H162	119.6	C382-C372-H372	121.4
C162-C172-C182	120(2)	C392-C382-C372	120(2)
C162-C172-H172	120.2	C392-C382-H382	120.2
C182-C172-H172	120.2	C372-C382-H382	120.2
C192-C182-C172	123(2)	C402-C392-C382	121(2)
C192-C182-H182	118.5	C402-C392-C412	126(2)
C172-C182-H182	118.5	C382-C392-C412	113(2)
C182-C192-C202	120(2)	N312-C402-C392	125(2)
C182-C192-C212	118.2(19)	N312-C402-C352	117.4(18)
C202-C192-C212	121(2)	C392-C402-C352	118(2)
N112-C202-C192	121.5(19)	C432-C412-C392	111(2)
N112-C202-C152	123.8(17)	C432-C412-C422	113(2)
C192-C202-C152	114.1(19)	C392-C412-C422	112(2)
C192-C212-C232	112(2)	C432-C412-H412	107.1
C192-C212-C222	114(3)	C392-C412-H412	107.1
C232-C212-C222	113(2)	C422-C412-H412	107.1
C192-C212-H212	105.5	C412-C422-H42A2	109.5
C232-C212-H212	105.5	C412-C422-H42B2	109.5
C222-C212-H212	105.5	H42A2-C422-H42B2	109.5
C212-C222-H22A2	109.5	C412-C422-H42C2	109.5
C212-C222-H22B2	109.5	H42A2-C422-H42C2	109.5
H22A2-C222-H22B2	109.5	H42B2-C422-H42C2	109.5
C212-C222-H22C2	109.5	C412-C432-H43A2	109.5
H22A2-C222-H22C2	109.5	C412-C432-H43B2	109.5
H22B2-C222-H22C2	109.5	H43A2-C432-H43B2	109.5
C212-C232-H23A2	109.5	C412-C432-H43C2	109.5
C212-C232-H23B2	109.5	H43A2-C432-H43C2	109.5
H23A2-C232-H23B2	109.5	H43B2-C432-H43C2	109.5
C212-C232-H23C2	109.5	N522-C442-C322	124.8(18)
H23A2-C232-H23C2	109.5	N522-C442-H442	117.6
H23B2-C232-H23C2	109.5	C322-C442-H442	117.6
N512-C242-C122	121.1(19)	C242-N512-C512	116.9(16)
N512-C242-H242	119.5	C242-N512-Zn42	109.8(15)
C122-C242-H242	119.5	C512-N512-Zn42	133.2(13)

C442-N522-C522	120.2(17)	H53A2-C532-H53B2	107.6
C442-N522-Zn32	106.0(14)	C532-C542-C552	111.7(18)
C522-N522-Zn32	133.7(13)	C532-C542-H54A2	109.3
N512-C512-C522	110.4(15)	C552-C542-H54A2	109.3
N512-C512-C562	110.0(16)	C532-C542-H54B2	109.3
C522-C512-C562	109.9(17)	C552-C542-H54B2	109.3
N512-C512-H512	108.8	H54A2-C542-H54B2	108.0
C522-C512-H512	108.8	C562-C552-C542	106.6(17)
C562-C512-H512	108.8	C562-C552-H55A2	110.4
N522-C522-C532	109.8(17)	C542-C552-H55A2	110.4
N522-C522-C512	112.4(16)	C562-C552-H55B2	110.4
C532-C522-C512	107.8(16)	C542-C552-H55B2	110.4
N522-C522-H522	108.9	H55A2-C552-H55B2	108.6
C532-C522-H522	108.9	C552-C562-C512	112.3(19)
C512-C522-H522	108.9	C552-C562-H56A2	109.1
C522-C532-C542	114.1(18)	C512-C562-H56A2	109.1
C522-C532-H53A2	108.7	C552-C562-H56B2	109.1
C542-C532-H53A2	108.7	C512-C562-H56B2	109.1
C522-C532-H53B2	108.7	H56A2-C562-H56B2	107.9
C542-C532-H53B2	108.7		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R,R*)-**62**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn11	68(2)	35(2)	43(2)	16(1)	17(2)	36(2)
Cl11	95(6)	40(4)	50(4)	12(3)	22(4)	49(4)
Cl21	67(5)	82(5)	74(5)	43(4)	19(4)	49(4)
Zn21	54(2)	25(1)	45(2)	18(1)	14(1)	22(1)
Cl31	69(5)	37(4)	53(4)	24(3)	20(3)	30(3)
Cl41	68(5)	40(3)	50(4)	29(3)	21(3)	24(3)
N111	55(8)	19(9)	26(9)	8(8)	17(9)	18(7)
C121	64(12)	27(10)	40(13)	17(11)	22(13)	26(10)
C131	67(10)	18(10)	53(13)	1(10)	9(13)	31(10)
C141	65(10)	16(10)	24(11)	-9(9)	-9(12)	8(9)
C151	44(9)	33(10)	10(9)	9(10)	1(9)	3(8)
C161	56(11)	40(13)	47(14)	22(12)	18(13)	6(10)
C171	42(12)	68(15)	16(10)	13(12)	9(11)	15(11)
C181	60(10)	40(14)	37(12)	2(12)	14(12)	20(12)
C191	58(10)	40(13)	37(12)	14(11)	8(12)	20(10)
C201	58(9)	34(11)	34(12)	18(11)	25(12)	20(9)
C211	44(17)	66(18)	89(14)	51(16)	5(14)	19(14)
C221	60(20)	42(19)	220(30)	50(20)	20(20)	12(16)
C231	80(20)	80(20)	99(14)	70(17)	-11(17)	-2(17)
C241	60(18)	26(13)	38(13)	18(11)	25(12)	25(14)
N311	53(13)	33(12)	24(10)	7(9)	6(8)	14(10)
C321	32(13)	35(12)	16(10)	0(9)	-5(8)	15(11)

C331	54(17)	42(14)	46(14)	23(11)	16(10)	26(13)
C341	44(15)	42(13)	42(13)	21(11)	9(9)	32(12)
C351	41(15)	30(13)	30(12)	10(10)	2(8)	15(11)
C361	49(15)	32(12)	37(12)	6(9)	9(9)	16(11)
C371	70(20)	80(20)	56(17)	47(16)	32(13)	40(17)
C381	80(20)	43(15)	73(18)	37(14)	36(14)	33(14)
C391	72(18)	40(14)	5(10)	2(9)	-1(9)	35(14)
C401	66(17)	16(11)	25(11)	0(9)	10(9)	22(12)
C411	50(16)	13(11)	30(12)	14(10)	12(11)	1(11)
C421	90(20)	15(13)	61(19)	5(13)	-9(17)	11(15)
C431	51(18)	58(18)	66(17)	10(14)	-13(14)	41(16)
C441	49(15)	40(13)	20(11)	12(10)	17(10)	31(12)
N511	41(12)	34(10)	22(9)	13(8)	17(8)	17(10)
N521	74(14)	29(10)	12(8)	1(8)	8(9)	26(10)
C511	54(15)	42(14)	52(14)	9(11)	21(10)	42(13)
C531	78(18)	56(16)	45(14)	22(12)	18(12)	48(15)
C541	56(16)	40(14)	110(20)	53(15)	33(16)	24(13)
C551	57(17)	39(14)	61(15)	25(13)	14(13)	33(13)
C561	50(20)	50(18)	100(20)	45(18)	16(18)	30(17)
Zn32	65(2)	33(2)	37(2)	15(1)	12(1)	33(2)
Cl12	80(5)	24(3)	45(4)	15(3)	16(3)	25(3)
Cl22	92(6)	74(5)	48(4)	25(4)	21(4)	63(5)
Zn42	45(2)	28(2)	48(2)	22(1)	9(1)	20(1)
Cl32	67(5)	40(4)	56(4)	21(3)	16(3)	37(4)
Cl42	66(5)	54(4)	69(4)	41(4)	15(4)	27(4)
N112	25(7)	48(11)	40(11)	23(10)	-4(9)	16(8)
C122	32(10)	21(10)	34(12)	12(10)	3(10)	9(8)
C132	41(10)	38(13)	110(20)	41(15)	14(16)	19(11)
C142	43(10)	32(13)	100(20)	39(14)	29(14)	15(9)
C152	50(9)	26(11)	58(14)	21(11)	25(12)	21(9)
C162	35(10)	19(12)	85(19)	15(12)	8(14)	-3(9)
C172	50(13)	50(15)	77(17)	29(15)	26(14)	24(11)
C182	53(10)	52(13)	50(14)	24(12)	23(12)	41(11)
C192	47(10)	44(13)	41(12)	23(12)	22(11)	30(10)
C202	20(8)	40(12)	44(13)	27(12)	-13(10)	1(8)
C212	28(16)	62(18)	100(20)	47(17)	-18(14)	11(13)
C222	60(20)	41(18)	150(30)	1(19)	20(20)	23(17)
C232	100(30)	100(30)	180(40)	110(30)	-40(30)	-30(20)
C242	51(18)	39(15)	52(14)	15(12)	14(13)	32(14)
N312	42(13)	32(11)	32(11)	15(9)	11(9)	16(10)
C322	37(13)	27(11)	21(10)	19(9)	13(9)	17(10)
C332	46(15)	22(12)	29(13)	6(10)	8(11)	13(11)
C342	52(16)	28(12)	25(11)	13(10)	9(10)	12(11)
C352	59(18)	44(15)	24(12)	7(11)	6(12)	33(14)
C362	70(20)	70(19)	32(13)	22(14)	8(13)	43(17)
C372	80(20)	130(30)	34(15)	15(17)	4(14)	80(20)
C382	100(20)	59(17)	41(15)	32(14)	6(14)	43(17)
C392	42(15)	45(14)	40(14)	29(12)	14(12)	28(13)
C402	61(17)	37(14)	27(12)	23(12)	6(11)	26(13)
C412	90(20)	90(20)	16(12)	10(14)	3(14)	60(20)
C422	160(40)	60(20)	60(20)	11(18)	0(20)	50(30)
C432	55(18)	59(19)	110(20)	58(18)	22(17)	17(15)
C442	48(15)	17(11)	55(15)	17(11)	23(12)	15(11)
N512	40(12)	31(11)	27(9)	16(9)	6(8)	21(10)

N522	41(12)	18(9)	22(9)	4(8)	7(8)	9(8)
C512	60(14)	19(9)	27(10)	5(8)	12(9)	26(9)
C532	53(15)	15(11)	60(16)	13(10)	-4(11)	7(10)
C542	44(15)	47(14)	65(15)	34(13)	14(12)	18(12)
C552	43(16)	32(13)	92(18)	22(13)	19(13)	33(13)
C562	31(15)	16(11)	69(17)	25(12)	24(12)	8(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-**62**.

	x	y	z	U(eq)
H(1A)	5482	180	1530	464
H(1B)	4353	-477	568	464
H(2A)	5924	464	-207	464
H(2B)	4636	-261	-965	464
H(3A)	7389	3363	-498	464
H(3B)	6323	3401	-1014	464
H131	7675	3708	3833	59
H141	5697	2608	3630	58
H161	3727	2515	3653	65
H171	2548	3310	3421	61
H181	3313	5044	3219	67
H211	6228	7082	3509	77
H22A1	4944	7989	3504	182
H22B1	4859	7696	4477	182
H22C1	3850	6758	3368	182
H23A1	5428	5485	1591	137
H23B1	5327	6700	1811	137
H23C1	4211	5471	1652	137
H241	9370	5695	4189	46
H331	9201	10397	8166	55
H341	8032	10130	9252	46
H36A1	6873	8659	9961	55
H36B1	8046	9619	10914	55
H371	6891	7560	10886	74
H381	8154	6795	10527	73
H411	9842	6649	8741	42
H42A1	8960	4593	8487	104
H42B1	8023	4807	7994	104
H42C1	8045	4862	9140	104
H43A1	10789	7729	10512	94
H43B1	10566	6311	9960	94
H43C1	9782	6727	10727	94
H441	10199	9456	6835	40
H511	10737	8963	5210	58
H521	11137	7220	5521	38
H53A1	12850	9039	6857	66
H53B1	12574	9885	6499	66

H54A1	13837	9223	5468	74
H54B1	12908	7775	5023	74
H551	12806	9042	3992	58
H56A1	11002	6913	3623	76
H56B1	10864	7928	3432	76
H132	2910	6578	6143	72
H142	4848	7499	6476	71
H162	6669	7321	6490	70
H172	7582	6208	6447	73
H182	6582	4343	6522	56
H212	3625	2679	6298	80
H22A2	4626	1793	5152	161
H22B2	4400	1330	6019	161
H22C2	5661	2402	6179	161
H23A2	4449	4143	8196	216
H23B2	5483	3810	8136	216
H23C2	4179	2753	7886	216
H242	1072	4803	5819	56
H332	1147	-293	1672	44
H342	2152	48	464	46
H362	3092	1355	-426	66
H372	2808	2225	-1288	95
H382	1915	3606	-418	74
H412	189	3491	1421	82
H42A2	1063	5576	1634	155
H42B2	1907	5251	904	155
H42C2	2022	5343	2065	155
H43A2	-958	2297	-381	106
H43B2	-61	3304	-660	106
H43C2	-798	3690	179	106
H442	-161	113	2704	48
H512	-613	3221	5051	42
H522	-841	720	4081	41
H53A2	-2622	60	2980	59
H53B2	-2402	1477	3574	59
H54A2	-2888	-58	4570	61
H54B2	-3738	395	4301	61
H55A2	-2440	2595	5766	64
H55B2	-2664	1731	6307	64
H56A2	-931	1675	6044	46
H56B2	-644	3114	6732	46

Table 6. Torsion angles [°] for (*R,R*)-**62**.

N511-Zn21-N111-C201	169.2(19)	Cl41-Zn21-N111-C121	101.9(12)
Cl31-Zn21-N111-C201	58.1(18)	C201-N111-C121-C241	-177(2)
Cl41-Zn21-N111-C201	-87.9(18)	Zn21-N111-C121-C241	-6(3)
N511-Zn21-N111-C121	-1.0(13)	C201-N111-C121-C131	6(3)
Cl31-Zn21-N111-C121	-112.1(12)	Zn21-N111-C121-C131	176.3(17)

N111-C121-C131-C141	-9(3)	C361-C351-C401-N311	-177(2)
C241-C121-C131-C141	174(2)	C341-C351-C401-N311	0(3)
C121-C131-C141-C151	4(3)	C361-C351-C401-C391	3(3)
C131-C141-C151-C161	-172(2)	C341-C351-C401-C391	-179.9(19)
C131-C141-C151-C201	3(3)	C381-C391-C401-N311	178(3)
C141-C151-C161-C171	-177(2)	C411-C391-C401-N311	6(3)
C201-C151-C161-C171	8(3)	C381-C391-C401-C351	-2(4)
C151-C161-C171-C181	0(3)	C411-C391-C401-C351	-174.4(19)
C161-C171-C181-C191	-2(4)	C381-C391-C411-C431	-58(3)
C171-C181-C191-C201	-3(4)	C401-C391-C411-C431	115(2)
C171-C181-C191-C211	176(2)	C381-C391-C411-C421	67(3)
C181-C191-C201-N111	-172(2)	C401-C391-C411-C421	-120(2)
C211-C191-C201-N111	9(4)	N311-C321-C441-N521	-4(3)
C181-C191-C201-C151	10(3)	C331-C321-C441-N521	-178(2)
C211-C191-C201-C151	-168(2)	C121-C241-N511-C511	176.7(18)
C121-N111-C201-C191	-176(2)	C121-C241-N511-Zn21	-14(3)
Zn21-N111-C201-C191	16(3)	N111-Zn21-N511-C241	8.2(16)
C121-N111-C201-C151	2(3)	Cl31-Zn21-N511-C241	118.4(15)
Zn21-N111-C201-C151	-166.1(13)	Cl41-Zn21-N511-C241	-107.0(15)
C141-C151-C201-C191	172(2)	N111-Zn21-N511-C511	176.3(16)
C161-C151-C201-C191	-13(3)	Cl31-Zn21-N511-C511	-73.4(15)
C141-C151-C201-N111	-6(3)	Cl41-Zn21-N511-C511	61.2(15)
C161-C151-C201-N111	169.2(18)	C321-C441-N521-C521	178.7(18)
C201-C191-C211-C231	100(3)	C321-C441-N521-Zn11	-1(3)
C181-C191-C211-C231	-79(3)	N311-Zn11-N521-C441	3.4(16)
C201-C191-C211-C221	-144(2)	Cl21-Zn11-N521-C441	-116.9(15)
C181-C191-C211-C221	37(3)	Cl11-Zn11-N521-C441	112.7(15)
N111-C121-C241-N511	15(3)	N311-Zn11-N521-C521	-176.3(17)
C131-C121-C241-N511	-168(2)	Cl21-Zn11-N521-C521	63.4(16)
N521-Zn11-N311-C321	-5.1(14)	Cl11-Zn11-N521-C521	-67.0(16)
Cl21-Zn11-N311-C321	104.7(13)	C241-N511-C511-C521	-58(2)
Cl11-Zn11-N311-C321	-105.2(14)	Zn21-N511-C511-C521	134.9(14)
N521-Zn11-N311-C401	171(2)	C241-N511-C511-C561	69(2)
Cl21-Zn11-N311-C401	-79(2)	Zn21-N511-C511-C561	-98.6(18)
Cl11-Zn11-N311-C401	71(2)	C441-N521-C521-C531	88(2)
C401-N311-C321-C441	-171(2)	Zn11-N521-C521-C531	-92.1(19)
Zn11-N311-C321-C441	6(2)	C441-N521-C521-C511	-39(3)
C401-N311-C321-C331	3(3)	Zn11-N521-C521-C511	140.9(15)
Zn11-N311-C321-C331	180.0(17)	N511-C511-C521-N521	-46(2)
N311-C321-C331-C341	-5(3)	C561-C511-C521-N521	-174.3(18)
C441-C321-C331-C341	169(2)	N511-C511-C521-C531	-173.5(16)
C321-C331-C341-C351	5(4)	C561-C511-C521-C531	58(2)
C331-C341-C351-C361	175(2)	N521-C521-C531-C541	168.7(15)
C331-C341-C351-C401	-2(3)	C511-C521-C531-C541	-61(2)
C401-C351-C361-C371	-9(4)	C521-C531-C541-C551	59(2)
C341-C351-C361-C371	174(2)	C531-C541-C551-C561	-56(3)
C351-C361-C371-C381	15(4)	C541-C551-C561-C511	52(3)
C361-C371-C381-C391	-16(5)	N511-C511-C561-C551	-179.2(18)
C371-C381-C391-C401	10(5)	C521-C511-C561-C551	-51(3)
C371-C381-C391-C411	-178(3)	N512-Zn42-N112-C202	-168(2)
C321-N311-C401-C351	-1(3)	Cl32-Zn42-N112-C202	-53(2)
Zn11-N311-C401-C351	-176.8(17)	Cl42-Zn42-N112-C202	84(2)
C321-N311-C401-C391	179(2)	N512-Zn42-N112-C122	0.0(14)
Zn11-N311-C401-C391	3(4)	Cl32-Zn42-N112-C122	115.8(13)

Cl42-Zn42-N112-C122	-107.7(13)	C372-C382-C392-C412	-178(2)
C202-N112-C122-C242	174(2)	C322-N312-C402-C392	176(2)
Zn42-N112-C122-C242	3(2)	Zn32-N312-C402-C392	-9(3)
C202-N112-C122-C132	3(3)	C322-N312-C402-C352	-1(3)
Zn42-N112-C122-C132	-168.2(19)	Zn32-N312-C402-C352	174.5(15)
N112-C122-C132-C142	-1(4)	C382-C392-C402-N312	177(2)
C242-C122-C132-C142	-172(3)	C412-C392-C402-N312	2(4)
C122-C132-C142-C152	4(4)	C382-C392-C402-C352	-7(3)
C132-C142-C152-C162	173(3)	C412-C392-C402-C352	179(2)
C132-C142-C152-C202	-9(4)	C342-C352-C402-N312	-2(3)
C142-C152-C162-C172	-179(3)	C362-C352-C402-N312	-173(2)
C202-C152-C162-C172	3(4)	C342-C352-C402-C392	-178(2)
C152-C162-C172-C182	-5(4)	C362-C352-C402-C392	10(3)
C162-C172-C182-C192	3(4)	C402-C392-C412-C432	-115(3)
C172-C182-C192-C202	0(4)	C382-C392-C412-C432	70(3)
C172-C182-C192-C212	-173(2)	C402-C392-C412-C422	118(3)
C122-N112-C202-C192	-179(2)	C382-C392-C412-C422	-57(3)
Zn42-N112-C202-C192	-11(3)	N312-C322-C442-N522	-10(3)
C122-N112-C202-C152	-8(3)	C332-C322-C442-N522	168(2)
Zn42-N112-C202-C152	159.2(17)	C122-C242-N512-C512	-178(2)
C182-C192-C202-N112	170(2)	C122-C242-N512-Zn42	6(3)
C212-C192-C202-N112	-18(3)	N112-Zn42-N512-C242	-3.0(16)
C182-C192-C202-C152	-1(3)	Cl32-Zn42-N512-C242	-112.9(16)
C212-C192-C202-C152	171(2)	Cl42-Zn42-N512-C242	113.8(16)
C162-C152-C202-N112	-171(2)	N112-Zn42-N512-C512	-178.6(18)
C142-C152-C202-N112	11(3)	Cl32-Zn42-N512-C512	71.6(18)
C162-C152-C202-C192	0(3)	Cl42-Zn42-N512-C512	-61.8(18)
C142-C152-C202-C192	-178(2)	C322-C442-N522-C522	-173.6(19)
C182-C192-C212-C232	84(3)	C322-C442-N522-Zn32	10(3)
C202-C192-C212-C232	-89(3)	N312-Zn32-N522-C442	-5.1(14)
C182-C192-C212-C222	-46(3)	Cl22-Zn32-N522-C442	108.3(14)
C202-C192-C212-C222	141(2)	Cl12-Zn32-N522-C442	-114.9(13)
N112-C122-C242-N512	-6(3)	N312-Zn32-N522-C522	178.7(19)
C132-C122-C242-N512	165(2)	Cl22-Zn32-N522-C522	-67.9(18)
N522-Zn32-N312-C322	1.0(14)	Cl12-Zn32-N522-C522	68.9(18)
Cl22-Zn32-N312-C322	-107.2(13)	C242-N512-C512-C522	131(2)
Cl12-Zn32-N312-C322	111.4(13)	Zn42-N512-C512-C522	-54(2)
N522-Zn32-N312-C402	-175(2)	C242-N512-C512-C562	-107(2)
Cl22-Zn32-N312-C402	77(2)	Zn42-N512-C512-C562	68(2)
Cl12-Zn32-N312-C402	-64(2)	C442-N522-C522-C532	-113(2)
C402-N312-C322-C442	180(2)	Zn32-N522-C522-C532	63(2)
Zn32-N312-C322-C442	4(2)	C442-N522-C522-C512	127(2)
C402-N312-C322-C332	3(3)	Zn32-N522-C522-C512	-57(2)
Zn32-N312-C322-C332	-173.7(17)	N512-C512-C522-N522	-58(2)
N312-C322-C332-C342	-2(3)	C562-C512-C522-N522	-179.3(16)
C442-C322-C332-C342	-179.2(19)	N512-C512-C522-C532	-179.0(16)
C322-C332-C342-C352	-1(4)	C562-C512-C522-C532	60(2)
C332-C342-C352-C362	172(2)	N522-C522-C532-C542	-179.8(16)
C332-C342-C352-C402	2(4)	C512-C522-C532-C542	-57(2)
C342-C352-C362-C372	173(3)	C522-C532-C542-C552	54(2)
C402-C352-C362-C372	-18(4)	C532-C542-C552-C562	-52(2)
C352-C362-C372-C382	18(5)	C542-C552-C562-C512	58(2)
C362-C372-C382-C392	-12(4)	N512-C512-C562-C552	173.8(16)
C372-C382-C392-C402	7(4)	C522-C512-C562-C552	-65(2)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**63**.

Identification code	(*R*)-**63**	
Empirical formula	C74 H70 Cl4 N4 Zn2	
Formula weight	1287.88	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 17.5549(10) Å	α = 90°.
	b = 11.7013(7) Å	β = 116.636(3)°.
	c = 17.5582(11) Å	γ = 90°.
Volume	3223.9(3) $Å^3$	
Z	2	
Density (calculated)	1.327 g/cm^3	
Absorption coefficient	0.956 mm^{-1}	
F(000)	1340	
Crystal size	0.40 x 0.25 x 0.20 mm^3	
Theta range for data collection	2.21 to 28.22°.	
Index ranges	-23<=h<=22, -15<=k<=15, -22<=l<=22	
Reflections collected	24032	
Independent reflections	12541 [R(int) = 0.0550]	
Completeness to theta = 28.22°	93.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12541 / 1 / 757	
Goodness-of-fit on F^2	0.903	
Final R indices [I>2sigma(I)]	R1 = 0.0360, wR2 = 0.0761	
R indices (all data)	R1 = 0.0535, wR2 = 0.0806	
Absolute structure parameter	0.003(7)	
Largest diff. peak and hole	0.413 and -0.463 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**63**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(61)	4923(2)	5601(3)	-2074(2)	41(1)
C(62)	4966(3)	5035(3)	-1355(3)	47(1)
C(63)	5726(3)	4627(3)	-758(3)	54(1)
C(64)	6455(3)	4773(4)	-841(3)	54(1)
C(65)	6426(3)	5347(4)	-1526(3)	57(1)
C(66)	5667(2)	5750(3)	-2137(2)	47(1)
C(67)	4098(3)	6004(3)	-2771(3)	63(1)
C(71)	8984(4)	1339(9)	-363(4)	110(2)
C(72)	9328(4)	865(7)	-903(4)	115(3)
C(73)	9649(4)	1641(10)	-1275(5)	128(4)
C(74)	9608(4)	2774(10)	-1150(5)	138(4)
C(75)	9275(5)	3237(9)	-652(5)	138(3)
C(76)	9000(4)	2501(7)	-293(4)	98(2)

C(77)	8704(6)	531(9)	4(6)	202(5)
C(81)	9257(3)	2350(4)	6049(3)	63(1)
C(82)	9045(4)	3197(5)	6498(3)	82(2)
C(83)	8250(5)	3680(6)	6118(5)	102(2)
C(84)	7690(4)	3361(6)	5344(5)	100(2)
C(85)	7885(4)	2540(5)	4877(4)	86(2)
C(86)	8670(3)	2063(4)	5250(3)	65(1)
C(87)	10096(4)	1820(5)	6472(4)	101(2)
C(91)	7367(3)	7940(5)	-1871(3)	75(2)
C(92)	7171(3)	7411(6)	-2645(4)	83(2)
C(93)	7636(4)	6489(6)	-2708(4)	89(2)
C(94)	8312(4)	6106(6)	-1997(5)	95(2)
C(95)	8520(4)	6613(7)	-1228(4)	95(2)
C(96)	8060(4)	7531(5)	-1160(3)	84(2)
C(97)	6846(5)	8901(6)	-1800(4)	128(3)
Zn(1)	5663(1)	5618(1)	3667(1)	27(1)
Zn(2)	8089(1)	3141(1)	2360(1)	28(1)
Cl(1)	5672(1)	3845(1)	3322(1)	57(1)
Cl(2)	6765(1)	6424(1)	4737(1)	42(1)
Cl(3)	8073(1)	1376(1)	2788(1)	56(1)
Cl(4)	8016(1)	3439(1)	1100(1)	51(1)
C(01)	6375(2)	6488(2)	1969(2)	22(1)
C(02)	6131(2)	7154(2)	2463(2)	23(1)
N(02)	5498(2)	6751(2)	2706(2)	22(1)
C(03)	6513(2)	8223(3)	2780(2)	26(1)
C(04)	7131(2)	8610(3)	2591(2)	28(1)
C(05)	7386(2)	7982(3)	2069(2)	26(1)
C(06)	8015(2)	8402(3)	1836(2)	34(1)
C(07)	8240(2)	7810(3)	1311(2)	41(1)
C(08)	7869(2)	6742(3)	994(2)	40(1)
C(09)	7257(2)	6305(3)	1202(2)	32(1)
C(10)	7006(2)	6907(3)	1748(2)	24(1)
N(11)	4445(2)	6208(2)	3419(2)	26(1)
C(12)	4197(2)	6979(3)	2795(2)	29(1)
C(13)	3385(2)	7446(3)	2403(3)	44(1)
C(14)	2792(2)	7043(4)	2640(3)	52(1)
C(15)	3008(2)	6231(3)	3272(2)	40(1)
C(16)	2399(3)	5802(4)	3508(3)	56(1)
C(17)	2621(3)	5014(4)	4129(3)	59(1)
C(18)	3466(3)	4637(3)	4560(3)	46(1)
C(19)	4102(2)	5022(3)	4377(2)	34(1)
C(20)	3869(2)	5822(3)	3688(2)	30(1)
C(21)	4819(2)	7332(3)	2504(2)	27(1)
C(22)	4996(2)	4595(3)	4919(2)	44(1)
C(23)	5328(3)	5009(5)	5814(3)	72(1)
C(24)	5046(3)	3285(3)	4891(3)	61(1)
C(31)	5941(2)	5367(2)	1622(2)	23(1)
C(32)	6356(2)	4338(3)	1866(2)	24(1)
N(32)	7220(2)	4218(2)	2474(2)	22(1)
C(33)	5944(2)	3304(3)	1491(2)	27(1)
C(34)	5113(2)	3300(3)	913(2)	29(1)
C(35)	4659(2)	4327(3)	639(2)	25(1)
C(36)	3796(2)	4347(3)	5(2)	33(1)
C(37)	3382(2)	5354(3)	-286(2)	38(1)

C(38)	3796(2)	6396(3)	34(2)	35(1)
C(39)	4623(2)	6403(3)	647(2)	28(1)
C(40)	5076(2)	5372(3)	978(2)	24(1)
N(41)	8922(2)	3982(2)	3493(2)	23(1)
C(42)	8451(2)	4609(3)	3761(2)	26(1)
C(43)	8768(2)	5066(3)	4580(2)	36(1)
C(44)	9586(2)	4852(3)	5135(2)	39(1)
C(45)	10100(2)	4184(3)	4894(2)	33(1)
C(46)	10942(2)	3916(3)	5469(2)	41(1)
C(47)	11428(2)	3275(3)	5227(2)	43(1)
C(48)	11104(2)	2906(3)	4374(2)	36(1)
C(49)	10294(2)	3156(3)	3771(2)	29(1)
C(50)	9755(2)	3772(3)	4041(2)	25(1)
C(51)	7551(2)	4766(3)	3171(2)	26(1)
C(52)	10041(2)	2829(3)	2855(2)	38(1)
C(53)	10147(3)	1551(4)	2741(3)	61(1)
C(54)	10521(3)	3550(4)	2496(3)	66(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**63**.

C(61)-C(66)	1.370(5)	Zn(1)-N(11)	2.098(3)
C(61)-C(62)	1.398(5)	Zn(1)-Cl(1)	2.1635(10)
C(61)-C(67)	1.492(6)	Zn(1)-Cl(2)	2.2140(10)
C(62)-C(63)	1.361(6)	Zn(2)-N(32)	2.056(2)
C(63)-C(64)	1.363(6)	Zn(2)-N(41)	2.111(2)
C(64)-C(65)	1.359(6)	Zn(2)-Cl(4)	2.1852(10)
C(65)-C(66)	1.367(5)	Zn(2)-Cl(3)	2.2017(10)
C(71)-C(77)	1.355(10)	C(01)-C(02)	1.370(4)
C(71)-C(76)	1.365(10)	C(01)-C(10)	1.415(4)
C(71)-C(72)	1.443(9)	C(01)-C(31)	1.503(4)
C(72)-C(73)	1.378(11)	C(02)-C(03)	1.410(4)
C(73)-C(74)	1.351(12)	C(02)-N(02)	1.436(4)
C(74)-C(75)	1.363(10)	N(02)-C(21)	1.276(4)
C(75)-C(76)	1.282(9)	C(03)-C(04)	1.348(4)
C(81)-C(86)	1.358(6)	C(04)-C(05)	1.396(4)
C(81)-C(82)	1.416(7)	C(05)-C(10)	1.417(4)
C(81)-C(87)	1.457(7)	C(05)-C(06)	1.428(4)
C(82)-C(83)	1.371(8)	C(06)-C(07)	1.345(5)
C(83)-C(84)	1.324(8)	C(07)-C(08)	1.403(5)
C(84)-C(85)	1.402(8)	C(08)-C(09)	1.379(5)
C(85)-C(86)	1.352(7)	C(09)-C(10)	1.411(4)
C(91)-C(96)	1.381(7)	N(11)-C(12)	1.333(4)
C(91)-C(92)	1.389(7)	N(11)-C(20)	1.370(4)
C(91)-C(97)	1.489(8)	C(12)-C(13)	1.388(5)
C(92)-C(93)	1.386(8)	C(12)-C(21)	1.457(4)
C(93)-C(94)	1.356(8)	C(13)-C(14)	1.367(5)
C(94)-C(95)	1.366(8)	C(14)-C(15)	1.379(5)
C(95)-C(96)	1.382(8)	C(15)-C(16)	1.402(5)
Zn(1)-N(02)	2.062(2)	C(15)-C(20)	1.435(5)

C(16)-C(17)	1.345(6)	C(82)-C(81)-C(87)	118.2(5)
C(17)-C(18)	1.401(6)	C(83)-C(82)-C(81)	118.9(6)
C(18)-C(19)	1.368(5)	C(84)-C(83)-C(82)	120.6(6)
C(19)-C(20)	1.437(5)	C(83)-C(84)-C(85)	122.0(6)
C(19)-C(22)	1.511(5)	C(86)-C(85)-C(84)	117.5(6)
C(22)-C(23)	1.491(6)	C(85)-C(86)-C(81)	122.4(5)
C(22)-C(24)	1.537(5)	C(96)-C(91)-C(92)	117.4(6)
C(31)-C(32)	1.374(4)	C(96)-C(91)-C(97)	120.7(6)
C(31)-C(40)	1.430(4)	C(92)-C(91)-C(97)	121.8(5)
C(32)-C(33)	1.411(4)	C(93)-C(92)-C(91)	121.9(5)
C(32)-N(32)	1.417(4)	C(94)-C(93)-C(92)	119.1(6)
N(32)-C(51)	1.270(4)	C(93)-C(94)-C(95)	120.2(7)
C(33)-C(34)	1.353(4)	C(94)-C(95)-C(96)	121.0(6)
C(34)-C(35)	1.404(4)	C(91)-C(96)-C(95)	120.3(6)
C(35)-C(40)	1.413(4)	N(02)-Zn(1)-N(11)	82.10(10)
C(35)-C(36)	1.421(4)	N(02)-Zn(1)-Cl(1)	113.79(7)
C(36)-C(37)	1.358(5)	N(11)-Zn(1)-Cl(1)	113.06(7)
C(37)-C(38)	1.402(5)	N(02)-Zn(1)-Cl(2)	99.73(7)
C(38)-C(39)	1.365(4)	N(11)-Zn(1)-Cl(2)	117.24(7)
C(39)-C(40)	1.417(4)	Cl(1)-Zn(1)-Cl(2)	122.20(4)
N(41)-C(42)	1.339(4)	N(32)-Zn(2)-N(41)	81.54(10)
N(41)-C(50)	1.366(4)	N(32)-Zn(2)-Cl(4)	106.92(7)
C(42)-C(43)	1.395(4)	N(41)-Zn(2)-Cl(4)	125.50(7)
C(42)-C(51)	1.461(4)	N(32)-Zn(2)-Cl(3)	114.72(7)
C(43)-C(44)	1.350(5)	N(41)-Zn(2)-Cl(3)	103.00(7)
C(44)-C(45)	1.395(5)	Cl(4)-Zn(2)-Cl(3)	119.43(4)
C(45)-C(46)	1.402(5)	C(02)-C(01)-C(10)	118.9(3)
C(45)-C(50)	1.424(4)	C(02)-C(01)-C(31)	120.5(3)
C(46)-C(47)	1.340(5)	C(10)-C(01)-C(31)	120.5(3)
C(47)-C(48)	1.411(5)	C(01)-C(02)-C(03)	121.7(3)
C(48)-C(49)	1.370(4)	C(01)-C(02)-N(02)	120.3(3)
C(49)-C(50)	1.430(4)	C(03)-C(02)-N(02)	117.9(3)
C(49)-C(52)	1.513(4)	C(21)-N(02)-C(02)	119.6(3)
C(52)-C(54)	1.516(5)	C(21)-N(02)-Zn(1)	109.9(2)
C(52)-C(53)	1.531(5)	C(02)-N(02)-Zn(1)	127.59(19)
		C(04)-C(03)-C(02)	119.6(3)
C(66)-C(61)-C(62)	117.7(4)	C(03)-C(04)-C(05)	121.0(3)
C(66)-C(61)-C(67)	120.2(4)	C(04)-C(05)-C(10)	119.8(3)
C(62)-C(61)-C(67)	122.1(4)	C(04)-C(05)-C(06)	121.6(3)
C(63)-C(62)-C(61)	120.0(4)	C(10)-C(05)-C(06)	118.6(3)
C(62)-C(63)-C(64)	121.1(4)	C(07)-C(06)-C(05)	121.4(3)
C(65)-C(64)-C(63)	119.5(4)	C(06)-C(07)-C(08)	120.3(3)
C(64)-C(65)-C(66)	120.1(4)	C(09)-C(08)-C(07)	120.2(3)
C(65)-C(66)-C(61)	121.5(4)	C(08)-C(09)-C(10)	120.9(3)
C(77)-C(71)-C(76)	130.5(9)	C(09)-C(10)-C(01)	122.4(3)
C(77)-C(71)-C(72)	113.1(10)	C(09)-C(10)-C(05)	118.6(3)
C(76)-C(71)-C(72)	116.4(6)	C(01)-C(10)-C(05)	119.0(3)
C(73)-C(72)-C(71)	116.0(8)	C(12)-N(11)-C(20)	119.2(3)
C(74)-C(73)-C(72)	120.5(7)	C(12)-N(11)-Zn(1)	108.7(2)
C(73)-C(74)-C(75)	124.3(10)	C(20)-N(11)-Zn(1)	131.4(2)
C(76)-C(75)-C(74)	114.3(10)	N(11)-C(12)-C(13)	123.9(3)
C(75)-C(76)-C(71)	128.5(8)	N(11)-C(12)-C(21)	117.4(3)
C(86)-C(81)-C(82)	118.7(5)	C(13)-C(12)-C(21)	118.7(3)
C(86)-C(81)-C(87)	123.2(5)	C(14)-C(13)-C(12)	117.9(3)

C(13)-C(14)-C(15)	120.6(4)	C(37)-C(36)-C(35)	120.7(3)
C(14)-C(15)-C(16)	120.9(4)	C(36)-C(37)-C(38)	120.7(3)
C(14)-C(15)-C(20)	119.2(3)	C(39)-C(38)-C(37)	119.8(3)
C(16)-C(15)-C(20)	120.0(3)	C(38)-C(39)-C(40)	121.4(3)
C(17)-C(16)-C(15)	120.2(4)	C(35)-C(40)-C(39)	118.3(3)
C(16)-C(17)-C(18)	120.4(4)	C(35)-C(40)-C(31)	119.7(3)
C(19)-C(18)-C(17)	123.2(4)	C(39)-C(40)-C(31)	122.0(3)
C(18)-C(19)-C(20)	117.3(3)	C(42)-N(41)-C(50)	119.1(3)
C(18)-C(19)-C(22)	118.1(3)	C(42)-N(41)-Zn(2)	108.13(19)
C(20)-C(19)-C(22)	124.6(3)	C(50)-N(41)-Zn(2)	130.6(2)
N(11)-C(20)-C(15)	119.1(3)	N(41)-C(42)-C(43)	123.3(3)
N(11)-C(20)-C(19)	122.1(3)	N(41)-C(42)-C(51)	117.5(3)
C(15)-C(20)-C(19)	118.9(3)	C(43)-C(42)-C(51)	119.2(3)
N(02)-C(21)-C(12)	120.3(3)	C(44)-C(43)-C(42)	118.5(3)
C(23)-C(22)-C(19)	111.1(4)	C(43)-C(44)-C(45)	120.5(3)
C(23)-C(22)-C(24)	110.9(3)	C(44)-C(45)-C(46)	121.5(3)
C(19)-C(22)-C(24)	111.6(3)	C(44)-C(45)-C(50)	118.7(3)
C(32)-C(31)-C(40)	118.5(3)	C(46)-C(45)-C(50)	119.7(3)
C(32)-C(31)-C(01)	122.5(3)	C(47)-C(46)-C(45)	120.8(3)
C(40)-C(31)-C(01)	118.9(3)	C(46)-C(47)-C(48)	119.8(3)
C(31)-C(32)-C(33)	121.1(3)	C(49)-C(48)-C(47)	122.7(3)
C(31)-C(32)-N(32)	124.1(3)	C(48)-C(49)-C(50)	117.6(3)
C(33)-C(32)-N(32)	114.7(3)	C(48)-C(49)-C(52)	118.4(3)
C(51)-N(32)-C(32)	123.3(3)	C(50)-C(49)-C(52)	123.9(3)
C(51)-N(32)-Zn(2)	111.4(2)	N(41)-C(50)-C(45)	119.8(3)
C(32)-N(32)-Zn(2)	125.27(19)	N(41)-C(50)-C(49)	121.1(3)
C(34)-C(33)-C(32)	120.5(3)	C(45)-C(50)-C(49)	119.1(3)
C(33)-C(34)-C(35)	120.7(3)	N(32)-C(51)-C(42)	120.1(3)
C(34)-C(35)-C(40)	119.3(3)	C(49)-C(52)-C(54)	110.3(3)
C(34)-C(35)-C(36)	121.6(3)	C(49)-C(52)-C(53)	113.0(3)
C(40)-C(35)-C(36)	119.0(3)	C(54)-C(52)-C(53)	111.5(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**63**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(61)	49(2)	30(2)	47(2)	-5(2)	23(2)	-7(2)
C(62)	66(3)	38(2)	55(3)	-16(2)	41(2)	-16(2)
C(63)	91(4)	40(2)	35(2)	-10(2)	31(3)	-19(2)
C(64)	60(3)	53(2)	36(2)	-6(2)	11(2)	-7(2)
C(65)	46(3)	78(3)	50(3)	-13(2)	25(2)	-21(2)
C(66)	52(2)	55(2)	36(2)	1(2)	22(2)	-13(2)
C(67)	69(3)	34(2)	88(3)	-2(2)	37(3)	-4(2)
C(71)	77(4)	182(8)	68(4)	24(5)	32(3)	-31(5)
C(72)	87(5)	169(8)	95(5)	-49(5)	45(4)	2(5)
C(73)	56(4)	239(11)	92(5)	-79(6)	35(4)	-5(5)
C(74)	71(4)	262(13)	85(5)	-63(7)	39(4)	-34(6)

C(75)	116(6)	169(9)	97(6)	20(6)	20(5)	-38(6)
C(76)	96(5)	103(5)	94(5)	-34(4)	40(4)	5(4)
C(77)	155(8)	218(12)	212(11)	64(9)	63(8)	-33(8)
C(81)	54(3)	60(3)	73(3)	15(2)	27(3)	1(2)
C(82)	125(5)	57(3)	72(3)	-1(3)	51(3)	-4(4)
C(83)	130(6)	87(4)	118(6)	34(4)	81(5)	34(4)
C(84)	82(4)	101(5)	130(6)	48(5)	59(5)	23(4)
C(85)	70(4)	80(4)	104(5)	24(3)	35(4)	-1(3)
C(86)	76(4)	53(3)	68(3)	-5(2)	32(3)	-12(3)
C(87)	86(4)	78(4)	124(5)	7(4)	32(4)	-4(3)
C(91)	80(4)	81(4)	61(3)	16(3)	28(3)	-11(3)
C(92)	54(3)	115(5)	70(4)	31(3)	19(3)	-18(3)
C(93)	73(4)	128(5)	76(4)	9(4)	43(3)	-20(4)
C(94)	65(4)	127(6)	108(5)	25(4)	51(4)	3(3)
C(95)	61(4)	132(6)	74(4)	28(4)	14(3)	-19(4)
C(96)	86(4)	86(4)	63(4)	9(3)	17(3)	-17(3)
C(97)	165(7)	100(5)	129(6)	33(4)	77(6)	35(5)
Zn(1)	28(1)	26(1)	30(1)	4(1)	15(1)	4(1)
Zn(2)	22(1)	27(1)	33(1)	-8(1)	11(1)	0(1)
Cl(1)	100(1)	27(1)	66(1)	3(1)	57(1)	11(1)
Cl(2)	28(1)	57(1)	35(1)	0(1)	10(1)	-3(1)
Cl(3)	53(1)	25(1)	99(1)	-4(1)	42(1)	-8(1)
Cl(4)	42(1)	79(1)	29(1)	-5(1)	13(1)	17(1)
C(01)	17(2)	23(2)	25(2)	-2(1)	8(1)	0(1)
C(02)	20(2)	23(2)	22(2)	2(1)	7(1)	3(1)
N(02)	23(1)	24(1)	21(1)	-3(1)	10(1)	-3(1)
C(03)	28(2)	21(2)	28(2)	-4(1)	13(1)	-1(1)
C(04)	24(2)	23(2)	29(2)	0(1)	4(2)	-2(1)
C(05)	18(2)	28(2)	27(2)	6(1)	5(1)	2(1)
C(06)	24(2)	33(2)	37(2)	4(1)	8(2)	-8(1)
C(07)	33(2)	49(2)	47(2)	4(2)	23(2)	-9(2)
C(08)	40(2)	46(2)	46(2)	-8(2)	29(2)	-5(2)
C(09)	35(2)	35(2)	36(2)	-2(2)	23(2)	-1(2)
C(10)	20(2)	27(2)	22(2)	1(1)	6(1)	-1(1)
N(11)	30(2)	24(1)	28(1)	-1(1)	17(1)	-3(1)
C(12)	24(2)	29(2)	33(2)	2(1)	13(2)	4(1)
C(13)	34(2)	49(2)	56(3)	17(2)	25(2)	9(2)
C(14)	33(2)	60(3)	71(3)	19(2)	29(2)	16(2)
C(15)	29(2)	49(2)	51(2)	2(2)	27(2)	2(2)
C(16)	41(2)	64(3)	78(3)	8(2)	39(2)	2(2)
C(17)	55(3)	61(3)	87(4)	6(2)	54(3)	-9(2)
C(18)	54(3)	44(2)	54(3)	6(2)	36(2)	-4(2)
C(19)	41(2)	33(2)	36(2)	-1(2)	23(2)	-5(2)
C(20)	35(2)	27(2)	35(2)	-9(1)	21(2)	-4(1)
C(21)	28(2)	25(2)	29(2)	4(1)	12(2)	0(1)
C(22)	44(2)	45(2)	44(2)	13(2)	21(2)	-4(2)
C(23)	77(4)	86(3)	47(3)	0(2)	22(3)	-10(3)
C(24)	67(3)	46(3)	79(3)	17(2)	42(2)	10(2)
C(31)	20(2)	27(2)	23(2)	-3(1)	12(1)	-1(1)
C(32)	19(2)	30(2)	24(2)	-1(1)	11(1)	0(1)
N(32)	15(1)	23(1)	26(1)	0(1)	6(1)	1(1)
C(33)	29(2)	24(2)	29(2)	-3(1)	14(1)	4(1)
C(34)	28(2)	29(2)	30(2)	-6(1)	14(1)	-7(1)
C(35)	24(2)	30(2)	21(2)	-1(1)	11(1)	-3(1)

C(36)	21(2)	39(2)	33(2)	-3(2)	6(2)	-8(2)
C(37)	23(2)	47(2)	34(2)	-1(2)	3(2)	1(2)
C(38)	29(2)	37(2)	34(2)	6(2)	9(2)	7(2)
C(39)	29(2)	31(2)	24(2)	0(1)	11(2)	-1(1)
C(40)	18(2)	33(2)	21(2)	0(1)	8(1)	0(1)
N(41)	20(1)	21(1)	25(1)	0(1)	8(1)	-3(1)
C(42)	22(2)	27(2)	27(2)	-2(1)	10(1)	-1(1)
C(43)	27(2)	41(2)	37(2)	-9(2)	13(2)	3(2)
C(44)	36(2)	44(2)	28(2)	-10(2)	7(2)	1(2)
C(45)	30(2)	34(2)	30(2)	1(1)	9(2)	-3(2)
C(46)	35(2)	51(2)	28(2)	-6(2)	6(2)	-2(2)
C(47)	24(2)	52(2)	40(2)	5(2)	3(2)	2(2)
C(48)	27(2)	38(2)	41(2)	3(2)	14(2)	6(2)
C(49)	22(2)	34(2)	31(2)	2(2)	11(1)	-2(2)
C(50)	21(2)	24(2)	28(2)	2(1)	9(1)	-2(1)
C(51)	25(2)	25(2)	30(2)	-3(1)	12(2)	4(1)
C(52)	21(2)	61(3)	32(2)	-1(2)	13(2)	7(2)
C(53)	69(3)	66(3)	56(3)	-16(2)	34(2)	0(2)
C(54)	78(3)	82(4)	49(3)	12(2)	39(3)	3(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**63**.

	x	y	z	U(eq)
H(62)	4465	4935	-1283	57
H(63)	5748	4233	-275	65
H(64)	6980	4477	-422	65
H(65)	6934	5469	-1581	68
H(66)	5654	6142	-2616	56
H(67A)	3635	5838	-2621	94
H(67B)	3991	5609	-3302	94
H(67C)	4128	6830	-2848	94
H(72)	9334	66	-995	138
H(73)	9900	1378	-1622	154
H(74)	9826	3282	-1427	166
H(75)	9249	4038	-577	165
H(76)	8778	2805	68	118
H(77A)	8801	-229	-170	303
H(77B)	8093	638	-178	303
H(77C)	9014	599	625	303
H(82)	9447	3426	7052	99
H(83)	8099	4249	6412	123
H(84)	7140	3700	5098	120
H(85)	7481	2326	4319	103
H(86)	8815	1507	4943	78
H(87A)	10417	2162	7037	152
H(87B)	10403	1943	6131	152
H(87C)	10031	998	6533	152

H(92)	6706	7688	-3146	99
H(93)	7484	6131	-3242	107
H(94)	8641	5483	-2034	114
H(95)	8989	6330	-732	114
H(96)	8220	7882	-622	101
H(97A)	6388	9080	-2365	191
H(97B)	7209	9575	-1568	191
H(97C)	6599	8679	-1420	191
H(03)	6335	8667	3125	31
H(04)	7398	9321	2817	34
H(06)	8281	9116	2056	40
H(07)	8651	8115	1155	49
H(08)	8040	6320	635	48
H(09)	7002	5588	975	39
H(13)	3245	8026	1984	53
H(14)	2225	7326	2367	63
H(16)	1828	6069	3229	68
H(17)	2202	4711	4275	71
H(18)	3604	4088	5001	55
H(21)	4719	7998	2163	33
H(22)	5370	4916	4678	53
H(23A)	5285	5844	5816	108
H(23B)	5926	4781	6138	108
H(23C)	4991	4675	6076	108
H(24A)	4796	3030	4296	91
H(24B)	4731	2947	5175	91
H(24C)	5644	3044	5182	91
H(33)	6253	2606	1645	32
H(34)	4834	2594	692	34
H(36)	3506	3648	-218	40
H(37)	2805	5352	-709	46
H(38)	3502	7096	-176	42
H(39)	4900	7113	856	34
H(43)	8416	5517	4743	43
H(44)	9815	5158	5695	46
H(46)	11172	4193	6038	49
H(47)	11989	3068	5629	52
H(48)	11462	2467	4211	43
H(51)	7213	5279	3311	32
H(52)	9422	3012	2519	45
H(53A)	9827	1109	2976	92
H(53B)	10752	1347	3041	92
H(53C)	9930	1377	2134	92
H(54A)	11133	3397	2814	99
H(54B)	10413	4361	2548	99
H(54C)	10328	3359	1894	99

Table 6. Torsion angles [°] for (*R*)-**63**.

C(66)-C(61)-C(62)-C(63)	-1.7(5)	C(04)-C(05)-C(06)-C(07)	-178.0(3)
C(67)-C(61)-C(62)-C(63)	176.4(4)	C(10)-C(05)-C(06)-C(07)	1.1(5)
C(61)-C(62)-C(63)-C(64)	0.9(6)	C(05)-C(06)-C(07)-C(08)	-1.4(5)
C(62)-C(63)-C(64)-C(65)	0.7(6)	C(06)-C(07)-C(08)-C(09)	1.5(6)
C(63)-C(64)-C(65)-C(66)	-1.5(6)	C(07)-C(08)-C(09)-C(10)	-1.3(5)
C(64)-C(65)-C(66)-C(61)	0.7(6)	C(08)-C(09)-C(10)-C(01)	179.5(3)
C(62)-C(61)-C(66)-C(65)	0.9(6)	C(08)-C(09)-C(10)-C(05)	1.0(5)
C(67)-C(61)-C(66)-C(65)	-177.2(4)	C(02)-C(01)-C(10)-C(09)	-176.3(3)
C(77)-C(71)-C(72)-C(73)	-178.1(7)	C(31)-C(01)-C(10)-C(09)	-0.2(4)
C(76)-C(71)-C(72)-C(73)	1.1(9)	C(02)-C(01)-C(10)-C(05)	2.2(4)
C(71)-C(72)-C(73)-C(74)	-2.0(10)	C(31)-C(01)-C(10)-C(05)	178.3(3)
C(72)-C(73)-C(74)-C(75)	1.2(12)	C(04)-C(05)-C(10)-C(09)	178.2(3)
C(73)-C(74)-C(75)-C(76)	0.5(11)	C(06)-C(05)-C(10)-C(09)	-0.9(4)
C(74)-C(75)-C(76)-C(71)	-1.5(12)	C(04)-C(05)-C(10)-C(01)	-0.3(4)
C(77)-C(71)-C(76)-C(75)	179.7(8)	C(06)-C(05)-C(10)-C(01)	-179.4(3)
C(72)-C(71)-C(76)-C(75)	0.7(11)	N(02)-Zn(1)-N(11)-C(12)	0.0(2)
C(86)-C(81)-C(82)-C(83)	1.3(8)	Cl(1)-Zn(1)-N(11)-C(12)	-112.58(19)
C(87)-C(81)-C(82)-C(83)	-178.2(5)	Cl(2)-Zn(1)-N(11)-C(12)	96.9(2)
C(81)-C(82)-C(83)-C(84)	-0.1(9)	N(02)-Zn(1)-N(11)-C(20)	169.2(3)
C(82)-C(83)-C(84)-C(85)	-1.1(10)	Cl(1)-Zn(1)-N(11)-C(20)	56.7(3)
C(83)-C(84)-C(85)-C(86)	0.9(9)	Cl(2)-Zn(1)-N(11)-C(20)	-93.8(3)
C(84)-C(85)-C(86)-C(81)	0.3(8)	C(20)-N(11)-C(12)-C(13)	1.4(5)
C(82)-C(81)-C(86)-C(85)	-1.4(7)	Zn(1)-N(11)-C(12)-C(13)	172.2(3)
C(87)-C(81)-C(86)-C(85)	178.1(5)	C(20)-N(11)-C(12)-C(21)	-177.5(3)
C(96)-C(91)-C(92)-C(93)	1.4(8)	Zn(1)-N(11)-C(12)-C(21)	-6.8(3)
C(97)-C(91)-C(92)-C(93)	-177.6(5)	N(11)-C(12)-C(13)-C(14)	-3.7(6)
C(91)-C(92)-C(93)-C(94)	-1.3(8)	C(21)-C(12)-C(13)-C(14)	175.2(3)
C(92)-C(93)-C(94)-C(95)	1.0(9)	C(12)-C(13)-C(14)-C(15)	2.4(6)
C(93)-C(94)-C(95)-C(96)	-1.0(9)	C(13)-C(14)-C(15)-C(16)	-179.0(4)
C(92)-C(91)-C(96)-C(95)	-1.3(8)	C(13)-C(14)-C(15)-C(20)	0.9(6)
C(97)-C(91)-C(96)-C(95)	177.7(6)	C(14)-C(15)-C(16)-C(17)	-179.7(4)
C(94)-C(95)-C(96)-C(91)	1.2(9)	C(20)-C(15)-C(16)-C(17)	0.5(6)
C(10)-C(01)-C(02)-C(03)	-2.3(4)	C(15)-C(16)-C(17)-C(18)	1.7(7)
C(31)-C(01)-C(02)-C(03)	-178.4(3)	C(16)-C(17)-C(18)-C(19)	-0.9(7)
C(10)-C(01)-C(02)-N(02)	-179.5(3)	C(17)-C(18)-C(19)-C(20)	-2.1(6)
C(31)-C(01)-C(02)-N(02)	4.4(4)	C(17)-C(18)-C(19)-C(22)	176.9(4)
C(01)-C(02)-N(02)-C(21)	-121.9(3)	C(12)-N(11)-C(20)-C(15)	2.0(4)
C(03)-C(02)-N(02)-C(21)	60.8(4)	Zn(1)-N(11)-C(20)-C(15)	-166.3(2)
C(01)-C(02)-N(02)-Zn(1)	79.6(3)	C(12)-N(11)-C(20)-C(19)	-177.8(3)
C(03)-C(02)-N(02)-Zn(1)	-97.7(3)	Zn(1)-N(11)-C(20)-C(19)	13.9(4)
N(11)-Zn(1)-N(02)-C(21)	7.3(2)	C(14)-C(15)-C(20)-N(11)	-3.1(5)
Cl(1)-Zn(1)-N(02)-C(21)	119.1(2)	C(16)-C(15)-C(20)-N(11)	176.7(3)
Cl(2)-Zn(1)-N(02)-C(21)	-109.1(2)	C(14)-C(15)-C(20)-C(19)	176.7(4)
N(11)-Zn(1)-N(02)-C(02)	167.6(2)	C(16)-C(15)-C(20)-C(19)	-3.5(5)
Cl(1)-Zn(1)-N(02)-C(02)	-80.6(2)	C(18)-C(19)-C(20)-N(11)	-176.0(3)
Cl(2)-Zn(1)-N(02)-C(02)	51.2(2)	C(22)-C(19)-C(20)-N(11)	5.1(5)
C(01)-C(02)-C(03)-C(04)	0.4(4)	C(18)-C(19)-C(20)-C(15)	4.2(5)
N(02)-C(02)-C(03)-C(04)	177.6(3)	C(22)-C(19)-C(20)-C(15)	-174.7(3)
C(02)-C(03)-C(04)-C(05)	1.6(4)	C(02)-N(02)-C(21)-C(12)	-175.7(3)
C(03)-C(04)-C(05)-C(10)	-1.6(4)	Zn(1)-N(02)-C(21)-C(12)	-13.6(4)
C(03)-C(04)-C(05)-C(06)	177.4(3)	N(11)-C(12)-C(21)-N(02)	14.7(4)

C(13)-C(12)-C(21)-N(02)	-164.3(3)	C(01)-C(31)-C(40)-C(39)	1.3(4)
C(18)-C(19)-C(22)-C(23)	-65.9(4)	N(32)-Zn(2)-N(41)-C(42)	9.82(19)
C(20)-C(19)-C(22)-C(23)	113.0(4)	Cl(4)-Zn(2)-N(41)-C(42)	114.62(18)
C(18)-C(19)-C(22)-C(24)	58.4(5)	Cl(3)-Zn(2)-N(41)-C(42)	-103.73(19)
C(20)-C(19)-C(22)-C(24)	-122.6(4)	N(32)-Zn(2)-N(41)-C(50)	172.4(3)
C(02)-C(01)-C(31)-C(32)	-114.6(3)	Cl(4)-Zn(2)-N(41)-C(50)	-82.8(3)
C(10)-C(01)-C(31)-C(32)	69.4(4)	Cl(3)-Zn(2)-N(41)-C(50)	58.8(3)
C(02)-C(01)-C(31)-C(40)	69.1(4)	C(50)-N(41)-C(42)-C(43)	0.0(4)
C(10)-C(01)-C(31)-C(40)	-107.0(3)	Zn(2)-N(41)-C(42)-C(43)	164.9(3)
C(40)-C(31)-C(32)-C(33)	0.2(4)	C(50)-N(41)-C(42)-C(51)	-176.9(3)
C(01)-C(31)-C(32)-C(33)	-176.2(3)	Zn(2)-N(41)-C(42)-C(51)	-11.9(3)
C(40)-C(31)-C(32)-N(32)	177.8(3)	N(41)-C(42)-C(43)-C(44)	-1.0(5)
C(01)-C(31)-C(32)-N(32)	1.4(5)	C(51)-C(42)-C(43)-C(44)	175.8(3)
C(31)-C(32)-N(32)-C(51)	43.6(4)	C(42)-C(43)-C(44)-C(45)	-0.3(5)
C(33)-C(32)-N(32)-C(51)	-138.7(3)	C(43)-C(44)-C(45)-C(46)	-177.7(4)
C(31)-C(32)-N(32)-Zn(2)	-137.3(3)	C(43)-C(44)-C(45)-C(50)	2.5(5)
C(33)-C(32)-N(32)-Zn(2)	40.4(3)	C(44)-C(45)-C(46)-C(47)	-179.9(4)
N(41)-Zn(2)-N(32)-C(51)	-6.3(2)	C(50)-C(45)-C(46)-C(47)	-0.1(5)
Cl(4)-Zn(2)-N(32)-C(51)	-130.9(2)	C(45)-C(46)-C(47)-C(48)	3.0(6)
Cl(3)-Zn(2)-N(32)-C(51)	94.2(2)	C(46)-C(47)-C(48)-C(49)	-1.5(6)
N(41)-Zn(2)-N(32)-C(32)	174.5(2)	C(47)-C(48)-C(49)-C(50)	-2.9(5)
Cl(4)-Zn(2)-N(32)-C(32)	49.9(2)	C(47)-C(48)-C(49)-C(52)	173.6(3)
Cl(3)-Zn(2)-N(32)-C(32)	-85.0(2)	C(42)-N(41)-C(50)-C(45)	2.3(4)
C(31)-C(32)-C(33)-C(34)	-3.6(5)	Zn(2)-N(41)-C(50)-C(45)	-158.7(2)
N(32)-C(32)-C(33)-C(34)	178.6(3)	C(42)-N(41)-C(50)-C(49)	-176.8(3)
C(32)-C(33)-C(34)-C(35)	3.8(5)	Zn(2)-N(41)-C(50)-C(49)	22.2(4)
C(33)-C(34)-C(35)-C(40)	-0.7(5)	C(44)-C(45)-C(50)-N(41)	-3.5(5)
C(33)-C(34)-C(35)-C(36)	177.1(3)	C(46)-C(45)-C(50)-N(41)	176.7(3)
C(34)-C(35)-C(36)-C(37)	-176.4(3)	C(44)-C(45)-C(50)-C(49)	175.5(3)
C(40)-C(35)-C(36)-C(37)	1.4(5)	C(46)-C(45)-C(50)-C(49)	-4.3(5)
C(35)-C(36)-C(37)-C(38)	0.0(5)	C(48)-C(49)-C(50)-N(41)	-175.3(3)
C(36)-C(37)-C(38)-C(39)	-0.4(5)	C(52)-C(49)-C(50)-N(41)	8.4(5)
C(37)-C(38)-C(39)-C(40)	-0.6(5)	C(48)-C(49)-C(50)-C(45)	5.6(5)
C(34)-C(35)-C(40)-C(39)	175.5(3)	C(52)-C(49)-C(50)-C(45)	-170.7(3)
C(36)-C(35)-C(40)-C(39)	-2.3(4)	C(32)-N(32)-C(51)-C(42)	-179.0(3)
C(34)-C(35)-C(40)-C(31)	-2.7(4)	Zn(2)-N(32)-C(51)-C(42)	1.7(4)
C(36)-C(35)-C(40)-C(31)	179.4(3)	N(41)-C(42)-C(51)-N(32)	7.6(4)
C(38)-C(39)-C(40)-C(35)	2.0(4)	C(43)-C(42)-C(51)-N(32)	-169.4(3)
C(38)-C(39)-C(40)-C(31)	-179.8(3)	C(48)-C(49)-C(52)-C(54)	-68.4(4)
C(32)-C(31)-C(40)-C(35)	2.9(4)	C(50)-C(49)-C(52)-C(54)	107.9(4)
C(01)-C(31)-C(40)-C(35)	179.5(3)	C(48)-C(49)-C(52)-C(53)	57.2(4)
C(32)-C(31)-C(40)-C(39)	-175.3(3)	C(50)-C(49)-C(52)-C(53)	-126.5(4)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R,R*)-**75**·py.

Identification code	(*R,R*)-**75**·py	
Empirical formula	C53.50 H44.50 N3.50 O3 Zn	
Formula weight	849.80	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P6(5)	
Unit cell dimensions	a = 26.3597(6) Å	α= 90°.
	b = 26.3597(6) Å	β= 90°.
	c = 10.2518(5) Å	γ = 120°.
Volume	6169.0(4) $Å^3$	
Z	6	
Density (calculated)	1.372 g/cm^3	
Absorption coefficient	0.649 mm^{-1}	
F(000)	2664	
Crystal size	0.44 x 0.24 x 0.22 mm^3	
Theta range for data collection	0.89 to 30.10°.	
Index ranges	-37<=h<=37, -36<=k<=36, -14<=l<=14	
Reflections collected	71849	
Independent reflections	12068 [R(int) = 0.0304]	
Completeness to theta = 30.10°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.800	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12068 / 8 / 527	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0996	
R indices (all data)	R1 = 0.0395, wR2 = 0.1016	
Absolute structure parameter	-0.003(6)	
Largest diff. peak and hole	0.580 and -0.444 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-**75**·py. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1S)	1634(3)	1532(3)	2486(8)	100(2)
C(1S)	1965(5)	1234(5)	2230(11)	101(3)
C(2S)	2064(3)	940(3)	3386(7)	61(2)
O(2S)	-222(8)	146(8)	2081(17)	200
C(3S)	215(11)	289(8)	1090(30)	200
C(4S)	433(10)	-120(11)	770(20)	200
C(41)	2404(6)	1417(6)	2207(18)	204(4)
C(42)	2463(6)	1032(8)	3032(16)	204(4)
C(43)	1997(8)	467(7)	3208(16)	204(4)
C(44)	1471(6)	287(6)	2560(20)	204(4)
C(45)	1411(6)	673(9)	1735(18)	204(4)

C(46)	1878(8)	1238(8)	1559(16)	204(4)
N(42)	2463(6)	1032(8)	3032(16)	204(4)
N(43)	1997(8)	467(7)	3208(16)	204(4)
N(44)	1471(6)	287(6)	2560(20)	204(4)
Zn(1)	2447(1)	3829(1)	5933(1)	17(1)
C(11)	2881(1)	3090(1)	4854(2)	21(1)
C(12)	2868(1)	2531(1)	4434(2)	27(1)
C(13)	3485(1)	2657(1)	4133(2)	30(1)
C(14)	3900(1)	2942(1)	5287(2)	30(1)
C(15)	3902(1)	3497(1)	5733(2)	27(1)
C(16)	3277(1)	3356(1)	6059(2)	21(1)
N(21)	2488(1)	4253(1)	4143(2)	19(1)
C(22)	2612(1)	4815(1)	4135(2)	22(1)
C(23)	2624(1)	5103(1)	2990(2)	26(1)
C(24)	2503(1)	4806(1)	1817(2)	25(1)
C(25)	2379(1)	4229(1)	1826(2)	25(1)
C(26)	2377(1)	3970(1)	2998(2)	23(1)
C(101)	605(1)	2712(1)	6735(2)	20(1)
C(102)	1190(1)	2892(1)	6246(2)	20(1)
O(102)	1619(1)	3412(1)	6500(1)	22(1)
C(103)	1267(1)	2479(1)	5494(2)	22(1)
C(104)	785(1)	1920(1)	5207(2)	25(1)
C(105)	229(1)	1764(1)	5595(2)	26(1)
C(106)	132(1)	2159(1)	6351(2)	23(1)
C(107)	-461(1)	1990(1)	6690(2)	27(1)
C(108)	-583(1)	2345(1)	7396(2)	29(1)
C(109)	-124(1)	2891(1)	7910(2)	24(1)
C(110)	-266(1)	3228(1)	8708(2)	26(1)
C(111)	162(1)	3744(1)	9279(2)	23(1)
C(112)	23(1)	4094(1)	10105(2)	27(1)
C(113)	459(1)	4594(1)	10675(2)	29(1)
C(114)	1057(1)	4765(1)	10468(2)	27(1)
C(115)	1201(1)	4438(1)	9675(2)	24(1)
C(116)	761(1)	3925(1)	9039(2)	21(1)
C(117)	907(1)	3595(1)	8195(2)	20(1)
C(118)	481(1)	3078(1)	7599(2)	20(1)
C(119)	1832(1)	2570(1)	5075(2)	22(1)
N(119)	2319(1)	3050(1)	5166(2)	21(1)
C(201)	3124(1)	5288(1)	8610(2)	18(1)
C(202)	3101(1)	4810(1)	7871(2)	18(1)
O(202)	2698(1)	4542(1)	7005(1)	23(1)
C(203)	3535(1)	4645(1)	8127(2)	21(1)
C(204)	3966(1)	4943(1)	9093(2)	25(1)
C(205)	3991(1)	5396(1)	9786(2)	26(1)
C(206)	3575(1)	5574(1)	9559(2)	22(1)
C(207)	3600(1)	6044(1)	10328(2)	24(1)
C(208)	3205(1)	6221(1)	10196(2)	23(1)
C(209)	2738(1)	5948(1)	9258(2)	19(1)
C(210)	2324(1)	6128(1)	9168(2)	20(1)
C(211)	1856(1)	5870(1)	8279(2)	19(1)
C(212)	1397(1)	6010(1)	8258(2)	22(1)
C(213)	940(1)	5729(1)	7408(2)	24(1)
C(214)	915(1)	5301(1)	6522(2)	24(1)
C(215)	1351(1)	5162(1)	6525(2)	22(1)

C(216)	1829(1)	5435(1)	7417(2)	18(1)
C(217)	2248(1)	5255(1)	7501(2)	17(1)
C(218)	2699(1)	5487(1)	8427(2)	17(1)
C(219)	3552(1)	4168(1)	7471(2)	22(1)
N(219)	3227(1)	3860(1)	6520(2)	21(1)

Table 3. Bond lengths [Å] and angles [°] for (*R,R*)-**75**·py.

