Fluorinated Phthalonitriles and Phthalocyanines: Synthesis and Spectroscopic Properties

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This work is dedicated to:

Marieana and Ion Pelmuş, my parents, for their love and sacrifices,

and

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for having the honor to work with them

"*Science promised us truth*, or at least a knowledge of such relations as our intelligence can seize: *it never promised us peace or happiness*. Sovereignly indifferent to our feelings, it is deaf to our lamentations. *It is for us to endeavour to live with science*, since nothing can bring back the illusions it has destroyed."

— Gustave Le Bon, *The Crowd; study of the popular mind*

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ABSTRACT

Since their discovery at the beginning of the 20th century, phthalocyanines (Pc) have come a long way; today they are replacing the porphyrins (natural products) in most of their applications. The functionalization of the organic macrocycle, the use of different metals, and the change of the axial ligands resulted in Pc applications in a wide range of fields, ranging from photochemistry, paints, catalysis, to fuel cells and cosmetic products.

In Dr. Gorun's group was developed a series of electron-deficient Pcs that benefit from a Teflon-like chemical shield, meant also to break the π-π interactions, namely the F_{64}PcM series. The present work is focused on (*i*) the redox properties of complexes with main group trivalent metals, namely non-functionalized F_{64}PcGaCl and F_{64}PcInCl, studied using classical electrochemical methods, cyclic voltammetry, and differential pulse polarography, (*ii*) the synthesis and photo-catalytical properties of a series of functionalized PcZn, and (*iii*) heterogenization strategies to produce functionalized Pc-based hybrid materials via bioconjugation or immobilization on solid supports.

Amido phthalonitriles and Pcs were produced to reveal the influence of exocyclic conjugation on the spectroscopic and photochemical properties of the Pcs. The phthalonitrile precursors and Pc, 20 new compounds, were synthesized using conventional and non-conventional methods (microwave), purified by chromatographic techniques, characterized by spectral methods (UV-Vis, FT-IR, ^{1}H-, ^{19}F-NMR, HRMS). 16 of the newly synthesized compounds were analyzed by single-crystal X-ray crystallography confirming the spectral data and providing new structural information at the molecular and state-state levels, especially spectroscopically and catalytically relevant aggregation.

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List of Abbreviations, Symbols, and Acronyms

-ve	negative
Å	angstrom
Ac	acetyl
AcOH	acetic acid
Ac2O	acetic anhydride
amu	atomic mass units
anhyd.	anhydrous
aq	aqueous
Ar	aryl
atm	atmosphere
°C	degrees Celsius
calcd	calculated (for MS analysis)
cat.	catalytic
$CHCl_3$	chloroform
cm^{-1}	wavenumbers(s)
^{13}C NMR	carbon NMR
CV	cyclic voltammetry
δ	chemical shift (ppm)
d	doublet (spectral)
DCM	dichloromethane
DPP	differential pulse polarography
DPV	differential pulse voltammetry
ε	molar absorptivity
EDG	electron-donating group
ESI	electrospray ionization
Et	ethyl
EtOAc	ethyl acetate
EtOH	ethanol
et al.	and others (co-authors)
EWG	electron-withdrawing group
^{19}F NMR	fluorine NMR
^{1}H NMR	proton NMR
HOMO	highest occupied molecular orbital
HPLC	high-performance liquid chromatography
HRMS	high-resolution mass spectrometry
i.e.	that is
IR	infrared
J	coupling constant in NMR

λ, λ_{max}	UV-vis wavelength, max UV-vis wavelength
LUMO	lowest unoccupied molecular orbital
MHz	megahertz
MPc	metal phthalocyanine
m.p.	melting point
MS	mass spectrometry
m/z	mass to charge ratio (in MS)
obsd	observed
Pc	phthalocyanine
Ph	phenyl
$PhNO_2$	nitrobenzene
PN	phthalonitrile
pp	pages
ppm	part per million
q	quartet (spectral)
redox	reduction-oxidation
rt	room temperature
sat.	saturated
SEC	spectroelectrochemistry
t	triplet (spectral)
TFA	trifluoroacetic acid
TFT	trifluorotoluene
THF	tetrahydrofuran
TLC	thin-layer chromatography
Tol	toluene
UV-vis	ultraviolet-visible absorption spectroscopy
vs.	versus

List of Publications and Conferences

Publications

1. Nguyen, T. H. Q.; Pelmuş, M.; Colomier, C.; Gorun, S.; Schlettwein, D. The influence of intermolecular coupling on electron and ion transport in differently substituted phthalocyanine thin films as electrochromic materials: a chemistry application of the Goldilocks principle. *Phys. Chem. Chem. Phys.* 2020, *22*(15), 7699-7709.

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2. Pelmuş, M.; Colomier, C.; Patel, H. H.; Xiao, O.; Foglia, R.; Suazo, M.; Gorun, S. M. Synthesis, X-ray structures, photo-physics and singlet oxygen production of fluorinated phthalocyanines. *ACS Spring 2020 National Meeting & Expo, SciMeetings.* **2020**. https://doi.org/10.1021/scimeetings.0c02234

3. Pelmuş, M.; Colomier, C.; Patel, H. H.; Xiao, O.; Foglia, R.; Suazo, M.; Gorun, S. M. Fluorinated phthalonitriles and phthalocyanines: synthesis, X-ray structures and exocyclic conjugation effects on reactivity. *46th NOS, ACS Division of Organic Chemistry*, Bloomington, **2019**, W-70.

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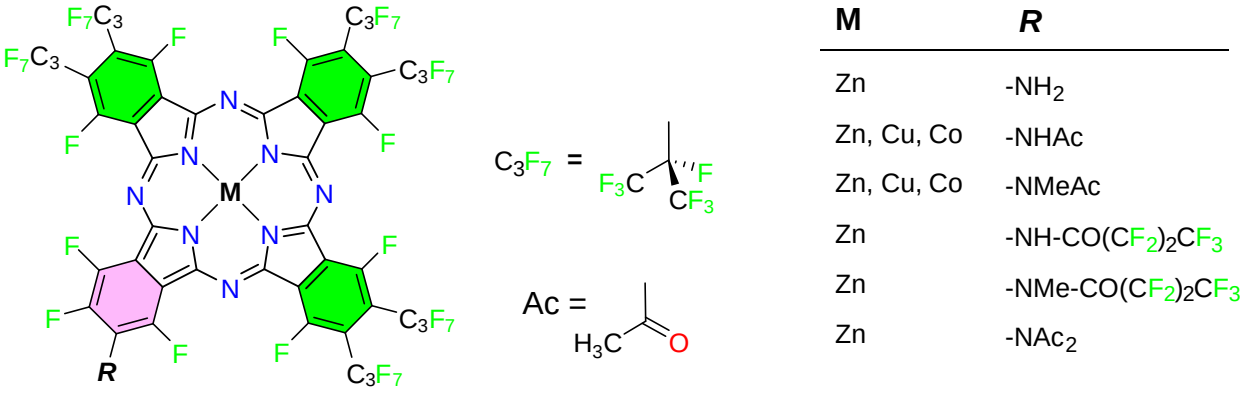
CHAPTER 1

INTRODUCTION

The present dissertation focus is the synthesis and characterization of fluorinated metal phthalocyanine (MPcs) (frequently used as metal catalysts and/or photosensitizers) functionalized with amido groups as an alternative to amino derivatives, Figure 1.1. The MPcs bearing perfluoroisopropyl (*i*-C_3F_7) groups as strong electron-withdrawing groups were initially functionalized with amino groups (Patel, 2015). The amino group is a highly reactive functionality and can serve very well also as a nucleophile replacing easily aromatic fluorine atoms from a fluorinated phthalocyanine (Leznoff *et al*., 2004). The downside of adding amino groups was a decrease in the photochemical activity due to its conjugation with the Pc macrocycle (Patel, 2015). The simultaneous presence of a strong electron-donating group (amino) and strong electron-withdrawing groups (perfluoroisopropyl) on the same macrocycle produces a *push-pull* effect within the molecule. While this effect can be beneficial in the production of solar cells (Ragoussi and Torres, 2015) in the case of amino-substituted F_{51}PcZn series diminishes the singlet oxygen production. It was hypothesized that the participation of the electron lone pair of the amino group in exocyclic conjugation will decrease this push-pull effect and result in an increase in the photochemical activity. Conversely, the methylation of the amino group, including anchoring fluorinated Pcs *via* alkylamino linkers is expected to increase its electron-donating capacities. Both effects are worth studying considering their homogeneous and heterogeneous photocatalytic relevance.

The amido group is indeed a weaker electron-donating group in comparison with the amino group, which has a resonance structure with the nitrogen lone pair conjugated with a carbonyl group from the acyl fragment (usually acetyl). Further, the amidation with two acyl groups

instead of a single one (as a bis-acetyl or succinyl) or perfluorobutiryl could provide insights regarding the degree of exocyclic conjugation.



M	R
Zn	-NH_2
Zn, Cu, Co	-NHAc
Zn, Cu, Co	-NMeAc
Zn	-NH-CO(CF_2)$_2$$CF_3$
Zn	-NMe-CO(CF_2)$_2$$CF_3$
Zn	-NAc_2

Figure 1.1 Structural representation of the amino and amido functionalized (acylated) MPc series.

The production of acylated MPcs was accomplished by following two main paths: (*i*) acylation of amino MPcs, and (*ii*) acylation of amino phthalonitriles (PNs) followed by the Pc synthesis. The synthesis and characterization of perfluoroalkyl- and amino-substituted PNs, together with their acylation (to produce the amido PNs shown in Figure 2.1) is being described in chapter 3.

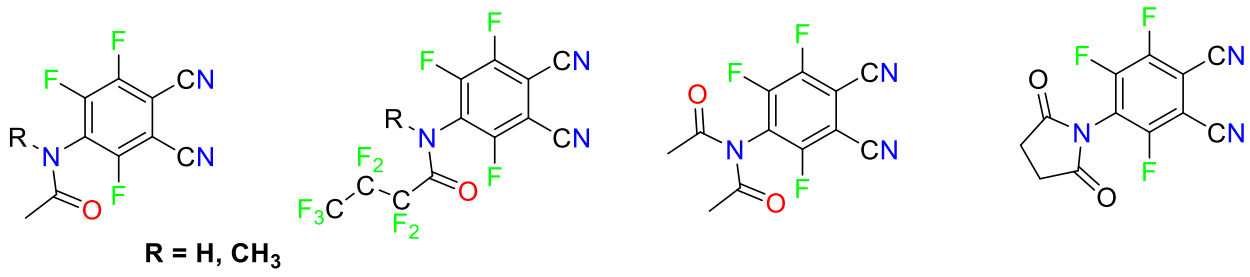


Figure 1.2 Chemical structures of the amido functionalized (acylated) PN series.

In chapter 4 covers the synthesis and characterization of 3 derivatives of the F_{64}PcM series (M = Ni, Ga-Cl, In-Cl) and the standard materials (M = Co, Cu, Zn) together with the partially perfluoroalkylated, F_{52}PcCu and F_{40}PcCu, derivatives, Figure 3.1. The partially perfluoroalkylated

perfluoro CuPcs could serve as starting materials for nucleophilic substitutions with amino derivatives, as was shown in the case of $F_{16}PcCu$ (DeOliveira *et al.*, 2008).

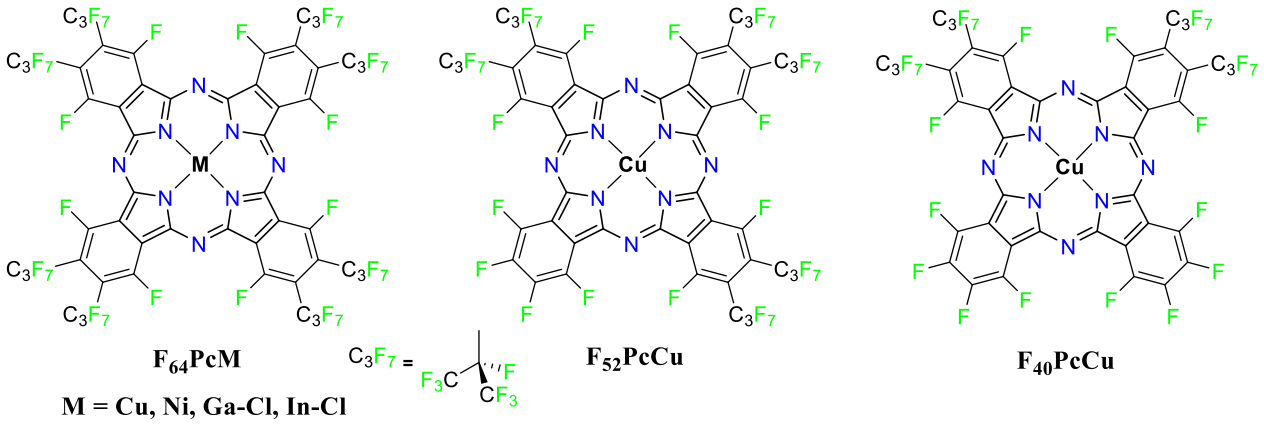


Figure 1.3 Chemical structures of MPcs with different degrees of perfluoroalkyl substitutions.

Chapter 5 presents the synthesis and characterization of amino and amido MPcs derivatives. The acylated phthalocyanines were synthesized in correlation with the phthalonitriles that contain as acyl groups acetyl and perfluorobutiryl.

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CHAPTER 2

EXPERIMENTAL TECHNIQUES, APPARATUSES, AND MATERIALS

2.1 Inert Atmosphere Techniques

Reactions that involved air- and/or moisture-sensitive reagents were set up in an inert atmosphere using the following instruments: glove box, Schlenk line, inert gas tanks (nitrogen or argon).

A glove box from Vigor Gas Purification Technologies Co., Ltd (Houston, TX), model VG1200/750TS, equipped with two antechamber entries (large Ø = 370 mm, and small Ø = 150 mm), was used for the set up (loading of the reagents) of the perfluoroalkyl phthalonitriles and group III phthalocyanine reactions. The inert atmosphere (99.99% nitrogen) inside the box contained less than 1 ppm of oxygen and 0.1 ppm water. A three-port glass stopcock, Schlenk line (Chemglass Life Sciences, Vineland, NJ) was used for distillations under inert and air-sensitive reactions. Nitrogen and argon gases (99.99% purity, AirGas, NJ) were used for the syntheses.

2.2 Syntheses techniques

The production of the modified phthalonitriles and metal phthalocyanines was accomplished using conventional and non-conventional (microwave) synthetic techniques. The chemical structures and reactions were drawn using ChemDraw Professional software version 19.1 (PerkinElmer, Akron, OH).

2.2.1 Conventional syntheses

Conventional reaction setups were composed of round bottom flasks connected to water or air condensers, under inert or ambient atmosphere, magnetic stirring, without or with heating (using

a high-temperature silicone oil bath on a hot plate with a temperature probe, IKA-Works, Wilmington, NC). These installations were used for the syntheses of amino phthalonitriles and their further acylation, and a part of the acylated metal phthalocyanines.

2.2.2 Microwave-assisted syntheses

Some MPcs syntheses were performed using a CEM Discover system (CEM Corporation, Matthews, NC) microwave oven. The temperature was controlled using a non-contact infrared probe. The oven was controlled using the ChemDriver v. 3.6.0 Discover software. The reactions were performed in 10 mL Pyrex glass reaction vials (microwave resistant) that were sealed with Teflon septa caps. The reactions were run at 180 – 200 °C, under magnetic stirring, using 300 W power.

2.3 Purification techniques

Purification techniques were necessary for some starting materials and crude reaction mixtures. The solvents were purified by distillation over a drying agent under an inert atmosphere, followed by storage over activated molecular sieves (5% w/v) (Armarego and Chai, 2013). The crude reaction mixtures were purified using liquid-liquid extractions, chromatography, crystallization, trituration, and sublimation.

Thin-layer chromatography (TLC) was performed using pre-coated aluminum-backed silica gel 60 plates, normal gravitational chromatography used silica gel 60 from Scientific Adsorbents Inc. (Atlanta, GA), 63–200 μm particle size, 60 Å pore size, while flash chromatography employed normal phase columns and a Teledyne Isco (Lincoln, NE) CombiFlash system.

2.4 Spectroscopy

2.4.1 Infrared Spectroscopy

Samples were prepared by mixing the solid compound with KBr (0.1-0.3 mg compound to 20 mg KBr), grinding to a fine powder, and pressing to obtain clear KBr pellets. A Nicolet FT-IR spectrophotometer (Thermo Fisher Scientific) controlled by OMNIC Spectra software was used to obtain data in the mid-infrared region 4000-400 cm^{-1} with a resolution of 2 cm^{-1} by averaging 16-32 scans.

2.4.2 UV-Vis Spectroscopy

Electronic absorption spectra were collected using an HP Diode array spectrophotometer 8425A, connected to a computer, and controlled using the Olis Global Works software and a Cary 500 UV-Vis-NIR spectrophotometer (Model EL01044985) controlled with the Varian Cary Win UV 3.0 software. The typical scanning range was 200–800 nm for the UV-Vis domain and 200-1100 nm for the UV-Vis-NIR experiments. Liquid samples were prepared as dilute solutions of the analyte in 1.0 cm and 1.0 mm quartz cells. Solutions were prepared freshly on the day of absorbance measurement unless stated otherwise. All measurements were corrected with the blank solvents. Concentrated phthalocyanine samples (10–50 μM) were measured in 1.0 mm cells, while dilute samples (0.5–5 μM) were measured in 1.0 cm cells. Gradually lower concentrations for determination of molar extinction coefficients were achieved by successive volume dilutions of an initial 50.0 mL 50 μM stock solution in a series of 10 mL volumetric flasks to reach the concentrations 40, 30, 25, 20, and 10 μM.

2.4.3 NMR Spectroscopy

FT NMR spectra were obtained at 25 °C on a Varian Inova 400 MHz instrument (^{1}H, 400 MHz; ^{13}C, 101 MHz; ^{19}F, 375.6 MHz). ^{13}C and ^{19}F spectra were acquired with proton decoupling un-

less otherwise stated. The assignment of all chemical shifts was based on 1D spectral data. Chemical shifts (δ) for ^{1}H spectra are reported in ppm relative to the residual proton signals from deuterated solvents (Fulmer *et al*., 2010). ^{19}F chemical shifts were referenced to the internal $CFCl_3$ (δ = 0.00 ppm) standard. ^{13}C chemical shifts are reported *vs*. the carbon peak of the solvent (Fulmer *et al*., 2010). Spectral data were processed by phase optimization and baseline correction using the MNOVA suite 12.0 software from Mestrelab Research, S.L. (Santiago de Compostela, Spain). To avoid cross-contamination solvent ampules were used from Alfa-Aesar and Millipore-Sigma.

2.4.4 Mass Spectrometry

Low-resolution mass spectra (MS) and high-resolution mass spectra (HRMS) were acquired at Rutgers University (Newark, NJ). The concentrations of the samples were ~5 μM in 100% ethanol for HRMS and 1 mg/mL for MS. The solutions were injected directly in an Apex-ultra 70 hybrid Fourier Transform mass spectrometer. The experimental isotopic splitting patterns were compared with the calculated ones for the proposed structures, using the software Bruker Compass Data Analysis 4.0.

2.4.5 X-ray Spectroscopy

Single-crystals suitable for X-ray diffraction were obtained by the slow evaporation of phthalocyanine and phthalonitrile solutions under ambient conditions (room temperature, air atmosphere, and in the dark). The data were collected at 100 K using a Bruker Smart Apex CCD diffractometer using Cu Kα (1.54178 Å) radiation at Rutgers University (Newark, NJ) and on a Bruker Kappa X8 Apex II diffractometer using Mo radiation at Hunter College (New York City, NY). Absorption corrections were performed using the software SADABS (Sheldrick, 2008 SADABS). Direct methods and refining with full-matrix least-squares on *F2* were used in solv-

ing the structures (Sheldrick, 1981). Non-hydrogen atoms were refined anisotropically while H atoms were placed at calculated positions and refined using a riding model. Computations were carried out using the SHELXTL package (Sheldrick, 2008 & 2015). TWINABS (Version 2012/1) was used to account for non-merohedral twinning (Sheldrick, 2012). Structures were visualized as ORTEP representations at 50% probability. Packing diagrams and all other structural representations were obtained with the Mercury suite (Macrae *et al*., 2020). Access to the ConQuest software, Cambridge Structural Database was provided through the Center for Functional Materials.

2.5 Electrochemical and spectroelectrochemical techniques

2.5.1 Electrochemical apparatus

Electrochemical measurements were performed using a conventional three-electrode cell that contained a glassy carbon (GCE) (Ø = 3 mm) working electrode, a Pt wire counter electrode, and a Ag/AgCl (3 M NaCl) reference electrode having E^0 = 0.206 V vs. the Standard Hydrogen Electrode (SHE). The cell was connected to a CV-50W BASi potentiostat and controlled by the software CV-50. Before cyclic voltammetry (CV) and differential pulse voltammetry (DPV) experiments, the active surface of the GCE was polished and subsequently washed with ACN. All experiments were performed at 25 ºC using 1 mM substrate and 0.1 M TBATFB supporting electrolyte solution under Ar. Blank CV and DPV scans were run for the bear electrolyte solution before adding the samples. A fixed scan rate, 0.1 V/s, and/or variable scan rates, 0.05 – 1 V/s, were used for CV, while 20 mV/s scan rate was used for DPV. For Differential Pulse Polarography (DPP) 4 mV/s scan rates with 50 mV pulse amplitude and 50 ms pulse width were used. Ultra-high purity (UHP) argon (>99.999%) was used for electrochemical experiments, including

purging solutions and maintaining an inert atmosphere blanket. gas to the electrochemistry apparatus was done using a regulator for pressure and flow.