O(1S)-C(1S)	1.461(10)	C(14)-C(15)	1.530(3)
C(1S)-C(2S)	1.508(10)	C(14)-H(14A)	0.9900
C(1S)-H(1A)	0.9900	C(14)-H(14B)	0.9900
C(1S)-H(1B)	0.9900	C(15)-C(16)	1.534(2)
C(2S)-H(2A)	0.9800	C(15)-H(15A)	0.9900
C(2S)-H(2B)	0.9800	C(15)-H(15B)	0.9900
C(2S)-H(2C)	0.9800	C(16)-N(219)	1.478(2)
O(2S)-C(3S)	1.435(13)	C(16)-H(16)	1.0000
C(3S)-C(4S)	1.491(13)	N(21)-C(26)	1.343(2)
C(3S)-H(3A)	0.9900	N(21)-C(22)	1.346(2)
C(3S)-H(3B)	0.9900	C(22)-C(23)	1.390(3)
C(4S)-H(4A)	0.9800	C(22)-H(22)	0.9500
C(4S)-H(4B)	0.9800	C(23)-C(24)	1.383(3)
C(4S)-H(4C)	0.9800	C(23)-H(23)	0.9500
C(41)-C(42)	1.3900	C(24)-C(25)	1.384(3)
C(41)-C(46)	1.3900	C(24)-H(24)	0.9500
C(41)-H(41)	0.9500	C(25)-C(26)	1.383(3)
C(42)-C(43)	1.3900	C(25)-H(25)	0.9500
C(42)-H(42)	0.9500	C(26)-H(26)	0.9500
C(43)-C(44)	1.3900	C(101)-C(106)	1.420(3)
C(43)-H(43)	0.9500	C(101)-C(102)	1.456(2)
C(44)-C(45)	1.3900	C(101)-C(118)	1.463(2)
C(44)-H(44)	0.9500	C(102)-O(102)	1.294(2)
C(45)-C(46)	1.3900	C(102)-C(103)	1.431(2)
C(45)-H(45)	0.9500	C(103)-C(104)	1.414(3)
C(46)-H(46)	0.9500	C(103)-C(119)	1.451(2)
Zn(1)-O(102)	1.9784(13)	C(104)-C(105)	1.369(3)
Zn(1)-O(202)	1.9839(13)	C(104)-H(104)	0.9500
Zn(1)-N(119)	2.0631(16)	C(105)-C(106)	1.418(3)
Zn(1)-N(219)	2.1046(15)	C(105)-H(105)	0.9500
Zn(1)-N(21)	2.1233(16)	C(106)-C(107)	1.438(3)
C(11)-N(119)	1.465(2)	C(107)-C(108)	1.343(3)
C(11)-C(12)	1.520(3)	C(107)-H(107)	0.9500
C(11)-C(16)	1.542(3)	C(108)-C(109)	1.438(3)
C(11)-H(11)	1.0000	C(108)-H(108)	0.9500
C(12)-C(13)	1.520(3)	C(109)-C(110)	1.389(3)
C(12)-H(12A)	0.9900	C(109)-C(118)	1.451(2)
C(12)-H(12B)	0.9900	C(110)-C(111)	1.389(3)
C(13)-C(14)	1.529(3)	C(110)-H(110)	0.9500
C(13)-H(13A)	0.9900	C(111)-C(116)	1.425(2)
C(13)-H(13B)	0.9900	C(111)-C(112)	1.429(3)

C(112)-C(113)	1.372(3)
C(112)-H(112)	0.9500
C(113)-C(114)	1.421(3)
C(113)-H(113)	0.9500
C(114)-C(115)	1.371(3)
C(114)-H(114)	0.9500
C(115)-C(116)	1.424(3)
C(115)-H(115)	0.9500
C(116)-C(117)	1.410(2)
C(117)-C(118)	1.400(2)
C(117)-H(117)	0.9500
C(119)-N(119)	1.278(2)
C(119)-H(119)	0.9500
C(201)-C(206)	1.425(2)
C(201)-C(202)	1.446(2)
C(201)-C(218)	1.467(2)
C(202)-O(202)	1.290(2)
C(202)-C(203)	1.435(2)
C(203)-C(204)	1.413(3)
C(203)-C(219)	1.447(3)
C(204)-C(205)	1.363(3)
C(204)-H(204)	0.9500
C(205)-C(206)	1.410(3)
C(205)-H(205)	0.9500
C(206)-C(207)	1.441(3)
C(207)-C(208)	1.345(3)
C(207)-H(207)	0.9500
C(208)-C(209)	1.439(2)
C(208)-H(208)	0.9500
C(209)-C(210)	1.394(2)
C(209)-C(218)	1.445(2)
C(210)-C(211)	1.405(2)
C(210)-H(210)	0.9500
C(211)-C(216)	1.421(2)
C(211)-C(212)	1.430(2)
C(212)-C(213)	1.367(3)
C(212)-H(212)	0.9500
C(213)-C(214)	1.423(3)
C(213)-H(213)	0.9500
C(214)-C(215)	1.369(2)
C(214)-H(214)	0.9500
C(215)-C(216)	1.426(2)
C(215)-H(215)	0.9500
C(216)-C(217)	1.406(2)
C(217)-C(218)	1.402(2)
C(217)-H(217)	0.9500
C(219)-N(219)	1.283(2)
C(219)-H(219)	0.9500

O(1S)-C(1S)-C(2S)	116.0(8)
O(1S)-C(1S)-H(1A)	108.3
C(2S)-C(1S)-H(1A)	108.3
O(1S)-C(1S)-H(1B)	108.3
C(2S)-C(1S)-H(1B)	108.3
H(1A)-C(1S)-H(1B)	107.4
C(1S)-C(2S)-H(2A)	109.5
C(1S)-C(2S)-H(2B)	109.5
H(2A)-C(2S)-H(2B)	109.5
C(1S)-C(2S)-H(2C)	109.5
H(2A)-C(2S)-H(2C)	109.5
H(2B)-C(2S)-H(2C)	109.5
O(2S)-C(3S)-C(4S)	120.9(15)
O(2S)-C(3S)-H(3A)	107.1
C(4S)-C(3S)-H(3A)	107.1
O(2S)-C(3S)-H(3B)	107.1
C(4S)-C(3S)-H(3B)	107.1
H(3A)-C(3S)-H(3B)	106.8
C(3S)-C(4S)-H(4A)	109.5
C(3S)-C(4S)-H(4B)	109.5
H(4A)-C(4S)-H(4B)	109.5
C(3S)-C(4S)-H(4C)	109.5
H(4A)-C(4S)-H(4C)	109.5
H(4B)-C(4S)-H(4C)	109.5
C(42)-C(41)-C(46)	120.0
C(42)-C(41)-H(41)	120.0
C(46)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	120.0
C(41)-C(42)-H(42)	120.0
C(43)-C(42)-H(42)	120.0
C(44)-C(43)-C(42)	120.0
C(44)-C(43)-H(43)	120.0
C(42)-C(43)-H(43)	120.0
C(43)-C(44)-C(45)	120.0
C(43)-C(44)-H(44)	120.0
C(45)-C(44)-H(44)	120.0
C(46)-C(45)-C(44)	120.0
C(46)-C(45)-H(45)	120.0
C(44)-C(45)-H(45)	120.0
C(45)-C(46)-C(41)	120.0
C(45)-C(46)-H(46)	120.0
C(41)-C(46)-H(46)	120.0
O(102)-Zn(1)-O(202)	96.66(6)
O(102)-Zn(1)-N(119)	88.51(6)
O(202)-Zn(1)-N(119)	164.81(6)
O(102)-Zn(1)-N(219)	136.33(6)
O(202)-Zn(1)-N(219)	86.97(6)
N(119)-Zn(1)-N(219)	79.52(6)
O(102)-Zn(1)-N(21)	107.30(6)
O(202)-Zn(1)-N(21)	94.29(6)
N(119)-Zn(1)-N(21)	97.79(6)
N(219)-Zn(1)-N(21)	115.82(6)
N(119)-C(11)-C(12)	117.40(16)
N(119)-C(11)-C(16)	106.78(14)
C(12)-C(11)-C(16)	110.40(14)
N(119)-C(11)-H(11)	107.3
C(12)-C(11)-H(11)	107.3
C(16)-C(11)-H(11)	107.3
C(13)-C(12)-C(11)	110.04(17)

C(13)-C(12)-H(12A)	109.7	C(104)-C(103)-C(102)	120.60(17)
C(11)-C(12)-H(12A)	109.7	C(104)-C(103)-C(119)	115.14(16)
C(13)-C(12)-H(12B)	109.7	C(102)-C(103)-C(119)	124.04(17)
C(11)-C(12)-H(12B)	109.7	C(105)-C(104)-C(103)	121.51(18)
H(12A)-C(12)-H(12B)	108.2	C(105)-C(104)-H(104)	119.2
C(12)-C(13)-C(14)	112.00(17)	C(103)-C(104)-H(104)	119.2
C(12)-C(13)-H(13A)	109.2	C(104)-C(105)-C(106)	119.74(18)
C(14)-C(13)-H(13A)	109.2	C(104)-C(105)-H(105)	120.1
C(12)-C(13)-H(13B)	109.2	C(106)-C(105)-H(105)	120.1
C(14)-C(13)-H(13B)	109.2	C(105)-C(106)-C(101)	121.21(17)
H(13A)-C(13)-H(13B)	107.9	C(105)-C(106)-C(107)	118.14(17)
C(13)-C(14)-C(15)	111.17(16)	C(101)-C(106)-C(107)	120.63(17)
C(13)-C(14)-H(14A)	109.4	C(108)-C(107)-C(106)	121.20(18)
C(15)-C(14)-H(14A)	109.4	C(108)-C(107)-H(107)	119.4
C(13)-C(14)-H(14B)	109.4	C(106)-C(107)-H(107)	119.4
C(15)-C(14)-H(14B)	109.4	C(107)-C(108)-C(109)	121.31(18)
H(14A)-C(14)-H(14B)	108.0	C(107)-C(108)-H(108)	119.3
C(14)-C(15)-C(16)	110.03(17)	C(109)-C(108)-H(108)	119.3
C(14)-C(15)-H(15A)	109.7	C(110)-C(109)-C(108)	119.71(17)
C(16)-C(15)-H(15A)	109.7	C(110)-C(109)-C(118)	120.85(17)
C(14)-C(15)-H(15B)	109.7	C(108)-C(109)-C(118)	119.43(17)
C(16)-C(15)-H(15B)	109.7	C(111)-C(110)-C(109)	121.91(17)
H(15A)-C(15)-H(15B)	108.2	C(111)-C(110)-H(110)	119.0
N(219)-C(16)-C(15)	114.79(16)	C(109)-C(110)-H(110)	119.0
N(219)-C(16)-C(11)	108.65(13)	C(110)-C(111)-C(116)	118.45(17)
C(15)-C(16)-C(11)	109.76(15)	C(110)-C(111)-C(112)	122.56(17)
N(219)-C(16)-H(16)	107.8	C(116)-C(111)-C(112)	118.98(17)
C(15)-C(16)-H(16)	107.8	C(113)-C(112)-C(111)	120.71(18)
C(11)-C(16)-H(16)	107.8	C(113)-C(112)-H(112)	119.6
C(26)-N(21)-C(22)	118.22(16)	C(111)-C(112)-H(112)	119.6
C(26)-N(21)-Zn(1)	121.44(12)	C(112)-C(113)-C(114)	120.34(19)
C(22)-N(21)-Zn(1)	120.32(12)	C(112)-C(113)-H(113)	119.8
N(21)-C(22)-C(23)	122.15(17)	C(114)-C(113)-H(113)	119.8
N(21)-C(22)-H(22)	118.9	C(115)-C(114)-C(113)	120.04(19)
C(23)-C(22)-H(22)	118.9	C(115)-C(114)-H(114)	120.0
C(24)-C(23)-C(22)	119.31(18)	C(113)-C(114)-H(114)	120.0
C(24)-C(23)-H(23)	120.3	C(114)-C(115)-C(116)	121.26(18)
C(22)-C(23)-H(23)	120.3	C(114)-C(115)-H(115)	119.4
C(23)-C(24)-C(25)	118.48(17)	C(116)-C(115)-H(115)	119.4
C(23)-C(24)-H(24)	120.8	C(117)-C(116)-C(115)	121.55(16)
C(25)-C(24)-H(24)	120.8	C(117)-C(116)-C(111)	119.83(16)
C(26)-C(25)-C(24)	119.29(18)	C(115)-C(116)-C(111)	118.62(16)
C(26)-C(25)-H(25)	120.4	C(118)-C(117)-C(116)	122.37(16)
C(24)-C(25)-H(25)	120.4	C(118)-C(117)-H(117)	118.8
N(21)-C(26)-C(25)	122.54(18)	C(116)-C(117)-H(117)	118.8
N(21)-C(26)-H(26)	118.7	C(117)-C(118)-C(109)	116.48(16)
C(25)-C(26)-H(26)	118.7	C(117)-C(118)-C(101)	124.90(15)
C(106)-C(101)-C(102)	118.81(16)	C(109)-C(118)-C(101)	118.59(16)
C(106)-C(101)-C(118)	118.40(16)	N(119)-C(119)-C(103)	125.57(17)
C(102)-C(101)-C(118)	122.79(16)	N(119)-C(119)-H(119)	117.2
O(102)-C(102)-C(103)	122.23(16)	C(103)-C(119)-H(119)	117.2
O(102)-C(102)-C(101)	119.90(16)	C(119)-N(119)-C(11)	122.24(16)
C(103)-C(102)-C(101)	117.86(16)	C(119)-N(119)-Zn(1)	126.65(13)
C(102)-O(102)-Zn(1)	131.76(12)	C(11)-N(119)-Zn(1)	110.79(12)

C(206)-C(201)-C(202)	118.62(15)	C(210)-C(211)-C(216)	118.19(15)
C(206)-C(201)-C(218)	118.73(16)	C(210)-C(211)-C(212)	122.42(16)
C(202)-C(201)-C(218)	122.65(14)	C(216)-C(211)-C(212)	119.32(16)
O(202)-C(202)-C(203)	121.55(16)	C(213)-C(212)-C(211)	120.07(16)
O(202)-C(202)-C(201)	120.03(15)	C(213)-C(212)-H(212)	120.0
C(203)-C(202)-C(201)	118.42(15)	C(211)-C(212)-H(212)	120.0
C(202)-O(202)-Zn(1)	133.88(12)	C(212)-C(213)-C(214)	120.91(17)
C(204)-C(203)-C(202)	120.08(17)	C(212)-C(213)-H(213)	119.5
C(204)-C(203)-C(219)	116.33(16)	C(214)-C(213)-H(213)	119.5
C(202)-C(203)-C(219)	123.56(16)	C(215)-C(214)-C(213)	119.95(17)
C(205)-C(204)-C(203)	121.59(17)	C(215)-C(214)-H(214)	120.0
C(205)-C(204)-H(204)	119.2	C(213)-C(214)-H(214)	120.0
C(203)-C(204)-H(204)	119.2	C(214)-C(215)-C(216)	120.90(17)
C(204)-C(205)-C(206)	120.11(17)	C(214)-C(215)-H(215)	119.6
C(204)-C(205)-H(205)	119.9	C(216)-C(215)-H(215)	119.6
C(206)-C(205)-H(205)	119.9	C(217)-C(216)-C(211)	120.17(15)
C(205)-C(206)-C(201)	121.16(17)	C(217)-C(216)-C(215)	120.91(16)
C(205)-C(206)-C(207)	119.02(16)	C(211)-C(216)-C(215)	118.81(16)
C(201)-C(206)-C(207)	119.79(17)	C(218)-C(217)-C(216)	122.26(15)
C(208)-C(207)-C(206)	122.13(17)	C(218)-C(217)-H(217)	118.9
C(208)-C(207)-H(207)	118.9	C(216)-C(217)-H(217)	118.9
C(206)-C(207)-H(207)	118.9	C(217)-C(218)-C(209)	116.96(15)
C(207)-C(208)-C(209)	120.77(17)	C(217)-C(218)-C(201)	124.32(15)
C(207)-C(208)-H(208)	119.6	C(209)-C(218)-C(201)	118.72(15)
C(209)-C(208)-H(208)	119.6	N(219)-C(219)-C(203)	127.02(16)
C(210)-C(209)-C(208)	119.58(16)	N(219)-C(219)-H(219)	116.5
C(210)-C(209)-C(218)	120.63(15)	C(203)-C(219)-H(219)	116.5
C(208)-C(209)-C(218)	119.79(15)	C(219)-N(219)-C(16)	118.68(15)
C(209)-C(210)-C(211)	121.67(16)	C(219)-N(219)-Zn(1)	124.91(12)
C(209)-C(210)-H(210)	119.2	C(16)-N(219)-Zn(1)	113.46(11)
C(211)-C(210)-H(210)	119.2		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R,R*)-**75**·py. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	17(1)	20(1)	18(1)	-1(1)	-1(1)	12(1)
C(11)	23(1)	26(1)	21(1)	3(1)	3(1)	17(1)
C(12)	29(1)	27(1)	31(1)	1(1)	5(1)	19(1)
C(13)	35(1)	36(1)	32(1)	2(1)	7(1)	27(1)
C(14)	32(1)	39(1)	35(1)	5(1)	5(1)	29(1)
C(15)	24(1)	34(1)	33(1)	2(1)	1(1)	21(1)
C(16)	24(1)	25(1)	22(1)	4(1)	1(1)	18(1)
N(21)	17(1)	23(1)	20(1)	1(1)	1(1)	12(1)
C(22)	21(1)	22(1)	22(1)	-1(1)	0(1)	11(1)
C(23)	26(1)	23(1)	26(1)	5(1)	2(1)	11(1)
C(24)	21(1)	30(1)	23(1)	7(1)	3(1)	11(1)

C(25)	24(1)	33(1)	20(1)	-3(1)	-1(1)	17(1)
C(26)	25(1)	27(1)	22(1)	-2(1)	-1(1)	17(1)
C(101)	19(1)	23(1)	20(1)	2(1)	-1(1)	11(1)
C(102)	19(1)	23(1)	19(1)	2(1)	-2(1)	13(1)
O(102)	17(1)	22(1)	26(1)	-2(1)	1(1)	9(1)
C(103)	21(1)	23(1)	24(1)	0(1)	-2(1)	13(1)
C(104)	28(1)	23(1)	26(1)	-2(1)	-5(1)	14(1)
C(105)	23(1)	23(1)	28(1)	-3(1)	-5(1)	10(1)
C(106)	21(1)	25(1)	20(1)	1(1)	-2(1)	11(1)
C(107)	19(1)	30(1)	24(1)	-3(1)	-3(1)	6(1)
C(108)	16(1)	37(1)	27(1)	-2(1)	0(1)	8(1)
C(109)	19(1)	31(1)	21(1)	0(1)	-1(1)	12(1)
C(110)	17(1)	35(1)	24(1)	1(1)	2(1)	12(1)
C(111)	22(1)	30(1)	18(1)	2(1)	3(1)	15(1)
C(112)	25(1)	36(1)	24(1)	1(1)	4(1)	17(1)
C(113)	32(1)	31(1)	26(1)	2(1)	7(1)	17(1)
C(114)	30(1)	22(1)	26(1)	1(1)	6(1)	11(1)
C(115)	21(1)	24(1)	22(1)	3(1)	6(1)	9(1)
C(116)	21(1)	23(1)	18(1)	3(1)	3(1)	11(1)
C(117)	18(1)	23(1)	18(1)	2(1)	2(1)	10(1)
C(118)	17(1)	26(1)	17(1)	2(1)	0(1)	11(1)
C(119)	26(1)	24(1)	22(1)	0(1)	-1(1)	17(1)
N(119)	23(1)	26(1)	22(1)	1(1)	1(1)	17(1)
C(201)	15(1)	19(1)	14(1)	3(1)	0(1)	6(1)
C(202)	15(1)	21(1)	17(1)	1(1)	0(1)	9(1)
O(202)	23(1)	28(1)	21(1)	-6(1)	-6(1)	17(1)
C(203)	18(1)	24(1)	20(1)	3(1)	0(1)	12(1)
C(204)	19(1)	31(1)	25(1)	2(1)	-3(1)	13(1)
C(205)	19(1)	30(1)	25(1)	-1(1)	-7(1)	11(1)
C(206)	17(1)	22(1)	21(1)	0(1)	-2(1)	6(1)
C(207)	21(1)	25(1)	20(1)	-4(1)	-5(1)	6(1)
C(208)	23(1)	21(1)	20(1)	-4(1)	-2(1)	7(1)
C(209)	18(1)	18(1)	16(1)	1(1)	2(1)	6(1)
C(210)	22(1)	19(1)	18(1)	-3(1)	1(1)	9(1)
C(211)	21(1)	17(1)	19(1)	2(1)	2(1)	9(1)
C(212)	26(1)	22(1)	22(1)	-1(1)	2(1)	15(1)
C(213)	26(1)	27(1)	26(1)	1(1)	1(1)	18(1)
C(214)	24(1)	26(1)	25(1)	-4(1)	-5(1)	15(1)
C(215)	23(1)	22(1)	24(1)	-3(1)	-4(1)	13(1)
C(216)	19(1)	18(1)	16(1)	2(1)	1(1)	9(1)
C(217)	17(1)	17(1)	16(1)	-1(1)	1(1)	8(1)
C(218)	15(1)	17(1)	16(1)	1(1)	2(1)	6(1)
C(219)	20(1)	28(1)	23(1)	3(1)	0(1)	15(1)
N(219)	22(1)	24(1)	23(1)	2(1)	2(1)	16(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R,R*)-**75**·py.

	x	y	z	U(eq)
H(1A)	2352	1523	1869	122
H(1B)	1756	934	1549	122
H(2A)	2281	746	3107	91
H(2B)	1685	648	3751	91
H(2C)	2290	1234	4052	91
H(3A)	560	667	1345	240
H(3B)	60	360	277	240
H(4A)	777	77	205	300
H(4B)	124	-466	327	300
H(4C)	542	-242	1581	300
H(41)	2723	1803	2086	244
H(42)	2823	1154	3475	244
H(43)	2037	203	3772	244
H(44)	1152	-99	2681	244
H(45)	1052	551	1292	244
H(46)	1838	1502	995	244
H(11)	3061	3378	4125	26
H(12A)	2697	2236	5139	32
H(12B)	2619	2369	3650	32
H(13A)	3637	2921	3368	36
H(13B)	3473	2287	3906	36
H(14A)	4302	3042	5031	36
H(14B)	3776	2661	6020	36
H(15A)	4065	3796	5033	33
H(15B)	4154	3660	6514	33
H(16)	3124	3053	6764	25
H(22)	2693	5020	4939	26
H(23)	2715	5500	3013	31
H(24)	2506	4993	1023	30
H(25)	2295	4015	1034	30
H(26)	2294	3575	2995	28
H(104)	848	1647	4735	30
H(105)	-92	1393	5359	31
H(107)	-771	1621	6411	33
H(108)	-980	2234	7558	35
H(110)	-667	3102	8868	31
H(112)	-375	3980	10262	33
H(113)	361	4826	11210	35
H(114)	1357	5107	10880	32
H(115)	1602	4555	9547	28
H(117)	1308	3728	8023	24
H(119)	1841	2244	4701	26
H(204)	4246	4825	9264	30
H(205)	4288	5593	10423	31
H(207)	3906	6235	10948	29
H(208)	3234	6529	10727	28
H(210)	2358	6433	9722	24
H(212)	1410	6298	8835	27

H(213)	633	5820	7408	29
H(214)	597	5113	5929	29
H(215)	1334	4880	5925	27
H(217)	2224	4966	6911	21
H(219)	3833	4071	7778	26

Table 6. Torsion angles [°] for (*R,R*)-**75**·py.

C(46)-C(41)-C(42)-C(43)	0.0	N(219)-Zn(1)-O(102)-C(102)	-82.94(17)
C(41)-C(42)-C(43)-C(44)	0.0	N(21)-Zn(1)-O(102)-C(102)	87.85(16)
C(42)-C(43)-C(44)-C(45)	0.0	O(102)-C(102)-C(103)-C(104)	-178.32(17)
C(43)-C(44)-C(45)-C(46)	0.0	C(101)-C(102)-C(103)-C(104)	1.8(3)
C(44)-C(45)-C(46)-C(41)	0.0	O(102)-C(102)-C(103)-C(119)	7.4(3)
C(42)-C(41)-C(46)-C(45)	0.0	C(101)-C(102)-C(103)-C(119)	-172.42(17)
N(119)-C(11)-C(12)-C(13)	179.19(16)	C(102)-C(103)-C(104)-C(105)	2.4(3)
C(16)-C(11)-C(12)-C(13)	-58.2(2)	C(119)-C(103)-C(104)-C(105)	177.12(18)
C(11)-C(12)-C(13)-C(14)	56.0(2)	C(103)-C(104)-C(105)-C(106)	-2.8(3)
C(12)-C(13)-C(14)-C(15)	-55.2(2)	C(104)-C(105)-C(106)-C(101)	-1.1(3)
C(13)-C(14)-C(15)-C(16)	55.8(2)	C(104)-C(105)-C(106)-C(107)	177.27(18)
C(14)-C(15)-C(16)-N(219)	179.23(16)	C(102)-C(101)-C(106)-C(105)	5.2(3)
C(14)-C(15)-C(16)-C(11)	-58.1(2)	C(118)-C(101)-C(106)-C(105)	-175.24(17)
N(119)-C(11)-C(16)-N(219)	-45.30(18)	C(102)-C(101)-C(106)-C(107)	-173.07(17)
C(12)-C(11)-C(16)-N(219)	-173.97(15)	C(118)-C(101)-C(106)-C(107)	6.5(3)
N(119)-C(11)-C(16)-C(15)	-171.55(14)	C(105)-C(106)-C(107)-C(108)	-179.51(19)
C(12)-C(11)-C(16)-C(15)	59.78(19)	C(101)-C(106)-C(107)-C(108)	-1.2(3)
O(102)-Zn(1)-N(21)-C(26)	-84.40(14)	C(106)-C(107)-C(108)-C(109)	-4.0(3)
O(202)-Zn(1)-N(21)-C(26)	177.24(14)	C(107)-C(108)-C(109)-C(110)	-175.7(2)
N(119)-Zn(1)-N(21)-C(26)	6.46(14)	C(107)-C(108)-C(109)-C(118)	3.6(3)
N(219)-Zn(1)-N(21)-C(26)	88.54(14)	C(108)-C(109)-C(110)-C(111)	176.86(19)
O(102)-Zn(1)-N(21)-C(22)	93.89(13)	C(118)-C(109)-C(110)-C(111)	-2.4(3)
O(202)-Zn(1)-N(21)-C(22)	-4.47(13)	C(109)-C(110)-C(111)-C(116)	-0.5(3)
N(119)-Zn(1)-N(21)-C(22)	-175.25(13)	C(109)-C(110)-C(111)-C(112)	-179.82(19)
N(219)-Zn(1)-N(21)-C(22)	-93.17(13)	C(110)-C(111)-C(112)-C(113)	178.5(2)
C(26)-N(21)-C(22)-C(23)	0.4(3)	C(116)-C(111)-C(112)-C(113)	-0.9(3)
Zn(1)-N(21)-C(22)-C(23)	-177.93(14)	C(111)-C(112)-C(113)-C(114)	-1.0(3)
N(21)-C(22)-C(23)-C(24)	0.3(3)	C(112)-C(113)-C(114)-C(115)	1.3(3)
C(22)-C(23)-C(24)-C(25)	-0.6(3)	C(113)-C(114)-C(115)-C(116)	0.3(3)
C(23)-C(24)-C(25)-C(26)	0.2(3)	C(114)-C(115)-C(116)-C(117)	178.25(18)
C(22)-N(21)-C(26)-C(25)	-0.9(3)	C(114)-C(115)-C(116)-C(111)	-2.2(3)
Zn(1)-N(21)-C(26)-C(25)	177.47(14)	C(110)-C(111)-C(116)-C(117)	2.6(3)
C(24)-C(25)-C(26)-N(21)	0.6(3)	C(112)-C(111)-C(116)-C(117)	-178.00(17)
C(106)-C(101)-C(102)-O(102)	174.67(16)	C(110)-C(111)-C(116)-C(115)	-176.90(18)
C(118)-C(101)-C(102)-O(102)	-4.8(3)	C(112)-C(111)-C(116)-C(115)	2.5(3)
C(106)-C(101)-C(102)-C(103)	-5.5(2)	C(115)-C(116)-C(117)-C(118)	177.59(17)
C(118)-C(101)-C(102)-C(103)	174.99(16)	C(111)-C(116)-C(117)-C(118)	-1.9(3)
C(103)-C(102)-O(102)-Zn(1)	4.5(3)	C(116)-C(117)-C(118)-C(109)	-0.9(3)
C(101)-C(102)-O(102)-Zn(1)	-175.69(12)	C(116)-C(117)-C(118)-C(101)	-178.78(17)
O(202)-Zn(1)-O(102)-C(102)	-175.53(16)	C(110)-C(109)-C(118)-C(117)	3.0(3)
N(119)-Zn(1)-O(102)-C(102)	-9.85(16)	C(108)-C(109)-C(118)-C(117)	-176.23(18)

C(110)-C(109)-C(118)-C(101)	-178.91(18)	C(206)-C(207)-C(208)-C(209)	-0.7(3)
C(108)-C(109)-C(118)-C(101)	1.8(3)	C(207)-C(208)-C(209)-C(210)	178.09(17)
C(106)-C(101)-C(118)-C(117)	171.21(17)	C(207)-C(208)-C(209)-C(218)	-1.4(3)
C(102)-C(101)-C(118)-C(117)	-9.3(3)	C(208)-C(209)-C(210)-C(211)	-179.25(16)
C(106)-C(101)-C(118)-C(109)	-6.7(2)	C(218)-C(209)-C(210)-C(211)	0.3(3)
C(102)-C(101)-C(118)-C(109)	172.86(16)	C(209)-C(210)-C(211)-C(216)	-3.0(3)
C(104)-C(103)-C(119)-N(119)	175.70(18)	C(209)-C(210)-C(211)-C(212)	173.93(17)
C(102)-C(103)-C(119)-N(119)	-9.7(3)	C(210)-C(211)-C(212)-C(213)	-177.34(17)
C(103)-C(119)-N(119)-C(11)	173.11(17)	C(216)-C(211)-C(212)-C(213)	-0.4(3)
C(103)-C(119)-N(119)-Zn(1)	0.3(3)	C(211)-C(212)-C(213)-C(214)	-0.9(3)
C(12)-C(11)-N(119)-C(119)	-1.1(3)	C(212)-C(213)-C(214)-C(215)	0.8(3)
C(16)-C(11)-N(119)-C(119)	-125.59(19)	C(213)-C(214)-C(215)-C(216)	0.7(3)
C(12)-C(11)-N(119)-Zn(1)	172.75(13)	C(210)-C(211)-C(216)-C(217)	2.6(2)
C(16)-C(11)-N(119)-Zn(1)	48.25(16)	C(212)-C(211)-C(216)-C(217)	-174.42(16)
O(102)-Zn(1)-N(119)-C(119)	7.18(16)	C(210)-C(211)-C(216)-C(215)	178.88(16)
O(202)-Zn(1)-N(119)-C(119)	117.5(2)	C(212)-C(211)-C(216)-C(215)	1.9(2)
N(219)-Zn(1)-N(119)-C(119)	144.98(17)	C(214)-C(215)-C(216)-C(217)	174.25(18)
N(21)-Zn(1)-N(119)-C(119)	-100.08(16)	C(214)-C(215)-C(216)-C(211)	-2.0(3)
O(102)-Zn(1)-N(119)-C(11)	-166.33(12)	C(211)-C(216)-C(217)-C(218)	0.6(3)
O(202)-Zn(1)-N(119)-C(11)	-56.0(3)	C(215)-C(216)-C(217)-C(218)	-175.64(16)
N(219)-Zn(1)-N(119)-C(11)	-28.53(12)	C(216)-C(217)-C(218)-C(209)	-3.2(2)
N(21)-Zn(1)-N(119)-C(11)	86.41(12)	C(216)-C(217)-C(218)-C(201)	175.85(15)
C(206)-C(201)-C(202)-O(202)	-179.97(16)	C(210)-C(209)-C(218)-C(217)	2.8(2)
C(218)-C(201)-C(202)-O(202)	0.3(2)	C(208)-C(209)-C(218)-C(217)	-177.65(16)
C(206)-C(201)-C(202)-C(203)	0.0(2)	C(210)-C(209)-C(218)-C(201)	-176.30(15)
C(218)-C(201)-C(202)-C(203)	-179.75(15)	C(208)-C(209)-C(218)-C(201)	3.2(2)
C(203)-C(202)-O(202)-Zn(1)	8.1(3)	C(206)-C(201)-C(218)-C(217)	177.96(16)
C(201)-C(202)-O(202)-Zn(1)	-171.92(12)	C(202)-C(201)-C(218)-C(217)	-2.3(3)
O(102)-Zn(1)-O(202)-C(202)	123.90(17)	C(206)-C(201)-C(218)-C(209)	-3.0(2)
N(119)-Zn(1)-O(202)-C(202)	14.6(3)	C(202)-C(201)-C(218)-C(209)	176.75(15)
N(219)-Zn(1)-O(202)-C(202)	-12.41(17)	C(204)-C(203)-C(219)-N(219)	-175.79(18)
N(21)-Zn(1)-O(202)-C(202)	-128.10(17)	C(202)-C(203)-C(219)-N(219)	6.3(3)
O(202)-C(202)-C(203)-C(204)	-179.23(17)	C(203)-C(219)-N(219)-C(16)	-174.69(17)
C(201)-C(202)-C(203)-C(204)	0.8(2)	C(203)-C(219)-N(219)-Zn(1)	-15.4(3)
O(202)-C(202)-C(203)-C(219)	-1.4(3)	C(15)-C(16)-N(219)-C(219)	-52.4(2)
C(201)-C(202)-C(203)-C(219)	178.70(16)	C(11)-C(16)-N(219)-C(219)	-175.74(16)
C(202)-C(203)-C(204)-C(205)	-1.2(3)	C(15)-C(16)-N(219)-Zn(1)	146.03(13)
C(219)-C(203)-C(204)-C(205)	-179.27(18)	C(11)-C(16)-N(219)-Zn(1)	22.74(17)
C(203)-C(204)-C(205)-C(206)	0.8(3)	O(102)-Zn(1)-N(219)-C(219)	-81.42(17)
C(204)-C(205)-C(206)-C(201)	0.0(3)	O(202)-Zn(1)-N(219)-C(219)	15.06(16)
C(204)-C(205)-C(206)-C(207)	178.37(18)	N(119)-Zn(1)-N(219)-C(219)	-157.99(16)
C(202)-C(201)-C(206)-C(205)	-0.4(3)	N(21)-Zn(1)-N(219)-C(219)	108.36(15)
C(218)-C(201)-C(206)-C(205)	179.33(16)	O(102)-Zn(1)-N(219)-C(16)	78.77(14)
C(202)-C(201)-C(206)-C(207)	-178.74(16)	O(202)-Zn(1)-N(219)-C(16)	175.25(12)
C(218)-C(201)-C(206)-C(207)	1.0(2)	N(119)-Zn(1)-N(219)-C(16)	2.20(12)
C(205)-C(206)-C(207)-C(208)	-177.51(18)	N(21)-Zn(1)-N(219)-C(16)	-91.45(12)
C(201)-C(206)-C(207)-C(208)	0.9(3)		

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*,*R*)-**76**·py.

Identification code	(*R*,*R*)-**76**·py	
Empirical formula	C49 H37 Fe N3 O2	
Formula weight	755.67	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 10.7342(11) Å	α= 90°.
	b = 19.595(2) Å	β= 105.904(2)°.
	c = 17.7357(19) Å	γ = 90°.
Volume	3587.8(7) $Å^3$	
Z	4	
Density (calculated)	1.399 g/cm^3	
Absorption coefficient	0.468 mm^{-1}	
F(000)	1576	
Crystal size	0.33 x 0.18 x 0.09 mm^3	
Theta range for data collection	2.01 to 30.03°.	
Index ranges	-15<=h<=15, -27<=k<=27, -24<=l<=24	
Reflections collected	41757	
Independent reflections	20505 [R(int) = 0.0322]	
Completeness to theta = 30.03°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.833	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20505 / 1 / 991	
Goodness-of-fit on F^2	0.998	
Final R indices [I>2sigma(I)]	R1 = 0.0455, wR2 = 0.1107	
R indices (all data)	R1 = 0.0539, wR2 = 0.1159	
Absolute structure parameter	0.002(9)	
Largest diff. peak and hole	1.157 and -0.422 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*,*R*)-**76**·py. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6355(1)	749(1)	995(1)	20(1)
Fe(2)	8652(1)	1331(1)	9003(1)	19(1)
C(11)	5018(2)	239(1)	-642(1)	22(1)
C(12)	4988(3)	-86(1)	-1428(1)	27(1)
C(13)	3751(3)	125(1)	-2053(1)	33(1)
C(14)	3659(3)	901(1)	-2122(1)	34(1)
C(15)	3667(2)	1226(1)	-1334(1)	28(1)
C(16)	4895(2)	1018(1)	-714(1)	23(1)
C(31)	9448(2)	1590(1)	10757(1)	23(1)
C(32)	9771(3)	2087(2)	11441(2)	31(1)
C(33)	10740(3)	1756(2)	12148(1)	35(1)
C(34)	11969(2)	1540(1)	11950(1)	31(1)
C(35)	11666(2)	1048(1)	11261(1)	29(1)

C(36)	10678(2)	1352(1)	10552(1)	21(1)
N(21)	5152(2)	382(1)	1696(1)	25(1)
C(22)	4273(2)	-105(1)	1443(2)	25(1)
C(23)	3589(3)	-405(2)	1913(2)	31(1)
C(24)	3811(3)	-189(2)	2677(2)	33(1)
C(25)	4715(3)	321(2)	2949(2)	33(1)
C(26)	5356(3)	591(1)	2447(2)	27(1)
N(41)	9817(2)	1712(1)	8281(1)	23(1)
C(42)	10684(3)	2211(1)	8516(2)	28(1)
C(43)	11355(3)	2507(2)	8037(2)	31(1)
C(44)	11124(3)	2274(2)	7277(2)	34(1)
C(45)	10244(3)	1751(2)	7026(2)	33(1)
C(46)	9610(3)	1483(2)	7537(2)	31(1)
C(101)	9499(2)	-675(1)	1897(2)	21(1)
C(102)	8484(2)	-322(1)	1326(1)	19(1)
O(102)	7820(2)	166(1)	1541(1)	23(1)
C(103)	8203(2)	-526(1)	524(2)	21(1)
C(104)	9034(3)	-992(1)	287(2)	25(1)
C(105)	10053(3)	-1273(1)	811(2)	28(1)
C(106)	10287(2)	-1137(1)	1620(2)	25(1)
C(107)	11319(2)	-1499(1)	2161(2)	26(1)
C(108)	11620(3)	-1383(1)	2945(2)	27(1)
C(109)	10852(3)	-920(1)	3259(2)	24(1)
C(110)	11172(2)	-818(1)	4063(2)	25(1)
C(111)	10391(2)	-436(1)	4420(2)	23(1)
C(112)	10712(3)	-325(1)	5248(2)	27(1)
C(113)	9868(3)	9(1)	5570(2)	30(1)
C(114)	8686(3)	265(2)	5093(2)	31(1)
C(115)	8371(3)	184(1)	4297(2)	26(1)
C(116)	9224(2)	-158(1)	3932(2)	23(1)
C(117)	8950(2)	-223(1)	3112(1)	20(1)
C(118)	9742(2)	-587(1)	2746(2)	20(1)
C(119)	7072(2)	-307(1)	-70(1)	23(1)
N(119)	6178(2)	101(1)	25(1)	22(1)
C(201)	5853(2)	2541(1)	2243(1)	19(1)
C(202)	5698(2)	2099(1)	1572(1)	19(1)
O(202)	6565(2)	1634(1)	1556(1)	21(1)
C(203)	4599(2)	2195(1)	907(1)	20(1)
C(204)	3695(3)	2718(1)	916(2)	25(1)
C(205)	3820(3)	3122(1)	1557(2)	24(1)
C(206)	4895(2)	3043(1)	2217(2)	22(1)
C(207)	5007(3)	3501(1)	2872(2)	26(1)
C(208)	6025(3)	3460(1)	3516(2)	28(1)
C(209)	7025(3)	2966(1)	3575(2)	25(1)
C(210)	8049(3)	2937(1)	4248(2)	27(1)
C(211)	9035(3)	2458(1)	4362(2)	23(1)
C(212)	10102(3)	2431(1)	5052(2)	30(1)
C(213)	11033(3)	1941(2)	5131(2)	31(1)
C(214)	10969(3)	1462(1)	4524(2)	29(1)
C(215)	9962(2)	1480(1)	3858(1)	24(1)
C(216)	8974(2)	1977(1)	3750(1)	21(1)
C(217)	7944(2)	2000(1)	3060(1)	19(1)
C(218)	6953(2)	2486(1)	2946(1)	20(1)
C(219)	4413(2)	1822(1)	188(1)	20(1)

N(219)	5056(2)	1292(1)	82(1)	21(1)
C(301)	5495(2)	2752(1)	8042(1)	19(1)
C(302)	6489(2)	2396(1)	8630(1)	19(1)
O(302)	7156(2)	1907(1)	8438(1)	21(1)
C(303)	6705(2)	2589(1)	9432(1)	20(1)
C(304)	5904(2)	3079(1)	9649(2)	24(1)
C(305)	4903(2)	3384(1)	9102(2)	24(1)
C(306)	4713(2)	3236(1)	8301(2)	22(1)
C(307)	3687(2)	3585(1)	7743(2)	26(1)
C(308)	3414(3)	3458(1)	6978(2)	27(1)
C(309)	4166(2)	2981(1)	6672(2)	22(1)
C(310)	3859(3)	2859(1)	5872(2)	26(1)
C(311)	4628(3)	2456(1)	5527(2)	24(1)
C(312)	4334(3)	2333(1)	4708(2)	30(1)
C(313)	5146(3)	1966(1)	4396(2)	29(1)
C(314)	6319(3)	1708(1)	4894(2)	28(1)
C(315)	6616(3)	1792(1)	5684(2)	27(1)
C(316)	5784(2)	2169(1)	6037(2)	22(1)
C(317)	6055(2)	2256(1)	6854(2)	22(1)
C(318)	5264(2)	2642(1)	7194(2)	19(1)
C(319)	7674(2)	2287(1)	10067(1)	21(1)
N(319)	8551(2)	1849(1)	10018(1)	22(1)
C(401)	9196(2)	-498(1)	7841(2)	21(1)
C(402)	9379(2)	-37(1)	8499(1)	20(1)
O(402)	8512(2)	429(1)	8505(1)	22(1)
C(403)	10520(2)	-99(1)	9129(2)	24(1)
C(404)	11406(3)	-629(1)	9140(2)	26(1)
C(405)	11235(3)	-1074(1)	8525(2)	29(1)
C(406)	10151(3)	-1010(1)	7867(2)	25(1)
C(407)	10036(3)	-1464(1)	7219(2)	30(1)
C(408)	9034(3)	-1434(1)	6578(2)	29(1)
C(409)	8024(2)	-932(1)	6500(2)	23(1)
C(410)	7019(3)	-900(1)	5823(2)	27(1)
C(411)	6014(3)	-419(1)	5713(2)	23(1)
C(412)	4998(3)	-371(1)	5010(2)	29(1)
C(413)	4043(3)	104(2)	4945(2)	31(1)
C(414)	4062(3)	559(2)	5573(2)	31(1)
C(415)	5039(2)	530(1)	6249(2)	25(1)
C(416)	6055(2)	43(1)	6339(1)	20(1)
C(417)	7081(2)	15(1)	7030(1)	19(1)
C(418)	8092(2)	-458(1)	7140(1)	20(1)
C(419)	10843(2)	362(1)	9794(2)	24(1)
N(419)	10244(2)	917(1)	9855(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*,*R*)-**76**·py.

Fe(1)-O(102)	1.9704(17)	Fe(1)-N(219)	2.1132(19)
Fe(1)-O(202)	1.9817(17)	Fe(1)-N(21)	2.147(2)
Fe(1)-N(119)	2.105(2)	Fe(2)-O(402)	1.9642(17)

Fe(2)-O(302)	1.9930(16)	C(42)-H(42)	0.9500
Fe(2)-N(319)	2.095(2)	C(43)-C(44)	1.380(4)
Fe(2)-N(419)	2.1083(19)	C(43)-H(43)	0.9500
Fe(2)-N(41)	2.154(2)	C(44)-C(45)	1.382(4)
C(11)-N(119)	1.489(3)	C(44)-H(44)	0.9500
C(11)-C(12)	1.524(3)	C(45)-C(46)	1.379(4)
C(11)-C(16)	1.535(3)	C(45)-H(45)	0.9500
C(11)-H(11)	1.0000	C(46)-H(46)	0.9500
C(12)-C(13)	1.535(4)	C(101)-C(106)	1.416(3)
C(12)-H(12A)	0.9900	C(101)-C(102)	1.444(3)
C(12)-H(12B)	0.9900	C(101)-C(118)	1.466(3)
C(13)-C(14)	1.528(3)	C(102)-O(102)	1.310(3)
C(13)-H(13A)	0.9900	C(102)-C(103)	1.428(3)
C(13)-H(13B)	0.9900	C(103)-C(104)	1.418(3)
C(14)-C(15)	1.533(3)	C(103)-C(119)	1.437(3)
C(14)-H(14A)	0.9900	C(104)-C(105)	1.344(4)
C(14)-H(14B)	0.9900	C(104)-H(104)	0.9500
C(15)-C(16)	1.523(3)	C(105)-C(106)	1.414(4)
C(15)-H(15A)	0.9900	C(105)-H(105)	0.9500
C(15)-H(15B)	0.9900	C(106)-C(107)	1.438(4)
C(16)-N(219)	1.474(3)	C(107)-C(108)	1.358(4)
C(16)-H(16)	1.0000	C(107)-H(107)	0.9500
C(31)-N(319)	1.487(3)	C(108)-C(109)	1.436(4)
C(31)-C(32)	1.520(3)	C(108)-H(108)	0.9500
C(31)-C(36)	1.535(3)	C(109)-C(110)	1.386(4)
C(31)-H(31)	1.0000	C(109)-C(118)	1.441(3)
C(32)-C(33)	1.536(3)	C(110)-C(111)	1.399(4)
C(32)-H(32A)	0.9900	C(110)-H(110)	0.9500
C(32)-H(32B)	0.9900	C(111)-C(116)	1.422(4)
C(33)-C(34)	1.516(4)	C(111)-C(112)	1.430(4)
C(33)-H(33A)	0.9900	C(112)-C(113)	1.363(4)
C(33)-H(33B)	0.9900	C(112)-H(112)	0.9500
C(34)-C(35)	1.521(3)	C(113)-C(114)	1.410(4)
C(34)-H(34A)	0.9900	C(113)-H(113)	0.9500
C(34)-H(34B)	0.9900	C(114)-C(115)	1.369(4)
C(35)-C(36)	1.527(3)	C(114)-H(114)	0.9500
C(35)-H(35A)	0.9900	C(115)-C(116)	1.425(4)
C(35)-H(35B)	0.9900	C(115)-H(115)	0.9500
C(36)-N(419)	1.468(3)	C(116)-C(117)	1.408(3)
C(36)-H(36)	1.0000	C(117)-C(118)	1.398(3)
N(21)-C(22)	1.331(3)	C(117)-H(117)	0.9500
N(21)-C(26)	1.352(3)	C(119)-N(119)	1.295(3)
C(22)-C(23)	1.385(4)	C(119)-H(119)	0.9500
C(22)-H(22)	0.9500	C(201)-C(206)	1.415(3)
C(23)-C(24)	1.377(4)	C(201)-C(202)	1.444(3)
C(23)-H(23)	0.9500	C(201)-C(218)	1.467(3)
C(24)-C(25)	1.384(4)	C(202)-O(202)	1.309(3)
C(24)-H(24)	0.9500	C(202)-C(203)	1.433(3)
C(25)-C(26)	1.373(4)	C(203)-C(204)	1.413(3)
C(25)-H(25)	0.9500	C(203)-C(219)	1.437(3)
C(26)-H(26)	0.9500	C(204)-C(205)	1.362(4)
N(41)-C(42)	1.335(3)	C(204)-H(204)	0.9500
N(41)-C(46)	1.353(3)	C(205)-C(206)	1.409(4)
C(42)-C(43)	1.381(4)	C(205)-H(205)	0.9500

C(206)-C(207)	1.446(4)	C(316)-C(317)	1.408(3)
C(207)-C(208)	1.350(4)	C(317)-C(318)	1.392(3)
C(207)-H(207)	0.9500	C(317)-H(317)	0.9500
C(208)-C(209)	1.428(4)	C(319)-N(319)	1.294(3)
C(208)-H(208)	0.9500	C(319)-H(319)	0.9500
C(209)-C(210)	1.385(4)	C(401)-C(406)	1.425(3)
C(209)-C(218)	1.444(3)	C(401)-C(402)	1.446(3)
C(210)-C(211)	1.386(4)	C(401)-C(418)	1.466(3)
C(210)-H(210)	0.9500	C(402)-O(402)	1.306(3)
C(211)-C(216)	1.425(3)	C(402)-C(403)	1.419(4)
C(211)-C(212)	1.430(4)	C(403)-C(404)	1.405(3)
C(212)-C(213)	1.364(4)	C(403)-C(419)	1.449(4)
C(212)-H(212)	0.9500	C(404)-C(405)	1.368(4)
C(213)-C(214)	1.416(4)	C(404)-H(404)	0.9500
C(213)-H(213)	0.9500	C(405)-C(406)	1.410(4)
C(214)-C(215)	1.366(3)	C(405)-H(405)	0.9500
C(214)-H(214)	0.9500	C(406)-C(407)	1.433(4)
C(215)-C(216)	1.414(3)	C(407)-C(408)	1.334(4)
C(215)-H(215)	0.9500	C(407)-H(407)	0.9500
C(216)-C(217)	1.408(3)	C(408)-C(409)	1.443(4)
C(217)-C(218)	1.400(3)	C(408)-H(408)	0.9500
C(217)-H(217)	0.9500	C(409)-C(410)	1.378(4)
C(219)-N(219)	1.288(3)	C(409)-C(418)	1.453(3)
C(219)-H(219)	0.9500	C(410)-C(411)	1.406(4)
C(301)-C(306)	1.423(3)	C(410)-H(410)	0.9500
C(301)-C(302)	1.450(3)	C(411)-C(412)	1.417(4)
C(301)-C(318)	1.473(3)	C(411)-C(416)	1.423(3)
C(302)-O(302)	1.297(3)	C(412)-C(413)	1.366(4)
C(302)-C(303)	1.429(3)	C(412)-H(412)	0.9500
C(303)-C(304)	1.410(3)	C(413)-C(414)	1.423(4)
C(303)-C(319)	1.434(3)	C(413)-H(413)	0.9500
C(304)-C(305)	1.373(4)	C(414)-C(415)	1.361(4)
C(304)-H(304)	0.9500	C(414)-H(414)	0.9500
C(305)-C(306)	1.411(4)	C(415)-C(416)	1.424(3)
C(305)-H(305)	0.9500	C(415)-H(415)	0.9500
C(306)-C(307)	1.436(3)	C(416)-C(417)	1.407(3)
C(307)-C(308)	1.330(4)	C(417)-C(418)	1.398(3)
C(307)-H(307)	0.9500	C(417)-H(417)	0.9500
C(308)-C(309)	1.436(4)	C(419)-N(419)	1.284(3)
C(308)-H(308)	0.9500	C(419)-H(419)	0.9500
C(309)-C(310)	1.386(4)		
C(309)-C(318)	1.445(3)	O(102)-Fe(1)-O(202)	107.19(7)
C(310)-C(311)	1.399(4)	O(102)-Fe(1)-N(119)	86.16(7)
C(310)-H(310)	0.9500	O(202)-Fe(1)-N(119)	155.59(7)
C(311)-C(312)	1.420(4)	O(102)-Fe(1)-N(219)	159.92(7)
C(311)-C(316)	1.435(3)	O(202)-Fe(1)-N(219)	84.48(7)
C(312)-C(313)	1.360(4)	N(119)-Fe(1)-N(219)	77.54(7)
C(312)-H(312)	0.9500	O(102)-Fe(1)-N(21)	92.70(8)
C(313)-C(314)	1.418(4)	O(202)-Fe(1)-N(21)	90.38(8)
C(313)-H(313)	0.9500	N(119)-Fe(1)-N(21)	109.73(8)
C(314)-C(315)	1.359(4)	N(219)-Fe(1)-N(21)	103.73(8)
C(314)-H(314)	0.9500	O(402)-Fe(2)-O(302)	109.36(7)
C(315)-C(316)	1.428(3)	O(402)-Fe(2)-N(319)	143.84(8)
C(315)-H(315)	0.9500	O(302)-Fe(2)-N(319)	86.19(7)

O(402)-Fe(2)-N(419)	85.60(7)	H(32A)-C(32)-H(32B)	108.2
O(302)-Fe(2)-N(419)	163.94(7)	C(34)-C(33)-C(32)	111.4(2)
N(319)-Fe(2)-N(419)	78.07(8)	C(34)-C(33)-H(33A)	109.3
O(402)-Fe(2)-N(41)	91.69(8)	C(32)-C(33)-H(33A)	109.3
O(302)-Fe(2)-N(41)	91.37(7)	C(34)-C(33)-H(33B)	109.3
N(319)-Fe(2)-N(41)	121.21(8)	C(32)-C(33)-H(33B)	109.3
N(419)-Fe(2)-N(41)	94.05(8)	H(33A)-C(33)-H(33B)	108.0
N(119)-C(11)-C(12)	117.04(19)	C(33)-C(34)-C(35)	110.8(2)
N(119)-C(11)-C(16)	106.31(16)	C(33)-C(34)-H(34A)	109.5
C(12)-C(11)-C(16)	111.16(18)	C(35)-C(34)-H(34A)	109.5
N(119)-C(11)-H(11)	107.3	C(33)-C(34)-H(34B)	109.5
C(12)-C(11)-H(11)	107.3	C(35)-C(34)-H(34B)	109.5
C(16)-C(11)-H(11)	107.3	H(34A)-C(34)-H(34B)	108.1
C(11)-C(12)-C(13)	110.2(2)	C(34)-C(35)-C(36)	111.15(19)
C(11)-C(12)-H(12A)	109.6	C(34)-C(35)-H(35A)	109.4
C(13)-C(12)-H(12A)	109.6	C(36)-C(35)-H(35A)	109.4
C(11)-C(12)-H(12B)	109.6	C(34)-C(35)-H(35B)	109.4
C(13)-C(12)-H(12B)	109.6	C(36)-C(35)-H(35B)	109.4
H(12A)-C(12)-H(12B)	108.1	H(35A)-C(35)-H(35B)	108.0
C(14)-C(13)-C(12)	110.5(2)	N(419)-C(36)-C(35)	117.08(18)
C(14)-C(13)-H(13A)	109.6	N(419)-C(36)-C(31)	106.29(16)
C(12)-C(13)-H(13A)	109.6	C(35)-C(36)-C(31)	111.83(18)
C(14)-C(13)-H(13B)	109.6	N(419)-C(36)-H(36)	107.0
C(12)-C(13)-H(13B)	109.6	C(35)-C(36)-H(36)	107.0
H(13A)-C(13)-H(13B)	108.1	C(31)-C(36)-H(36)	107.0
C(13)-C(14)-C(15)	110.9(2)	C(22)-N(21)-C(26)	117.3(2)
C(13)-C(14)-H(14A)	109.5	C(22)-N(21)-Fe(1)	121.85(18)
C(15)-C(14)-H(14A)	109.5	C(26)-N(21)-Fe(1)	120.52(17)
C(13)-C(14)-H(14B)	109.5	N(21)-C(22)-C(23)	123.0(3)
C(15)-C(14)-H(14B)	109.5	N(21)-C(22)-H(22)	118.5
H(14A)-C(14)-H(14B)	108.1	C(23)-C(22)-H(22)	118.5
C(16)-C(15)-C(14)	109.55(19)	C(24)-C(23)-C(22)	119.0(3)
C(16)-C(15)-H(15A)	109.8	C(24)-C(23)-H(23)	120.5
C(14)-C(15)-H(15A)	109.8	C(22)-C(23)-H(23)	120.5
C(16)-C(15)-H(15B)	109.8	C(23)-C(24)-C(25)	118.8(3)
C(14)-C(15)-H(15B)	109.8	C(23)-C(24)-H(24)	120.6
H(15A)-C(15)-H(15B)	108.2	C(25)-C(24)-H(24)	120.6
N(219)-C(16)-C(15)	116.42(18)	C(26)-C(25)-C(24)	118.7(3)
N(219)-C(16)-C(11)	107.40(16)	C(26)-C(25)-H(25)	120.7
C(15)-C(16)-C(11)	111.35(18)	C(24)-C(25)-H(25)	120.7
N(219)-C(16)-H(16)	107.1	N(21)-C(26)-C(25)	123.2(2)
C(15)-C(16)-H(16)	107.1	N(21)-C(26)-H(26)	118.4
C(11)-C(16)-H(16)	107.1	C(25)-C(26)-H(26)	118.4
N(319)-C(31)-C(32)	115.83(19)	C(42)-N(41)-C(46)	117.4(2)
N(319)-C(31)-C(36)	106.62(17)	C(42)-N(41)-Fe(2)	122.53(19)
C(32)-C(31)-C(36)	111.15(18)	C(46)-N(41)-Fe(2)	119.84(17)
N(319)-C(31)-H(31)	107.6	N(41)-C(42)-C(43)	123.5(3)
C(32)-C(31)-H(31)	107.6	N(41)-C(42)-H(42)	118.2
C(36)-C(31)-H(31)	107.6	C(43)-C(42)-H(42)	118.2
C(31)-C(32)-C(33)	109.7(2)	C(44)-C(43)-C(42)	118.5(3)
C(31)-C(32)-H(32A)	109.7	C(44)-C(43)-H(43)	120.7
C(33)-C(32)-H(32A)	109.7	C(42)-C(43)-H(43)	120.7
C(31)-C(32)-H(32B)	109.7	C(43)-C(44)-C(45)	118.9(3)
C(33)-C(32)-H(32B)	109.7	C(43)-C(44)-H(44)	120.5

C(45)-C(44)-H(44)	120.5	C(117)-C(116)-C(115)	122.2(2)
C(46)-C(45)-C(44)	119.2(3)	C(111)-C(116)-C(115)	118.2(2)
C(46)-C(45)-H(45)	120.4	C(118)-C(117)-C(116)	122.9(2)
C(44)-C(45)-H(45)	120.4	C(118)-C(117)-H(117)	118.5
N(41)-C(46)-C(45)	122.4(3)	C(116)-C(117)-H(117)	118.5
N(41)-C(46)-H(46)	118.8	C(117)-C(118)-C(109)	116.2(2)
C(45)-C(46)-H(46)	118.8	C(117)-C(118)-C(101)	125.2(2)
C(106)-C(101)-C(102)	118.1(2)	C(109)-C(118)-C(101)	118.6(2)
C(106)-C(101)-C(118)	118.4(2)	N(119)-C(119)-C(103)	126.6(2)
C(102)-C(101)-C(118)	123.5(2)	N(119)-C(119)-H(119)	116.7
O(102)-C(102)-C(103)	120.7(2)	C(103)-C(119)-H(119)	116.7
O(102)-C(102)-C(101)	120.7(2)	C(119)-N(119)-C(11)	119.80(19)
C(103)-C(102)-C(101)	118.5(2)	C(119)-N(119)-Fe(1)	125.06(16)
C(102)-O(102)-Fe(1)	134.81(16)	C(11)-N(119)-Fe(1)	114.13(14)
C(104)-C(103)-C(102)	119.8(2)	C(206)-C(201)-C(202)	118.1(2)
C(104)-C(103)-C(119)	116.6(2)	C(206)-C(201)-C(218)	119.2(2)
C(102)-C(103)-C(119)	123.5(2)	C(202)-C(201)-C(218)	122.8(2)
C(105)-C(104)-C(103)	121.2(2)	O(202)-C(202)-C(203)	120.2(2)
C(105)-C(104)-H(104)	119.4	O(202)-C(202)-C(201)	120.9(2)
C(103)-C(104)-H(104)	119.4	C(203)-C(202)-C(201)	118.9(2)
C(104)-C(105)-C(106)	120.6(2)	C(202)-O(202)-Fe(1)	129.55(15)
C(104)-C(105)-H(105)	119.7	C(204)-C(203)-C(202)	119.9(2)
C(106)-C(105)-H(105)	119.7	C(204)-C(203)-C(219)	116.8(2)
C(105)-C(106)-C(101)	121.1(2)	C(202)-C(203)-C(219)	123.1(2)
C(105)-C(106)-C(107)	118.4(2)	C(205)-C(204)-C(203)	121.4(2)
C(101)-C(106)-C(107)	120.5(2)	C(205)-C(204)-H(204)	119.3
C(108)-C(107)-C(106)	121.6(2)	C(203)-C(204)-H(204)	119.3
C(108)-C(107)-H(107)	119.2	C(204)-C(205)-C(206)	120.0(2)
C(106)-C(107)-H(107)	119.2	C(204)-C(205)-H(205)	120.0
C(107)-C(108)-C(109)	120.1(2)	C(206)-C(205)-H(205)	120.0
C(107)-C(108)-H(108)	119.9	C(205)-C(206)-C(201)	121.8(2)
C(109)-C(108)-H(108)	119.9	C(205)-C(206)-C(207)	117.9(2)
C(110)-C(109)-C(108)	118.8(2)	C(201)-C(206)-C(207)	120.3(2)
C(110)-C(109)-C(118)	120.9(2)	C(208)-C(207)-C(206)	120.9(2)
C(108)-C(109)-C(118)	120.3(2)	C(208)-C(207)-H(207)	119.6
C(109)-C(110)-C(111)	122.2(2)	C(206)-C(207)-H(207)	119.6
C(109)-C(110)-H(110)	118.9	C(207)-C(208)-C(209)	121.3(2)
C(111)-C(110)-H(110)	118.9	C(207)-C(208)-H(208)	119.4
C(110)-C(111)-C(116)	117.8(2)	C(209)-C(208)-H(208)	119.4
C(110)-C(111)-C(112)	122.7(2)	C(210)-C(209)-C(208)	119.6(2)
C(116)-C(111)-C(112)	119.4(2)	C(210)-C(209)-C(218)	120.0(2)
C(113)-C(112)-C(111)	120.1(3)	C(208)-C(209)-C(218)	120.4(2)
C(113)-C(112)-H(112)	119.9	C(209)-C(210)-C(211)	123.2(2)
C(111)-C(112)-H(112)	119.9	C(209)-C(210)-H(210)	118.4
C(112)-C(113)-C(114)	120.8(3)	C(211)-C(210)-H(210)	118.4
C(112)-C(113)-H(113)	119.6	C(210)-C(211)-C(216)	117.6(2)
C(114)-C(113)-H(113)	119.6	C(210)-C(211)-C(212)	123.4(2)
C(115)-C(114)-C(113)	120.3(3)	C(216)-C(211)-C(212)	119.0(2)
C(115)-C(114)-H(114)	119.8	C(213)-C(212)-C(211)	120.5(2)
C(113)-C(114)-H(114)	119.8	C(213)-C(212)-H(212)	119.8
C(114)-C(115)-C(116)	121.0(2)	C(211)-C(212)-H(212)	119.8
C(114)-C(115)-H(115)	119.5	C(212)-C(213)-C(214)	120.4(3)
C(116)-C(115)-H(115)	119.5	C(212)-C(213)-H(213)	119.8
C(117)-C(116)-C(111)	119.6(2)	C(214)-C(213)-H(213)	119.8

C(215)-C(214)-C(213)	120.1(2)	C(312)-C(311)-C(316)	119.3(2)
C(215)-C(214)-H(214)	119.9	C(313)-C(312)-C(311)	121.3(3)
C(213)-C(214)-H(214)	119.9	C(313)-C(312)-H(312)	119.4
C(214)-C(215)-C(216)	121.4(2)	C(311)-C(312)-H(312)	119.4
C(214)-C(215)-H(215)	119.3	C(312)-C(313)-C(314)	119.6(3)
C(216)-C(215)-H(215)	119.3	C(312)-C(313)-H(313)	120.2
C(217)-C(216)-C(215)	121.4(2)	C(314)-C(313)-H(313)	120.2
C(217)-C(216)-C(211)	120.1(2)	C(315)-C(314)-C(313)	121.1(2)
C(215)-C(216)-C(211)	118.5(2)	C(315)-C(314)-H(314)	119.4
C(218)-C(217)-C(216)	122.1(2)	C(313)-C(314)-H(314)	119.4
C(218)-C(217)-H(217)	118.9	C(314)-C(315)-C(316)	121.1(2)
C(216)-C(217)-H(217)	118.9	C(314)-C(315)-H(315)	119.5
C(217)-C(218)-C(209)	117.0(2)	C(316)-C(315)-H(315)	119.5
C(217)-C(218)-C(201)	125.1(2)	C(317)-C(316)-C(315)	122.4(2)
C(209)-C(218)-C(201)	117.9(2)	C(317)-C(316)-C(311)	120.0(2)
N(219)-C(219)-C(203)	126.2(2)	C(315)-C(316)-C(311)	117.6(2)
N(219)-C(219)-H(219)	116.9	C(318)-C(317)-C(316)	122.2(2)
C(203)-C(219)-H(219)	116.9	C(318)-C(317)-H(317)	118.9
C(219)-N(219)-C(16)	120.42(19)	C(316)-C(317)-H(317)	118.9
C(219)-N(219)-Fe(1)	124.13(16)	C(317)-C(318)-C(309)	117.4(2)
C(16)-N(219)-Fe(1)	115.45(13)	C(317)-C(318)-C(301)	124.8(2)
C(306)-C(301)-C(302)	118.2(2)	C(309)-C(318)-C(301)	117.8(2)
C(306)-C(301)-C(318)	118.5(2)	N(319)-C(319)-C(303)	127.3(2)
C(302)-C(301)-C(318)	123.3(2)	N(319)-C(319)-H(319)	116.3
O(302)-C(302)-C(303)	120.4(2)	C(303)-C(319)-H(319)	116.3
O(302)-C(302)-C(301)	121.2(2)	C(319)-N(319)-C(31)	118.4(2)
C(303)-C(302)-C(301)	118.4(2)	C(319)-N(319)-Fe(2)	126.04(16)
C(302)-O(302)-Fe(2)	135.51(16)	C(31)-N(319)-Fe(2)	114.71(14)
C(304)-C(303)-C(302)	120.5(2)	C(406)-C(401)-C(402)	118.4(2)
C(304)-C(303)-C(319)	115.6(2)	C(406)-C(401)-C(418)	118.2(2)
C(302)-C(303)-C(319)	123.8(2)	C(402)-C(401)-C(418)	123.4(2)
C(305)-C(304)-C(303)	121.4(2)	O(402)-C(402)-C(403)	121.1(2)
C(305)-C(304)-H(304)	119.3	O(402)-C(402)-C(401)	120.2(2)
C(303)-C(304)-H(304)	119.3	C(403)-C(402)-C(401)	118.7(2)
C(304)-C(305)-C(306)	119.4(2)	C(402)-O(402)-Fe(2)	131.79(16)
C(304)-C(305)-H(305)	120.3	C(404)-C(403)-C(402)	120.5(2)
C(306)-C(305)-H(305)	120.3	C(404)-C(403)-C(419)	116.1(2)
C(305)-C(306)-C(301)	121.8(2)	C(402)-C(403)-C(419)	123.4(2)
C(305)-C(306)-C(307)	117.9(2)	C(405)-C(404)-C(403)	121.2(2)
C(301)-C(306)-C(307)	120.3(2)	C(405)-C(404)-H(404)	119.4
C(308)-C(307)-C(306)	121.7(2)	C(403)-C(404)-H(404)	119.4
C(308)-C(307)-H(307)	119.1	C(404)-C(405)-C(406)	120.1(2)
C(306)-C(307)-H(307)	119.1	C(404)-C(405)-H(405)	119.9
C(307)-C(308)-C(309)	121.2(2)	C(406)-C(405)-H(405)	119.9
C(307)-C(308)-H(308)	119.4	C(405)-C(406)-C(401)	120.9(2)
C(309)-C(308)-H(308)	119.4	C(405)-C(406)-C(407)	118.6(2)
C(310)-C(309)-C(308)	119.9(2)	C(401)-C(406)-C(407)	120.5(3)
C(310)-C(309)-C(318)	120.0(2)	C(408)-C(407)-C(406)	121.9(2)
C(308)-C(309)-C(318)	120.1(2)	C(408)-C(407)-H(407)	119.1
C(309)-C(310)-C(311)	122.8(2)	C(406)-C(407)-H(407)	119.1
C(309)-C(310)-H(310)	118.6	C(407)-C(408)-C(409)	121.4(2)
C(311)-C(310)-H(310)	118.6	C(407)-C(408)-H(408)	119.3
C(310)-C(311)-C(312)	123.4(2)	C(409)-C(408)-H(408)	119.3
C(310)-C(311)-C(316)	117.3(2)	C(410)-C(409)-C(408)	120.2(2)

C(410)-C(409)-C(418)	120.7(2)	C(414)-C(415)-H(415)	119.7
C(408)-C(409)-C(418)	119.1(2)	C(416)-C(415)-H(415)	119.7
C(409)-C(410)-C(411)	122.6(2)	C(417)-C(416)-C(411)	120.2(2)
C(409)-C(410)-H(410)	118.7	C(417)-C(416)-C(415)	121.2(2)
C(411)-C(410)-H(410)	118.7	C(411)-C(416)-C(415)	118.6(2)
C(410)-C(411)-C(412)	122.9(2)	C(418)-C(417)-C(416)	122.7(2)
C(410)-C(411)-C(416)	117.4(2)	C(418)-C(417)-H(417)	118.7
C(412)-C(411)-C(416)	119.7(2)	C(416)-C(417)-H(417)	118.7
C(413)-C(412)-C(411)	119.9(3)	C(417)-C(418)-C(409)	116.3(2)
C(413)-C(412)-H(412)	120.1	C(417)-C(418)-C(401)	124.7(2)
C(411)-C(412)-H(412)	120.1	C(409)-C(418)-C(401)	118.9(2)
C(412)-C(413)-C(414)	120.8(3)	N(419)-C(419)-C(403)	125.7(2)
C(412)-C(413)-H(413)	119.6	N(419)-C(419)-H(419)	117.2
C(414)-C(413)-H(413)	119.6	C(403)-C(419)-H(419)	117.2
C(415)-C(414)-C(413)	120.3(3)	C(419)-N(419)-C(36)	120.8(2)
C(415)-C(414)-H(414)	119.8	C(419)-N(419)-Fe(2)	126.29(17)
C(413)-C(414)-H(414)	119.8	C(36)-N(419)-Fe(2)	112.83(13)
C(414)-C(415)-C(416)	120.6(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*,*R*)-**76**·py. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	22(1)	16(1)	21(1)	0(1)	6(1)	3(1)
Fe(2)	18(1)	17(1)	23(1)	-1(1)	6(1)	3(1)
C(11)	23(1)	20(1)	23(1)	0(1)	7(1)	-1(1)
C(12)	33(1)	24(1)	24(1)	-6(1)	8(1)	3(1)
C(13)	40(1)	34(1)	23(1)	-4(1)	4(1)	1(1)
C(14)	45(1)	34(1)	22(1)	1(1)	5(1)	10(1)
C(15)	32(1)	27(1)	24(1)	1(1)	3(1)	6(1)
C(16)	27(1)	20(1)	21(1)	1(1)	9(1)	1(1)
C(31)	22(1)	26(1)	21(1)	2(1)	7(1)	1(1)
C(32)	31(1)	38(1)	23(1)	-1(1)	4(1)	7(1)
C(33)	41(1)	42(1)	21(1)	1(1)	6(1)	7(1)
C(34)	34(1)	33(1)	23(1)	1(1)	1(1)	3(1)
C(35)	27(1)	27(1)	30(1)	2(1)	3(1)	4(1)
C(36)	22(1)	19(1)	22(1)	2(1)	5(1)	0(1)
N(21)	24(1)	18(1)	34(1)	2(1)	12(1)	3(1)
C(22)	21(1)	21(1)	32(1)	0(1)	7(1)	1(1)
C(23)	26(1)	26(1)	41(2)	1(1)	9(1)	-2(1)
C(24)	29(1)	30(1)	43(2)	6(1)	17(1)	-3(1)
C(25)	33(2)	34(1)	33(2)	0(1)	14(1)	-2(1)
C(26)	24(1)	25(1)	33(1)	-2(1)	9(1)	-5(1)
N(41)	17(1)	24(1)	26(1)	3(1)	4(1)	2(1)
C(42)	26(1)	24(1)	34(1)	4(1)	5(1)	2(1)
C(43)	24(1)	28(1)	43(2)	7(1)	11(1)	-5(1)
C(44)	29(1)	40(2)	36(2)	7(1)	12(1)	-1(1)

C(45)	33(1)	37(2)	32(2)	3(1)	13(1)	-4(1)
C(46)	30(1)	33(2)	31(1)	1(1)	12(1)	0(1)
C(101)	22(1)	16(1)	28(1)	-2(1)	11(1)	-4(1)
C(102)	20(1)	13(1)	27(1)	1(1)	10(1)	0(1)
O(102)	25(1)	19(1)	25(1)	-3(1)	7(1)	5(1)
C(103)	22(1)	16(1)	29(1)	0(1)	12(1)	-1(1)
C(104)	28(1)	23(1)	28(1)	-2(1)	14(1)	2(1)
C(105)	27(1)	26(1)	34(1)	-4(1)	15(1)	5(1)
C(106)	21(1)	20(1)	35(1)	0(1)	12(1)	1(1)
C(107)	21(1)	23(1)	38(1)	-1(1)	14(1)	3(1)
C(108)	20(1)	22(1)	39(2)	4(1)	8(1)	4(1)
C(109)	24(1)	18(1)	31(1)	4(1)	10(1)	0(1)
C(110)	24(1)	21(1)	31(1)	7(1)	6(1)	5(1)
C(111)	25(1)	18(1)	25(1)	6(1)	7(1)	-1(1)
C(112)	31(1)	25(1)	25(1)	5(1)	5(1)	2(1)
C(113)	39(2)	25(1)	27(1)	5(1)	9(1)	0(1)
C(114)	35(1)	29(1)	33(1)	0(1)	17(1)	-1(1)
C(115)	23(1)	25(1)	29(1)	0(1)	8(1)	0(1)
C(116)	25(1)	17(1)	29(1)	2(1)	10(1)	-2(1)
C(117)	19(1)	16(1)	25(1)	3(1)	6(1)	1(1)
C(118)	19(1)	15(1)	28(1)	3(1)	8(1)	0(1)
C(119)	29(1)	17(1)	24(1)	0(1)	10(1)	-3(1)
N(119)	24(1)	16(1)	24(1)	1(1)	6(1)	0(1)
C(201)	21(1)	13(1)	23(1)	-1(1)	8(1)	0(1)
C(202)	18(1)	17(1)	25(1)	3(1)	9(1)	-3(1)
O(202)	21(1)	18(1)	25(1)	-2(1)	7(1)	3(1)
C(203)	20(1)	15(1)	24(1)	1(1)	6(1)	1(1)
C(204)	24(1)	21(1)	30(1)	2(1)	7(1)	4(1)
C(205)	27(1)	18(1)	30(1)	1(1)	11(1)	6(1)
C(206)	25(1)	16(1)	29(1)	3(1)	13(1)	1(1)
C(207)	31(1)	18(1)	33(1)	-4(1)	14(1)	1(1)
C(208)	36(2)	21(1)	29(1)	-6(1)	12(1)	1(1)
C(209)	31(1)	18(1)	29(1)	-3(1)	14(1)	-1(1)
C(210)	33(1)	24(1)	24(1)	-5(1)	8(1)	-6(1)
C(211)	28(1)	19(1)	24(1)	-2(1)	11(1)	-6(1)
C(212)	34(1)	29(1)	23(1)	-5(1)	4(1)	-5(1)
C(213)	30(1)	34(1)	24(1)	1(1)	0(1)	-3(1)
C(214)	27(1)	29(1)	29(1)	3(1)	5(1)	2(1)
C(215)	28(1)	22(1)	24(1)	0(1)	7(1)	-3(1)
C(216)	22(1)	19(1)	23(1)	1(1)	9(1)	-7(1)
C(217)	22(1)	15(1)	22(1)	-2(1)	9(1)	-5(1)
C(218)	23(1)	16(1)	23(1)	1(1)	10(1)	-4(1)
C(219)	19(1)	18(1)	22(1)	2(1)	4(1)	0(1)
N(219)	22(1)	17(1)	24(1)	0(1)	8(1)	-1(1)
C(301)	16(1)	14(1)	28(1)	3(1)	7(1)	2(1)
C(302)	15(1)	16(1)	27(1)	-1(1)	9(1)	-3(1)
O(302)	20(1)	18(1)	24(1)	0(1)	7(1)	5(1)
C(303)	19(1)	17(1)	26(1)	-1(1)	8(1)	0(1)
C(304)	27(1)	20(1)	29(1)	-3(1)	15(1)	-2(1)
C(305)	22(1)	17(1)	35(1)	2(1)	13(1)	3(1)
C(306)	19(1)	15(1)	33(1)	2(1)	11(1)	-1(1)
C(307)	21(1)	18(1)	39(1)	5(1)	11(1)	4(1)
C(308)	23(1)	21(1)	39(1)	8(1)	10(1)	5(1)
C(309)	18(1)	18(1)	31(1)	7(1)	8(1)	3(1)

C(310)	25(1)	23(1)	31(1)	9(1)	7(1)	3(1)
C(311)	24(1)	21(1)	29(1)	6(1)	7(1)	0(1)
C(312)	30(1)	28(1)	29(1)	7(1)	6(1)	1(1)
C(313)	36(1)	27(1)	25(1)	2(1)	9(1)	-5(1)
C(314)	28(1)	28(1)	31(1)	-1(1)	11(1)	3(1)
C(315)	25(1)	27(1)	30(1)	-1(1)	8(1)	3(1)
C(316)	20(1)	19(1)	27(1)	3(1)	6(1)	0(1)
C(317)	18(1)	18(1)	32(1)	1(1)	8(1)	0(1)
C(318)	18(1)	15(1)	26(1)	2(1)	7(1)	-3(1)
C(319)	21(1)	19(1)	24(1)	-2(1)	10(1)	-4(1)
N(319)	20(1)	22(1)	24(1)	2(1)	6(1)	0(1)
C(401)	21(1)	18(1)	26(1)	3(1)	8(1)	1(1)
C(402)	22(1)	15(1)	24(1)	2(1)	8(1)	2(1)
O(402)	20(1)	21(1)	26(1)	-3(1)	6(1)	3(1)
C(403)	24(1)	19(1)	29(1)	2(1)	8(1)	2(1)
C(404)	23(1)	20(1)	33(1)	3(1)	5(1)	6(1)
C(405)	25(1)	20(1)	40(2)	1(1)	7(1)	6(1)
C(406)	27(1)	17(1)	34(1)	0(1)	13(1)	2(1)
C(407)	33(2)	23(1)	35(1)	-3(1)	13(1)	9(1)
C(408)	39(2)	19(1)	33(1)	-4(1)	17(1)	4(1)
C(409)	26(1)	18(1)	26(1)	-2(1)	11(1)	-2(1)
C(410)	36(1)	19(1)	27(1)	-5(1)	14(1)	1(1)
C(411)	27(1)	22(1)	22(1)	1(1)	8(1)	-6(1)
C(412)	36(1)	27(1)	25(1)	-3(1)	8(1)	-8(1)
C(413)	30(1)	35(1)	24(1)	1(1)	1(1)	-6(1)
C(414)	26(1)	32(1)	32(1)	0(1)	2(1)	0(1)
C(415)	22(1)	25(1)	27(1)	-2(1)	7(1)	-1(1)
C(416)	22(1)	17(1)	23(1)	0(1)	8(1)	-2(1)
C(417)	21(1)	17(1)	22(1)	0(1)	9(1)	-2(1)
C(418)	21(1)	17(1)	23(1)	1(1)	10(1)	0(1)
C(419)	22(1)	21(1)	27(1)	3(1)	5(1)	3(1)
N(419)	22(1)	21(1)	22(1)	-1(1)	7(1)	-1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for (*R*,*R*)-**76**·py.

	x	y	z	U(eq)
H(11)	4246	67	-488	26
H(12A)	5017	-589	-1374	32
H(12B)	5757	60	-1591	32
H(13A)	3757	-74	-2565	39
H(13B)	2984	-55	-1910	39
H(14A)	2852	1029	-2522	41
H(14B)	4400	1078	-2295	41
H(15A)	3630	1729	-1386	34
H(15B)	2896	1074	-1175	34
H(16)	5645	1185	-894	27
H(31)	9037	1179	10923	27

H(32A)	8970	2212	11583	37
H(32B)	10150	2508	11289	37
H(33A)	10959	2085	12589	42
H(33B)	10335	1352	12319	42
H(34A)	12562	1318	12412	38
H(34B)	12410	1949	11817	38
H(35A)	11320	617	11415	34
H(35B)	12473	939	11118	34
H(36)	11085	1766	10390	26
H(22)	4107	-254	914	30
H(23)	2975	-755	1712	37
H(24)	3353	-386	3011	39
H(25)	4888	481	3474	39
H(26)	5973	943	2635	32
H(42)	10850	2371	9039	34
H(43)	11961	2862	8228	37
H(44)	11563	2470	6932	41
H(45)	10078	1579	6507	40
H(46)	9005	1124	7361	37
H(104)	8868	-1107	-252	30
H(105)	10622	-1566	635	33
H(107)	11803	-1827	1965	31
H(108)	12340	-1608	3287	33
H(110)	11948	-1015	4382	30
H(112)	11515	-485	5575	33
H(113)	10079	70	6122	36
H(114)	8107	496	5326	37
H(115)	7571	358	3982	31
H(117)	8193	-10	2793	24
H(119)	6970	-479	-584	27
H(204)	2986	2788	466	30
H(205)	3181	3457	1560	29
H(207)	4355	3835	2848	31
H(208)	6077	3767	3939	33
H(210)	8078	3261	4651	32
H(212)	10163	2755	5458	36
H(213)	11728	1922	5597	37
H(214)	11629	1127	4580	34
H(215)	9924	1151	3459	29
H(217)	7920	1676	2658	23
H(219)	3754	1980	-251	24
H(304)	6062	3200	10186	29
H(305)	4342	3693	9263	29
H(307)	3190	3915	7925	31
H(308)	2708	3687	6628	33
H(310)	3093	3057	5544	32
H(312)	3555	2511	4372	35
H(313)	4930	1884	3847	35
H(314)	6906	1472	4672	34
H(315)	7390	1598	6007	33
H(317)	6802	2043	7184	27
H(319)	7673	2425	10580	25
H(404)	12137	-679	9582	31
H(405)	11849	-1427	8542	35

H(407)	10691	-1797	7245	36
H(408)	8986	-1750	6165	35
H(410)	7005	-1216	5415	32
H(412)	4982	-668	4585	35
H(413)	3359	131	4475	37
H(414)	3388	885	5520	37
H(415)	5044	836	6664	29
H(417)	7088	329	7439	23
H(419)	11562	243	10221	28

Table 6. Torsion angles [°] for (*R*,*R*)-**76**·py.

N(119)-C(11)-C(12)-C(13)	-178.33(19)	C(24)-C(25)-C(26)-N(21)	-0.2(4)
C(16)-C(11)-C(12)-C(13)	-55.9(3)	O(402)-Fe(2)-N(41)-C(42)	-152.0(2)
C(11)-C(12)-C(13)-C(14)	57.0(3)	O(302)-Fe(2)-N(41)-C(42)	98.6(2)
C(12)-C(13)-C(14)-C(15)	-58.4(3)	N(319)-Fe(2)-N(41)-C(42)	12.2(2)
C(13)-C(14)-C(15)-C(16)	57.9(3)	N(419)-Fe(2)-N(41)-C(42)	-66.3(2)
C(14)-C(15)-C(16)-N(219)	179.68(19)	O(402)-Fe(2)-N(41)-C(46)	33.3(2)
C(14)-C(15)-C(16)-C(11)	-56.8(2)	O(302)-Fe(2)-N(41)-C(46)	-76.1(2)
N(119)-C(11)-C(16)-N(219)	-46.4(2)	N(319)-Fe(2)-N(41)-C(46)	-162.45(18)
C(12)-C(11)-C(16)-N(219)	-174.81(18)	N(419)-Fe(2)-N(41)-C(46)	119.1(2)
N(119)-C(11)-C(16)-C(15)	-174.94(17)	C(46)-N(41)-C(42)-C(43)	1.1(4)
C(12)-C(11)-C(16)-C(15)	56.7(2)	Fe(2)-N(41)-C(42)-C(43)	-173.7(2)
N(319)-C(31)-C(32)-C(33)	-178.0(2)	N(41)-C(42)-C(43)-C(44)	-0.3(4)
C(36)-C(31)-C(32)-C(33)	-56.1(3)	C(42)-C(43)-C(44)-C(45)	-0.6(4)
C(31)-C(32)-C(33)-C(34)	58.0(3)	C(43)-C(44)-C(45)-C(46)	0.8(4)
C(32)-C(33)-C(34)-C(35)	-57.6(3)	C(42)-N(41)-C(46)-C(45)	-0.9(4)
C(33)-C(34)-C(35)-C(36)	55.1(3)	Fe(2)-N(41)-C(46)-C(45)	174.1(2)
C(34)-C(35)-C(36)-N(419)	-176.94(19)	C(44)-C(45)-C(46)-N(41)	-0.1(4)
C(34)-C(35)-C(36)-C(31)	-54.0(3)	C(106)-C(101)-C(102)-O(102)	-172.3(2)
N(319)-C(31)-C(36)-N(419)	-49.0(2)	C(118)-C(101)-C(102)-O(102)	8.7(4)
C(32)-C(31)-C(36)-N(419)	-176.10(18)	C(106)-C(101)-C(102)-C(103)	8.8(3)
N(319)-C(31)-C(36)-C(35)	-177.91(18)	C(118)-C(101)-C(102)-C(103)	-170.2(2)
C(32)-C(31)-C(36)-C(35)	55.0(2)	C(103)-C(102)-O(102)-Fe(1)	1.4(3)
O(102)-Fe(1)-N(21)-C(22)	-98.27(19)	C(101)-C(102)-O(102)-Fe(1)	-177.44(16)
O(202)-Fe(1)-N(21)-C(22)	154.50(19)	O(202)-Fe(1)-O(102)-C(102)	-149.0(2)
N(119)-Fe(1)-N(21)-C(22)	-11.4(2)	N(119)-Fe(1)-O(102)-C(102)	10.2(2)
N(219)-Fe(1)-N(21)-C(22)	70.1(2)	N(219)-Fe(1)-O(102)-C(102)	-25.4(4)
O(102)-Fe(1)-N(21)-C(26)	74.9(2)	N(21)-Fe(1)-O(102)-C(102)	119.8(2)
O(202)-Fe(1)-N(21)-C(26)	-32.3(2)	O(102)-C(102)-C(103)-C(104)	171.9(2)
N(119)-Fe(1)-N(21)-C(26)	161.81(19)	C(101)-C(102)-C(103)-C(104)	-9.2(3)
N(219)-Fe(1)-N(21)-C(26)	-116.71(19)	O(102)-C(102)-C(103)-C(119)	-11.0(4)
C(26)-N(21)-C(22)-C(23)	-0.9(4)	C(101)-C(102)-C(103)-C(119)	167.9(2)
Fe(1)-N(21)-C(22)-C(23)	172.5(2)	C(102)-C(103)-C(104)-C(105)	3.2(4)
N(21)-C(22)-C(23)-C(24)	0.6(4)	C(119)-C(103)-C(104)-C(105)	-174.1(2)
C(22)-C(23)-C(24)-C(25)	-0.1(4)	C(103)-C(104)-C(105)-C(106)	3.2(4)
C(23)-C(24)-C(25)-C(26)	-0.1(4)	C(104)-C(105)-C(106)-C(101)	-3.4(4)
C(22)-N(21)-C(26)-C(25)	0.7(4)	C(104)-C(105)-C(106)-C(107)	174.4(3)
Fe(1)-N(21)-C(26)-C(25)	-172.8(2)	C(102)-C(101)-C(106)-C(105)	-2.7(4)

C(118)-C(101)-C(106)-C(105)	176.3(2)	C(218)-C(201)-C(202)-C(203)	-179.3(2)
C(102)-C(101)-C(106)-C(107)	179.5(2)	C(203)-C(202)-O(202)-Fe(1)	-30.7(3)
C(118)-C(101)-C(106)-C(107)	-1.4(4)	C(201)-C(202)-O(202)-Fe(1)	151.72(17)
C(105)-C(106)-C(107)-C(108)	178.4(3)	O(102)-Fe(1)-O(202)-C(202)	-157.74(18)
C(101)-C(106)-C(107)-C(108)	-3.8(4)	N(119)-Fe(1)-O(202)-C(202)	81.5(3)
C(106)-C(107)-C(108)-C(109)	3.8(4)	N(219)-Fe(1)-O(202)-C(202)	38.97(19)
C(107)-C(108)-C(109)-C(110)	179.2(3)	N(21)-Fe(1)-O(202)-C(202)	-64.8(2)
C(107)-C(108)-C(109)-C(118)	1.3(4)	O(202)-C(202)-C(203)-C(204)	-177.3(2)
C(108)-C(109)-C(110)-C(111)	-172.8(2)	C(201)-C(202)-C(203)-C(204)	0.3(3)
C(118)-C(109)-C(110)-C(111)	5.1(4)	O(202)-C(202)-C(203)-C(219)	-2.9(3)
C(109)-C(110)-C(111)-C(116)	1.1(4)	C(201)-C(202)-C(203)-C(219)	174.7(2)
C(109)-C(110)-C(111)-C(112)	-179.8(2)	C(202)-C(203)-C(204)-C(205)	-2.2(4)
C(110)-C(111)-C(112)-C(113)	-175.2(2)	C(219)-C(203)-C(204)-C(205)	-176.9(2)
C(116)-C(111)-C(112)-C(113)	3.9(4)	C(203)-C(204)-C(205)-C(206)	2.7(4)
C(111)-C(112)-C(113)-C(114)	-1.7(4)	C(204)-C(205)-C(206)-C(201)	-1.3(4)
C(112)-C(113)-C(114)-C(115)	-0.2(4)	C(204)-C(205)-C(206)-C(207)	177.8(2)
C(113)-C(114)-C(115)-C(116)	-0.2(4)	C(202)-C(201)-C(206)-C(205)	-0.5(4)
C(110)-C(111)-C(116)-C(117)	-5.5(3)	C(218)-C(201)-C(206)-C(205)	179.8(2)
C(112)-C(111)-C(116)-C(117)	175.4(2)	C(202)-C(201)-C(206)-C(207)	-179.7(2)
C(110)-C(111)-C(116)-C(115)	174.9(2)	C(218)-C(201)-C(206)-C(207)	0.6(4)
C(112)-C(111)-C(116)-C(115)	-4.1(4)	C(205)-C(206)-C(207)-C(208)	-178.9(2)
C(114)-C(115)-C(116)-C(117)	-177.2(2)	C(201)-C(206)-C(207)-C(208)	0.3(4)
C(114)-C(115)-C(116)-C(111)	2.3(4)	C(206)-C(207)-C(208)-C(209)	0.0(4)
C(111)-C(116)-C(117)-C(118)	3.9(4)	C(207)-C(208)-C(209)-C(210)	-179.5(3)
C(115)-C(116)-C(117)-C(118)	-176.6(2)	C(207)-C(208)-C(209)-C(218)	-1.3(4)
C(116)-C(117)-C(118)-C(109)	2.1(3)	C(208)-C(209)-C(210)-C(211)	177.8(2)
C(116)-C(117)-C(118)-C(101)	179.6(2)	C(218)-C(209)-C(210)-C(211)	-0.5(4)
C(110)-C(109)-C(118)-C(117)	-6.6(4)	C(209)-C(210)-C(211)-C(216)	0.0(4)
C(108)-C(109)-C(118)-C(117)	171.3(2)	C(209)-C(210)-C(211)-C(212)	179.3(3)
C(110)-C(109)-C(118)-C(101)	175.8(2)	C(210)-C(211)-C(212)-C(213)	179.3(3)
C(108)-C(109)-C(118)-C(101)	-6.4(3)	C(216)-C(211)-C(212)-C(213)	-1.5(4)
C(106)-C(101)-C(118)-C(117)	-171.1(2)	C(211)-C(212)-C(213)-C(214)	1.3(4)
C(102)-C(101)-C(118)-C(117)	7.9(4)	C(212)-C(213)-C(214)-C(215)	-1.0(4)
C(106)-C(101)-C(118)-C(109)	6.3(3)	C(213)-C(214)-C(215)-C(216)	1.0(4)
C(102)-C(101)-C(118)-C(109)	-174.7(2)	C(214)-C(215)-C(216)-C(217)	179.3(2)
C(104)-C(103)-C(119)-N(119)	178.3(2)	C(214)-C(215)-C(216)-C(211)	-1.2(4)
C(102)-C(103)-C(119)-N(119)	1.1(4)	C(210)-C(211)-C(216)-C(217)	0.2(4)
C(103)-C(119)-N(119)-C(11)	-175.8(2)	C(212)-C(211)-C(216)-C(217)	-179.1(2)
C(103)-C(119)-N(119)-Fe(1)	16.4(3)	C(210)-C(211)-C(216)-C(215)	-179.3(2)
C(12)-C(11)-N(119)-C(119)	-3.3(3)	C(212)-C(211)-C(216)-C(215)	1.4(4)
C(16)-C(11)-N(119)-C(119)	-128.1(2)	C(215)-C(216)-C(217)-C(218)	179.5(2)
C(12)-C(11)-N(119)-Fe(1)	165.83(16)	C(211)-C(216)-C(217)-C(218)	0.0(4)
C(16)-C(11)-N(119)-Fe(1)	41.0(2)	C(216)-C(217)-C(218)-C(209)	-0.4(3)
O(102)-Fe(1)-N(119)-C(119)	-18.19(19)	C(216)-C(217)-C(218)-C(201)	179.9(2)
O(202)-Fe(1)-N(119)-C(119)	106.5(2)	C(210)-C(209)-C(218)-C(217)	0.7(4)
N(219)-Fe(1)-N(119)-C(119)	150.0(2)	C(208)-C(209)-C(218)-C(217)	-177.6(2)
N(21)-Fe(1)-N(119)-C(119)	-109.69(19)	C(210)-C(209)-C(218)-C(201)	-179.6(2)
O(102)-Fe(1)-N(119)-C(11)	173.37(15)	C(208)-C(209)-C(218)-C(201)	2.1(3)
O(202)-Fe(1)-N(119)-C(11)	-62.0(2)	C(206)-C(201)-C(218)-C(217)	177.9(2)
N(219)-Fe(1)-N(119)-C(11)	-18.43(14)	C(202)-C(201)-C(218)-C(217)	-1.8(4)
N(21)-Fe(1)-N(119)-C(11)	81.88(15)	C(206)-C(201)-C(218)-C(209)	-1.8(3)
C(206)-C(201)-C(202)-O(202)	178.6(2)	C(202)-C(201)-C(218)-C(209)	178.5(2)
C(218)-C(201)-C(202)-O(202)	-1.7(3)	C(204)-C(203)-C(219)-N(219)	-173.4(2)
C(206)-C(201)-C(202)-C(203)	1.0(3)	C(202)-C(203)-C(219)-N(219)	12.0(4)

C(203)-C(219)-N(219)-C(16)	-171.1(2)	C(312)-C(311)-C(316)-C(317)	-176.6(2)
C(203)-C(219)-N(219)-Fe(1)	10.1(3)	C(310)-C(311)-C(316)-C(315)	-176.2(2)
C(15)-C(16)-N(219)-C(219)	-19.6(3)	C(312)-C(311)-C(316)-C(315)	2.6(4)
C(11)-C(16)-N(219)-C(219)	-145.2(2)	C(315)-C(316)-C(317)-C(318)	177.8(2)
C(15)-C(16)-N(219)-Fe(1)	159.29(15)	C(311)-C(316)-C(317)-C(318)	-3.1(4)
C(11)-C(16)-N(219)-Fe(1)	33.7(2)	C(316)-C(317)-C(318)-C(309)	-2.5(3)
O(102)-Fe(1)-N(219)-C(219)	-154.1(2)	C(316)-C(317)-C(318)-C(301)	-179.9(2)
O(202)-Fe(1)-N(219)-C(219)	-27.18(18)	C(310)-C(309)-C(318)-C(317)	6.5(3)
N(119)-Fe(1)-N(219)-C(219)	169.44(19)	C(308)-C(309)-C(318)-C(317)	-171.8(2)
N(21)-Fe(1)-N(219)-C(219)	61.86(19)	C(310)-C(309)-C(318)-C(301)	-175.9(2)
O(102)-Fe(1)-N(219)-C(16)	27.0(3)	C(308)-C(309)-C(318)-C(301)	5.9(3)
O(202)-Fe(1)-N(219)-C(16)	153.93(15)	C(306)-C(301)-C(318)-C(317)	171.2(2)
N(119)-Fe(1)-N(219)-C(16)	-9.45(14)	C(302)-C(301)-C(318)-C(317)	-8.3(4)
N(21)-Fe(1)-N(219)-C(16)	-117.02(15)	C(306)-C(301)-C(318)-C(309)	-6.2(3)
C(306)-C(301)-C(302)-O(302)	173.8(2)	C(302)-C(301)-C(318)-C(309)	174.3(2)
C(318)-C(301)-C(302)-O(302)	-6.7(3)	C(304)-C(303)-C(319)-N(319)	-177.2(2)
C(306)-C(301)-C(302)-C(303)	-5.2(3)	C(302)-C(303)-C(319)-N(319)	6.0(4)
C(318)-C(301)-C(302)-C(303)	174.3(2)	C(303)-C(319)-N(319)-C(31)	-178.7(2)
C(303)-C(302)-O(302)-Fe(2)	-6.2(3)	C(303)-C(319)-N(319)-Fe(2)	-9.9(3)
C(301)-C(302)-O(302)-Fe(2)	174.85(16)	C(32)-C(31)-N(319)-C(319)	-31.6(3)
O(402)-Fe(2)-O(302)-C(302)	149.1(2)	C(36)-C(31)-N(319)-C(319)	-155.88(19)
N(319)-Fe(2)-O(302)-C(302)	2.6(2)	C(32)-C(31)-N(319)-Fe(2)	158.34(16)
N(419)-Fe(2)-O(302)-C(302)	-8.8(4)	C(36)-C(31)-N(319)-Fe(2)	34.1(2)
N(41)-Fe(2)-O(302)-C(302)	-118.6(2)	O(402)-Fe(2)-N(319)-C(319)	-112.8(2)
O(302)-C(302)-C(303)-C(304)	-174.4(2)	O(302)-Fe(2)-N(319)-C(319)	5.32(19)
C(301)-C(302)-C(303)-C(304)	4.6(3)	N(419)-Fe(2)-N(319)-C(319)	-177.9(2)
O(302)-C(302)-C(303)-C(319)	2.3(4)	N(41)-Fe(2)-N(319)-C(319)	94.6(2)
C(301)-C(302)-C(303)-C(319)	-178.7(2)	O(402)-Fe(2)-N(319)-C(31)	56.3(2)
C(302)-C(303)-C(304)-C(305)	-0.2(4)	O(302)-Fe(2)-N(319)-C(31)	174.47(15)
C(319)-C(303)-C(304)-C(305)	-177.1(2)	N(419)-Fe(2)-N(319)-C(31)	-8.73(14)
C(303)-C(304)-C(305)-C(306)	-3.6(4)	N(41)-Fe(2)-N(319)-C(31)	-96.24(16)
C(304)-C(305)-C(306)-C(301)	3.0(4)	C(406)-C(401)-C(402)-O(402)	-178.5(2)
C(304)-C(305)-C(306)-C(307)	-177.6(2)	C(418)-C(401)-C(402)-O(402)	2.8(4)
C(302)-C(301)-C(306)-C(305)	1.5(3)	C(406)-C(401)-C(402)-C(403)	2.1(4)
C(318)-C(301)-C(306)-C(305)	-178.0(2)	C(418)-C(401)-C(402)-C(403)	-176.6(2)
C(302)-C(301)-C(306)-C(307)	-177.9(2)	C(403)-C(402)-O(402)-Fe(2)	27.7(3)
C(318)-C(301)-C(306)-C(307)	2.6(3)	C(401)-C(402)-O(402)-Fe(2)	-151.63(18)
C(305)-C(306)-C(307)-C(308)	-177.7(2)	O(302)-Fe(2)-O(402)-C(402)	157.2(2)
C(301)-C(306)-C(307)-C(308)	1.7(4)	N(319)-Fe(2)-O(402)-C(402)	-91.6(2)
C(306)-C(307)-C(308)-C(309)	-2.2(4)	N(419)-Fe(2)-O(402)-C(402)	-28.8(2)
C(307)-C(308)-C(309)-C(310)	-180.0(3)	N(41)-Fe(2)-O(402)-C(402)	65.2(2)
C(307)-C(308)-C(309)-C(318)	-1.7(4)	O(402)-C(402)-C(403)-C(404)	176.0(2)
C(308)-C(309)-C(310)-C(311)	173.2(2)	C(401)-C(402)-C(403)-C(404)	-4.7(4)
C(318)-C(309)-C(310)-C(311)	-5.1(4)	O(402)-C(402)-C(403)-C(419)	-3.4(4)
C(309)-C(310)-C(311)-C(312)	-179.3(3)	C(401)-C(402)-C(403)-C(419)	175.9(2)
C(309)-C(310)-C(311)-C(316)	-0.5(4)	C(402)-C(403)-C(404)-C(405)	3.9(4)
C(310)-C(311)-C(312)-C(313)	176.6(3)	C(419)-C(403)-C(404)-C(405)	-176.7(2)
C(316)-C(311)-C(312)-C(313)	-2.1(4)	C(403)-C(404)-C(405)-C(406)	-0.5(4)
C(311)-C(312)-C(313)-C(314)	-0.8(4)	C(404)-C(405)-C(406)-C(401)	-2.1(4)
C(312)-C(313)-C(314)-C(315)	3.2(4)	C(404)-C(405)-C(406)-C(407)	177.1(3)
C(313)-C(314)-C(315)-C(316)	-2.6(4)	C(402)-C(401)-C(406)-C(405)	1.3(4)
C(314)-C(315)-C(316)-C(317)	178.9(3)	C(418)-C(401)-C(406)-C(405)	180.0(2)
C(314)-C(315)-C(316)-C(311)	-0.3(4)	C(402)-C(401)-C(406)-C(407)	-177.9(2)
C(310)-C(311)-C(316)-C(317)	4.6(4)	C(418)-C(401)-C(406)-C(407)	0.8(4)

C(405)-C(406)-C(407)-C(408)	179.8(3)	C(410)-C(409)-C(418)-C(417)	1.0(4)
C(401)-C(406)-C(407)-C(408)	-1.0(4)	C(408)-C(409)-C(418)-C(417)	-179.7(2)
C(406)-C(407)-C(408)-C(409)	1.1(4)	C(410)-C(409)-C(418)-C(401)	-178.4(2)
C(407)-C(408)-C(409)-C(410)	178.2(3)	C(408)-C(409)-C(418)-C(401)	0.9(3)
C(407)-C(408)-C(409)-C(418)	-1.1(4)	C(406)-C(401)-C(418)-C(417)	179.9(2)
C(408)-C(409)-C(410)-C(411)	-179.6(2)	C(402)-C(401)-C(418)-C(417)	-1.4(4)
C(418)-C(409)-C(410)-C(411)	-0.3(4)	C(406)-C(401)-C(418)-C(409)	-0.8(3)
C(409)-C(410)-C(411)-C(412)	178.1(3)	C(402)-C(401)-C(418)-C(409)	177.9(2)
C(409)-C(410)-C(411)-C(416)	-0.6(4)	C(404)-C(403)-C(419)-N(419)	171.9(2)
C(410)-C(411)-C(412)-C(413)	179.3(3)	C(402)-C(403)-C(419)-N(419)	-8.7(4)
C(416)-C(411)-C(412)-C(413)	-2.0(4)	C(403)-C(419)-N(419)-C(36)	-178.7(2)
C(411)-C(412)-C(413)-C(414)	0.7(4)	C(403)-C(419)-N(419)-Fe(2)	-1.6(3)
C(412)-C(413)-C(414)-C(415)	0.4(4)	C(35)-C(36)-N(419)-C(419)	-12.8(3)
C(413)-C(414)-C(415)-C(416)	-0.2(4)	C(31)-C(36)-N(419)-C(419)	-138.5(2)
C(410)-C(411)-C(416)-C(417)	0.8(3)	C(35)-C(36)-N(419)-Fe(2)	169.76(15)
C(412)-C(411)-C(416)-C(417)	-177.9(2)	C(31)-C(36)-N(419)-Fe(2)	43.99(18)
C(410)-C(411)-C(416)-C(415)	-179.1(2)	O(402)-Fe(2)-N(419)-C(419)	14.7(2)
C(412)-C(411)-C(416)-C(415)	2.2(4)	O(302)-Fe(2)-N(419)-C(419)	173.9(2)
C(414)-C(415)-C(416)-C(417)	179.0(2)	N(319)-Fe(2)-N(419)-C(419)	162.3(2)
C(414)-C(415)-C(416)-C(411)	-1.1(4)	N(41)-Fe(2)-N(419)-C(419)	-76.7(2)
C(411)-C(416)-C(417)-C(418)	-0.1(4)	O(402)-Fe(2)-N(419)-C(36)	-167.98(14)
C(415)-C(416)-C(417)-C(418)	179.8(2)	O(302)-Fe(2)-N(419)-C(36)	-8.8(3)
C(416)-C(417)-C(418)-C(409)	-0.7(3)	N(319)-Fe(2)-N(419)-C(36)	-20.42(14)
C(416)-C(417)-C(418)-C(401)	178.6(2)	N(41)-Fe(2)-N(419)-C(36)	100.64(14)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**77**.

Identification code	(*R*)-**77**	
Empirical formula	C122 H82 Cl4 N4 O5 Zn2	
Formula weight	1956.46	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 12.5693(17) Å	α= 90°.
	b = 32.926(4) Å	β= 119.512(2)°.
	c = 12.6967(17) Å	γ = 90°.
Volume	4572.9(11) $Å^3$	
Z	2	
Density (calculated)	1.421 g/cm^3	
Absorption coefficient	0.705 mm^{-1}	
F(000)	2020	
Crystal size	0.56 x 0.18 x 0.12 mm^3	
Theta range for data collection	1.94 to 26.18°.	
Index ranges	-15<=h<=15, -40<=k<=38, -15<=l<=15	
Reflections collected	29596	
Independent reflections	15636 [R(int) = 0.0270]	
Completeness to theta = 26.18°	91.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.761	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15636 / 1 / 1235	
Goodness-of-fit on F^2	1.335	
Final R indices [I>2sigma(I)]	R1 = 0.0547, wR2 = 0.1475	
R indices (all data)	R1 = 0.0572, wR2 = 0.1504	
Absolute structure parameter	0.029(11)	
Largest diff. peak and hole	0.936 and -0.572 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**77**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn(1)	1272(1)	1479(1)	1863(1)	22(1)
Zn(2)	226(1)	3973(1)	7(1)	23(1)
C(1S)	2377(6)	2508(2)	4408(6)	29(1)
Cl(1)	3144(2)	2211(1)	3824(2)	38(1)
Cl(2)	1753(2)	2199(1)	5091(2)	53(1)
C(2S)	2508(8)	2790(2)	1095(7)	39(2)
Cl(3)	1699(2)	3093(1)	1612(2)	48(1)
Cl(4)	3237(2)	3072(1)	494(2)	59(1)
O(1S)	-1708(5)	5251(2)	205(5)	44(1)
C(3S)	-1146(8)	5163(4)	1371(8)	67(3)
C(4S)	-316(7)	4809(2)	1613(6)	37(2)

C(5S)	-2475(8)	5603(2)	-135(8)	48(2)
C(6S)	-2993(7)	5696(2)	-1391(8)	46(2)
C(101)	2670(6)	1000(2)	5330(5)	21(1)
C(102)	1784(5)	1155(2)	4165(5)	22(1)
O(102)	2057(4)	1170(1)	3309(4)	24(1)
C(103)	625(5)	1295(2)	3992(5)	22(1)
C(104)	305(6)	1222(2)	4902(6)	25(1)
C(105)	1125(6)	1068(2)	5981(5)	25(1)
C(106)	2323(6)	967(2)	6225(5)	23(1)
C(107)	3183(6)	834(2)	7421(5)	25(1)
C(108)	4353(6)	737(2)	7732(6)	30(1)
C(109)	4762(5)	757(2)	6858(5)	24(1)
C(110)	5965(6)	657(2)	7217(6)	28(1)
C(111)	6416(6)	680(2)	6418(6)	24(1)
C(112)	7677(6)	590(2)	6757(6)	30(1)
C(113)	8062(6)	606(2)	5949(7)	36(2)
C(114)	7247(6)	716(2)	4734(6)	34(2)
C(115)	6085(6)	808(2)	4371(6)	28(1)
C(116)	5616(5)	798(2)	5199(5)	24(1)
C(117)	4395(5)	900(2)	4844(5)	21(1)
C(118)	3931(5)	888(2)	5640(6)	23(1)
C(119)	-218(5)	1525(2)	2990(5)	22(1)
N(119)	-34(4)	1699(2)	2170(4)	23(1)
C(120)	-2726(5)	1922(2)	-842(5)	20(1)
C(121)	-1892(5)	1712(2)	201(6)	23(1)
C(122)	-975(5)	1917(2)	1186(5)	20(1)
C(123)	-898(6)	2348(2)	1148(6)	27(1)
C(124)	-1682(6)	2554(2)	160(6)	28(1)
C(125)	-2624(5)	2358(2)	-851(6)	22(1)
C(126)	-3485(6)	2565(2)	-1913(6)	28(1)
C(127)	-4378(6)	2368(2)	-2878(5)	27(1)
C(128)	-4475(5)	1944(2)	-2865(5)	28(1)
C(129)	-3674(5)	1728(2)	-1867(5)	24(1)
C(201)	3089(6)	1927(2)	79(6)	23(1)
C(202)	2112(5)	1749(2)	237(5)	21(1)
O(202)	2290(4)	1717(1)	1323(4)	27(1)
C(203)	987(6)	1634(2)	-817(6)	27(1)
C(204)	789(6)	1724(2)	-1961(5)	29(1)
C(205)	1651(6)	1925(2)	-2140(5)	32(2)
C(206)	2798(6)	2025(2)	-1122(6)	28(1)
C(207)	3696(6)	2231(2)	-1334(6)	30(1)
C(208)	4796(6)	2325(2)	-421(6)	27(1)
C(209)	5157(6)	2208(2)	805(5)	24(1)
C(210)	6364(5)	2271(2)	1709(6)	26(1)
C(211)	6791(6)	2151(2)	2902(6)	24(1)
C(212)	8008(6)	2210(2)	3856(6)	27(1)
C(213)	8374(5)	2089(2)	4985(6)	27(1)
C(214)	7528(6)	1889(2)	5266(6)	28(1)
C(215)	6364(5)	1825(2)	4400(5)	25(1)
C(216)	5944(6)	1949(2)	3180(6)	26(1)
C(217)	4739(5)	1886(2)	2267(5)	21(1)
C(218)	4307(5)	2006(2)	1076(5)	21(1)
C(219)	47(5)	1399(2)	-751(5)	21(1)
N(219)	52(4)	1268(2)	185(4)	22(1)

C(220)	-2691(5)	1026(2)	483(5)	19(1)
C(221)	-1853(5)	1254(2)	251(5)	19(1)
C(222)	-941(5)	1045(2)	168(5)	19(1)
C(223)	-867(5)	617(2)	221(5)	22(1)
C(224)	-1661(5)	395(2)	455(5)	24(1)
C(225)	-2565(5)	598(2)	613(5)	24(1)
C(226)	-3322(6)	379(2)	961(6)	28(1)
C(227)	-4162(6)	580(2)	1161(6)	30(1)
C(228)	-4296(6)	1000(2)	1012(6)	30(1)
C(229)	-3597(6)	1222(2)	668(5)	24(1)
C(301)	-1638(5)	3535(2)	1742(5)	22(1)
C(302)	-1456(5)	3708(2)	795(5)	20(1)
O(302)	-338(4)	3753(1)	1017(4)	26(1)
C(303)	-2489(5)	3817(2)	-329(5)	21(1)
C(304)	-3668(5)	3716(2)	-570(5)	23(1)
C(305)	-3856(5)	3530(2)	293(5)	24(1)
C(306)	-2873(5)	3447(2)	1441(5)	22(1)
C(307)	-3107(6)	3276(2)	2351(6)	24(1)
C(308)	-2200(6)	3195(2)	3463(6)	24(1)
C(309)	-950(6)	3276(2)	3822(6)	24(1)
C(310)	-60(6)	3192(2)	4979(5)	22(1)
C(311)	1194(6)	3270(2)	5417(5)	23(1)
C(312)	2131(6)	3173(2)	6595(6)	30(1)
C(313)	3339(6)	3250(2)	6942(5)	28(1)
C(314)	3654(6)	3432(2)	6129(6)	28(1)
C(315)	2765(6)	3530(2)	4974(6)	26(1)
C(316)	1497(6)	3456(2)	4583(5)	24(1)
C(317)	586(5)	3541(2)	3388(5)	22(1)
C(318)	-647(5)	3454(2)	2969(5)	20(1)
C(319)	-2424(5)	4050(2)	-1264(5)	21(1)
N(319)	-1434(4)	4191(1)	-1213(4)	20(1)
C(320)	-1087(5)	4438(2)	-3877(5)	18(1)
C(321)	-1328(5)	4211(2)	-3060(5)	20(1)
C(322)	-1450(5)	4415(2)	-2176(5)	21(1)
C(323)	-1376(5)	4842(2)	-2092(5)	22(1)
C(324)	-1159(5)	5062(2)	-2867(5)	21(1)
C(325)	-975(5)	4872(2)	-3766(5)	21(1)
C(326)	-666(5)	5088(2)	-4535(5)	25(1)
C(327)	-489(6)	4897(2)	-5379(6)	26(1)
C(328)	-616(6)	4473(2)	-5514(5)	24(1)
C(329)	-913(5)	4248(2)	-4782(5)	24(1)
C(401)	3771(5)	4443(2)	1576(5)	24(1)
C(402)	2602(5)	4273(2)	658(5)	22(1)
O(402)	1720(4)	4261(1)	878(4)	27(1)
C(403)	2533(5)	4121(2)	-432(5)	22(1)
C(404)	3491(6)	4186(2)	-683(6)	26(1)
C(405)	4548(6)	4377(2)	143(6)	27(1)
C(406)	4716(6)	4493(2)	1286(6)	27(1)
C(407)	5872(6)	4664(2)	2150(6)	28(1)
C(408)	6099(6)	4764(2)	3273(6)	28(1)
C(409)	5208(6)	4710(2)	3643(6)	26(1)
C(410)	5526(6)	4791(2)	4845(6)	28(1)
C(411)	4699(6)	4717(2)	5256(5)	24(1)
C(412)	5035(6)	4777(2)	6507(6)	29(1)

C(413)	4192(6)	4703(2)	6881(6)	31(1)
C(414)	3013(6)	4588(2)	6051(6)	30(1)
C(415)	2662(6)	4526(2)	4867(6)	26(1)
C(416)	3497(6)	4583(2)	4429(5)	24(1)
C(417)	3195(5)	4507(2)	3227(5)	23(1)
C(418)	4012(5)	4553(2)	2790(6)	24(1)
C(419)	1518(5)	3891(2)	-1321(5)	23(1)
N(419)	590(5)	3754(2)	-1243(5)	25(1)
C(420)	-2437(5)	3548(2)	-3951(5)	19(1)
C(421)	-1368(6)	3756(2)	-3092(5)	21(1)
C(422)	-395(5)	3537(2)	-2219(5)	23(1)
C(423)	-449(6)	3112(2)	-2154(5)	24(1)
C(424)	-1470(6)	2902(2)	-2966(6)	27(1)
C(425)	-2492(6)	3116(2)	-3876(5)	24(1)
C(426)	-3576(5)	2907(2)	-4716(5)	22(1)
C(427)	-4550(6)	3114(2)	-5580(6)	31(2)
C(428)	-4496(5)	3544(2)	-5659(6)	24(1)
C(429)	-3471(5)	3752(2)	-4873(5)	21(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**77**.

Zn(1)-O(202)	1.894(4)	C(6S)-H(6B)	0.9800
Zn(1)-O(102)	1.896(4)	C(6S)-H(6C)	0.9800
Zn(1)-N(119)	2.001(5)	C(101)-C(106)	1.408(8)
Zn(1)-N(219)	2.038(5)	C(101)-C(102)	1.437(8)
Zn(2)-O(302)	1.889(4)	C(101)-C(118)	1.479(8)
Zn(2)-O(402)	1.897(4)	C(102)-O(102)	1.292(7)
Zn(2)-N(419)	1.991(5)	C(102)-C(103)	1.438(8)
Zn(2)-N(319)	2.020(5)	C(103)-C(119)	1.410(9)
C(1S)-Cl(2)	1.755(6)	C(103)-C(104)	1.419(8)
C(1S)-Cl(1)	1.772(6)	C(104)-C(105)	1.344(9)
C(1S)-H(1A)	0.9900	C(104)-H(104)	0.9500
C(1S)-H(1B)	0.9900	C(105)-C(106)	1.419(8)
C(2S)-Cl(4)	1.725(7)	C(105)-H(105)	0.9500
C(2S)-Cl(3)	1.767(7)	C(106)-C(107)	1.432(9)
C(2S)-H(2A)	0.9900	C(107)-C(108)	1.360(9)
C(2S)-H(2B)	0.9900	C(107)-H(107)	0.9500
O(1S)-C(3S)	1.321(10)	C(108)-C(109)	1.436(9)
O(1S)-C(5S)	1.433(9)	C(108)-H(108)	0.9500
C(3S)-C(4S)	1.492(12)	C(109)-C(110)	1.387(9)
C(3S)-H(3A)	0.9900	C(109)-C(118)	1.440(9)
C(3S)-H(3B)	0.9900	C(110)-C(111)	1.387(9)
C(4S)-H(4A)	0.9800	C(110)-H(110)	0.9500
C(4S)-H(4B)	0.9800	C(111)-C(116)	1.423(9)
C(4S)-H(4C)	0.9800	C(111)-C(112)	1.453(9)
C(5S)-C(6S)	1.427(12)	C(112)-C(113)	1.333(10)
C(5S)-H(5A)	0.9900	C(112)-H(112)	0.9500
C(5S)-H(5B)	0.9900	C(113)-C(114)	1.415(10)
C(6S)-H(6A)	0.9800	C(113)-H(113)	0.9500

C(114)-C(115)	1.332(9)	C(214)-C(215)	1.345(9)
C(114)-H(114)	0.9500	C(214)-H(214)	0.9500
C(115)-C(116)	1.438(8)	C(215)-C(216)	1.428(9)
C(115)-H(115)	0.9500	C(215)-H(215)	0.9500
C(116)-C(117)	1.410(8)	C(216)-C(217)	1.397(9)
C(117)-C(118)	1.394(8)	C(217)-C(218)	1.390(8)
C(117)-H(117)	0.9500	C(217)-H(217)	0.9500
C(119)-N(119)	1.304(8)	C(219)-N(219)	1.262(8)
C(119)-H(119)	0.9500	C(219)-H(219)	0.9500
N(119)-C(122)	1.421(8)	N(219)-C(222)	1.439(7)
C(120)-C(121)	1.402(8)	C(220)-C(225)	1.421(8)
C(120)-C(129)	1.412(8)	C(220)-C(229)	1.426(8)
C(120)-C(125)	1.442(8)	C(220)-C(221)	1.436(8)
C(121)-C(122)	1.389(9)	C(221)-C(222)	1.386(8)
C(121)-C(221)	1.509(8)	C(222)-C(223)	1.411(8)
C(122)-C(123)	1.425(8)	C(223)-C(224)	1.382(8)
C(123)-C(124)	1.336(9)	C(223)-H(223)	0.9500
C(123)-H(123)	0.9500	C(224)-C(225)	1.414(8)
C(124)-C(125)	1.402(9)	C(224)-H(224)	0.9500
C(124)-H(124)	0.9500	C(225)-C(226)	1.425(8)
C(125)-C(126)	1.420(9)	C(226)-C(227)	1.372(9)
C(126)-C(127)	1.353(10)	C(226)-H(226)	0.9500
C(126)-H(126)	0.9500	C(227)-C(228)	1.395(9)
C(127)-C(128)	1.400(9)	C(227)-H(227)	0.9500
C(127)-H(127)	0.9500	C(228)-C(229)	1.370(8)
C(128)-C(129)	1.367(9)	C(228)-H(228)	0.9500
C(128)-H(128)	0.9500	C(229)-H(229)	0.9500
C(129)-H(129)	0.9500	C(301)-C(306)	1.434(8)
C(201)-C(206)	1.419(8)	C(301)-C(302)	1.445(8)
C(201)-C(218)	1.450(9)	C(301)-C(318)	1.462(8)
C(201)-C(202)	1.461(8)	C(302)-O(302)	1.299(7)
C(202)-O(202)	1.288(7)	C(302)-C(303)	1.424(8)
C(202)-C(203)	1.439(9)	C(303)-C(304)	1.398(8)
C(203)-C(204)	1.380(9)	C(303)-C(319)	1.448(8)
C(203)-C(219)	1.449(8)	C(304)-C(305)	1.374(8)
C(204)-C(205)	1.381(9)	C(304)-H(304)	0.9500
C(204)-H(204)	0.9500	C(305)-C(306)	1.396(9)
C(205)-C(206)	1.421(9)	C(305)-H(305)	0.9500
C(205)-H(205)	0.9500	C(306)-C(307)	1.441(8)
C(206)-C(207)	1.451(8)	C(307)-C(308)	1.333(9)
C(207)-C(208)	1.331(9)	C(307)-H(307)	0.9500
C(207)-H(207)	0.9500	C(308)-C(309)	1.430(8)
C(208)-C(209)	1.443(9)	C(308)-H(308)	0.9500
C(208)-H(208)	0.9500	C(309)-C(310)	1.367(9)
C(209)-C(210)	1.395(9)	C(309)-C(318)	1.438(8)
C(209)-C(218)	1.437(8)	C(310)-C(311)	1.414(9)
C(210)-C(211)	1.392(9)	C(310)-H(310)	0.9500
C(210)-H(210)	0.9500	C(311)-C(312)	1.411(9)
C(211)-C(212)	1.421(9)	C(311)-C(316)	1.428(8)
C(211)-C(216)	1.440(9)	C(312)-C(313)	1.381(9)
C(212)-C(213)	1.332(9)	C(312)-H(312)	0.9500
C(212)-H(212)	0.9500	C(313)-C(314)	1.409(9)
C(213)-C(214)	1.437(9)	C(313)-H(313)	0.9500
C(213)-H(213)	0.9500	C(314)-C(315)	1.374(9)

C(314)-H(314)	0.9500	C(414)-H(414)	0.9500
C(315)-C(316)	1.438(9)	C(415)-C(416)	1.422(9)
C(315)-H(315)	0.9500	C(415)-H(415)	0.9500
C(316)-C(317)	1.406(8)	C(416)-C(417)	1.402(8)
C(317)-C(318)	1.398(8)	C(417)-C(418)	1.395(8)
C(317)-H(317)	0.9500	C(417)-H(417)	0.9500
C(319)-N(319)	1.299(7)	C(419)-N(419)	1.298(8)
C(319)-H(319)	0.9500	C(419)-H(419)	0.9500
N(319)-C(322)	1.419(7)	N(419)-C(422)	1.437(8)
C(320)-C(329)	1.418(8)	C(420)-C(429)	1.419(8)
C(320)-C(321)	1.428(8)	C(420)-C(421)	1.422(8)
C(320)-C(325)	1.434(8)	C(420)-C(425)	1.427(8)
C(321)-C(322)	1.381(8)	C(421)-C(422)	1.382(8)
C(321)-C(421)	1.497(8)	C(422)-C(423)	1.405(9)
C(322)-C(323)	1.409(8)	C(423)-C(424)	1.374(9)
C(323)-C(324)	1.355(8)	C(423)-H(423)	0.9500
C(323)-H(323)	0.9500	C(424)-C(425)	1.422(9)
C(324)-C(325)	1.418(8)	C(424)-H(424)	0.9500
C(324)-H(324)	0.9500	C(425)-C(426)	1.428(9)
C(325)-C(326)	1.409(8)	C(426)-C(427)	1.358(9)
C(326)-C(327)	1.352(9)	C(426)-H(426)	0.9500
C(326)-H(326)	0.9500	C(427)-C(428)	1.423(9)
C(327)-C(328)	1.405(9)	C(427)-H(427)	0.9500
C(327)-H(327)	0.9500	C(428)-C(429)	1.363(8)
C(328)-C(329)	1.376(8)	C(428)-H(428)	0.9500
C(328)-H(328)	0.9500	C(429)-H(429)	0.9500
C(329)-H(329)	0.9500		
C(401)-C(406)	1.415(9)	O(202)-Zn(1)-O(102)	116.78(18)
C(401)-C(418)	1.463(9)	O(202)-Zn(1)-N(119)	133.4(2)
C(401)-C(402)	1.464(8)	O(102)-Zn(1)-N(119)	95.21(19)
C(402)-O(402)	1.270(7)	O(202)-Zn(1)-N(219)	93.31(18)
C(402)-C(403)	1.435(8)	O(102)-Zn(1)-N(219)	126.38(19)
C(403)-C(404)	1.405(8)	N(119)-Zn(1)-N(219)	93.45(19)
C(403)-C(419)	1.434(9)	O(302)-Zn(2)-O(402)	112.96(17)
C(404)-C(405)	1.373(9)	O(302)-Zn(2)-N(419)	135.4(2)
C(404)-H(404)	0.9500	O(402)-Zn(2)-N(419)	95.49(19)
C(405)-C(406)	1.412(9)	O(302)-Zn(2)-N(319)	93.72(18)
C(405)-H(405)	0.9500	O(402)-Zn(2)-N(319)	128.49(19)
C(406)-C(407)	1.435(9)	N(419)-Zn(2)-N(319)	94.2(2)
C(407)-C(408)	1.351(9)	Cl(2)-C(1S)-Cl(1)	110.8(4)
C(407)-H(407)	0.9500	Cl(2)-C(1S)-H(1A)	109.5
C(408)-C(409)	1.423(9)	Cl(1)-C(1S)-H(1A)	109.5
C(408)-H(408)	0.9500	Cl(2)-C(1S)-H(1B)	109.5
C(409)-C(410)	1.399(9)	Cl(1)-C(1S)-H(1B)	109.5
C(409)-C(418)	1.448(9)	H(1A)-C(1S)-H(1B)	108.1
C(410)-C(411)	1.396(9)	Cl(4)-C(2S)-Cl(3)	112.8(4)
C(410)-H(410)	0.9500	Cl(4)-C(2S)-H(2A)	109.0
C(411)-C(416)	1.420(9)	Cl(3)-C(2S)-H(2A)	109.0
C(411)-C(412)	1.442(9)	Cl(4)-C(2S)-H(2B)	109.0
C(412)-C(413)	1.379(10)	Cl(3)-C(2S)-H(2B)	109.0
C(412)-H(412)	0.9500	H(2A)-C(2S)-H(2B)	107.8
C(413)-C(414)	1.382(10)	C(3S)-O(1S)-C(5S)	115.1(7)
C(413)-H(413)	0.9500	O(1S)-C(3S)-C(4S)	109.6(7)
C(414)-C(415)	1.357(9)	O(1S)-C(3S)-H(3A)	109.8

C(4S)-C(3S)-H(3A)	109.8	C(110)-C(111)-C(112)	123.5(6)
O(1S)-C(3S)-H(3B)	109.8	C(116)-C(111)-C(112)	117.4(6)
C(4S)-C(3S)-H(3B)	109.8	C(113)-C(112)-C(111)	121.4(6)
H(3A)-C(3S)-H(3B)	108.2	C(113)-C(112)-H(112)	119.3
C(3S)-C(4S)-H(4A)	109.5	C(111)-C(112)-H(112)	119.3
C(3S)-C(4S)-H(4B)	109.5	C(112)-C(113)-C(114)	120.4(6)
H(4A)-C(4S)-H(4B)	109.5	C(112)-C(113)-H(113)	119.8
C(3S)-C(4S)-H(4C)	109.5	C(114)-C(113)-H(113)	119.8
H(4A)-C(4S)-H(4C)	109.5	C(115)-C(114)-C(113)	121.2(6)
H(4B)-C(4S)-H(4C)	109.5	C(115)-C(114)-H(114)	119.4
C(6S)-C(5S)-O(1S)	112.2(6)	C(113)-C(114)-H(114)	119.4
C(6S)-C(5S)-H(5A)	109.2	C(114)-C(115)-C(116)	121.0(6)
O(1S)-C(5S)-H(5A)	109.2	C(114)-C(115)-H(115)	119.5
C(6S)-C(5S)-H(5B)	109.2	C(116)-C(115)-H(115)	119.5
O(1S)-C(5S)-H(5B)	109.2	C(117)-C(116)-C(111)	119.2(5)
H(5A)-C(5S)-H(5B)	107.9	C(117)-C(116)-C(115)	122.3(6)
C(5S)-C(6S)-H(6A)	109.5	C(111)-C(116)-C(115)	118.5(5)
C(5S)-C(6S)-H(6B)	109.5	C(118)-C(117)-C(116)	122.7(5)
H(6A)-C(6S)-H(6B)	109.5	C(118)-C(117)-H(117)	118.7
C(5S)-C(6S)-H(6C)	109.5	C(116)-C(117)-H(117)	118.7
H(6A)-C(6S)-H(6C)	109.5	C(117)-C(118)-C(109)	116.5(5)
H(6B)-C(6S)-H(6C)	109.5	C(117)-C(118)-C(101)	125.1(6)
C(106)-C(101)-C(102)	117.8(5)	C(109)-C(118)-C(101)	118.4(5)
C(106)-C(101)-C(118)	118.9(5)	N(119)-C(119)-C(103)	127.3(5)
C(102)-C(101)-C(118)	123.3(5)	N(119)-C(119)-H(119)	116.3
O(102)-C(102)-C(101)	119.1(5)	C(103)-C(119)-H(119)	116.3
O(102)-C(102)-C(103)	121.9(5)	C(119)-N(119)-C(122)	121.8(5)
C(101)-C(102)-C(103)	119.0(5)	C(119)-N(119)-Zn(1)	118.8(4)
C(102)-O(102)-Zn(1)	127.4(4)	C(122)-N(119)-Zn(1)	114.7(4)
C(119)-C(103)-C(104)	115.9(5)	C(121)-C(120)-C(129)	123.0(5)
C(119)-C(103)-C(102)	124.4(5)	C(121)-C(120)-C(125)	118.2(5)
C(104)-C(103)-C(102)	119.6(6)	C(129)-C(120)-C(125)	118.8(5)
C(105)-C(104)-C(103)	120.7(6)	C(122)-C(121)-C(120)	120.8(5)
C(105)-C(104)-H(104)	119.6	C(122)-C(121)-C(221)	116.9(5)
C(103)-C(104)-H(104)	119.6	C(120)-C(121)-C(221)	121.9(6)
C(104)-C(105)-C(106)	120.7(5)	C(121)-C(122)-N(119)	120.6(5)
C(104)-C(105)-H(105)	119.7	C(121)-C(122)-C(123)	119.6(5)
C(106)-C(105)-H(105)	119.7	N(119)-C(122)-C(123)	119.5(5)
C(101)-C(106)-C(105)	121.5(6)	C(124)-C(123)-C(122)	120.4(6)
C(101)-C(106)-C(107)	120.5(5)	C(124)-C(123)-H(123)	119.8
C(105)-C(106)-C(107)	118.0(5)	C(122)-C(123)-H(123)	119.8
C(108)-C(107)-C(106)	121.6(5)	C(123)-C(124)-C(125)	121.7(6)
C(108)-C(107)-H(107)	119.2	C(123)-C(124)-H(124)	119.1
C(106)-C(107)-H(107)	119.2	C(125)-C(124)-H(124)	119.1
C(107)-C(108)-C(109)	120.8(6)	C(124)-C(125)-C(126)	123.7(5)
C(107)-C(108)-H(108)	119.6	C(124)-C(125)-C(120)	119.2(5)
C(109)-C(108)-H(108)	119.6	C(126)-C(125)-C(120)	117.1(6)
C(110)-C(109)-C(108)	118.8(6)	C(127)-C(126)-C(125)	122.3(6)
C(110)-C(109)-C(118)	121.4(6)	C(127)-C(126)-H(126)	118.9
C(108)-C(109)-C(118)	119.8(6)	C(125)-C(126)-H(126)	118.9
C(111)-C(110)-C(109)	121.3(6)	C(126)-C(127)-C(128)	120.4(6)
C(111)-C(110)-H(110)	119.4	C(126)-C(127)-H(127)	119.8
C(109)-C(110)-H(110)	119.4	C(128)-C(127)-H(127)	119.8
C(110)-C(111)-C(116)	119.1(6)	C(129)-C(128)-C(127)	120.0(6)