2.5.2 Spectroelectrochemical apparatus

For spectroelectrochemical (SEC) measurements the UV-vis-NIR spectrophotometer was equipped with a BAS LC-4C amperometric controller (general-purpose potentiostat). The thin-layer quartz cell contained a transparent Pt gauze working electrode, Pt wire as a counter electrode, and a Ag/AgCl (3 M NaCl) reference electrode. The working electrode was cleaned by being immersed for 30 minutes in concentrated nitric acid after the determinations. All spectroelectrochemical equipment was acquired from Bioanalytical Systems, Inc. (West Lafayette, IN).

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CHAPTER 3

SYNTHESIS AND CHARACTERIZATION OF FLUORINATED PHTHALONITRILES

3.1 Introduction

Isolated first in 1896 from the diazotization process of 2-aminobenzonitrile (Lorz *et al*., 2007), the phthalonitrile *abbr*. PN or the nitrile of phthalic acid, a member of the benzonitriles class started to receive attention after Linstead in 1934, used it together with its derivatives in the synthesis of phthalocyanines (Pcs) (Linstead, 1934; Byrne *et al*., 1934). PNs together with phthalic anhydrides are the most used starting materials to produce Pcs (Löbbert, 2000). Through alterations of the precursors and/or on the Pcs' skeleton, different substituents can be introducing on the organic macrocycle. The tailoring of the macrocycle together with the chelation of different metallic ions and/or coordination of axial ligands fine-tunes the Pcs' properties increasing the number of applications (Claessens *et al*., 2008).

This work is focused on the introduction of substituents on the Pc organic macrocycle via modifications of the PN precursors as an alternative to the direct functionalization of the Pcs. Fluorinated Pcs are of interest as they exhibit high thermal stability and resistance to oxidation (Hudlicky and Pavlah, 1995; Stuzhin, 2014). Perfluorinated phthalonitrile (tetrafluorophthalonitrille, **[3-1]**), abbreviated perfluorinated-PN or F_4PN, commercially available, proved to be a versatile starting material for the production of substituted PNs as it is the subject of facile aromatic nucleophilic substitutions, thus offering options to produce an entire range of C, N, O, S and/or P derivatives (Stuzhin, 2014). The main substitution processes that are followed in this work are the introduction of bulky perfluoroalkyl substituents and reactive functional groups. Bulky perfluoroalkyl substituents are of interest for increasing the Pcs' electron deficiency, breaking their

π-π interactions, and, as shown below, constructing a Teflon-like shield around Pc molecules. The reactive functional groups are important for Pcs' conjugation with linkers (further functionalization), biological vectors (bioconjugation), and solid materials (covalent immobilization).

3.1.1 Perfluoroalkyl-substituted PNs

To produce perfluoroalkyl-substituted benzonitriles, the reported strategies are based on the introduction of cyano groups in perfluoroalkyl halogenated aromatics and perfluoroalkylation of halogenated phthalonitriles. For the introduction of cyano groups, metal cyanides are used to substitute the halogen atoms (Inukai and Maki, 1965) or, by starting from *o*-xylene perfluoroalkyl derivatives through oxidation, amidation, and dehydration (Loas, 2012; Gorun *et al*., 2012). The second strategy, more common, is to perform a nucleophilic substitution on halogenated phthalonitriles using perfluoroalkylating agents such as CF_3SiR_3 derivatives in the presence of potassium iodide and copper(I) iodide (Kuwahara *et al*., 2003) or diphenyl(trifluoromethyl)sulfonium trifluoromethanesulfonate in the presence of Cu^0 (Shibata *et al*., 2014). All described strategies provided trifluoroalkylated PNs with different degrees of substitution but neither gave completely fluorinated (perfluorinated) alkyl-substituted PNs.

The Pc mixture obtained from trifluoromethyl-disubstituted PN showed aggregation in solution, indicating the need for bulkier substituents to prevent the π-π stacking (Laos, 2012). The introduction of perfluoroalkyl substituents in the PN's structure by nucleophilic substitution of **[3-1]** with perfluorisopropyl carbanions, Figure 3.1 (Gorun *et al*., 1989), proved that these groups are big enough (bulky) to hinder the aggregation in solution between the resulted Pcs (Bench, Beveridge *et al*., 2002). The perfluorisopropyl carbanions were generated from perfluoropropene and catalytic amounts of cesium fluoride as the reaction mixture was let to reach

room temperature from -78 °C (Gorun *et al*., 1989). Excess perfluoropropene resulted in the production of di- and tri-perfluoroisopropyl-substituted PNs: **[3-2] - [3-4]**, Figure 3.1.

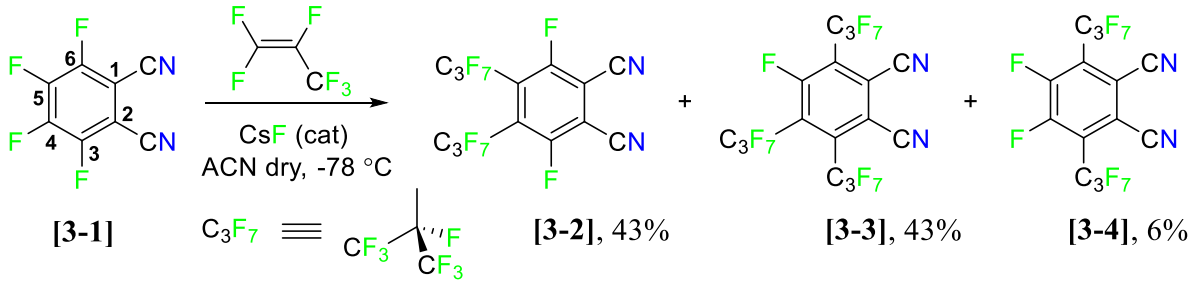


Figure 3.1 Reaction scheme of the synthesis of perfluoroalkyl-substituted PNs **[3-2] – [3-4]**. (Gorun *et al*., 1998)

3.1.2 Amino-substituted PNs

The derivatization strategies which were developed over the years for the functionalization of tetrafluorophthalonitrile **[3-1]** were summarized in a recent review (Stuzhin, 2014). The fluorine atom at position 4 (*para*) of the PN **[3-1]** is easier to be replaced by nucleophiles because in positions 1 and 2 there are 2 nitrile groups (strong electron-withdrawing substituents) and polar solvents are used (Birchall *et al*., 1970; Chambers, 1973).

Mechanistic studies suggest that nucleophilic substitutions on polyfluobenzenes proceed *via* an addition-elimination mechanism (S_NAr) *via* an intermediate Meisenheimer complex (MC) where the addition, rather than the breaking of the C-F bond, is the rate-limiting step (Chambers, 1973). *Ab initio* studies confirmed the proposed mechanism (Tanaka *et al*., 1999). Further studies on polyfluoroaromatics were reviewed by Chambers (Chambers, 2004).

The present study is focused on the production of amino-substituted PNs **[3-5] – [3-7]**, derivatives with reactive functional groups. Well-established preparation procedures were followed for their production, Figure 3.2 (Birchall *et al*., 1967; Ikeno *et al*., 2000; Patel, 2015). The reactions with methyl and dimethyl amines, taking into consideration their increased nucleo-

philicity, were performed at room temperature to avoid multiple substitutions under reflux conditions.

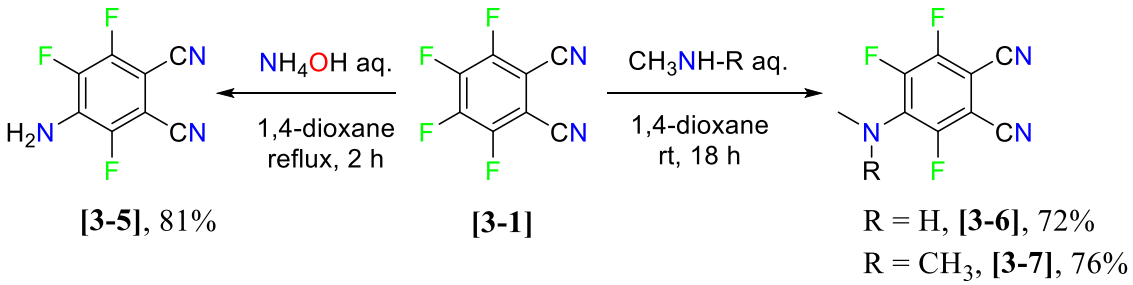


Figure 3.2 Reaction scheme of the synthesis of amino-substituted PNs **[3-5] - [3-7]**.

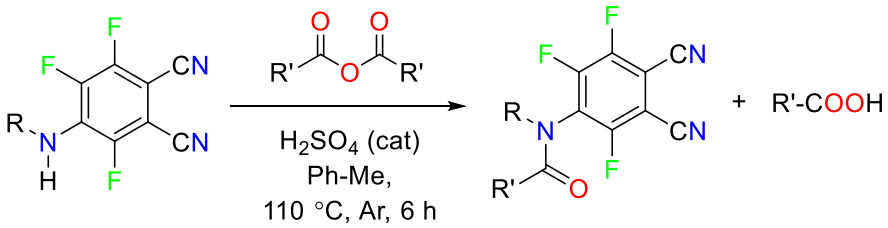
3.1.2 Acylated (amido- and imido-substituted) PNs

Further functionalization of the amino-substituted PNs was considered for conjugation purposes (to organic molecules, biological vectors, functionalized solid substrates) as well as for testing substituent's electronic effects as the strong electron donor effect of the amino group is being tempered by the exocyclic conjugation of the amino electron lone pair. The acylated derivatives can be synthesized using a variety of agents, the main ones being organic acid anhydrides and chlorides. Previous reports on the acylation of amino-substituted nitriles indicate the need for strong mineral acids as catalysts for the reaction with anhydrides, taking into consideration the low pK_a of these derivatives (Michálková Nečedová *et al*., 2017; Laev *et al*., 2001).

Acetic anhydride and heptafluorobutyric anhydride were used for the acylation of PNs **[3-5]** and **[3-6]** in the presence of sulfuric acid, Figure 3.3. Another strategy was to use an excess of acetyl chloride as solvent and reagent, without adding sulfuric acid. The second strategy was rationalized by the fact that the hydrochloric acid by-product can act also as a catalyst, Figure 3.4.

Imido derivatives were under consideration also to be produced and, for this purpose the substrate **[3-5]** was used. The bis-acetylated derivative **[3-12]** was not isolated using the previous

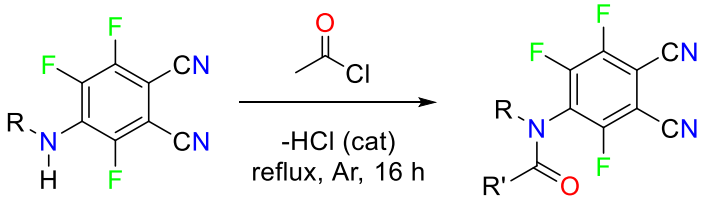
strategies, indicating that more energic conditions are necessary. Toluene was used as a high boiling solvent to obtain the necessary product, Figure 3.5.



R = H, **[3-5]**
R = CH_3, **[3-6]**

R = H, R' = CH_3, **[3-8]**, 80%
R = R' = CH_3, **[3-9]**, 82%
R = H, R' = $CF_2CF_2CF_3$, **[3-10]**,71%
R = CH_3, R' = $CF_2CF_2CF_3$, **[3-11]**, 75%

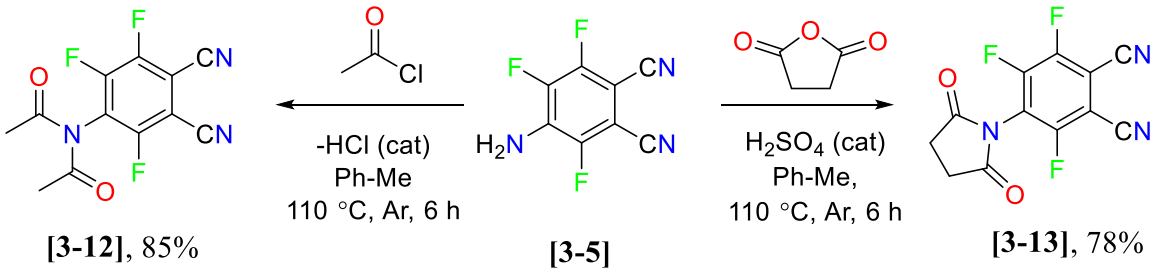
Figure 3.3 Reaction scheme of the synthesis of amido-substituted PNs **[3-8] - [3-11]** using anhydrides.



R = H, **[3-5]**
R = CH_3, **[3-6]**

R = H, R' = CH_3, **[3-8]**, 95%
R = R' = CH_3, **[3-9]**, 93%

Figure 3.4 Reaction scheme of the synthesis of amido-substituted PNs **[3-8]** and **[3-9]** using acetyl chloride.



[3-12], 85%

[3-5]

[3-13], 78%

Figure 3.5 Reaction scheme of the synthesis of imido-substituted PNs **[3-12]** and **[3-13]**.

3.2 Experimental

3.2.1 Synthesis and characterization of perfluoroalkyl-substituted PNs [3-2] – [3-4]

Perfluoroalkyl derivatives: 3,6-difluoro-4,5-bis(perfluoropropan-2-yl)phthalonitrile **[3-2]**, 4-fluoro-3,5,6-tris(perfluoropropan-2-yl)phthalonitrile **[3-3]**, and 4,5-difluoro-3,6-bis(perfluoropropan-2-yl)phthalonitrile **[3-4]**, were prepared according to the previously reported procedure, see Figure 3.1 (Gorun, 1998), using 3,4,5,6-tetrafluorophthalonitrile **[3-1]** as starting material. Spectroscopic data, including FT-IR and UV-Vis are consistent with the proposed structures.

3,6-difluoro-4,5-bis(perfluoropropan-2-yl)phthalonitrile **[3-2]**:

FT-IR (KBr disk) *v*, cm^{-1} (intensity): 2253 (w) C≡N; 1625 (w), 1457 (w), 1430 (m) C=C; 1293 (s), 1250 (s), 1174 (s) C-F of CF_3 and C-F aromatic, overlapped; 1066 (m) C-F of **CF**$(CF_3)_2$; 980 (s), 963 (s), 814 (m), 731 (s), 714 (s), 555 (w). UV-Vis (acetonitrile) λ, nm: 204 (λ_{max}), 240, 248, 310, 320.

4-fluoro-3,5,6-tris(perfluoropropan-2-yl)phthalonitrile **[3-3]**:

FT-IR (KBr disk) *v*, cm^{-1} (intensity): 1554 (w), 1423 (w) C=C; 1278 (s), 1234 (s), 1172 (m), 1144 (m), 1117 (m) C-F from CF_3 and C-F aromatic, overlapped; 1074 (m) C-F from **CF**$(CF_3)_2$; 1002 (m), 965 (m), 766 (m), 736 (w), 669 (w), 552 (w), 505 (w). UV (acetonitrile) λ, nm: 216 (λ_{max}), 242, 249, 303, 312.

4,5-difluoro-3,6-bis(perfluoropropan-2-yl)phthalonitrile **[3-4]**:

FT-IR (KBr disk) *v*, cm^{-1} (intensity): 2246 (w) C≡N; 1600 (w), 1480 (s) C=C; 1345 (m), 1297 (s), 1237 (s), 1171 (m) C-F from CF_3 and C-F aromatic, overlapped; 1094 (m) C-F from **CF**$(CF_3)_2$; 1009 (s), 983 (s), 940 (m), 738 (m), 711 (m), 548 (w). UV-Vis (acetonitrile) λ, nm: 200 (λ_{max}), 251, 300.

3.2.2 Synthesis and characterization of amino-substituted PNs [3-5] - [3-7]

The fluorinated amino-phthalonitriles: 4-amino-3,5,6-trifluorophthalonitrile **[3-5]**, 5-(*N*-methylamino)-3,5,6-trifluorophthalonitrile **[3-6]**, and 4-(*N*,*N*-dimethylamino)-3,5,6-trifluorophthalonitrile **[3-7]** were prepared following previously reported protocols (Birchall, 1970; Ikeno, 2000; Patel, 2015) using 3,4,5,6-tetrafluorophthalonitrile **[3-1]** as starting material. Spectroscopic data, including ^{13}C and $^{13}C\{^{19}F\}$ NMR and UV-Vis are consistent with the proposed structures.

3,4,5,6-tetrafluorophthalonitrile **[3-1]**:

^{13}C NMR (101 MHz, acetone-d_6) δ, ppm: 150.98 (J = 261.0 Hz)*, 145.57 (dtd, J =266.8, 14.1, 5.2 Hz), 109.95, 102.66 – 101.92 (m). (* average value) $^{13}C\{^{19}F\}$ NMR (101 MHz, acetone-d_6) δ, ppm: 151.24, 145.54, 109.95, 102.29. UV-Vis (acetonitrile) λ, nm: 204 (λ_{max}), 238, 247, 289, 297.

4-amino-3,5,6-trifluorophthalonitrile **[3-5]**:

^{13}C NMR (101 MHz, acetone-d_6) δ, ppm: 150.75 (ddd, J = 254.1, 12.9, 1.8 Hz), 149.47 (ddd, J = 255.0*, 12.6*, 2.02 Hz), 141.93 (ddd, J = 250.0, 14.7, 9.6 Hz), 134.95 (ddd, J = 16.2, 13.5, 4.5 Hz), 111.58 (dd, J = 3.9, 2.9 Hz), 111.22 – 110.98 (m), 99.97 (dt, J = 16.9, 3.5 Hz), 88.64 (ddd, J = 17.1, 3.6, 1.5 Hz). (* average value) $^{13}C\{^{19}F\}$ NMR (101 MHz, acetone-d_6) δ, ppm: 150.80, 149.63, 141.98, 134.99, 111.63, 111.18, 100.03, 88.71. UV-Vis (acetonitrile) λ, nm: 206, 234 (λ_{max}), 278, 320.

4-(N-methylamino)-3,5,6-trifluoro-phthalonitrile **[3-6]**:

^{13}C NMR (101 MHz, acetone-d_6) δ, ppm: 151.18 (ddd, J = 253.6, 13.9, 1.6 Hz), 150.11 (dd, J = 251.6, 9.3 Hz), 142.27 (ddd, J = 248.6, 15.2, 9.7 Hz), 136.87 – 133.71 (m), 111.62 (dd, J = 4.0, 2.8 Hz), 111.14 (ddd, J = 3.1, 2.0, 1.3 Hz), 100.08 (ddd, J = 18.1, 4.3, 2.8 Hz), 87.77 (ddd, J =

17.3, 3.8, 1.4 Hz), 34.11 – 29.88 (m). $^{13}C\{^{19}F\}$ NMR (101 MHz, acetone-d_6) δ, ppm: 151.17, 150.08, 142.26, 135.60, 111.61, 111.14, 100.08, 87.76, 34.11 – 29.88 (m). UV-Vis (acetonitrile) λ, nm: 206, 244 (λ_{max}), 290, 334.

4-(N,N-dimethylamino)-3,5,6-trifluorophthalonitrile **[3-7]**:

^{13}C NMR (101 MHz, acetone-d_6) δ, ppm: 154.09 (ddd, *J* = 255.3, 8.4, 1.4 Hz), 151.33 (ddd, *J* = 255.7, 15.5, 2.1 Hz), 146.88 (ddd, *J* = 254.2, 13.8, 9.5 Hz), 137.40 (ddd, *J* = 12.1, 9.3, 3.3 Hz), 111.35 – 111.25 (m), 111.24 – 111.17 (m), 100.83 (ddd, *J* = 20.0, 4.2, 3.4 Hz), 92.36 (ddd, *J* = 17.2, 4.0, 2.0 Hz), 44.66 – 41.02 (m). $^{13}C\{^{19}F\}$ NMR (101 MHz, acetone-d_6) δ, ppm: 154.09, 151.33, 146.88, 137.40, 111.29, 111.21, 100.83, 92.36, 45.19 – 41.04 (m). UV-Vis (acetonitrile) λ, nm: 208, 252 (λ_{max}), 304, 348.

3.2.3 General procedure for the synthesis and purification of acylated PNs

Step 1: Synthesis

Method A: *Acid anhydrides as acylating agents*. One equivalent of a solid amino-substituted PN was added while stirring to dry toluene in a round bottom flask. The suspension was purged with argon and 2 equivalents of the acid anhydride were added. The mixture was refluxed at 110 °C for 15 min and then 3 drops of concentrated sulfuric per 1 mmol of PN were added and the stirring was continued for 1 hour while refluxing. The reaction progress was monitored by TLC.