C(129)-C(128)-H(128)	120.0	C(218)-C(217)-C(216)	122.9(5)
C(127)-C(128)-H(128)	120.0	C(218)-C(217)-H(217)	118.6
C(128)-C(129)-C(120)	121.3(5)	C(216)-C(217)-H(217)	118.6
C(128)-C(129)-H(129)	119.3	C(217)-C(218)-C(209)	117.0(5)
C(120)-C(129)-H(129)	119.3	C(217)-C(218)-C(201)	125.3(5)
C(206)-C(201)-C(218)	120.0(5)	C(209)-C(218)-C(201)	117.6(5)
C(206)-C(201)-C(202)	116.7(6)	N(219)-C(219)-C(203)	127.7(5)
C(218)-C(201)-C(202)	123.3(5)	N(219)-C(219)-H(219)	116.1
O(202)-C(202)-C(203)	123.2(5)	C(203)-C(219)-H(219)	116.1
O(202)-C(202)-C(201)	117.7(5)	C(219)-N(219)-C(222)	124.0(5)
C(203)-C(202)-C(201)	119.1(5)	C(219)-N(219)-Zn(1)	121.3(4)
C(202)-O(202)-Zn(1)	129.0(4)	C(222)-N(219)-Zn(1)	113.0(3)
C(204)-C(203)-C(202)	120.5(5)	C(225)-C(220)-C(229)	118.9(5)
C(204)-C(203)-C(219)	116.5(6)	C(225)-C(220)-C(221)	119.4(5)
C(202)-C(203)-C(219)	122.9(5)	C(229)-C(220)-C(221)	121.6(5)
C(203)-C(204)-C(205)	121.8(6)	C(222)-C(221)-C(220)	118.4(5)
C(203)-C(204)-H(204)	119.1	C(222)-C(221)-C(121)	120.2(5)
C(205)-C(204)-H(204)	119.1	C(220)-C(221)-C(121)	121.2(5)
C(204)-C(205)-C(206)	119.2(5)	C(221)-C(222)-C(223)	122.0(5)
C(204)-C(205)-H(205)	120.4	C(221)-C(222)-N(219)	119.3(5)
C(206)-C(205)-H(205)	120.4	C(223)-C(222)-N(219)	118.2(5)
C(201)-C(206)-C(205)	122.2(5)	C(224)-C(223)-C(222)	120.0(5)
C(201)-C(206)-C(207)	119.6(6)	C(224)-C(223)-H(223)	120.0
C(205)-C(206)-C(207)	118.2(5)	C(222)-C(223)-H(223)	120.0
C(208)-C(207)-C(206)	121.0(6)	C(223)-C(224)-C(225)	119.9(6)
C(208)-C(207)-H(207)	119.5	C(223)-C(224)-H(224)	120.1
C(206)-C(207)-H(207)	119.5	C(225)-C(224)-H(224)	120.1
C(207)-C(208)-C(209)	121.2(6)	C(224)-C(225)-C(220)	120.2(5)
C(207)-C(208)-H(208)	119.4	C(224)-C(225)-C(226)	120.8(6)
C(209)-C(208)-H(208)	119.4	C(220)-C(225)-C(226)	119.0(5)
C(210)-C(209)-C(218)	120.5(6)	C(227)-C(226)-C(225)	120.4(6)
C(210)-C(209)-C(208)	119.0(6)	C(227)-C(226)-H(226)	119.8
C(218)-C(209)-C(208)	120.4(6)	C(225)-C(226)-H(226)	119.8
C(211)-C(210)-C(209)	122.2(6)	C(226)-C(227)-C(228)	120.4(6)
C(211)-C(210)-H(210)	118.9	C(226)-C(227)-H(227)	119.8
C(209)-C(210)-H(210)	118.9	C(228)-C(227)-H(227)	119.8
C(210)-C(211)-C(212)	124.4(6)	C(229)-C(228)-C(227)	121.3(6)
C(210)-C(211)-C(216)	117.5(6)	C(229)-C(228)-H(228)	119.4
C(212)-C(211)-C(216)	118.0(6)	C(227)-C(228)-H(228)	119.4
C(213)-C(212)-C(211)	122.1(6)	C(228)-C(229)-C(220)	120.0(5)
C(213)-C(212)-H(212)	118.9	C(228)-C(229)-H(229)	120.0
C(211)-C(212)-H(212)	118.9	C(220)-C(229)-H(229)	120.0
C(212)-C(213)-C(214)	120.0(6)	C(306)-C(301)-C(302)	116.8(5)
C(212)-C(213)-H(213)	120.0	C(306)-C(301)-C(318)	119.3(5)
C(214)-C(213)-H(213)	120.0	C(302)-C(301)-C(318)	123.9(5)
C(215)-C(214)-C(213)	120.5(6)	O(302)-C(302)-C(303)	122.8(5)
C(215)-C(214)-H(214)	119.7	O(302)-C(302)-C(301)	117.6(5)
C(213)-C(214)-H(214)	119.7	C(303)-C(302)-C(301)	119.6(5)
C(214)-C(215)-C(216)	121.0(6)	C(302)-O(302)-Zn(2)	128.7(4)
C(214)-C(215)-H(215)	119.5	C(304)-C(303)-C(302)	120.2(5)
C(216)-C(215)-H(215)	119.5	C(304)-C(303)-C(319)	115.4(5)
C(217)-C(216)-C(215)	121.9(5)	C(302)-C(303)-C(319)	124.4(5)
C(217)-C(216)-C(211)	119.8(6)	C(305)-C(304)-C(303)	120.8(6)
C(215)-C(216)-C(211)	118.3(6)	C(305)-C(304)-H(304)	119.6

C(303)-C(304)-H(304)	119.6	C(320)-C(321)-C(421)	121.4(5)
C(304)-C(305)-C(306)	120.5(5)	C(321)-C(322)-C(323)	121.2(5)
C(304)-C(305)-H(305)	119.8	C(321)-C(322)-N(319)	119.2(5)
C(306)-C(305)-H(305)	119.8	C(323)-C(322)-N(319)	118.7(5)
C(305)-C(306)-C(301)	121.6(5)	C(324)-C(323)-C(322)	120.6(5)
C(305)-C(306)-C(307)	119.2(5)	C(324)-C(323)-H(323)	119.7
C(301)-C(306)-C(307)	119.1(5)	C(322)-C(323)-H(323)	119.7
C(308)-C(307)-C(306)	121.5(5)	C(323)-C(324)-C(325)	121.2(5)
C(308)-C(307)-H(307)	119.3	C(323)-C(324)-H(324)	119.4
C(306)-C(307)-H(307)	119.3	C(325)-C(324)-H(324)	119.4
C(307)-C(308)-C(309)	122.2(5)	C(326)-C(325)-C(324)	122.9(5)
C(307)-C(308)-H(308)	118.9	C(326)-C(325)-C(320)	118.8(5)
C(309)-C(308)-H(308)	118.9	C(324)-C(325)-C(320)	118.2(5)
C(310)-C(309)-C(308)	119.6(5)	C(327)-C(326)-C(325)	121.6(6)
C(310)-C(309)-C(318)	120.8(5)	C(327)-C(326)-H(326)	119.2
C(308)-C(309)-C(318)	119.6(6)	C(325)-C(326)-H(326)	119.2
C(309)-C(310)-C(311)	123.3(5)	C(326)-C(327)-C(328)	120.3(5)
C(309)-C(310)-H(310)	118.3	C(326)-C(327)-H(327)	119.8
C(311)-C(310)-H(310)	118.3	C(328)-C(327)-H(327)	119.8
C(312)-C(311)-C(310)	124.2(5)	C(329)-C(328)-C(327)	120.3(5)
C(312)-C(311)-C(316)	119.7(6)	C(329)-C(328)-H(328)	119.8
C(310)-C(311)-C(316)	116.0(5)	C(327)-C(328)-H(328)	119.8
C(313)-C(312)-C(311)	120.6(6)	C(328)-C(329)-C(320)	120.8(5)
C(313)-C(312)-H(312)	119.7	C(328)-C(329)-H(329)	119.6
C(311)-C(312)-H(312)	119.7	C(320)-C(329)-H(329)	119.6
C(312)-C(313)-C(314)	120.5(6)	C(406)-C(401)-C(418)	118.8(5)
C(312)-C(313)-H(313)	119.8	C(406)-C(401)-C(402)	118.6(5)
C(314)-C(313)-H(313)	119.8	C(418)-C(401)-C(402)	122.6(5)
C(315)-C(314)-C(313)	120.5(6)	O(402)-C(402)-C(403)	123.8(5)
C(315)-C(314)-H(314)	119.8	O(402)-C(402)-C(401)	118.7(5)
C(313)-C(314)-H(314)	119.8	C(403)-C(402)-C(401)	117.5(5)
C(314)-C(315)-C(316)	120.6(6)	C(402)-O(402)-Zn(2)	127.5(4)
C(314)-C(315)-H(315)	119.7	C(404)-C(403)-C(419)	115.6(5)
C(316)-C(315)-H(315)	119.7	C(404)-C(403)-C(402)	120.9(5)
C(317)-C(316)-C(311)	120.8(6)	C(419)-C(403)-C(402)	123.5(5)
C(317)-C(316)-C(315)	120.9(5)	C(405)-C(404)-C(403)	120.8(6)
C(311)-C(316)-C(315)	118.1(5)	C(405)-C(404)-H(404)	119.6
C(318)-C(317)-C(316)	122.1(5)	C(403)-C(404)-H(404)	119.6
C(318)-C(317)-H(317)	118.9	C(404)-C(405)-C(406)	120.5(5)
C(316)-C(317)-H(317)	118.9	C(404)-C(405)-H(405)	119.8
C(317)-C(318)-C(309)	116.8(5)	C(406)-C(405)-H(405)	119.8
C(317)-C(318)-C(301)	124.9(5)	C(405)-C(406)-C(401)	121.1(6)
C(309)-C(318)-C(301)	118.3(5)	C(405)-C(406)-C(407)	118.3(6)
N(319)-C(319)-C(303)	126.0(5)	C(401)-C(406)-C(407)	120.7(6)
N(319)-C(319)-H(319)	117.0	C(408)-C(407)-C(406)	120.7(6)
C(303)-C(319)-H(319)	117.0	C(408)-C(407)-H(407)	119.7
C(319)-N(319)-C(322)	122.4(5)	C(406)-C(407)-H(407)	119.7
C(319)-N(319)-Zn(2)	120.9(4)	C(407)-C(408)-C(409)	121.8(6)
C(322)-N(319)-Zn(2)	114.6(4)	C(407)-C(408)-H(408)	119.1
C(329)-C(320)-C(321)	122.0(5)	C(409)-C(408)-H(408)	119.1
C(329)-C(320)-C(325)	118.1(5)	C(410)-C(409)-C(408)	119.2(6)
C(321)-C(320)-C(325)	119.8(5)	C(410)-C(409)-C(418)	121.1(6)
C(322)-C(321)-C(320)	118.9(5)	C(408)-C(409)-C(418)	119.6(6)
C(322)-C(321)-C(421)	119.6(5)	C(411)-C(410)-C(409)	120.6(6)

C(411)-C(410)-H(410)	119.7	C(422)-N(419)-Zn(2)	115.4(4)
C(409)-C(410)-H(410)	119.7	C(429)-C(420)-C(421)	122.6(5)
C(410)-C(411)-C(416)	119.6(5)	C(429)-C(420)-C(425)	118.2(5)
C(410)-C(411)-C(412)	121.4(6)	C(421)-C(420)-C(425)	119.2(5)
C(416)-C(411)-C(412)	119.0(5)	C(422)-C(421)-C(420)	119.5(5)
C(413)-C(412)-C(411)	119.8(6)	C(422)-C(421)-C(321)	119.6(5)
C(413)-C(412)-H(412)	120.1	C(420)-C(421)-C(321)	120.6(5)
C(411)-C(412)-H(412)	120.1	C(421)-C(422)-C(423)	121.1(6)
C(412)-C(413)-C(414)	120.2(6)	C(421)-C(422)-N(419)	118.6(5)
C(412)-C(413)-H(413)	119.9	C(423)-C(422)-N(419)	119.3(5)
C(414)-C(413)-H(413)	119.9	C(424)-C(423)-C(422)	120.9(6)
C(415)-C(414)-C(413)	121.8(6)	C(424)-C(423)-H(423)	119.6
C(415)-C(414)-H(414)	119.1	C(422)-C(423)-H(423)	119.6
C(413)-C(414)-H(414)	119.1	C(423)-C(424)-C(425)	119.6(6)
C(414)-C(415)-C(416)	120.9(6)	C(423)-C(424)-H(424)	120.2
C(414)-C(415)-H(415)	119.6	C(425)-C(424)-H(424)	120.2
C(416)-C(415)-H(415)	119.6	C(424)-C(425)-C(420)	119.7(5)
C(417)-C(416)-C(411)	118.7(5)	C(424)-C(425)-C(426)	121.0(5)
C(417)-C(416)-C(415)	123.0(6)	C(420)-C(425)-C(426)	119.4(5)
C(411)-C(416)-C(415)	118.2(5)	C(427)-C(426)-C(425)	120.6(5)
C(418)-C(417)-C(416)	123.7(6)	C(427)-C(426)-H(426)	119.7
C(418)-C(417)-H(417)	118.1	C(425)-C(426)-H(426)	119.7
C(416)-C(417)-H(417)	118.1	C(426)-C(427)-C(428)	120.1(6)
C(417)-C(418)-C(409)	116.0(6)	C(426)-C(427)-H(427)	120.0
C(417)-C(418)-C(401)	125.5(6)	C(428)-C(427)-H(427)	120.0
C(409)-C(418)-C(401)	118.4(5)	C(429)-C(428)-C(427)	120.6(6)
N(419)-C(419)-C(403)	127.4(5)	C(429)-C(428)-H(428)	119.7
N(419)-C(419)-H(419)	116.3	C(427)-C(428)-H(428)	119.7
C(403)-C(419)-H(419)	116.3	C(428)-C(429)-C(420)	121.1(5)
C(419)-N(419)-C(422)	122.1(5)	C(428)-C(429)-H(429)	119.4
C(419)-N(419)-Zn(2)	120.2(4)	C(420)-C(429)-H(429)	119.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**77**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zn(1)	17(1)	31(1)	18(1)	3(1)	9(1)	-1(1)
Zn(2)	18(1)	37(1)	16(1)	0(1)	9(1)	-4(1)
C(1S)	33(4)	31(3)	28(3)	0(3)	19(3)	-1(3)
Cl(1)	46(1)	34(1)	39(1)	-5(1)	24(1)	1(1)
Cl(2)	92(2)	39(1)	56(1)	-15(1)	57(1)	-25(1)
C(2S)	62(5)	27(4)	40(4)	4(3)	35(4)	10(3)
Cl(3)	72(1)	35(1)	59(1)	9(1)	50(1)	18(1)
Cl(4)	54(1)	52(1)	93(2)	33(1)	54(1)	22(1)
O(1S)	55(3)	42(3)	52(3)	-9(2)	40(3)	-12(2)
C(3S)	44(5)	109(8)	34(4)	7(5)	9(4)	21(5)
C(4S)	40(4)	49(4)	25(3)	-6(3)	17(3)	1(3)

C(5S)	58(5)	40(4)	65(5)	-7(4)	45(5)	-1(4)
C(6S)	44(4)	28(4)	76(6)	-2(4)	37(4)	2(3)
C(101)	30(3)	12(3)	24(3)	0(2)	15(3)	3(2)
C(102)	21(3)	22(3)	25(3)	0(2)	12(3)	-2(2)
O(102)	23(2)	29(2)	25(2)	4(2)	15(2)	3(2)
C(103)	21(3)	22(3)	27(3)	-5(2)	15(3)	-4(2)
C(104)	28(3)	23(3)	31(3)	-7(2)	20(3)	-4(2)
C(105)	29(3)	29(3)	25(3)	4(2)	20(3)	-1(2)
C(106)	28(3)	20(3)	25(3)	-7(2)	16(3)	-5(2)
C(107)	36(4)	21(3)	25(3)	0(2)	19(3)	-1(3)
C(108)	43(4)	22(3)	21(3)	-1(2)	14(3)	-3(3)
C(109)	25(3)	16(3)	22(3)	1(2)	5(3)	-3(2)
C(110)	31(4)	21(3)	23(3)	-4(2)	6(3)	2(3)
C(111)	27(3)	12(3)	30(3)	-5(2)	12(3)	-1(2)
C(112)	23(3)	22(3)	31(3)	-2(3)	2(3)	6(2)
C(113)	28(3)	31(4)	52(4)	-3(3)	23(3)	2(3)
C(114)	32(4)	35(4)	38(4)	-4(3)	21(3)	-1(3)
C(115)	26(3)	33(3)	25(3)	-2(3)	12(3)	-3(3)
C(116)	23(3)	19(3)	26(3)	-6(2)	10(3)	-3(2)
C(117)	26(3)	14(3)	17(3)	2(2)	6(2)	1(2)
C(118)	27(3)	16(3)	35(3)	-5(2)	23(3)	-7(2)
C(119)	14(3)	26(3)	23(3)	-8(3)	9(2)	0(2)
N(119)	16(2)	27(3)	22(2)	-4(2)	6(2)	0(2)
C(120)	22(3)	20(3)	20(3)	3(2)	12(2)	4(2)
C(121)	22(3)	20(3)	31(3)	4(2)	17(3)	1(2)
C(122)	21(3)	19(3)	25(3)	2(2)	16(3)	1(2)
C(123)	25(3)	27(3)	24(3)	-8(2)	9(3)	-10(2)
C(124)	31(3)	18(3)	37(4)	-1(3)	19(3)	0(2)
C(125)	26(3)	15(3)	32(3)	3(2)	19(3)	1(2)
C(126)	34(4)	27(3)	35(3)	15(3)	25(3)	11(3)
C(127)	30(3)	30(3)	17(3)	13(2)	8(3)	7(3)
C(128)	18(3)	44(4)	20(3)	-5(3)	8(3)	-4(3)
C(129)	24(3)	21(3)	30(3)	1(2)	17(3)	1(2)
C(201)	31(3)	16(3)	29(3)	0(2)	20(3)	4(2)
C(202)	20(3)	17(3)	24(3)	0(2)	11(2)	-4(2)
O(202)	26(2)	35(2)	25(2)	4(2)	17(2)	-7(2)
C(203)	25(3)	27(3)	32(3)	5(3)	17(3)	9(2)
C(204)	18(3)	43(4)	17(3)	2(3)	2(2)	-6(3)
C(205)	34(4)	48(4)	16(3)	4(3)	15(3)	-1(3)
C(206)	35(4)	28(3)	29(3)	7(3)	23(3)	2(3)
C(207)	28(4)	44(4)	23(3)	-1(3)	18(3)	2(3)
C(208)	31(3)	25(3)	33(3)	6(3)	22(3)	3(3)
C(209)	26(3)	23(3)	26(3)	-1(2)	13(3)	6(2)
C(210)	20(3)	22(3)	41(4)	-1(3)	20(3)	0(2)
C(211)	29(3)	15(3)	32(3)	-3(2)	18(3)	9(2)
C(212)	25(3)	18(3)	35(3)	-3(3)	12(3)	-1(2)
C(213)	13(3)	24(3)	35(3)	-9(3)	5(3)	2(2)
C(214)	35(4)	19(3)	27(3)	1(2)	13(3)	7(3)
C(215)	25(3)	22(3)	28(3)	0(2)	13(3)	5(2)
C(216)	27(3)	19(3)	33(3)	-2(2)	17(3)	0(2)
C(217)	25(3)	16(3)	29(3)	-2(2)	17(3)	0(2)
C(218)	25(3)	14(3)	28(3)	2(2)	16(3)	7(2)
C(219)	16(3)	22(3)	21(3)	1(2)	5(2)	3(2)
N(219)	18(2)	25(3)	17(2)	-3(2)	5(2)	-2(2)

C(220)	17(3)	21(3)	14(3)	0(2)	3(2)	-2(2)
C(221)	17(3)	18(3)	10(3)	0(2)	-1(2)	-5(2)
C(222)	12(3)	20(3)	16(3)	1(2)	0(2)	1(2)
C(223)	14(3)	26(3)	22(3)	2(2)	5(2)	0(2)
C(224)	23(3)	19(3)	25(3)	2(2)	8(3)	-1(2)
C(225)	27(3)	22(3)	22(3)	-3(2)	12(3)	-4(2)
C(226)	26(3)	23(3)	28(3)	3(2)	8(3)	-5(2)
C(227)	31(3)	23(3)	39(4)	3(3)	21(3)	-3(3)
C(228)	33(4)	32(3)	30(3)	2(3)	21(3)	1(3)
C(229)	31(3)	16(3)	28(3)	-3(2)	17(3)	-1(2)
C(301)	22(3)	16(3)	25(3)	-1(2)	10(3)	0(2)
C(302)	21(3)	17(3)	22(3)	-8(2)	10(2)	-7(2)
O(302)	17(2)	38(2)	23(2)	6(2)	11(2)	-2(2)
C(303)	26(3)	17(3)	25(3)	-2(2)	16(3)	-2(2)
C(304)	18(3)	25(3)	22(3)	-3(2)	6(2)	2(2)
C(305)	22(3)	25(3)	29(3)	-2(2)	15(3)	-5(2)
C(306)	28(3)	15(3)	27(3)	-2(2)	17(3)	-3(2)
C(307)	26(3)	22(3)	31(3)	-4(2)	19(3)	-6(2)
C(308)	34(3)	18(3)	32(3)	-1(2)	26(3)	-5(2)
C(309)	35(3)	15(3)	32(3)	-4(2)	23(3)	4(2)
C(310)	39(4)	15(3)	26(3)	0(2)	27(3)	1(2)
C(311)	33(3)	20(3)	20(3)	-2(2)	16(3)	1(2)
C(312)	41(4)	27(3)	25(3)	2(3)	19(3)	2(3)
C(313)	34(4)	27(3)	17(3)	-1(2)	7(3)	1(3)
C(314)	23(3)	24(3)	32(3)	-5(3)	10(3)	-6(2)
C(315)	27(3)	26(3)	26(3)	3(3)	14(3)	-1(3)
C(316)	31(3)	24(3)	21(3)	-2(2)	16(3)	-3(2)
C(317)	26(3)	21(3)	20(3)	-1(2)	14(3)	2(2)
C(318)	32(3)	11(3)	21(3)	-7(2)	16(3)	-5(2)
C(319)	20(3)	20(3)	16(3)	-4(2)	5(2)	2(2)
N(319)	20(2)	22(2)	19(2)	-1(2)	10(2)	-2(2)
C(320)	17(3)	21(3)	14(3)	2(2)	6(2)	-1(2)
C(321)	17(3)	20(3)	22(3)	-3(2)	7(2)	-2(2)
C(322)	16(3)	26(3)	15(3)	0(2)	4(2)	-4(2)
C(323)	25(3)	27(3)	14(3)	-3(2)	8(2)	-1(2)
C(324)	26(3)	11(3)	22(3)	-2(2)	11(3)	-1(2)
C(325)	21(3)	22(3)	19(3)	-1(2)	11(2)	1(2)
C(326)	25(3)	23(3)	25(3)	5(2)	11(3)	1(2)
C(327)	32(3)	22(3)	37(3)	2(3)	26(3)	-3(3)
C(328)	29(3)	27(3)	23(3)	-1(2)	17(3)	2(2)
C(329)	25(3)	21(3)	27(3)	1(2)	13(3)	-2(2)
C(401)	21(3)	16(3)	25(3)	7(2)	4(3)	3(2)
C(402)	25(3)	21(3)	21(3)	0(2)	12(3)	-1(2)
O(402)	26(2)	39(3)	21(2)	-2(2)	15(2)	-4(2)
C(403)	28(3)	18(3)	24(3)	-2(2)	15(3)	3(2)
C(404)	31(3)	20(3)	33(3)	-2(3)	21(3)	-2(2)
C(405)	26(3)	28(3)	30(3)	5(3)	17(3)	0(3)
C(406)	26(3)	20(3)	34(3)	5(3)	16(3)	1(2)
C(407)	21(3)	28(3)	38(4)	-1(3)	17(3)	-6(3)
C(408)	21(3)	20(3)	34(3)	4(3)	7(3)	-1(2)
C(409)	25(3)	22(3)	32(3)	9(3)	16(3)	5(2)
C(410)	20(3)	19(3)	24(3)	-2(2)	-5(3)	1(2)
C(411)	29(3)	18(3)	26(3)	0(2)	14(3)	1(2)
C(412)	34(4)	21(3)	26(3)	-5(2)	10(3)	1(3)

C(413)	43(4)	26(3)	20(3)	1(3)	13(3)	8(3)
C(414)	43(4)	27(3)	30(3)	2(3)	24(3)	8(3)
C(415)	26(3)	22(3)	29(3)	0(2)	13(3)	5(2)
C(416)	32(3)	15(3)	26(3)	0(2)	15(3)	2(2)
C(417)	21(3)	24(3)	22(3)	-2(2)	9(3)	-2(2)
C(418)	24(3)	16(3)	27(3)	5(2)	9(3)	3(2)
C(419)	30(3)	20(3)	22(3)	4(2)	17(3)	3(2)
N(419)	27(3)	26(3)	25(3)	3(2)	16(2)	2(2)
C(420)	21(3)	24(3)	15(3)	0(2)	12(2)	-2(2)
C(421)	29(3)	20(3)	16(3)	1(2)	14(3)	-3(2)
C(422)	27(3)	30(3)	16(3)	-3(2)	15(3)	-3(2)
C(423)	31(3)	23(3)	25(3)	6(2)	19(3)	6(2)
C(424)	35(4)	25(3)	28(3)	1(3)	22(3)	-1(3)
C(425)	37(3)	22(3)	27(3)	0(2)	26(3)	0(2)
C(426)	28(3)	16(3)	27(3)	-3(2)	17(3)	-3(2)
C(427)	29(3)	35(4)	33(4)	-8(3)	18(3)	-12(3)
C(428)	21(3)	19(3)	28(3)	-4(2)	10(3)	0(2)
C(429)	24(3)	21(3)	18(3)	2(2)	11(2)	2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**77**.

	x	y	z	U(eq)
H(1A)	2959	2703	5011	35
H(1B)	1717	2666	3743	35
H(2A)	3123	2626	1779	46
H(2B)	1931	2600	471	46
H(3A)	-1758	5097	1622	80
H(3B)	-668	5401	1846	80
H(4A)	94	4743	2478	56
H(4B)	298	4878	1379	56
H(4C)	-793	4575	1143	56
H(5A)	-3142	5557	53	57
H(5B)	-1989	5838	349	57
H(6A)	-3513	5937	-1584	69
H(6B)	-3485	5466	-1874	69
H(6C)	-2336	5749	-1578	69
H(104)	-498	1283	4747	30
H(105)	901	1025	6586	30
H(107)	2930	813	8012	30
H(108)	4907	654	8537	36
H(110)	6489	570	8025	34
H(112)	8238	518	7570	36
H(113)	8889	544	6191	43
H(114)	7533	723	4168	40
H(115)	5559	883	3551	34
H(117)	3867	979	4030	25
H(119)	-1010	1556	2901	26

H(123)	-286	2490	1829	32
H(124)	-1599	2840	143	34
H(126)	-3432	2852	-1946	34
H(127)	-4942	2517	-3569	33
H(128)	-5098	1807	-3550	33
H(129)	-3757	1441	-1862	28
H(204)	39	1645	-2644	34
H(205)	1480	1996	-2933	38
H(207)	3496	2300	-2138	36
H(208)	5353	2471	-580	32
H(210)	6912	2400	1503	31
H(212)	8581	2339	3682	33
H(213)	9192	2135	5603	32
H(214)	7793	1801	6071	34
H(215)	5814	1696	4603	30
H(217)	4191	1754	2470	26
H(219)	-656	1336	-1501	25
H(223)	-272	481	95	27
H(224)	-1600	108	510	29
H(226)	-3245	92	1054	33
H(227)	-4655	432	1403	36
H(228)	-4884	1135	1151	36
H(229)	-3715	1507	553	29
H(304)	-4347	3776	-1341	28
H(305)	-4661	3457	108	29
H(307)	-3926	3220	2155	29
H(308)	-2391	3079	4035	28
H(310)	-296	3074	5515	27
H(312)	1928	3053	7154	36
H(313)	3963	3180	7734	34
H(314)	4488	3488	6381	34
H(315)	2991	3647	4429	31
H(317)	816	3660	2849	26
H(319)	-3173	4104	-1981	25
H(323)	-1480	4976	-1486	27
H(324)	-1129	5350	-2807	25
H(326)	-581	5375	-4459	30
H(327)	-276	5050	-5882	32
H(328)	-498	4342	-6115	29
H(329)	-1001	3962	-4885	29
H(404)	3406	4098	-1432	31
H(405)	5171	4431	-55	32
H(407)	6483	4707	1928	34
H(408)	6875	4873	3832	33
H(410)	6312	4898	5385	34
H(412)	5835	4867	7073	35
H(413)	4421	4732	7710	37
H(414)	2434	4551	6317	36
H(415)	1848	4443	4324	31
H(417)	2388	4418	2679	28
H(419)	1525	3831	-2050	27
H(423)	229	2969	-1540	29
H(424)	-1493	2614	-2921	32
H(426)	-3616	2620	-4669	26

H(427)	-5268	2972	-6133	38
H(428)	-5180	3687	-6264	29
H(429)	-3448	4039	-4944	25

Table 6. Torsion angles [°] for (*R*)-**77**.

C(5S)-O(1S)-C(3S)-C(4S)	-176.1(7)	C(114)-C(115)-C(116)-C(111)	-0.9(9)
C(3S)-O(1S)-C(5S)-C(6S)	176.3(8)	C(111)-C(116)-C(117)-C(118)	-0.3(8)
C(106)-C(101)-C(102)-O(102)	-176.6(5)	C(115)-C(116)-C(117)-C(118)	179.6(6)
C(118)-C(101)-C(102)-O(102)	5.6(8)	C(116)-C(117)-C(118)-C(109)	-1.2(8)
C(106)-C(101)-C(102)-C(103)	4.2(8)	C(116)-C(117)-C(118)-C(101)	178.5(5)
C(118)-C(101)-C(102)-C(103)	-173.6(5)	C(110)-C(109)-C(118)-C(117)	1.3(8)
C(101)-C(102)-O(102)-Zn(1)	-162.3(4)	C(108)-C(109)-C(118)-C(117)	180.0(5)
C(103)-C(102)-O(102)-Zn(1)	16.8(8)	C(110)-C(109)-C(118)-C(101)	-178.4(5)
O(202)-Zn(1)-O(102)-C(102)	141.2(5)	C(108)-C(109)-C(118)-C(101)	0.2(8)
N(119)-Zn(1)-O(102)-C(102)	-3.7(5)	C(106)-C(101)-C(118)-C(117)	179.0(5)
N(219)-Zn(1)-O(102)-C(102)	-101.9(5)	C(102)-C(101)-C(118)-C(117)	-3.1(9)
O(102)-C(102)-C(103)-C(119)	-12.3(9)	C(106)-C(101)-C(118)-C(109)	-1.3(8)
C(101)-C(102)-C(103)-C(119)	166.9(5)	C(102)-C(101)-C(118)-C(109)	176.6(5)
O(102)-C(102)-C(103)-C(104)	171.5(5)	C(104)-C(103)-C(119)-N(119)	165.2(6)
C(101)-C(102)-C(103)-C(104)	-9.4(8)	C(102)-C(103)-C(119)-N(119)	-11.1(10)
C(119)-C(103)-C(104)-C(105)	-168.7(6)	C(103)-C(119)-N(119)-C(122)	178.7(6)
C(102)-C(103)-C(104)-C(105)	7.9(9)	C(103)-C(119)-N(119)-Zn(1)	24.5(8)
C(103)-C(104)-C(105)-C(106)	-1.2(9)	O(202)-Zn(1)-N(119)-C(119)	-150.9(4)
C(102)-C(101)-C(106)-C(105)	2.4(8)	O(102)-Zn(1)-N(119)-C(119)	-15.8(5)
C(118)-C(101)-C(106)-C(105)	-179.6(5)	N(219)-Zn(1)-N(119)-C(119)	111.2(4)
C(102)-C(101)-C(106)-C(107)	-176.9(5)	O(202)-Zn(1)-N(119)-C(122)	53.1(5)
C(118)-C(101)-C(106)-C(107)	1.1(8)	O(102)-Zn(1)-N(119)-C(122)	-171.8(4)
C(104)-C(105)-C(106)-C(101)	-4.1(9)	N(219)-Zn(1)-N(119)-C(122)	-44.8(4)
C(104)-C(105)-C(106)-C(107)	175.2(6)	C(129)-C(120)-C(121)-C(122)	180.0(5)
C(101)-C(106)-C(107)-C(108)	0.1(9)	C(125)-C(120)-C(121)-C(122)	-1.6(8)
C(105)-C(106)-C(107)-C(108)	-179.2(6)	C(129)-C(120)-C(121)-C(221)	7.4(9)
C(106)-C(107)-C(108)-C(109)	-1.2(9)	C(125)-C(120)-C(121)-C(221)	-174.3(5)
C(107)-C(108)-C(109)-C(110)	179.7(6)	C(120)-C(121)-C(122)-N(119)	-171.4(5)
C(107)-C(108)-C(109)-C(118)	1.0(9)	C(221)-C(121)-C(122)-N(119)	1.6(8)
C(108)-C(109)-C(110)-C(111)	-178.4(6)	C(120)-C(121)-C(122)-C(123)	1.6(8)
C(118)-C(109)-C(110)-C(111)	0.2(9)	C(221)-C(121)-C(122)-C(123)	174.5(5)
C(109)-C(110)-C(111)-C(116)	-1.9(9)	C(119)-N(119)-C(122)-C(121)	-77.5(7)
C(109)-C(110)-C(111)-C(112)	178.1(6)	Zn(1)-N(119)-C(122)-C(121)	77.7(6)
C(110)-C(111)-C(112)-C(113)	178.2(6)	C(119)-N(119)-C(122)-C(123)	109.5(6)
C(116)-C(111)-C(112)-C(113)	-1.8(9)	Zn(1)-N(119)-C(122)-C(123)	-95.3(5)
C(111)-C(112)-C(113)-C(114)	0.5(10)	C(121)-C(122)-C(123)-C(124)	-1.8(9)
C(112)-C(113)-C(114)-C(115)	0.7(11)	N(119)-C(122)-C(123)-C(124)	171.3(5)
C(113)-C(114)-C(115)-C(116)	-0.5(10)	C(122)-C(123)-C(124)-C(125)	2.1(9)
C(110)-C(111)-C(116)-C(117)	1.9(8)	C(123)-C(124)-C(125)-C(126)	179.3(6)
C(112)-C(111)-C(116)-C(117)	-178.1(5)	C(123)-C(124)-C(125)-C(120)	-2.1(9)
C(110)-C(111)-C(116)-C(115)	-178.1(6)	C(121)-C(120)-C(125)-C(124)	1.9(8)
C(112)-C(111)-C(116)-C(115)	1.9(8)	C(129)-C(120)-C(125)-C(124)	-179.7(5)
C(114)-C(115)-C(116)-C(117)	179.1(6)	C(121)-C(120)-C(125)-C(126)	-179.5(5)

C(129)-C(120)-C(125)-C(126)	-1.0(8)	C(210)-C(209)-C(218)-C(217)	1.0(8)
C(124)-C(125)-C(126)-C(127)	179.4(6)	C(208)-C(209)-C(218)-C(217)	177.1(5)
C(120)-C(125)-C(126)-C(127)	0.8(8)	C(210)-C(209)-C(218)-C(201)	-176.3(5)
C(125)-C(126)-C(127)-C(128)	-0.7(9)	C(208)-C(209)-C(218)-C(201)	-0.2(8)
C(126)-C(127)-C(128)-C(129)	0.8(9)	C(206)-C(201)-C(218)-C(217)	-172.9(5)
C(127)-C(128)-C(129)-C(120)	-1.1(9)	C(202)-C(201)-C(218)-C(217)	7.1(9)
C(121)-C(120)-C(129)-C(128)	179.6(5)	C(206)-C(201)-C(218)-C(209)	4.2(8)
C(125)-C(120)-C(129)-C(128)	1.2(8)	C(202)-C(201)-C(218)-C(209)	-175.9(5)
C(206)-C(201)-C(202)-O(202)	-169.3(5)	C(204)-C(203)-C(219)-N(219)	176.8(6)
C(218)-C(201)-C(202)-O(202)	10.7(8)	C(202)-C(203)-C(219)-N(219)	0.9(9)
C(206)-C(201)-C(202)-C(203)	8.0(8)	C(203)-C(219)-N(219)-C(222)	178.2(5)
C(218)-C(201)-C(202)-C(203)	-172.0(5)	C(203)-C(219)-N(219)-Zn(1)	14.4(8)
C(203)-C(202)-O(202)-Zn(1)	6.3(9)	O(202)-Zn(1)-N(219)-C(219)	-15.5(5)
C(201)-C(202)-O(202)-Zn(1)	-176.5(4)	O(102)-Zn(1)-N(219)-C(219)	-142.6(4)
O(102)-Zn(1)-O(202)-C(202)	139.8(5)	N(119)-Zn(1)-N(219)-C(219)	118.3(5)
N(119)-Zn(1)-O(202)-C(202)	-92.1(5)	O(202)-Zn(1)-N(219)-C(222)	179.0(4)
N(219)-Zn(1)-O(202)-C(202)	5.8(5)	O(102)-Zn(1)-N(219)-C(222)	51.9(4)
O(202)-C(202)-C(203)-C(204)	171.5(6)	N(119)-Zn(1)-N(219)-C(222)	-47.2(4)
C(201)-C(202)-C(203)-C(204)	-5.7(9)	C(225)-C(220)-C(221)-C(222)	-0.3(8)
O(202)-C(202)-C(203)-C(219)	-12.7(9)	C(229)-C(220)-C(221)-C(222)	175.3(5)
C(201)-C(202)-C(203)-C(219)	170.1(5)	C(225)-C(220)-C(221)-C(121)	-175.3(5)
C(202)-C(203)-C(204)-C(205)	0.0(10)	C(229)-C(220)-C(221)-C(121)	0.3(9)
C(219)-C(203)-C(204)-C(205)	-176.1(6)	C(122)-C(121)-C(221)-C(222)	-69.5(7)
C(203)-C(204)-C(205)-C(206)	3.2(10)	C(120)-C(121)-C(221)-C(222)	103.4(6)
C(218)-C(201)-C(206)-C(205)	174.9(6)	C(122)-C(121)-C(221)-C(220)	105.4(6)
C(202)-C(201)-C(206)-C(205)	-5.1(9)	C(120)-C(121)-C(221)-C(220)	-81.7(7)
C(218)-C(201)-C(206)-C(207)	-4.7(9)	C(220)-C(221)-C(222)-C(223)	4.4(8)
C(202)-C(201)-C(206)-C(207)	175.3(6)	C(121)-C(221)-C(222)-C(223)	179.5(5)
C(204)-C(205)-C(206)-C(201)	-0.5(10)	C(220)-C(221)-C(222)-N(219)	-167.4(5)
C(204)-C(205)-C(206)-C(207)	179.1(6)	C(121)-C(221)-C(222)-N(219)	7.7(8)
C(201)-C(206)-C(207)-C(208)	1.0(10)	C(219)-N(219)-C(222)-C(221)	-90.6(7)
C(205)-C(206)-C(207)-C(208)	-178.6(6)	Zn(1)-N(219)-C(222)-C(221)	74.4(6)
C(206)-C(207)-C(208)-C(209)	3.0(10)	C(219)-N(219)-C(222)-C(223)	97.3(7)
C(207)-C(208)-C(209)-C(210)	172.7(6)	Zn(1)-N(219)-C(222)-C(223)	-97.7(5)
C(207)-C(208)-C(209)-C(218)	-3.5(9)	C(221)-C(222)-C(223)-C(224)	-5.1(9)
C(218)-C(209)-C(210)-C(211)	-1.3(9)	N(219)-C(222)-C(223)-C(224)	166.7(5)
C(208)-C(209)-C(210)-C(211)	-177.4(6)	C(222)-C(223)-C(224)-C(225)	1.5(9)
C(209)-C(210)-C(211)-C(212)	-179.9(6)	C(223)-C(224)-C(225)-C(220)	2.6(9)
C(209)-C(210)-C(211)-C(216)	1.2(9)	C(223)-C(224)-C(225)-C(226)	-174.4(6)
C(210)-C(211)-C(212)-C(213)	-179.9(6)	C(229)-C(220)-C(225)-C(224)	-178.9(6)
C(216)-C(211)-C(212)-C(213)	-1.0(9)	C(221)-C(220)-C(225)-C(224)	-3.2(8)
C(211)-C(212)-C(213)-C(214)	0.6(9)	C(229)-C(220)-C(225)-C(226)	-1.8(8)
C(212)-C(213)-C(214)-C(215)	-0.5(9)	C(221)-C(220)-C(225)-C(226)	173.9(5)
C(213)-C(214)-C(215)-C(216)	0.8(9)	C(224)-C(225)-C(226)-C(227)	177.3(6)
C(214)-C(215)-C(216)-C(217)	180.0(6)	C(220)-C(225)-C(226)-C(227)	0.2(9)
C(214)-C(215)-C(216)-C(211)	-1.1(9)	C(225)-C(226)-C(227)-C(228)	0.9(10)
C(210)-C(211)-C(216)-C(217)	-0.9(8)	C(226)-C(227)-C(228)-C(229)	-0.2(10)
C(212)-C(211)-C(216)-C(217)	-179.9(5)	C(227)-C(228)-C(229)-C(220)	-1.4(10)
C(210)-C(211)-C(216)-C(215)	-179.8(5)	C(225)-C(220)-C(229)-C(228)	2.5(9)
C(212)-C(211)-C(216)-C(215)	1.2(8)	C(221)-C(220)-C(229)-C(228)	-173.1(6)
C(215)-C(216)-C(217)-C(218)	179.6(5)	C(306)-C(301)-C(302)-O(302)	-173.7(5)
C(211)-C(216)-C(217)-C(218)	0.7(8)	C(318)-C(301)-C(302)-O(302)	7.2(8)
C(216)-C(217)-C(218)-C(209)	-0.7(8)	C(306)-C(301)-C(302)-C(303)	6.1(8)
C(216)-C(217)-C(218)-C(201)	176.3(5)	C(318)-C(301)-C(302)-C(303)	-173.0(5)

C(303)-C(302)-O(302)-Zn(2)	1.3(8)	O(302)-Zn(2)-N(319)-C(319)	-19.6(4)
C(301)-C(302)-O(302)-Zn(2)	-178.9(4)	O(402)-Zn(2)-N(319)-C(319)	-143.0(4)
O(402)-Zn(2)-O(302)-C(302)	145.9(5)	N(419)-Zn(2)-N(319)-C(319)	116.5(4)
N(419)-Zn(2)-O(302)-C(302)	-88.8(5)	O(302)-Zn(2)-N(319)-C(322)	176.8(4)
N(319)-Zn(2)-O(302)-C(302)	11.1(5)	O(402)-Zn(2)-N(319)-C(322)	53.3(4)
O(302)-C(302)-C(303)-C(304)	172.2(5)	N(419)-Zn(2)-N(319)-C(322)	-47.1(4)
C(301)-C(302)-C(303)-C(304)	-7.6(8)	C(329)-C(320)-C(321)-C(322)	178.0(5)
O(302)-C(302)-C(303)-C(319)	-10.6(9)	C(325)-C(320)-C(321)-C(322)	0.1(8)
C(301)-C(302)-C(303)-C(319)	169.6(5)	C(329)-C(320)-C(321)-C(421)	2.0(9)
C(302)-C(303)-C(304)-C(305)	3.7(9)	C(325)-C(320)-C(321)-C(421)	-175.8(5)
C(319)-C(303)-C(304)-C(305)	-173.7(5)	C(320)-C(321)-C(322)-C(323)	1.8(9)
C(303)-C(304)-C(305)-C(306)	1.6(9)	C(421)-C(321)-C(322)-C(323)	177.9(5)
C(304)-C(305)-C(306)-C(301)	-2.9(9)	C(320)-C(321)-C(322)-N(319)	-167.0(5)
C(304)-C(305)-C(306)-C(307)	176.1(5)	C(421)-C(321)-C(322)-N(319)	9.1(8)
C(302)-C(301)-C(306)-C(305)	-0.9(8)	C(319)-N(319)-C(322)-C(321)	-90.9(7)
C(318)-C(301)-C(306)-C(305)	178.2(5)	Zn(2)-N(319)-C(322)-C(321)	72.5(6)
C(302)-C(301)-C(306)-C(307)	-179.9(5)	C(319)-N(319)-C(322)-C(323)	100.0(7)
C(318)-C(301)-C(306)-C(307)	-0.8(8)	Zn(2)-N(319)-C(322)-C(323)	-96.6(5)
C(305)-C(306)-C(307)-C(308)	-179.5(6)	C(321)-C(322)-C(323)-C(324)	-1.3(9)
C(301)-C(306)-C(307)-C(308)	-0.5(9)	N(319)-C(322)-C(323)-C(324)	167.6(5)
C(306)-C(307)-C(308)-C(309)	0.6(9)	C(322)-C(323)-C(324)-C(325)	-1.3(9)
C(307)-C(308)-C(309)-C(310)	179.2(6)	C(323)-C(324)-C(325)-C(326)	-175.6(6)
C(307)-C(308)-C(309)-C(318)	0.5(8)	C(323)-C(324)-C(325)-C(320)	3.2(9)
C(308)-C(309)-C(310)-C(311)	-178.6(5)	C(329)-C(320)-C(325)-C(326)	-1.7(8)
C(318)-C(309)-C(310)-C(311)	0.1(8)	C(321)-C(320)-C(325)-C(326)	176.3(5)
C(309)-C(310)-C(311)-C(312)	-177.8(6)	C(329)-C(320)-C(325)-C(324)	179.5(5)
C(309)-C(310)-C(311)-C(316)	1.4(8)	C(321)-C(320)-C(325)-C(324)	-2.5(8)
C(310)-C(311)-C(312)-C(313)	178.2(6)	C(324)-C(325)-C(326)-C(327)	179.5(6)
C(316)-C(311)-C(312)-C(313)	-0.9(9)	C(320)-C(325)-C(326)-C(327)	0.8(9)
C(311)-C(312)-C(313)-C(314)	0.8(9)	C(325)-C(326)-C(327)-C(328)	0.4(10)
C(312)-C(313)-C(314)-C(315)	-1.0(9)	C(326)-C(327)-C(328)-C(329)	-0.6(10)
C(313)-C(314)-C(315)-C(316)	1.3(9)	C(327)-C(328)-C(329)-C(320)	-0.3(9)
C(312)-C(311)-C(316)-C(317)	177.3(6)	C(321)-C(320)-C(329)-C(328)	-176.4(6)
C(310)-C(311)-C(316)-C(317)	-1.9(8)	C(325)-C(320)-C(329)-C(328)	1.5(9)
C(312)-C(311)-C(316)-C(315)	1.2(8)	C(406)-C(401)-C(402)-O(402)	-174.0(5)
C(310)-C(311)-C(316)-C(315)	-178.0(5)	C(418)-C(401)-C(402)-O(402)	7.7(8)
C(314)-C(315)-C(316)-C(317)	-177.5(6)	C(406)-C(401)-C(402)-C(403)	7.5(8)
C(314)-C(315)-C(316)-C(311)	-1.5(9)	C(418)-C(401)-C(402)-C(403)	-170.8(5)
C(311)-C(316)-C(317)-C(318)	1.1(9)	C(403)-C(402)-O(402)-Zn(2)	10.8(8)
C(315)-C(316)-C(317)-C(318)	177.0(5)	C(401)-C(402)-O(402)-Zn(2)	-167.6(4)
C(316)-C(317)-C(318)-C(309)	0.4(8)	O(302)-Zn(2)-O(402)-C(402)	143.1(5)
C(316)-C(317)-C(318)-C(301)	179.7(5)	N(419)-Zn(2)-O(402)-C(402)	-1.8(5)
C(310)-C(309)-C(318)-C(317)	-1.0(8)	N(319)-Zn(2)-O(402)-C(402)	-101.6(5)
C(308)-C(309)-C(318)-C(317)	177.6(5)	O(402)-C(402)-C(403)-C(404)	172.5(6)
C(310)-C(309)-C(318)-C(301)	179.6(5)	C(401)-C(402)-C(403)-C(404)	-9.1(8)
C(308)-C(309)-C(318)-C(301)	-1.7(8)	O(402)-C(402)-C(403)-C(419)	-8.4(9)
C(306)-C(301)-C(318)-C(317)	-177.5(5)	C(401)-C(402)-C(403)-C(419)	170.0(5)
C(302)-C(301)-C(318)-C(317)	1.6(9)	C(419)-C(403)-C(404)-C(405)	-175.2(5)
C(306)-C(301)-C(318)-C(309)	1.9(8)	C(402)-C(403)-C(404)-C(405)	3.9(9)
C(302)-C(301)-C(318)-C(309)	-179.0(5)	C(403)-C(404)-C(405)-C(406)	3.1(9)
C(304)-C(303)-C(319)-N(319)	177.0(5)	C(404)-C(405)-C(406)-C(401)	-4.5(9)
C(302)-C(303)-C(319)-N(319)	-0.3(9)	C(404)-C(405)-C(406)-C(407)	175.5(6)
C(303)-C(319)-N(319)-C(322)	179.7(5)	C(418)-C(401)-C(406)-C(405)	177.4(5)
C(303)-C(319)-N(319)-Zn(2)	17.3(8)	C(402)-C(401)-C(406)-C(405)	-0.9(9)

C(418)-C(401)-C(406)-C(407)	-2.6(9)	O(302)-Zn(2)-N(419)-C(419)	-142.0(4)
C(402)-C(401)-C(406)-C(407)	179.1(5)	O(402)-Zn(2)-N(419)-C(419)	-11.0(5)
C(405)-C(406)-C(407)-C(408)	-177.1(6)	N(319)-Zn(2)-N(419)-C(419)	118.3(5)
C(401)-C(406)-C(407)-C(408)	2.9(9)	O(302)-Zn(2)-N(419)-C(422)	55.1(5)
C(406)-C(407)-C(408)-C(409)	-0.8(10)	O(402)-Zn(2)-N(419)-C(422)	-173.9(4)
C(407)-C(408)-C(409)-C(410)	175.5(6)	N(319)-Zn(2)-N(419)-C(422)	-44.5(4)
C(407)-C(408)-C(409)-C(418)	-1.5(9)	C(429)-C(420)-C(421)-C(422)	180.0(5)
C(408)-C(409)-C(410)-C(411)	-175.9(6)	C(425)-C(420)-C(421)-C(422)	1.3(8)
C(418)-C(409)-C(410)-C(411)	1.0(9)	C(429)-C(420)-C(421)-C(321)	5.2(8)
C(409)-C(410)-C(411)-C(416)	-4.2(9)	C(425)-C(420)-C(421)-C(321)	-173.4(5)
C(409)-C(410)-C(411)-C(412)	176.4(6)	C(322)-C(321)-C(421)-C(422)	-72.0(8)
C(410)-C(411)-C(412)-C(413)	179.6(6)	C(320)-C(321)-C(421)-C(422)	104.0(7)
C(416)-C(411)-C(412)-C(413)	0.1(9)	C(322)-C(321)-C(421)-C(420)	102.8(6)
C(411)-C(412)-C(413)-C(414)	-2.5(9)	C(320)-C(321)-C(421)-C(420)	-81.3(7)
C(412)-C(413)-C(414)-C(415)	3.0(10)	C(420)-C(421)-C(422)-C(423)	-0.8(8)
C(413)-C(414)-C(415)-C(416)	-0.9(10)	C(321)-C(421)-C(422)-C(423)	174.0(5)
C(410)-C(411)-C(416)-C(417)	3.6(8)	C(420)-C(421)-C(422)-N(419)	-169.9(5)
C(412)-C(411)-C(416)-C(417)	-176.9(5)	C(321)-C(421)-C(422)-N(419)	4.9(8)
C(410)-C(411)-C(416)-C(415)	-177.6(6)	C(419)-N(419)-C(422)-C(421)	-88.2(7)
C(412)-C(411)-C(416)-C(415)	1.9(8)	Zn(2)-N(419)-C(422)-C(421)	74.3(6)
C(414)-C(415)-C(416)-C(417)	177.2(6)	C(419)-N(419)-C(422)-C(423)	102.5(7)
C(414)-C(415)-C(416)-C(411)	-1.5(9)	Zn(2)-N(419)-C(422)-C(423)	-95.0(5)
C(411)-C(416)-C(417)-C(418)	0.2(9)	C(421)-C(422)-C(423)-C(424)	0.6(8)
C(415)-C(416)-C(417)-C(418)	-178.5(6)	N(419)-C(422)-C(423)-C(424)	169.5(5)
C(416)-C(417)-C(418)-C(409)	-3.3(9)	C(422)-C(423)-C(424)-C(425)	-0.8(8)
C(416)-C(417)-C(418)-C(401)	174.4(5)	C(423)-C(424)-C(425)-C(420)	1.3(8)
C(410)-C(409)-C(418)-C(417)	2.7(8)	C(423)-C(424)-C(425)-C(426)	-178.6(5)
C(408)-C(409)-C(418)-C(417)	179.6(6)	C(429)-C(420)-C(425)-C(424)	179.7(5)
C(410)-C(409)-C(418)-C(401)	-175.2(5)	C(421)-C(420)-C(425)-C(424)	-1.6(8)
C(408)-C(409)-C(418)-C(401)	1.8(8)	C(429)-C(420)-C(425)-C(426)	-0.4(8)
C(406)-C(401)-C(418)-C(417)	-177.4(6)	C(421)-C(420)-C(425)-C(426)	178.3(5)
C(402)-C(401)-C(418)-C(417)	0.9(9)	C(424)-C(425)-C(426)-C(427)	179.8(5)
C(406)-C(401)-C(418)-C(409)	0.3(8)	C(420)-C(425)-C(426)-C(427)	0.0(8)
C(402)-C(401)-C(418)-C(409)	178.5(5)	C(425)-C(426)-C(427)-C(428)	0.2(9)
C(404)-C(403)-C(419)-N(419)	172.2(6)	C(426)-C(427)-C(428)-C(429)	0.1(9)
C(402)-C(403)-C(419)-N(419)	-6.9(10)	C(427)-C(428)-C(429)-C(420)	-0.6(9)
C(403)-C(419)-N(419)-C(422)	177.9(5)	C(421)-C(420)-C(429)-C(428)	-177.9(5)
C(403)-C(419)-N(419)-Zn(2)	16.2(8)	C(425)-C(420)-C(429)-C(428)	0.7(8)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for (*R*)-**78**.

Identification code	(*R*)-**78**	
Empirical formula	C62 H44 Fe N2 O3	
Formula weight	920.84	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	P3(2)	
Unit cell dimensions	a = 12.6954(3) Å	α= 90°.
	b = 12.6954(3) Å	β= 90°.
	c = 24.3493(10) Å	γ = 120°.
Volume	3398.68(18) $Å^3$	
Z	3	
Density (calculated)	1.350 g/cm^3	
Absorption coefficient	0.385 mm^{-1}	
F(000)	1440	
Crystal size	0.30 x 0.24 x 0.03 mm^3	
Theta range for data collection	0.84 to 30.02°.	
Index ranges	-17<=h<=17, -17<=k<=17, -34<=l<=34	
Reflections collected	39455	
Independent reflections	13200 [R(int) = 0.0447]	
Completeness to theta = 30.02°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.734	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13200 / 1 / 614	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0524, wR2 = 0.1178	
R indices (all data)	R1 = 0.0622, wR2 = 0.1231	
Absolute structure parameter	0.004(14)	
Largest diff. peak and hole	0.718 and -0.299 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**78**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	9252(1)	309(1)	5000(1)	24(1)
O(1S)	7207(3)	8409(3)	3280(1)	50(1)
C(1S)	6784(4)	7686(5)	2791(2)	48(1)
C(2S)	7527(5)	7148(5)	2662(2)	51(1)
C(3S)	6593(5)	8999(5)	3401(2)	57(1)
C(4S)	7176(3)	9860(4)	3892(2)	29(1)
C(101)	5656(3)	-1746(3)	5609(1)	19(1)
C(102)	6807(3)	-1508(3)	5387(1)	21(1)
O(102)	7710(2)	-391(2)	5349(1)	25(1)
C(103)	6945(3)	-2504(3)	5206(1)	20(1)
C(104)	6022(3)	-3714(3)	5316(1)	22(1)
C(105)	4951(3)	-3944(3)	5563(1)	24(1)
C(106)	4740(3)	-2980(3)	5685(1)	22(1)

C(107)	3564(3)	-3270(3)	5893(2)	27(1)
C(108)	3300(3)	-2416(4)	6021(2)	28(1)
C(109)	4184(3)	-1140(4)	5963(1)	23(1)
C(110)	3881(3)	-272(4)	6110(1)	27(1)
C(111)	4698(3)	985(4)	6051(1)	26(1)
C(112)	4402(4)	1897(4)	6193(2)	32(1)
C(113)	5212(4)	3074(4)	6133(2)	36(1)
C(114)	6405(4)	3462(4)	5924(2)	36(1)
C(115)	6706(4)	2609(4)	5783(2)	30(1)
C(116)	5883(3)	1352(3)	5837(1)	24(1)
C(117)	6191(3)	460(3)	5701(1)	22(1)
C(118)	5392(3)	-780(3)	5754(1)	22(1)
C(119)	7976(3)	-2372(3)	4901(1)	20(1)
N(119)	8866(3)	-1357(3)	4727(1)	22(1)
C(120)	11903(3)	-952(3)	4389(1)	18(1)
C(121)	10848(3)	-1192(3)	4692(1)	18(1)
C(122)	9836(3)	-1321(3)	4416(1)	20(1)
C(123)	9812(3)	-1272(3)	3837(1)	22(1)
C(124)	10822(3)	-1047(3)	3537(1)	21(1)
C(125)	11891(3)	-854(3)	3804(1)	19(1)
C(126)	12968(3)	-551(3)	3510(1)	22(1)
C(127)	13982(3)	-388(3)	3772(2)	25(1)
C(128)	13994(3)	-508(3)	4344(2)	25(1)
C(129)	12984(3)	-769(3)	4649(1)	22(1)
C(201)	11198(3)	3906(3)	4390(1)	21(1)
C(202)	11026(3)	2777(3)	4611(1)	21(1)
O(202)	9919(2)	1833(2)	4640(1)	28(1)
C(203)	12051(3)	2695(3)	4795(1)	22(1)
C(204)	13230(3)	3665(3)	4702(1)	24(1)
C(205)	13414(3)	4699(3)	4456(1)	25(1)
C(206)	12413(3)	4844(3)	4309(1)	24(1)
C(207)	12647(4)	5992(3)	4083(2)	29(1)
C(208)	11735(4)	6192(3)	3949(2)	28(1)
C(209)	10497(3)	5295(3)	4038(1)	24(1)
C(210)	9579(4)	5568(3)	3930(1)	26(1)
C(211)	8357(4)	4752(3)	4034(1)	26(1)
C(212)	7415(4)	5035(4)	3945(1)	30(1)
C(213)	6234(4)	4203(4)	4064(2)	33(1)
C(214)	5921(4)	3029(4)	4265(2)	31(1)
C(215)	6802(3)	2741(4)	4355(2)	28(1)
C(216)	8057(3)	3588(3)	4249(1)	24(1)
C(217)	8965(3)	3296(3)	4352(1)	25(1)
C(218)	10203(3)	4119(3)	4259(1)	22(1)
C(219)	11944(3)	1681(3)	5112(1)	23(1)
N(219)	10939(3)	767(3)	5284(1)	21(1)
C(220)	10567(3)	-2269(3)	5605(1)	19(1)
C(221)	10830(3)	-1196(3)	5309(1)	20(1)
C(222)	10932(3)	-208(3)	5590(1)	21(1)
C(223)	10838(3)	-206(3)	6167(1)	23(1)
C(224)	10584(3)	-1218(4)	6453(1)	26(1)
C(225)	10412(3)	-2288(3)	6186(1)	21(1)
C(226)	10058(3)	-3392(3)	6471(1)	27(1)
C(227)	9874(4)	-4406(4)	6199(2)	31(1)
C(228)	10044(3)	-4371(3)	5627(1)	26(1)

C(229)	10390(3)	-3331(3)	5340(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for (*R*)-**78**.

Fe(1)-O(202)	1.895(2)	C(114)-H(114)	0.9500
Fe(1)-O(102)	1.897(2)	C(115)-C(116)	1.410(5)
Fe(1)-N(119)	2.030(3)	C(115)-H(115)	0.9500
Fe(1)-N(219)	2.040(3)	C(116)-C(117)	1.411(5)
O(1S)-C(3S)	1.357(6)	C(117)-C(118)	1.388(5)
O(1S)-C(1S)	1.433(6)	C(117)-H(117)	0.9500
C(1S)-C(2S)	1.450(8)	C(119)-N(119)	1.289(4)
C(1S)-H(1SA)	0.9900	C(119)-H(119)	0.9500
C(1S)-H(1SB)	0.9900	N(119)-C(122)	1.426(4)
C(2S)-H(2SA)	0.9800	C(120)-C(129)	1.422(4)
C(2S)-H(2SB)	0.9800	C(120)-C(121)	1.423(4)
C(2S)-H(2SC)	0.9800	C(120)-C(125)	1.430(4)
C(3S)-C(4S)	1.536(6)	C(121)-C(122)	1.385(4)
C(3S)-H(3SA)	0.9900	C(121)-C(221)	1.502(4)
C(3S)-H(3SB)	0.9900	C(122)-C(123)	1.414(5)
C(4S)-H(4SA)	0.9800	C(123)-C(124)	1.376(5)
C(4S)-H(4SB)	0.9800	C(123)-H(123)	0.9500
C(4S)-H(4SC)	0.9800	C(124)-C(125)	1.412(4)
C(101)-C(106)	1.420(5)	C(124)-H(124)	0.9500
C(101)-C(102)	1.442(5)	C(125)-C(126)	1.415(4)
C(101)-C(118)	1.466(5)	C(126)-C(127)	1.357(5)
C(102)-O(102)	1.308(4)	C(126)-H(126)	0.9500
C(102)-C(103)	1.430(5)	C(127)-C(128)	1.404(5)
C(103)-C(104)	1.416(4)	C(127)-H(127)	0.9500
C(103)-C(119)	1.439(4)	C(128)-C(129)	1.371(5)
C(104)-C(105)	1.377(5)	C(128)-H(128)	0.9500
C(104)-H(104)	0.9500	C(129)-H(129)	0.9500
C(105)-C(106)	1.410(5)	C(201)-C(206)	1.414(5)
C(105)-H(105)	0.9500	C(201)-C(202)	1.442(4)
C(106)-C(107)	1.438(5)	C(201)-C(218)	1.453(5)
C(107)-C(108)	1.323(5)	C(202)-O(202)	1.316(4)
C(107)-H(107)	0.9500	C(202)-C(203)	1.429(5)
C(108)-C(109)	1.444(5)	C(203)-C(204)	1.401(5)
C(108)-H(108)	0.9500	C(203)-C(219)	1.447(5)
C(109)-C(110)	1.383(5)	C(204)-C(205)	1.353(5)
C(109)-C(118)	1.456(4)	C(204)-H(204)	0.9500
C(110)-C(111)	1.411(6)	C(205)-C(206)	1.418(5)
C(110)-H(110)	0.9500	C(205)-H(205)	0.9500
C(111)-C(112)	1.427(5)	C(206)-C(207)	1.443(5)
C(111)-C(116)	1.432(5)	C(207)-C(208)	1.345(6)
C(112)-C(113)	1.333(6)	C(207)-H(207)	0.9500
C(112)-H(112)	0.9500	C(208)-C(209)	1.422(5)
C(113)-C(114)	1.432(6)	C(208)-H(208)	0.9500
C(113)-H(113)	0.9500	C(209)-C(210)	1.396(5)
C(114)-C(115)	1.361(5)	C(209)-C(218)	1.451(5)

C(210)-C(211)	1.392(5)
C(210)-H(210)	0.9500
C(211)-C(212)	1.427(5)
C(211)-C(216)	1.428(5)
C(212)-C(213)	1.365(6)
C(212)-H(212)	0.9500
C(213)-C(214)	1.423(6)
C(213)-H(213)	0.9500
C(214)-C(215)	1.358(5)
C(214)-H(214)	0.9500
C(215)-C(216)	1.431(5)
C(215)-H(215)	0.9500
C(216)-C(217)	1.399(5)
C(217)-C(218)	1.404(5)
C(217)-H(217)	0.9500
C(219)-N(219)	1.292(4)
C(219)-H(219)	0.9500
N(219)-C(222)	1.441(4)
C(220)-C(229)	1.408(5)
C(220)-C(221)	1.425(4)
C(220)-C(225)	1.428(4)
C(221)-C(222)	1.376(4)
C(222)-C(223)	1.411(4)
C(223)-C(224)	1.351(5)
C(223)-H(223)	0.9500
C(224)-C(225)	1.420(5)
C(224)-H(224)	0.9500
C(225)-C(226)	1.420(5)
C(226)-C(227)	1.361(5)
C(226)-H(226)	0.9500
C(227)-C(228)	1.406(5)
C(227)-H(227)	0.9500
C(228)-C(229)	1.358(5)
C(228)-H(228)	0.9500
C(229)-H(229)	0.9500
O(202)-Fe(1)-O(102)	121.03(10)
O(202)-Fe(1)-N(119)	131.62(12)
O(102)-Fe(1)-N(119)	90.21(11)
O(202)-Fe(1)-N(219)	89.78(11)
O(102)-Fe(1)-N(219)	132.23(11)
N(119)-Fe(1)-N(219)	94.54(10)
C(3S)-O(1S)-C(1S)	113.5(4)
O(1S)-C(1S)-C(2S)	111.0(4)
O(1S)-C(1S)-H(1SA)	109.4
C(2S)-C(1S)-H(1SA)	109.4
O(1S)-C(1S)-H(1SB)	109.4
C(2S)-C(1S)-H(1SB)	109.4
H(1SA)-C(1S)-H(1SB)	108.0
C(1S)-C(2S)-H(2SA)	109.5
C(1S)-C(2S)-H(2SB)	109.5
H(2SA)-C(2S)-H(2SB)	109.5
C(1S)-C(2S)-H(2SC)	109.5
H(2SA)-C(2S)-H(2SC)	109.5
H(2SB)-C(2S)-H(2SC)	109.5
O(1S)-C(3S)-C(4S)	110.9(4)
O(1S)-C(3S)-H(3SA)	109.5
C(4S)-C(3S)-H(3SA)	109.5
O(1S)-C(3S)-H(3SB)	109.5
C(4S)-C(3S)-H(3SB)	109.5
H(3SA)-C(3S)-H(3SB)	108.1
C(3S)-C(4S)-H(4SA)	109.5
C(3S)-C(4S)-H(4SB)	109.5
H(4SA)-C(4S)-H(4SB)	109.5
C(3S)-C(4S)-H(4SC)	109.5
H(4SA)-C(4S)-H(4SC)	109.5
H(4SB)-C(4S)-H(4SC)	109.5
C(106)-C(101)-C(102)	117.7(3)
C(106)-C(101)-C(118)	119.2(3)
C(102)-C(101)-C(118)	123.1(3)
O(102)-C(102)-C(103)	120.6(3)
O(102)-C(102)-C(101)	120.1(3)
C(103)-C(102)-C(101)	119.4(3)
C(102)-O(102)-Fe(1)	132.8(2)
C(104)-C(103)-C(102)	120.0(3)
C(104)-C(103)-C(119)	115.8(3)
C(102)-C(103)-C(119)	124.2(3)
C(105)-C(104)-C(103)	120.4(3)
C(105)-C(104)-H(104)	119.8
C(103)-C(104)-H(104)	119.8
C(104)-C(105)-C(106)	120.3(3)
C(104)-C(105)-H(105)	119.9
C(106)-C(105)-H(105)	119.9
C(105)-C(106)-C(101)	121.6(3)
C(105)-C(106)-C(107)	118.4(3)
C(101)-C(106)-C(107)	120.1(3)
C(108)-C(107)-C(106)	121.9(3)
C(108)-C(107)-H(107)	119.1
C(106)-C(107)-H(107)	119.1
C(107)-C(108)-C(109)	121.6(3)
C(107)-C(108)-H(108)	119.2
C(109)-C(108)-H(108)	119.2
C(110)-C(109)-C(108)	119.9(3)
C(110)-C(109)-C(118)	120.6(3)
C(108)-C(109)-C(118)	119.5(3)
C(109)-C(110)-C(111)	122.3(3)
C(109)-C(110)-H(110)	118.8
C(111)-C(110)-H(110)	118.8
C(110)-C(111)-C(112)	123.4(3)
C(110)-C(111)-C(116)	117.6(3)
C(112)-C(111)-C(116)	119.0(4)
C(113)-C(112)-C(111)	121.0(4)
C(113)-C(112)-H(112)	119.5
C(111)-C(112)-H(112)	119.5
C(112)-C(113)-C(114)	121.0(4)
C(112)-C(113)-H(113)	119.5
C(114)-C(113)-H(113)	119.5
C(115)-C(114)-C(113)	119.1(4)