Method B: *Organic acid chlorides as acylating agents*. One equivalent of a solid amino-substituted PN was added to a round bottom flask under argon. An excess of 7 equivalents of organic acid chloride, which served also as a solvent, was added to the flask and the reaction mixture was refluxed for 6 hours.

Step 2: Reactions work-up

After cooling to room temperature, reaction mixtures were extracted with ethyl acetate and washed in a separatory funnel with 5% sodium bicarbonate, followed by brine. The organic layer was dried over anhydrous magnesium sulfate, filtered and the solvent was removed under vacuum. The resulting residue (a solid material or oil) was further purified chromatographically.

Step 3: Normal phase flash chromatography

The residue was dissolved in a minimum amount of acetone and adsorbed onto silica gel (on average, 100-200 mg of residue per gram of silica) and the loaded silica was added to a cartridge half prefilled with silica gel. A gradient of ethyl acetate 0-30% in hexane was used for the fractionation of the crude reaction product.

3.2.4 Synthesis and characterization of amido-substituted PNs [3-8] – [3-11]

***4-(acetamido)-3,5,6-trifluorophthalonitrile* [3-8]**:

Method A: 197 mg (1 mmol) of **[3-5]** were mixed with 5 mL of dry toluene in a 10 mL round bottom flask under argon. 190 µL (2 mmoles) of acetic anhydride were added following the general procedure described in **section 3.2.3** for synthesis, reaction work-up, and purification.

Method B: 197 mg (1 mmol) of **[3-5]** were added to a 5 mL round bottom flask under argon. 500 µL (7 mmoles) of acetic chloride were added following the general procedure described in **section 3.2.3** for synthesis, reaction work-up, and purification.

After flash chromatography the solid material was recrystallized from acetone; the slow evaporation of the solvent yielded colorless crystals of **[3-8]** in 80% (method A) and 95% (method B) yields based on the limiting reagent **[3-5]**; m.p. 150-151 °C. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 2.24 (d, J = 0.4 Hz, CH_3, 3H), 9.71 (s, N-H, 1H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -110.96 (dd, J = 10.7, 8.4 Hz, 1F), -125.46 (dd, J = 20.9, 8.4 Hz, 1F), -131.01 (dd, J =

20.8, 10.7 Hz, 1F). FT-IR (KBr disk) *v*, cm^{-1} (intensity): 3237 (m) N-H; 2986 (w) C-H; 2247 (w) C≡N; 1682 (s) C=O; 1623 (m), 1533 (m) C=C aromatic; 1475.18 (s), 1371 (w) CH_3 bend; 1320, 1293, 1259 C-F aromatic; 1151 (w), 1107 (w), 1041 (w), 1012 (w), 985 (w), 939 (w). HRMS (+ve ESI) for $C_{10}H_4ON_3F_3Na^+$ [M + Na^+] calcd. 262.01987, found 262.02091. UV-Vis (acetonitrile) λ, nm: 210, 224 (λ_{max}), 270, 289, 308.

4-(N-methylacetamido)-3,5,6-trifluorophthalonitrile **[3-9]** (mixture of rotamers in 1:1 ratio as determined by NMR):

Method A: 211 mg (1 mmol) of **[3-6]** were suspended under argon in 5 mL of dry toluene in a 10 mL round bottom flask. 190 µL (2 mmoles) of acetic anhydride were added following the general procedure described in **section 3.2.3** for synthesis, reaction workup, and purification.

Method B: 211 mg (1 mmol) of **[3-6]** were added to a 5 mL round bottom flask under argon. 500 µL (7 mmoles) of acetic chloride were added following the general procedure described in **section 3.2.3** for synthesis, reaction work-up, and purification.

After solvent removal the resulted dense oil was dried in a stream of air overnight. **[3-9]** appears as a mixture of *cis* and *trans* rotamers (1:1 molar ratio), at the NMR time scale. **[3-9]** was obtained in 82% (method A) and 92% (method B) overall yields based on the limiting reagent **[3-6]**. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 3.49 (s, N-CH_3, 3H), 3.22 (s, N-CH_3, 3H), 2.34 (s, CO-CH_3, 3H), 1.96 (s, CO-CH_3, 3H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -110.05 (t, *J* = 9.3 Hz, 1F), -112.05 (t, *J* = 9.3 Hz, 1F), -124.98 (dd, *J* = 20.5, 6.8 Hz, 1F), -126.84 (dd, *J* = 21.2, 6.8 Hz, 1F), -128.84 (dd, *J* = 21.1, 11.5 Hz, 1F), -130.61 (dd, *J* = 20.5, 11.0 Hz, 1F). FT-IR (KBr disk) *v*, cm^{-1} (intensity): 2957 (w) C-H; 2243 (w) C≡N; 1690 (s) C=O; 1621 (w), 1497 (s), 1480 (s), 1427 (m), 1404 (m), 1378 (m) C=C overlapped with CH_3 bending; 1340, 1311,

1218, 1152, 1131, 1068, 1001 (m), 955 (s). HRMS (+ve ESI) for $C_{11}H_6ON_3F_3Na^+$ [M + Na^+] calcd. 276.03552, found 276.03633. UV-Vis (acetonitrile) λ, nm: 206 (λ_{max}), 228, 280, 308.

4-(perfluoro-n-butyramido)-3,5,6-trifluorophthalonitrile **[3-10]**:

Method A: 197 mg of **[3-5]** (1 mmol) were suspended under argon in 5 mL of dry toluene in a 10 mL round bottom flask. 490 µL (2 mmoles) of heptafluorobutyric anhydride were added following the general procedure described in **section 3.2.3** for synthesis, reaction work-up, and purification. After flash chromatography and removal of the solvents the obtained solid material was dissolved in acetone and the solvent was let to evaporate slowly yielding colorless crystals of **[3-10]** in 71% yield based on the limiting reagent **[3-5]**; m.p. 118-120 °C. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 5.60 (s, N-H, 1H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -80.37 (t, J = 8.6 Hz, CF_3, 3F), -110.33 (dd, J = 11.2, 5.9 Hz, 1F), -119.56 (q, J = 8.7 Hz, CF_3-C**F**$_2$, 2F), -124.51 (dd, J = 20.4, 5.7 Hz, 1F), -126.61 (s, CF_3-CF_2-C**F**$_2$, 2F), -129.56 (dd, J = 20.4, 11.4 Hz, 1F). FT-IR (KBr disk) ν, cm^{-1} (intensity): 3265 (m) N-H; 2916 (w); 2246 (m) C≡N; 1738 (s) C=O; 1623 (w), 1482 (s), 1407 (m) C=C; 1233 (s), 1124 (m), 1073 (m), 1038 (w) C-F aliphatic and aromatic, overlapped; 982, 965, 938, 858. MS for $C_{12}HF_{10}N_3OH^+$ [M + H^+] calcd. 394.00, found 393.9. UV-Vis (acetonitrile) λ, nm: 210 (λ_{max}), 250, 296, 306, 334.

4-(N-methyl-perfluoro-n-butyramido)-3,5,6-trifluorophthalonitrile **[3-11]** (mixture of rotamers in 1:1.5 ratio):

Method A: 211 mg of **[3-6]** (1 mmol) were suspended under argon in 5 mL of dry toluene in a 10 mL round bottom flask. 490 µL (2 mmoles) of heptafluorobutyric anhydride were added following the general procedure described in **section 3.2.3** for synthesis, reaction work-up, and purification. After solvent removal the oily residue was dried in a stream of air overnight. **[3-11]** appears as a mixture of *cis* and *trans* rotamers (1:1.5 molar ratio), at the NMR time scale, 75%

overall yield based on the limiting reagent **[3-6]**. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 3.73 (s, N-CH_3, 3H), 3.49 (s, N-CH_3, 3H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -79.69 (t, J = 9.2 Hz, CF_3, 3F), -79.81 (t, J = 9.1 Hz, CF_3, 3F), -110.98 (dd, J = 11.9, 5.2 Hz, 1F), -112.65 (dd, J = 8.6, 4.4 Hz, 1F), -112.90 (d, J = 10.0 Hz, CF_3-C**F**$_2$, 2F), -113.24 (qt, J = 9.1, 4.6 Hz, CF_3-C**F**$_2$, 2F), -125.20 (dd, J = 20.5, 4.5 Hz, 1F), -125.28 (s, CF_3-CF_2-C**F**$_2$, 2F), -125.44 (s, CF_3-CF_2-C**F**$_2$, 2F), -126.63 (dd, J = 20.2, 4.2 Hz, 1F), -128.26 (dd, J = 20.8, 11.9 Hz, 1F), -129.05 (dd, J = 20.4, 11.6 Hz, 1F). FT-IR (KBr disk) ν, cm^{-1} (intensity): 2246 (w) C≡N; 1716 (s) C=O; 1622 (s), 1484 (s), 1408 (w), 1379 (m) C=C aromatic; 1343 (m), 1323 (m), 1235 (s), 1127 (s), 1038 (w), 1010 (w) C-F aliphatic and aromatic, overlapped; 965 (s), 871 (w), 771 (w). MS (+ve EI) for $C_{13}H_3F_{10}N_3OH^+$ [M + H^+] calcd. 408.02, found 408.1. UV-Vis (acetonitrile) λ, nm: 210 (λ_{max}), 248, 296, 306.

3.2.5 Synthesis and characterization of imido-substituted PNs [3-12] and **[3-13]**

4-(N-acetyl-acetamido)-3,5,6-trifluorophthalonitrile **[3-12]**:

197 mg (1 mmol) of **[3-5]** were dissolved under argon in 5 mL of dry toluene in a 10 mL round bottom flask. 500 µL (7 mmoles) of acetic chloride were added and the reaction mixture was heated to 110 °C for 6 hours. The general procedure described in **section 3.2.3** for reaction work-up and purification was followed.

Following flash chromatography the solid material was dissolved in acetone and the solvent was let to slowly evaporate yielding colorless crystals of **[3-12]**, in 85% yield based on the limiting reagent **[3-5]**; m.p. 131-133 °C. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 2.25 (s, CH_3, 6H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -111.78 (dd, J = 11.9, 5.4 Hz, 1F), -125.73 (dd, J = 21.2, 5.3 Hz, 1F), -128.60 (dd, J = 21.5, 12.0 Hz, 1F). FT-IR (KBr disk) ν, cm^{-1} (intensity): 2949 (w) C-H; 2245 (m) C≡N; 1739 (s), 1722 (s) C=O; 1621 (m), 1497 (s), 1478 (s) C=C aromatic; 1424

(m), 1399 (s), 1368 (s) CH_3 bending; 1326 (m), 1276 (s), 1250 (s), 1212 (s), 1127 (m), 1050 (w), 1013 (m) C-F aromatic; 960, 931, 791. MS (+ve EI) for $C_{12}H_6F_3N_3O_2$ calcd. 281.04, found 281.1. UV-Vis (acetonitrile) λ, nm: 208 (λ_{max}), 250, 296, 306.

4-(succinimidyl)-3,5,6-trifluorophthalonitrile **[3-13]**:

Method A: 197 mg of **[3-5]** (1 mmol) were mixed with 5 mL of dry toluene in a 10 mL round bottom flask under argon; 200 mg (2 mmoles) of succinic anhydride were added following the general procedure described in **section 3.2.3** for synthesis, reaction workup, and purification. Following flash chromatography the solid material was dissolved in acetone and the solvent was let to slowly evaporate yielding colorless crystals of **[3-13]** were obtained in 71% yield based on the limiting reagent **[3-5]**; m.p. 118-120 °C. ^{1}H NMR (400 MHz, acetone-d_6) δ, ppm: 3.13 (s, CH_2, 4H). ^{19}F NMR (376.5 MHz, acetone-d_6) δ, ppm: -108.73 (dd, J = 11.8, 4.9 Hz), -122.88 (dd, J = 20.5, 4.7 Hz), -129.31 (dd, J = 20.5, 12.1 Hz). FT-IR (KBr disk) ν, cm^{-1} (intensity): 2954 (w) C-H; 2251 (m) C≡N; 1797, 1738 (s) C=O; 1625 (w), 1597 (w), 1504 (s), 1489 (s) C=C aromatic; 1412 (s), 1360 (m), C-N; 1300 (s), 1254 (s), 1179 (m), 1141 (s), 1103 (m), 1043 (m), 1006 (m), C-F aromatic; 972 (s). MS (+ve EI) for $C_{12}H_4F_3N_3O_2$ calcd. 279.03, found 279.1. UV-Vis (acetonitrile) λ, nm: 208 (λ_{max}), 236, 254, 282, 396, 306.

3.2.6 Electrochemical characterization of the PNs [3-1] – [3-7]

The electrochemical characterization of the PNs **[3-1]** – **[3-7]** was performed using a three-electrode conventional cell connected to a potentiostat. The potential of the working electrode was varied while monitoring the change in current intensity by CV and DPV. Before each experiment, the active surface of the GCE was polished and subsequently washed with ACN. All the experiments were performed at 20 ºC, in 0.1 M TBATFB in acetonitrile supporting electrolyte solution, under an inert atmosphere, argon. The electrochemical system was purged by bubbling

argon under magnetic stirring for 30 min before starting the experiment and 10 min between measurements. The working concentration for the PNs was 1 mM.

The supporting electrolyte solution was scanned using CV and DPV methods to make sure that the electrochemical cell is clean, before the PN addition; this scan is represented in voltammograms by a dotted blue line, 0 mM. CV was performed at a scan rate of 0.1 V/s or between 0.05 – 1 V/s for experiments that underwent with a variation of the scan rate. Successive scans were done for 10 cycles at 0.1 V/s. DPV was performed at a scan rate of 20 mV/s.

3.2.7 X-ray characterization of the PNs [3-8], [3-10], [3-12], and [3-13]

Single crystals of PNs **[3-8]**, **[3-10]**, **[3-12],** and **[3-13]** suitable for X-ray analysis were grown by the slow evaporation of their acetone solutions. X-ray diffraction intensities data were collected at Hunter College, New York at 100 K using a Bruker X8 Kappa Apex II diffractometer, MoKα (0.7107 Å) radiation for **[3-8]** and **[3-13]**, and at Rutgers University (Newark, NJ) at 100 K using a Bruker SMART APEX II CCD Diffractometer, CuKα (1.54178 Å) radiation for **[3-10]** and **[3-12]**.

3.3. Results and discussion

3.3.1 Synthesis

Perfluoroalkyl-substituted PNs **[3-2]** – **[3-4]** (Gorun *et al*., 1989) and amino-substituted PNs **[3-5]** – **[3-7]** (Birchall *et al*., 1970; Ikeno *et al*., 2000; Patel, 2015) Pc precursors were synthesized using the reported procedures to be used as starting materials for future functionalization and/or for the synthesis of symmetric and asymmetric MPcs. Acylated PNs **[3-8]** – **[3-13]** are new compounds, synthesized from the amino-substituted PNs **[3-5]** or **[3-6]**. For their production, two different acylation procedures used different reagents: organic acid anhydrides (Method A) and or-

ganic acid chlorides (Method B). The basicity of the PN amino group is lowered due to the conjugation of the N-lone pair with the benzene ring as well as the electron-withdrawing effect of the nitrile groups and fluorine atoms. The nucleophilicity of the amino N atom decreases for the same reasons. Thus, the reactions between the organic acid anhydrides and the amino-substituted PNs **[3-5]** or **[3-6]**, in the absence of acids do not occur. Sulfuric acid activates the carbonyl group, thus increasing its susceptibility to nucleophilic attack, leading to the formation of amides, Figure 3.6.

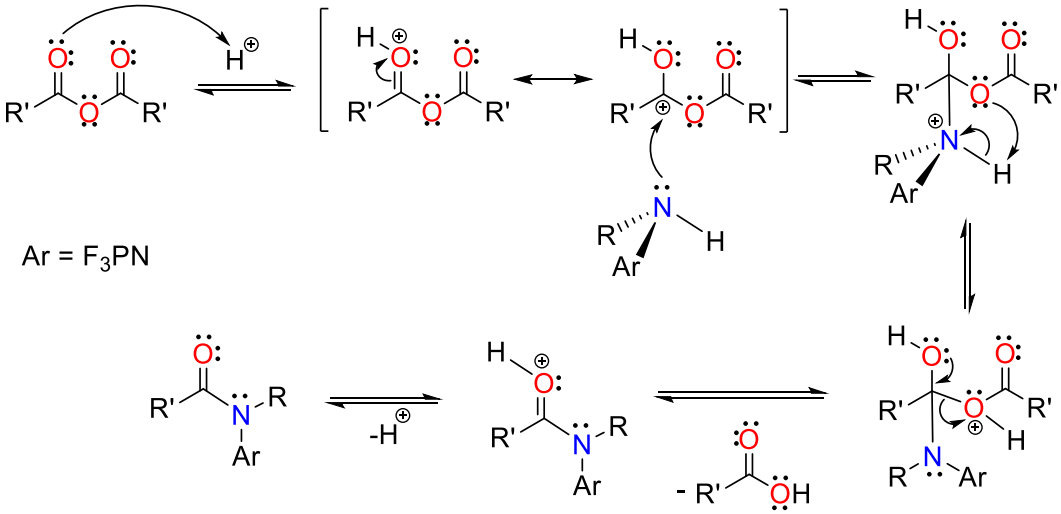


Figure 3.6 Reaction mechanism of acid-catalyzed formation of amides from amino PNs (Bruckner, 2002).

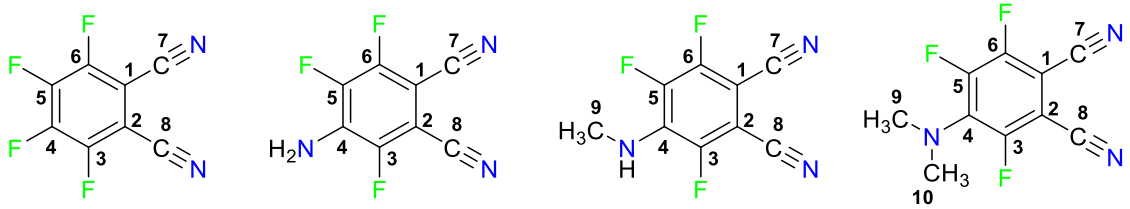
In the case of Method B, the acyl chloride produces as a side product hydrochloric acid, which catalyzes the reaction by activating the carbonyl group the same way sulfuric acid does (Bruckner, 2002).

Method A was used in the synthesis of amido-substituted PNs **[3-8]** – **[3-11]** and succinimidyl-substituted PN **[3-13]** in good yields, ~70%. Both methods were used for the synthesis of acetylated PNs **[3-8]** and **[3-9]**, but higher yields (>90%) and fewer side products were obtained when the acetyl chloride was used. Modification of Method B was considered in the production of **[3-12]**, namely, toluene was added as a high boiling point solvent and the reaction temperature

was increased to 110 °C. These modifications were needed as higher energy is necessary for introducing the second acetyl group.

3.3.2 NMR spectroscopy

The magnetic resonance spectra are shown in Figures A.1 to A.20. Previously reported PNs **[3-1]** and **[3-5]** – **[3-7]** were analyzed by fluorine-decoupled carbon NMR, $^{13}C\{^{19}F\}$, and proton decoupled carbon NMR, $^{13}C\{^{1}H\}$, both data information unreported for these compounds. Fluorine carbon coupling constants were extracted from the spectra and they correspond to the expected values for polyfluorinated aromatics (~250 Hz for 1 bond distance, ~20 Hz for 2 bond distance *ortho*, ~8 Hz for 3 bond distance *meta*, ~3 Hz for 4 bond distance *para*). Assignments of the $^{13}C\{^{19}F\}$ NMR spectra follow chemical structures (Figure 3.7), previously reported data for polyfluorinated aromatics, and electronegativity influence on the chemical shift, Table 3.1.



[3-1] **[3-5]** **[3-6]** **[3-7]**

Figure 3.7 Labeling scheme for carbon atoms of the structures of PNs **[3-1]** and **[3-5]** – **[3-7]**.

Table 3.1 Assignments of the $^{13}C\{^{19}F\}$ NMR chemical shifts of the PNs **[3-1]** and **[3-5]** – **[3-7]**

PN / Assignment	[3-1]	[3-5]	[3-6]	[3-7]
	δ, ppm			
C1	102.29	88.71	87.76	92.36
C2	102.29	100.03	100.08	100.83
C3	145.54	150.8	151.17	154.09
C4	151.24	134.99	135.60	137.40
C5	151.24	141.98	142.26	146.88
C6	145.54	149.63	150.08	151.33
C7	109.95	111.18	111.14	111.21
C8	109.95	111.63	111.61	111.29
C9	-	-	34.11 – 29.88	45.19 – 41.04
C10	-	-	-	

The newly synthesized acylated PNs **[3-8]** – **[3-13]** were characterized by carbon decoupled ^{1}H and ^{19}F NMR. The assignments for the hydrogen atoms, Table 3.2, correspond to expected chemical shift values of the N-H (5 – 10 ppm), N-CH_3 (2 – 4 ppm), O=C-CH_3 (1.5 – 2.5 ppm) from amides (Abraham *et al*., 2013).

Table 3.2 Assignments of the ^{1}H NMR chemical shifts of the PNs **[3-8]** – **[3-13]**

PN / Assignment	[3-8]	[3-9][a]	[3-10]	[3-11][b]	[3-12]	[3-13]
	δ, ppm					
N-H	9.71	-	5.6	-	-	-
N-CH_3	-	3.48	-	3.73	-	-
N-CH_3’		3.22		3.49		
CO-CH_3	2.24	2.34	-	-	2.25	-
CO-CH_3’		1.96				
CO-CH_2	-	-	-	-	-	3.13

a – rotamer mixture, molar ratio N-CH_3 : N-CH_3’ and CO-CH_3 : CO-CH_3’ 1: 1
b – rotamer mixture, molar ratio N-CH_3 : N-CH_3’ 1: 1.5

Assignments of the fluorine NMR signals follow the labeling scheme Figure 3.8. The reported trend in the chemical shifts of the amino PNs **[3-5]** – **[3-7]** (Tanabe *et al*., 1971; Bolton *et*

al., 1978; Kitazume and Nakajima, 2004; Patel, 2015) was used for the aromatic fluorine atoms' assignment. Electronic effects and reported data on perfluorinated carboxylic acids derivatives (Jackson, 2013) were considered for the assignment of the perfluoro-*n*-propyl tails of **[3-10]** and **[3-11]**. Table 3.3 summarizes the assignments of fluorine chemical shits of the PNs **[3-8]** – **[3-13]**.

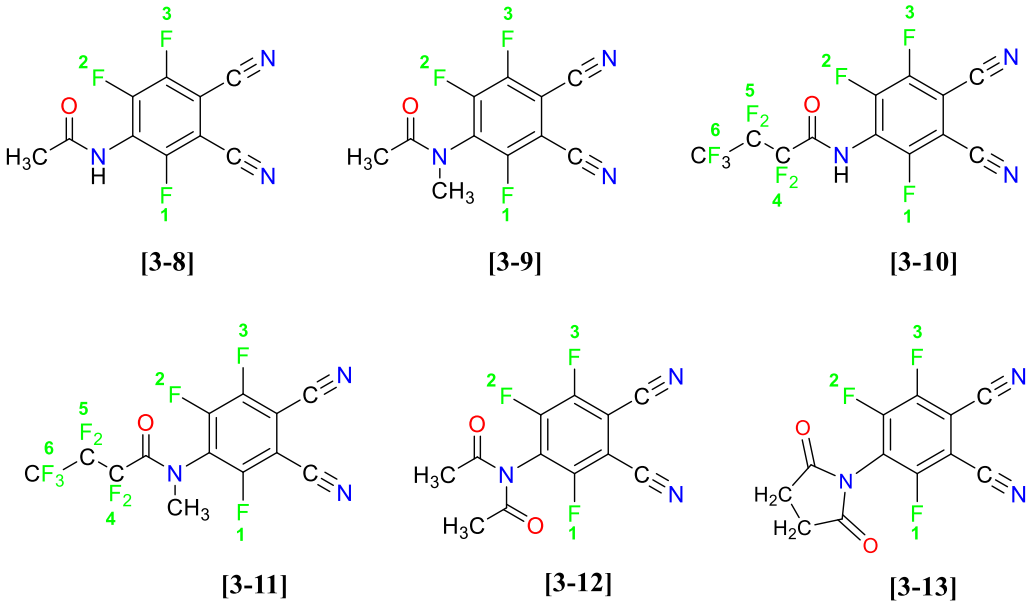


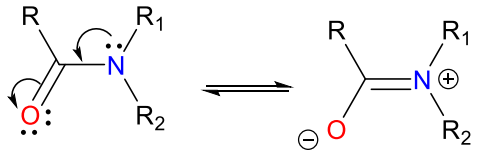
Figure 3.8 Labeling scheme for fluorine atoms from the structures of PNs **[3-8]** – **[3-13]**.

Table 3.3 Assignments of the ^{19}F NMR chemical shifts of the PNs **[3-8]** – **[3-13]**

PN / Assignment	**[3-8]**	**[3-9]**[a]	**[3-10]**	**[3-11]**[b]	**[3-12]**	**[3-13]**
	δ, ppm					
F1	-110.96	-110.05	-110.33	-110.98	-111.78	-108.73
F1’		-112.05		-112.65		
F2	-131.01	-130.61	-129.56	-129.05	-128.60	-129.31
F2’		-128.84		-128.26		
F3	-125.46	-124.98	-124.51	-125.20	-125.73	-122.88
F3’		-126.84		-126.63		
F4	-	-	-119.56	-112.90	-	-
F4’				-113.24		
F5	-	-	-126.61	-125.28	-	-
F5’				-125.44		
F6	-	-	-80.37	-79.69	-	-
F6’				-79.81		

a – rotamer mixture, molar ratio F: F’ 1: 1
b – rotamer mixture, molar ratio F: F’ 1: 1.5

In the case of *N*-methyl derivatives **[3-9]** and **[3-11]** at the NMR time scale a mixture of rotamers was observed at 25 °C. This is common for amido derivatives due to the conjugation of nitrogen with the carbonyl group that hinders the rotation, Figure 3.9 (Stewart and Siddall, 1970; Abraham *et al*., 2013). The hindered rotation is not observed at room temperature in the case of *N*-H derivatives **[3-8]** and **[3-10]** indicating that the methyl group favors the conjugation. Methyl groups have a *+I* inductive effect and, in the *N*-Me derivatives, this effect increases the electron donor capacity of the nitrogen.



I *II*

Figure 3.9 Resonance structures in amide derivatives, *I* – free rotation, *II* – hindered rotation (Smith and March, 2006).

Considering the ^{1}H and ^{19}F NMR chemical shifts of the *N*-H derivatives **[3-8]** and **[3-10]** it was possible to distinguish between the rotamer peaks of *N*-methyl derivatives **[3-9]** and **[3-11]**. Furthermore, in the case of **[3-11]** the ratio between rotamers is 1: 1.5, a value that confirms the assignments and the rationalized trend.

3.3.3 FT-IR spectroscopy

The FT-IR spectra are presented in Figures B.1 to B.9. Spectral data confirms the proposed structures. Vibrations of C-F corresponding to polyfluoroaromatics and polyfluoroaliphatics (1350 – 1100 cm^{-1}), and of C=C aromatic (1600-1575 and 1500-1450 cm^{-1}) are observed for the perfluoroalkyl-substituted PNs **[3-2]** – **[3-4]**. Vibrations of N-H (3325 – 3050 cm^{-1}), C-H aliphatic (3000 – 2800 cm^{-1}) and C=O (1750 – 1650 cm^{-1}) corresponding to amides or imides (2 asymmetric C=O stretches) together with C≡N (2300 – 2200 cm^{-1}) and aromatic C-F (~1250 cm^{-1}) vibrations are being observed for the acylated PNs **[3-8]** – **[3-13]**. Some aspects regarding the nitrile vibrations are under consideration for the following discussion.

The perfluoroalkyl-substituted PNs **[3-2]** – **[3-4]** lack almost completely the nitrile stretch present in the fluorinated PN **[3-1]**, a fact attributed to the presence of perfluoro-*iso*-propyl groups, strong EWG. Medium to weak intensities were observed for the nitrile vibrations also in the case of acylated PNs **[3-8]** – **[3-13]** compared to the strong intensities seen for the corresponding amino PNs **[3-5]** and **[3-6]** (Patel, 2015), as the electron donor effect of the nitrogen decreases upon acylation. Acylation resulted also in a small increase in the wavenumber of the nitrile stretch by ~10 cm^{-1} vs. the parent amino PNs.

3.3.4 UV-Vis spectroscopy

The wavelengths of the main absorptions are compared with perfluorinated PN **[3-1]**, Table 3.4 considering bathochromic and hypsochromic shifts for 4 main absorption bands (*I* - *IV*). The

UV-Vis spectra of all tested PNs, Figures D.1 and D.2, show strong similarities between the PNs **[3-1]** – **[3-4]** and **[3-8]** – **[3-13]**, while the amino-substituted PNs **[3-5]** – **[3-7]** present big separations for the 4 absorption bands, as well as a gradual bathochromic shift. The wavelength values are summarized in Table 3.4 and a graphic representation is given in Figure 3.10.

Table 3.4 Main absorption bands for the PNs **[3-1]** – **[3-13]** in the UV region

Band / PN	*I*	*II*	*III*	*IV*
	λ, nm			
[3-1]	204	238	247	297
[3-2]	204	240	248	320
[3-3]	216	242	249	312
[3-4]	<200	-	251	300
[3-5]	206	234	278	320
[3-6]	206	244	290	334
[3-7]	208	252	304	348
[3-8]	210	224	289	308
[3-9]	206	228	280	308
[3-10]	210	250	296	306
[3-11]	210	248	296	306
[3-12]	208	250	296	306
[3-13]	208	254	296	306

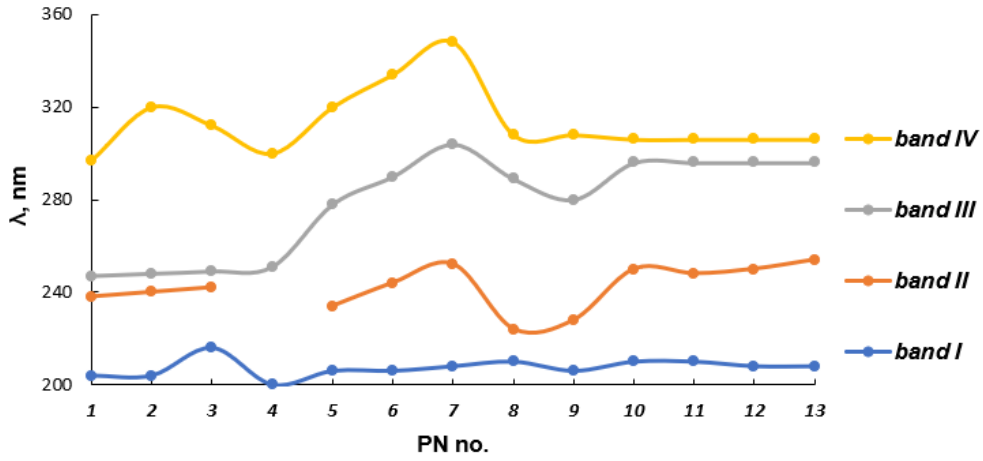


Figure 3.10 Graphic representation of the absorption bands' variation depending on the PN type.

Very small variations are being noticed for band *I* for all tested PNs. Bands *II* and *III* show small variations for the perfluoroalkyl PNs **[3-2]** – **[3-4]**, band *IV* shows a bathochromic shift of 20 nm for **[3-2]**, which is decreasing to half that value for **[3-3]**; no variation is seen for **[3-4]**. The conjugation of the amino group with the aromatic ring shows a bathochromic shift, for the bands *II-IV* of the PNs **[3-5]** – **[3-7]**, which increases linearly with the nitrogen methylation degree. Acylation breaks the conjugation between the amino group and the aromatic ring as the carbonyl group is a strong electron-withdrawing group; this can be seen in the variation of the bands *I-III* for PNs **[3-8]** and **[3-9]**. The addition of the perfluoro-*n*-propyl radical or 2 acyl groups, PNs **[3-10]** – **[3-13]**, does not have any more influence on the absorption bands, as the spectra are similar to those observed for PNs **[3-1]**. This indicates a break in the amino group conjugation with the aromatic ring.

3.3.5 Electrochemistry

CV and DPV characterizations were performed for the PNs **[3-1]** – **[3-7]**, the voltammograms are present in Figures E.1 to E.28 and the redox potential data are listed in Table 3.4 for the reduction reactions, and in Table 3.5 for the oxidation reactions, respectively. An electrochemical potential of -1.21 V, irreversible process, was reported previously for the 1st reduction wave of PN **[3-1]**, the CV measurements were performed in ACN, saturated calomel electrode (SCE) was used as a reference, the working and counter electrodes are not being specified, (Petit *et al*., 1991). Half-wave potentials ($E_{1/2}$) and the difference between the coupled redox potentials (ΔE) were calculated for the reversible reductions of the PNs **[3-2]** and **[3-3]** and the semi-reversible reduction of **[3-7]**, Table 3.5. PNs **[3-1]** – **[3-4]** showed only reduction behavior, as the molecules, structurally, present nitrile groups, but do not contain functional groups susceptible to

oxidation. On another part, the amino-substituted PNs **[3-5]** – **[3-7]** show both reduction and oxidation behavior as they present nitrile and amino groups.

Table 3.5 Reduction potentials (***E*$_{red}$**) from CV (0.1 V/s) and DPV of PNs **[3-1] – [3-7]**

	E*$_{red}$, *V								
Method:	***CV***				***DPV***				
Wave / PN	***I***	***II***	***III***	***IV***	***I***	***II***	***III***	***IV***	***V***
[3-1]	-1.12*	-1.28	-	-	-1.05	-	-	-	-
[3-2]	$E_{1/2}$ = -0.41 ΔE = 0.08	-1.34	-1.52	-1.83	-0.39	-1.23	-1.45	-1.77	-
[3-3]	$E_{1/2}$ = -0.40 ΔE = 0.08	-1.32	-1.67	-	-0.39	-0.68	-1.23	-1.49	-1.90
[3-4]	-0.93	-1.32	-1.61	-	-0.85	-1.54	-	-	-
[3-5]	-1.36	-1.56	-	-	-1.47	-	-	-	-
[3-6]	-1.35	-1.54	-	-	-1.48	-	-	-	-
[3-7]	$E_{1/2}$ = -1.38 ΔE = 0.10	-1.88	-	-	-1.35	-1.72	-1.81	-	-

* -1.21 V (Petit *et al.*, 1991)

Table 3.6 Oxidation potentials (***E*$_{ox}$**) from CV (0.1 V/s) and DPV of PNs **[3-1] – [3-7]**

	E*$_{ox}$, *V		
Method	***CV***	***DPV***	
Wave / PN	***I***	***I***	***II***
[3-1]	-	-	-
[3-2]	-	-	-
[3-3]	-	-	-
[3-4]	-	-	-
[3-5]	1.81	1.82	-
[3-6]	1.80	1.70	-
[3-7]	1.88	1.69	1.76

CV measurements were performed for identifying the redox coupled transformations, while DPV measurements quantify the redox potentials with higher precision. Analyzing the first reduction

potentials (E_{red}) of the PNs, extracted from the DPV measurements (Table 3.5), the following trend **[3-2]** ~ **[3-3]** < **[3-4]** ~ **[3-1]** < **[3-7]** ~ **[3-5]** ~ **[3-6]** is noted. The E_{red} agrees with the electronic effects of the *para* (σ_p) and *meta* (σ_m) substituents, a good correlation (R^2 ~ 0.98) with the sum of the Hammett constants ($\Sigma\sigma$) (Hammett, 1937; Hansch, 1991) was obtained, Figure 3.11.

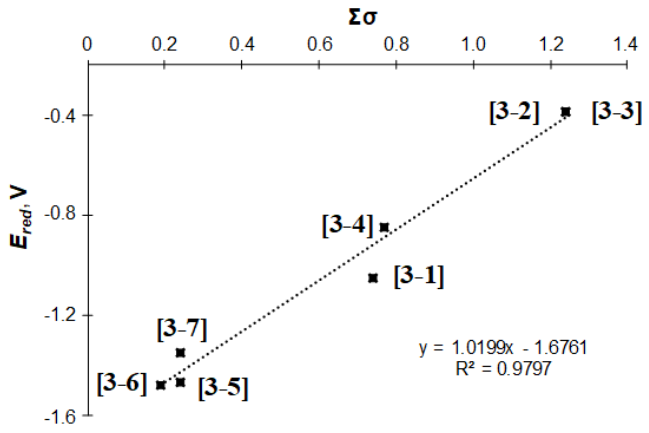


Figure 3.11 E_{red} correlation with the Hammett constants.

Considering the tetrafluoro-PN **[3-1]** as the reference point we can see how the introduction of perfluoroisopropyl substituents (electron-withdrawing groups) in the *para* position vs. the first cyano group decrease substantially the reduction potential of the resulted PNs **[3-2]** and **[3-3]** while the same substituents introduced in *ortho* and *meta*, PN **[3-4]**, has only a minor influence. The introduction of an amino substituent (electron donor group) in the *para* position vs. the first cyano group shifts the potential in the other direction strongly increasing the reduction potential. These observations reinforce the correlation of the electrochemical potential with the Hammett constants specific for the nature and position of the substituents.

3.3.6 Crystal structures

Out of the 6 newly synthesized PNs, only 4 were solids at room temperature. All 4 solid PNs crystallized from acetone solutions offering X-ray quality crystals. Their X-ray structures con-

firmed the proposed chemical composition and revealed detailed geometrical features. The color code used for the crystal representations of **[3-8]**, **[3-10]**, **[3-12]**, and **[3-13]** is the same as in their structural formulas, Figure 3.8

[3-8]: Crystal data, data collection, and refinement parameters are summarized in Table F.1. The structure was solved using direct methods and standard difference map techniques and was refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 2014/7) (Sheldrick, 1981; 2008; 2015). TWINABS (Version 2012/1) was used to account for non-merohedral twinning (Sheldrick, 2012).

[3-10]: Crystal data, data collection, and refinement parameters are summarized in Table G.1. **[3-12]**: Crystal data, data collection, and refinement parameters are summarized in Table H.1. The structures of **[3-10]** and **[3-12]** were refined by full-matrix least-squares based on F^2 with all reflections (SHELXTL V5.10; G. Sheldrick, Siemens XRD, Madison, WI) (Bruker 2005; 2016). Non-hydrogen atoms were refined with anisotropic displacement coefficients, and hydrogen atoms were treated as an idealized contribution. SADABS (Sheldrick, SADABS 2008), 12 G.M. SADABS (2.01), Bruker/Siemens Area Detector Absorption Correction Program; (Bruker AXS: Madison, WI, 1998) absorption correction was applied (Sheldrick, 2008 & 2015).

[3-13]: Crystal data, data collection, and refinement parameters are summarized in Table I.1. The structure was solved using direct methods and standard difference map techniques and was refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 2017/1) (Sheldrick, 1981, 2008 & 2015). All hydrogen atoms were placed in calculated positions and refined with a riding model [U_{iso}(H) = 1.2–1.5U_{eq}(C)].

The crystal formed by PN **[3-8]**, Figure 3.12 was a non-merohedral twin. However, it refined well using *TWINABS* for the absorption correction and HKLF 5 data. The X-ray structure

of **[3-8]** represented as ORTEP in Figure F.1 and full data are listed in Tables F.2 to F.7. There are 4 molecules per unit cell, Figure 3.12. The molecules form one-dimensional chains along the b-axis due to hydrogen bonding between the amino and the carbonyl on another molecule, N-H···O=C-, at 2.029 Å, Figure 3.13.

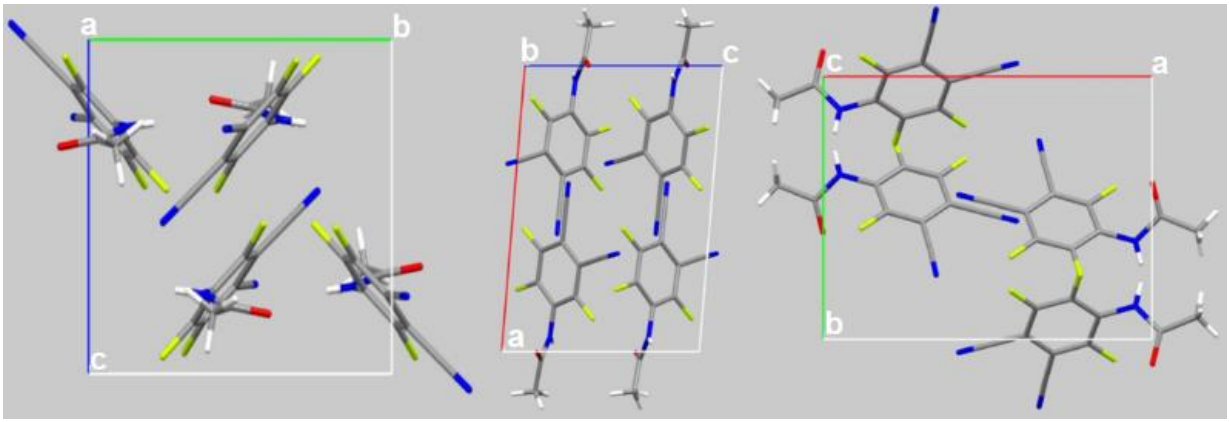


Figure 3.12. Packing diagrams viewed along the crystallographic a-axis (left), b-axis (center), and c-axis (right).

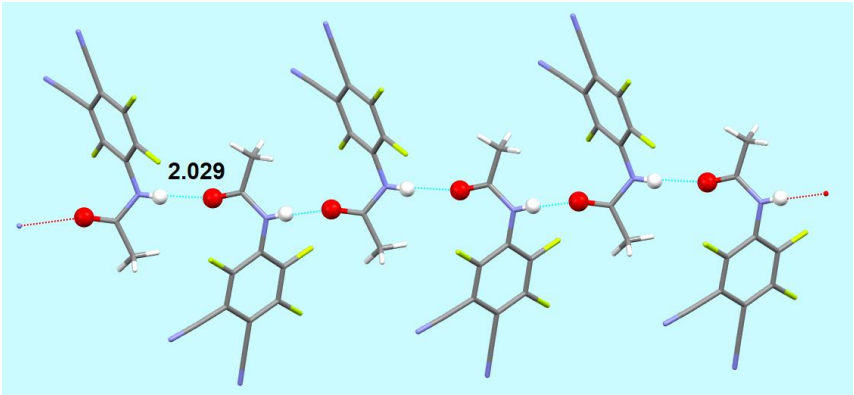


Figure 3.13 Representation of the hydrogen bonding network present in the crystal of **[3-8]**.