C(115)-C(114)-H(114)	120.5	O(202)-C(202)-C(201)	119.2(3)
C(113)-C(114)-H(114)	120.5	C(203)-C(202)-C(201)	119.9(3)
C(114)-C(115)-C(116)	122.2(4)	C(202)-O(202)-Fe(1)	133.1(2)
C(114)-C(115)-H(115)	118.9	C(204)-C(203)-C(202)	119.8(3)
C(116)-C(115)-H(115)	118.9	C(204)-C(203)-C(219)	116.9(3)
C(115)-C(116)-C(117)	122.7(3)	C(202)-C(203)-C(219)	123.2(3)
C(115)-C(116)-C(111)	117.8(3)	C(205)-C(204)-C(203)	121.0(3)
C(117)-C(116)-C(111)	119.5(3)	C(205)-C(204)-H(204)	119.5
C(118)-C(117)-C(116)	123.4(3)	C(203)-C(204)-H(204)	119.5
C(118)-C(117)-H(117)	118.3	C(204)-C(205)-C(206)	120.4(3)
C(116)-C(117)-H(117)	118.3	C(204)-C(205)-H(205)	119.8
C(117)-C(118)-C(109)	116.5(3)	C(206)-C(205)-H(205)	119.8
C(117)-C(118)-C(101)	125.7(3)	C(201)-C(206)-C(205)	121.8(3)
C(109)-C(118)-C(101)	117.8(3)	C(201)-C(206)-C(207)	119.4(3)
N(119)-C(119)-C(103)	125.3(3)	C(205)-C(206)-C(207)	118.8(3)
N(119)-C(119)-H(119)	117.3	C(208)-C(207)-C(206)	121.4(3)
C(103)-C(119)-H(119)	117.3	C(208)-C(207)-H(207)	119.3
C(119)-N(119)-C(122)	121.2(3)	C(206)-C(207)-H(207)	119.3
C(119)-N(119)-Fe(1)	124.6(2)	C(207)-C(208)-C(209)	121.6(3)
C(122)-N(119)-Fe(1)	112.7(2)	C(207)-C(208)-H(208)	119.2
C(129)-C(120)-C(121)	122.1(3)	C(209)-C(208)-H(208)	119.2
C(129)-C(120)-C(125)	118.8(3)	C(210)-C(209)-C(208)	119.9(3)
C(121)-C(120)-C(125)	119.1(3)	C(210)-C(209)-C(218)	120.5(3)
C(122)-C(121)-C(120)	119.4(3)	C(208)-C(209)-C(218)	119.5(3)
C(122)-C(121)-C(221)	118.2(3)	C(211)-C(210)-C(209)	122.7(3)
C(120)-C(121)-C(221)	122.1(3)	C(211)-C(210)-H(210)	118.7
C(121)-C(122)-C(123)	121.2(3)	C(209)-C(210)-H(210)	118.7
C(121)-C(122)-N(119)	118.8(3)	C(210)-C(211)-C(212)	123.2(3)
C(123)-C(122)-N(119)	119.6(3)	C(210)-C(211)-C(216)	117.3(3)
C(124)-C(123)-C(122)	120.1(3)	C(212)-C(211)-C(216)	119.5(4)
C(124)-C(123)-H(123)	120.0	C(213)-C(212)-C(211)	120.5(4)
C(122)-C(123)-H(123)	120.0	C(213)-C(212)-H(212)	119.7
C(123)-C(124)-C(125)	120.5(3)	C(211)-C(212)-H(212)	119.7
C(123)-C(124)-H(124)	119.8	C(212)-C(213)-C(214)	120.5(4)
C(125)-C(124)-H(124)	119.8	C(212)-C(213)-H(213)	119.8
C(124)-C(125)-C(126)	121.9(3)	C(214)-C(213)-H(213)	119.8
C(124)-C(125)-C(120)	119.6(3)	C(215)-C(214)-C(213)	120.1(4)
C(126)-C(125)-C(120)	118.5(3)	C(215)-C(214)-H(214)	120.0
C(127)-C(126)-C(125)	121.2(3)	C(213)-C(214)-H(214)	120.0
C(127)-C(126)-H(126)	119.4	C(214)-C(215)-C(216)	121.7(4)
C(125)-C(126)-H(126)	119.4	C(214)-C(215)-H(215)	119.2
C(126)-C(127)-C(128)	120.7(3)	C(216)-C(215)-H(215)	119.2
C(126)-C(127)-H(127)	119.6	C(217)-C(216)-C(211)	120.7(3)
C(128)-C(127)-H(127)	119.6	C(217)-C(216)-C(215)	121.6(3)
C(129)-C(128)-C(127)	120.3(3)	C(211)-C(216)-C(215)	117.7(3)
C(129)-C(128)-H(128)	119.8	C(216)-C(217)-C(218)	122.6(3)
C(127)-C(128)-H(128)	119.8	C(216)-C(217)-H(217)	118.7
C(128)-C(129)-C(120)	120.5(3)	C(218)-C(217)-H(217)	118.7
C(128)-C(129)-H(129)	119.8	C(217)-C(218)-C(209)	116.2(3)
C(120)-C(129)-H(129)	119.8	C(217)-C(218)-C(201)	125.5(3)
C(206)-C(201)-C(202)	116.6(3)	C(209)-C(218)-C(201)	118.2(3)
C(206)-C(201)-C(218)	119.8(3)	N(219)-C(219)-C(203)	125.7(3)
C(202)-C(201)-C(218)	123.6(3)	N(219)-C(219)-H(219)	117.1
O(202)-C(202)-C(203)	120.9(3)	C(203)-C(219)-H(219)	117.1

C(219)-N(219)-C(222)	121.3(3)	C(225)-C(224)-H(224)	119.2
C(219)-N(219)-Fe(1)	124.8(2)	C(226)-C(225)-C(224)	122.8(3)
C(222)-N(219)-Fe(1)	112.1(2)	C(226)-C(225)-C(220)	118.3(3)
C(229)-C(220)-C(221)	122.2(3)	C(224)-C(225)-C(220)	118.9(3)
C(229)-C(220)-C(225)	118.9(3)	C(227)-C(226)-C(225)	121.0(3)
C(221)-C(220)-C(225)	118.8(3)	C(227)-C(226)-H(226)	119.5
C(222)-C(221)-C(220)	119.4(3)	C(225)-C(226)-H(226)	119.5
C(222)-C(221)-C(121)	120.0(3)	C(226)-C(227)-C(228)	120.1(3)
C(220)-C(221)-C(121)	120.3(3)	C(226)-C(227)-H(227)	119.9
C(221)-C(222)-C(223)	121.8(3)	C(228)-C(227)-H(227)	119.9
C(221)-C(222)-N(219)	118.9(3)	C(229)-C(228)-C(227)	120.6(3)
C(223)-C(222)-N(219)	118.6(3)	C(229)-C(228)-H(228)	119.7
C(224)-C(223)-C(222)	119.5(3)	C(227)-C(228)-H(228)	119.7
C(224)-C(223)-H(223)	120.3	C(228)-C(229)-C(220)	121.0(3)
C(222)-C(223)-H(223)	120.3	C(228)-C(229)-H(229)	119.5
C(223)-C(224)-C(225)	121.6(3)	C(220)-C(229)-H(229)	119.5
C(223)-C(224)-H(224)	119.2		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (*R*)-**78**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	17(1)	17(1)	39(1)	6(1)	7(1)	10(1)
O(1S)	47(2)	59(2)	42(2)	8(2)	-4(1)	25(2)
C(1S)	40(2)	48(3)	50(3)	2(2)	-7(2)	19(2)
C(2S)	48(3)	49(3)	41(2)	5(2)	-4(2)	14(2)
C(3S)	53(3)	46(3)	68(3)	-7(3)	-8(2)	23(3)
C(4S)	22(2)	43(2)	31(2)	-2(2)	-6(1)	21(2)
C(101)	19(2)	20(2)	18(1)	0(1)	-3(1)	10(1)
C(102)	20(2)	22(2)	21(2)	1(1)	1(1)	11(1)
O(102)	18(1)	20(1)	38(1)	4(1)	8(1)	10(1)
C(103)	18(1)	18(2)	21(2)	-2(1)	-2(1)	8(1)
C(104)	21(2)	18(2)	25(2)	-2(1)	1(1)	8(1)
C(105)	24(2)	18(2)	24(2)	-2(1)	0(1)	6(1)
C(106)	18(2)	28(2)	16(1)	1(1)	-1(1)	8(1)
C(107)	19(2)	27(2)	28(2)	-2(1)	-4(1)	7(1)
C(108)	15(2)	36(2)	26(2)	5(1)	2(1)	9(1)
C(109)	20(2)	34(2)	20(1)	-1(1)	-1(1)	16(1)
C(110)	20(2)	40(2)	25(2)	1(1)	0(1)	19(2)
C(111)	24(2)	37(2)	22(2)	-8(1)	-5(1)	19(2)
C(112)	30(2)	45(2)	33(2)	-10(2)	-5(2)	26(2)
C(113)	44(2)	46(2)	38(2)	-10(2)	-6(2)	36(2)
C(114)	42(2)	30(2)	41(2)	-5(2)	-6(2)	23(2)
C(115)	32(2)	28(2)	34(2)	-2(2)	1(2)	18(2)
C(116)	27(2)	30(2)	22(2)	-1(1)	-1(1)	20(2)
C(117)	20(2)	22(2)	26(2)	-2(1)	-1(1)	11(1)
C(118)	20(2)	28(2)	19(1)	1(1)	1(1)	13(1)

C(119)	23(2)	21(2)	20(1)	-4(1)	-1(1)	13(1)
N(119)	20(1)	25(1)	25(1)	5(1)	4(1)	13(1)
C(120)	20(1)	20(1)	22(1)	3(1)	2(1)	15(1)
C(121)	22(2)	20(1)	16(1)	3(1)	1(1)	13(1)
C(122)	20(2)	20(2)	25(2)	2(1)	0(1)	14(1)
C(123)	24(2)	21(2)	25(2)	2(1)	-1(1)	14(1)
C(124)	27(2)	21(1)	20(2)	1(1)	0(1)	15(1)
C(125)	24(2)	14(1)	22(2)	2(1)	1(1)	12(1)
C(126)	26(2)	22(2)	20(2)	4(1)	5(1)	12(1)
C(127)	19(2)	25(2)	30(2)	3(1)	8(1)	11(1)
C(128)	20(2)	31(2)	26(2)	0(1)	2(1)	13(1)
C(129)	23(2)	27(2)	18(1)	-1(1)	-2(1)	16(1)
C(201)	22(2)	16(1)	23(2)	0(1)	3(1)	8(1)
C(202)	20(2)	20(2)	22(1)	1(1)	4(1)	8(1)
O(202)	18(1)	20(1)	47(2)	10(1)	5(1)	9(1)
C(203)	22(2)	21(2)	23(2)	0(1)	3(1)	11(1)
C(204)	21(2)	27(2)	23(2)	0(1)	3(1)	10(1)
C(205)	19(2)	23(2)	25(2)	-3(1)	4(1)	3(1)
C(206)	21(2)	19(2)	25(2)	-3(1)	3(1)	6(1)
C(207)	34(2)	16(2)	27(2)	2(1)	5(1)	6(1)
C(208)	38(2)	14(1)	28(2)	0(1)	3(1)	9(1)
C(209)	33(2)	17(2)	19(2)	-1(1)	3(1)	11(1)
C(210)	40(2)	19(2)	21(2)	-1(1)	-1(1)	17(2)
C(211)	39(2)	27(2)	19(2)	-4(1)	-3(1)	23(2)
C(212)	47(2)	31(2)	25(2)	0(1)	-7(2)	29(2)
C(213)	41(2)	48(2)	25(2)	-7(2)	-8(2)	34(2)
C(214)	30(2)	42(2)	29(2)	-1(2)	-3(1)	24(2)
C(215)	27(2)	30(2)	32(2)	-1(1)	0(1)	17(2)
C(216)	32(2)	24(2)	18(1)	-2(1)	-3(1)	16(2)
C(217)	29(2)	20(2)	27(2)	-1(1)	-1(1)	14(1)
C(218)	26(2)	17(2)	22(2)	-3(1)	0(1)	11(1)
C(219)	20(2)	25(2)	27(2)	-3(1)	2(1)	14(1)
N(219)	22(1)	20(1)	27(1)	1(1)	3(1)	14(1)
C(220)	18(1)	24(2)	17(1)	1(1)	2(1)	12(1)
C(221)	21(2)	22(2)	19(1)	3(1)	4(1)	13(1)
C(222)	17(1)	24(2)	24(2)	2(1)	5(1)	11(1)
C(223)	24(2)	26(2)	24(2)	-5(1)	1(1)	16(1)
C(224)	25(2)	38(2)	19(2)	1(1)	4(1)	18(2)
C(225)	22(2)	24(2)	18(1)	6(1)	6(1)	13(1)
C(226)	32(2)	36(2)	20(2)	10(1)	8(1)	22(2)
C(227)	33(2)	30(2)	33(2)	11(1)	10(2)	18(2)
C(228)	33(2)	22(2)	27(2)	-1(1)	1(1)	15(2)
C(229)	23(2)	24(2)	22(2)	1(1)	1(1)	15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (*R*)-**78**.

	x	y	z	U(eq)
H(1SA)	6809	8202	2481	57
H(1SB)	5929	7034	2843	57
H(2SA)	7218	6655	2328	76
H(2SB)	7496	6631	2968	76
H(2SC)	8370	7793	2603	76
H(3SA)	5737	8398	3489	68
H(3SB)	6595	9473	3078	68
H(4SA)	6719	10276	3972	44
H(4SB)	8019	10463	3803	44
H(4SC)	7162	9390	4214	44
H(104)	6142	-4372	5220	27
H(105)	4352	-4756	5651	29
H(107)	2960	-4100	5940	32
H(108)	2510	-2647	6153	33
H(110)	3094	-533	6256	32
H(112)	3615	1661	6332	39
H(113)	4995	3666	6231	44
H(114)	6979	4304	5884	43
H(115)	7497	2869	5642	36
H(117)	6986	721	5565	27
H(119)	8003	-3091	4822	24
H(123)	9098	-1395	3654	27
H(124)	10799	-1020	3147	26
H(126)	12980	-460	3122	27
H(127)	14692	-191	3565	30
H(128)	14705	-407	4521	30
H(129)	13007	-829	5037	26
H(204)	13909	3594	4813	29
H(205)	14219	5333	4382	30
H(207)	13464	6621	4028	35
H(208)	11921	6951	3792	34
H(210)	9798	6341	3780	31
H(212)	7611	5808	3802	36
H(213)	5618	4409	4012	39
H(214)	5094	2447	4335	37
H(215)	6580	1956	4493	34
H(217)	8735	2509	4489	29
H(219)	12676	1688	5200	27
H(223)	10953	501	6353	28
H(224)	10518	-1215	6842	31
H(226)	9948	-3423	6858	32
H(227)	9630	-5139	6395	37
H(228)	9915	-5082	5440	32
H(229)	10515	-3320	4955	26

Table 6. Torsion angles [°] for (*R*)-**78**.

C(3S)-O(1S)-C(1S)-C(2S)	176.0(4)	C(108)-C(109)-C(118)-C(101)	0.0(4)
C(1S)-O(1S)-C(3S)-C(4S)	-174.0(4)	C(106)-C(101)-C(118)-C(117)	-179.7(3)
C(106)-C(101)-C(102)-O(102)	-174.8(3)	C(102)-C(101)-C(118)-C(117)	-0.3(5)
C(118)-C(101)-C(102)-O(102)	5.8(5)	C(106)-C(101)-C(118)-C(109)	-0.8(4)
C(106)-C(101)-C(102)-C(103)	5.8(4)	C(102)-C(101)-C(118)-C(109)	178.6(3)
C(118)-C(101)-C(102)-C(103)	-173.7(3)	C(104)-C(103)-C(119)-N(119)	174.9(3)
C(103)-C(102)-O(102)-Fe(1)	9.3(5)	C(102)-C(103)-C(119)-N(119)	-4.2(5)
C(101)-C(102)-O(102)-Fe(1)	-170.1(2)	C(103)-C(119)-N(119)-C(122)	-178.4(3)
O(202)-Fe(1)-O(102)-C(102)	141.6(3)	C(103)-C(119)-N(119)-Fe(1)	16.5(5)
N(119)-Fe(1)-O(102)-C(102)	0.6(3)	O(202)-Fe(1)-N(119)-C(119)	-147.1(3)
N(219)-Fe(1)-O(102)-C(102)	-95.7(3)	O(102)-Fe(1)-N(119)-C(119)	-13.3(3)
O(102)-C(102)-C(103)-C(104)	171.5(3)	N(219)-Fe(1)-N(119)-C(119)	119.1(3)
C(101)-C(102)-C(103)-C(104)	-9.0(4)	O(202)-Fe(1)-N(119)-C(122)	46.7(3)
O(102)-C(102)-C(103)-C(119)	-9.5(5)	O(102)-Fe(1)-N(119)-C(122)	-179.5(2)
C(101)-C(102)-C(103)-C(119)	169.9(3)	N(219)-Fe(1)-N(119)-C(122)	-47.0(2)
C(102)-C(103)-C(104)-C(105)	4.7(5)	C(129)-C(120)-C(121)-C(122)	177.8(3)
C(119)-C(103)-C(104)-C(105)	-174.4(3)	C(125)-C(120)-C(121)-C(122)	-0.2(5)
C(103)-C(104)-C(105)-C(106)	2.9(5)	C(129)-C(120)-C(121)-C(221)	3.7(5)
C(104)-C(105)-C(106)-C(101)	-6.2(5)	C(125)-C(120)-C(121)-C(221)	-174.4(3)
C(104)-C(105)-C(106)-C(107)	174.1(3)	C(120)-C(121)-C(122)-C(123)	2.8(5)
C(102)-C(101)-C(106)-C(105)	1.7(5)	C(221)-C(121)-C(122)-C(123)	177.2(3)
C(118)-C(101)-C(106)-C(105)	-178.8(3)	C(120)-C(121)-C(122)-N(119)	-169.6(3)
C(102)-C(101)-C(106)-C(107)	-178.5(3)	C(221)-C(121)-C(122)-N(119)	4.8(4)
C(118)-C(101)-C(106)-C(107)	0.9(5)	C(119)-N(119)-C(122)-C(121)	-90.6(4)
C(105)-C(106)-C(107)-C(108)	179.5(3)	Fe(1)-N(119)-C(122)-C(121)	76.1(3)
C(101)-C(106)-C(107)-C(108)	-0.2(5)	C(119)-N(119)-C(122)-C(123)	96.9(4)
C(106)-C(107)-C(108)-C(109)	-0.6(5)	Fe(1)-N(119)-C(122)-C(123)	-96.4(3)
C(107)-C(108)-C(109)-C(110)	-178.9(3)	C(121)-C(122)-C(123)-C(124)	-2.5(5)
C(107)-C(108)-C(109)-C(118)	0.7(5)	N(119)-C(122)-C(123)-C(124)	169.9(3)
C(108)-C(109)-C(110)-C(111)	-178.5(3)	C(122)-C(123)-C(124)-C(125)	-0.5(5)
C(118)-C(109)-C(110)-C(111)	1.9(5)	C(123)-C(124)-C(125)-C(126)	-176.3(3)
C(109)-C(110)-C(111)-C(112)	179.2(3)	C(123)-C(124)-C(125)-C(120)	3.0(5)
C(109)-C(110)-C(111)-C(116)	-0.9(5)	C(129)-C(120)-C(125)-C(124)	179.2(3)
C(110)-C(111)-C(112)-C(113)	179.4(4)	C(121)-C(120)-C(125)-C(124)	-2.6(4)
C(116)-C(111)-C(112)-C(113)	-0.5(5)	C(129)-C(120)-C(125)-C(126)	-1.4(4)
C(111)-C(112)-C(113)-C(114)	0.1(6)	C(121)-C(120)-C(125)-C(126)	176.7(3)
C(112)-C(113)-C(114)-C(115)	0.3(6)	C(124)-C(125)-C(126)-C(127)	-178.9(3)
C(113)-C(114)-C(115)-C(116)	-0.3(6)	C(120)-C(125)-C(126)-C(127)	1.8(5)
C(114)-C(115)-C(116)-C(117)	-178.9(4)	C(125)-C(126)-C(127)-C(128)	-0.5(5)
C(114)-C(115)-C(116)-C(111)	-0.1(6)	C(126)-C(127)-C(128)-C(129)	-1.2(5)
C(110)-C(111)-C(116)-C(115)	-179.4(3)	C(127)-C(128)-C(129)-C(120)	1.5(5)
C(112)-C(111)-C(116)-C(115)	0.5(5)	C(121)-C(120)-C(129)-C(128)	-178.3(3)
C(110)-C(111)-C(116)-C(117)	-0.5(5)	C(125)-C(120)-C(129)-C(128)	-0.2(5)
C(112)-C(111)-C(116)-C(117)	179.4(3)	C(206)-C(201)-C(202)-O(202)	-172.8(3)
C(115)-C(116)-C(117)-C(118)	179.8(3)	C(218)-C(201)-C(202)-O(202)	8.3(5)
C(111)-C(116)-C(117)-C(118)	1.0(5)	C(206)-C(201)-C(202)-C(203)	7.2(4)
C(116)-C(117)-C(118)-C(109)	0.0(5)	C(218)-C(201)-C(202)-C(203)	-171.7(3)
C(116)-C(117)-C(118)-C(101)	178.9(3)	C(203)-C(202)-O(202)-Fe(1)	12.3(5)
C(110)-C(109)-C(118)-C(117)	-1.4(5)	C(201)-C(202)-O(202)-Fe(1)	-167.7(2)
C(108)-C(109)-C(118)-C(117)	179.0(3)	O(102)-Fe(1)-O(202)-C(202)	140.1(3)
C(110)-C(109)-C(118)-C(101)	179.6(3)	N(119)-Fe(1)-O(202)-C(202)	-97.2(3)

N(219)-Fe(1)-O(202)-C(202)	-1.3(3)	C(206)-C(201)-C(218)-C(209)	1.2(5)
O(202)-C(202)-C(203)-C(204)	172.6(3)	C(202)-C(201)-C(218)-C(209)	-179.9(3)
C(201)-C(202)-C(203)-C(204)	-7.4(5)	C(204)-C(203)-C(219)-N(219)	172.8(3)
O(202)-C(202)-C(203)-C(219)	-11.7(5)	C(202)-C(203)-C(219)-N(219)	-3.0(5)
C(201)-C(202)-C(203)-C(219)	168.3(3)	C(203)-C(219)-N(219)-C(222)	179.0(3)
C(202)-C(203)-C(204)-C(205)	2.3(5)	C(203)-C(219)-N(219)-Fe(1)	15.9(5)
C(219)-C(203)-C(204)-C(205)	-173.7(3)	O(202)-Fe(1)-N(219)-C(219)	-12.5(3)
C(203)-C(204)-C(205)-C(206)	2.7(5)	O(102)-Fe(1)-N(219)-C(219)	-146.4(2)
C(202)-C(201)-C(206)-C(205)	-2.2(5)	N(119)-Fe(1)-N(219)-C(219)	119.2(3)
C(218)-C(201)-C(206)-C(205)	176.7(3)	O(202)-Fe(1)-N(219)-C(222)	-177.0(2)
C(202)-C(201)-C(206)-C(207)	179.4(3)	O(102)-Fe(1)-N(219)-C(222)	49.2(3)
C(218)-C(201)-C(206)-C(207)	-1.7(5)	N(119)-Fe(1)-N(219)-C(222)	-45.2(2)
C(204)-C(205)-C(206)-C(201)	-2.8(5)	C(229)-C(220)-C(221)-C(222)	176.7(3)
C(204)-C(205)-C(206)-C(207)	175.6(3)	C(225)-C(220)-C(221)-C(222)	0.2(5)
C(201)-C(206)-C(207)-C(208)	0.2(5)	C(229)-C(220)-C(221)-C(121)	4.0(5)
C(205)-C(206)-C(207)-C(208)	-178.3(3)	C(225)-C(220)-C(221)-C(121)	-172.5(3)
C(206)-C(207)-C(208)-C(209)	1.8(6)	C(122)-C(121)-C(221)-C(222)	-72.6(4)
C(207)-C(208)-C(209)-C(210)	175.4(3)	C(120)-C(121)-C(221)-C(222)	101.6(4)
C(207)-C(208)-C(209)-C(218)	-2.2(5)	C(122)-C(121)-C(221)-C(220)	100.1(4)
C(208)-C(209)-C(210)-C(211)	-176.7(3)	C(120)-C(121)-C(221)-C(220)	-85.7(4)
C(218)-C(209)-C(210)-C(211)	0.9(5)	C(220)-C(221)-C(222)-C(223)	3.0(5)
C(209)-C(210)-C(211)-C(212)	177.6(3)	C(121)-C(221)-C(222)-C(223)	175.7(3)
C(209)-C(210)-C(211)-C(216)	-1.2(5)	C(220)-C(221)-C(222)-N(219)	-166.9(3)
C(210)-C(211)-C(212)-C(213)	-178.9(3)	C(121)-C(221)-C(222)-N(219)	5.8(4)
C(216)-C(211)-C(212)-C(213)	-0.1(5)	C(219)-N(219)-C(222)-C(221)	-90.6(4)
C(211)-C(212)-C(213)-C(214)	-1.6(6)	Fe(1)-N(219)-C(222)-C(221)	74.5(3)
C(212)-C(213)-C(214)-C(215)	2.0(6)	C(219)-N(219)-C(222)-C(223)	99.2(4)
C(213)-C(214)-C(215)-C(216)	-0.6(6)	Fe(1)-N(219)-C(222)-C(223)	-95.7(3)
C(210)-C(211)-C(216)-C(217)	0.2(5)	C(221)-C(222)-C(223)-C(224)	-3.2(5)
C(212)-C(211)-C(216)-C(217)	-178.6(3)	N(219)-C(222)-C(223)-C(224)	166.7(3)
C(210)-C(211)-C(216)-C(215)	-179.8(3)	C(222)-C(223)-C(224)-C(225)	0.3(5)
C(212)-C(211)-C(216)-C(215)	1.4(5)	C(223)-C(224)-C(225)-C(226)	-175.3(3)
C(214)-C(215)-C(216)-C(217)	178.9(3)	C(223)-C(224)-C(225)-C(220)	2.8(5)
C(214)-C(215)-C(216)-C(211)	-1.1(5)	C(229)-C(220)-C(225)-C(226)	-1.4(5)
C(211)-C(216)-C(217)-C(218)	1.1(5)	C(221)-C(220)-C(225)-C(226)	175.2(3)
C(215)-C(216)-C(217)-C(218)	-179.0(3)	C(229)-C(220)-C(225)-C(224)	-179.6(3)
C(216)-C(217)-C(218)-C(209)	-1.3(5)	C(221)-C(220)-C(225)-C(224)	-3.0(5)
C(216)-C(217)-C(218)-C(201)	175.7(3)	C(224)-C(225)-C(226)-C(227)	178.4(3)
C(210)-C(209)-C(218)-C(217)	0.4(5)	C(220)-C(225)-C(226)-C(227)	0.2(5)
C(208)-C(209)-C(218)-C(217)	178.0(3)	C(225)-C(226)-C(227)-C(228)	0.5(6)
C(210)-C(209)-C(218)-C(201)	-176.9(3)	C(226)-C(227)-C(228)-C(229)	-0.1(6)
C(208)-C(209)-C(218)-C(201)	0.7(5)	C(227)-C(228)-C(229)-C(220)	-1.2(5)
C(206)-C(201)-C(218)-C(217)	-175.8(3)	C(221)-C(220)-C(229)-C(228)	-174.6(3)
C(202)-C(201)-C(218)-C(217)	3.1(5)	C(225)-C(220)-C(229)-C(228)	1.9(5)

Symmetry transformations used to generate equivalent atoms:

Appendix V

Computational Data

(Numerical order)

Computational Methods

All DFT computations relating to CD spectroscopy were carried out using version 2005.01b, of the Amsterdam Density Functional (ADF) software suite. Initial geometries were either obtained as is from crystal data, or generated by removal/replacement of atoms, as specified in chapters 2-4. Thereafter, minimized geometries were calculated employing a triple-ζ Slater-type basis set, including one polarization function (TZP), and the Vosko-Wilk-Nusair (VWN) local density approximation. Addition of a second polarization function yielded minimal, if any, improvement in the computational results. For Zn and Fe the 1s, 2s, and 2p orbitals were kept frozen. For C, N, and O only the 1s orbital was kept frozen. Post SCF energies of *P* and *M* (*R,R*)-**75**·py, and *P* and *M* (*R,R*)-**76**·py were computed using various functionals (see below). To account for unpaired electons, those of (*R,R*)-**76**·py were calculated in spin unrestricted mode, and with a spin polarization value of 4. The same TZP basis set and other parameters, excluding the energy functionals, were utilized in the spectroscopic computations. Excitation energies and rotational strengths were calculated for the first 175 non-zero strength transitions of (*R*,*R*)-**52** (cyclohexyl-phenanthryl zinc complex), and for the first 250 non-zero strength transitions of (*R*,*R*)-**75** (cyclo-benza zinc complex). Rotary strengths are reported in the dipole-length format. Gaussian shaped distributions were subsequently generated from the computed data using a line width ($\Delta\lambda_{1/2}$) of 11 nm, and the simulated spectra obtained by superposition of the individual Gaussian curves.

(*R*,*R*)-**53** *M*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	Zn	-2.8941	2.0885	-0.4788	30.00	20.00	63.9291
2	C	-4.7764	2.9563	-2.5213	6.00	4.00	12.0000
3	C	-1.9135	0.6691	-3.2468	6.00	4.00	12.0000
4	C	-1.7013	-0.1634	-4.3658	6.00	4.00	12.0000
5	N	-3.5300	2.2460	-2.3717	7.00	5.00	14.0031
6	C	-0.6880	-1.0624	-4.3907	6.00	4.00	12.0000
7	C	0.2121	-1.1410	-3.3070	6.00	4.00	12.0000
8	C	1.2430	-2.1096	-3.3658	6.00	4.00	12.0000
9	C	2.1554	-2.2223	-2.3737	6.00	4.00	12.0000
10	C	2.1235	-1.3499	-1.2612	6.00	4.00	12.0000
11	C	3.1243	-1.4425	-0.2832	6.00	4.00	12.0000
12	C	3.1543	-0.5817	0.7832	6.00	4.00	12.0000
13	H	-6.7298	3.2152	2.9406	1.00	1.00	1.0078
14	C	2.1609	0.3920	0.8948	6.00	4.00	12.0000
15	C	1.1518	0.4882	-0.0353	6.00	4.00	12.0000
16	C	1.0950	-0.3717	-1.1489	6.00	4.00	12.0000
17	C	-4.9068	3.9511	-1.3639	6.00	4.00	12.0000
18	C	-3.0631	1.4903	-3.3115	6.00	4.00	12.0000
19	C	-3.3973	1.2515	3.6178	6.00	4.00	12.0000
20	C	-3.6556	1.8039	2.3120	6.00	4.00	12.0000
21	O	-2.8003	1.6141	1.3616	8.00	6.00	15.9949
22	C	-4.8524	2.5573	2.1128	6.00	4.00	12.0000
23	C	-5.8073	2.6596	3.1452	6.00	4.00	12.0000
24	H	-4.9573	1.0700	6.6678	1.00	1.00	1.0078
25	C	-5.5928	2.0942	4.3578	6.00	4.00	12.0000
26	C	-4.3829	1.4168	4.6174	6.00	4.00	12.0000
27	C	-4.1645	0.9248	5.9263	6.00	4.00	12.0000
28	C	-3.0029	0.3175	6.2587	6.00	4.00	12.0000
29	N	-4.4641	3.2940	-0.1651	7.00	5.00	14.0031
30	C	-1.9844	0.1262	5.2977	6.00	4.00	12.0000
31	C	-0.7921	-0.5056	5.6806	6.00	4.00	12.0000
32	C	0.2081	-0.7365	4.7729	6.00	4.00	12.0000
33	C	0.0229	-0.3392	3.4493	6.00	4.00	12.0000
34	C	-1.1285	0.2977	3.0485	6.00	4.00	12.0000
35	H	-2.8260	-0.0405	7.2787	1.00	1.00	1.0078
36	C	-2.1730	0.5647	3.9554	6.00	4.00	12.0000
37	C	-5.1771	3.2341	0.9117	6.00	4.00	12.0000
38	H	-5.6083	2.2274	-2.3913	1.00	1.00	1.0078
39	H	-4.1747	4.7617	-1.5758	1.00	1.00	1.0078
40	H	-6.4022	5.2581	-0.5212	1.00	1.00	1.0078
41	C	-6.2890	4.5527	-1.3631	6.00	4.00	12.0000
42	H	-7.0325	3.7445	-1.2085	1.00	1.00	1.0078
43	H	-7.5774	5.6661	-2.6932	1.00	1.00	1.0078
44	H	-5.8696	6.1235	-2.7642	1.00	1.00	1.0078
45	H	-7.1156	3.5473	-3.8591	1.00	1.00	1.0078