PN **[3-10]** formed crystals that had multiple domains, the main one in 50% proportion. The perfluoro-*n*-propyl tail was disordered and was modeled in part using a 20:80 occupancy of 2 sites. The software feature "Cellnow" was used for the structural elucidation. Some of the minor components were refined isotropically. The ORTEP representation shows the molecule being mirrored, Figure G.1. Full data are listed in Tables G.2 to F.5. Same as for the PN **[3-8]** the ami-

no group is interacting with the carbonyl on another molecule by H-bonding, N-H···O=C, 2.742 Å intermolecular interactions, Figure 3.14. The unit cell of the crystal has 8 molecules, the arrangement along the axes is showed in Figure 3.15.

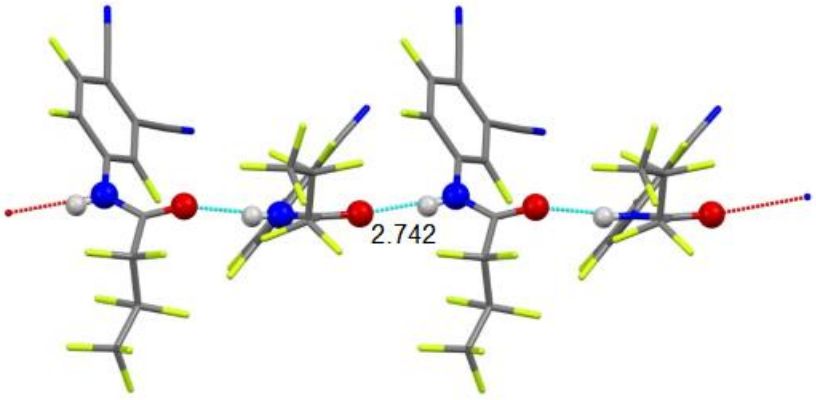


Figure 3.14 Graphic representation of the hydrogen bonding present in the crystal of **[3-10]**.

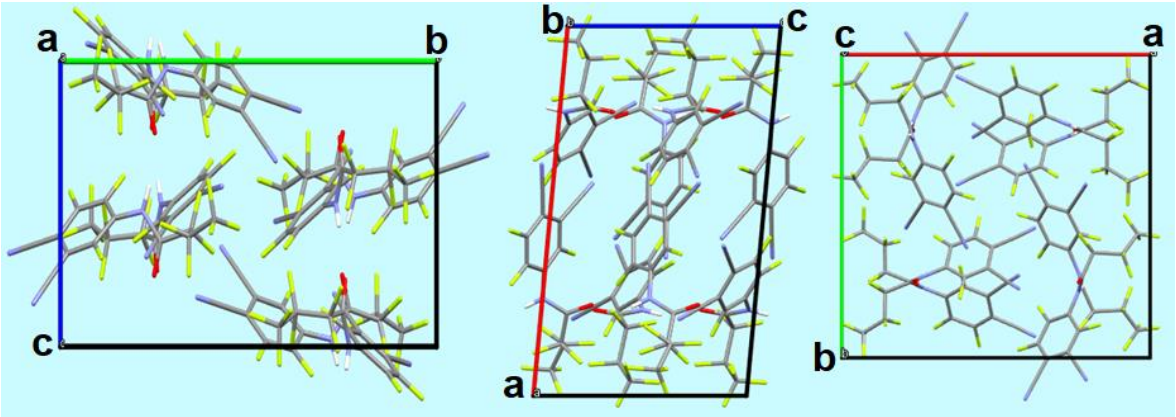


Figure 3.15 Graphic representation of the unit cell of the crystal of **[3-10]**, views along **a**-axis (left), **b**-axis (center), and **c**-axis (right).

In the case of **[3-12]** structure, the solid-state X-ray analysis of the crystals shows very good planarity for the acylated nitrogen atom. Van der Waals interactions are being established between molecules, Figure 3.16. The X-ray structure of **[3-12]** represented as ORTEP in Figure H.1 and full data are listed in Tables H.2 to H.5. The unit cell of the crystal contains 8 molecules; their arrangement is showed in Figure 3.17.

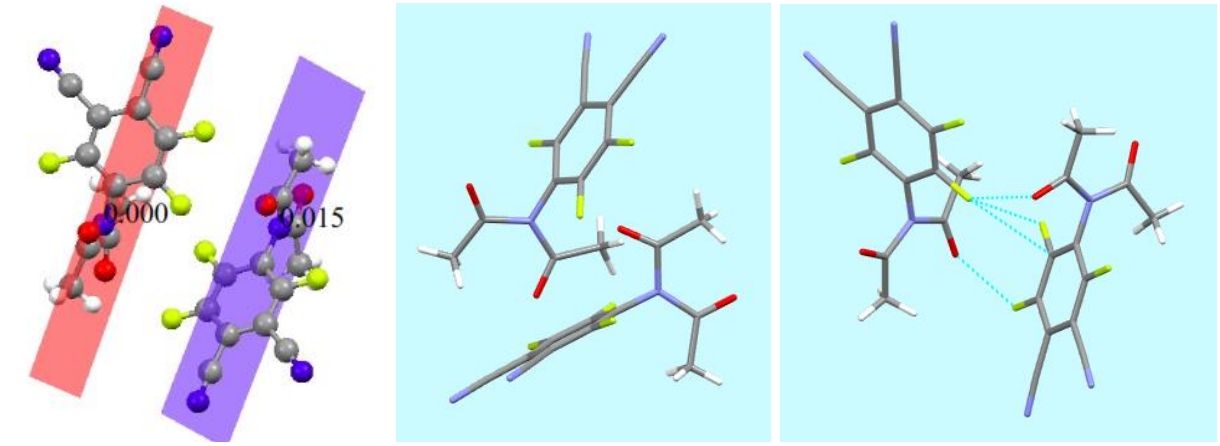


Figure 3.16 Graphic representations for the planarity of the acylated nitrogen atom (left and center) and short contact (Van der Waals) interactions in the crystal of **[3-12]**.

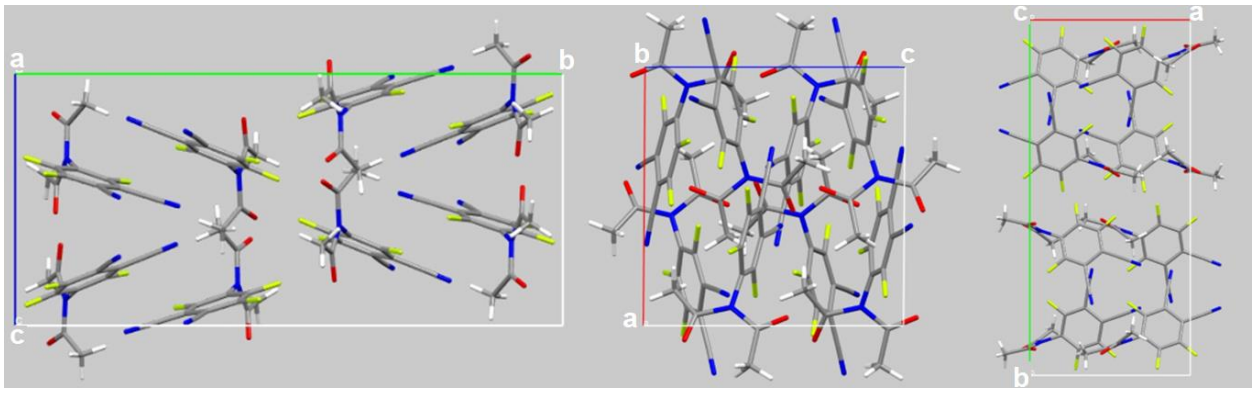


Figure 3.17 Graphic representation of the unit cell of the crystal of **[3-12]**, views along **a**-axis (left), **b**-axis (center), and **c**-axis (right).

The data recorded for the **[3-13]** PN's crystal had no complications. The X-ray structure of **[3-13]** represented as ORTEP is present in Figure I.1 and full data are listed in Tables I.2 to I.6. The succinimidyl substituent *vs.* the aromatic ring is tilted with a 60.56° angle and Van der Waals interactions are being established between these 2 different rings, Figure 3.18. The unit cell of the crystal contains 8 molecules, shown in Figure 3.19.

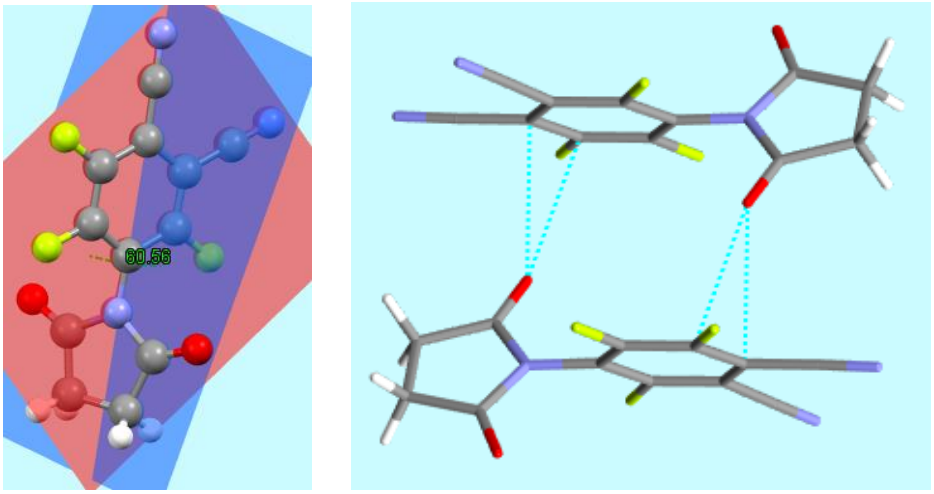


Figure 3.18 Graphic representations for the succinimidyl ring's position vs. the aromatic ring, 60.56° angle (left) and short contact (Van der Waals) interactions (right) in the crystal of **[3-13]**.

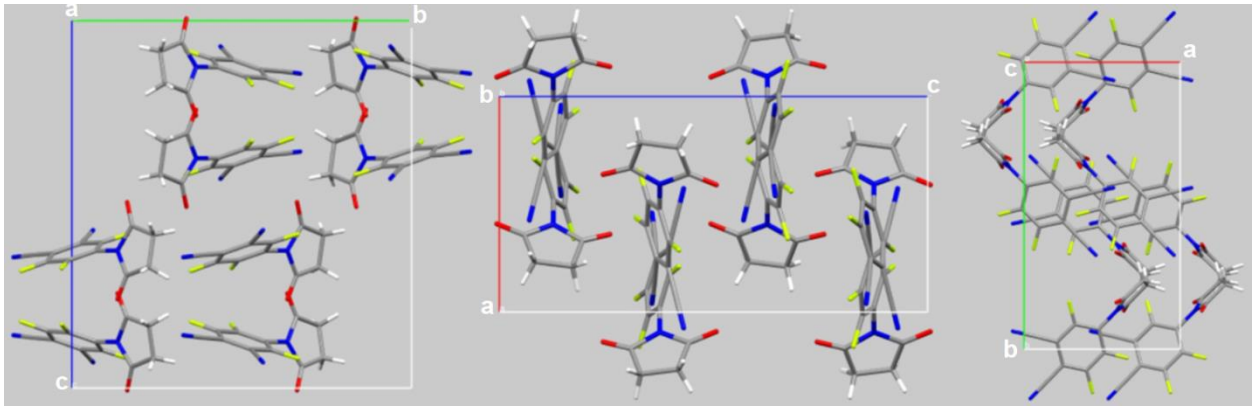


Figure 3.19 Graphic representation of the unit cell of the crystal of **[3-13]**, views along **a**-axis (left), **b**-axis (center), and **c**-axis (right).

The planarity of the nitrogen and the angles of the amides **[3-8]** and **[3-10]** as well as imides **[3-12]** and **[3-13]** are evidence of the exocyclic N sp^2 hybridization. By acylation, the position of nitrogen's lone pair relative to the aromatic ring is being changed from perpendicular in the aromatic amines, as was shown in the X-ray structure of **[3-6]** (Patel, 2015), to different angles, Figures 3.19 and 3.20. The exocyclic N lone pair is thus not available for conjugating with the aromatic ring.

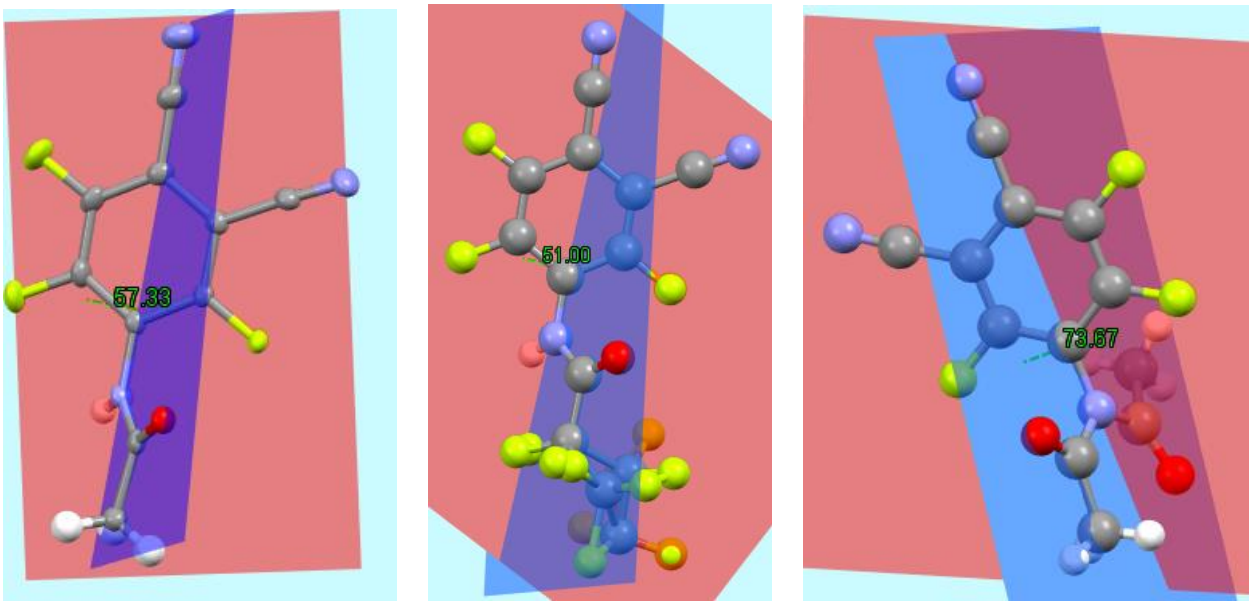


Figure 3.20 Graphic representations for the amide position (blue plane) vs. the aromatic ring (red plane), 57.33° angle for **[3-8]** (left), 51.00° angle for **[3-10]** (center), 73.67° angle for **[3-12]** (right).

3.4. Conclusions

Perfluoroalkyl- and amino-substituted PNs were synthesized by aromatic nucleophilic substitution. Spectral and electrochemical characterizations were performed to complete the previously reported data. The perfluoroisopropyl groups have a strong influence on the nitrile stretch in the FT-IR measurements, reducing almost completely the vibration. A good correlation was found between the reduction potentials and Hammett constants, reinforcing the influence of the substituents' position and nature on the reduction potential.

Acylated derivatives were obtained from the amino-substituted PNs, characterized by spectral techniques, and X-ray quality crystals were obtained for the solid materials. The newly synthesized PNs belong to 2 classes, amido, and imido derivatives. The *N*-methyl acylated derivatives were produced as a mixture of rotamers, oils in ambient conditions. The rotamer ratios in acetone solution were determined by ^{1}H and ^{19}F NMR and it is influenced by the acylating agent's nature.

The change in the electron donor capacity, as we go from amines to amides, has a great influence on the UV-Vis absorption. The main absorption bands are similar to the ones obtained for the perfluoroalkylated PNs and can be interpreted as a loss in conjugation between the nitrogen and the aromatic ring. This idea is being supported also by the X-ray analysis of the solid-state crystals of 4 of the acylated PNs that indicate the exocyclic conjugation and a change in angle for the lone pair of the nitrogen.

The present study brings valuable information for the synthesis and characterization of MPc as the described PN structures will represent between one and 4 quarters of the Pc ligand.

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CHAPTER 4

SYNTHESIS AND CHARACTERIZATION OF FIRST GENERATION, NON-FUNCTIONALIZED PERFLUORINATED METAL PHTHALOCYANINES

4.1 Introduction

The large family of perfluorinated phthalocyanines (Pcs) can be divided, based on the nature of the substituents, into two categories: (i) Pcs substituted only with aromatic fluorine atoms, and (ii) Pcs with both aromatic fluorine atoms and aliphatic fluorinated substituents attached on the Pc ligand (Bench, Beveridge *et al.*, 2002; Bench, Brennessel *et al.*, 2002; Loas, 2012; Stuzhin, 2014; Patel, 2015). The present chapter is focused on the perfluorinated metal Pcs, F_{16}PcM series, and perfluorinated alkyl-substituted metal Pcs, F_nPcM series (n = 40, 52, 64).

Perfluorinated or hexadecafluoro metal phthalocyanines, F_{16}PcM, introduced in the 1960s, started to receive attention in the early ’90s mainly due to their applications in molecular electronics and catalysis. A large number of metal complexes were described for the ligand $F_{16}Pc^{2-}$ starting with the first and second 3*d* and 4*d* transition metals and expanding towards post-transition metals and metalloids.

The Zn(II), Cu(II), Co(II), Fe(II), O=Ti(IV), O=V(IV), Ru(II), Sn(IV), Zr(IV) F_{16}Pc complexes were recently reviewed (Stuzhin, 2014). Complexes that were not included in the review are those of Ni(II) (Muzikante *et al.*, 2007), Ge(IV) (Slodek *et al.*, 2006; Slodek, 2010), and Al(III) (Basova *et al.*, 2013). Complexes of Co(III) (Goodwin *et al.*, 2015), Cd(II) (Baréa *et al.*, 2017), Pd(II) (Parkhomenko *et al.*, 2017; Sukhikh *et al.*, 2018), Mn(II) (Denekamp *et al.*, 2019), and Pb(II) (Kuprikova *et al.*, 2020), with applications in catalysis and thin films, have been reported since 2014. A few theoretical studies on the influence of fluorination and metal type on Pc

properties were aimed at the yet unreported complexes of Sc, Cr, Ca, Ag (Cárdenas-Jirón *et al.*, 2012; Arillo-Flores *et al.*, 2013; Fadlallah *et al.*, 2016; Klyamer *et al.*, 2019).

The synthesis of perfluorinated metal Pcs starts with the perfluorinated phthalonitrile PN **[3-1]**, which reacts with a metal source (metal salt or even metal powder), with or without solvent to produce the desired F_{16}PcM, Figure 4.1.

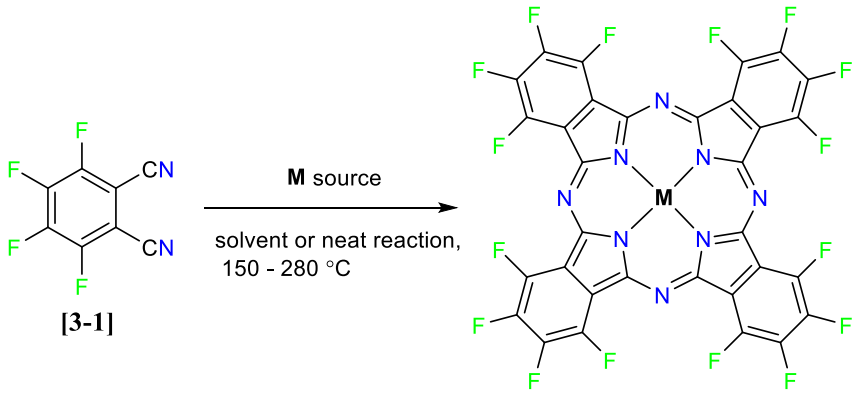

Figure 4.1 Reaction scheme for the synthesis of hexadecafluoro metal Pcs, F_{16}PcM. Additional metal ligands needed to render the complexes neutral are shown in parentheses.

The F_{16}PcM derivatives, relative to the parent H_{16}PcM complexes benefit from the electronegativity of aromatic fluorine atoms by exhibiting increased thermal stability, increased solubility in organic solvents, and higher resistance to oxidation, but suffer easily nucleophilic substitutions and still aggregate by π-π stacking (Stuzhin, 2014; Leznoff *et al.*, 2004; Nemykin and Lukyanets, 2010). To decrease the nucleophilic susceptibility, hinder aggregation, and enhance the solubility further, the introduction of bulky perfluoroalkyl substituents proved to be a good strategy regardless of the type of metal (Bench, Beveridge *et al.*, 2002; Carrión *et al.*, 2018).