46	H	-0.6853	-0.8133	6.7270	1.00	1.00	1.0078
47	H	-6.4702	4.8941	-4.8099	1.00	1.00	1.0078
48	H	-4.1748	4.4410	-3.9313	1.00	1.00	1.0078
49	H	-4.8620	2.9858	-4.6824	1.00	1.00	1.0078
50	H	-6.3315	2.1714	5.1605	1.00	1.00	1.0078
51	H	0.8001	-0.5365	2.7022	1.00	1.00	1.0078
52	H	-1.2526	0.5993	2.0087	1.00	1.00	1.0078
53	C	-6.5529	5.2564	-2.6802	6.00	4.00	12.0000
54	H	-6.1517	3.7594	0.9330	1.00	1.00	1.0078
55	H	-3.6119	1.4340	-4.2731	1.00	1.00	1.0078
56	H	-2.4022	-0.0857	-5.2051	1.00	1.00	1.0078
57	H	1.1339	-1.2328	5.0795	1.00	1.00	1.0078
58	H	-0.5463	-1.7373	-5.2395	1.00	1.00	1.0078
59	H	1.2766	-2.7692	-4.2392	1.00	1.00	1.0078
60	H	2.9461	-2.9791	-2.4197	1.00	1.00	1.0078
61	H	3.8931	-2.2140	-0.4040	1.00	1.00	1.0078
62	H	3.9483	-0.6531	1.5323	1.00	1.00	1.0078
63	H	2.1778	1.0951	1.7334	1.00	1.00	1.0078
64	H	0.3713	1.2405	0.0692	1.00	1.00	1.0078
65	C	-6.3395	4.3374	-3.8668	6.00	4.00	12.0000
66	C	-4.9737	3.6801	-3.8326	6.00	4.00	12.0000
67	C	0.0950	-0.2901	-2.1849	6.00	4.00	12.0000
68	C	-1.0357	0.6032	-2.1193	6.00	4.00	12.0000
69	O	-1.2390	1.3004	-1.0506	8.00	6.00	15.9949

```
*****************************************************************************
*                                                                           *
*   Final excitation energies from Davidson algorithm                       *
*                                                                           *
*****************************************************************************
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Number of loops in Davidson routine = 242
Number of matrix-vector multiplications = 416
Type of excitations = SINGLET-SINGLET

Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.81001E-01	2.2041	0.12189E-01	0.13E-10
2	0.90212E-01	2.4548	0.97649E-03	0.20E-08
3	0.93914E-01	2.5555	0.23533E-03	0.25E-09
4	0.94845E-01	2.5809	0.14354E-01	0.15E-08
5	0.10113	2.7520	0.66796E-03	0.21E-08
6	0.10584	2.8802	0.60686E-02	0.27E-08
7	0.10805	2.9401	0.62898E-01	0.28E-07
8	0.10880	2.9605	0.28471E-01	0.26E-07
9	0.11286	3.0711	0.13399E-01	0.68E-09
10	0.11555	3.1443	0.20215	0.12E-07
11	0.11982	3.2603	0.27129E-02	0.74E-08

12	0.12088	3.2892	0.76351E-02	0.64E-09
13	0.12446	3.3867	0.91980E-02	0.19E-10
14	0.12535	3.4109	0.48017E-02	0.16E-08
15	0.12699	3.4555	0.28692E-03	0.37E-11
16	0.13040	3.5482	0.10334E-01	0.46E-08
17	0.13270	3.6110	0.45579E-03	0.36E-08
18	0.13340	3.6301	0.16221E-01	0.53E-09
19	0.13464	3.6636	0.46403E-02	0.80E-08
20	0.13478	3.6676	0.29187E-03	0.68E-07
21	0.13585	3.6967	0.84780E-02	0.27E-08
22	0.13856	3.7705	0.41328E-02	0.14E-07
23	0.13884	3.7780	0.16575E-02	0.25E-07
24	0.13975	3.8027	0.13966E-01	0.77E-08
25	0.13985	3.8056	0.54984E-03	0.51E-07
26	0.14257	3.8796	0.14610E-01	0.38E-07
27	0.14424	3.9249	0.89342E-03	0.35E-08
28	0.14537	3.9556	0.17702E-01	0.39E-08
29	0.14579	3.9672	0.74179E-01	0.11E-08
30	0.14713	4.0035	0.19489E-01	0.63E-09
31	0.14772	4.0195	0.32270E-01	0.74E-09
32	0.14921	4.0601	0.13333	0.88E-07
33	0.15372	4.1828	0.20900E-01	0.46E-09
34	0.15462	4.2074	0.71095E-01	0.36E-08
35	0.15703	4.2731	0.20677E-02	0.61E-09
36	0.15980	4.3484	0.40761E-03	0.71E-12
37	0.16052	4.3679	0.56759E-02	0.10E-06
38	0.16202	4.4087	0.66965E-02	0.15E-07
39	0.16213	4.4119	0.62767E-01	0.41E-07
40	0.16380	4.4572	0.28523E-02	0.85E-09
41	0.16440	4.4735	0.92117E-02	0.15E-07
42	0.16464	4.4802	0.20961E-01	0.53E-09
43	0.16536	4.4996	0.11648E-01	0.26E-06
44	0.16563	4.5071	0.41068E-01	0.15E-07
45	0.16586	4.5134	0.80005E-01	0.69E-07
46	0.16626	4.5243	0.24722	0.42E-06
47	0.16690	4.5415	0.40795E-01	0.39E-08
48	0.16780	4.5661	0.56576E-01	0.30E-07
49	0.16850	4.5850	0.14291	0.28E-06
50	0.16920	4.6041	0.98261E-02	0.52E-06
51	0.16956	4.6141	0.11394E-01	0.25E-08
52	0.17028	4.6336	0.15040E-01	0.13E-06
53	0.17049	4.6392	0.14430E-01	0.20E-08
54	0.17247	4.6932	0.32922E-02	0.20E-07
55	0.17282	4.7028	0.46703E-02	0.60E-08
56	0.17347	4.7205	0.11887E-01	0.16E-07
57	0.17382	4.7299	0.63057E-01	0.11E-10
58	0.17584	4.7848	0.21534E-02	0.17E-09
59	0.17590	4.7866	0.29391E-02	0.23E-07
60	0.17647	4.8019	0.17024E-01	0.31E-07
61	0.17672	4.8089	0.67461E-02	0.57E-09
62	0.17681	4.8112	0.47791E-02	0.21E-08
63	0.17711	4.8193	0.81259E-02	0.32E-07
64	0.17769	4.8351	0.50672E-02	0.54E-12
65	0.17857	4.8591	0.13142E-02	0.21E-08
66	0.17972	4.8904	0.10110E-01	0.44E-11
67	0.18102	4.9257	0.11042E-02	0.14E-07

68	0.18121	4.9308	0.95329E-02	0.27E-08
69	0.18200	4.9525	0.16079E-01	0.27E-07
70	0.18210	4.9552	0.27005E-01	0.49E-09
71	0.18248	4.9656	0.38977E-01	0.15E-07
72	0.18291	4.9774	0.32104E-01	0.48E-08
73	0.18313	4.9832	0.45394E-02	0.54E-08
74	0.18350	4.9932	0.44666E-01	0.83E-08
75	0.18398	5.0063	0.12668E-01	0.46E-08
76	0.18438	5.0172	0.53498E-02	0.43E-08
77	0.18525	5.0408	0.64734E-01	0.20E-06
78	0.18562	5.0510	0.13410	0.24E-07
79	0.18595	5.0600	0.26734E-01	0.19E-08
80	0.18600	5.0612	0.16511	0.19E-08
81	0.18663	5.0784	0.59235E-02	0.28E-10
82	0.18701	5.0889	0.17609E-01	0.12E-09
83	0.18760	5.1049	0.94258E-02	0.37E-07
84	0.18794	5.1142	0.52997E-01	0.45E-07
85	0.18840	5.1267	0.35974E-02	0.32E-09
86	0.18867	5.1341	0.52158E-02	0.18E-07
87	0.18922	5.1488	0.24102E-01	0.16E-08
88	0.19055	5.1851	0.15448E-02	0.14E-08
89	0.19087	5.1939	0.35386E-01	0.45E-07
90	0.19116	5.2018	0.94487E-03	0.26E-09
91	0.19168	5.2158	0.76386E-02	0.10E-10
92	0.19203	5.2254	0.77440E-02	0.60E-08
93	0.19215	5.2287	0.12055	0.11E-06
94	0.19234	5.2339	0.34389E-02	0.70E-08
95	0.19279	5.2461	0.10456	0.34E-08
96	0.19314	5.2556	0.16581E-02	0.21E-08
97	0.19386	5.2752	0.16107E-02	0.26E-08
98	0.19440	5.2898	0.64774E-01	0.11E-06
99	0.19465	5.2968	0.91643E-01	0.43E-08
100	0.19490	5.3036	0.33149E-01	0.16E-08
101	0.19516	5.3107	0.22114E-02	0.18E-07
102	0.19567	5.3243	0.25617E-01	0.37E-08
103	0.19600	5.3334	0.69202E-02	0.13E-08
104	0.19620	5.3389	0.55109E-02	0.98E-09
105	0.19645	5.3456	0.91391E-02	0.76E-10
106	0.19704	5.3619	0.12359E-02	0.70E-08
107	0.19829	5.3957	0.21652E-02	0.38E-08
108	0.19908	5.4173	0.24098E-02	0.75E-09
109	0.19938	5.4253	0.13732E-01	0.21E-08
110	0.19956	5.4302	0.18042E-02	0.39E-08
111	0.19970	5.4342	0.14739E-02	0.43E-08
112	0.20023	5.4486	0.98300E-02	0.19E-07
113	0.20146	5.4820	0.40052E-01	0.19E-10
114	0.20182	5.4918	0.41263E-01	0.19E-08
115	0.20225	5.5035	0.89266E-01	0.29E-09
116	0.20275	5.5170	0.19442E-02	0.43E-08
117	0.20281	5.5187	0.10157E-01	0.20E-08
118	0.20299	5.5236	0.58383E-02	0.17E-07
119	0.20307	5.5259	0.36303E-02	0.30E-10
120	0.20371	5.5431	0.17533E-01	0.54E-08
121	0.20412	5.5545	0.10915	0.61E-07
122	0.20424	5.5578	0.82667E-03	0.50E-09
123	0.20458	5.5668	0.25083E-01	0.11E-09

124	0.20523	5.5846	0.54749E-02	0.49E-08
125	0.20547	5.5912	0.97797E-01	0.10E-06
126	0.20589	5.6025	0.13012E-01	0.10E-08
127	0.20617	5.6103	0.80632E-02	0.12E-07
128	0.20668	5.6240	0.29201E-01	0.16E-07
129	0.20710	5.6356	0.18857E-01	0.37E-08
130	0.20767	5.6509	0.27714E-01	0.37E-07
131	0.20790	5.6573	0.22038E-01	0.57E-07
132	0.20806	5.6617	0.43111E-01	0.21E-06
133	0.20860	5.6763	0.10684E-01	0.88E-08
134	0.20863	5.6771	0.92146E-02	0.27E-08
135	0.20886	5.6834	0.35924E-01	0.30E-08
136	0.20893	5.6852	0.15930E-01	0.27E-07
137	0.20922	5.6932	0.45811E-02	0.32E-08
138	0.20960	5.7036	0.13850E-01	0.63E-08
139	0.21001	5.7147	0.14953E-01	0.37E-07
140	0.21015	5.7185	0.84863E-02	0.63E-07
141	0.21043	5.7261	0.11069E-01	0.90E-08
142	0.21093	5.7396	0.10534E-01	0.36E-07
143	0.21118	5.7465	0.78863E-01	0.78E-07
144	0.21167	5.7598	0.52342E-02	0.53E-07
145	0.21196	5.7676	0.19728E-01	0.88E-09
146	0.21209	5.7713	0.83639E-02	0.21E-06
147	0.21219	5.7739	0.47492E-02	0.87E-09
148	0.21227	5.7762	0.17913E-01	0.14E-06
149	0.21243	5.7806	0.11622E-02	0.45E-09
150	0.21278	5.7901	0.14175E-01	0.16E-07
151	0.21314	5.7997	0.19206E-01	0.20E-06
152	0.21355	5.8110	0.68693E-01	0.19E-07
153	0.21418	5.8281	0.28784E-01	0.36E-06
154	0.21438	5.8337	0.25168E-01	0.42E-07
155	0.21450	5.8368	0.14313E-01	0.12E-09
156	0.21485	5.8464	0.91160E-02	0.10E-06
157	0.21531	5.8590	0.42899E-02	0.43E-07
158	0.21558	5.8662	0.12145E-02	0.25E-09
159	0.21615	5.8819	0.10733E-01	0.27E-07
160	0.21664	5.8951	0.33460E-02	0.45E-07
161	0.21672	5.8974	0.70302E-02	0.13E-06
162	0.21714	5.9086	0.14189E-02	0.56E-07
163	0.21752	5.9189	0.46484E-02	0.17E-06
164	0.21766	5.9229	0.30809E-01	0.43E-09
165	0.21799	5.9318	0.76605E-02	0.36E-07
166	0.21803	5.9330	0.51322E-02	0.39E-06
167	0.21814	5.9360	0.78367E-03	0.56E-06
168	0.21820	5.9375	0.31900E-02	0.66E-06
169	0.21826	5.9391	0.12422E-01	0.32E-06
170	0.21871	5.9515	0.20303E-02	0.74E-07
171	0.21932	5.9681	0.78713E-02	0.36E-08
172	0.21962	5.9762	0.47473E-01	0.11E-07
173	0.21985	5.9825	0.11392E-01	0.50E-07
174	0.22000	5.9865	0.21628E-02	0.50E-09
175	0.22016	5.9910	0.10227E-02	0.56E-08

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	2.2041	1.22E-02	-0.25245	5.96E-02	0.39804
2	2.4548	9.76E-04	0.11461	3.24E-02	-4.53E-02
3	2.5555	2.35E-04	-1.79E-02	5.86E-02	3.18E-04
4	2.5809	1.44E-02	-4.96E-02	4.30E-02	0.47192
5	2.752	6.68E-04	-4.27E-02	-6.41E-02	6.30E-02
6	2.8802	6.07E-03	0.10049	8.02E-02	0.26358
7	2.9401	6.29E-02	-0.84937	0.23586	-0.31007
8	2.9605	2.85E-02	-0.46369	0.37027	-0.20107
9	3.0711	1.34E-02	-0.187	-8.16E-02	0.36939
10	3.1443	0.20215	-1.1524	0.732	-0.87197
11	3.2603	2.71E-03	-0.17566	2.95E-02	4.73E-02
12	3.2892	7.64E-03	-0.25567	0.16348	5.15E-02
13	3.3867	9.20E-03	0.17714	-0.10756	0.26059
14	3.4109	4.80E-03	-0.11703	0.11067	0.17753
15	3.4555	2.87E-04	4.15E-02	-3.57E-02	1.98E-02
16	3.5482	1.03E-02	-1.33E-02	2.69E-02	-0.34348
17	3.611	4.56E-04	-2.11E-02	2.97E-02	6.19E-02
18	3.6301	1.62E-02	-0.38705	0.17552	-4.22E-02
19	3.6636	4.64E-03	0.19155	-9.76E-02	-7.40E-02
20	3.6676	2.92E-04	-3.93E-02	-1.88E-02	-3.67E-02
21	3.6967	8.48E-03	-0.20559	8.80E-02	0.20879
22	3.7705	4.13E-03	-1.95E-03	-1.93E-02	0.21063
23	3.778	1.66E-03	2.59E-02	-5.28E-02	-0.12021
24	3.8027	1.40E-02	-0.14928	0.11707	-0.33752
25	3.8056	5.50E-04	-8.28E-03	-6.57E-02	3.90E-02
26	3.8796	1.46E-02	-0.28518	0.24022	0.12115
27	3.9249	8.93E-04	6.91E-02	-6.12E-02	-2.78E-02
28	3.9556	1.77E-02	0.30232	-0.10217	-0.28431
29	3.9672	7.42E-02	-0.74559	0.34767	0.29398
30	4.0035	1.95E-02	-0.216	0.18125	-0.34524
31	4.0195	3.23E-02	0.41681	-0.2707	0.28406
32	4.0601	0.13333	0.53161	-0.52665	0.88344
33	4.1828	2.09E-02	0.38134	-0.20904	0.12176
34	4.2074	7.11E-02	-0.71985	0.40692	-7.71E-02
35	4.2731	2.07E-03	-0.11292	7.37E-02	-3.97E-02
36	4.3484	4.08E-04	-4.27E-02	-3.83E-02	2.31E-02
37	4.3679	5.68E-03	0.1672	0.11885	-0.10468
38	4.4087	6.70E-03	-0.22708	-7.08E-02	7.37E-02
39	4.4119	6.28E-02	0.28397	3.60E-02	0.70623
40	4.4572	2.85E-03	-0.10452	7.44E-02	-9.83E-02
41	4.4735	9.21E-03	-0.15581	9.14E-02	-0.22676
42	4.4802	2.10E-02	0.10494	1.02E-02	0.42409
43	4.4996	1.16E-02	0.12756	-0.15355	0.25655
44	4.5071	4.11E-02	-0.46882	0.33531	0.19924
45	4.5134	8.00E-02	8.16E-02	-0.20081	-0.82252
46	4.5243	0.24722	1.0919	-0.80125	0.62943
47	4.5415	4.08E-02	-0.56354	0.22006	2.51E-02
48	4.5661	5.66E-02	-0.57371	0.39992	-0.12907
49	4.585	0.14291	-0.75473	0.44115	-0.71276
50	4.6041	9.83E-03	0.21691	8.52E-02	-0.18114
51	4.6141	1.14E-02	8.96E-02	0.2701	-0.14077

52	4.6336	1.50E-02	-0.11224	1.88E-02	-0.34574
53	4.6392	1.44E-02	0.10885	-9.51E-02	-0.32568
54	4.6932	3.29E-03	-0.12235	0.10891	4.24E-02
55	4.7028	4.67E-03	0.15864	0.1216	2.41E-02
56	4.7205	1.19E-02	-3.08E-02	2.75E-02	-0.31793
57	4.7299	6.31E-02	0.50798	-0.36818	-0.38802
58	4.7848	2.15E-03	-0.10571	8.20E-02	-2.17E-02
59	4.7866	2.94E-03	7.70E-02	2.99E-02	-0.13505
60	4.8019	1.70E-02	0.27851	-0.2546	-4.82E-02
61	4.8089	6.75E-03	-0.22045	8.17E-02	4.47E-02
62	4.8112	4.78E-03	-0.11841	-4.48E-02	0.15656
63	4.8193	8.13E-03	9.21E-02	-6.27E-03	-0.24556
64	4.8351	5.07E-03	0.11634	-7.49E-02	0.15371
65	4.8591	1.31E-03	6.49E-02	3.17E-02	7.63E-02
66	4.8904	1.01E-02	-0.10147	-2.67E-03	-0.27217
67	4.9257	1.10E-03	5.49E-04	-4.18E-02	-8.60E-02
68	4.9308	9.53E-03	0.19612	-0.1166	0.16387
69	4.9525	1.61E-02	-0.16715	0.24595	-0.20997
70	4.9552	2.70E-02	-0.41562	0.22079	-3.10E-02
71	4.9656	3.90E-02	0.262	-0.34242	0.36674
72	4.9774	3.21E-02	-0.17233	0.10414	-0.47194
73	4.9832	4.54E-03	-0.1892	-3.68E-02	5.59E-03
74	4.9932	4.47E-02	0.18118	-0.35216	0.45638
75	5.0063	1.27E-02	0.1395	5.05E-02	-0.2851
76	5.0172	5.35E-03	-0.16431	0.12839	6.48E-03
77	5.0408	6.47E-02	0.53405	-0.47251	0.12529
78	5.051	0.1341	-0.66191	0.31479	-0.73922
79	5.06	2.67E-02	-0.39154	0.24941	1.21E-02
80	5.0612	0.16511	0.79103	-0.44213	0.7144
81	5.0784	5.92E-03	-6.72E-02	-4.05E-02	-0.20361
82	5.0889	1.76E-02	0.28848	-0.19966	0.13473
83	5.1049	9.43E-03	-0.24115	0.12796	-2.90E-02
84	5.1142	5.30E-02	0.52346	-0.3283	0.20293
85	5.1267	3.60E-03	0.11989	-0.11399	3.57E-02
86	5.1341	5.22E-03	0.10147	-6.01E-02	-0.166
87	5.1488	2.41E-02	0.26772	-0.23457	0.25371
88	5.1851	1.54E-03	-6.78E-02	-7.22E-02	4.85E-02
89	5.1939	3.54E-02	-0.43944	0.23156	-0.17708
90	5.2018	9.45E-04	-8.01E-02	6.78E-03	-3.09E-02
91	5.2158	7.64E-03	6.69E-02	-4.68E-02	0.23047
92	5.2254	7.74E-03	-0.16551	7.01E-02	-0.16786
93	5.2287	0.12055	0.68519	-0.37325	0.57642
94	5.2339	3.44E-03	3.72E-03	-2.69E-02	-0.1615
95	5.2461	0.10456	-0.54498	0.27472	-0.66414
96	5.2556	1.66E-03	-7.59E-02	6.72E-02	-5.11E-02
97	5.2752	1.61E-03	-5.52E-02	-4.92E-02	-8.37E-02
98	5.2898	6.48E-02	0.58574	-0.39456	3.23E-02
99	5.2968	9.16E-02	0.58701	-0.20021	0.56704
100	5.3036	3.31E-02	-0.34427	4.52E-02	-0.36681
101	5.3107	2.21E-03	5.46E-02	-7.46E-02	-9.19E-02
102	5.3243	2.56E-02	-0.29328	0.14243	-0.30014
103	5.3334	6.92E-03	0.20175	-9.04E-02	6.39E-02
104	5.3389	5.51E-03	-0.13295	9.33E-02	-0.12555
105	5.3456	9.14E-03	-0.23815	0.1046	-4.61E-02
106	5.3619	1.24E-03	-8.41E-02	1.78E-02	4.49E-02
107	5.3957	2.17E-03	5.15E-02	-0.10881	-4.35E-02

108	5.4173	2.41E-03	-8.39E-02	8.95E-02	5.58E-02
109	5.4253	1.37E-02	0.19391	-0.11664	-0.22827
110	5.4302	1.80E-03	6.40E-02	6.53E-02	-7.21E-02
111	5.4342	1.47E-03	1.42E-02	-1.21E-02	0.10356
112	5.4486	9.83E-03	3.62E-02	-5.20E-02	-0.26387
113	5.482	4.01E-02	-0.42786	0.30051	-0.15762
114	5.4918	4.13E-02	-0.47377	0.27928	6.49E-02
115	5.5035	8.93E-02	0.50832	-0.29303	-0.56373
116	5.517	1.94E-03	0.1071	-4.34E-02	3.20E-02
117	5.5187	1.02E-02	-4.14E-02	3.49E-02	0.26869
118	5.5236	5.84E-03	-2.48E-02	-7.61E-02	-0.19166
119	5.5259	3.63E-03	0.15506	-4.58E-02	2.59E-02
120	5.5431	1.75E-02	-0.2319	0.13057	0.24141
121	5.5545	0.10915	0.54211	-0.50422	-0.50399
122	5.5578	8.27E-04	-1.05E-02	-6.74E-03	7.69E-02
123	5.5668	2.51E-02	-0.35995	0.20976	0.10173
124	5.5846	5.47E-03	-0.16181	-2.91E-02	-0.11395
125	5.5912	9.78E-02	0.44347	0.11385	0.71015
126	5.6025	1.30E-02	0.28112	-0.11983	-3.75E-02
127	5.6103	8.06E-03	-0.13864	9.88E-02	0.17227
128	5.624	2.92E-02	-0.43777	0.14231	5.93E-03
129	5.6356	1.89E-02	0.28321	-5.55E-02	-0.23084
130	5.6509	2.77E-02	0.22579	-0.17911	-0.34223
131	5.6573	2.20E-02	-0.38313	0.10431	3.65E-02
132	5.6617	4.31E-02	-0.42645	-1.24E-03	-0.35908
133	5.6763	1.07E-02	-3.94E-02	9.96E-02	0.25564
134	5.6771	9.21E-03	-3.23E-02	-4.61E-02	-0.25117
135	5.6834	3.59E-02	-0.47478	0.17179	-5.54E-02
136	5.6852	1.59E-02	-0.32525	9.21E-02	1.01E-02
137	5.6932	4.58E-03	-9.16E-02	0.15562	1.57E-02
138	5.7036	1.39E-02	-0.25477	0.1398	0.12112
139	5.7147	1.50E-02	-0.24417	0.1873	-0.10999
140	5.7185	8.49E-03	-0.21768	0.11464	6.63E-03
141	5.7261	1.11E-02	-0.19424	0.20066	3.01E-02
142	5.7396	1.05E-02	0.2002	-7.43E-02	0.17121
143	5.7465	7.89E-02	-0.559	0.23872	-0.43668
144	5.7598	5.23E-03	0.17936	5.79E-02	3.97E-02
145	5.7676	1.97E-02	-0.11856	-1.44E-02	-0.35405
146	5.7713	8.36E-03	-0.18613	1.35E-05	-0.15655
147	5.7739	4.75E-03	7.74E-02	0.11685	0.11805
148	5.7762	1.79E-02	-0.13286	3.09E-03	0.33003
149	5.7806	1.16E-03	-8.69E-02	-3.85E-03	-2.53E-02
150	5.7901	1.42E-02	-6.91E-02	0.26197	0.16286
151	5.7997	1.92E-02	0.24596	1.56E-02	0.27282
152	5.811	6.87E-02	0.47542	-0.22183	-0.45528
153	5.8281	2.88E-02	-0.36323	-0.13942	-0.22409
154	5.8337	2.52E-02	0.12873	8.47E-02	-0.39033
155	5.8368	1.43E-02	-6.56E-02	-2.58E-02	-0.30842
156	5.8464	9.12E-03	0.10833	0.10324	0.2031
157	5.859	4.29E-03	0.12144	4.60E-03	0.12296
158	5.8662	1.21E-03	-8.39E-02	-2.79E-02	2.52E-02
159	5.8819	1.07E-02	-0.17747	-3.18E-02	-0.20488
160	5.8951	3.35E-03	4.38E-02	0.1056	0.1005
161	5.8974	7.03E-03	9.40E-02	-8.07E-02	-0.18254
162	5.9086	1.42E-03	6.54E-02	7.23E-02	1.75E-02
163	5.9189	4.65E-03	7.52E-02	1.66E-02	-0.16163

164	5.9229	3.08E-02	-0.12147	3.48E-02	0.44312
165	5.9318	7.66E-03	0.19977	-2.80E-02	0.10964
166	5.933	5.13E-03	5.03E-02	7.20E-02	0.16615
167	5.936	7.84E-04	-6.61E-02	1.66E-02	-2.72E-02
168	5.9375	3.19E-03	-2.99E-02	9.07E-02	0.11321
169	5.9391	1.24E-02	0.28205	-7.63E-02	-1.80E-03
170	5.9515	2.03E-03	1.74E-02	-0.11427	2.37E-02
171	5.9681	7.87E-03	-0.21998	6.48E-02	3.52E-02
172	5.9762	4.75E-02	0.11063	-0.18614	-0.52664
173	5.9825	1.14E-02	0.25795	-0.10574	-2.42E-03
174	5.9865	2.16E-03	3.43E-02	-2.75E-02	-0.1132
175	5.991	1.02E-03	3.87E-02	-6.24E-02	-3.96E-02

Rotatory strengths R in 10**(-40) esu**2 * cm**2 ,
(multiply by 1.07827 to obtain reduced rotatory strengths),
magnetic transition dipole vectors m in a.u.:

no.	R	m (x,y,z)		
1	-21.602	0.53258	0.76975	-7.66E-03
2	-16.44	-0.39753	-0.72579	1.40E-02
3	0.11942	9.27E-02	3.65E-02	6.48E-02
4	18.829	0.29603	0.24745	0.17778
5	-20.304	0.65579	1.0072	0.10212
6	-14.675	-0.38442	-0.57866	8.64E-02
7	-82.441	0.91098	1.4009	-0.30189
8	-30.952	-0.86796	-1.5803	-0.25546
9	-84.82	1.2829	2.2116	0.16408
10	79.802	-0.32419	-0.70745	-0.5537
11	-6.292	0.11522	6.97E-02	-0.17994
12	-2.7683	0.11895	0.13252	-5.82E-02
13	6.8442	0.17726	0.36384	0.1411
14	-1.2545	1.72E-02	-1.41E-02	-9.87E-03
15	1.6254	0.15748	-5.51E-03	8.44E-03
16	2.7925	-0.34788	-0.45358	-5.66E-02
17	1.2659	1.68E-02	4.01E-02	7.33E-02
18	-7.6382	0.43756	0.7779	-9.94E-03
19	-2.7304	-0.13529	-0.15618	1.24E-02
20	-1.0688	5.04E-02	0.11819	8.90E-03
21	-1.7998	0.34414	0.52276	8.19E-02
22	3.8815	0.22814	0.42794	0.11951
23	-1.6319	1.30E-02	0.13744	5.28E-05
24	11.476	-0.3015	-0.56456	-0.20671
25	-2.0899	9.12E-03	0.17454	6.85E-02
26	-2.5738	0.1006	0.10242	-5.64E-02
27	-5.9212	0.31497	0.70172	0.14159
28	-25.745	-0.87745	-1.2952	-8.34E-02
29	-60.395	1.1394	1.7295	-2.71E-02
30	16.278	-0.17474	-0.22576	-0.20921
31	19.245	-0.12572	-0.32242	0.16464
32	19.359	1.1633	1.8296	0.48363
33	-2.7633	-0.37547	-0.57209	9.75E-02
34	-35.973	0.68959	0.80275	-0.22228
35	4.0639	-0.12907	8.51E-02	9.09E-02

36	-5.7715	0.24832	0.26454	-0.16196
37	-136.36	-1.4746	-2.5975	0.22171
38	-66.417	0.84322	1.4014	0.12093
39	81.129	0.42137	0.48492	0.29317
40	0.67354	-8.74E-03	-5.14E-02	-5.87E-02
41	6.2358	4.55E-02	0.21815	-6.00E-02
42	18.501	0.24341	0.20516	0.11992
43	-13.259	0.92542	1.7367	0.36005
44	-42.707	3.75E-02	-0.37804	-0.18489
45	58.277	-0.34255	-0.22015	-0.28079
46	38.33	0.57816	0.83271	0.31543
47	-3.2506	-9.52E-02	-0.30469	-1.61E-02
48	-21.415	-0.1786	-0.5967	-0.35115
49	58.683	-0.41724	-0.72493	-0.35614
50	-26.574	-0.36838	-0.71433	-0.15461
51	14.542	0.10437	0.12288	-0.13602
52	23.959	-0.17627	-0.23775	-0.24969
53	-17.92	-0.27246	1.05E-02	0.13931
54	-2.181	-0.10426	-0.18699	-3.87E-02
55	-1.6707	4.77E-02	-0.10069	-0.10011
56	17.235	-2.11E-02	1.83E-02	-0.22634
57	-14.795	-0.51463	-0.56598	2.51E-02
58	-3.2954	-0.34649	-0.64107	-9.07E-02
59	0.61684	-1.04E-02	-0.11897	-5.17E-02
60	3.3157	-0.23981	-0.3402	0.11958
61	-4.161	0.20374	0.29579	6.96E-02
62	0.82611	0.12007	3.33E-02	0.12272
63	-1.266	-0.21483	-8.08E-02	-5.67E-02
64	2.5462	0.10576	0.16229	6.94E-02
65	-6.526	-0.145	-0.28762	-0.11994
66	3.3999	0.22852	0.58272	-0.14389
67	13.067	-0.62478	-0.9941	-0.16547
68	5.4869	-0.43848	-0.94086	-2.63E-03
69	0.12784	-0.27841	-0.3186	-0.15414
70	-8.6558	2.49E-02	-0.10311	0.11613
71	-40.778	0.65082	1.2596	0.23946
72	15.737	-0.42384	-0.68319	-0.13745
73	-16.943	0.24055	0.74375	0.17872
74	-66.15	1.2317	1.846	0.32062
75	-21.459	-0.61804	-0.82625	-0.12935
76	1.7491	-6.44E-02	-2.24E-02	-4.56E-02
77	-26.03	0.32252	0.65214	0.20335
78	98.675	0.14684	0.43632	-0.51195
79	6.7756	0.37319	0.70243	-2.72E-02
80	103.54	-5.17E-02	-0.19645	0.55053
81	-6.953	0.37673	0.47051	-7.31E-02
82	-8.0057	0.74126	1.3223	0.1204
83	-9.4926	0.18554	-1.25E-02	-0.20994
84	-4.1558	0.24817	0.63307	0.29715
85	-6.714	-0.20207	4.19E-02	1.46E-02
86	3.7593	-0.3588	-0.79599	-2.71E-02
87	-31.819	1.2987	2.2758	0.20173
88	-17.994	0.42001	0.668	7.96E-03
89	13.633	-0.71323	-1.1359	-4.20E-02
90	-2.4369	9.90E-02	7.51E-02	9.45E-02
91	10.623	-0.19005	-0.18892	0.21228

92	5.8568	-0.23032	-0.48203	-0.12232
93	74.552	-0.16619	-0.21274	0.60846
94	4.5336	-8.24E-02	-0.16062	-9.43E-02
95	81.466	-0.2104	-0.15357	-0.41124
96	3.4898	-0.14796	-3.12E-02	-0.11107
97	2.9777	-8.40E-02	-6.48E-02	-5.75E-02
98	-19.282	0.19035	0.50781	0.21929
99	67.56	-2.56E-02	0.18701	0.59801
100	27.061	4.85E-02	0.25734	-0.32677
101	-3.8645	-0.10768	6.07E-02	6.51E-02
102	22.998	-5.80E-02	-0.14107	-0.33537
103	1.3846	0.18299	0.52205	0.25307
104	3.7273	1.35E-02	6.84E-02	-8.94E-02
105	4.9395	-0.19531	-0.25183	-1.70E-02
106	1.7265	-3.06E-02	-0.10275	0.1466
107	-3.8187	-8.85E-02	9.25E-02	3.62E-02
108	-1.3781	-9.73E-02	-0.1577	1.69E-03
109	-10.992	-4.66E-02	0.3173	2.55E-03
110	-8.0548	-0.22142	-0.17184	0.12175
111	0.66924	8.07E-02	6.03E-02	2.34E-02
112	-2.969	-9.67E-02	0.30149	-2.49E-02
113	-0.90315	-3.68E-02	-7.27E-03	0.11032
114	-14.338	-0.25716	-0.63529	-8.06E-02
115	-45.883	-9.07E-02	0.58019	-3.81E-02
116	1.1125	6.10E-02	8.70E-03	-4.47E-02
117	-4.2851	6.10E-02	-0.15458	-3.82E-02
118	-2.5884	0.30779	0.41528	-0.14745
119	-0.36064	-8.30E-02	-7.66E-02	0.30224
120	8.9608	-0.23404	-0.60199	0.25825
121	-129.01	0.26508	1.1671	0.20342
122	-1.141	7.18E-02	2.84E-02	-5.07E-02
123	5.1163	-0.29086	-0.42504	6.06E-02
124	7.0993	-0.13794	-0.29371	6.57E-03
125	81.657	0.30331	0.29604	0.25092
126	3.8511	0.18444	0.28078	4.98E-02
127	13.227	-0.16869	-0.17508	0.29039
128	-13.064	-2.69E-02	-0.45635	-0.37751
129	-10.958	8.53E-02	0.59103	0.16401
130	-34.516	1.78E-02	0.61821	0.11603
131	-7.5573	2.33E-02	-0.19127	-8.73E-02
132	41.241	-0.47185	-0.74141	7.57E-02
133	-0.34037	-9.25E-02	-0.20897	6.15E-02
134	1.4168	-1.06E-02	0.19247	-5.79E-02
135	10.667	-0.16133	-0.21915	-0.11388
136	-10.216	6.51E-02	-0.20814	-0.29902
137	-2.5319	-6.77E-02	-8.28E-02	-0.25915
138	-1.0055	-6.09E-02	-7.98E-02	-7.12E-02
139	-4.2028	-0.17763	-0.31958	1.22E-02
140	-5.3435	-5.54E-02	-0.3051	3.62E-02
141	-19.349	0.13045	-0.26301	-0.13183
142	7.7541	0.24121	4.58E-02	-7.00E-02
143	-20.136	-0.13464	-0.22496	0.24499
144	6.9728	0.13504	0.23139	-0.20246
145	8.3067	-0.36859	-0.27235	3.49E-02
146	3.3115	-0.11864	-0.13699	5.13E-02
147	-1.7383	0.15921	-7.73E-03	-0.15914

148	7.9016	0.11775	0.13303	0.14772
149	1.7987	-8.48E-02	-0.15655	1.35E-02
150	-16.25	3.10E-02	-0.20703	-7.71E-02
151	18.739	0.28622	0.24548	1.93E-02
152	-27.852	-0.30208	-1.28E-02	-4.97E-02
153	9.9241	-7.70E-02	-0.17392	4.52E-02
154	-6.6078	-0.24434	-0.18168	-4.82E-02
155	-6.9099	-0.32152	-0.19406	0.17966
156	10.991	0.11252	0.21575	5.99E-02
157	-2.4504	-2.33E-02	-0.32673	-4.93E-02
158	-1.9563	0.201	-7.60E-02	0.25577
159	-6.9374	0.13951	0.45041	-4.70E-02
160	-1.6062	3.66E-02	7.11E-02	-0.1584
161	2.8509	0.19521	0.2364	-7.02E-02
162	-6.7332	-3.77E-03	-0.33392	-0.23849
163	7.8289	9.34E-02	0.42551	-0.11823
164	14.793	0.11702	8.21E-02	0.16725
165	7.1573	0.13673	6.73E-02	4.50E-02
166	-6.5612	8.73E-02	-1.27E-02	-0.18841
167	0.54335	6.95E-02	0.10761	-0.18792
168	-6.9961	0.18196	-0.20348	-5.11E-02
169	12.525	0.262	0.27323	-4.73E-02
170	-8.3319	0.35162	0.34843	-6.97E-02
171	-6.9375	0.1203	5.20E-02	-0.18004
172	34.944	-0.38421	-0.294	-0.25828
173	6.8421	7.46E-02	-9.81E-02	0.24265
174	3.9932	0.48559	0.70223	-0.17329
175	1.0011	-0.20293	-0.33037	0.21474

(*R*,*R*)-**53** *P*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	Zn	6.1159	15.6334	-0.5146	30.00	20.00	63.9291
2	C	4.8952	15.3900	-3.1282	6.00	4.00	12.0000
3	C	7.3088	11.7792	4.9583	6.00	4.00	12.0000
4	C	6.6155	12.7551	4.2398	6.00	4.00	12.0000
5	C	4.8087	14.8558	-4.5347	6.00	4.00	12.0000
6	C	6.7222	12.8382	2.8701	6.00	4.00	12.0000
7	C	7.5032	11.9207	2.1401	6.00	4.00	12.0000
8	C	6.1450	13.4607	-2.4330	6.00	4.00	12.0000
9	C	5.5399	16.7765	-3.1347	6.00	4.00	12.0000
10	C	7.3807	18.6914	2.0939	6.00	4.00	12.0000
11	C	6.7929	18.0757	0.9287	6.00	4.00	12.0000
12	O	6.5128	16.8147	0.9408	8.00	6.00	15.9949
13	C	7.5246	11.5269	-2.0968	6.00	4.00	12.0000
14	C	6.5514	18.8862	-0.2249	6.00	4.00	12.0000
15	C	6.8425	20.2687	-0.1979	6.00	4.00	12.0000
16	C	7.3713	20.8530	0.9038	6.00	4.00	12.0000
17	C	8.0917	10.8829	4.2796	6.00	4.00	12.0000
18	C	7.6544	20.0766	2.0481	6.00	4.00	12.0000
19	C	8.2423	20.7315	3.1575	6.00	4.00	12.0000
20	C	8.5495	20.0500	4.2866	6.00	4.00	12.0000
21	C	8.2990	18.6614	4.3852	6.00	4.00	12.0000
22	N	5.8041	17.1673	-1.7666	7.00	5.00	14.0031
23	C	8.6408	17.9897	5.5657	6.00	4.00	12.0000
24	C	8.2483	10.6741	-1.3279	6.00	4.00	12.0000
25	C	8.4439	16.6414	5.6929	6.00	4.00	12.0000
26	C	7.8990	15.9336	4.6213	6.00	4.00	12.0000
27	C	7.5393	16.5694	3.4538	6.00	4.00	12.0000
28	C	7.7196	17.9584	3.2900	6.00	4.00	12.0000
29	O	6.5281	13.9929	0.4011	8.00	6.00	15.9949
30	C	6.1022	18.3902	-1.4663	6.00	4.00	12.0000
31	H	3.8599	15.5351	-2.7480	1.00	1.00	1.0078
32	H	6.5224	16.6462	-3.6418	1.00	1.00	1.0078
33	H	3.7132	17.8315	-3.4763	1.00	1.00	1.0078
34	H	5.1588	18.7335	-3.9718	1.00	1.00	1.0078
35	N	5.5831	14.5895	-2.1527	7.00	5.00	14.0031
36	C	4.7056	17.7281	-3.9575	6.00	4.00	12.0000
37	H	3.9236	17.8859	-5.9658	1.00	1.00	1.0078
38	H	5.5549	17.2085	-5.8577	1.00	1.00	1.0078
39	H	3.9541	15.4239	-6.4369	1.00	1.00	1.0078
40	H	2.9540	15.8169	-5.0314	1.00	1.00	1.0078
41	C	6.8691	12.6412	-1.5327	6.00	4.00	12.0000
42	H	4.3606	13.8468	-4.5350	1.00	1.00	1.0078
43	H	5.8323	14.7542	-4.9477	1.00	1.00	1.0078
44	H	7.4560	11.3844	-3.1812	1.00	1.00	1.0078
45	H	8.7982	9.8381	-1.7675	1.00	1.00	1.0078

46	C	8.2624	10.8338	0.0741	6.00	4.00	12.0000
47	H	9.5345	9.1093	0.3281	1.00	1.00	1.0078
48	H	9.4966	9.1996	2.8041	1.00	1.00	1.0078
49	C	4.5590	17.2066	-5.3734	6.00	4.00	12.0000
50	H	8.6411	10.0989	4.8144	1.00	1.00	1.0078
51	H	7.2205	11.7263	6.0475	1.00	1.00	1.0078
52	H	5.9719	13.4657	4.7665	1.00	1.00	1.0078
53	C	7.5741	11.8943	0.7018	6.00	4.00	12.0000
54	H	6.1955	13.6139	2.3162	1.00	1.00	1.0078
55	H	6.0733	13.0664	-3.4657	1.00	1.00	1.0078
56	H	6.6394	20.8531	-1.1018	1.00	1.00	1.0078
57	C	8.9741	9.8883	0.8533	6.00	4.00	12.0000
58	H	7.6046	21.9205	0.9244	1.00	1.00	1.0078
59	H	8.4456	21.8023	3.0734	1.00	1.00	1.0078
60	H	9.0059	20.5561	5.1430	1.00	1.00	1.0078
61	H	9.0804	18.5747	6.3832	1.00	1.00	1.0078
62	C	3.9975	15.7995	-5.4008	6.00	4.00	12.0000
63	H	8.7186	16.1213	6.6161	1.00	1.00	1.0078
64	H	7.7606	14.8503	4.6916	1.00	1.00	1.0078
65	C	6.9670	12.8988	-0.1320	6.00	4.00	12.0000
66	H	7.1199	16.0000	2.6262	1.00	1.00	1.0078
67	H	6.0437	19.1584	-2.2633	1.00	1.00	1.0078
68	C	8.9515	9.9374	2.2059	6.00	4.00	12.0000
69	C	8.1909	10.9210	2.8823	6.00	4.00	12.0000

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* *
* Final excitation energies from Davidson algorithm *
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Number of loops in Davidson routine = 322
Number of matrix-vector multiplications = 496
Type of excitations = SINGLET-SINGLET

Symmetry A

Excitation energies E in a.u. and eV, dE wrt prev. cycle,
oscillator strengths f in a.u.

no.	E/a.u.	E/eV	f	dE/a.u.
1	0.84672E-01	2.3040	0.66383E-02	0.40E-09
2	0.86928E-01	2.3654	0.59206E-03	0.12E-10
3	0.94383E-01	2.5683	0.10549E-01	0.31E-11
4	0.98919E-01	2.6917	0.49132E-02	0.90E-11
5	0.10054	2.7359	0.10668E-02	0.38E-10
6	0.10165	2.7659	0.18531E-02	0.49E-09
7	0.10630	2.8925	0.27228E-01	0.49E-08
8	0.10818	2.9438	0.25953E-01	0.22E-08
9	0.11173	3.0404	0.99913E-01	0.50E-08
10	0.11750	3.1975	0.11448	0.16E-09
11	0.12189	3.3169	0.40609E-03	0.32E-11

12	0.12325	3.3539	0.20308E-01	0.11E-08
13	0.12718	3.4608	0.11341E-01	0.17E-08
14	0.12732	3.4645	0.14388E-02	0.19E-09
15	0.12796	3.4820	0.33733E-02	0.93E-10
16	0.12899	3.5099	0.10405E-01	0.10E-08
17	0.13111	3.5676	0.74458E-02	0.11E-09
18	0.13171	3.5839	0.35802E-02	0.13E-09
19	0.13273	3.6118	0.82626E-03	0.13E-09
20	0.13606	3.7025	0.17247E-02	0.25E-08
21	0.13631	3.7091	0.17401E-02	0.21E-08
22	0.13721	3.7337	0.13816E-02	0.12E-09
23	0.13828	3.7629	0.55933E-02	0.51E-09
24	0.13930	3.7905	0.59972E-02	0.76E-12
25	0.14177	3.8577	0.20321E-01	0.19E-09
26	0.14256	3.8793	0.97480E-03	0.67E-10
27	0.14313	3.8947	0.81493E-03	0.89E-09
28	0.14429	3.9262	0.89298E-04	0.18E-10
29	0.14450	3.9319	0.24282E-03	0.30E-09
30	0.14621	3.9785	0.60041E-01	0.21E-07
31	0.14838	4.0376	0.15224	0.28E-09
32	0.14972	4.0742	0.92715E-02	0.68E-09
33	0.15078	4.1031	0.71797E-01	0.37E-08
34	0.15262	4.1531	0.23612E-01	0.43E-09
35	0.15670	4.2639	0.13901E-01	0.38E-09
36	0.16022	4.3597	0.13868E-01	0.17E-07
37	0.16093	4.3790	0.42929E-02	0.16E-09
38	0.16198	4.4077	0.54600E-01	0.28E-07
39	0.16263	4.4255	0.20695E-02	0.43E-08
40	0.16377	4.4564	0.79188E-01	0.28E-08
41	0.16493	4.4879	0.19065E-01	0.49E-09
42	0.16526	4.4971	0.13224E-01	0.11E-08
43	0.16597	4.5162	0.25387E-01	0.35E-11
44	0.16615	4.5212	0.11343	0.11E-07
45	0.16709	4.5466	0.14759E-01	0.16E-08
46	0.16731	4.5528	0.89315E-02	0.42E-11
47	0.16762	4.5611	0.15184	0.35E-09
48	0.16829	4.5795	0.13668	0.20E-07
49	0.16851	4.5855	0.22838E-01	0.19E-08
50	0.16901	4.5989	0.50038E-01	0.14E-07
51	0.16941	4.6098	0.55470E-01	0.15E-08
52	0.17128	4.6608	0.14256E-01	0.67E-09
53	0.17159	4.6691	0.71685E-02	0.55E-09
54	0.17238	4.6908	0.84071E-03	0.80E-09
55	0.17288	4.7042	0.80470E-02	0.29E-09
56	0.17328	4.7153	0.14540E-02	0.26E-08
57	0.17348	4.7205	0.12670E-01	0.57E-08
58	0.17398	4.7344	0.17303E-01	0.18E-08
59	0.17446	4.7472	0.77707E-02	0.44E-09
60	0.17516	4.7664	0.10027E-02	0.47E-08
61	0.17612	4.7924	0.10703E-02	0.98E-09
62	0.17641	4.8003	0.24451E-01	0.14E-09
63	0.17696	4.8155	0.18132E-02	0.11E-10
64	0.17714	4.8202	0.44554E-02	0.25E-09
65	0.17785	4.8396	0.33866E-02	0.12E-09
66	0.17848	4.8568	0.75343E-02	0.44E-08
67	0.17863	4.8608	0.10146E-01	0.18E-07

68	0.17943	4.8826	0.75925E-03	0.25E-09
69	0.18040	4.9090	0.15399E-01	0.66E-10
70	0.18052	4.9123	0.19943E-02	0.81E-09
71	0.18117	4.9300	0.68638E-03	0.26E-08
72	0.18140	4.9361	0.49241E-02	0.36E-09
73	0.18301	4.9799	0.32874E-01	0.43E-08
74	0.18377	5.0006	0.18175E-01	0.63E-09
75	0.18392	5.0047	0.10286E-02	0.32E-08
76	0.18412	5.0100	0.52410E-01	0.18E-08
77	0.18446	5.0194	0.10136	0.23E-07
78	0.18463	5.0240	0.23290E-02	0.47E-08
79	0.18532	5.0428	0.97257E-01	0.37E-08
80	0.18582	5.0564	0.14578E-01	0.89E-09
81	0.18636	5.0711	0.22905	0.37E-07
82	0.18735	5.0980	0.18223E-01	0.22E-09
83	0.18775	5.1090	0.15347E-01	0.16E-07
84	0.18821	5.1215	0.20982E-02	0.49E-08
85	0.18858	5.1314	0.35523E-02	0.25E-08
86	0.18877	5.1366	0.27903E-01	0.13E-08
87	0.18937	5.1529	0.17612E-01	0.11E-07
88	0.18942	5.1545	0.92388E-02	0.49E-08
89	0.18956	5.1581	0.10204E-02	0.65E-08
90	0.19022	5.1763	0.46783E-02	0.70E-08
91	0.19073	5.1899	0.54614E-02	0.35E-08
92	0.19156	5.2125	0.23229E-01	0.25E-08
93	0.19232	5.2333	0.13714	0.18E-08
94	0.19274	5.2448	0.26835E-02	0.39E-08
95	0.19293	5.2499	0.31340E-01	0.60E-11
96	0.19334	5.2611	0.91194E-01	0.76E-08
97	0.19341	5.2630	0.11505E-01	0.35E-09
98	0.19398	5.2783	0.38658E-01	0.15E-09
99	0.19500	5.3063	0.50059E-02	0.45E-08
100	0.19519	5.3115	0.17232E-02	0.12E-08
101	0.19540	5.3170	0.87337E-02	0.11E-12
102	0.19596	5.3324	0.30727E-01	0.89E-09
103	0.19621	5.3392	0.98409E-02	0.20E-09
104	0.19626	5.3405	0.44462E-02	0.66E-09
105	0.19660	5.3496	0.66415E-02	0.40E-08
106	0.19673	5.3532	0.23063E-02	0.37E-09
107	0.19740	5.3715	0.25906E-02	0.20E-08
108	0.19770	5.3797	0.86766E-02	0.71E-12
109	0.19869	5.4066	0.64938E-02	0.36E-09
110	0.19917	5.4196	0.32201E-01	0.99E-08
111	0.19970	5.4342	0.52179E-01	0.47E-08
112	0.20052	5.4565	0.14086E-01	0.18E-08
113	0.20088	5.4662	0.16612E-02	0.26E-08
114	0.20092	5.4672	0.90026E-03	0.82E-08
115	0.20149	5.4829	0.39847E-01	0.20E-09
116	0.20214	5.5005	0.22549E-01	0.22E-07
117	0.20275	5.5171	0.26618E-01	0.87E-10
118	0.20317	5.5286	0.24477E-01	0.18E-07
119	0.20357	5.5394	0.30221E-02	0.12E-08
120	0.20381	5.5459	0.27244E-02	0.90E-09
121	0.20405	5.5524	0.10152E-01	0.27E-08
122	0.20479	5.5725	0.14055E-01	0.46E-07
123	0.20512	5.5815	0.72621E-01	0.11E-07

124	0.20534	5.5876	0.11590E-01	0.24E-11
125	0.20550	5.5921	0.38524E-02	0.91E-10
126	0.20562	5.5953	0.33642E-02	0.35E-09
127	0.20581	5.6003	0.37593E-02	0.12E-07
128	0.20595	5.6041	0.69340E-01	0.18E-07
129	0.20615	5.6097	0.99424E-01	0.47E-08
130	0.20659	5.6215	0.48381E-01	0.64E-09
131	0.20679	5.6271	0.29726E-02	0.28E-08
132	0.20756	5.6479	0.75115E-02	0.33E-09
133	0.20819	5.6651	0.66426E-01	0.20E-07
134	0.20852	5.6741	0.17904E-01	0.59E-08
135	0.20873	5.6798	0.31326E-02	0.13E-08
136	0.20896	5.6860	0.65478E-02	0.32E-08
137	0.20903	5.6880	0.12480E-01	0.74E-08
138	0.20916	5.6915	0.94263E-02	0.48E-08
139	0.20928	5.6948	0.89397E-02	0.17E-08
140	0.20967	5.7055	0.30955E-02	0.43E-11
141	0.21008	5.7166	0.68938E-01	0.37E-08
142	0.21082	5.7368	0.70192E-02	0.49E-08
143	0.21096	5.7405	0.86253E-02	0.21E-09
144	0.21148	5.7547	0.15997E-01	0.23E-09
145	0.21185	5.7647	0.28221E-01	0.14E-07
146	0.21217	5.7734	0.57451E-02	0.42E-08
147	0.21233	5.7779	0.17453E-01	0.40E-09
148	0.21252	5.7830	0.50766E-01	0.25E-08
149	0.21287	5.7924	0.58483E-01	0.23E-09
150	0.21303	5.7968	0.38854E-01	0.26E-08
151	0.21343	5.8076	0.67229E-02	0.16E-07
152	0.21354	5.8107	0.21819E-03	0.59E-09
153	0.21408	5.8255	0.16074E-02	0.21E-12
154	0.21430	5.8313	0.69994E-02	0.69E-08
155	0.21450	5.8369	0.35586E-01	0.81E-08
156	0.21461	5.8397	0.18625E-02	0.91E-09
157	0.21513	5.8539	0.16213E-01	0.16E-07
158	0.21542	5.8619	0.41858E-02	0.79E-08
159	0.21608	5.8798	0.15950E-01	0.10E-08
160	0.21622	5.8837	0.17144E-01	0.46E-09
161	0.21643	5.8894	0.38198E-03	0.40E-09
162	0.21653	5.8922	0.76802E-02	0.60E-09
163	0.21726	5.9119	0.49002E-02	0.82E-07
164	0.21750	5.9184	0.64161E-02	0.52E-10
165	0.21783	5.9273	0.56413E-02	0.84E-11
166	0.21799	5.9318	0.11305E-01	0.13E-09
167	0.21820	5.9374	0.11724E-03	0.65E-07
168	0.21830	5.9402	0.26531E-02	0.80E-09
169	0.21839	5.9427	0.53203E-02	0.90E-07
170	0.21860	5.9483	0.91473E-02	0.25E-07
171	0.21882	5.9543	0.25290E-01	0.71E-09
172	0.21891	5.9569	0.39910E-02	0.10E-10
173	0.21953	5.9738	0.13167E-01	0.36E-09
174	0.21968	5.9778	0.11706E-01	0.71E-10
175	0.22025	5.9932	0.59284E-02	0.42E-08

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	2.304	6.64E-03	7.63E-03	0.33039	9.16E-02
2	2.3654	5.92E-04	-7.56E-03	-0.10049	7.75E-03
3	2.5683	1.05E-02	7.24E-02	0.36404	0.17286
4	2.6917	4.91E-03	-4.95E-02	-0.22718	-0.14298
5	2.7359	1.07E-03	2.20E-02	-0.11517	4.66E-02
6	2.7659	1.85E-03	3.99E-02	-0.16004	1.19E-02
7	2.8925	2.72E-02	0.14915	-0.174	0.57594
8	2.9438	2.60E-02	1.16E-02	-0.2653	0.53789
9	3.0404	9.99E-02	0.3265	5.66E-02	1.1097
10	3.1975	0.11448	0.32235	-0.45211	1.0738
11	3.3169	4.06E-04	-1.29E-02	1.59E-02	6.77E-02
12	3.3539	2.03E-02	8.95E-02	-0.4225	0.24624
13	3.4608	1.13E-02	-7.51E-02	-0.2634	-0.24235
14	3.4645	1.44E-03	5.24E-02	-5.61E-02	0.10518
15	3.482	3.37E-03	-5.77E-02	0.11849	-0.14889
16	3.5099	1.04E-02	-3.44E-02	0.32143	0.12846
17	3.5676	7.45E-03	-7.25E-02	0.18917	-0.21011
18	3.5839	3.58E-03	2.07E-02	-0.19621	-4.30E-02
19	3.6118	8.26E-04	-8.82E-03	7.52E-02	-6.00E-02
20	3.7025	1.72E-03	6.96E-03	8.08E-02	0.11156
21	3.7091	1.74E-03	-9.18E-03	-9.48E-02	-0.10034
22	3.7337	1.38E-03	3.24E-02	5.96E-02	0.10249
23	3.7629	5.59E-03	8.18E-02	-3.69E-02	0.22938
24	3.7905	6.00E-03	-2.37E-02	0.25	-3.89E-02
25	3.8577	2.03E-02	0.12205	-0.38149	0.23362
26	3.8793	9.75E-04	2.16E-02	-4.72E-02	8.69E-02
27	3.8947	8.15E-04	-1.37E-02	-8.91E-02	-2.03E-02
28	3.9262	8.93E-05	-2.50E-03	3.03E-02	2.30E-03
29	3.9319	2.43E-04	-1.30E-02	-4.53E-02	-1.73E-02
30	3.9785	6.00E-02	-0.12641	-0.66174	-0.40263
31	4.0376	0.15224	-0.40881	0.59333	-1.0099
32	4.0742	9.27E-03	7.39E-02	-0.20346	0.21456
33	4.1031	7.18E-02	0.29616	0.19259	0.76775
34	4.1531	2.36E-02	0.13595	-0.30554	0.34674
35	4.2639	1.39E-02	-0.14601	-8.27E-02	-0.3239
36	4.3597	1.39E-02	-0.29076	-0.14676	-0.15414
37	4.379	4.29E-03	-6.39E-02	-0.13389	-0.13418
38	4.4077	5.46E-02	0.20851	6.13E-02	0.67703
39	4.4255	2.07E-03	0.10457	-8.76E-02	-2.21E-02
40	4.4564	7.92E-02	8.40E-02	0.27321	0.80225
41	4.4879	1.91E-02	5.66E-02	-1.35E-02	-0.41231
42	4.4971	1.32E-02	3.67E-02	0.20576	-0.27632
43	4.5162	2.54E-02	-0.11378	-0.16132	-0.43643
44	4.5212	0.11343	0.14557	6.01E-02	0.99961
45	4.5466	1.48E-02	-5.71E-02	-2.83E-02	0.35838
46	4.5528	8.93E-03	-1.59E-02	6.64E-02	-0.27461
47	4.5611	0.15184	0.18476	-0.68987	0.92128
48	4.5795	0.13668	-0.16257	1.072	-0.20642
49	4.5855	2.28E-02	0.18494	-4.94E-02	0.40822
50	4.5989	5.00E-02	4.07E-02	-0.28293	-0.602
51	4.6098	5.55E-02	0.51441	-0.17119	0.4441

52	4.6608	1.43E-02	2.24E-02	-0.28378	0.20932
53	4.6691	7.17E-03	1.38E-02	0.22119	-0.11641
54	4.6908	8.41E-04	4.33E-03	-7.28E-02	-4.46E-02
55	4.7042	8.05E-03	0.10343	0.19095	0.15054
56	4.7153	1.45E-03	6.75E-02	-8.66E-02	-2.31E-02
57	4.7205	1.27E-02	5.05E-02	0.24034	0.22191
58	4.7344	1.73E-02	-9.08E-02	0.33453	-0.17037
59	4.7472	7.77E-03	-0.14307	5.57E-02	-0.20795
60	4.7664	1.00E-03	-7.23E-03	8.85E-02	-2.67E-02
61	4.7924	1.07E-03	2.68E-02	-5.43E-02	-7.38E-02
62	4.8003	2.45E-02	-8.88E-02	0.41031	-0.17797
63	4.8155	1.81E-03	-3.36E-02	3.89E-02	-0.11282
64	4.8202	4.46E-03	7.43E-02	6.60E-02	-0.16688
65	4.8396	3.39E-03	-0.127	4.92E-02	-0.10007
66	4.8568	7.53E-03	0.12824	-0.21581	1.73E-02
67	4.8608	1.01E-02	-3.12E-02	8.86E-02	-0.27635
68	4.8826	7.59E-04	2.23E-02	-7.64E-02	-3.87E-03
69	4.909	1.54E-02	-0.21027	-0.13202	-0.25768
70	4.9123	1.99E-03	8.77E-03	-8.58E-02	-9.56E-02
71	4.93	6.86E-04	4.73E-02	1.34E-02	5.71E-02
72	4.9361	4.92E-03	7.00E-02	5.95E-02	0.17964
73	4.9799	3.29E-02	-9.47E-02	-0.27747	-0.42835
74	5.0006	1.82E-02	0.2059	-0.18104	0.27053
75	5.0047	1.03E-03	-4.55E-03	-2.92E-02	-8.67E-02
76	5.01	5.24E-02	0.14804	-0.15147	0.61817
77	5.0194	0.10136	-0.3997	0.3839	-0.71912
78	5.024	2.33E-03	0.12005	3.85E-02	5.50E-02
79	5.0428	9.73E-02	-0.26637	8.63E-02	-0.84191
80	5.0564	1.46E-02	-6.95E-02	0.24543	-0.22938
81	5.0711	0.22905	-0.41652	0.33293	-1.2487
82	5.098	1.82E-02	0.10936	-0.15725	0.33047
83	5.109	1.53E-02	-0.12516	-4.23E-02	-0.32429
84	5.1215	2.10E-03	-3.59E-02	0.11522	-4.65E-02
85	5.1314	3.55E-03	-6.24E-02	-0.10789	0.1128
86	5.1366	2.79E-02	0.12151	-0.3682	0.2672
87	5.1529	1.76E-02	-6.03E-02	1.81E-02	-0.36816
88	5.1545	9.24E-03	6.73E-02	-5.54E-02	0.25605
89	5.1581	1.02E-03	-1.12E-02	-8.90E-02	5.96E-03
90	5.1763	4.68E-03	-2.72E-02	-0.16825	8.86E-02
91	5.1899	5.46E-03	6.58E-02	-0.19616	1.20E-02
92	5.2125	2.32E-02	-2.30E-02	0.21353	0.36848
93	5.2333	0.13714	-0.1464	-5.50E-03	-1.0238
94	5.2448	2.68E-03	-2.31E-02	3.89E-02	-0.13725
95	5.2499	3.13E-02	-3.60E-02	0.21386	-0.44343
96	5.2611	9.12E-02	0.15992	-0.23381	0.792
97	5.263	1.15E-02	9.03E-02	-0.20209	0.20056
98	5.2783	3.87E-02	-0.1505	-9.97E-03	-0.52554
99	5.3063	5.01E-03	-1.70E-02	-1.72E-02	-0.19473
100	5.3115	1.72E-03	-4.89E-02	-5.98E-02	-8.53E-02
101	5.317	8.73E-03	2.62E-02	-7.71E-02	0.24578
102	5.3324	3.07E-02	-0.1337	0.21309	-0.41463
103	5.3392	9.84E-03	4.09E-02	-0.20431	0.17838
104	5.3405	4.45E-03	1.72E-03	-0.11568	0.14352
105	5.3496	6.64E-03	6.50E-03	-0.10413	-0.19947
106	5.3532	2.31E-03	1.14E-02	-1.03E-02	0.13172
107	5.3715	2.59E-03	3.17E-02	4.87E-03	0.13659

108	5.3797	8.68E-03	-0.10217	7.25E-02	-0.22391
109	5.4066	6.49E-03	-5.20E-02	0.21073	-4.37E-02
110	5.4196	3.22E-02	8.78E-02	-0.45398	0.16946
111	5.4342	5.22E-02	9.71E-02	-0.61499	-6.54E-02
112	5.4565	1.41E-02	-6.15E-03	0.15416	0.2856
113	5.4662	1.66E-03	-5.81E-02	-8.14E-02	-4.91E-02
114	5.4672	9.00E-04	-2.57E-02	6.73E-03	7.76E-02
115	5.4829	3.98E-02	-0.21194	-9.71E-02	-0.49224
116	5.5005	2.25E-02	-8.98E-02	0.39894	1.08E-02
117	5.5171	2.66E-02	0.11491	-0.35449	0.24096
118	5.5286	2.45E-02	0.13143	-0.26	-0.30957
119	5.5394	3.02E-03	-6.39E-03	1.21E-02	-0.1486
120	5.5459	2.72E-03	-5.67E-02	2.33E-02	0.12766
121	5.5524	1.02E-02	-0.19122	0.19156	-3.71E-02
122	5.5725	1.41E-02	-0.1637	0.27587	-6.93E-03
123	5.5815	7.26E-02	2.29E-02	2.18E-02	-0.72806
124	5.5876	1.16E-02	1.63E-02	-0.25514	0.13894
125	5.5921	3.85E-03	3.59E-02	-0.10106	0.12891
126	5.5953	3.36E-03	-8.48E-02	4.64E-02	0.12324
127	5.6003	3.76E-03	-1.95E-02	-8.66E-02	-0.13974
128	5.6041	6.93E-02	-6.23E-02	5.18E-02	0.70602
129	5.6097	9.94E-02	-4.25E-02	-0.41827	0.73937
130	5.6215	4.84E-02	-8.68E-02	-0.42116	0.40789
131	5.6271	2.97E-03	-0.10546	8.71E-03	0.10181
132	5.6479	7.51E-03	5.93E-02	-0.20064	-0.10251
133	5.6651	6.64E-02	-8.79E-02	0.6805	-8.83E-02
134	5.6741	1.79E-02	-0.10398	0.33128	-9.07E-02
135	5.6798	3.13E-03	-9.30E-02	3.48E-02	0.11248
136	5.686	6.55E-03	-7.24E-02	-1.93E-02	0.20343
137	5.688	1.25E-02	-5.26E-02	2.79E-02	-0.29328
138	5.6915	9.43E-03	0.11761	-0.23107	-1.93E-02
139	5.6948	8.94E-03	4.00E-02	-0.11953	0.21952
140	5.7055	3.10E-03	7.63E-02	-7.09E-02	0.10629
141	5.7166	6.89E-02	-0.2451	0.14463	-0.64128
142	5.7368	7.02E-03	7.42E-02	-3.84E-02	-0.20725
143	5.7405	8.63E-03	-4.26E-02	-0.15811	0.18579
144	5.7547	1.60E-02	-2.23E-02	0.33558	1.89E-02
145	5.7647	2.82E-02	3.07E-02	0.31444	0.31624
146	5.7734	5.75E-03	7.83E-02	0.16663	8.20E-02
147	5.7779	1.75E-02	3.45E-02	0.31529	-0.15065
148	5.783	5.08E-02	-0.10776	0.49729	0.31529
149	5.7924	5.85E-02	5.36E-02	0.23076	-0.59665
150	5.7968	3.89E-02	0.14693	0.32065	-0.38624
151	5.8076	6.72E-03	-8.40E-02	8.72E-02	-0.18054
152	5.8107	2.18E-04	2.61E-02	-2.80E-02	-8.21E-03
153	5.8255	1.61E-03	-8.16E-02	-3.80E-02	-5.61E-02
154	5.8313	7.00E-03	-0.14473	0.14901	-7.65E-02
155	5.8369	3.56E-02	-0.11678	-0.37245	-0.31064
156	5.8397	1.86E-03	6.55E-02	1.01E-03	-9.34E-02
157	5.8539	1.62E-02	0.12381	-0.3072	-5.78E-02
158	5.8619	4.19E-03	-7.21E-03	0.14695	8.66E-02
159	5.8798	1.60E-02	-1.89E-02	0.24487	-0.22451
160	5.8837	1.71E-02	-5.92E-02	0.21121	0.26613
161	5.8894	3.82E-04	-3.74E-03	4.97E-02	1.28E-02
162	5.8922	7.68E-03	-5.21E-02	-4.93E-03	0.22465
163	5.9119	4.90E-03	-4.16E-02	1.76E-02	-0.17829

164	5.9184	6.42E-03	5.59E-02	0.13831	-0.14832
165	5.9273	5.64E-03	2.07E-02	0.13827	-0.13892
166	5.9318	1.13E-02	5.84E-02	-0.26957	-4.14E-02
167	5.9374	1.17E-04	-1.07E-02	-1.70E-03	2.63E-02
168	5.9402	2.65E-03	2.29E-02	-6.82E-02	-0.11423
169	5.9427	5.32E-03	-2.79E-02	0.16333	9.53E-02
170	5.9483	9.15E-03	-0.18401	0.13522	0.10307
171	5.9543	2.53E-02	-0.21118	0.35833	-1.93E-02
172	5.9569	3.99E-03	-5.48E-03	0.12269	-0.11074
173	5.9738	1.32E-02	2.96E-02	0.18634	-0.23318
174	5.9778	1.17E-02	7.37E-02	1.59E-02	0.27249
175	5.9932	5.93E-03	8.61E-02	-0.12891	-0.12786

Rotatory strengths R in 10**(-40) esu**2 * cm**2 ,
(multiply by 1.07827 to obtain reduced rotatory strengths),
magnetic transition dipole vectors m in a.u.:

no.	R	m (x,y,z)		
1	4.0759	1.3103	1.45E-02	2.75E-02
2	3.7028	-0.4236	-0.12321	1.58E-02
3	8.24E-02	0.73115	-0.1258	-3.92E-02
4	0.79525	-0.485	0.1485	-9.17E-02
5	-0.61419	-0.14681	-9.57E-02	-0.22328
6	-1.106	-7.95E-02	-9.95E-03	-0.26127
7	-10.734	3.5808	-0.78016	-1.2421
8	85.476	-0.30944	-1.3794	4.23E-04
9	-33.812	5.3445	-1.6782	-1.6161
10	14.267	2.4524	-2.1173	-1.5713
11	-1.4601	0.30624	-0.34906	4.88E-02
12	16.974	0.36165	-0.56021	-0.80021
13	1.3261	-1.2787	0.3879	-4.86E-02
14	-2.7681	0.36114	-0.18145	-0.38831
15	1.5847	-0.8066	0.29837	0.50514
16	-7.4005	0.96039	-0.17192	0.44263
17	3.783	-0.63021	0.46147	0.55657
18	-3.6237	-0.25623	0.12342	-0.32876
19	0.75453	1.44E-02	5.66E-02	1.55E-02
20	-2.7855	0.53611	-0.23665	3.19E-02
21	-0.8217	-0.45721	0.14281	-5.84E-02
22	3.6573	0.72207	-3.02E-02	-5.91E-02
23	2.456	1.2566	-0.4195	-0.47037
24	5.8105	0.18828	0.16961	0.34142
25	-4.1879	0.58896	-0.4503	-1.119
26	-5.65E-02	0.71577	-0.15639	-0.26547
27	0.77235	-0.11838	8.41E-03	-0.11852
28	0.42674	-0.61663	-9.59E-03	0.24194
29	-1.1491	0.53101	2.02E-02	-0.16969
30	54.3	-4.0862	0.37295	9.78E-02
31	31.231	-3.2107	2.3698	2.5608
32	6.7089	0.50971	-0.58527	-0.59777
33	0.2087	4.2994	-1.4849	-1.2849
34	1.4194	0.77063	-0.83175	-1.0177
35	-11.756	-1.7597	0.6958	0.76951

36	127.55	-2.7539	0.24201	1.454
37	2.3735	-0.71763	0.23248	3.47E-02
38	15.426	5.5565	-1.2529	-1.5011
39	11.962	0.8589	0.64846	-0.80246
40	-86.117	3.3364	-1.8947	-0.15932
41	-3.4318	-1.6064	1.0589	-0.22
42	14.083	-0.98573	0.88421	0.31141
43	-25.376	-1.7538	1.0861	0.30243
44	-43.837	4.1518	-2.4269	-0.64472
45	-54.396	2.6983	-0.80212	-0.27737
46	4.0104	-0.62431	0.69035	0.14122
47	16.915	4.4507	-2.2988	-2.5361
48	39.359	-1.1751	0.48127	2.616
49	-1.1558	2.1037	-1.0405	-1.0911
50	-52.662	-3.3192	1.3583	-0.49195
51	10.687	2.1327	-0.98705	-2.7488
52	-5.9905	1.178	-0.41373	-0.80829
53	0.67601	-0.68364	0.24857	0.36648
54	0.70727	-0.35822	4.71E-02	-0.17885
55	-1.3231	1.0599	-0.28021	-0.41004
56	3.2199	0.25337	0.16505	-0.4704
57	-21.267	0.8115	-0.63414	9.57E-02
58	8.3535	-1.6514	0.3	1.2612
59	-3.6022	-0.88447	0.52695	0.82318
60	1.459	0.37408	0.19431	0.31107
61	-5.2589	-0.70638	0.17374	-8.25E-02
62	21.962	-0.29717	0.59619	0.99924
63	-0.25727	-0.94728	8.25E-02	0.32003
64	11.383	-0.57964	0.50042	-0.34945
65	-2.4024	-0.51019	0.18695	0.84118
66	8.2842	0.36036	-3.97E-02	-1.1349
67	-12.737	-2.548	0.58736	0.67174
68	-0.63719	-3.25E-02	3.65E-02	-0.20846
69	39.725	-2.336	0.3868	1.054
70	0.59532	-0.93807	8.11E-02	-0.18526
71	12.381	1.546	0.16796	-0.40105
72	-10.252	-0.33005	-0.6095	8.85E-02
73	-5.0733	-2.9278	0.87719	0.12929
74	4.4001	1.3512	-0.58349	-1.3499
75	-0.10091	-0.87875	0.21108	-2.01E-02
76	-17.016	2.006	-1.5594	-0.97925
77	-4.0254	-3.9204	1.8968	3.2154
78	12.49	0.65337	4.43E-02	-0.49339
79	0.22769	-4.1638	2.1745	1.539
80	12.285	-0.75123	0.72881	0.78021
81	21.022	-7.1596	3.2709	3.1888
82	1.6714	0.90793	-1.009	-0.7591
83	31.212	-4.3876	0.49322	1.2208
84	4.2447	-0.48042	0.19352	0.46299
85	20.742	6.90E-02	-0.53348	0.30795
86	20.086	0.94288	-0.94958	-1.4184
87	-8.4782	-0.97236	1.0985	0.31106
88	-3.2383	0.99658	-0.71818	-0.47104
89	6.2897	-0.48188	-0.24839	-0.13652
90	5.8906	0.32753	-0.3387	-0.26082
91	11.062	0.82972	-1.55E-02	-0.89136

92	-24.647	1.0332	-1.3634	0.57085
93	-120.44	-5.6428	2.9551	1.2901
94	0.17257	-0.68893	0.32541	0.20269
95	4.2298	-2.6034	1.2903	0.79337
96	-14.648	4.3291	-2.3421	-1.644
97	3.1815	1.3307	-0.62857	-1.1654
98	-25.651	-3.249	1.4482	1.11
99	-11.274	-0.63722	0.64532	0.2442
100	-0.84702	-0.16569	0.16127	2.41E-02
101	-3.9886	1.421	-0.81193	-0.47532
102	9.1341	-2.2886	1.3896	1.3587
103	4.1455	1.3044	-0.54279	-0.82226
104	0.42285	0.68059	-0.37457	-0.29756
105	-12.888	-0.52761	0.75724	-0.1384
106	-2.9281	0.69082	-0.40573	-0.1857
107	-2.1878	0.58755	-0.51254	-0.18599
108	-0.70511	-1.3062	0.81176	0.87218
109	-2.0957	-0.4225	3.64E-02	0.88081
110	23.835	1.9596	-0.47387	-1.6879
111	-5.6245	0.99383	0.40837	-1.9999
112	-11.363	0.96985	-0.92682	0.35236
113	0.40308	2.52E-03	-8.81E-02	0.10824
114	5.3398	-0.24784	-0.43951	0.2481
115	-10.146	-2.5593	1.1764	0.95734
116	21.544	-0.77611	1.64E-02	1.4087
117	23.729	2.4078	-0.81669	-1.932
118	13.825	-1.0443	0.95015	-1.4308
119	0.2162	-0.76372	0.19602	4.27E-02
120	1.9924	0.54452	-0.28881	0.3606
121	16.262	-0.96527	-0.28232	1.6581
122	19.295	-1.0305	-0.2736	1.6389
123	-65.709	-4.4444	2.0963	0.30571
124	-5.2835	1.1453	-0.34399	-0.92718
125	-4.8977	1.0967	-0.18442	-0.61095
126	-5.208	0.74828	-0.46082	0.50943
127	-12.62	-0.76443	0.63786	9.46E-02
128	-67.413	4.1976	-2.3587	0.13839
129	-34.131	4.628	-2.1076	-1.1223
130	-35.843	3.2585	-0.98832	-0.69958
131	-0.58778	0.46264	-0.53736	0.50066
132	-16.528	-0.62485	0.61081	-0.87315
133	56.668	-1.7993	0.43567	2.4241
134	17.66	-1.0638	0.28804	1.4452
135	-7.18E-02	0.48998	-0.23539	0.47526
136	-3.8668	1.265	-0.60435	0.31245
137	-15.429	-1.9694	0.66635	0.63973
138	-3.4705	0.11274	0.21422	-1.114
139	-3.198	1.6095	-0.63696	-0.70172
140	6.1629	0.88663	-0.37558	-0.64089
141	-9.4183	-4.0571	1.7691	2.0119
142	-1.3164	-1.1112	0.6502	-0.49169
143	0.10332	1.2558	-0.49561	-0.1315
144	-1.4353	-0.27822	-8.74E-02	0.90302
145	-39.319	1.318	-1.0033	0.34231
146	8.0128	0.38095	-7.58E-03	6.62E-02
147	1.6918	-1.1962	0.42284	0.56303

148	-8.5863	1.3366	-0.90513	1.7689
149	-28.114	-3.5664	1.6495	0.51727
150	-20.031	-2.4139	1.0175	0.14651
151	2.951	-1.0489	0.30098	0.56398
152	-1.292	-0.14165	0.10911	-0.15494
153	-3.6382	-7.60E-02	0.16243	0.27541
154	14.201	-0.81363	0.24284	1.2255
155	-5.3313	-1.8053	0.76247	-0.16272
156	3.8116	-0.44433	0.26104	-0.48145
157	-2.4966	-0.24709	0.22785	-1.5557
158	5.4175	0.55032	-7.96E-02	0.44636
159	12.756	-1.4275	0.80396	0.75611
160	6.3427	1.2808	-0.75235	0.98289
161	0.31874	4.56E-03	6.89E-02	-0.16032
162	-5.6183	1.5316	-0.49254	0.23826
163	-3.641	-0.66772	0.41339	0.28341
164	-7.0592	-1.3634	0.46259	0.11959
165	-9.4254	-1.194	0.41566	0.52358
166	11.851	0.72365	0.13928	-1.1019
167	-1.4602	0.42772	-5.07E-02	-6.56E-02
168	-1.97	-0.33902	0.34237	-0.19938
169	-4.2172	0.48688	-0.26438	0.40798
170	-10.451	0.89073	-0.16573	1.3775
171	18.192	-1.1644	-0.35834	2.0853
172	-1.7722	-0.72807	0.23096	0.35984
173	-14.331	-2.4753	0.73185	0.53187
174	-7.4245	1.292	-0.87847	-0.41358
175	-4.0357	-0.65256	0.43251	-0.74153

(*R,R*)-**75**·py *M*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	Zn	1.3987	8.7388	6.0854	30.00	20.00	63.9291
2	C	3.4878	7.0797	4.9729	6.00	4.00	12.0000
3	C	4.1856	5.8127	4.5507	6.00	4.00	12.0000
4	C	5.6474	6.0842	4.2590	6.00	4.00	12.0000
5	C	6.3401	6.7262	5.4433	6.00	4.00	12.0000
6	C	5.6176	7.9754	5.9023	6.00	4.00	12.0000
7	C	4.1679	7.6743	6.2084	6.00	4.00	12.0000
8	N	0.9558	9.6953	4.3019	7.00	5.00	14.0031
9	C	0.5487	10.9671	4.3014	6.00	4.00	12.0000
10	C	0.2042	11.6236	3.1350	6.00	4.00	12.0000
11	C	0.2967	10.9464	1.9317	6.00	4.00	12.0000
12	C	0.7262	9.6284	1.9361	6.00	4.00	12.0000
13	C	1.0390	9.0383	3.1446	6.00	4.00	12.0000
14	C	-1.9626	6.2285	6.9052	6.00	4.00	12.0000
15	C	-0.6672	6.6304	6.4177	6.00	4.00	12.0000
16	O	-0.2234	7.8183	6.6811	8.00	6.00	15.9949
17	C	0.0923	5.6843	5.6596	6.00	4.00	12.0000
18	C	-0.4384	4.4102	5.3683	6.00	4.00	12.0000
19	C	-1.6902	4.0681	5.7535	6.00	4.00	12.0000
20	C	-2.4673	4.9692	6.5067	6.00	4.00	12.0000
21	C	-3.7860	4.5764	6.8537	6.00	4.00	12.0000
22	C	-4.5888	5.3797	7.5824	6.00	4.00	12.0000
23	C	-4.1130	6.6187	8.0802	6.00	4.00	12.0000
24	C	-4.9358	7.3767	8.8974	6.00	4.00	12.0000
25	C	-4.4944	8.5512	9.4956	6.00	4.00	12.0000
26	C	-5.3144	9.3263	10.3464	6.00	4.00	12.0000
27	C	-4.8238	10.4509	10.9454	6.00	4.00	12.0000
28	C	-3.4872	10.8421	10.7359	6.00	4.00	12.0000
29	C	-2.6713	10.1129	9.9133	6.00	4.00	12.0000
30	C	-3.1515	8.9613	9.2529	6.00	4.00	12.0000
31	C	-2.3401	8.2268	8.3782	6.00	4.00	12.0000
32	C	-2.7795	7.0541	7.7705	6.00	4.00	12.0000
33	C	1.4244	5.8977	5.2179	6.00	4.00	12.0000
34	N	2.0857	6.9969	5.2702	7.00	5.00	14.0031
35	C	1.2466	12.0601	8.7948	6.00	4.00	12.0000
36	C	1.8120	10.9854	8.0150	6.00	4.00	12.0000
37	O	1.1086	10.3936	7.1260	8.00	6.00	15.9949
38	C	3.1705	10.6086	8.2752	6.00	4.00	12.0000
39	C	3.9178	11.2766	9.2595	6.00	4.00	12.0000
40	C	3.3865	12.2997	9.9818	6.00	4.00	12.0000
41	C	2.0534	12.6951	9.7577	6.00	4.00	12.0000
42	C	1.5280	13.7541	10.5504	6.00	4.00	12.0000
43	C	0.2460	14.1535	10.4255	6.00	4.00	12.0000
44	C	-0.6226	13.5392	9.4877	6.00	4.00	12.0000
45	C	-1.9438	13.9428	9.4059	6.00	4.00	12.0000

46	C	-2.8375	13.3764	8.5020	6.00	4.00	12.0000
47	C	-4.1998	13.7352	8.4427	6.00	4.00	12.0000
48	C	-5.0414	13.1252	7.5564	6.00	4.00	12.0000
49	C	-4.5540	12.1335	6.6792	6.00	4.00	12.0000
50	C	-3.2407	11.7658	6.7131	6.00	4.00	12.0000
51	C	-2.3455	12.3673	7.6244	6.00	4.00	12.0000
52	C	-1.0151	11.9562	7.7127	6.00	4.00	12.0000
53	C	-0.1240	12.4948	8.6317	6.00	4.00	12.0000
54	C	3.8320	9.5440	7.6216	6.00	4.00	12.0000
55	N	3.3787	8.7929	6.6638	7.00	5.00	14.0031
56	H	3.6151	7.8400	4.1686	1.00	1.00	1.0078
57	H	4.0985	5.0684	5.3671	1.00	1.00	1.0078
58	H	3.6882	5.3731	3.6684	1.00	1.00	1.0078
59	H	5.7211	6.7605	3.3854	1.00	1.00	1.0078
60	H	6.1590	5.1498	3.9734	1.00	1.00	1.0078
61	H	7.3880	6.9631	5.1927	1.00	1.00	1.0078
62	H	6.3747	6.0018	6.2801	1.00	1.00	1.0078
63	H	5.6492	8.7516	5.1128	1.00	1.00	1.0078
64	H	6.1181	8.4004	6.7886	1.00	1.00	1.0078
65	H	4.1263	6.8778	6.9850	1.00	1.00	1.0078
66	H	0.5125	11.4451	5.2890	1.00	1.00	1.0078
67	H	-0.1346	12.6628	3.1790	1.00	1.00	1.0078
68	H	0.0345	11.4409	0.9912	1.00	1.00	1.0078
69	H	0.8134	9.0564	1.0084	1.00	1.00	1.0078
70	H	1.3666	7.9926	3.2181	1.00	1.00	1.0078
71	H	0.1919	3.7085	4.8093	1.00	1.00	1.0078
72	H	-2.1177	3.0900	5.5067	1.00	1.00	1.0078
73	H	-4.1372	3.6021	6.4965	1.00	1.00	1.0078
74	H	-5.6129	5.0837	7.8309	1.00	1.00	1.0078
75	H	-5.9526	7.0189	9.0987	1.00	1.00	1.0078
76	H	-6.3469	9.0009	10.5153	1.00	1.00	1.0078
77	H	-5.4671	11.0506	11.5981	1.00	1.00	1.0078
78	H	-3.0971	11.7404	11.2245	1.00	1.00	1.0078
79	H	-1.6331	10.4191	9.7434	1.00	1.00	1.0078
80	H	-1.3257	8.5724	8.1732	1.00	1.00	1.0078
81	H	1.9136	4.9921	4.8020	1.00	1.00	1.0078
82	H	4.9486	10.9461	9.4345	1.00	1.00	1.0078
83	H	3.9673	12.8177	10.7478	1.00	1.00	1.0078
84	H	2.1978	14.2270	11.2754	1.00	1.00	1.0078
85	H	-0.1558	14.9620	11.0471	1.00	1.00	1.0078
86	H	-2.2951	14.7300	10.0857	1.00	1.00	1.0078
87	H	-4.5717	14.4988	9.1359	1.00	1.00	1.0078
88	H	-6.1007	13.3950	7.5295	1.00	1.00	1.0078
89	H	-5.2401	11.6481	5.9785	1.00	1.00	1.0078
90	H	-2.8575	10.9783	6.0518	1.00	1.00	1.0078
91	H	-0.6695	11.1381	7.0788	1.00	1.00	1.0078
92	H	4.8486	9.3422	8.0116	1.00	1.00	1.0078

TOTAL BONDING ENERGIES FROM VARIOUS XC FUNCTIONALS

XC	Energy Functional	hartree	eV	kcal/mol
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FR:	KCIS-modified	-17.951403	-488.48254	-11264.677
FR:	KCIS-original	-17.924493	-487.75027	-11247.79

FR:	PKZB	-42.651964	-1160.619	-26764.515
FR:	VS98	1.2096635	32.916618	759.07537
FR:	LDA(VWN)	-24.357843	-662.81063	-15284.779
FR:	PW91	-22.68922	-617.40508	-14237.702
FR:	BLYP	-21.343936	-580.79804	-13393.523
FR:	BP	-22.277433	-606.1998	-13979.302
FR:	PBE	-22.586257	-614.60333	-14173.092
FR:	RPBE	-21.727532	-591.23624	-13634.234
FR:	revPBE	-21.836237	-594.19425	-13702.447
FR:	OLYP	-21.654647	-589.25294	-13588.498
FR:	FT97	-21.37252	-581.57585	-13411.46
FR:	BLAP3	-23.211547	-631.61832	-14565.467
FR:	HCTH/93	-21.769915	-592.38953	-13660.829
FR:	HCTH/120	-22.117606	-601.85069	-13879.009
FR:	HCTH/147	-22.094781	-601.22959	-13864.686
FR:	HCTH/407	-21.913461	-596.2956	-13750.906
FR:	BmTau1	-23.052614	-627.29355	-14465.735
FR:	BOP	-21.057548	-573.00503	-13213.812
FR:	PKZBx-KCIScor	-17.708957	-481.88525	-11112.54
FR:	VS98-x(xc)	-19.532041	-531.49388	-12256.542
FR:	VS98-x-only	-21.655258	-589.26956	-13588.881
FR:	Becke00	-22.97564	-625.19898	-14417.433
FR:	Becke00x(xc)	-20.98086	-570.91824	-13165.69
FR:	Becke00-x-only	-23.036688	-626.86018	-14455.742
FR:	Becke88x+BR89c	-22.467268	-611.36546	-14098.425
FR:	OLAP3	-23.522258	-640.07322	-14760.442
FR:	TPSS	1125236.3	30619239	6096537.5
FR:	mPBE	-22.356189	-608.34287	-14028.722
FR:	OPBE	-22.56555	-614.03987	-14160.098
FR:	OPerdew	-22.588145	-614.6547	-14174.276
FR:	mPBEKCIS	-18.476475	-502.77048	-11594.165
FR:	mPW	-22.337273	-607.82812	-14016.852
FR:	tau-HCTH	-21.374679	-581.63461	-13412.815
FR:	XLYP	-21.252234	-578.3027	-13335.979
FR:	KT1	-23.014576	-626.25847	-14441.866
FR:	KT2	-23.839179	-648.69706	-14959.312
FR:	TPSSh	1125234.8	30619197	6095572.7
FR:	B3LYP(VWN5)	-25.415907	-691.60202	-15948.724
FR:	O3LYP(VWN5)	-24.92153	-678.14934	-15638.498
FR:	KMLYP(VWN5)	-33.464727	-910.62154	-20999.435
FR:	PBE0	-27.373276	-744.86475	-17176.992
FR:	B3LYP*(VWN5)	-24.622191	-670.00392	-15450.66
FR:	BHandH	-32.886274	-894.88105	-20636.451
FR:	BHandHLYP	-31.083683	-845.83006	-19505.308
FR:	B97	-25.620666	-697.1738	-16077.212
FR:	B97-1	-26.064093	-709.24005	-16355.467
FR:	B97-2	-26.196043	-712.8306	-16438.267
FR:	mPBE0KCIS	-23.321012	-634.59702	-14634.157
FR:	mPBE1KCIS	-21.906407	-596.10367	-13746.479
FR:	B1LYP(VWN5)	-26.21381	-713.31405	-16449.416
FR:	B1PW91(VWN5)	-27.106484	-737.60496	-17009.577
FR:	mPW1PW	-27.181981	-739.65934	-17056.953
FR:	mPW1K	-30.631413	-833.52317	-19221.504
FR:	tau-HCTH-hybrid	-25.053822	-681.74918	-15721.512
FR:	X3LYP(VWN5)	-25.852781	-703.48997	-16222.867
FR:	OPBE0	-27.357746	-744.44216	-17167.247

(*R,R*)-**75**·py *P*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	C	-5.7163	-1.9433	9.2546	6.00	4.00	12.0000
2	C	-4.5155	-2.3995	8.4539	6.00	4.00	12.0000
3	C	-3.3675	-1.4345	8.6170	6.00	4.00	12.0000
4	C	-6.1310	-0.5398	8.8677	6.00	4.00	12.0000
5	Zn	-0.8209	-0.1614	7.8178	30.00	20.00	63.9291
6	C	-3.7919	-0.0277	8.1962	6.00	4.00	12.0000
7	C	0.5201	3.8685	7.7200	6.00	4.00	12.0000
8	C	-0.4010	2.7625	7.8246	6.00	4.00	12.0000
9	O	-0.1248	1.6225	7.2850	8.00	6.00	15.9949
10	C	-1.6278	2.9857	8.5252	6.00	4.00	12.0000
11	C	-1.9065	4.2284	9.1175	6.00	4.00	12.0000
12	C	-1.0207	5.2562	9.0483	6.00	4.00	12.0000
13	C	0.1867	5.0903	8.3462	6.00	4.00	12.0000
14	C	1.0634	6.2061	8.2699	6.00	4.00	12.0000
15	C	2.2262	6.1401	7.5885	6.00	4.00	12.0000
16	C	2.6150	4.9451	6.9317	6.00	4.00	12.0000
17	C	3.8066	4.9134	6.2295	6.00	4.00	12.0000
18	C	4.2435	3.7687	5.5696	6.00	4.00	12.0000
19	C	5.4591	3.7150	4.8541	6.00	4.00	12.0000
20	C	5.8468	2.5626	4.2323	6.00	4.00	12.0000
21	C	5.0327	1.4129	4.2877	6.00	4.00	12.0000
22	C	3.8443	1.4399	4.9619	6.00	4.00	12.0000
23	C	3.4173	2.6093	5.6265	6.00	4.00	12.0000
24	C	2.2101	2.6432	6.3314	6.00	4.00	12.0000
25	C	1.7697	3.7827	6.9957	6.00	4.00	12.0000
26	C	-2.6735	2.0309	8.5932	6.00	4.00	12.0000
27	N	-2.6219	0.8063	8.1999	7.00	5.00	14.0031
28	C	1.4594	-3.2494	5.8622	6.00	4.00	12.0000
29	C	0.3277	-2.5480	6.4215	6.00	4.00	12.0000
30	O	0.4478	-1.3414	6.8552	8.00	6.00	15.9949
31	C	-0.9135	-3.2558	6.4839	6.00	4.00	12.0000
32	C	-1.0669	-4.5001	5.8472	6.00	4.00	12.0000
33	C	-0.0299	-5.0953	5.2038	6.00	4.00	12.0000
34	C	1.2411	-4.4915	5.2310	6.00	4.00	12.0000
35	C	2.3151	-5.1830	4.6073	6.00	4.00	12.0000
36	C	3.5680	-4.6844	4.6091	6.00	4.00	12.0000
37	C	3.8619	-3.4716	5.2808	6.00	4.00	12.0000
38	C	5.1663	-3.0107	5.3207	6.00	4.00	12.0000
39	C	5.5242	-1.8805	6.0484	6.00	4.00	12.0000
40	C	6.8484	-1.3948	6.0992	6.00	4.00	12.0000
41	C	7.1625	-0.3117	6.8705	6.00	4.00	12.0000
42	C	6.1668	0.3322	7.6324	6.00	4.00	12.0000
43	C	4.8735	-0.1025	7.5848	6.00	4.00	12.0000
44	C	4.5065	-1.2084	6.7858	6.00	4.00	12.0000
45	C	3.1798	-1.6368	6.6907	6.00	4.00	12.0000

46	C	2.8120	-2.7490	5.9443	6.00	4.00	12.0000
47	C	-2.0404	-2.8110	7.2123	6.00	4.00	12.0000
48	N	-2.1415	-1.7420	7.9279	7.00	5.00	14.0031
49	C	-4.9806	0.4361	9.0029	6.00	4.00	12.0000
50	N	0.3227	-0.1224	9.5419	7.00	5.00	14.0031
51	C	0.0309	-0.8404	10.6244	6.00	4.00	12.0000
52	C	0.8511	-0.8669	11.7350	6.00	4.00	12.0000
53	C	2.0258	-0.1330	11.7110	6.00	4.00	12.0000
54	C	2.3329	0.6037	10.5804	6.00	4.00	12.0000
55	C	1.4517	0.5900	9.5164	6.00	4.00	12.0000
56	H	-6.5543	-2.6466	9.1156	1.00	1.00	1.0078
57	H	-5.4635	-1.9657	10.3325	1.00	1.00	1.0078
58	H	-4.7859	-2.4535	7.3802	1.00	1.00	1.0078
59	H	-4.2090	-3.4157	8.7569	1.00	1.00	1.0078
60	H	-3.1262	-1.3611	9.7019	1.00	1.00	1.0078
61	H	-6.4744	-0.5423	7.8149	1.00	1.00	1.0078
62	H	-6.9895	-0.2068	9.4744	1.00	1.00	1.0078
63	H	-4.1089	-0.1254	7.1333	1.00	1.00	1.0078
64	H	-2.8653	4.3473	9.6362	1.00	1.00	1.0078
65	H	-1.2319	6.2248	9.5100	1.00	1.00	1.0078
66	H	0.7582	7.1281	8.7754	1.00	1.00	1.0078
67	H	2.8928	7.0062	7.5226	1.00	1.00	1.0078
68	H	4.4208	5.8213	6.1931	1.00	1.00	1.0078
69	H	6.0794	4.6174	4.8077	1.00	1.00	1.0078
70	H	6.7935	2.5274	3.6843	1.00	1.00	1.0078
71	H	5.3591	0.4901	3.7978	1.00	1.00	1.0078
72	H	3.2079	0.5484	5.0154	1.00	1.00	1.0078
73	H	1.5696	1.7594	6.3387	1.00	1.00	1.0078
74	H	-3.6197	2.4259	9.0122	1.00	1.00	1.0078
75	H	-2.0511	-4.9807	5.8928	1.00	1.00	1.0078
76	H	-0.1457	-6.0575	4.6980	1.00	1.00	1.0078
77	H	2.0898	-6.1387	4.1231	1.00	1.00	1.0078
78	H	4.3889	-5.2185	4.1194	1.00	1.00	1.0078
79	H	5.9406	-3.5729	4.7844	1.00	1.00	1.0078
80	H	7.6169	-1.9100	5.5126	1.00	1.00	1.0078
81	H	8.1918	0.0586	6.9023	1.00	1.00	1.0078
82	H	6.4339	1.1951	8.2483	1.00	1.00	1.0078
83	H	4.0873	0.4063	8.1552	1.00	1.00	1.0078
84	H	2.3943	-1.0913	7.2193	1.00	1.00	1.0078
85	H	-2.9011	-3.5030	7.1634	1.00	1.00	1.0078
86	H	-4.6778	0.5247	10.0661	1.00	1.00	1.0078
87	H	-5.2993	1.4413	8.6779	1.00	1.00	1.0078
88	H	-0.9001	-1.4181	10.5826	1.00	1.00	1.0078
89	H	0.5710	-1.4637	12.6067	1.00	1.00	1.0078
90	H	2.7008	-0.1366	12.5728	1.00	1.00	1.0078
91	H	3.2482	1.1984	10.5172	1.00	1.00	1.0078
92	H	1.6274	1.1718	8.6004	1.00	1.00	1.0078

TOTAL BONDING ENERGIES FROM VARIOUS XC FUNCTIONALS

XC	Energy Functional	hartree	eV	kcal/mol
===	==========			
FR:	KCIS-modified	-17.94929623	-488.4252018	-11263.35462
FR:	KCIS-original	-17.92230802	-487.6908151	-11246.41926

FR:	PKZB	-42.6347862	-1160.151561	-26753.73508
FR:	VS98	1.172435691	31.90359842	735.7145812
FR:	LDA(VWN)	-24.35359906	-662.6951487	-15282.11575
FR:	PW91	-22.68411364	-617.2661389	-14234.49772
FR:	BLYP	-21.33763578	-580.6266122	-13389.57002
FR:	BP	-22.27169591	-606.0436816	-13975.70166
FR:	PBE	-22.58131432	-614.4688269	-14169.99016
FR:	RPBE	-21.72187671	-591.0823399	-13630.68487
FR:	revPBE	-21.83040489	-594.0355417	-13698.78733
FR:	OLYP	-21.64754685	-589.0597212	-13584.04216
FR:	FT97	-21.36451443	-581.3580174	-13406.43663
FR:	BLAP3	-23.31812037	-634.5183397	-14632.34299
FR:	HCTH/93	-21.7630287	-592.2021424	-13656.50813
FR:	HCTH/120	-22.111832	-601.6935632	-13875.38553
FR:	HCTH/147	-22.0886471	-601.0626698	-13860.83678
FR:	HCTH/407	-21.90702879	-596.1205842	-13746.86956
FR:	BmTau1	-23.15908829	-630.1908566	-14532.54884
FR:	BOP	-21.05080163	-572.8214578	-13209.57885
FR:	PKZBx-KCIScor	-17.7067857	-481.8261543	-11111.17695
FR:	VS98-x(xc)	-19.51598233	-531.0568995	-12246.46509
FR:	VS98-x-only	-21.65309068	-589.2105768	-13587.52098
FR:	Becke00	-22.97246451	-625.1125652	-14415.44064
FR:	Becke00x(xc)	-20.97742342	-570.824735	-13163.53332
FR:	Becke00-x-only	-23.03406082	-626.7886862	-14454.09291
FR:	Becke88x+BR89c	-22.46398431	-611.2761151	-14096.36446
FR:	OLAP3	-23.62803143	-642.9514487	-14826.81513
FR:	TPSS	1132883.539	30827329.61	10895228.64
FR:	mPBE	-22.35109817	-608.2043269	-14025.52733
FR:	OPBE	-22.55876643	-613.8552677	-14155.84115
FR:	OPerdew	-22.58160698	-614.4767906	-14170.17381
FR:	mPBEKCIS	-18.47324491	-502.6825707	-11592.13742
FR:	mPW	-22.33161404	-607.6741368	-14013.30086
FR:	tau-HCTH	-21.36703493	-581.4266036	-13408.01826
FR:	XLYP	-21.2460513	-578.1344715	-13332.09988
FR:	KT1	-23.01004677	-626.1352306	-14439.02387
FR:	KT2	-23.83469589	-648.5750748	-14956.49905
FR:	TPSSh	1132882.002	30827287.77	10894263.83
FR:	B3LYP(VWN5)	-25.41021192	-691.4470474	-15945.1504
FR:	O3LYP(VWN5)	-24.91506652	-677.9734555	-15634.44193
FR:	KMLYP(VWN5)	-33.46070602	-910.5121381	-20996.91225
FR:	PBE0	-27.36872299	-744.7408453	-17174.13478
FR:	B3LYP*(VWN5)	-24.61650525	-669.8491899	-15447.09189
FR:	BHandH	-32.8826627	-894.7827789	-20634.18455
FR:	BHandHLYP	-31.07868261	-845.6939831	-19502.16983
FR:	B97	-25.61596365	-697.0458368	-16074.26157
FR:	B97-1	-26.05988495	-709.1255502	-16352.82642
FR:	B97-2	-26.19053875	-712.680821	-16434.81293
FR:	mPBE0KCIS	-23.31820763	-634.5207141	-14632.39774
FR:	mPBE1KCIS	-21.90347851	-596.0239763	-13744.64173
FR:	B1LYP(VWN5)	-26.2081592	-713.1602976	-16445.86992
FR:	B1PW91(VWN5)	-27.10113629	-737.4594407	-17006.22157
FR:	mPW1PW	-27.17688717	-739.5207268	-17053.75597
FR:	mPW1K	-30.62672163	-833.395499	-19218.56
FR:	tau-HCTH-hybrid	-25.04902206	-681.6185711	-15718.50031
FR:	X3LYP(VWN5)	-25.84730573	-703.340975	-16219.43093
FR:	OPBE0	-27.35181208	-744.2806759	-17163.52302

(*R*,*R*)-**75**·THF *M*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	O	2.0170	10.8364	4.1879	8.00	6.00	15.9949
2	C	1.6233	10.2521	2.9354	6.00	4.00	12.0000
3	C	6.5671	9.1261	5.6550	6.00	4.00	12.0000
4	C	5.1262	8.8101	5.9828	6.00	4.00	12.0000
5	C	1.6856	11.3815	1.9251	6.00	4.00	12.0000
6	H	5.9160	12.1177	9.1916	1.00	1.00	1.0078
7	H	3.1514	15.3840	11.0227	1.00	1.00	1.0078
8	H	0.7897	16.1037	10.7998	1.00	1.00	1.0078
9	H	-1.3376	15.8768	9.8350	1.00	1.00	1.0078
10	H	-3.6059	15.6584	8.8831	1.00	1.00	1.0078
11	H	-5.1435	14.5565	7.2829	1.00	1.00	1.0078
12	C	-1.0275	7.3549	6.6500	6.00	4.00	12.0000
13	H	0.5252	12.8099	3.0835	1.00	1.00	1.0078
14	C	0.2701	7.7582	6.1702	6.00	4.00	12.0000
15	O	0.7068	8.9399	6.4376	8.00	6.00	15.9949
16	C	1.0332	6.8115	5.4113	6.00	4.00	12.0000
17	C	1.5732	12.6226	2.7939	6.00	4.00	12.0000
18	C	0.4981	5.5459	5.1060	6.00	4.00	12.0000
19	C	-0.7591	5.2031	5.4851	6.00	4.00	12.0000
20	C	-1.5327	6.1018	6.2457	6.00	4.00	12.0000
21	C	-2.8512	5.7071	6.6001	6.00	4.00	12.0000
22	C	-3.6465	6.5088	7.3386	6.00	4.00	12.0000
23	C	-3.1697	7.7470	7.8370	6.00	4.00	12.0000
24	H	3.4598	12.2896	3.8106	1.00	1.00	1.0078
25	C	-3.9858	8.5050	8.6598	6.00	4.00	12.0000
26	C	-3.5399	9.6771	9.2605	6.00	4.00	12.0000
27	C	-4.3540	10.4535	10.1139	6.00	4.00	12.0000
28	C	-3.8577	11.5743	10.7163	6.00	4.00	12.0000
29	C	2.3704	12.2141	3.9994	6.00	4.00	12.0000
30	C	-2.5185	11.9594	10.5049	6.00	4.00	12.0000
31	C	-1.7095	11.2310	9.6782	6.00	4.00	12.0000
32	C	-2.1957	10.0829	9.0145	6.00	4.00	12.0000
33	C	-1.3914	9.3491	8.1350	6.00	4.00	12.0000
34	C	-1.8357	8.1817	7.5235	6.00	4.00	12.0000
35	H	2.1262	12.7380	4.9362	1.00	1.00	1.0078
36	C	2.3639	7.0295	4.9746	6.00	4.00	12.0000
37	N	3.0333	8.1279	5.0647	7.00	5.00	14.0031
38	C	2.2008	13.1987	8.5554	6.00	4.00	12.0000
39	C	2.7691	12.1114	7.8017	6.00	4.00	12.0000
40	O	2.0528	11.4872	6.9345	8.00	6.00	15.9949
41	H	0.6043	9.8481	3.0624	1.00	1.00	1.0078
42	C	4.1299	11.7492	8.0516	6.00	4.00	12.0000
43	C	4.8816	12.4382	9.0210	6.00	4.00	12.0000
44	C	4.3453	13.4641	9.7314	6.00	4.00	12.0000
45	C	3.0092	13.8492	9.5109	6.00	4.00	12.0000

46	Zn	2.3654	9.8194	5.9518	30.00	20.00	63.9291
47	C	2.4818	14.9072	10.2998	6.00	4.00	12.0000
48	C	1.1964	15.2986	10.1788	6.00	4.00	12.0000
49	C	0.3312	14.6768	9.2430	6.00	4.00	12.0000
50	C	-0.9894	15.0843	9.1612	6.00	4.00	12.0000
51	C	-1.8828	14.5136	8.2610	6.00	4.00	12.0000
52	C	-3.2427	14.8838	8.1984	6.00	4.00	12.0000
53	H	2.3053	9.4152	2.7009	1.00	1.00	1.0078
54	C	-4.0870	14.2738	7.3154	6.00	4.00	12.0000
55	C	-3.6077	13.2697	6.4502	6.00	4.00	12.0000
56	C	-2.2948	12.8931	6.4863	6.00	4.00	12.0000
57	C	4.4281	8.2232	4.7510	6.00	4.00	12.0000
58	C	-1.3950	13.4981	7.3903	6.00	4.00	12.0000
59	C	-0.0618	13.0876	7.4722	6.00	4.00	12.0000
60	C	0.8290	13.6306	8.3916	6.00	4.00	12.0000
61	C	4.7987	10.6837	7.3993	6.00	4.00	12.0000
62	N	4.3381	9.9186	6.4689	7.00	5.00	14.0031
63	H	4.5355	8.9929	3.9521	1.00	1.00	1.0078
64	H	5.0542	6.2137	5.1185	1.00	1.00	1.0078
65	H	0.8915	11.3050	1.1673	1.00	1.00	1.0078
66	H	4.6233	6.5318	3.4269	1.00	1.00	1.0078
67	H	6.6439	7.9316	3.1314	1.00	1.00	1.0078
68	C	5.1292	6.9654	4.3073	6.00	4.00	12.0000
69	H	7.0991	6.3184	3.6992	1.00	1.00	1.0078
70	H	8.3354	8.1242	4.9215	1.00	1.00	1.0078
71	H	7.3334	7.1552	6.0128	1.00	1.00	1.0078
72	H	6.5780	9.9042	4.8664	1.00	1.00	1.0078
73	H	7.0783	9.5542	6.5335	1.00	1.00	1.0078
74	H	5.1042	8.0036	6.7496	1.00	1.00	1.0078
75	H	4.9245	13.9964	10.4908	1.00	1.00	1.0078
76	H	-4.2976	12.7819	5.7557	1.00	1.00	1.0078
77	H	2.6556	11.3794	1.3996	1.00	1.00	1.0078
78	H	-1.9200	12.0956	5.8348	1.00	1.00	1.0078
79	C	6.5858	7.2471	3.9999	6.00	4.00	12.0000
80	H	0.2899	12.2808	6.8280	1.00	1.00	1.0078
81	H	5.8297	10.5096	7.7709	1.00	1.00	1.0078
82	H	1.1265	4.8451	4.5437	1.00	1.00	1.0078
83	H	-1.1885	4.2308	5.2288	1.00	1.00	1.0078
84	H	-3.2030	4.7328	6.2463	1.00	1.00	1.0078
85	H	-4.6672	6.2102	7.5995	1.00	1.00	1.0078
86	H	-5.0027	8.1491	8.8655	1.00	1.00	1.0078
87	H	-5.3880	10.1325	10.2829	1.00	1.00	1.0078
88	H	-4.4957	12.1742	11.3724	1.00	1.00	1.0078
89	H	1.9668	13.5293	2.3101	1.00	1.00	1.0078
90	C	7.2907	7.8838	5.1800	6.00	4.00	12.0000
91	H	-2.1245	12.8537	10.9988	1.00	1.00	1.0078
92	H	-0.6695	11.5326	9.5060	1.00	1.00	1.0078
93	H	-0.3763	9.6938	7.9281	1.00	1.00	1.0078
94	H	2.8516	6.1406	4.5281	1.00	1.00	1.0078

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*************************************************************************
*                                                                       *
*   Final excitation energies from Davidson algorithm                   *
*                                                                       *
*************************************************************************

   Number of loops in Davidson routine     =  322
   Number of matrix-vector multiplications =  571
   Type of excitations = SINGLET-SINGLET


 Symmetry A

 Excitation energies E in a.u. and eV, dE wrt prev. cycle,
 oscillator strengths f in a.u.

 no.      E/a.u.          E/eV            f            dE/a.u.
 ---------------------------------------------------------------
   1 0.66735E-01  1.8160    0.14203E-03  0.42E-11
   2 0.75362E-01  2.0507    0.39614E-02  0.19E-08
   3 0.83956E-01  2.2846    0.12577E-01  0.38E-08
   4 0.84692E-01  2.3046    0.71750E-02  0.44E-08
   5 0.88274E-01  2.4021    0.73565E-02  0.70E-09
   6 0.89592E-01  2.4379    0.29269E-02  0.17E-08
   7 0.90025E-01  2.4497    0.21698E-02  0.19E-08
   8 0.95522E-01  2.5993    0.10572E-02  0.48E-09
   9 0.97933E-01  2.6649    0.35674E-02  0.40E-10
  10 0.10085       2.7442    0.53152E-01  0.23E-07
  11 0.10368       2.8212    0.50316E-01  0.35E-08
  12 0.10436       2.8399    0.15441      0.50E-07
  13 0.11047       3.0059    0.10278E-01  0.33E-08
  14 0.11159       3.0365    0.26231E-02  0.32E-08
  15 0.11413       3.1057    0.13043E-02  0.92E-09
  16 0.11465       3.1198    0.29751E-02  0.21E-08
  17 0.11714       3.1876    0.11766E-02  0.19E-08
  18 0.11756       3.1991    0.19834E-02  0.18E-08
  19 0.11843       3.2225    0.18707E-02  0.12E-07
  20 0.11924       3.2447    0.43729E-03  0.89E-10
  21 0.11991       3.2629    0.30692E-02  0.25E-08
  22 0.12132       3.3013    0.38948E-02  0.52E-07
  23 0.12298       3.3466    0.15067E-01  0.15E-07
  24 0.12576       3.4222    0.15253E-01  0.63E-07
  25 0.12667       3.4469    0.82987E-02  0.16E-06
  26 0.12778       3.4771    0.13262E-01  0.23E-08
  27 0.12825       3.4900    0.75727E-02  0.40E-08
  28 0.12993       3.5356    0.45544E-01  0.31E-07
  29 0.13084       3.5604    0.15463E-01  0.14E-10
  30 0.13151       3.5785    0.59637E-01  0.26E-07
  31 0.13282       3.6141    0.32055E-02  0.30E-08
  32 0.13412       3.6495    0.80083E-02  0.14E-08
  33 0.13590       3.6980    0.34004E-02  0.11E-07
  34 0.13711       3.7311    0.56960E-01  0.14E-07
  35 0.13827       3.7625    0.16361E-01  0.92E-09
  36 0.13879       3.7765    0.68112E-02  0.75E-09
  37 0.13916       3.7868    0.67418E-02  0.15E-08
  38 0.13960       3.7986    0.60510E-02  0.87E-08
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39	0.14094	3.8353	0.25035E-01	0.28E-08
40	0.14185	3.8598	0.53031E-02	0.40E-08
41	0.14221	3.8698	0.55937E-02	0.33E-09
42	0.14285	3.8871	0.16857E-01	0.24E-08
43	0.14552	3.9598	0.20292	0.35E-09
44	0.14684	3.9957	0.39396E-01	0.19E-09
45	0.14697	3.9993	0.33798E-01	0.51E-09
46	0.14703	4.0009	0.39774E-03	0.56E-09
47	0.14719	4.0051	0.31083E-01	0.21E-07
48	0.14824	4.0337	0.10984E-01	0.43E-09
49	0.14930	4.0627	0.11178E-01	0.38E-08
50	0.14950	4.0681	0.41243E-01	0.13E-08
51	0.15073	4.1015	0.11590E-01	0.15E-08
52	0.15106	4.1105	0.10647E-01	0.61E-08
53	0.15201	4.1364	0.76485E-01	0.14E-07
54	0.15256	4.1513	0.33364E-01	0.18E-07
55	0.15329	4.1713	0.86714E-03	0.13E-08
56	0.15478	4.2117	0.65388E-03	0.25E-09
57	0.15544	4.2298	0.37492E-02	0.75E-09
58	0.15559	4.2338	0.13089E-03	0.14E-09
59	0.15584	4.2408	0.10265E-02	0.20E-08
60	0.15604	4.2461	0.10299E-01	0.16E-12
61	0.15757	4.2878	0.22620E-01	0.84E-11
62	0.15843	4.3111	0.11982E-01	0.91E-10
63	0.15891	4.3243	0.31860E-02	0.71E-08
64	0.15929	4.3344	0.72068E-03	0.24E-09
65	0.16024	4.3604	0.37366E-02	0.54E-09
66	0.16049	4.3671	0.32036E-01	0.32E-09
67	0.16138	4.3913	0.22398E-02	0.13E-09
68	0.16151	4.3949	0.53738E-02	0.35E-08
69	0.16169	4.3999	0.58541E-02	0.27E-08
70	0.16190	4.4056	0.64761E-02	0.49E-08
71	0.16259	4.4244	0.12807E-02	0.43E-08
72	0.16266	4.4262	0.26937E-02	0.18E-08
73	0.16315	4.4396	0.53979E-03	0.71E-08
74	0.16342	4.4468	0.56021E-02	0.26E-08
75	0.16374	4.4557	0.10711E-01	0.18E-07
76	0.16395	4.4613	0.63132E-02	0.11E-07
77	0.16430	4.4707	0.17850E-01	0.24E-09
78	0.16463	4.4797	0.83038E-02	0.37E-07
79	0.16571	4.5092	0.15382E-01	0.25E-08
80	0.16647	4.5300	0.55011E-01	0.29E-07
81	0.16667	4.5354	0.52843E-01	0.17E-07
82	0.16685	4.5402	0.16037E-01	0.76E-08
83	0.16809	4.5740	0.56203E-01	0.29E-11
84	0.16842	4.5830	0.12634	0.25E-08
85	0.16855	4.5866	0.91713E-01	0.30E-09
86	0.16938	4.6090	0.12219E-01	0.11E-08
87	0.16968	4.6172	0.22471E-01	0.11E-07
88	0.17012	4.6293	0.13926E-01	0.81E-10
89	0.17088	4.6499	0.47409E-01	0.20E-08
90	0.17091	4.6506	0.20979E-01	0.13E-07
91	0.17154	4.6678	0.99924E-02	0.11E-07
92	0.17170	4.6723	0.90649E-02	0.61E-07
93	0.17231	4.6889	0.77486E-01	0.33E-07
94	0.17250	4.6940	0.53768E-02	0.29E-10

95	0.17324	4.7142	0.54706E-02	0.17E-08
96	0.17332	4.7163	0.17086E-01	0.68E-09
97	0.17419	4.7400	0.46821E-01	0.13E-07
98	0.17429	4.7426	0.66035E-02	0.78E-08
99	0.17473	4.7547	0.93638E-02	0.17E-07
100	0.17501	4.7622	0.31378E-01	0.81E-07
101	0.17540	4.7729	0.61708E-02	0.19E-07
102	0.17553	4.7765	0.72466E-02	0.13E-09
103	0.17625	4.7960	0.33017E-01	0.57E-09
104	0.17643	4.8010	0.72920E-01	0.35E-08
105	0.17693	4.8144	0.20582E-02	0.57E-09
106	0.17715	4.8204	0.60123E-01	0.53E-07
107	0.17755	4.8313	0.11848E-01	0.33E-07
108	0.17787	4.8401	0.51026E-01	0.71E-07
109	0.17821	4.8492	0.50623E-01	0.20E-06
110	0.17862	4.8606	0.36731E-01	0.11E-07
111	0.17901	4.8712	0.10868	0.11E-07
112	0.17945	4.8830	0.48861E-02	0.13E-10
113	0.17976	4.8916	0.23430E-01	0.39E-07
114	0.18007	4.9000	0.94565E-01	0.95E-08
115	0.18016	4.9023	0.14136E-01	0.37E-08
116	0.18088	4.9220	0.97820E-02	0.12E-08
117	0.18107	4.9272	0.21396E-01	0.63E-08
118	0.18169	4.9440	0.46830E-01	0.28E-07
119	0.18177	4.9462	0.26923E-01	0.13E-08
120	0.18200	4.9526	0.14776	0.36E-07
121	0.18208	4.9546	0.21969E-01	0.16E-08
122	0.18273	4.9723	0.67082E-01	0.73E-08
123	0.18296	4.9785	0.42267E-01	0.69E-08
124	0.18332	4.9884	0.47239E-01	0.30E-07
125	0.18340	4.9907	0.20364E-01	0.74E-10
126	0.18381	5.0018	0.47746E-01	0.89E-08
127	0.18413	5.0105	0.31992E-01	0.31E-07
128	0.18442	5.0182	0.80592E-02	0.21E-08
129	0.18458	5.0228	0.35341E-01	0.98E-08
130	0.18474	5.0270	0.55470E-01	0.60E-09
131	0.18492	5.0318	0.50756E-02	0.24E-08
132	0.18499	5.0338	0.21107E-01	0.29E-08
133	0.18529	5.0420	0.39701E-02	0.12E-07
134	0.18543	5.0457	0.16661E-03	0.34E-07
135	0.18557	5.0495	0.56648E-02	0.45E-09
136	0.18574	5.0542	0.39743E-01	0.13E-07
137	0.18586	5.0575	0.92131E-03	0.66E-08
138	0.18648	5.0742	0.56477E-01	0.55E-07
139	0.18673	5.0813	0.17270E-01	0.22E-09
140	0.18713	5.0920	0.21324E-01	0.29E-07
141	0.18753	5.1029	0.15910E-01	0.17E-07
142	0.18784	5.1114	0.10200	0.37E-08
143	0.18801	5.1159	0.18067E-01	0.88E-07
144	0.18839	5.1263	0.83526E-01	0.25E-06
145	0.18861	5.1324	0.12508E-01	0.48E-08
146	0.18964	5.1603	0.98719E-02	0.95E-08
147	0.18981	5.1651	0.11429E-01	0.22E-07
148	0.18996	5.1692	0.16416E-01	0.12E-09
149	0.19012	5.1734	0.31732E-03	0.50E-08
150	0.19027	5.1775	0.11619E-01	0.15E-07

151	0.19072	5.1898	0.21390E-02	0.11E-07
152	0.19080	5.1921	0.99960E-02	0.88E-09
153	0.19128	5.2050	0.92615E-02	0.78E-10
154	0.19130	5.2054	0.13859E-02	0.86E-09
155	0.19147	5.2101	0.11935E-01	0.17E-08
156	0.19172	5.2169	0.14755E-01	0.10E-08
157	0.19206	5.2263	0.52598E-02	0.60E-08
158	0.19277	5.2456	0.22454E-02	0.35E-08
159	0.19292	5.2496	0.98008E-02	0.88E-08
160	0.19324	5.2584	0.11779E-01	0.83E-08
161	0.19337	5.2617	0.80108E-03	0.14E-08
162	0.19345	5.2639	0.51491E-02	0.47E-08
163	0.19354	5.2665	0.24787E-01	0.15E-07
164	0.19392	5.2769	0.61343E-03	0.70E-10
165	0.19401	5.2793	0.26278E-01	0.28E-08
166	0.19459	5.2951	0.26335E-01	0.74E-08
167	0.19489	5.3033	0.53155E-02	0.65E-08
168	0.19508	5.3085	0.61803E-02	0.55E-09
169	0.19559	5.3224	0.34696E-02	0.32E-07
170	0.19583	5.3289	0.11824E-02	0.17E-08
171	0.19598	5.3330	0.36599E-03	0.82E-08
172	0.19619	5.3387	0.23896E-02	0.50E-08
173	0.19635	5.3428	0.41970E-02	0.12E-08
174	0.19656	5.3486	0.10694E-01	0.21E-07
175	0.19686	5.3568	0.83858E-02	0.48E-10
176	0.19691	5.3582	0.14312E-02	0.29E-10
177	0.19751	5.3745	0.12775E-02	0.30E-08
178	0.19763	5.3778	0.10105E-01	0.37E-08
179	0.19770	5.3796	0.61988E-03	0.56E-08
180	0.19792	5.3857	0.56640E-02	0.20E-08
181	0.19796	5.3869	0.20613E-03	0.34E-09
182	0.19811	5.3909	0.88582E-02	0.13E-08
183	0.19873	5.4077	0.29521E-01	0.13E-08
184	0.19910	5.4179	0.10397E-01	0.20E-07
185	0.19928	5.4226	0.11196E-02	0.48E-08
186	0.19932	5.4239	0.24638E-01	0.13E-07
187	0.19988	5.4391	0.92610E-02	0.49E-08
188	0.20018	5.4471	0.31466E-02	0.88E-12
189	0.20030	5.4503	0.32529E-01	0.46E-08
190	0.20048	5.4553	0.46970E-02	0.11E-07
191	0.20058	5.4581	0.13246E-01	0.27E-08
192	0.20096	5.4684	0.27977E-02	0.85E-09
193	0.20109	5.4720	0.15128E-01	0.49E-08
194	0.20137	5.4796	0.15331E-01	0.69E-11
195	0.20142	5.4810	0.11472E-01	0.29E-10
196	0.20155	5.4846	0.89496E-03	0.86E-09
197	0.20182	5.4918	0.23197E-02	0.27E-08
198	0.20196	5.4956	0.30407E-01	0.23E-07
199	0.20202	5.4972	0.22671E-02	0.18E-07
200	0.20215	5.5007	0.98735E-02	0.41E-07
201	0.20265	5.5144	0.72292E-02	0.27E-07
202	0.20293	5.5221	0.19432	0.23E-08
203	0.20312	5.5271	0.11990E-01	0.53E-07
204	0.20353	5.5382	0.87443E-01	0.26E-07
205	0.20372	5.5436	0.77692E-03	0.68E-08
206	0.20393	5.5492	0.19268E-02	0.26E-08

207	0.20407	5.5532	0.87240E-02	0.13E-08
208	0.20417	5.5558	0.93212E-02	0.35E-08
209	0.20428	5.5588	0.10361E-01	0.29E-08
210	0.20448	5.5641	0.24225E-01	0.15E-08
211	0.20466	5.5691	0.28277E-02	0.43E-08
212	0.20479	5.5726	0.11286E-01	0.76E-09
213	0.20494	5.5766	0.27118E-02	0.19E-07
214	0.20516	5.5828	0.32047E-01	0.14E-07
215	0.20521	5.5841	0.13048E-01	0.30E-07
216	0.20558	5.5941	0.16352E-01	0.17E-07
217	0.20569	5.5970	0.73134E-02	0.40E-08
218	0.20599	5.6052	0.93995E-03	0.32E-08
219	0.20615	5.6096	0.50985E-02	0.13E-08
220	0.20637	5.6157	0.10846E-01	0.17E-07
221	0.20672	5.6252	0.29843E-01	0.16E-07
222	0.20683	5.6282	0.66940E-03	0.11E-08
223	0.20770	5.6517	0.14487E-01	0.79E-09
224	0.20798	5.6596	0.31030E-02	0.19E-07
225	0.20814	5.6637	0.71236E-02	0.26E-07
226	0.20823	5.6663	0.50147E-03	0.26E-09
227	0.20848	5.6731	0.30705E-02	0.17E-08
228	0.20858	5.6758	0.22513E-02	0.47E-09
229	0.20887	5.6836	0.21224E-02	0.33E-08
230	0.20901	5.6874	0.56743E-03	0.19E-11
231	0.20920	5.6926	0.34924E-01	0.53E-07
232	0.20940	5.6980	0.78626E-02	0.76E-07
233	0.20971	5.7064	0.61948E-02	0.22E-08
234	0.21001	5.7146	0.17998E-01	0.56E-07
235	0.21011	5.7174	0.10703E-02	0.16E-08
236	0.21037	5.7246	0.76114E-02	0.21E-08
237	0.21126	5.7488	0.58644E-02	0.91E-07
238	0.21137	5.7516	0.18248E-01	0.13E-06
239	0.21148	5.7547	0.35176E-02	0.13E-06
240	0.21151	5.7554	0.40157E-02	0.83E-08
241	0.21187	5.7654	0.53217E-02	0.67E-08
242	0.21194	5.7672	0.16960E-01	0.81E-07
243	0.21200	5.7688	0.45866E-02	0.14E-06
244	0.21216	5.7731	0.50326E-02	0.42E-07
245	0.21236	5.7786	0.48756E-02	0.22E-06
246	0.21243	5.7806	0.14355E-01	0.81E-07
247	0.21259	5.7847	0.23763E-01	0.36E-07
248	0.21266	5.7868	0.61058E-02	0.92E-07
249	0.21277	5.7898	0.52247E-02	0.33E-06
250	0.21285	5.7920	0.20967E-01	0.47E-07

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	1.816	1.42E-04	4.10E-02	-1.68E-02	3.51E-02
2	2.0507	3.96E-03	5.70E-02	0.27217	-3.90E-02
3	2.2846	1.26E-02	0.34389	0.32229	-5.08E-02
4	2.3046	7.18E-03	-0.27159	-2.40E-02	0.22965

5	2.4021	7.36E-03	5.15E-03	0.31802	0.15442
6	2.4379	2.93E-03	-8.92E-02	9.10E-02	0.181
7	2.4497	2.17E-03	1.58E-02	-0.15669	0.10654
8	2.5993	1.06E-03	2.25E-02	0.12501	2.16E-02
9	2.6649	3.57E-03	0.15334	-4.24E-02	-0.17125
10	2.7442	5.32E-02	-0.68855	0.46875	-0.31106
11	2.8212	5.03E-02	-0.73194	0.23431	0.3706
12	2.8399	0.15441	-1.2101	0.61244	0.61628
13	3.0059	1.03E-02	-0.27503	0.24753	5.15E-02
14	3.0365	2.62E-03	-0.1417	9.51E-02	7.84E-02
15	3.1057	1.30E-03	-8.21E-02	-9.52E-02	-3.65E-02
16	3.1198	2.98E-03	-0.14191	-0.12052	-6.53E-02
17	3.1876	1.18E-03	-0.12212	-1.18E-02	-3.73E-03
18	3.1991	1.98E-03	0.15683	1.38E-02	2.28E-02
19	3.2225	1.87E-03	-8.28E-02	-3.38E-02	0.12529
20	3.2447	4.37E-04	-6.35E-02	-3.65E-02	-1.13E-02
21	3.2629	3.07E-03	-8.51E-02	0.15982	7.49E-02
22	3.3013	3.89E-03	-0.18559	-9.41E-02	-6.96E-02
23	3.3466	1.51E-02	-0.16622	0.3691	0.14107
24	3.4222	1.53E-02	-6.75E-02	-0.26619	-0.32637
25	3.4469	8.30E-03	0.29869	-7.78E-02	5.47E-02
26	3.4771	1.33E-02	-0.11348	3.34E-02	0.37641
27	3.49	7.57E-03	-0.10258	-0.15992	0.22906
28	3.5356	4.55E-02	-0.54238	0.43875	0.19778
29	3.5604	1.55E-02	0.41833	1.28E-02	-4.59E-02
30	3.5785	5.96E-02	-0.75728	0.31192	9.72E-02
31	3.6141	3.21E-03	0.14352	-7.82E-02	-9.74E-02
32	3.6495	8.01E-03	-0.18019	-0.21816	-9.75E-02
33	3.698	3.40E-03	-3.74E-02	-0.15577	-0.10896
34	3.7311	5.70E-02	-0.60116	0.29658	0.41686
35	3.7625	1.64E-02	0.36981	-0.20179	2.91E-03
36	3.7765	6.81E-03	0.14503	-0.22862	1.77E-02
37	3.7868	6.74E-03	-6.74E-02	-0.21644	0.14587
38	3.7986	6.05E-03	0.14923	-9.75E-02	-0.18235
39	3.8353	2.50E-02	0.31904	-0.37931	0.1441
40	3.8598	5.30E-03	0.16027	0.17023	-3.76E-02
41	3.8698	5.59E-03	0.23782	-4.74E-02	-1.40E-02
42	3.8871	1.69E-02	-0.14734	0.38877	-6.45E-02
43	3.9598	0.20292	1.2427	-0.42579	-0.60493
44	3.9957	3.94E-02	-0.46711	0.30511	0.30192
45	3.9993	3.38E-02	-0.19443	0.44722	0.32732
46	4.0009	3.98E-04	-1.54E-02	3.74E-02	-4.92E-02
47	4.0051	3.11E-02	8.60E-02	-0.52571	-0.18169
48	4.0337	1.10E-02	0.14763	0.23036	0.19048
49	4.0627	1.12E-02	-0.32442	-2.92E-04	8.40E-02
50	4.0681	4.12E-02	0.59917	-0.10368	-0.20989
51	4.1015	1.16E-02	0.32419	4.64E-02	-8.99E-02
52	4.1105	1.06E-02	3.10E-02	0.25866	0.19458
53	4.1364	7.65E-02	-0.49256	-0.5488	-0.45928
54	4.1513	3.34E-02	0.54045	-2.73E-02	0.18763
55	4.1713	8.67E-04	-1.36E-02	-7.01E-02	-5.82E-02
56	4.2117	6.54E-04	4.38E-02	4.08E-02	5.25E-02
57	4.2298	3.75E-03	-0.16663	-6.89E-02	6.06E-02
58	4.2338	1.31E-04	2.78E-02	1.47E-02	1.66E-02
59	4.2408	1.03E-03	-3.35E-02	1.31E-02	9.27E-02
60	4.2461	1.03E-02	0.17912	8.82E-02	-0.24319

61	4.2878	2.26E-02	0.30294	-0.32911	-0.12344
62	4.3111	1.20E-02	0.18129	-0.1272	-0.25377
63	4.3243	3.19E-03	1.87E-04	0.13376	0.11037
64	4.3344	7.21E-04	3.57E-02	6.08E-02	-4.26E-02
65	4.3604	3.74E-03	-0.10957	-4.85E-02	-0.1436
66	4.3671	3.20E-02	-1.48E-02	-0.23993	-0.49157
67	4.3913	2.24E-03	-6.48E-02	0.11338	-6.13E-02
68	4.3949	5.37E-03	0.1899	-9.37E-02	7.12E-02
69	4.3999	5.85E-03	-0.17118	-8.14E-02	-0.13555
70	4.4056	6.48E-03	0.20493	-3.73E-02	-0.1289
71	4.4244	1.28E-03	3.61E-02	-2.95E-02	9.82E-02
72	4.4262	2.69E-03	-9.77E-02	-6.08E-02	-0.10767
73	4.4396	5.40E-04	-5.24E-02	3.15E-03	4.70E-02
74	4.4468	5.60E-03	7.38E-02	-0.1986	-8.08E-02
75	4.4557	1.07E-02	0.15136	-0.27377	-1.61E-02
76	4.4613	6.31E-03	-0.13525	0.19866	1.87E-03
77	4.4707	1.79E-02	0.30922	0.15967	0.20458
78	4.4797	8.30E-03	6.93E-02	0.26521	2.29E-02
79	4.5092	1.54E-02	1.24E-03	-0.29859	-0.22378
80	4.53	5.50E-02	-0.60963	0.34111	8.76E-02
81	4.5354	5.28E-02	0.55899	-0.395	-8.41E-02
82	4.5402	1.60E-02	-7.34E-02	6.42E-02	-0.36697
83	4.574	5.62E-02	-0.66601	8.36E-02	0.22579
84	4.583	0.12634	0.99304	-0.17024	-0.33178
85	4.5866	9.17E-02	0.74549	-0.46673	-0.20634
86	4.609	1.22E-02	-0.16954	0.21241	0.18534
87	4.6172	2.25E-02	0.17844	-0.25784	-0.31674
88	4.6293	1.39E-02	-0.2783	0.19058	9.50E-02
89	4.6499	4.74E-02	-0.55599	-0.23557	-0.22703
90	4.6506	2.10E-02	-0.26391	0.20755	0.26721
91	4.6678	9.99E-03	-0.271	6.48E-02	-9.87E-02
92	4.6723	9.06E-03	-4.55E-02	0.16227	-0.22536
93	4.6889	7.75E-02	-0.75802	7.06E-02	0.30813
94	4.694	5.38E-03	0.19519	-2.14E-02	-9.05E-02
95	4.7142	5.47E-03	-0.12807	0.14688	9.69E-02
96	4.7163	1.71E-02	7.97E-02	-0.22908	-0.29839
97	4.74	4.68E-02	0.56821	-0.24734	0.13836
98	4.7426	6.60E-03	0.12313	7.36E-02	0.19041
99	4.7547	9.36E-03	0.28277	-5.33E-03	-1.99E-02
100	4.7622	3.14E-02	0.47682	-0.13547	-0.15241
101	4.7729	6.17E-03	-0.10164	0.20502	2.02E-02
102	4.7765	7.25E-03	-0.22191	-4.63E-02	0.10265
103	4.796	3.30E-02	-0.38255	0.2422	0.27567
104	4.801	7.29E-02	-0.66028	0.20338	0.37764
105	4.8144	2.06E-03	2.48E-02	-0.10982	-6.91E-02
106	4.8204	6.01E-02	-0.69227	-1.21E-02	0.17238
107	4.8313	1.18E-02	0.21122	-0.23442	-2.30E-02
108	4.8401	5.10E-02	-0.65018	2.83E-03	-8.70E-02
109	4.8492	5.06E-02	0.3679	-0.39619	-0.36577
110	4.8606	3.67E-02	-5.58E-02	0.20055	0.51489
111	4.8712	0.10868	-0.9023	0.3019	7.36E-02
112	4.883	4.89E-03	-0.17323	0.10332	-1.27E-02
113	4.8916	2.34E-02	0.27765	-0.28685	-0.1901
114	4.9	9.46E-02	-0.80351	0.34325	0.15584
115	4.9023	1.41E-02	-0.3269	9.31E-02	-4.66E-02
116	4.922	9.78E-03	-1.93E-02	-0.23083	-0.16572

117	4.9272	2.14E-02	-0.1193	0.27872	0.29211
118	4.944	4.68E-02	0.49542	-0.27562	-0.25537
119	4.9462	2.69E-02	0.36535	-0.12319	-0.27114
120	4.9526	0.14776	-1.0348	0.26687	0.27533
121	4.9546	2.20E-02	-2.86E-02	0.26341	0.33284
122	4.9723	6.71E-02	0.673	-0.28445	-0.12975
123	4.9785	4.23E-02	-0.53639	0.23211	7.03E-02
124	4.9884	4.72E-02	0.42732	-0.39102	-0.22588
125	4.9907	2.04E-02	0.21155	-0.28139	-0.20644
126	5.0018	4.77E-02	0.58833	-0.17509	-0.1133
127	5.0105	3.20E-02	0.40557	-0.2366	-0.20039
128	5.0182	8.06E-03	-4.76E-02	0.22088	0.12043
129	5.0228	3.53E-02	-0.31032	0.36907	0.23385
130	5.027	5.55E-02	-0.25761	0.51799	0.34019
131	5.0318	5.08E-03	-0.1332	-0.15306	-2.34E-03
132	5.0338	2.11E-02	-0.378	0.10875	0.1282
133	5.042	3.97E-03	-8.41E-03	-8.93E-02	-0.15523
134	5.0457	1.67E-04	1.42E-02	-3.39E-02	8.33E-04
135	5.0495	5.66E-03	8.99E-03	0.20095	7.30E-02
136	5.0542	3.97E-02	-0.36743	0.37552	0.21197
137	5.0575	9.21E-04	-1.27E-02	8.46E-02	1.07E-02
138	5.0742	5.65E-02	0.4292	-0.46347	-0.23512
139	5.0813	1.73E-02	-0.23832	-0.21328	-0.1909
140	5.092	2.13E-02	0.27713	-0.29056	-9.85E-02
141	5.1029	1.59E-02	-0.25832	-0.20102	-0.14185
142	5.1114	0.102	0.60139	0.49544	0.45543
143	5.1159	1.81E-02	0.22111	-0.2734	-0.14321
144	5.1263	8.35E-02	0.14668	-0.72554	-0.34225
145	5.1324	1.25E-02	0.14177	-0.22576	-0.16853
146	5.1603	9.87E-03	-0.15855	-0.10645	-0.204
147	5.1651	1.14E-02	0.18242	0.12419	0.20401
148	5.1692	1.64E-02	-0.32608	-8.23E-02	-0.12857
149	5.1734	3.17E-04	2.76E-02	-1.44E-02	3.92E-02
150	5.1775	1.16E-02	-0.24353	-9.76E-02	-0.1509
151	5.1898	2.14E-03	8.59E-02	9.09E-02	-3.46E-02
152	5.1921	1.00E-02	0.23931	1.00E-01	0.10641
153	5.205	9.26E-03	9.15E-02	-0.20216	-0.15292
154	5.2054	1.39E-03	-2.39E-02	7.73E-05	0.10147
155	5.2101	1.19E-02	-0.10458	0.22554	0.17803
156	5.2169	1.48E-02	-0.32771	-3.87E-02	-8.09E-02
157	5.2263	5.26E-03	-0.139	0.11422	9.33E-02
158	5.2456	2.25E-03	4.07E-02	0.10845	6.36E-02
159	5.2496	9.80E-03	-0.20957	-9.25E-02	-0.15406
160	5.2584	1.18E-02	0.27186	-0.10651	-7.86E-02
161	5.2617	8.01E-04	-6.05E-03	-6.41E-02	-4.54E-02
162	5.2639	5.15E-03	-0.10199	9.30E-02	0.14451
163	5.2665	2.48E-02	-0.11529	-0.3707	-0.20345
164	5.2769	6.13E-04	6.61E-03	6.74E-02	-1.24E-02
165	5.2793	2.63E-02	-0.38503	0.22276	7.28E-02
166	5.2951	2.63E-02	-0.42813	-0.13231	-4.69E-02
167	5.3033	5.32E-03	0.11404	0.11492	-0.12124
168	5.3085	6.18E-03	-0.14903	3.05E-02	0.15615
169	5.3224	3.47E-03	3.69E-02	0.13269	8.74E-02
170	5.3289	1.18E-03	-5.58E-02	4.68E-02	6.13E-02
171	5.333	3.66E-04	-4.61E-02	-1.29E-02	2.25E-02
172	5.3387	2.39E-03	-4.74E-03	-7.67E-02	-0.11118

173	5.3428	4.20E-03	0.15623	7.50E-02	4.51E-02
174	5.3486	1.07E-02	2.38E-02	0.27724	6.47E-02
175	5.3568	8.39E-03	0.22458	-1.29E-02	0.11529
176	5.3582	1.43E-03	-7.72E-02	6.18E-02	3.34E-02
177	5.3745	1.28E-03	8.34E-02	5.18E-02	-8.34E-03
178	5.3778	1.01E-02	-2.28E-02	-0.13476	-0.24086
179	5.3796	6.20E-04	6.57E-02	-1.97E-02	1.89E-03
180	5.3857	5.66E-03	-0.19546	-6.58E-02	-1.97E-02
181	5.3869	2.06E-04	-1.18E-03	7.86E-03	3.87E-02
182	5.3909	8.86E-03	2.58E-02	-0.25682	-2.11E-02
183	5.4077	2.95E-02	0.20573	0.3836	0.18263
184	5.4179	1.04E-02	-0.24132	-3.51E-02	-0.13732
185	5.4226	1.12E-03	-1.26E-02	9.04E-02	1.02E-02
186	5.4239	2.46E-02	0.32555	0.15837	0.23312
187	5.4391	9.26E-03	-9.47E-03	0.23893	0.111
188	5.4471	3.15E-03	8.20E-02	-9.99E-02	-8.29E-02
189	5.4503	3.25E-02	0.42149	9.85E-02	0.23718
190	5.4553	4.70E-03	-6.41E-02	0.17117	4.16E-02
191	5.4581	1.32E-02	0.21462	0.17099	0.15414
192	5.4684	2.80E-03	8.09E-02	-0.11513	3.30E-02
193	5.472	1.51E-02	0.29435	-5.18E-02	0.15336
194	5.4796	1.53E-02	9.73E-02	0.18928	0.26248
195	5.481	1.15E-02	0.17058	0.21272	0.10529
196	5.4846	8.95E-04	-5.83E-02	1.89E-02	5.39E-02
197	5.4918	2.32E-03	0.11494	-4.52E-02	4.45E-02
198	5.4956	3.04E-02	0.16573	0.43782	8.17E-02
199	5.4972	2.27E-03	1.98E-02	-0.11777	5.07E-02
200	5.5007	9.87E-03	0.11039	-0.24172	-5.15E-02
201	5.5144	7.23E-03	1.27E-03	-0.14448	-0.18064
202	5.5221	0.19432	0.28867	0.92879	0.70025
203	5.5271	1.20E-02	3.86E-02	-0.14438	0.25731
204	5.5382	8.74E-02	-0.73279	-0.17244	-0.27882
205	5.5436	7.77E-04	-5.06E-02	-2.00E-02	-5.25E-02
206	5.5492	1.93E-03	8.95E-02	7.85E-02	-1.33E-03
207	5.5532	8.72E-03	0.16774	-0.12842	-0.13962
208	5.5558	9.32E-03	0.24197	9.86E-02	1.42E-02
209	5.5588	1.04E-02	0.21288	-0.16234	-6.64E-02
210	5.5641	2.42E-02	-0.12826	0.37375	0.14688
211	5.5691	2.83E-03	-0.11643	7.55E-02	3.84E-02
212	5.5726	1.13E-02	0.20592	0.11871	0.16177
213	5.5766	2.71E-03	-8.72E-02	-8.31E-02	7.31E-02
214	5.5828	3.20E-02	0.33837	0.29611	0.17925
215	5.5841	1.30E-02	-0.10072	0.29162	1.36E-02
216	5.5941	1.64E-02	0.34065	3.04E-02	4.84E-02
217	5.597	7.31E-03	0.19594	-0.10738	-5.84E-02
218	5.6052	9.40E-04	4.26E-02	-2.09E-02	6.78E-02
219	5.6096	5.10E-03	6.38E-03	0.17166	8.71E-02
220	5.6157	1.08E-02	-0.14345	-0.21916	-0.10111
221	5.6252	2.98E-02	-1.83E-02	-0.41143	-0.21665
222	5.6282	6.69E-04	6.87E-02	3.67E-03	1.13E-02
223	5.6517	1.45E-02	-0.2612	-0.15301	0.11398
224	5.6596	3.10E-03	-1.22E-02	-0.1419	-4.58E-02
225	5.6637	7.12E-03	7.30E-02	-0.20448	-6.48E-02
226	5.6663	5.01E-04	-1.90E-02	1.39E-02	-5.53E-02
227	5.6731	3.07E-03	0.12196	-1.65E-02	-8.34E-02
228	5.6758	2.25E-03	-1.32E-02	-8.39E-02	-9.47E-02

229	5.6836	2.12E-03	8.21E-03	9.37E-02	-7.99E-02
230	5.6874	5.67E-04	-3.86E-02	4.16E-02	-2.92E-02
231	5.6926	3.49E-02	4.18E-03	0.45849	0.20046
232	5.698	7.86E-03	-0.23239	-2.01E-02	-4.38E-02
233	5.7064	6.19E-03	0.15305	-2.01E-03	-0.14451
234	5.7146	1.80E-02	2.15E-02	0.282	0.22037
235	5.7174	1.07E-03	3.56E-02	-7.26E-02	-3.32E-02
236	5.7246	7.61E-03	1.14E-02	0.23239	1.16E-02
237	5.7488	5.86E-03	-1.64E-02	6.20E-02	0.19373
238	5.7516	1.82E-02	-0.27417	5.36E-02	0.22685
239	5.7547	3.52E-03	-0.13248	-6.42E-02	-5.72E-02
240	5.7554	4.02E-03	6.39E-02	0.14234	-6.43E-02
241	5.7654	5.32E-03	0.19336	3.47E-03	-1.67E-02
242	5.7672	1.70E-02	-0.1822	-0.18437	-0.22989
243	5.7688	4.59E-03	-0.10799	0.13229	-5.74E-02
244	5.7731	5.03E-03	-4.89E-02	-0.10614	-0.14808
245	5.7786	4.88E-03	-5.17E-02	-0.15114	-9.45E-02
246	5.7806	1.44E-02	-0.22681	-0.1825	-0.1289
247	5.7847	2.38E-02	-0.24263	-0.25618	-0.20779
248	5.7868	6.11E-03	0.13171	0.14382	-7.10E-02
249	5.7898	5.22E-03	9.05E-02	2.33E-02	-0.16764
250	5.792	2.10E-02	0.37629	6.62E-02	4.23E-02

Rotatory strengths R in 10**(-40) esu**2 * cm**2 ,
(multiply by 1.07827 to obtain reduced rotatory strengths),
magnetic transition dipole vectors m in a.u.:

no.	R	m (x,y,z)		
1	-0.81839	6.19E-02	1.00E-02	-0.16631
2	-30.918	-0.265	-0.33559	0.63332
3	-3.5242	-0.30379	0.25322	-0.15563
4	-14.904	0.35031	-0.16477	0.12173
5	-7.7887	5.18E-02	-0.3125	0.42788
6	-8.6047	7.55E-02	0.14054	-0.23511
7	-47.72	0.20401	0.55129	-1.1196
8	4.0556	-0.18656	0.19826	-0.15611
9	-9.0731	5.21E-02	-0.15527	0.3099
10	-410.29	-1.1259	-2.5595	4.2308
11	25.074	4.04E-04	-0.60067	0.66758
12	157.82	-0.37924	-1.5914	1.9232
13	4.8859	-0.47855	-0.63024	0.87614
14	2.261	-0.10575	-0.24773	0.23181
15	-1.7967	2.60E-02	2.36E-02	8.88E-02
16	4.1021	1.53E-02	-0.29416	0.24333
17	4.0381	-0.12969	-0.16452	0.17235
18	-1.1048	4.77E-02	0.51708	-0.84572
19	-26.704	0.18537	0.41078	-0.67084
20	-0.23318	-1.28E-02	-3.59E-02	0.27565
21	-4.1816	-5.10E-02	-0.3458	0.44286
22	4.8443	-9.45E-02	-0.50108	0.63392
23	-6.2153	-0.40166	-0.58366	0.86698
24	-50.05	-0.12189	-0.79213	1.3218
25	29.237	0.63309	0.40189	-0.61747
26	-138.25	0.46515	0.72319	-1.4821

27	-103.36	0.62763	0.46016	-1.312
28	33.261	-0.60247	-1.2173	1.7615
29	9.5304	-4.65E-02	0.69795	-1.1107
30	73.286	-0.78212	-1.6878	2.5203
31	0.74318	5.97E-02	0.30957	-0.19315
32	-6.4339	0.29245	-0.46877	0.78829
33	0.23404	4.20E-02	-0.37735	0.51598
34	25.119	-7.47E-02	-0.77084	0.69639
35	4.3128	0.57476	0.94384	-1.307
36	-17.63	0.53697	0.59901	-0.88617
37	-48.042	0.56241	0.25941	-0.75237
38	-9.384	-0.20334	0.21423	-6.26E-02
39	-189.59	0.84364	1.7009	-2.9719
40	5.35E-02	-0.35246	0.27105	-0.28117
41	8.7696	0.20621	0.3978	-0.49874
42	-101.96	-0.67226	-1.0407	1.9693
43	143.84	-0.28225	2.3993	-3.2774
44	30.369	6.64E-02	-1.3043	1.8475
45	-14.461	-0.13087	-0.46309	0.36756
46	-1.456	-0.22972	9.02E-02	0.2662
47	29.151	0.72815	2.82E-02	-0.41758
48	-5.437	0.18928	9.55E-02	-0.3833
49	3.834	0.13439	-0.51266	0.71087
50	21.172	-0.22892	1.1468	-1.6479
51	1.2839	-9.20E-02	0.28393	-0.24576
52	-2.1026	-4.69E-02	0.25102	-0.37207
53	-2.9952	-0.20866	-1.22	1.7093
54	21.312	0.97478	1.1529	-2.1579
55	-0.81272	5.06E-02	-0.14543	0.22261
56	0.49914	0.107	0.2146	-0.21539
57	-1.1331	-8.85E-02	3.44E-02	-0.28353
58	1.3037	0.10958	-0.3227	0.4378
59	6.5364	9.91E-02	-0.51052	0.40729
60	-48.901	-0.94531	-8.80E-02	0.12485
61	-26.169	0.24148	1.3414	-2.0845
62	-14.986	-0.37499	0.16882	-0.102
63	-8.3467	-0.36878	0.32707	-0.71654
64	-2.4814	-0.17206	2.64E-04	0.10333
65	-30.009	-0.14002	-0.8556	1.2822
66	-146.04	-0.60122	-0.49507	1.52
67	-24.937	-0.38956	-0.6034	1.0207
68	7.0407	0.54307	0.36222	-0.5525
69	-14.939	-0.26273	-0.54352	1.1259
70	11.486	-0.23041	0.56622	-0.90818
71	-20.922	0.22149	0.41684	-0.86007
72	12.616	-0.40929	0.16104	-0.21667
73	1.5106	0.11108	-0.24266	0.27678
74	-0.34477	0.28413	0.14312	-7.41E-02
75	-9.6687	0.72729	0.59839	-0.79078
76	8.7373	-0.65981	-0.26561	0.31542
77	-0.59111	0.43371	0.98887	-1.4396
78	-22.737	-0.28155	-0.36506	0.8668
79	-4.7385	0.18185	-0.13648	0.27294
80	4.112	-0.6532	-1.9469	3.2351
81	-25.365	0.74271	2.0129	-3.2376
82	-153.49	-1.018	-0.87296	1.8252

83	72.999	6.89E-03	-1.5671	1.9723
84	102.89	-0.13991	1.8536	-2.6855
85	93.393	1.01	1.9829	-2.7566
86	2.6325	1.92E-02	-0.43521	0.57659
87	-5.5075	-0.19169	0.45523	-0.40481
88	9.439	-0.26767	-0.81403	1.2709
89	11.372	-0.37698	-1.4072	2.1708
90	0.48173	0.10081	-0.51423	0.50661
91	13.407	-0.79902	-0.69362	1.1625
92	-35.333	-1.2263	-0.25876	0.72649
93	58.185	0.32614	-1.5402	1.9565
94	0.96576	-0.1449	0.30231	-0.42913
95	4.9164	-0.2953	-0.21001	0.14326
96	-6.2893	-0.29555	-1.59E-02	2.27E-02
97	-110.03	0.95176	2.1431	-3.451
98	-15.778	0.51942	0.5045	-0.88237
99	13.562	0.14618	0.60538	-0.97731
100	40.424	0.27628	0.88218	-1.045
101	1.0252	-0.57964	-0.34538	0.80374
102	-1.6545	0.19868	-0.17236	0.28339
103	11.981	-5.14E-02	-0.74808	0.7703
104	16.758	0.33589	-1.2327	1.4394
105	-0.28424	3.66E-02	-3.81E-02	9.11E-02
106	37.665	0.41277	-1.6351	2.4701
107	5.3978	0.71228	0.60728	-0.64335
108	20.308	-0.51104	-1.5715	2.7784
109	11.252	-4.21E-02	0.77957	-1.0172
110	-162.74	0.98054	0.29503	-1.3494
111	54.571	-0.86054	-2.8775	4.4005
112	-4.3711	-0.31326	-0.60608	0.80367
113	5.6464	0.23236	0.63783	-0.74909
114	86.43	-0.72403	-2.0827	3.2069
115	-12.9	-0.5436	-1.4376	2.1186
116	0.33624	0.13246	-0.11617	0.1378
117	-10.143	0.18676	7.08E-02	-0.13858
118	30.249	0.12678	1.0304	-1.3687
119	13.22	-0.25794	0.98942	-1.004
120	185.78	-0.43876	-2.55	3.685
121	-15.705	0.54575	6.68E-02	-0.20617
122	70.522	0.7381	1.9856	-2.8303
123	29.496	-0.57299	-1.4481	2.1889
124	38.296	0.54217	0.78128	-1.046
125	17.196	0.28434	0.43001	-0.64812
126	64.535	0.50171	1.664	-2.3826
127	53.794	0.37768	0.88946	-1.4246
128	-6.3435	-7.27E-02	-0.16197	4.49E-02
129	34.994	-0.56272	-0.70835	1.0061
130	31.946	-0.57761	-0.45541	0.65441
131	-0.67358	0.52348	-0.44707	0.66487
132	17.672	-6.54E-02	-1.0164	1.2542
133	-10.085	-0.43854	-8.06E-02	0.34576
134	0.5136	-6.55E-03	-6.87E-02	-6.63E-02
135	-1.3829	-0.28751	6.88E-02	-0.23446
136	41.477	-0.45811	-0.82108	1.4907
137	-7.1228	-0.36368	-0.4518	0.3176
138	73.282	0.94415	0.7994	-1.1745

139	0.7717	-0.27218	-0.63778	1.0352
140	27.008	0.8451	0.76851	-1.0524
141	-3.8961	-1.70E-02	-0.89009	1.409
142	-18.879	0.55659	1.9512	-3.0334
143	29.491	0.79372	0.47471	-0.55439
144	73.843	1.5241	-0.22571	0.2164
145	2.4029	4.66E-02	0.33251	-0.46674
146	-7.3191	-0.78622	-0.64916	1.102
147	-4.1728	0.643	0.55759	-1.0012
148	-5.0659	-0.3191	-0.78655	1.4799
149	-0.30462	0.3158	0.16439	-0.19568
150	-10.457	-0.23447	-0.91316	1.2627
151	1.8023	-0.38616	0.29624	-0.40156
152	-0.24995	0.18399	0.4948	-0.88848
153	0.85042	0.15594	0.25319	-0.26499
154	-0.88176	0.31112	-0.16332	3.65E-02
155	-0.62067	-0.12555	-0.39957	0.41767
156	2.7898	-0.28451	-0.86268	1.4185
157	5.654	-0.11804	-0.28171	0.42593
158	-1.2218	0.1344	2.86E-02	-0.21621
159	-4.4629	-0.46371	-0.4901	1.0478
160	2.3507	3.14E-02	0.95604	-1.3136
161	-0.32448	1.80E-02	-7.03E-03	3.78E-02
162	-0.52638	0.34073	-0.25392	0.38836
163	-4.9627	0.36388	-0.35863	0.55072
164	-2.327	-0.22496	-0.11824	3.31E-02
165	17.665	-0.38382	-0.88287	1.7007
166	-10.59	0.33823	-1.4208	1.8772
167	-12.361	-0.86723	0.17113	-0.22101
168	-10.142	0.77502	-0.14761	0.49294
169	-8.3397	-3.73E-02	-0.22047	-5.43E-02
170	4.4737	-0.14751	-0.27533	0.3855
171	-0.79401	0.25041	-0.17666	0.26243
172	-0.40742	-0.14822	4.10E-02	-6.41E-03
173	-0.81379	-5.08E-02	0.42905	-0.61339
174	-13.878	-0.70989	-0.20878	0.24563
175	2.6228	0.72657	0.67692	-1.243
176	-4.7768	0.14297	-0.38697	0.43962
177	-0.96288	-0.2702	0.29117	-0.40275
178	-15.314	-0.49942	8.18E-02	0.27124
179	-0.49027	6.68E-02	0.29136	-0.37838
180	-2.2106	0.13345	-0.4631	0.70044
181	0.12831	0.19141	-6.28E-03	2.12E-02
182	-8.2949	0.68295	0.23016	-0.29712
183	-5.9784	-0.24341	0.52972	-0.97729
184	11.741	-0.70376	-0.56323	1.018
185	0.43859	-0.32455	-2.53E-02	6.97E-03
186	-37.056	0.45452	0.82667	-1.8707
187	1.6065	-0.24222	-9.82E-03	6.19E-02
188	3.8734	9.95E-02	0.26939	-0.42427
189	22.676	1.034	1.1905	-1.9263
190	3.8344	-0.42943	-3.99E-02	-0.10688
191	-16.309	-2.71E-02	0.7512	-1.2445
192	-3.6286	0.61431	0.37591	-0.65972
193	2.9027	0.98384	0.78889	-1.5415
194	-19.287	0.55379	0.28208	-0.72052

195	-13.815	-0.37495	0.42891	-0.8157
196	-4.57E-02	0.22621	-0.2515	0.32979
197	3.4415	0.39383	0.11604	-0.57054
198	18.889	-0.92029	0.6683	-0.73343
199	8.505	0.55586	-0.16684	0.10686
200	14.78	0.5145	6.29E-02	-0.40975
201	-3.7741	-0.37231	2.16E-02	6.87E-02
202	-45.021	-4.15E-02	0.92956	-1.4886
203	-63.776	1.4737	0.47729	-1.0049
204	55.14	-1.067	-1.5543	2.9266
205	-2.2746	-0.2204	-0.29502	0.50862
206	6.3003	-4.27E-02	0.38034	-0.52754
207	2.4128	-0.19673	0.72202	-0.97379
208	2.1726	-0.10087	0.45233	-0.77285
209	1.486	0.28103	0.66137	-0.81103
210	-2.3007	-0.47556	-0.51114	0.81889
211	2.3151	-0.26553	-0.52077	0.47444
212	6.8397	0.41402	0.53444	-0.73984
213	-3.0905	0.54363	-0.19614	0.24581
214	-11.562	-7.30E-03	0.76742	-1.5276
215	12.616	-0.71362	-8.68E-02	0.51105
216	15.945	0.33844	1.0939	-1.6709
217	-6.8175	4.83E-02	0.74881	-0.71943
218	-0.21098	0.45074	0.17367	-0.24258
219	-3.1786	-0.27525	-0.13521	0.13178
220	1.9834	0.2775	-0.43575	0.4676
221	-12.045	0.18307	0.20988	-0.1782
222	0.33002	6.87E-02	0.12938	-0.33725
223	-11.424	0.89656	-0.60497	0.81724
224	-1.8298	0.15482	1.01E-02	9.71E-02
225	4.5362	0.30081	0.11766	-0.32939
226	0.62971	-0.36512	-9.49E-02	5.32E-02
227	9.03E-02	-0.35424	0.47477	-0.61668
228	-0.3164	-0.19566	-8.94E-02	0.12061
229	1.0279	-0.80003	0.11181	-5.60E-03
230	2.268	-0.44919	-5.62E-02	0.18422
231	1.2254	-0.44342	-8.44E-02	0.22832
232	5.2067	-0.23116	-0.65273	1.0222
233	0.43826	-0.16061	0.32954	-0.18755
234	5.0344	-1.64E-02	7.55E-02	1.95E-03
235	-0.74168	0.12661	0.1307	-5.51E-02
236	20.107	-0.50486	0.39668	-9.80E-02
237	1.322	1.0071	7.78E-02	8.92E-02
238	-12.132	0.8745	-0.58474	0.96811
239	6.0883	-0.2533	-0.45179	0.64192
240	0.93366	-0.62897	0.15675	-0.33973
241	-3.6645	-0.13836	0.28825	-0.61292
242	8.9961	-0.70831	-0.44158	0.74951
243	-1.0661	-0.3933	-4.93E-02	0.70542
244	-8.1435	-0.33294	-2.02E-02	0.35767
245	-3.4181	4.70E-02	-5.40E-02	0.21419
246	-9.6715	9.14E-02	-0.69109	1.136
247	0.18707	-0.26622	-0.6275	1.0806
248	-12.041	-0.76604	0.22958	-0.23673
249	-1.5225	-0.83969	0.28025	-0.37567
250	16.066	0.17914	1.0358	-1.6032

(*R*,*R*)-**75**·THF *P*

==========
G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	Zn	12.2125	0.3791	9.9226	30.00	20.00	63.9291
2	C	14.4929	-1.3359	10.6219	6.00	4.00	12.0000
3	C	15.7052	-1.7325	11.4259	6.00	4.00	12.0000
4	C	16.5873	-2.6765	10.6375	6.00	4.00	12.0000
5	C	16.9940	-2.0649	9.3144	6.00	4.00	12.0000
6	C	15.7844	-1.6569	8.5004	6.00	4.00	12.0000
7	C	14.9026	-0.7184	9.2868	6.00	4.00	12.0000
8	C	10.7536	1.9969	13.6232	6.00	4.00	12.0000
9	C	11.6420	1.3611	12.6822	6.00	4.00	12.0000
10	O	11.3223	1.2804	11.4354	8.00	6.00	15.9949
11	C	12.8600	0.8154	13.1952	6.00	4.00	12.0000
12	C	13.2581	1.0633	14.5207	6.00	4.00	12.0000
13	C	12.4798	1.7866	15.3660	6.00	4.00	12.0000
14	C	11.2164	2.2328	14.9355	6.00	4.00	12.0000
15	C	10.4009	2.9204	15.8750	6.00	4.00	12.0000
16	C	9.1613	3.3429	15.5526	6.00	4.00	12.0000
17	C	8.6155	3.0763	14.2712	6.00	4.00	12.0000
18	C	7.3150	3.4579	13.9907	6.00	4.00	12.0000
19	C	6.6995	3.1417	12.7837	6.00	4.00	12.0000
20	C	5.3712	3.5150	12.4856	6.00	4.00	12.0000
21	C	4.7919	3.1385	11.3071	6.00	4.00	12.0000
22	C	5.5150	2.3715	10.3721	6.00	4.00	12.0000
23	C	6.8106	2.0171	10.6226	6.00	4.00	12.0000
24	C	7.4444	2.3920	11.8277	6.00	4.00	12.0000
25	C	8.7772	2.0603	12.0878	6.00	4.00	12.0000
26	C	9.4006	2.3815	13.2879	6.00	4.00	12.0000
27	C	13.7165	-0.0392	12.4583	6.00	4.00	12.0000
28	N	13.5624	-0.4293	11.2404	7.00	5.00	14.0031
29	C	10.6014	1.7258	6.1966	6.00	4.00	12.0000
30	C	11.5074	1.0959	7.1294	6.00	4.00	12.0000
31	O	11.4292	1.3455	8.3903	8.00	6.00	15.9949
32	C	12.4985	0.2101	6.5959	6.00	4.00	12.0000
33	C	12.5371	-0.0898	5.2215	6.00	4.00	12.0000
34	C	11.6436	0.4564	4.3587	6.00	4.00	12.0000
35	C	10.6853	1.3739	4.8322	6.00	4.00	12.0000
36	C	9.8060	1.9562	3.8799	6.00	4.00	12.0000
37	C	8.8814	2.8683	4.2447	6.00	4.00	12.0000
38	C	8.7575	3.2751	5.5962	6.00	4.00	12.0000
39	C	7.8083	4.2240	5.9358	6.00	4.00	12.0000
40	C	7.6521	4.6729	7.2428	6.00	4.00	12.0000
41	C	6.6848	5.6334	7.6092	6.00	4.00	12.0000
42	C	6.5756	6.0474	8.9066	6.00	4.00	12.0000
43	C	7.4332	5.5254	9.8959	6.00	4.00	12.0000
44	C	8.3796	4.5952	9.5702	6.00	4.00	12.0000
45	C	8.5141	4.1343	8.2421	6.00	4.00	12.0000

46	C	9.4623	3.1655	7.9018	6.00	4.00	12.0000
47	C	9.6180	2.7074	6.5987	6.00	4.00	12.0000
48	C	13.5537	-0.3332	7.3653	6.00	4.00	12.0000
49	N	13.7061	-0.2432	8.6431	7.00	5.00	14.0031
50	H	13.9240	-2.2584	10.3653	1.00	1.00	1.0078
51	H	15.3968	-2.1952	12.3797	1.00	1.00	1.0078
52	H	16.2781	-0.8189	11.6842	1.00	1.00	1.0078
53	H	17.4774	-2.9491	11.2291	1.00	1.00	1.0078
54	H	16.0358	-3.6182	10.4492	1.00	1.00	1.0078
55	H	17.6244	-2.7634	8.7391	1.00	1.00	1.0078
56	H	17.6163	-1.1690	9.5069	1.00	1.00	1.0078
57	H	16.1077	-1.1805	7.5586	1.00	1.00	1.0078
58	H	15.1950	-2.5531	8.2190	1.00	1.00	1.0078
59	H	15.5032	0.1810	9.5510	1.00	1.00	1.0078
60	H	14.2179	0.6500	14.8530	1.00	1.00	1.0078
61	H	12.7918	1.9969	16.3929	1.00	1.00	1.0078
62	H	10.8129	3.0920	16.8746	1.00	1.00	1.0078
63	H	8.5379	3.8734	16.2801	1.00	1.00	1.0078
64	H	6.7492	4.0021	14.7573	1.00	1.00	1.0078
65	H	4.8172	4.1064	13.2233	1.00	1.00	1.0078
66	H	3.7616	3.4321	11.0844	1.00	1.00	1.0078
67	H	5.0392	2.0767	9.4323	1.00	1.00	1.0078
68	H	7.3898	1.4494	9.8850	1.00	1.00	1.0078
69	H	9.3592	1.5317	11.3289	1.00	1.00	1.0078
70	H	14.5828	-0.4140	13.0359	1.00	1.00	1.0078
71	H	13.3174	-0.7728	4.8651	1.00	1.00	1.0078
72	H	11.6648	0.2254	3.2899	1.00	1.00	1.0078
73	H	9.9102	1.6456	2.8352	1.00	1.00	1.0078
74	H	8.2114	3.3208	3.5058	1.00	1.00	1.0078
75	H	7.1675	4.6340	5.1454	1.00	1.00	1.0078
76	H	6.0303	6.0397	6.8300	1.00	1.00	1.0078
77	H	5.8209	6.7902	9.1824	1.00	1.00	1.0078
78	H	7.3336	5.8594	10.9336	1.00	1.00	1.0078
79	H	9.0436	4.1763	10.3359	1.00	1.00	1.0078
80	H	10.1127	2.7540	8.6753	1.00	1.00	1.0078
81	H	14.3240	-0.8573	6.7663	1.00	1.00	1.0078
82	O	10.6924	-1.0077	9.8581	8.00	6.00	15.9949
83	C	10.4433	-1.8538	8.7245	6.00	4.00	12.0000
84	H	9.7545	-3.9239	8.7689	1.00	1.00	1.0078
85	H	8.4783	-2.7080	9.0221	1.00	1.00	1.0078
86	H	8.9532	-3.3759	11.3155	1.00	1.00	1.0078
87	H	10.7114	-3.4554	10.9913	1.00	1.00	1.0078
88	H	8.9621	-0.9329	11.0094	1.00	1.00	1.0078
89	H	10.4997	-1.1881	11.8959	1.00	1.00	1.0078
90	C	9.5322	-2.9523	9.2349	6.00	4.00	12.0000
91	C	9.7747	-2.9303	10.7350	6.00	4.00	12.0000
92	C	9.9381	-1.4580	10.9882	6.00	4.00	12.0000
93	H	11.4196	-2.2346	8.3730	1.00	1.00	1.0078
94	H	9.9976	-1.2444	7.9186	1.00	1.00	1.0078