Perfluoro(octakis-*iso*-propyl) metal Pcs, F_{64}PcM series, exhibit enhanced solubility, increased stability to oxidative conditions, and higher electron deficiency *vs.* the F_{16}PcM analogs. Metal complexes of the $F_{64}Pc^{2-}$ ligand have been reported, starting with Zn(II) (Bench, 2001;

Bench, Beveridge *et al.*, 2002), Co(II) (Bench, 2001; Bench, Brennessel *et al.*, 2002), Fe(II) (Lee, 2003), Ru(II) (Lee, 2003; Gorun *et al.*, 2009), Cu(II) (Moons *et al.*, 2010), O=V(IV) (Łapok *et al.*, 2011), Mg(II) (Gorun *et al.*, 2009; Kopeć *et al.*, 2014), Pt(II) (Gerdes, 2008), Pd(II) (Gerdes, 2008), Al(III) (Gorun *et al.*, 2009; Łapok *et al.*, 2016 Al, Ga, In), Ga(III) (Gorun *et al.*, 2009; Łapok *et al.*, 2016 Al, Ga, In; Pelmuş *et al.*, 2016), In(III) (Gorun *et al.*, 2009; Łapok *et al.*, 2016 Al, Ga, In; Pelmuş *et al.*, 2016), Lu(III) (Graham, 2012; Gonidec *et al.*, 2013), Y(III) (Graham, 2012), Tb(III) (Graham, 2012; Gonidec *et al.*, 2013), and Dy(III) (Graham, 2012). A new member of the F_{64}PcM family, F_{64}PcNi(II), is reported here.

Part of the F_{64}PcM series was reviewed recently together with representatives of the functionalized perfluoroalkyl-substituted Pcs class to highlight its enhanced photoactivity vs. F_{16}PcM and H_{16}PcM series (Carrión *et al.*, 2018). The synthesis of the F_{64}PcM series starts with the perfluorinated phthalonitrile PN **[3-2]**, which reacts with a metal source (metal acetates, chlorides, carbonyls, or acetylacetonates), with or without solvent, under microwave irradiation, Figure 4.2.

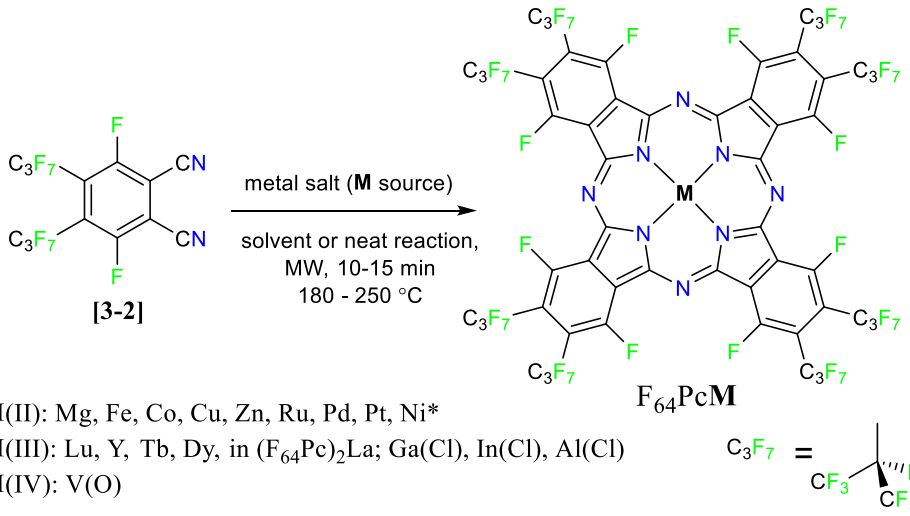

Figure 4.2 Reaction scheme for the synthesis of perfluoro(octakis-*iso*-propyl) metal Pcs, F_{64}PcM. Additional metal ligands needed to render the complexes neutral are shown in parentheses. MW = microwave radiation. *F_{64}PcNi - new compound.

By reacting the PNs **[3-1]** and **[3-2]** with different metal(II) acetates, mixed Pcs were produced for cobalt(II) and zinc(II) (Patel, 2015), and copper(II) (Nguyen *et al.*, 2020), Figure 4.3. These complexes are subject to aggregation and nucleophilic substitution due to the presence of one and two tetrafluoro-substituted quadrants in the structures of F_{52}PcM and F_{40}PcM, respectively.

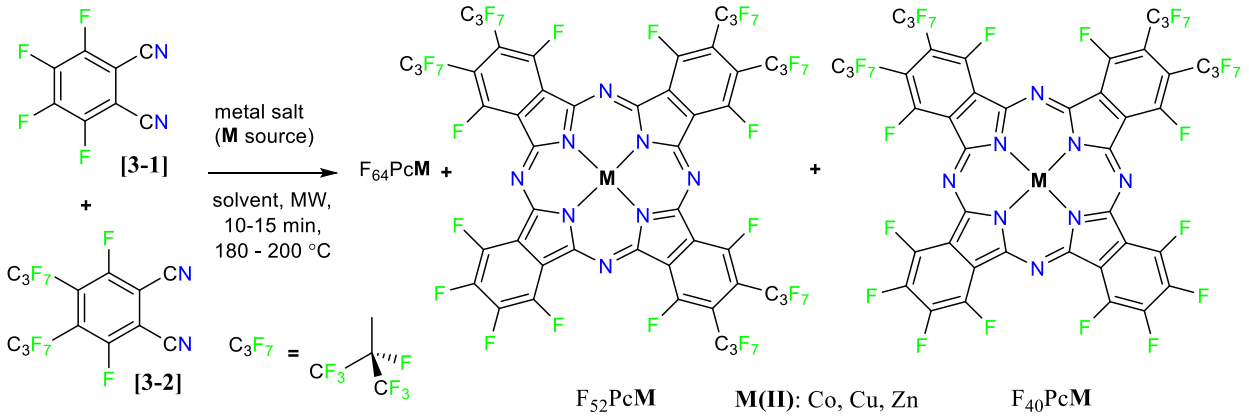

Figure 4.3 Reaction scheme for the synthesis of mixed perfluoro(octakis-*iso*-propyl) metal Pcs, F_nPcM, n = 40, 52, 64.

4.2 Experimental

4.2.1 General procedures for the synthesis and purification of fluorinated MPcs

Synthesis

Metal salt (excess) and PN(s) (a single type or a mixture of two different PNs) were suspended under magnetic stirring in a high boiling point solvent ($PhNO_2$, n-pentanol, or a mixture $PhNO_2$ with a few drops of DMF) in a 10 mL glass vial. The vial was sealed with a Teflon cap. The mixture was stirred for 5 min and heated stepwise, ramped from room temperature to 100 °C in max. 2 min, hold additional 2 min, ramped with additional 20 °C and hold every time for 2 min, in a microwave (MW) reactor, to the optimum reaction temperature, 180 – 200 °C range, where was held for an additional 10 min.

Purification

The purification process consists of a series of steps due to the complexity of the resulted reaction mixture: unreacted metal salts and PNs, organic impurities (side products), high boiling point solvents, and MPcs.

Step 1: Removal of unreacted metal salts.

The reaction mixture was dissolved in ethyl acetate, filtered, washed in a separatory funnel with water (2 times), and with brine. The organic layer was dried with anhydrous magnesium sulfate and the solvent was removed under reduced pressure to give a solid residue.

Step 2: Material recovery in powder form.

After the solvent removal, 3-5 mL of DCM or petroleum ether were added to the solid residue. The solid material, usually attached to the glass walls of the flask, was removed mechanically. The resulting suspension was refluxed, and the isolated solid was crushed into a fine powder.

Step 3: Removal of organic impurities and unreacted PNs.

The powder was placed on a filter paper and washed with hexanes, toluene, DCM, and ACN or ACN/water 10-60% mixtures. The process of removing the organic impurities was monitored by TLC and/or UV-vis analysis. If organic impurities were still present (after solvent washings), sublimation, recrystallization, and/or normal phase column chromatography were used for further purification.

Step 4: Separation of MPcs mixtures.

In the cases where two PNs were used, the resulting phthalocyanines were separated by normal phase column chromatography. The specific solvent mixtures are given for each compound.

4.2.2 Synthesis of hexadecafluoro zinc(II) Pc, F_{16}PcZn [4-1]

1,2,3,4,8,9,10,11,15,16,17,18,22,23,24,25-hexadecafluoro zinc(II) phthalocyanine, **F_{16}PcZn**, **[4-1]**: 200 mg (1 mmol) of **[3-1]** PN were mixed with 60 mg (0.33 mmoles) of anhydrous zinc acetate and 0.25 mL of nitrobenzene in a MW vial. The mixture was stirred for 5 min and heated (MW irradiation) stepwise, ramped from room temperature to 100 °C in max. 2 min, then held for an additional 2 min, followed by increasing the temperature to 200 °C in 20 °C steps and held every time for 2 min and, finally, keeping the temperature at 200 °C for an additional 10 minutes. After cooling, the material was washed with water and organic solvents (toluene, DCM, ACN) until no more impurities were detected by TLC (silica gel, acetone: hexane 1:1). The material was dissolved in hot ethyl acetate, filtered, and isolated as a blue powder, see section **4.2.1**. The powder was dried in the oven at 100 °C, yielding 143 mg (66% yield) of **[4-1]**. Spectroscopic data agreed with the literature (Birchall *et al.,* 1970). ^{19}F NMR (376 MHz, methanol-d_4, CF_3Cl 0.00 ppm) δ, ppm: -140.73 (d, J = 10.5 Hz, 8 F), -147.73 (d, J = 10.8 Hz, 8 F). Another 2 broad peaks, with low intensity, are present in the ^{19}F NMR spectrum at -142.19 and -154.02 ppm due to aggregation. In the conventional synthesis of F_{16}PcZn, the PN **[3-1]** was reacted with zinc dust in boiling α-chloronaphthalene or in neat conditions with ZnI_2, or $ZnBr_2$ to afford F_{16}PcZn in 67 – 87% yields after 1.5 h of heating at 250 °C (Birchall *et al.,* 1970).

4.2.3 Synthesis of octakis(perfluoroisopropyl) MPcs, F_{64}PcM(II) M = Zn [4-2], M = Cu [4-3], M = Co [4-4], M = Ni [4-5], and F_{64}PcM(III)Cl, M = Ga [4-6], M = In [4-7]

1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octakis(perfluoroisopropyl) metal(II) phthalocyanines, **F_{64}PcM**: F_{64}PcZn **[4-2]**, F_{64}PcCu **[4-3]**, and F_{64}PcCo **[4-4]** were synthesized and purified following reported procedures (Bench, Beveridg *et al.*, 2002; Gorun *et al.*, 2009). The spectroscopic data confirmed the identity and purity of the products. ^{19}F NMR was obtained

for the F_{64}PcZn **[4-2]** also in 10% acetone-*d_6* in ethyl acetate to compare with the data from F_{64}PcNi **[4-5]**, obtained in this solvent mixture due to its low solubility in acetone-*d_6*. ^{19}F NMR (376.5 MHz, 10% acetone-*d_6* in ethyl acetate, $CFCl_3$ 0.00 ppm) δ, ppm: -71.55 (dt, *J* = 33.6, 8.0 Hz, CF_3, 48 F), -103.30 (ddq, *J* = 67.5, 34.0, 16.2 Hz, aromatic F, 8F), -164.70 (s, aliphatic F, 8F).

1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octakis(perfluoroisopropyl) nickel(II) phthalocyanine, **F_{64}PcNi [4-5]**:

A mixture of nickel acetate hydrate, $Ni(AcO)_2 \cdot xH_2O$ (x = 0, 2, and 4) (50 mg, ~0.2 mmol), and perfluoro-(4,5-di-isopropyl)phthalonitrile **[3-2]**, (200 mg, 0.4 mmol) was placed in a 10 mL MW vial with 10 drops of $PhNO_2$ and 3 drops of DMF. The vial was sealed, heated stepwise, ramped from room temperature to 100 °C in max. 2 min, hold additional 2 min, ramped with additional 20 °C and hold every time for 2 min, and kept for 10 min at 200 °C (MW irradiation). The crude product was dissolved in ethyl acetate and washed with water and brine to remove the unreacted metal salt. After drying, with $MgSO_4$ anh. and solvent evaporation, the organic mixture was loaded on silica gel. The purification by column chromatography was performed using normal phase, silica gel, and a gradient of up to 30% ethyl acetate in hexanes as mobile phase. After solvent removal, the product was isolated as a fine greenish-blue powder, see section **4.2.1**. The solid was dried at 100 °C. F_{64}PcNi **[4-5]**, $C_{56}F_{64}N_8Ni$, 2059.26 g/mol, yield: 73 mg (35%), mp > 300 °C. UV-Vis (TFT) λ, nm (log ε): 680 (6.39), 611(5.65), 354 (5.72), 290 (5.75). ^{19}F NMR (376.5 MHz, acetone-*d_6*, $CFCl_3$ 0.00 ppm) δ, ppm: -71.56 (dt, *J* = 33.1, 7.9 Hz, CF_3, 48 F), -103.01 – -103.81 (m, aromatic F, 8F), -164.88 (s, aliphatic F, 8F). FT-IR (KBr disk) *ν*, cm^{-1}: 1605.59, 1535.38, 1460.37, 1253.59, 1169.63, 1103.80, 1061.64, 986.75, 959.31, 871.21, 785.95, 765.82,

755.60, 732.72, 723.68, 544.40, 458.27. HRMS (-ve ESI): calcd for [M+Cl$^-$] ($C_{56}F_{64}N_8NiCl^-$) 2092.8446; obsd: 2092.8260. $|M_{calcd}-M_{obsd}|/M_{calcd}\cdot 10^6$ = 9 ppm. The Cl was adventitious.

Chloro-(1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octakis(perfluoroisopropyl)) gallium(III) phthalocyanine, **F_{64}PcGaCl [4-6]**:

The synthesis of the Pc **[4-6]** was performed without solvent. The reactants were loaded in the reaction vessel in a glove box under N_2 due to the instability of $GaCl_3$ in the presence of atmospheric water vapors. A mixture of $GaCl_3$ (106 mg, 0.602 mmol) and perfluoro-(4,5-diisopropyl)phthalonitrile **[4-2]**, (250 mg, 0.5 mmol), PN:$GaCl_3$ ratio 1:1.2, was placed in a 10 mL glass vial. The vial was sealed with a septa Teflon cap, heated stepwise, ramp from room temperature to 100 °C in max. 2 min, hold additional 2 min, ramped with additional 20 °C and hold every time for 2 min, and held for 10 min at 200 °C (MW irradiation). After cooling, the powdered crude product was suspended in water to hydrolyze unreacted $GaCl_3$, filtered, and the solid material was washed with aq. AcOH 0-30%, followed by organic solvents (toluene, dichloromethane, ACN). After solvent washings, the purity of the material was tested by UV-Vis spectroscopy. Once there were no more changes in the UV region, the material was dissolved in ethyl acetate. The solution was filtered, the solvent was removed under vacuum, and the green solid material was recovered in powder form, see section **4.2.1**. The solid was dried at 100 °C. F_{64}PcGaCl **[4-6]**, $C_{56}F_{64}N_8GaCl$, 2105.73 g/mol, yield: 108 mg (41%), mp > 300 °C. UV-Vis (TFT) λ nm (log ε): 690 (5.03), 622 (4.19), 400 (4.22), 321 (4.16). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -71.22 (ddq, *J* = 45.1, 19.2, 17.9, 9.7 Hz, CF_3, 48F), -98.64 – -108.37 (m, aromatic F, 8F), -164.59 (dt, *J* = 17.6, 9.3 Hz, aliphatic F, 8F). FT-IR (KBr disk) *v*, cm^{-1}: 1453.46, 1209.77, 1167.28, 1102.55, 1055.79, 983.36, 960.20, 862.14, 785.14, 752.73,

729.10, 656.47, 542.49, 471.20. HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{56}F_{64}N_8GaCl_2^-$) 2138.7851; obsd: 2138.8170. $|M_{calcd}-M_{obsd}|/M_{calcd}\cdot 10^6$ = 15 ppm.

Chloro-(1,4,8,11,15,18,22,25-octafluoro-2,3,9,10,16,17,23,24-octakis(perfluoroisopropyl)) indium(III) phthalocyanine, **F_{64}PcInCl [4-7]**:

A mixture of $InCl_3$ (41.5 mg, 0.19 mmol), perfluoro-(4,5-di-isopropyl)-phthalonitrile **[4-2]**, (0.25 g, 0.5 mmol), PN: $InCl_3$ ratio 1:0.38, and $PhNO_2$ (0.25 mL) was placed in a 10 mL glass tube, sealed with a Teflon cap, under N_2, and heated stepwise, ramp from room temperature to 100 °C in max. 2 min, hold additional 2 min, ramp with additional 20 °C and hold every time for 2 min, to 200 °C for 20 min. The mixture was triturated with toluene, filtered and the solid material was washed with organic solvents (toluene, ACN) and water; the operation was repeated until no more changes were seen by UV-Vis spectroscopy in ethanol. The solid was dissolved in ethyl acetate and isolated as a fine powder, see section **4.2.1**. The green powdered solid was dried at 100 °C. **F_{64}PcInCl [4-7]**, $C_{56}F_{64}N_8InCl$, 2150.83 g/mol, yield: 120 mg (45 %), mp > 300 °C. UV-Vis (TFT) λ, nm (log ε): 700 (5.14), 631 (4.35), 414 (4.48), 333 (4.30). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$ 0.00 ppm) δ, ppm: -71.31 (dddd, J = 49.9, 33.4, 16.4, 8.2 Hz, CF_3, 48F), -103.00 (dtd, J = 67.8, 33.5, 32.7, 17.2 Hz, aromatic F, 8F), -164.64 (dp, J = 16.7, 8.3 Hz, aliphatic F, 8F). FT-IR (KBr disk) ν, cm^{-1}: 1453.29, 1210.53, 1168.20, 1101.16, 1055.01, 983.16, 966.08, 857.68, 783.47, 751.84, 729.45, 718.81, 656.61, 542.69, 469.48. HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{56}F_{64}N_8InCl_2^-$) 2184.7634; obsd: 2184.7446. $|M_{calcd}-M_{obsd}|/M_{calcd}\cdot 10^6$ = 8 ppm.

4.2.4 Synthesis of mixed perfluoroisopropyl metal Pcs, F_nPcCu, n = 40, 52, 64

0.016 g (0.08 mmol) of PN **[3-1]** was mixed with 0.1 g (0.2 mmol) of PN **[3-2]**, 0.015 g (0.08 mmol) copper(II) acetate monohydrate and a few drops of $PhNO_2$ in a 10 mL glass vial. The vial was sealed with a Teflon cap, stirred for 5 minutes, and heated stepwise, ramped from room

temperature to 100 °C in max. 2 min, hold additional 2 min, ramped with additional 20 °C and hold every time for 2 min, in a MW reactor to 185 °C and kept at this temperature for an additional 12 minutes. After cooling the reaction mixture was loaded on silica gel 60 (63–200 μm) and the products were separated via gravity column using a 0–30% gradient of ethyl acetate in hexanes, followed by an isocratic 30% ethyl acetate/hexanes mixture to yield a mixture of **F_{64}PcCu [4-3]**, **F_{52}PcCu [4-8]**, and **F_{40}PcCu [4-9]**. The mixture was next loaded on silica gel and, using flash chromatography with a 0-50% DCM/hexanes, the Pc **[4-3]** eluted as the first fraction, followed by Pc **[4-8]**. The solvent was switched to 0-30% ethyl acetate/hexane to isolate Pc **[4-9]** as a deep-blue fraction. The purity of the compounds was tested by TLC and UV-Vis. Solvent evaporation yielded blue fine powders, dried at 100 °C, see section **4.2.1**.

1,4,8,11,15,18,22,23,24,25-deca-fluoro-2,3,9,10,16,17-hexakis-perfluoroisopropyl copper(II) phthalocyanine, **F_{52}PcCu [4-8]**: $C_{50}F_{52}N_8Cu$, 1764.07 g/mol, yield: 14 mg (12 %), mp > 300 °C. UV-Vis ($CHCl_3$) λ, nm (log ε): 705 (5.25), 677 (5.18), 644 (4.62), 613 (4.50), 363 (4.81), 323 (4.57). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$ 0.00 ppm) δ, ppm: -71.54 (s, CF_3), -101.54 (s, aromatic F), -161.99 (s, aliphatic F). FT-IR (KBr disk) *ν*, cm^{-1}: 1490.76, 1250.21, 1170.53, 1103.79, 961.63, 790.04, 755.59, 730.33, 680.47. HRMS (-ve ESI): calcd for $[M+Cl^-]$ ($C_{50}F_{52}N_8CuCl^-$) 1797.8395; obsd 1797.8470. $|M_{calcd}-M_{obsd}|/M_{calcd}\cdot 10^6$ = 4.4 ppm.

1,4,8,11,15,16,17,18,22,23,24,25-dodecafluoro-2,3,9,10,16,17-tetrakis(perfluoroisopropyl) copper(II) phthalocyanine, **F_{40}PcCu [4-8]**: $C_{44}F_{40}N_8Cu$, 1464.02 g/mol, yield: 20 mg (17 %), mp > 300 °C. UV-Vis (TFT): λ, nm (log ε) 686 (5.33), 616 (4.64), 360 (4.85). ^{19}F NMR (376.5 MHz, ethyl acetate +10% acetone-d_6, $CFCl_3$ 0.00 ppm) δ, ppm: -71.70 (s, CF_3), -101.21 (s, aromatic F), -162.11 (s, aliphatic F). FT-IR (KBr disk) *ν*, cm^{-1}: 2918.53, 2850.76, 1527.97, 1491.21,

1251.43, 1171.29, 1104.90, 964.30, 752.33, 729.74, 470.64. HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{44}F_{40}N_8CuCl^-$) 1497.8586; obsd 1497.8611. $|M_{calcd}-M_{obsd}|/M_{calcd}\cdot 10^6$ = 1.7 ppm.

4.2.5 Electrochemical and spectroelectrochemical characterization of F_{64}PcM(III)Cl, M = Ga [4-6] and M = In [4-7], and F_{40}PcCu [4-9]

The electrochemical and spectroelectrochemical set-ups are described in **Chapter 2**.

Cyclic voltammetry (CV) measurements were performed using scan rates of 5 mV/s or 0.1 V/s, for single and/or successive (10 cycles) scans. Differential pulse polarography (DPP) measurements were performed using a 4 mV/s scan rate, pulsing with 50 mV amplitude for 50 ms width. All experiments were performed at 20 ºC, in trifluorotoluene (TFT) containing 0.1 M TBATFB (supporting electrolyte), under an argon atmosphere. The Pc concentration was 0.5 mM.

Spectroelectrochemistry (SEC). The concentration of Pcs in the supporting electrolyte solution, 0.1 M TBATFB in TFT, was adjusted to obtain an absorbance close to 1 at λ_{max}/Q-band 686 nm; consecutive spectra were acquired at constant redox potentials.

4.2.5 X-ray analysis

Single crystals of **F_{64}PcNi·2(acetone)**, **F_{64}PcNi·2(THF)**, **F_{64}PcGaCl·H_2O**, **F_{40}PcCu**, and **F_{52}PcCu** suitable for X-ray analysis were grown by the slow evaporation of their solutions under atmospheric conditions in the dark. The solvents used for growing the F_{64}PcNi crystals were acetone or THF, F_{52}PcCu crystals were grown from an acetone/methanol 1:1 mixture, and F_{64}PcGaCl crystals from ethyl acetate: TFT 1:1 mixture. X-ray diffraction data were collected at Hunter College, New York at 100 K using a Bruker X8 Kappa Apex II diffractometer, MoKα (0.7107 Å) radiation for **F_{64}PcNi·2(THF)** while the data for **F_{40}PcCu**, **F_{52}PcCu**, **F_{64}PcNi·2(acetone)** and **F_{64}PcGaCl·H_2O** was obtained at Rutgers University (Newark, NJ) at 100 K using a Bruker SMART APEX II CCD Diffractometer, CuKα (1.54178 Å) radiation.

4.3 Results and discussion

4.3.1 Synthesis

The Pcs **[4-1]** – **[4-9]** were synthesized in fair yields. F_{16}PcZn **[4-1]** was synthesized *vs*. being purchased due to the high cost of the commercially available material; the zinc acetate and PN **[3-1]** starting materials are inexpensive; **[3-1]** was also used in the production of substituted PNs **[3-2]** – **[3-13]**. Comparing the MW assisted with the conventional reaction, for the synthesis of **[4-1]** Pc, we can say that the reaction time was lowered, but also the yield is lower. For the synthesis and purification of the newly reported compounds **[4-5]** – **[4-9]**, the general procedure described in **section 4.2.1** was followed. Optimization was needed for the synthesis of Pcs **[4-5]** and **[4-6]** due to the low yields or no product formation when the standard procedure, see **section 4.2.1**, was followed. Solvent screening showed that Pc **[4-5]** forms in higher yield when nitrobenzene and DMF were combined. The combination of $GaCl_3$, organic solvents, and PN **[4-2]** was not successful in producing the Pc **[4-6]**; only the neat reaction was conducted to product formation. Different molar ratios of **[3-1]**: **[3-2]** PNs were tested to produce **[4-9]** Pc as a major product; the best result, 17% yield, was obtained for the 2:5 ratio.

4.3.2 NMR spectroscopic properties

The NMR spectra are shown in Figures A.21 to A.27. F_{16}PcZn was analyzed by ^{19}F NMR. The NMR data of this complex, to the best of our knowledge, has not been reported. In the case of F_{64}PcM derivatives **[4-5]** – **[4-9]**, the ^{19}F NMR spectra are very similar in terms of chemical shifts. For the ^{19}F NMR of Pc **[4-6]** a manual phase correction was necessary since the signals weren't properly phased using the auto phase correction, *aph* command, Figure A.24. The comparison between **[4-2]**, **[4-6]**, and **[4-7]** Pcs in acetone-d_6 (Pelmuş *et al.*, 2016) and the data of this report for **[4-2]** and **[4-5]** Pcs, in 10% acetone-d_6 in ethyl acetate, reveals similarly sharp

NMR spectra, excellent signal to noise ratios, quantitative integrations and similar values for the width at half heights, Table 4.1. The similarities establish the diamagnetism of **[4-2]** and **[4-5]** – **[4-7]** complexes, small variations, maximum of 1 ppm, in chemical shifts for equivalent aromatic fluorine atoms suggests that the type of metal, if diamagnetic, doesn't have a strong influence on the chemical shift of the Pc fluorine atoms. Similar splitting patterns and very close coupling constants are also observed for the CF_3 groups present in the following Pcs pairs **[4-2]** and **[4-5]**, and **[4-6]** and **[4-7]** (Pelmuş *et al*., 2016).

In the case of **[4-8]** and **[4-9]** Pc due to the paramagnetism of copper(II) ion, one can only distinguish 3 peaks for the -CF_3 groups, aromatic fluorine (from the perfluoroalkylated quadrants), and aliphatic fluorine (from the *iso* group). The signals for the aromatic fluorine atoms of the unsubstituted quadrants should have been in the 140-160 ppm region according to the NMR data obtained for the zinc(II) and cobalt(II) (Patel, 2015).

Table 4.1 ^{19}F NMR data comparison between $F_{64}PcZn$ **[4-2]** and $F_{64}PcNi$ **[4-5]**

Assignment / **Pc**	**CF_3 aliphatic**	**C-F aromatic**	**C-F aliphatic**
	δ (width at half height), ppm		
$F_{64}PcZn$ **[4-2]**	-71.55 (14)	-103.03 (0.24)	-164.70 (0.10)
$F_{64}PcNi$ **[4-5]**	-71.56 (14)	-103.39* (0.24)	-164.88 (0.10)

*highest central peak

4.3.3 Vibrational spectroscopic properties

The infrared spectra obtained for Pcs **[4-5]** – **[4-9]**, Figures B.10 to B.14, reveal strong vibrations that overlap in the 1300 – 1100 cm^{-1} region, confirming the presence of the C-F aliphatic and C-F aromatic bonds. The vibrations present around 1450 cm^{-1} correspond to C=C bonds.

4.3.4 Electronic spectroscopic properties

The UV-Vis spectra are shown in Figures D.3 to D.11. Complexes **[4-5]** – **[4-7]** exhibit typical electronic absorption spectra for symmetrical, non-aggregated Pcs in solution. The Q band (sharp peak, λ_{max}) appears in the visible, 650 – 750 nm region, while the B-bands appear in the UV region, 300 – 400 nm. The linear dependence of concentration *vs.* absorbance, Beer-Lambert law, Figures D.3 and D.4 for **[4-5]**, D.5 and D.7 for **[4-6]**, and D.6 for **[4-7]**, together with high extinction coefficients, Table 4.2, and sharp Q band absorption prove that the F_{64}PcM complexes do not aggregate in solution. In contrast, F_{16}PcM has low solubility in non-coordinative solvents and aggregate in solution (Bench, 2002 Co; Stuzhin, 2014; Patel, 2015). All complexes were tested in two different solvents, one coordinating (EtOH or EtOAc) and one non-coordinating ($CHCl_3$ or TFT).

Table 4.2 UV-Vis absorption maxima and molar extinction coefficients of **[4-5]** – **[4-9]** Pcs

Pc	**Solvent**	**λ_{max} (log ε) nm (L mol^{-1} cm^{-1})**
[4-5]	EtOAc	677 (6.31), 611 (5.58), 353 (5.77), 291 (5.69)
	TFT	680 (6.39), 611 (5.65), 354 (5.72), 290 (5.75)
[4-6]	EtOH	693 (5.08), 624 (4.37), 390 (4.56), 318 (4.55)
	TFT	690 (5.03), 622 (4.19), 400 (4.22), 321 (4.16)
	$CHCl_3$	709 (5.09), 646 (4.32), 382 (4.55), 321 (4.55)
[4-7]	EtOH	700 (5.33), 629 (4.56), 393 (4.73), 323 (4.59)
	TFT	700 (5.14), 631 (4.35), 414 (4.48), 333 (4.30)
[4-8]	EtOH	695 (5.16), 665 (5.14), 640 (4.75), 603 (4.66), 376 (4.54), 323 (4.45)
	$CHCl_3$	705 (5.25), 677 (5.18), 644 (4.62), 613 (4.50), 363 (4.81), 323 (4.57)
[4-9]	EtOH	676 (4.95), 640 (4.74), 612 (4.49), 372 (4.62), 316 (4.52)
	TFT	686 (5.33), 616 (4.64), 360 (4.85)

In the case of Pcs **[4-8]** and **[4-9]** due to the decrease in macrocycle symmetry, from D_{4h} to C_{2v}, the Q band is split (Mack *et al.*, 2011), Figure 4.4. The presence of non-alkylated quadrants in the Pc structures promotes the aggregation in solution, this being most visible for Pc **[4-9]**, see Table 4.2.

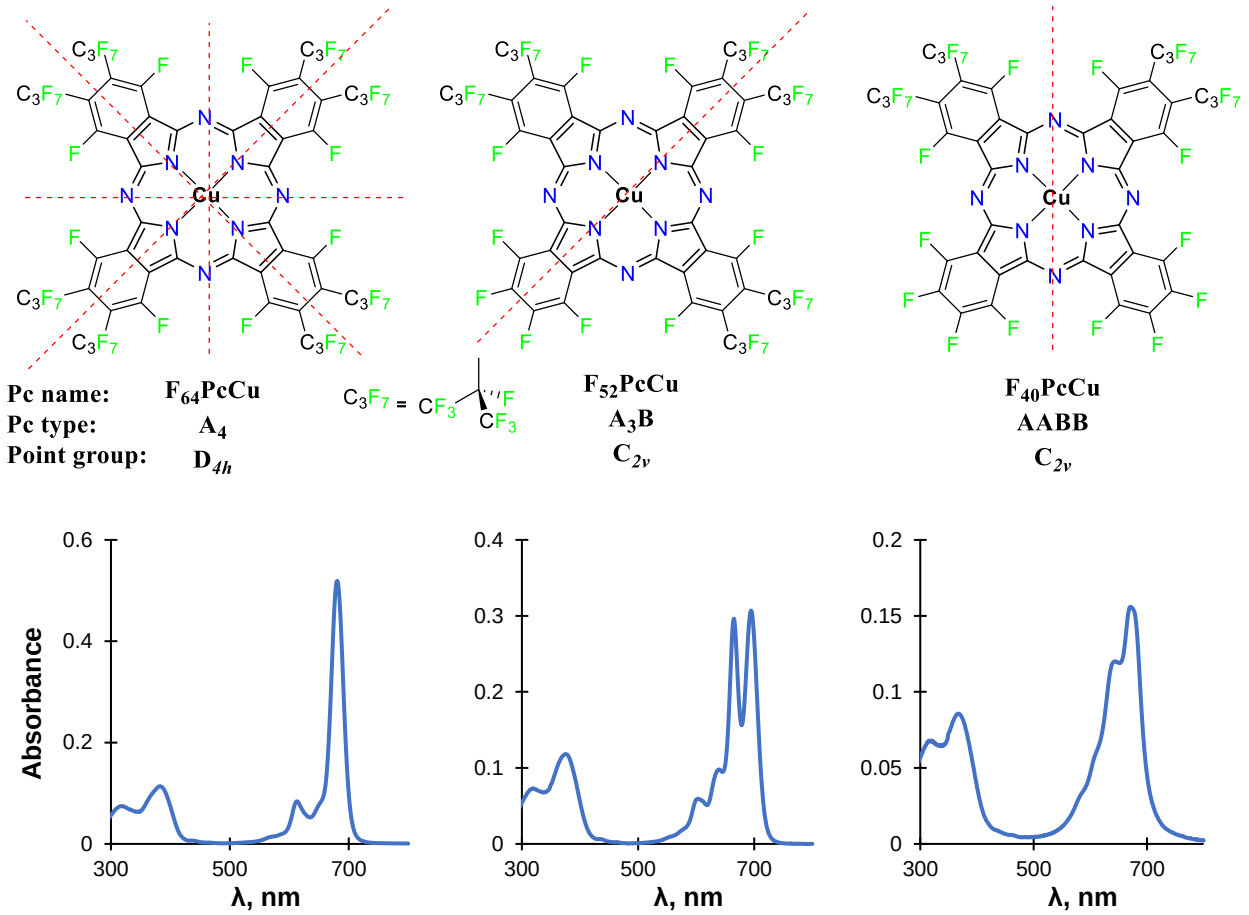

Figure 4.4 Variation of symmetry and Pc type for the F_nPcCu (n = 64, 52, 40) series, and its influence on the UV-Vis absorption spectra in ethanol at 20 µM Pc concentration, 1 mm light path-length.

4.3.5 Redox properties

The redox properties of compounds **[4-6]** and **[4-7]** were analyzed using electrochemical and spectroelectrochemical techniques, Figures 4.5 – 4.7. The Pcs have the best solubility and stability in a fluorinated solvent, TFT electrolyte solutions. No oxidations were observed in the scanning domain, up to 1 V. The reductions, revealed by DPP, proved to be reversible by CV, ΔE_p ~59 mV (ΔE_p = peak-to-peak potential separations), and quasi reversible ΔE_p 80 – 100 mV, Figure 4.5. The reduction potentials (E_{pc}), re-oxidation potentials (E_{pa}), half-wave potentials ($E_{1/2}$), and peak-to-peak potential separations (ΔE_p) extracted from CV and DPP are shown in Tables 4.3 and 4.4 (Pelmuş, 2016).

All reduction for complexes **[4-6]** and **[4-7]** are assigned to the $F_{64}Pc^{2-}$ ligand as the Cl-Ga(III) and Cl-In(III) centers are redox-inactive (Yenilmez *et al.*, 2015; Ertunç *et al.*, 2015). In(I) is not a viable oxidation state when the metal is coordinated by a Pc ligand, especially in the case of $F_{64}Pc^{2-}$, a very electronic deficient ligand. Looking at the reduction potentials obtained for the Pcs **[4-2]**, F_{64}PcZn, and **[4-4]**, F_{64}PcCo, corresponding low values (approx. 0.2 V vs. Ag/AgCl) were registered, even though they were obtained in DMF (Bench, 2001). These reduction potentials correspond to the Pc ligand. In the case of Ga(III) and In(III) complexes the first reduction of F_{64}Pc(2-)M(3+)Cl to F_{64}Pc(3-)M(3+)Cl is reversible as no shift of the potential or decrease in the current intensity have been observed in repetitive scans, Figures E.29 and E.30.

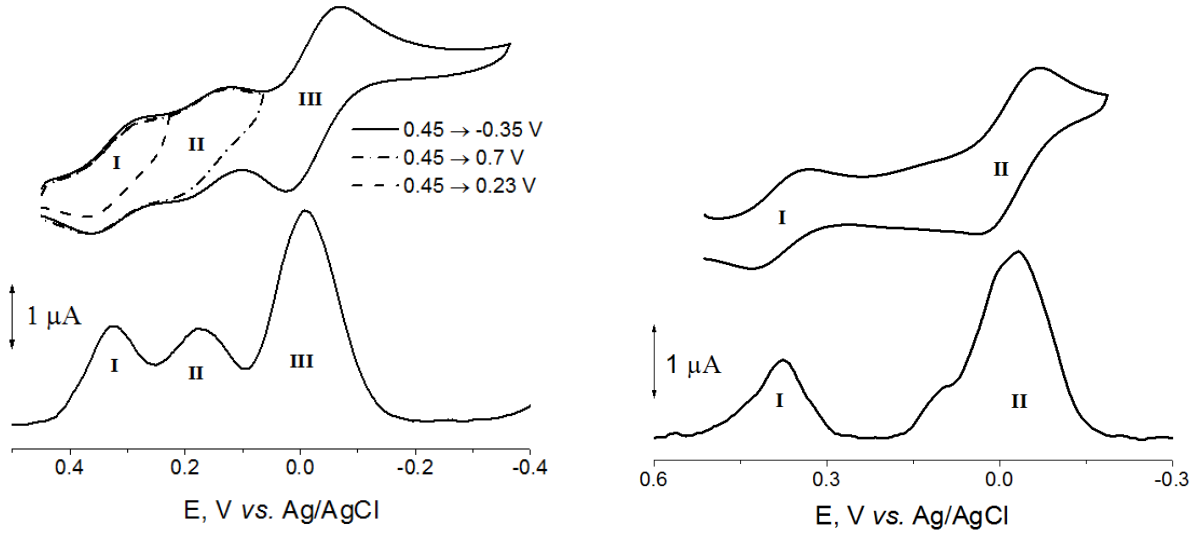

Figure 4.5 Traces of CV (top) and DPP (bottom) of F_{64}PcGaCl (left) and F_{64}PcInCl (right). The redox, $E_{1/2}$ for CV, and reduction, E_{pc} for DPP, processes are numbered *I-III*. Figure reproduced with permission from Pelmuş *et al.*, 2016.

Table 4.3 Redox processes from CV experiments (Pelmuş *et al.*, 2016)

Pc	$E_{1/2}$, V (ΔE_p, mV)		
	I	***II***	***III***
[4-6]	0.33 (79)	0.16 (60)	-0.01 (88)
[4-7]	0.37 (101)	-0.03 (104)	-

Table 4.4 Reduction processes from DPP experiments (Pelmuş *et al.*, 2016)

Pc	E_{pc} (V)		
	I	***II***	***III***
[4-6]	0.32	0.17	-0.01
[4-7]	0.38	-0.03	-

In situ spectroelectrochemical reductions of the Pcs **[4-6]** (13 spectra acquired in 1.5 h) and **[4-7]** (9 spectra acquired in 0.3 h) resulted in significant spectral changes in the UV-Vis-NIR domain. In the case of Pc **[4-6]** all major absorption bands (Q band region and B bands) decrease

upon reduction, and new peaks appear at 594 nm and in the NIR region at 862 and 1007 nm. Isosbestic points at 449, 609, 643, and 706 nm indicate a simple A→B reduction process, and the new bands are assigned to the $F_{64}Pc^{3-}$ anion, Figure 4.6A. Following the interruption of the electrical current, slow reversible oxidation of F_{64}Pc(3-)Ga(3+)Cl to F_{64}Pc(2-)Ga(3+)Cl was recorded. Traces of oxygen can be responsible for the re-oxidation process. The same isosbestic points are present, and process B→A was assigned as the re-oxidation back to the $F_{64}Pc^{2-}$ anion, viz. F_{64}Pc(2-)Ga(3+)Cl, Figure 4.6B (Pelmuş *et al.*, 2016).

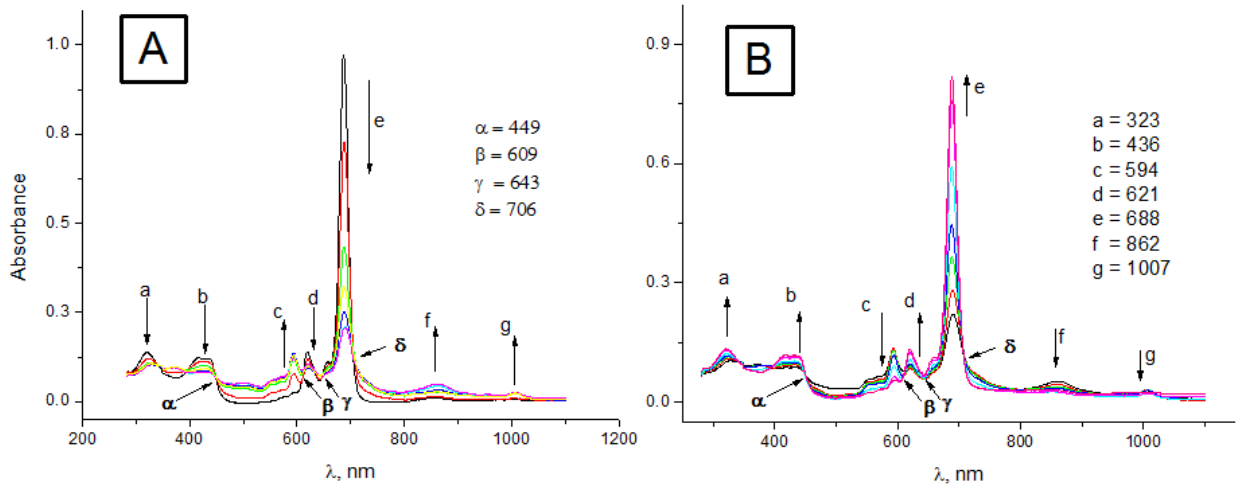

Figure 4.6 Time-dependent UV-Vis spectral variations of F_{64}PcGaCl **[4-6]** in TFT. **A**) *In situ* electrochemical reduction, **B**) Chemical, spontaneous re-oxidation in the absence of an electrical potential. The isosbestic points are marked with Greek letters. Figure reproduced with permission from Pelmuş *et al.*, 2016.