```
*************************************************************************
*                                                                       *
*   Final excitation energies from Davidson algorithm                   *
*                                                                       *
*************************************************************************

   Number of loops in Davidson routine     =  403
   Number of matrix-vector multiplications =  652
   Type of excitations = SINGLET-SINGLET


 Symmetry A

 Excitation energies E in a.u. and eV, dE wrt prev. cycle,
 oscillator strengths f in a.u.

 no.      E/a.u.          E/eV            f            dE/a.u.
 ---------------------------------------------------------------
   1 0.72805E-01  1.9811    0.22298E-02  0.25E-11
   2 0.80050E-01  2.1783    0.43965E-02  0.53E-10
   3 0.81930E-01  2.2294    0.29296E-02  0.75E-09
   4 0.86334E-01  2.3493    0.12833E-01  0.15E-07
   5 0.86944E-01  2.3659    0.59981E-02  0.24E-09
   6 0.90034E-01  2.4500    0.60335E-02  0.38E-07
   7 0.91351E-01  2.4858    0.31174E-02  0.18E-08
   8 0.95650E-01  2.6028    0.48640E-02  0.40E-08
   9 0.99643E-01  2.7114    0.66897E-02  0.31E-08
  10 0.10076      2.7417    0.10261E-01  0.45E-08
  11 0.10345      2.8150    0.22723      0.14E-06
  12 0.10801      2.9390    0.30347E-01  0.93E-08
  13 0.11245      3.0598    0.25277E-02  0.24E-09
  14 0.11320      3.0804    0.94389E-03  0.27E-11
  15 0.11614      3.1602    0.22554E-02  0.86E-10
  16 0.11689      3.1809    0.11587E-02  0.85E-10
  17 0.11711      3.1867    0.36928E-02  0.15E-07
  18 0.11874      3.2310    0.95296E-03  0.51E-10
  19 0.11958      3.2540    0.10864E-02  0.12E-09
  20 0.12187      3.3163    0.85701E-02  0.12E-07
  21 0.12211      3.3227    0.13927E-01  0.15E-08
  22 0.12318      3.3520    0.17032E-02  0.11E-07
  23 0.12428      3.3820    0.20988E-01  0.58E-07
  24 0.12498      3.4009    0.68401E-02  0.92E-07
  25 0.12557      3.4170    0.26125E-02  0.59E-08
  26 0.12657      3.4442    0.57657E-02  0.38E-08
  27 0.12699      3.4557    0.89391E-02  0.59E-09
  28 0.12789      3.4799    0.38166E-02  0.93E-09
  29 0.12959      3.5263    0.20634E-01  0.25E-07
  30 0.13108      3.5668    0.32635E-01  0.18E-07
  31 0.13162      3.5817    0.48289E-01  0.29E-07
  32 0.13324      3.6257    0.74862E-01  0.12E-07
  33 0.13399      3.6461    0.20556E-01  0.15E-07
  34 0.13562      3.6903    0.30581E-01  0.25E-08
  35 0.13612      3.7040    0.14444E-01  0.60E-08
  36 0.13761      3.7444    0.79315E-02  0.14E-08
  37 0.13917      3.7871    0.29825E-02  0.65E-08
  38 0.14009      3.8121    0.72382E-02  0.27E-09
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39	0.14118	3.8416	0.99810E-02	0.53E-08
40	0.14181	3.8587	0.93613E-02	0.64E-08
41	0.14256	3.8793	0.16260E-01	0.28E-08
42	0.14524	3.9521	0.25145	0.30E-07
43	0.14663	3.9900	0.24597E-01	0.22E-08
44	0.14691	3.9976	0.82997E-02	0.11E-09
45	0.14726	4.0072	0.56072E-01	0.21E-08
46	0.14877	4.0483	0.10832E-01	0.15E-08
47	0.14903	4.0554	0.70871E-02	0.25E-10
48	0.14992	4.0795	0.49026E-01	0.84E-08
49	0.15027	4.0890	0.10064	0.31E-09
50	0.15103	4.1099	0.10595E-01	0.12E-07
51	0.15215	4.1402	0.54778E-01	0.96E-08
52	0.15387	4.1870	0.19703E-02	0.27E-08
53	0.15423	4.1969	0.11235E-01	0.25E-08
54	0.15446	4.2032	0.13991E-01	0.23E-08
55	0.15526	4.2249	0.21938E-02	0.45E-12
56	0.15611	4.2481	0.30684E-03	0.25E-08
57	0.15632	4.2538	0.31477E-02	0.15E-08
58	0.15685	4.2682	0.31043E-02	0.25E-09
59	0.15688	4.2690	0.24821E-02	0.62E-09
60	0.15756	4.2874	0.31994E-02	0.47E-11
61	0.15888	4.3233	0.14534E-02	0.88E-09
62	0.15962	4.3434	0.14570E-01	0.58E-08
63	0.16041	4.3651	0.62543E-02	0.72E-10
64	0.16046	4.3664	0.31079E-02	0.16E-08
65	0.16072	4.3735	0.11282E-01	0.71E-09
66	0.16098	4.3806	0.42320E-04	0.23E-08
67	0.16185	4.4042	0.83672E-02	0.31E-08
68	0.16259	4.4243	0.57467E-02	0.27E-08
69	0.16270	4.4273	0.21163E-01	0.80E-12
70	0.16284	4.4312	0.72845E-03	0.16E-08
71	0.16306	4.4371	0.48149E-02	0.11E-07
72	0.16336	4.4453	0.52330E-01	0.18E-08
73	0.16346	4.4480	0.85064E-02	0.12E-08
74	0.16384	4.4583	0.93922E-02	0.85E-10
75	0.16416	4.4669	0.44268E-02	0.24E-09
76	0.16428	4.4703	0.19909E-01	0.18E-09
77	0.16471	4.4820	0.17444E-02	0.41E-10
78	0.16533	4.4989	0.10062E-01	0.29E-07
79	0.16547	4.5027	0.42026E-01	0.20E-07
80	0.16579	4.5113	0.96220E-02	0.13E-07
81	0.16612	4.5203	0.48391E-02	0.68E-08
82	0.16695	4.5428	0.27758E-01	0.19E-07
83	0.16752	4.5585	0.20538E-01	0.47E-08
84	0.16857	4.5872	0.12095E-01	0.65E-09
85	0.16871	4.5908	0.55290E-01	0.29E-07
86	0.16910	4.6016	0.70813E-01	0.10E-07
87	0.16931	4.6072	0.20054E-01	0.23E-07
88	0.16944	4.6108	0.18331E-01	0.19E-07
89	0.16970	4.6177	0.94982E-02	0.84E-09
90	0.16985	4.6219	0.19696E-01	0.14E-07
91	0.17048	4.6391	0.65515E-01	0.59E-08
92	0.17106	4.6548	0.45039E-02	0.20E-08
93	0.17148	4.6662	0.40788E-01	0.12E-07
94	0.17180	4.6750	0.73522E-01	0.12E-07

95	0.17248	4.6935	0.96378E-01	0.31E-07
96	0.17289	4.7045	0.11930E-01	0.26E-07
97	0.17296	4.7064	0.17194E-01	0.21E-07
98	0.17376	4.7283	0.12539E-01	0.61E-08
99	0.17448	4.7478	0.85732E-02	0.49E-08
100	0.17458	4.7506	0.14677E-01	0.12E-09
101	0.17492	4.7598	0.20757E-02	0.52E-07
102	0.17518	4.7670	0.29067E-01	0.18E-07
103	0.17558	4.7777	0.54135E-01	0.81E-07
104	0.17660	4.8056	0.81120E-01	0.21E-06
105	0.17692	4.8143	0.13912E-01	0.12E-07
106	0.17747	4.8292	0.66836E-01	0.77E-08
107	0.17821	4.8493	0.96621E-02	0.19E-07
108	0.17839	4.8542	0.31949E-01	0.13E-07
109	0.17858	4.8595	0.84135E-03	0.32E-07
110	0.17891	4.8684	0.19666E-01	0.32E-09
111	0.17898	4.8702	0.38603E-02	0.13E-08
112	0.17943	4.8826	0.20930E-01	0.26E-07
113	0.17979	4.8925	0.12422	0.18E-06
114	0.17987	4.8946	0.50822E-02	0.12E-08
115	0.18043	4.9097	0.17039	0.24E-08
116	0.18087	4.9216	0.32668E-01	0.22E-08
117	0.18119	4.9305	0.24298	0.72E-07
118	0.18153	4.9397	0.89724E-01	0.52E-07
119	0.18189	4.9494	0.11986	0.22E-10
120	0.18250	4.9660	0.16178E-02	0.65E-09
121	0.18290	4.9770	0.27223E-01	0.27E-07
122	0.18306	4.9814	0.14497E-02	0.33E-08
123	0.18381	5.0016	0.28341E-01	0.27E-07
124	0.18381	5.0018	0.39232E-02	0.10E-08
125	0.18386	5.0031	0.33170E-01	0.15E-07
126	0.18392	5.0048	0.14229E-01	0.24E-08
127	0.18418	5.0117	0.36088E-01	0.30E-07
128	0.18439	5.0176	0.26460E-01	0.23E-07
129	0.18465	5.0246	0.32352E-01	0.11E-08
130	0.18471	5.0262	0.47616E-02	0.35E-09
131	0.18480	5.0286	0.16782E-01	0.24E-09
132	0.18505	5.0356	0.97411E-01	0.13E-07
133	0.18545	5.0463	0.25837E-01	0.51E-08
134	0.18569	5.0529	0.11458	0.33E-07
135	0.18584	5.0570	0.17324E-01	0.94E-08
136	0.18663	5.0785	0.25072E-01	0.14E-07
137	0.18716	5.0928	0.11157E-01	0.12E-08
138	0.18766	5.1065	0.35144E-03	0.59E-08
139	0.18796	5.1146	0.72010E-01	0.39E-08
140	0.18840	5.1266	0.50525E-02	0.25E-08
141	0.18861	5.1323	0.56780E-01	0.20E-07
142	0.18938	5.1532	0.27769E-02	0.45E-09
143	0.18944	5.1549	0.29754E-02	0.77E-09
144	0.18955	5.1578	0.67824E-02	0.58E-08
145	0.18965	5.1605	0.19377E-01	0.22E-08
146	0.18967	5.1612	0.43063E-02	0.41E-12
147	0.19027	5.1775	0.12512E-01	0.98E-08
148	0.19057	5.1856	0.20652E-02	0.27E-08
149	0.19082	5.1924	0.14693E-01	0.81E-08
150	0.19116	5.2018	0.10912E-02	0.20E-07

151	0.19130	5.2055	0.61837E-02	0.32E-08
152	0.19180	5.2192	0.25434E-02	0.11E-09
153	0.19214	5.2283	0.14601E-01	0.60E-08
154	0.19223	5.2308	0.41948E-03	0.13E-08
155	0.19232	5.2334	0.82293E-02	0.37E-08
156	0.19261	5.2412	0.23275E-02	0.28E-08
157	0.19281	5.2466	0.36308E-02	0.90E-08
158	0.19287	5.2482	0.45153E-02	0.61E-09
159	0.19326	5.2589	0.86093E-02	0.84E-08
160	0.19345	5.2640	0.50921E-02	0.12E-07
161	0.19366	5.2699	0.64115E-02	0.18E-10
162	0.19407	5.2809	0.14838E-01	0.51E-09
163	0.19436	5.2888	0.12373E-01	0.38E-07
164	0.19466	5.2970	0.50876E-03	0.58E-10
165	0.19500	5.3061	0.22551E-02	0.87E-09
166	0.19505	5.3076	0.34380E-02	0.66E-07
167	0.19560	5.3227	0.68567E-03	0.46E-07
168	0.19575	5.3266	0.41118E-02	0.26E-08
169	0.19589	5.3305	0.15872E-01	0.52E-08
170	0.19610	5.3360	0.79102E-02	0.12E-08
171	0.19652	5.3476	0.19985E-01	0.62E-08
172	0.19659	5.3494	0.16531E-02	0.25E-07
173	0.19683	5.3560	0.27352E-02	0.54E-08
174	0.19712	5.3638	0.16442E-01	0.24E-09
175	0.19731	5.3692	0.26904E-02	0.69E-08
176	0.19765	5.3784	0.12864E-02	0.99E-09
177	0.19771	5.3799	0.11596E-01	0.31E-07
178	0.19790	5.3851	0.19633E-01	0.31E-07
179	0.19836	5.3977	0.34294E-02	0.17E-08
180	0.19872	5.4074	0.39940E-02	0.54E-10
181	0.19889	5.4121	0.19085E-02	0.18E-08
182	0.19925	5.4219	0.19854E-02	0.28E-09
183	0.19937	5.4252	0.18564E-01	0.12E-08
184	0.19975	5.4354	0.41076E-02	0.45E-09
185	0.19976	5.4357	0.36922E-01	0.15E-08
186	0.19999	5.4419	0.19988E-01	0.86E-10
187	0.20055	5.4572	0.72720E-01	0.15E-06
188	0.20079	5.4636	0.22423E-01	0.45E-08
189	0.20096	5.4685	0.85986E-01	0.44E-07
190	0.20133	5.4784	0.11231E-01	0.33E-08
191	0.20147	5.4822	0.22183E-01	0.17E-10
192	0.20166	5.4873	0.44230E-01	0.16E-08
193	0.20211	5.4996	0.83564E-02	0.98E-09
194	0.20227	5.5039	0.60462E-02	0.60E-08
195	0.20243	5.5084	0.56251E-01	0.18E-09
196	0.20288	5.5206	0.21193E-01	0.65E-07
197	0.20314	5.5276	0.20395E-01	0.49E-07
198	0.20335	5.5334	0.17022E-01	0.60E-07
199	0.20343	5.5357	0.39864E-01	0.35E-09
200	0.20353	5.5383	0.49935E-01	0.11E-08
201	0.20369	5.5428	0.36648E-02	0.15E-08
202	0.20372	5.5434	0.22239E-02	0.81E-08
203	0.20403	5.5519	0.75660E-02	0.63E-08
204	0.20439	5.5617	0.33228E-01	0.96E-07
205	0.20465	5.5689	0.11474E-02	0.49E-08
206	0.20519	5.5836	0.24600E-02	0.27E-09

207	0.20522	5.5843	0.10016E-01	0.65E-10
208	0.20543	5.5901	0.55670E-02	0.15E-07
209	0.20577	5.5994	0.34783E-02	0.20E-07
210	0.20580	5.6001	0.48779E-02	0.83E-08
211	0.20593	5.6037	0.31965E-02	0.16E-07
212	0.20617	5.6103	0.88372E-02	0.10E-08
213	0.20621	5.6113	0.27105E-02	0.22E-09
214	0.20635	5.6150	0.69426E-02	0.10E-07
215	0.20650	5.6192	0.74625E-02	0.29E-07
216	0.20655	5.6206	0.10575E-01	0.30E-07
217	0.20672	5.6251	0.11728E-02	0.32E-07
218	0.20675	5.6260	0.76275E-02	0.19E-08
219	0.20716	5.6371	0.25409E-01	0.19E-07
220	0.20727	5.6401	0.32602E-02	0.10E-07
221	0.20747	5.6455	0.46359E-02	0.94E-09
222	0.20804	5.6611	0.44386E-02	0.53E-08
223	0.20813	5.6635	0.35016E-02	0.27E-08
224	0.20850	5.6736	0.91843E-02	0.57E-08
225	0.20878	5.6812	0.96791E-02	0.18E-08
226	0.20896	5.6860	0.19714E-01	0.16E-08
227	0.20909	5.6897	0.27531E-01	0.19E-07
228	0.20938	5.6974	0.20969E-02	0.29E-10
229	0.20952	5.7013	0.11009E-01	0.17E-08
230	0.20966	5.7051	0.70219E-02	0.62E-07
231	0.20986	5.7107	0.14100E-01	0.74E-07
232	0.20996	5.7134	0.37666E-02	0.50E-09
233	0.21047	5.7272	0.67822E-02	0.33E-08
234	0.21056	5.7295	0.80213E-02	0.17E-06
235	0.21089	5.7385	0.12604E-01	0.11E-06
236	0.21117	5.7462	0.17957E-01	0.15E-07
237	0.21145	5.7540	0.22427E-02	0.23E-07
238	0.21157	5.7572	0.10876E-01	0.35E-08
239	0.21160	5.7580	0.49729E-02	0.25E-06
240	0.21177	5.7625	0.76442E-03	0.97E-10
241	0.21185	5.7647	0.97941E-02	0.10E-07
242	0.21199	5.7686	0.46798E-02	0.41E-06
243	0.21203	5.7697	0.18233E-02	0.17E-06
244	0.21216	5.7732	0.18554E-02	0.11E-06
245	0.21228	5.7765	0.97668E-02	0.31E-06
246	0.21243	5.7806	0.54408E-02	0.56E-07
247	0.21247	5.7816	0.23412E-02	0.23E-06
248	0.21253	5.7833	0.26646E-02	0.97E-06
249	0.21272	5.7884	0.36776E-02	0.30E-06
250	0.21281	5.7908	0.33428E-02	0.98E-07

Transition dipole moments mu (x,y,z) in a.u.
(weak excitations are not printed)

no.	E/eV	f	mu (x,y,z)		
1	1.9811	2.23E-03	-5.33E-02	-6.41E-03	0.20751
2	2.1783	4.40E-03	0.10285	5.15E-03	-0.26792
3	2.2294	2.93E-03	-7.16E-02	0.10194	-0.19525
4	2.3493	1.28E-02	0.18319	-0.17216	0.39971

5	2.3659	6.00E-03	8.06E-02	-0.12343	0.28593
6	2.45	6.03E-03	-9.34E-02	0.10624	0.28374
7	2.4858	3.12E-03	0.11136	-0.12413	-0.1529
8	2.6028	4.86E-03	0.22467	-0.15278	-4.96E-02
9	2.7114	6.69E-03	-0.29282	-8.80E-02	-8.49E-02
10	2.7417	1.03E-02	0.33048	0.11219	-0.17593
11	2.815	0.22723	1.5038	-1.0157	3.98E-02
12	2.939	3.03E-02	-0.4971	0.40848	8.66E-02
13	3.0598	2.53E-03	-7.00E-02	-2.21E-02	0.16834
14	3.0804	9.44E-04	9.57E-02	-2.52E-02	-5.21E-02
15	3.1602	2.26E-03	-0.15134	4.53E-02	6.46E-02
16	3.1809	1.16E-03	-4.55E-02	1.65E-02	-0.11189
17	3.1867	3.69E-03	0.18308	-0.10415	5.42E-02
18	3.231	9.53E-04	7.53E-02	-7.13E-02	-3.58E-02
19	3.254	1.09E-03	-7.80E-03	1.91E-03	0.11646
20	3.3163	8.57E-03	0.10123	-6.10E-03	0.30854
21	3.3227	1.39E-02	-0.30949	0.26163	8.28E-02
22	3.352	1.70E-03	2.80E-02	0.10605	-9.33E-02
23	3.382	2.10E-02	-8.50E-03	-0.14619	-0.48153
24	3.4009	6.84E-03	-0.1278	-0.10729	-0.23292
25	3.417	2.61E-03	0.11782	1.99E-02	-0.13012
26	3.4442	5.77E-03	0.22008	-8.70E-02	-0.11106
27	3.4557	8.94E-03	0.25951	-0.19404	2.43E-02
28	3.4799	3.82E-03	5.38E-02	-0.15361	0.13517
29	3.5263	2.06E-02	0.27284	-0.40487	-2.20E-02
30	3.5668	3.26E-02	0.5219	-0.21426	0.23491
31	3.5817	4.83E-02	-0.61668	0.34144	0.23116
32	3.6257	7.49E-02	0.73532	-0.54833	3.77E-02
33	3.6461	2.06E-02	0.38119	-0.28863	-3.88E-02
34	3.6903	3.06E-02	0.48597	-0.30478	-9.58E-02
35	3.704	1.44E-02	-0.38946	8.52E-02	1.51E-02
36	3.7444	7.93E-03	-0.24724	0.13534	8.38E-02
37	3.7871	2.98E-03	-4.72E-02	-0.11804	0.12644
38	3.8121	7.24E-03	-4.80E-03	-0.25408	0.11366
39	3.8416	9.98E-03	0.29011	8.13E-02	-0.12358
40	3.8587	9.36E-03	-0.21901	-0.2167	6.40E-02
41	3.8793	1.63E-02	-0.32706	0.21317	0.13663
42	3.9521	0.25145	-1.3065	0.90598	-0.26303
43	3.99	2.46E-02	0.12417	-0.16396	-0.45752
44	3.9976	8.30E-03	-0.13717	0.13979	0.21537
45	4.0072	5.61E-02	-0.55093	0.4989	0.13684
46	4.0483	1.08E-02	-0.19361	-2.02E-02	-0.26705
47	4.0554	7.09E-03	0.20576	0.12444	0.11623
48	4.0795	4.90E-02	0.23165	0.22412	0.6218
49	4.089	0.10064	-0.14798	0.35696	0.9248
50	4.1099	1.06E-02	0.20077	0.16917	0.19053
51	4.1402	5.48E-02	-0.37074	2.34E-03	-0.63451
52	4.187	1.97E-03	-4.73E-02	-0.13026	-1.14E-03
53	4.1969	1.12E-02	0.27982	-0.15317	8.67E-02
54	4.2032	1.40E-02	-0.19411	0.12725	-0.28634
55	4.2249	2.19E-03	1.16E-02	-3.86E-02	0.13989
56	4.2481	3.07E-04	2.72E-02	-4.36E-04	-4.70E-02
57	4.2538	3.15E-03	1.47E-02	-9.37E-03	-0.17292
58	4.2682	3.10E-03	7.44E-02	-0.11482	0.10475
59	4.269	2.48E-03	-7.28E-02	5.82E-02	-0.1227
60	4.2874	3.20E-03	-5.65E-02	0.14237	-8.36E-02

61	4.3233	1.45E-03	-8.57E-02	-4.51E-02	-6.59E-02
62	4.3434	1.46E-02	0.34055	-0.13721	-4.60E-02
63	4.3651	6.25E-03	0.11354	-0.20487	-6.02E-02
64	4.3664	3.11E-03	3.54E-02	-0.15676	-5.68E-02
65	4.3735	1.13E-02	3.75E-02	-0.21218	-0.24264
66	4.3806	4.23E-05	1.16E-02	1.59E-02	2.16E-03
67	4.4042	8.37E-03	-2.08E-02	0.16335	0.22456
68	4.4243	5.75E-03	0.15132	-8.26E-02	-0.15261
69	4.4273	2.12E-02	-0.43936	3.11E-02	-3.34E-02
70	4.4312	7.28E-04	-2.18E-02	-7.76E-02	1.45E-02
71	4.4371	4.81E-03	0.14723	-0.13987	-5.52E-02
72	4.4453	5.23E-02	0.58517	-0.3338	-0.16323
73	4.448	8.51E-03	0.12563	-0.24917	-1.38E-02
74	4.4583	9.39E-03	-0.28433	-5.41E-02	4.71E-02
75	4.4669	4.43E-03	-0.14412	-5.40E-02	-0.12948
76	4.4703	1.99E-02	-0.359	0.18632	-0.13487
77	4.482	1.74E-03	0.11147	-3.02E-03	5.87E-02
78	4.4989	1.01E-02	-0.11589	0.25472	-0.11392
79	4.5027	4.20E-02	-0.43575	0.30264	0.31544
80	4.5113	9.62E-03	0.13014	-0.23671	0.11869
81	4.5203	4.84E-03	7.55E-03	-0.1938	-7.80E-02
82	4.5428	2.78E-02	0.4197	-0.22398	-0.15193
83	4.5585	2.05E-02	0.39273	-0.16222	5.78E-02
84	4.5872	1.21E-02	-0.29398	7.49E-02	-0.12485
85	4.5908	5.53E-02	-0.57072	0.3631	-0.18446
86	4.6016	7.08E-02	-0.59815	0.51989	8.20E-03
87	4.6072	2.01E-02	-0.29586	0.28768	-8.59E-02
88	4.6108	1.83E-02	0.29852	-0.19319	0.18931
89	4.6177	9.50E-03	-6.62E-02	-0.10127	-0.26328
90	4.6219	1.97E-02	-0.34576	5.34E-02	-0.22701
91	4.6391	6.55E-02	0.39301	-0.4134	-0.50108
92	4.6548	4.50E-03	7.51E-02	-1.25E-02	-0.18355
93	4.6662	4.08E-02	-0.52005	0.22521	-0.18872
94	4.675	7.35E-02	0.65241	-0.46039	-6.57E-02
95	4.6935	9.64E-02	-0.7768	0.30928	-0.37296
96	4.7045	1.19E-02	0.2896	2.02E-02	0.13866
97	4.7064	1.72E-02	-0.20358	3.60E-02	-0.32615
98	4.7283	1.25E-02	-1.25E-02	0.15444	0.29023
99	4.7478	8.57E-03	0.22413	-1.70E-02	0.15226
100	4.7506	1.47E-02	0.1873	-4.50E-02	0.29833
101	4.7598	2.08E-03	3.47E-02	-2.34E-02	-0.12668
102	4.767	2.91E-02	0.36262	-2.23E-02	0.3419
103	4.7777	5.41E-02	0.61665	-7.00E-02	0.27809
104	4.8056	8.11E-02	-0.64609	0.43035	0.29389
105	4.8143	1.39E-02	0.22746	-0.2546	-3.73E-02
106	4.8292	6.68E-02	-0.51134	0.53257	-0.14071
107	4.8493	9.66E-03	-0.24827	0.1066	9.12E-02
108	4.8542	3.19E-02	0.39673	3.68E-02	0.33152
109	4.8595	8.41E-04	1.64E-02	8.06E-02	1.72E-02
110	4.8684	1.97E-02	0.33586	-0.2118	8.50E-02
111	4.8702	3.86E-03	0.12453	-0.10963	6.95E-02
112	4.8826	2.09E-02	0.32346	-0.24613	-9.88E-02
113	4.8925	0.12422	-0.88672	0.49586	-6.51E-02
114	4.8946	5.08E-03	0.11829	-0.15605	-6.35E-02
115	4.9097	0.17039	0.83569	-0.75188	-0.39093
116	4.9216	3.27E-02	0.42496	-0.19755	0.22653

117	4.9305	0.24298	-1.1967	0.71753	-0.25389
118	4.9397	8.97E-02	-0.70497	0.4862	8.96E-02
119	4.9494	0.11986	-0.84089	0.52972	2.80E-02
120	4.966	1.62E-03	-8.78E-02	5.73E-02	4.80E-02
121	4.977	2.72E-02	-5.12E-02	0.16615	0.43935
122	4.9814	1.45E-03	-4.74E-03	-2.49E-02	0.106
123	5.0016	2.83E-02	0.27852	-0.33296	-0.20701
124	5.0018	3.92E-03	2.27E-02	-5.21E-02	-0.16966
125	5.0031	3.32E-02	-0.39986	0.32698	6.17E-02
126	5.0048	1.42E-02	0.26006	-0.21375	-5.23E-02
127	5.0117	3.61E-02	0.44587	-0.29824	7.85E-02
128	5.0176	2.65E-02	-0.33972	0.29497	-0.11329
129	5.0246	3.24E-02	-0.4661	0.17508	-0.12209
130	5.0262	4.76E-03	6.30E-02	1.12E-02	0.18594
131	5.0286	1.68E-02	0.15286	-0.1306	-0.30951
132	5.0356	9.74E-02	-0.39973	0.55195	0.57023
133	5.0463	2.58E-02	0.38764	-0.12687	0.20645
134	5.0529	0.11458	-0.22891	-0.2165	-0.90902
135	5.057	1.73E-02	-0.31923	0.13684	0.13857
136	5.0785	2.51E-02	0.2414	-0.32679	-0.19089
137	5.0928	1.12E-02	6.26E-02	-0.13088	-0.26149
138	5.1065	3.51E-04	-3.00E-02	-1.55E-02	4.09E-02
139	5.1146	7.20E-02	0.39472	-0.38338	-0.52143
140	5.1266	5.05E-03	8.72E-02	-0.14524	-0.10734
141	5.1323	5.68E-02	-2.62E-02	0.15813	0.6526
142	5.1532	2.78E-03	0.12575	-2.82E-02	-7.34E-02
143	5.1549	2.98E-03	-0.10341	4.90E-02	-0.10232
144	5.1578	6.78E-03	0.1491	-0.14822	9.73E-02
145	5.1605	1.94E-02	-0.23357	0.17823	0.25873
146	5.1612	4.31E-03	-0.15021	-8.10E-02	7.02E-02
147	5.1775	1.25E-02	0.29908	-7.02E-02	6.53E-02
148	5.1856	2.07E-03	3.09E-02	-6.03E-02	-0.10801
149	5.1924	1.47E-02	-0.11322	-3.50E-02	-0.31853
150	5.2018	1.09E-03	2.22E-02	3.78E-02	8.15E-02
151	5.2055	6.18E-03	0.19061	-9.58E-02	5.46E-02
152	5.2192	2.54E-03	3.87E-02	-7.54E-02	-0.11276
153	5.2283	1.46E-02	-0.1992	-1.60E-02	-0.27212
154	5.2308	4.19E-04	3.76E-02	2.68E-02	3.38E-02
155	5.2334	8.23E-03	-4.70E-02	-1.68E-02	-0.24838
156	5.2412	2.33E-03	-0.11305	2.82E-02	6.75E-02
157	5.2466	3.63E-03	-8.54E-02	0.11681	8.55E-02
158	5.2482	4.52E-03	0.1608	-9.50E-02	-1.52E-02
159	5.2589	8.61E-03	7.63E-02	6.79E-02	0.23746
160	5.264	5.09E-03	-5.92E-02	-2.71E-02	-0.18772
161	5.2699	6.41E-03	0.14552	-0.15807	5.91E-02
162	5.2809	1.48E-02	0.2434	-0.17856	-0.1535
163	5.2888	1.24E-02	0.18237	-0.13051	-0.2126
164	5.297	5.09E-04	-5.23E-02	-3.28E-02	-1.04E-02
165	5.3061	2.26E-03	0.11242	-4.93E-02	-4.77E-02
166	5.3076	3.44E-03	-0.122	0.105	-2.30E-02
167	5.3227	6.86E-04	6.90E-02	1.19E-02	-1.89E-02
168	5.3266	4.11E-03	-7.01E-02	9.65E-02	-0.13144
169	5.3305	1.59E-02	-9.72E-02	0.12741	0.30962
170	5.336	7.91E-03	0.10846	-6.44E-02	-0.21117
171	5.3476	2.00E-02	0.33738	-0.19509	2.55E-02
172	5.3494	1.65E-03	-0.10779	2.41E-02	2.03E-02

173	5.356	2.74E-03	6.96E-02	-0.10156	-7.54E-02
174	5.3638	1.64E-02	-0.27578	-7.55E-02	-0.20825
175	5.3692	2.69E-03	0.12724	-1.74E-02	-6.29E-02
176	5.3784	1.29E-03	1.60E-02	5.01E-02	-8.36E-02
177	5.3799	1.16E-02	-0.23197	0.1507	0.10707
178	5.3851	1.96E-02	-1.55E-02	2.92E-02	0.38434
179	5.3977	3.43E-03	-0.14607	4.72E-02	-4.86E-02
180	5.4074	3.99E-03	-9.27E-02	0.12341	7.96E-02
181	5.4121	1.91E-03	0.11088	-2.39E-02	-3.91E-02
182	5.4219	1.99E-03	-6.04E-04	-2.86E-02	-0.11886
183	5.4252	1.86E-02	0.12587	1.33E-02	0.35163
184	5.4354	4.11E-03	0.16462	-1.89E-02	5.82E-02
185	5.4357	3.69E-02	-7.51E-02	-8.39E-02	-0.51435
186	5.4419	2.00E-02	0.23287	-0.17478	0.25523
187	5.4572	7.27E-02	-0.18883	-0.19712	-0.68512
188	5.4636	2.24E-02	-0.3891	4.21E-02	-0.11977
189	5.4685	8.60E-02	-0.22342	-0.24568	-0.72906
190	5.4784	1.12E-02	0.25024	-0.14469	1.09E-02
191	5.4822	2.22E-02	8.91E-02	-0.12792	-0.37532
192	5.4873	4.42E-02	0.22215	0.15095	0.50682
193	5.4996	8.36E-03	0.13673	-4.74E-02	-0.20268
194	5.5039	6.05E-03	-0.18518	9.95E-02	2.53E-02
195	5.5084	5.63E-02	0.23799	-0.3279	-0.50265
196	5.5206	2.12E-02	-0.35699	0.148	-8.57E-02
197	5.5276	2.04E-02	0.20006	-0.33173	2.31E-02
198	5.5334	1.70E-02	0.11423	1.84E-02	0.33493
199	5.5357	3.99E-02	0.10347	-0.17162	-0.50376
200	5.5383	4.99E-02	7.29E-02	-5.88E-02	-0.59938
201	5.5428	3.66E-03	8.10E-02	-8.99E-02	0.11112
202	5.5434	2.22E-03	8.20E-02	-6.23E-02	-7.59E-02
203	5.5519	7.57E-03	0.19191	-0.10354	-8.98E-02
204	5.5617	3.32E-02	-3.09E-02	0.24281	0.42889
205	5.5689	1.15E-03	-1.04E-02	7.37E-02	-5.36E-02
206	5.5836	2.46E-03	3.28E-02	3.78E-02	0.1244
207	5.5843	1.00E-02	-1.76E-02	-3.38E-02	0.26787
208	5.5901	5.57E-03	-2.88E-02	-4.69E-02	0.19395
209	5.5994	3.48E-03	6.07E-02	-8.12E-02	-0.12284
210	5.6001	4.88E-03	0.15115	-2.84E-03	0.11269
211	5.6037	3.20E-03	-0.12216	7.74E-02	4.86E-02
212	5.6103	8.84E-03	-0.1976	0.11334	-0.11136
213	5.6113	2.71E-03	-4.41E-02	-1.59E-02	-0.13234
214	5.615	6.94E-03	0.19299	-3.66E-02	-0.10902
215	5.6192	7.46E-03	0.18198	-8.04E-02	0.12093
216	5.6206	1.06E-02	-0.24439	8.10E-02	-0.10249
217	5.6251	1.17E-03	5.35E-02	4.20E-03	-7.51E-02
218	5.626	7.63E-03	-0.16805	0.13676	-9.16E-02
219	5.6371	2.54E-02	-0.12868	7.23E-02	-0.40273
220	5.6401	3.26E-03	0.14772	-4.21E-02	-1.40E-03
221	5.6455	4.64E-03	-4.88E-02	-8.70E-02	-0.15351
222	5.6611	4.44E-03	8.70E-02	-0.1406	-6.82E-02
223	5.6635	3.50E-03	0.11657	-1.68E-02	0.10661
224	5.6736	9.18E-03	-5.08E-03	1.45E-02	0.25659
225	5.6812	9.68E-03	9.30E-02	-5.82E-03	-0.24671
226	5.686	1.97E-02	0.14404	-9.50E-02	0.33427
227	5.6897	2.75E-02	-5.34E-02	8.73E-02	-0.43246
228	5.6974	2.10E-03	6.50E-02	-0.10069	-2.55E-02

229	5.7013	1.10E-02	0.1666	-2.60E-02	0.22448
230	5.7051	7.02E-03	0.10137	-9.01E-02	0.17845
231	5.7107	1.41E-02	0.14967	9.41E-02	0.26368
232	5.7134	3.77E-03	6.12E-02	2.05E-02	-0.15081
233	5.7272	6.78E-03	-9.92E-02	-9.85E-02	-0.16969
234	5.7295	8.02E-03	0.21398	-0.10656	-2.17E-04
235	5.7385	1.26E-02	-0.11333	4.95E-02	0.27268
236	5.7462	1.80E-02	0.29228	-9.08E-02	-0.18408
237	5.754	2.24E-03	-7.37E-02	3.05E-03	0.10233
238	5.7572	1.09E-02	0.21113	1.37E-02	0.17983
239	5.758	4.97E-03	-6.81E-03	9.37E-02	0.16255
240	5.7625	7.64E-04	-6.87E-02	2.55E-02	-6.44E-03
241	5.7647	9.79E-03	-8.47E-02	2.18E-02	-0.24839
242	5.7686	4.68E-03	0.11158	4.29E-03	0.14368
243	5.7697	1.82E-03	-7.29E-02	-5.37E-02	6.86E-02
244	5.7732	1.86E-03	-8.26E-02	-1.02E-03	-7.93E-02
245	5.7765	9.77E-03	0.21915	-0.13014	-6.37E-02
246	5.7806	5.44E-03	9.22E-02	3.60E-02	0.16917
247	5.7816	2.34E-03	-8.96E-02	6.29E-02	-6.75E-02
248	5.7833	2.66E-03	0.13263	-3.11E-02	1.58E-02
249	5.7884	3.68E-03	-1.39E-02	-7.11E-02	-0.1438
250	5.7908	3.34E-03	0.11584	-9.98E-02	1.33E-02

Rotatory strengths R in 10**(-40) esu**2 * cm**2 ,
(multiply by 1.07827 to obtain reduced rotatory strengths),
magnetic transition dipole vectors m in a.u.:

no.	R	m (x,y,z)		
1	-0.42205	0.25461	-5.52E-02	5.50E-02
2	21.26	0.4597	1.3905	-0.13345
3	1.2707	-0.24835	0.10794	0.1198
4	-0.25047	0.33804	-0.48374	-0.36594
5	20.373	-0.40637	-1.3348	-0.15946
6	0.33245	-2.22E-02	-0.42417	0.15648
7	-4.8222	6.64E-02	0.48072	-0.2081
8	-10.503	-7.69E-02	0.28217	-0.31912
9	159.17	-1.474	-3.0179	0.25878
10	172.41	1.012	3.0285	-0.32507
11	-154.15	1.425	2.6478	-2.7055
12	-17.759	-0.5314	-1.061	1.0841
13	0.20451	0.2778	-0.2498	8.78E-02
14	-0.67996	-4.52E-02	0.43926	-0.24014
15	-1.7361	-2.19E-02	-0.54199	0.21501
16	0.19794	5.95E-02	0.16743	-6.98E-03
17	-4.5616	-2.84E-02	-1.95E-02	-0.29876
18	-0.31848	8.02E-02	0.23965	-0.27076
19	1.2802	-0.19477	-0.63887	4.41E-02
20	-8.1265	-0.17641	-1.0132	-7.39E-02
21	-10.908	-0.91676	-1.5468	0.9024
22	13.634	8.77E-03	0.66273	0.13601
23	14.796	-0.35075	0.29754	-0.2145
24	37.08	-0.72675	-0.97029	0.17036
25	10.687	0.17418	1.3338	1.31E-02
26	-6.1801	8.20E-02	1.0086	-0.39119

27	-12.36	0.13436	0.37142	-0.62743
28	48.671	-0.65926	-1.7889	-0.24281
29	50.914	0.14286	-0.3812	-1.0328
30	8.4994	1.3881	2.1076	-1.0081
31	-36.942	-0.69948	-2.569	1.2506
32	-52.654	0.5592	1.0305	-1.8458
33	-12.49	0.48202	0.97212	-1.1312
34	-16.046	0.81578	1.8548	-1.0522
35	7.5339	-0.35991	-1.3416	0.40537
36	10.813	-0.54725	-1.0999	0.70956
37	26.257	-0.16133	-1.2224	-0.32045
38	26.407	0.26518	-0.79302	-0.77597
39	116.33	0.8677	3.0249	3.37E-02
40	161.34	-0.48827	-2.7419	-0.26034
41	-6.892	-0.67997	-1.7412	0.87499
42	-126.41	-2.0603	-2.5936	3.3396
43	2.8741	0.34462	1.9789	-0.6423
44	11.074	-9.79E-02	-0.66846	0.5896
45	9.3138	-1.0189	-1.52	1.7286
46	1.0522	-2.11E-02	-9.01E-02	5.41E-03
47	10.296	-0.25672	0.39912	0.40294
48	49.586	0.10812	-0.54552	0.49464
49	-15.185	-0.13035	-2.8417	1.0063
50	-5.6195	-0.4907	0.17122	0.23993
51	-13.919	-9.40E-02	0.54012	0.14995
52	15.137	0.23071	-0.57559	-0.12717
53	-15.558	0.34823	0.6745	-0.69379
54	-9.758	2.79E-02	0.72979	0.44994
55	-3.3911	0.33808	0.21587	-7.14E-02
56	0.89199	-3.12E-02	0.19511	-0.10029
57	-6.625	-9.49E-02	0.39407	0.13313
58	15.676	-0.14069	-0.94623	-0.30242
59	-0.53923	0.10673	0.54251	0.21246
60	8.0214	-0.37314	0.26419	0.29514
61	18.868	-0.47394	-1.0149	9.64E-02
62	35.7	1.5896	3.1329	-0.86943
63	8.5004	0.17536	0.1524	-0.7874
64	3.5692	0.31759	0.15409	-0.49399
65	63.351	-0.59562	-0.68494	-0.60062
66	1.5082	0.15005	0.30426	-9.17E-02
67	20.315	-0.12051	-0.24073	0.54771
68	-4.4294	-9.23E-02	0.69216	-0.34326
69	68.418	-0.90249	-2.8369	0.54471
70	0.94489	0.30573	-0.17702	-0.21062
71	-1.5534	0.30308	0.5913	-0.57008
72	-7.3598	1.4178	3.3557	-1.5884
73	21.965	0.26212	-0.19143	-0.91054
74	65.048	-0.49426	-2.3136	0.2177
75	26.97	-0.50048	-1.1537	0.15434
76	-18.344	-0.42065	-0.62165	0.83789
77	4.6955	0.27047	0.47298	-0.14986
78	58.43	-0.15449	1.1679	0.59275
79	-27.52	-8.18E-02	-1.7163	1.1635
80	31.367	-2.25E-03	-0.93295	-0.73702
81	-8.9728	0.62355	0.47873	-0.64118
82	-3.5324	1.1241	2.9558	-1.1535

83	-18.004	0.4855	1.3297	-0.88785
84	21.039	-0.88278	-1.485	0.47269
85	-30.296	-0.83786	-0.90572	1.5063
86	-27.947	-1.2064	-1.6528	2.3315
87	-18.027	-0.47253	-0.41688	1.1217
88	-13.398	0.59137	0.33534	-0.89056
89	22	-0.1054	-9.21E-02	-0.29255
90	7.0262	-0.30865	-0.31641	0.2644
91	5.2145	0.57446	2.4375	-1.6046
92	4.2564	0.13035	1.5584	-0.1515
93	-20.914	-0.81699	-1.3393	1.1232
94	-34.33	1.0786	2.1244	-1.9588
95	-64.722	-1.1279	-1.7352	1.6464
96	-2.267	-1.02E-02	0.88176	-0.17666
97	-11.118	-2.69E-02	0.60746	0.22847
98	3.4008	-0.18381	-0.82426	0.48041
99	4.5066	0.27124	0.50714	-0.2172
100	-8.0832	0.26019	-0.38501	-0.33635
101	2.4689	6.86E-02	0.59774	-0.17439
102	38.318	0.82208	1.0279	-0.3295
103	56.525	0.9746	2.3347	-0.71106
104	-41.594	-1.0384	-3.3766	2.0611
105	-15.207	1.0474	1.3242	-0.92257
106	50.205	-1.0769	-6.66E-02	2.1477
107	11.839	-0.62989	-1.6346	0.74631
108	59.618	0.76363	1.6595	-0.33502
109	-8.1132	-0.5839	-0.34687	0.18259
110	-17.376	0.74978	1.073	-1.156
111	6.5719	-2.94E-02	-0.48087	-0.3049
112	-5.6188	0.26744	0.80708	-0.89359
113	-24.248	-2.1041	-3.6269	2.6122
114	7.9023	0.30307	0.19027	-0.43069
115	-31.983	1.5252	3.5789	-3.2759
116	-37.587	0.54756	0.75933	-1.0689
117	-190.52	-2.1684	-3.4947	3.528
118	-45.092	-1.2638	-2.6368	2.2309
119	-116.12	-1.1923	-2.9532	2.4646
120	-2.1462	-4.97E-02	-0.43845	0.24326
121	10.371	-5.94E-02	-1.4777	0.65202
122	2.1272	0.4083	-0.307	3.12E-02
123	12.056	0.82462	1.3839	-1.3635
124	1.3624	0.23365	0.67055	-0.2088
125	-40.771	-0.54421	-1.4566	1.388
126	-15.577	0.50631	1.1824	-1.0521
127	-24.504	0.90923	1.328	-1.443
128	-0.18913	-0.98025	-0.66253	1.2215
129	-54.186	-0.30256	-1.3217	1.1426
130	2.4636	1.58E-02	-0.29165	6.84E-02
131	4.7669	0.16258	1.5085	-0.62159
132	18.91	-0.9433	-2.7752	2.1657
133	-19.823	0.45568	0.84162	-0.74574
134	-1.5571	-0.12718	1.5704	-0.33473
135	-4.8253	-0.23998	-1.5157	0.79624
136	6.2962	0.95344	1.3586	-1.26
137	5.6997	-9.83E-03	0.81951	-0.50498
138	-2.2921	0.33649	-5.07E-02	-1.05E-02

139	-56.983	-0.15383	2.8372	-1.7389
140	-2.2977	7.35E-02	0.47171	-0.48774
141	2.4111	0.32848	-1.7744	0.45879
142	-2.6513	-2.53E-02	0.75733	-0.18062
143	-1.0477	-0.3245	-0.14136	0.30375
144	-7.4548	0.40132	1.71E-02	-0.91356
145	-22.176	-2.75E-02	-1.6323	0.73602
146	11.98	0.14715	-0.96081	-7.00E-02
147	-10.677	0.18507	0.97332	-0.49507
148	0.53845	0.22705	0.44572	-0.20485
149	-3.1199	-0.2813	0.58399	7.73E-02
150	0.41195	-0.16298	-0.14606	0.13361
151	2.5412	0.39361	0.37142	-0.52501
152	2.3784	0.19689	0.40488	-0.29261
153	7.08E-02	-0.27293	-0.18399	0.20953
154	0.18597	-6.65E-02	-2.79E-02	0.11924
155	6.0895	-8.02E-02	0.55836	-0.12666
156	-1.0817	5.03E-02	-0.59127	0.26312
157	-1.7363	-0.29508	-0.65607	0.51535
158	-9.3866	5.63E-02	0.59298	-0.49185
159	1.7477	-6.04E-02	-0.32201	0.14274
160	1.9735	3.72E-02	0.30279	-0.1001
161	-0.90286	0.55047	0.32031	-0.56318
162	-24.813	0.14322	1.4878	-0.81782
163	-6.7326	0.17871	1.6491	-0.7247
164	1.9767	9.03E-02	-0.37363	-8.04E-02
165	-5.8358	-5.41E-02	0.45619	-8.01E-02
166	0.4851	-0.58418	-0.51699	0.64926
167	-0.94775	-0.14431	0.4292	-4.45E-02
168	-7.6934	-0.58286	6.69E-02	0.60845
169	-0.29594	-0.18537	-1.6601	0.62093
170	3.0799	6.84E-02	1.2758	-0.41611
171	-5.7833	0.76219	1.3179	-0.96267
172	-0.26341	-6.07E-02	-0.60029	0.33561
173	1.6247	8.65E-02	0.16329	-0.23158
174	12.246	-1.87E-02	-0.80747	6.79E-02
175	-1.5957	8.07E-02	1.0142	-9.41E-03
176	-0.86486	-0.32105	0.30652	0.16612
177	-16.254	-0.15419	-1.327	0.88969
178	2.9587	9.78E-03	-1.6344	0.15703
179	-12.451	0.1376	-0.35521	0.32778
180	0.23566	-0.29925	-0.65336	0.67737
181	4.6896	0.2671	0.70831	-0.18432
182	4.0386	-0.11123	0.54775	-0.27536
183	1.3328	-8.98E-02	-0.75781	7.69E-02
184	-10.157	-0.12437	0.49684	-0.22727
185	30.713	-0.32589	1.5281	-0.4551
186	-18.756	0.41132	-1.57E-02	-0.69779
187	15.466	0.26742	1.6643	-0.64834
188	-33.837	8.23E-02	-1.2382	0.49589
189	61.737	0.22955	1.4815	-0.92882
190	-15.232	0.27341	0.87081	-0.64546
191	-6.4888	-0.13885	1.4906	-0.46768
192	16.019	-8.85E-02	-0.62663	0.35949
193	3.99E-02	-1.17E-02	1.4616	-0.35059
194	-4.6593	-0.28656	-0.82898	0.38327

195	2.4566	0.25572	2.3939	-1.4612
196	-15.67	-0.50602	-1.153	0.8923
197	-1.1312	0.85133	0.42193	-1.5206
198	-17.829	-0.17362	-0.98214	-0.11263
199	8.8779	7.93E-02	2.3598	-0.86243
200	10.221	-0.31215	2.9741	-0.40196
201	3.1443	0.44447	-0.2991	-0.44594
202	1.8853	0.13068	0.45928	-0.34107
203	-13.767	0.30947	1.7978	-0.76081
204	24.182	-0.52005	-1.3394	0.95998
205	-2.6125	-0.50646	8.80E-02	0.42517
206	1.8089	-3.29E-02	-0.35122	0.1771
207	-1.9896	0.38581	-1.1983	-0.15716
208	0.36947	0.25889	-1.0062	-0.19705
209	0.99208	0.21868	0.75139	-0.42275
210	-3.6379	-6.95E-02	0.37434	-3.43E-02
211	-7.241	-7.23E-02	-0.79456	0.45165
212	-3.1123	-0.60821	-0.46095	0.72864
213	2.6426	0.22159	0.52935	-0.22231
214	1.9672	6.66E-02	1.1502	-0.34483
215	-6.9192	0.5905	0.74767	-0.63419
216	-7.0463	-0.41276	-0.85891	0.59712
217	4.6722	0.12118	0.74849	-0.13582
218	3.4564	-0.65489	-0.28953	0.60897
219	-1.7154	-0.48577	1.0922	0.36937
220	0.26856	0.13014	0.4332	-0.10776
221	8.3828	0.12318	0.29755	-0.43944
222	6.6679	0.56949	0.52862	-0.77716
223	3.5858	2.59E-02	-4.08E-02	0.10796
224	-0.43354	0.1809	-1.1733	6.26E-02
225	7.5909	-1.23E-02	1.5705	-0.17225
226	13.881	0.68673	-0.92807	-0.38354
227	3.083	-0.66708	1.7455	0.40461
228	-3.5684	0.35296	0.47122	-0.36619
229	-10.008	9.97E-02	-0.20286	-0.28662
230	-3.7923	0.3511	-0.25971	-0.42073
231	-9.1162	-0.16671	-0.35438	7.44E-02
232	1.8254	-6.56E-02	0.74007	2.25E-02
233	5.088	0.43629	0.22379	-0.51213
234	1.4136	0.41223	0.77256	-0.51873
235	-19.702	0.16645	-1.3408	6.13E-03
236	-24.829	0.1158	2.3096	-0.38289
237	-4.3438	0.44719	-0.38352	0.1533
238	10.827	0.24772	0.64374	-8.43E-02
239	2.0052	-0.3095	-0.56961	0.36778
240	-3.6632	0.11132	-0.26815	0.16248
241	0.78376	-0.38575	0.5307	0.16469
242	2.6757	0.27888	0.342	-0.14778
243	-1.3414	0.1871	-0.54737	-0.3123
244	-4.0063	-2.31E-02	-0.40042	0.24353
245	2.92E-02	0.45304	1.0712	-0.63211
246	5.9867	0.18241	-3.17E-02	5.75E-02
247	-4.174	-0.2401	-0.11839	0.47108
248	1.7446	0.24897	0.77188	-0.1035
249	-4.3274	0.3474	0.39112	-9.93E-02
250	-5.8426	0.2877	0.50426	-0.58384

(*R,R*)-**76**·py *P*

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	C	5.3114	6.6223	1.7460	6.00	4.00	12.0000
2	C	4.9597	7.3039	2.8671	6.00	4.00	12.0000
3	C	6.9576	4.1214	-2.0876	6.00	4.00	12.0000
4	C	7.7507	3.5582	-0.9324	6.00	4.00	12.0000
5	C	6.6724	6.4843	6.6337	6.00	4.00	12.0000
6	C	7.2251	6.2829	7.8865	6.00	4.00	12.0000
7	C	8.1967	5.3146	8.1174	6.00	4.00	12.0000
8	C	8.7726	5.1002	9.3881	6.00	4.00	12.0000
9	C	9.7380	4.1488	9.5602	6.00	4.00	12.0000
10	C	10.1777	3.3740	8.4684	6.00	4.00	12.0000
11	N	6.2159	1.8258	2.6442	7.00	5.00	14.0031
12	C	5.4885	0.9457	1.9555	6.00	4.00	12.0000
13	C	5.5442	6.9754	4.1040	6.00	4.00	12.0000
14	C	4.3861	0.3112	2.4963	6.00	4.00	12.0000
15	C	4.0281	0.5930	3.8048	6.00	4.00	12.0000
16	C	4.7897	1.4983	4.5238	6.00	4.00	12.0000
17	C	5.8717	2.0958	3.9082	6.00	4.00	12.0000
18	C	9.6389	3.5606	7.2267	6.00	4.00	12.0000
19	C	8.6296	4.5239	7.0138	6.00	4.00	12.0000
20	C	8.0582	4.7149	5.7519	6.00	4.00	12.0000
21	C	7.0816	5.6764	5.5168	6.00	4.00	12.0000
22	C	6.5820	4.9634	0.5729	6.00	4.00	12.0000
23	N	7.3558	3.9368	0.4040	7.00	5.00	14.0031
24	C	5.1699	7.7426	5.2391	6.00	4.00	12.0000
25	C	10.6014	-0.2169	3.6017	6.00	4.00	12.0000
26	C	9.9320	0.5499	2.5896	6.00	4.00	12.0000
27	O	9.0932	1.4899	2.8934	8.00	6.00	15.9949
28	C	10.1946	0.2421	1.2244	6.00	4.00	12.0000
29	C	11.2232	-0.6523	0.8809	6.00	4.00	12.0000
30	C	11.9562	-1.2746	1.8403	6.00	4.00	12.0000
31	C	11.6353	-1.0902	3.1987	6.00	4.00	12.0000
32	C	12.3669	-1.8323	4.1639	6.00	4.00	12.0000
33	C	12.0723	-1.7595	5.4788	6.00	4.00	12.0000
34	C	10.9942	-0.9597	5.9354	6.00	4.00	12.0000
35	Fe	7.9647	2.6893	1.9159	26.00	16.00	55.9349
36	C	10.6565	-0.9688	7.2779	6.00	4.00	12.0000
37	C	9.5557	-0.2713	7.7648	6.00	4.00	12.0000
38	C	9.1917	-0.2804	9.1292	6.00	4.00	12.0000
39	C	8.0811	0.3901	9.5576	6.00	4.00	12.0000
40	C	7.2810	1.0995	8.6390	6.00	4.00	12.0000
41	C	7.6174	1.1371	7.3156	6.00	4.00	12.0000
42	C	8.7614	0.4622	6.8358	6.00	4.00	12.0000
43	C	9.1337	0.5120	5.4897	6.00	4.00	12.0000
44	C	10.2346	-0.1781	4.9990	6.00	4.00	12.0000
45	C	9.4418	0.7789	0.1570	6.00	4.00	12.0000

46	C	5.7085	7.5080	6.4536	6.00	4.00	12.0000
47	N	8.4503	1.6155	0.2393	7.00	5.00	14.0031
48	C	6.4894	5.9311	4.2221	6.00	4.00	12.0000
49	C	6.8285	5.1880	3.0420	6.00	4.00	12.0000
50	O	7.6671	4.1979	3.0863	8.00	6.00	15.9949
51	C	6.2351	5.5657	1.8035	6.00	4.00	12.0000
52	H	4.8835	6.8828	0.7710	1.00	1.00	1.0078
53	H	4.2365	8.1239	2.8311	1.00	1.00	1.0078
54	H	4.4344	8.5403	5.0931	1.00	1.00	1.0078
55	H	5.4245	8.1094	7.3236	1.00	1.00	1.0078
56	H	6.7320	1.7050	-0.9138	1.00	1.00	1.0078
57	C	7.7916	2.0413	-0.9754	6.00	4.00	12.0000
58	H	8.3731	0.4564	-2.3232	1.00	1.00	1.0078
59	H	9.4140	1.8954	-2.3680	1.00	1.00	1.0078
60	H	6.5363	1.7123	-3.4176	1.00	1.00	1.0078
61	H	8.0040	1.7714	-4.4057	1.00	1.00	1.0078
62	H	6.9173	4.0216	-4.2451	1.00	1.00	1.0078
63	H	8.5389	4.0277	-3.5367	1.00	1.00	1.0078
64	H	5.8972	3.8156	-1.9836	1.00	1.00	1.0078
65	H	6.9765	5.2245	-2.0654	1.00	1.00	1.0078
66	H	8.8084	3.8838	-1.0527	1.00	1.00	1.0078
67	H	6.8918	6.9184	8.7165	1.00	1.00	1.0078
68	C	8.3607	1.5596	-2.2888	6.00	4.00	12.0000
69	H	8.4336	5.7183	10.2271	1.00	1.00	1.0078
70	H	10.1787	3.9885	10.5487	1.00	1.00	1.0078
71	H	10.9478	2.6106	8.6178	1.00	1.00	1.0078
72	H	5.8192	0.7520	0.9282	1.00	1.00	1.0078
73	H	3.8147	-0.3989	1.8923	1.00	1.00	1.0078
74	H	3.1591	0.1093	4.2621	1.00	1.00	1.0078
75	H	4.5524	1.7507	5.5613	1.00	1.00	1.0078
76	H	6.4988	2.8351	4.4243	1.00	1.00	1.0078
77	H	9.9696	2.9535	6.3755	1.00	1.00	1.0078
78	H	8.4157	4.1147	4.9126	1.00	1.00	1.0078
79	C	7.5673	2.1150	-3.4528	6.00	4.00	12.0000
80	H	6.1418	5.4551	-0.3127	1.00	1.00	1.0078
81	H	11.4168	-0.8332	-0.1827	1.00	1.00	1.0078
82	H	12.7694	-1.9586	1.5818	1.00	1.00	1.0078
83	H	13.1740	-2.4781	3.8026	1.00	1.00	1.0078
84	H	12.6343	-2.3410	6.2169	1.00	1.00	1.0078
85	H	11.2609	-1.5696	7.9687	1.00	1.00	1.0078
86	H	9.8161	-0.8431	9.8327	1.00	1.00	1.0078
87	H	7.8078	0.3778	10.6171	1.00	1.00	1.0078
88	H	6.3971	1.6363	8.9953	1.00	1.00	1.0078
89	H	7.0125	1.7055	6.5988	1.00	1.00	1.0078
90	C	7.5149	3.6264	-3.4065	6.00	4.00	12.0000
91	H	8.5342	1.0989	4.7894	1.00	1.00	1.0078
92	H	9.7484	0.4107	-0.8374	1.00	1.00	1.0078

TOTAL BONDING ENERGIES FROM VARIOUS XC FUNCTIONALS

XC	Energy Functional	hartree	eV	kcal/mol
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FR:	KCIS-modified	-18.20806707	-495.4667144	-11425.73579
FR:	KCIS-original	-18.18107753	-494.7322918	-11408.7996

FR:	PKZB	-42.97073925	-1169.293309	-26964.54883
FR:	VS98	1.082512609	29.45666685	679.2869893
FR:	LDA(VWN)	-24.61468263	-669.799594	-15445.94818
FR:	PW91	-22.94515472	-624.3694279	-14398.30348
FR:	BLYP	-22.53368947	-613.1728889	-14140.10511
FR:	PBE	-22.84194587	-621.5609725	-14333.53895
FR:	RPBE	-21.98291288	-598.1854954	-13794.48755
FR:	revPBE	-22.09138274	-601.1371106	-13862.55343
FR:	OLYP	-21.92410734	-596.5853153	-13757.58651
FR:	FT97	-21.63387612	-588.6877217	-13575.46365
FR:	BLAP3	-15.45362904	-420.5146422	-9697.299653
FR:	HCTH/93	-22.04827573	-599.9641091	-13835.50337
FR:	HCTH/120	-22.40072549	-609.5547549	-14056.66895
FR:	HCTH/147	-22.37695571	-608.9079464	-14041.75319
FR:	HCTH/407	-22.18991725	-603.818371	-13924.38477
FR:	BmTau1	-13.84254567	-376.6748329	-8686.329464
FR:	BOP	-21.30161612	-579.6464673	-13366.96734
FR:	PKZBx-KCIScor	-17.96484441	-488.8482893	-11273.11126
FR:	VS98-x(xc)	-19.81975747	-539.3230416	-12437.08689
FR:	VS98-x-only	-21.91151998	-596.2427958	-13749.68783
FR:	Becke00	-23.24711379	-632.5861523	-14587.78568
FR:	Becke00x(xc)	-21.26643147	-578.6890441	-13344.88863
FR:	Becke00-x-only	-23.39363345	-636.5731552	-14679.72817
FR:	Becke88x+BR89c	-22.72833425	-618.469443	-14262.24657
FR:	OLAP3	-15.78679008	-429.5804153	-9906.361383
FR:	TPSS	1403899.447	38202047.67	880960296.0
FR:	mPBE	-22.61174285	-615.2968296	-14189.08436
FR:	OPBE	-22.84356754	-621.6051003	-14334.55656
FR:	OPerdew	-22.86685051	-622.238662	-14349.16684
FR:	mPBEKCIS	-18.70834593	-509.0799948	-11739.66555
FR:	mPW	-22.59210955	-614.7625803	-14176.76428
FR:	tau-HCTH	-21.67270983	-589.7444409	-13599.83218
FR:	XLYP	-21.49857214	-585.0059132	-13490.55912
FR:	KT1	-23.28633124	-633.6533136	-14612.39501
FR:	KT2	-24.13333431	-656.7014398	-15143.89751
FR:	TPSSh	1403897.842	38202004.02	880959289.4
FR:	B3LYP(VWN5)	-25.81884456	-702.5665074	-16201.57128
FR:	O3LYP(VWN5)	-25.28853246	-688.135981	-15868.79538
FR:	KMLYP(VWN5)	-34.14884595	-929.2373784	-21428.72662
FR:	PBE0	-27.82333998	-757.111603	-17459.41128
FR:	B3LYP*(VWN5)	-24.98691368	-679.9285163	-15679.52671
FR:	BHandH	-33.52875332	-912.3637992	-21039.61257
FR:	BHandHLYP	-31.71950421	-863.1316259	-19904.2915
FR:	B97	-26.02525512	-708.1832245	-16331.09587
FR:	B97-1	-26.47999301	-720.5572721	-16616.44824
FR:	B97-2	-26.61931543	-724.348428	-16703.87438
FR:	mPBE0KCIS	-23.74729079	-646.1966611	-14901.65152
FR:	mPBE1KCIS	-22.27591889	-606.1585945	-13978.35162
FR:	B1LYP(VWN5)	-26.65522526	-725.325584	-16726.40814
FR:	B1PW91(VWN5)	-27.55611317	-749.8399914	-17291.7239
FR:	mPW1PW	-27.63131967	-751.8864645	-17338.9167
FR:	mPW1K	-31.21923727	-849.5186701	-19590.36922
FR:	tau-HCTH-hybrid[56]	-25.43433938	-692.1035889	-15960.2906
FR:	X3LYP(VWN5)	-26.26995363	-714.8418097	-16484.64652
FR:	OPBE0	-27.82455623	-757.1446989	-17460.17448

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G E O M E T R Y
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ATOMS

=====		X Y Z (Angstrom)			CHARGE Nucl	+Core	At.Mass
1	C	7.7189	-1.2452	15.6064	6.00	4.00	12.0000
2	C	7.0064	-1.9677	13.4371	6.00	4.00	12.0000
3	C	7.1899	-2.8737	12.3589	6.00	4.00	12.0000
4	C	6.4632	-2.7747	11.2267	6.00	4.00	12.0000
5	C	5.4679	-1.7740	11.0887	6.00	4.00	12.0000
6	Fe	4.9252	2.6355	15.3426	26.00	16.00	55.9349
7	C	4.7225	-1.7125	9.9242	6.00	4.00	12.0000
8	C	3.7070	-0.7782	9.7462	6.00	4.00	12.0000
9	C	2.9345	-0.7071	8.5671	6.00	4.00	12.0000
10	C	1.9288	0.2107	8.4511	6.00	4.00	12.0000
11	C	1.6455	1.0950	9.5107	6.00	4.00	12.0000
12	C	2.3792	1.0516	10.6629	6.00	4.00	12.0000
13	C	4.9286	3.1109	18.2781	6.00	4.00	12.0000
14	C	4.9320	4.0586	19.4545	6.00	4.00	12.0000
15	C	5.6230	3.4323	20.6468	6.00	4.00	12.0000
16	C	7.0262	2.9883	20.2987	6.00	4.00	12.0000
17	C	7.0208	2.0296	19.1269	6.00	4.00	12.0000
18	C	6.3310	2.6472	17.9354	6.00	4.00	12.0000
19	C	3.4335	0.1252	10.8139	6.00	4.00	12.0000
20	C	4.2022	0.0774	11.9818	6.00	4.00	12.0000
21	C	5.2275	-0.8450	12.1594	6.00	4.00	12.0000
22	C	7.8184	-2.1244	14.5742	6.00	4.00	12.0000
23	C	6.8594	0.7370	16.6413	6.00	4.00	12.0000
24	N	6.1786	1.8305	16.7581	7.00	5.00	14.0031
25	N	6.4538	3.4373	14.1667	7.00	5.00	14.0031
26	C	7.2744	4.4076	14.5711	6.00	4.00	12.0000
27	C	8.2491	4.9447	13.7513	6.00	4.00	12.0000
28	C	8.3795	4.4567	12.4611	6.00	4.00	12.0000
29	C	7.5271	3.4500	12.0409	6.00	4.00	12.0000
30	C	6.5806	2.9655	12.9219	6.00	4.00	12.0000
31	C	2.0138	5.3458	13.7186	6.00	4.00	12.0000
32	C	2.7948	4.6578	14.7115	6.00	4.00	12.0000
33	O	3.6078	3.6974	14.4027	8.00	6.00	15.9949
34	C	2.6389	5.0388	16.0760	6.00	4.00	12.0000
35	C	1.6951	6.0124	16.4487	6.00	4.00	12.0000
36	C	0.9232	6.6279	15.5181	6.00	4.00	12.0000
37	C	1.0720	6.3041	14.1564	6.00	4.00	12.0000
38	C	0.2267	6.9666	13.2273	6.00	4.00	12.0000
39	C	0.2853	6.6974	11.9071	6.00	4.00	12.0000
40	C	1.2427	5.7835	11.4004	6.00	4.00	12.0000
41	C	1.3215	5.5687	10.0354	6.00	4.00	12.0000
42	C	2.3107	4.7696	9.4727	6.00	4.00	12.0000
43	C	2.4142	4.5594	8.0803	6.00	4.00	12.0000
44	C	3.4404	3.8206	7.5635	6.00	4.00	12.0000
45	C	4.4105	3.2589	8.4184	6.00	4.00	12.0000

46	C	4.3197	3.4247	9.7716	6.00	4.00	12.0000
47	C	3.2691	4.1748	10.3445	6.00	4.00	12.0000
48	C	3.1476	4.3386	11.7282	6.00	4.00	12.0000
49	C	2.1507	5.1210	12.2969	6.00	4.00	12.0000
50	C	3.3757	4.4602	17.1285	6.00	4.00	12.0000
51	N	4.3577	3.6129	17.0424	7.00	5.00	14.0031
52	C	6.0433	-0.9345	13.3518	6.00	4.00	12.0000
53	C	5.9405	-0.0134	14.4460	6.00	4.00	12.0000
54	O	5.0839	0.9664	14.4214	8.00	6.00	15.9949
55	C	6.8148	-0.1723	15.5567	6.00	4.00	12.0000
56	H	8.3567	-1.3424	16.4925	1.00	1.00	1.0078
57	H	7.9520	-3.6514	12.4734	1.00	1.00	1.0078
58	H	6.6165	-3.4695	10.3942	1.00	1.00	1.0078
59	H	4.9345	-2.4345	9.1260	1.00	1.00	1.0078
60	H	3.1546	-1.4087	7.7546	1.00	1.00	1.0078
61	H	1.3356	0.2600	7.5330	1.00	1.00	1.0078
62	H	0.8418	1.8307	9.4048	1.00	1.00	1.0078
63	H	2.1731	1.7476	11.4848	1.00	1.00	1.0078
64	H	4.3697	2.1930	18.5659	1.00	1.00	1.0078
65	H	3.9038	4.3434	19.7326	1.00	1.00	1.0078
66	H	5.4506	4.9917	19.1551	1.00	1.00	1.0078
67	H	5.0377	2.5539	20.9824	1.00	1.00	1.0078
68	H	5.6354	4.1407	21.4922	1.00	1.00	1.0078
69	H	7.5137	2.5199	21.1702	1.00	1.00	1.0078
70	H	7.6340	3.8774	20.0396	1.00	1.00	1.0078
71	H	6.4872	1.0986	19.4047	1.00	1.00	1.0078
72	H	8.0541	1.7399	18.8693	1.00	1.00	1.0078
73	H	6.8910	3.5631	17.6408	1.00	1.00	1.0078
74	H	3.9696	0.7664	12.7961	1.00	1.00	1.0078
75	H	8.5339	-2.9514	14.5983	1.00	1.00	1.0078
76	H	7.5754	0.4602	17.4359	1.00	1.00	1.0078
77	H	7.1339	4.7574	15.6001	1.00	1.00	1.0078
78	H	8.9024	5.7361	14.1270	1.00	1.00	1.0078
79	H	9.1433	4.8580	11.7875	1.00	1.00	1.0078
80	H	7.5900	3.0293	11.0332	1.00	1.00	1.0078
81	H	5.8948	2.1531	12.6459	1.00	1.00	1.0078
82	H	1.5990	6.2565	17.5128	1.00	1.00	1.0078
83	H	0.1804	7.3796	15.7999	1.00	1.00	1.0078
84	H	-0.4877	7.6958	13.6232	1.00	1.00	1.0078
85	H	-0.3812	7.1977	11.1968	1.00	1.00	1.0078
86	H	0.6012	6.0737	9.3800	1.00	1.00	1.0078
87	H	1.6595	5.0116	7.4266	1.00	1.00	1.0078
88	H	3.5156	3.6666	6.4828	1.00	1.00	1.0078
89	H	5.2317	2.6746	7.9924	1.00	1.00	1.0078
90	H	5.0594	2.9713	10.4426	1.00	1.00	1.0078
91	H	3.8652	3.8508	12.3930	1.00	1.00	1.0078
92	H	3.0555	4.7967	18.1300	1.00	1.00	1.0078

TOTAL BONDING ENERGIES FROM VARIOUS XC FUNCTIONALS

XC	Energy Functional	hartree	eV	kcal/mol
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FR:	KCIS-modified	-18.20865315	-495.4826624	-11426.10356
FR:	KCIS-original	-18.18140693	-494.7412553	-11409.0063

FR:	PKZB	-42.96943826	-1169.257907	-26963.73244
FR:	VS98	1.08182677	29.43800421	678.8566186
FR:	LDA(VWN)	-24.6138257	-669.7762756	-15445.41044
FR:	PW91	-22.94503794	-624.3662504	-14398.23021
FR:	BLYP	-21.59135379	-587.5306304	-13548.78049
FR:	BP	-22.53354387	-613.168927	-14140.01375
FR:	PBE	-22.84185375	-621.5584656	-14333.48114
FR:	RPBE	-21.98319101	-598.1930637	-13794.66208
FR:	revPBE	-22.0915424	-601.1414549	-13862.65361
FR:	OLYP	-21.92442893	-596.594066	-13757.78831
FR:	FT97	-21.63332563	-588.6727424	-13575.11822
FR:	BLAP3	-15.33656454	-417.329155	-9623.840562
FR:	HCTH/93	-22.04871957	-599.9761865	-13835.78188
FR:	HCTH/120	-22.40123686	-609.5686699	-14056.98984
FR:	HCTH/147	-22.37739455	-608.9198878	-14042.02856
FR:	HCTH/407	-22.19045763	-603.8330755	-13924.72386
FR:	BmTau1	-13.72316216	-373.4262425	-8611.415178
FR:	BOP	-21.30214528	-579.6608665	-13367.29939
FR:	PKZBx-KCIScor	-17.96529351	-488.8605098	-11273.39307
FR:	VS98-x(xc)	-19.82067969	-539.3481365	-12437.66559
FR:	VS98-x-only	-21.91362966	-596.3002031	-13751.01167
FR:	Becke00	-23.2473081	-632.5914399	-14587.90761
FR:	Becke00x(xc)	-21.2676487	-578.7221666	-13345.65245
FR:	Becke00-x-only	-23.39510996	-636.6133331	-14680.65469
FR:	Becke88x+BR89c	-22.72854429	-618.4751584	-14262.37837
FR:	OLAP3	-15.66963968	-426.3925907	-9832.848389
FR:	TPSS	1403260.591	38184663.50	880559408.3
FR:	mPBE	-22.61175799	-615.2972415	-14189.09386
FR:	OPBE	-22.8433364	-621.5988106	-14334.41152
FR:	OPerdew	-22.86661901	-622.2323627	-14349.02158
FR:	mPBEKCIS	-18.70874079	-509.0907395	-11739.91333
FR:	mPW	-22.59206528	-614.7613755	-14176.73649
FR:	tau-HCTH	-21.67298232	-589.7518558	-13600.00317
FR:	XLYP	-21.4990873	-585.0199314	-13490.88238
FR:	KT1	-23.28572231	-633.6367437	-14612.0129
FR:	KT2	-24.13248532	-656.6783376	-15143.36476
FR:	TPSSh	1403258.987	38184619.88	880558401.7
FR:	B3LYP(VWN5)	-25.81898044	-702.5702047	-16201.65654
FR:	O3LYP(VWN5)	-25.28841329	-688.132738	-15868.72059
FR:	KMLYP(VWN5)	-34.14815963	-929.2187024	-21428.29594
FR:	PBE0	-27.82298044	-757.1018193	-17459.18566
FR:	B3LYP*(VWN5)	-24.98702223	-679.93147	-15679.59483
FR:	BHandH	-33.52787096	-912.339789	-21039.05889
FR:	BHandHLYP	-31.71940341	-863.128883	-19904.22824
FR:	B97	-26.02561436	-708.1929997	-16331.32129
FR:	B97-1	-26.48035322	-720.5670739	-16616.67427
FR:	B97-2	-26.61930269	-724.3480812	-16703.86639
FR:	mPBE0KCIS	-23.74739141	-646.1993992	-14901.71466
FR:	mPBE1KCIS	-22.27610543	-606.1636706	-13978.46867
FR:	B1LYP(VWN5)	-26.6553786	-725.3297567	-16726.50436
FR:	B1PW91(VWN5)	-27.55574278	-749.8299127	-17291.49148
FR:	mPW1PW	-27.63100326	-751.8778545	-17338.71815
FR:	mPW1K	-31.2187271	-849.5047876	-19590.04909
FR:	tau-HCTH-hybrid[56]	-25.43480137	-692.1161605	-15960.58051
FR:	X3LYP(VWN5)	-26.27006384	-714.8448086	-16484.71568
FR:	OPBE0	-27.82409242	-757.132078	-17459.88344