Similar spectral changes are observed in the spectroelectrochemical reduction of **[4-7]** Pc, the decrease in the intensity of Q and B bands is accompanied by the appearance of new absorption bands at 458 and 597 nm. Broad, unresolved absorptions in the 750 to 900 nm increase as a broad shoulder; the reduction process was stopped earlier *vs*. the case of **[4-6]** Pc. Isosbestic points are present at 430, 619, and 727 nm, Figure 4.7A, observed during the re-oxidation process, Figure 4.7B.

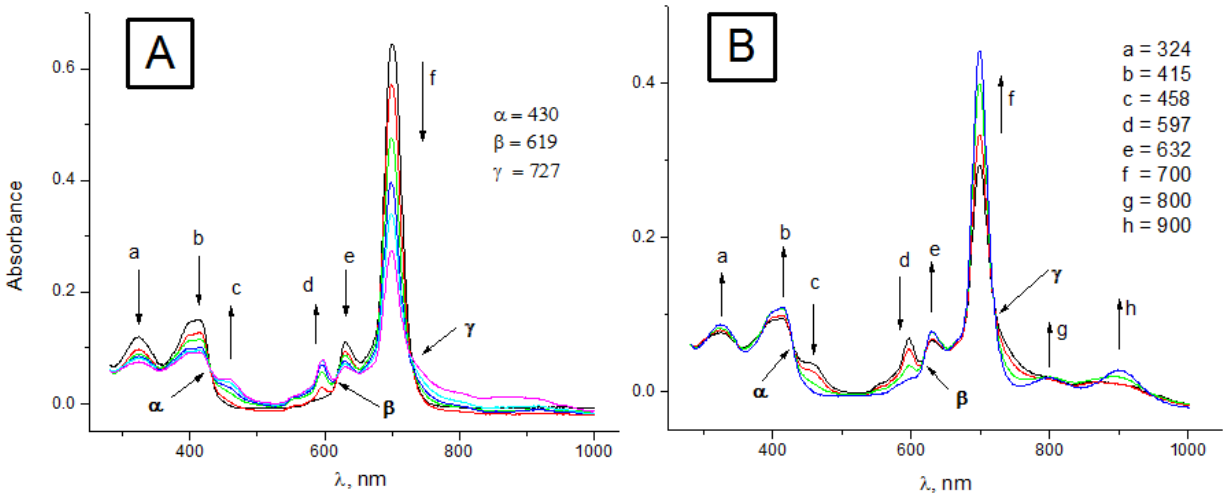

Figure 4.7 Time-dependent changes in the UV-Vis spectrum of F_{64}PcInCl **[4-7]** in TFT. **A**) *In situ* electrochemical reduction, **B**) Chemical, spontaneous re-oxidation in the absence of an electrical potential. The isosbestic points are marked with Greek letters. Figure reproduced with permission from Pelmuş *et al.*, 2016.

The time-dependent spectral changes in the Q bands observed for both compounds during their reduction and re-oxidation, Figure 4.8, suggest a slow, quasi-reversible reduction of Pc^{2-} to Pc^{3-}, attributed to the stabilization effect of the electron-deficient nature macrocycle. The re-oxidation yields approx. 80% F_{64}PcGaCl **[4-6]** and 70% F_{64}PcInCl **[4-7]**, Figure 4.8, relative to the initial amounts (Pelmuş *et al.*, 2016).

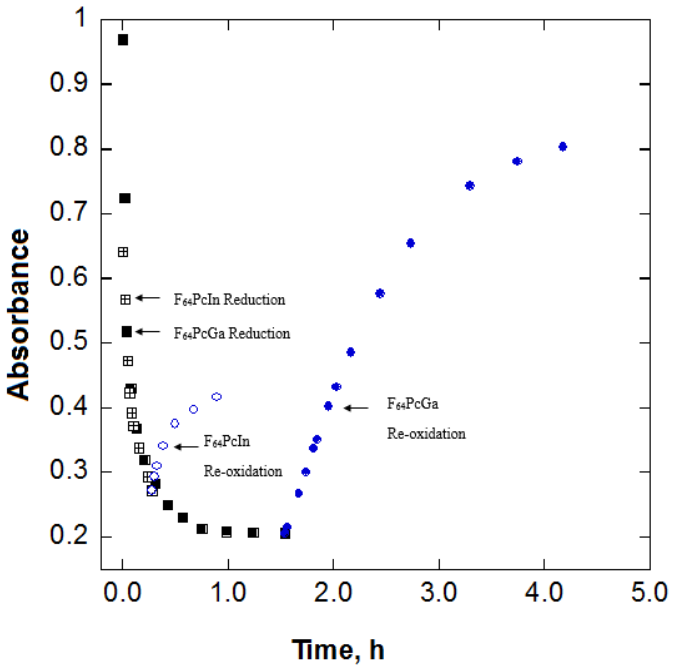

Figure 4.8 Time-dependent electrochemical reduction and spontaneous chemical re-oxidation of F_{64}PcGaCl and F_{64}PcInCl, measured by the Q bands' absorbance at 688 nm, and 700 nm, respectively. Figure reproduced with permission from Pelmuş *et al.*, 2016.

In the case of **[4-9]** Pc, the electrochemical reduction showed a first reduction process taking place -0.28 V on the GCE (Nguyen *et al.*, 2020). Spectroscopic changes were visible when the reduction potential of the Pt gauze was set at -0.22 V for a **[4-9]** solution in TFT, Figure 4.9. The material suffered a quick electrochemical reduction seen by a decrease, for the first 100 s, in the absorbance of the Q-band (682 nm) and B-bands region, together with the appearance of new peaks at 434 and 586 nm. After there were no more visible changes in the UV-vis spectra for F_{40}PcCu **[4-9]**, the current was stopped and a natural re-oxidation occurred, see Figure 4.10. The spectroscopic changes recorded in the case of reduction are now reversed with increases of the Q-band and in the B-bands region. Similar behavior was previously shown for the spectroelectrochemical reduction of **[4-2]** Pc (Keizer *et al.*, 2003).

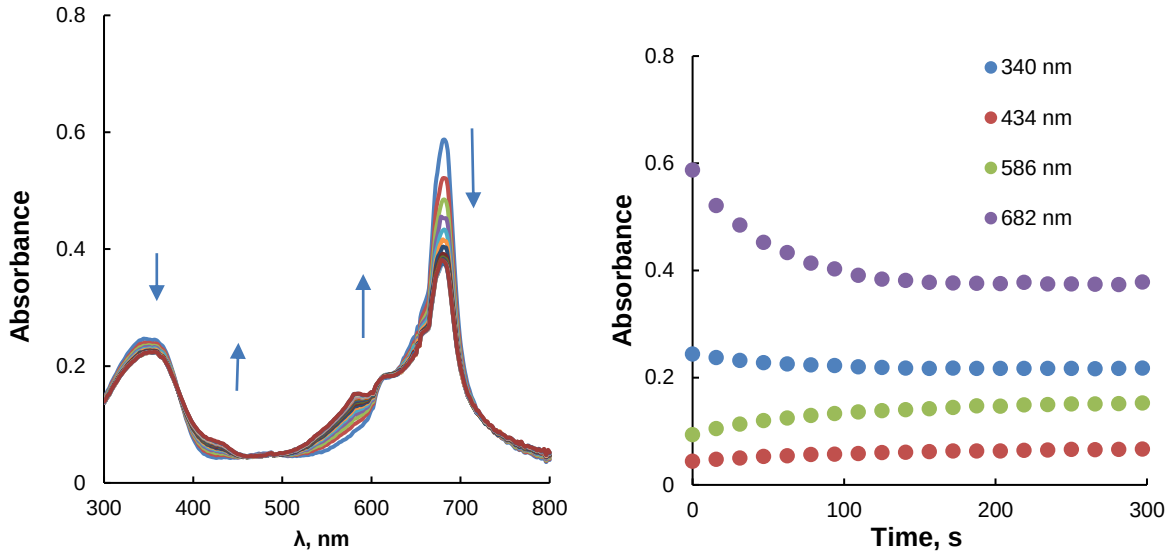

Figure 4.9 UV-Vis spectral changes in time for the reduction of F_{40}PcCu **[4-9]** at E_{red} -0.22 V, 300-800 nm domain (left), and selected wavelengths (right).

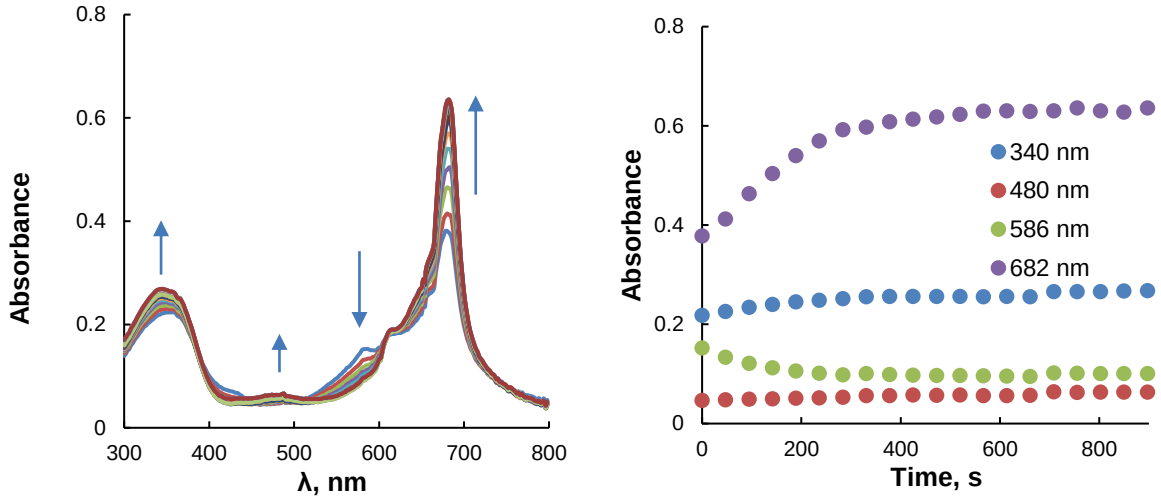

Figure 4.10 UV-Vis spectral changes in time for the re-oxidation to F_{40}PcCu **[4-9]** (no current applied), 300-800 nm domain (left), and selected wavelengths (right).

4.3.6 Crystal Structures

F_{64}PcNi·2(acetone): Diamond-shaped crystals were grown from acetone. Crystal data, data collection, and refinement parameters are summarized in Table J.1. The X-ray structure of **F_{64}PcNi·2(acetone)** represented as ORTEP is shown in Figure J.1 and full data are listed in Ta-

bles J.2 to J.5. A polyhedron view of the metal centers along with the views along the axes are included in Figures 4.11 and 4.12.

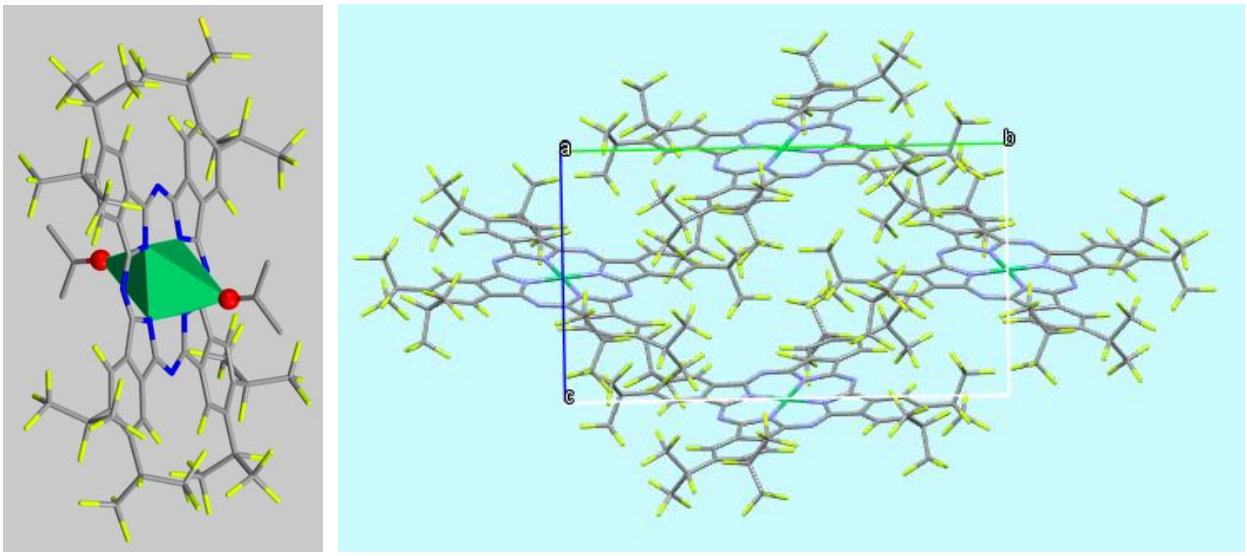

Figure 4.11 Graphic representation of the crystal of **F_{64}PcNi·2(acetone)** polyhedron view (left) and a view along **a**-axis of the unit cell (right).

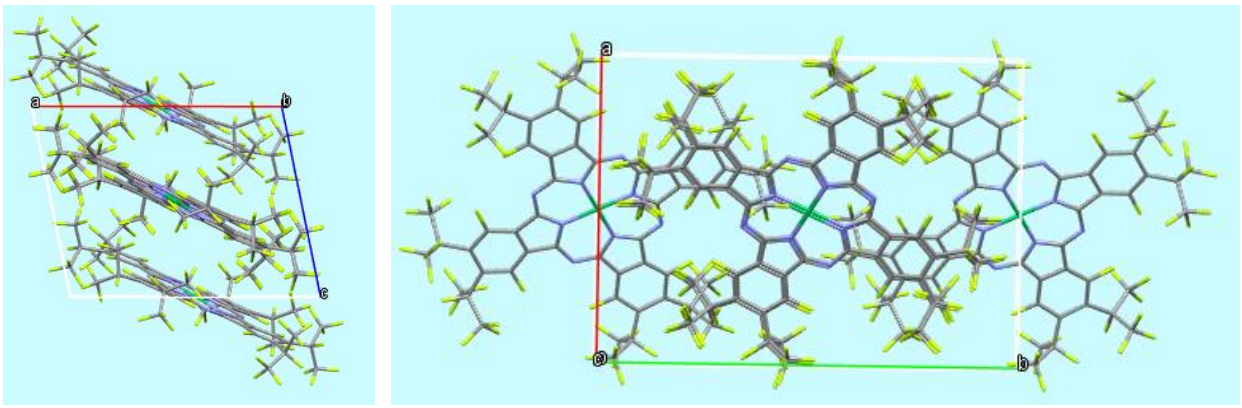

Figure 4.12 Graphic representation of the unit cell of the crystal of **F_{64}PcNi·2(acetone)**, views along **b**-axis (left), and **c**-axis (right).

The unit cell view along **a**-axis shows a 3D parallel arrangement of the Pc macrocycles, Figure 4.11. The views along **b**- and **c**-axes show how the Pc molecules are found in a parallel and linear arrangement, Figure 4.12. Acetone molecules have been removed from the unit cell for better visibility.

F_{64}PcNi·2(THF): Small crystals were grown from THF. Larger crystals were not formed even when a large amount of solution was used, and the evaporation rate was decreased. Crystal data, data collection, and refinement parameters are summarized in Table K.1. The X-ray structure of **F_{64}PcNi·2(THF)** represented as ORTEP is present in Figure K.1 and full data are listed in Tables K.2 to K.6. The polyhedron view of the metal center and the unit cell view along **a**-axis are shown in Figure 4.13. The views along **b**- and **c**-axes show how the Pc molecules are found in a parallel and linear arrangement, Figure 4.14.

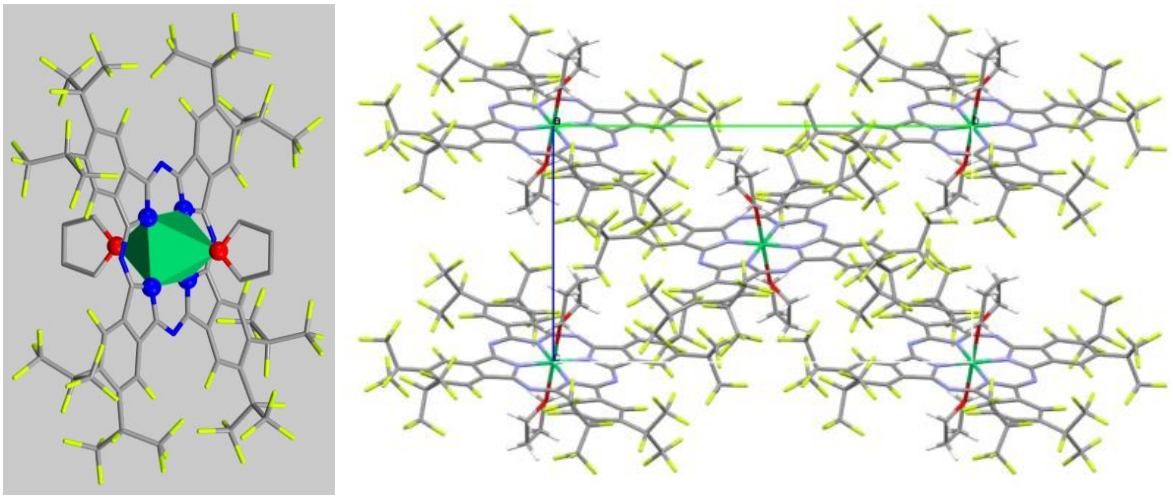

Figure 4.13 Graphic representation of the crystal of **F_{64}PcNi·2(THF)** polyhedron view (left) and a view along **a**-axis of the unit cell (right).

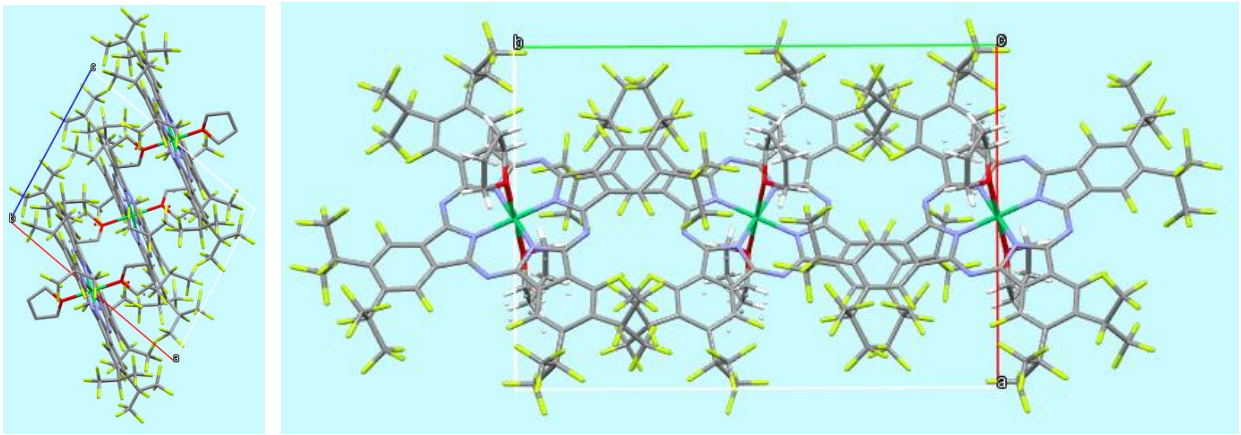

Figure 4.14 Graphic representation of the unit cell of the crystal of **F_{64}PcNi·2(THF)**, views along **b**-axis (left), and **c**-axis (right).

$F_{64}PcGaCl(H_2O)$: $F_{64}PcGaCl$ produced poor-quality crystals from ethyl acetate. A mixture of ethyl acetate: TFT 1:1 was used to slow the evaporation rate of the solvent. The crystals proved to break apart into powder when they got dried. As the evaporation process took place under atmospheric conditions, a water adduct was seen by X-ray. Crystal data, data collection, and refinement parameters are summarized in Table L.1. The X-ray structure of **$F_{64}PcGaCl(H_2O)$** represented as ORTEP is present in Figure L.1. Full details are listed in Tables L.2 to L.5. Packing diagrams and unit cell views along the axes shown in Figure 4.15 and 4.16. A polyhedron view of the metal center is also included in Figure 4.16.

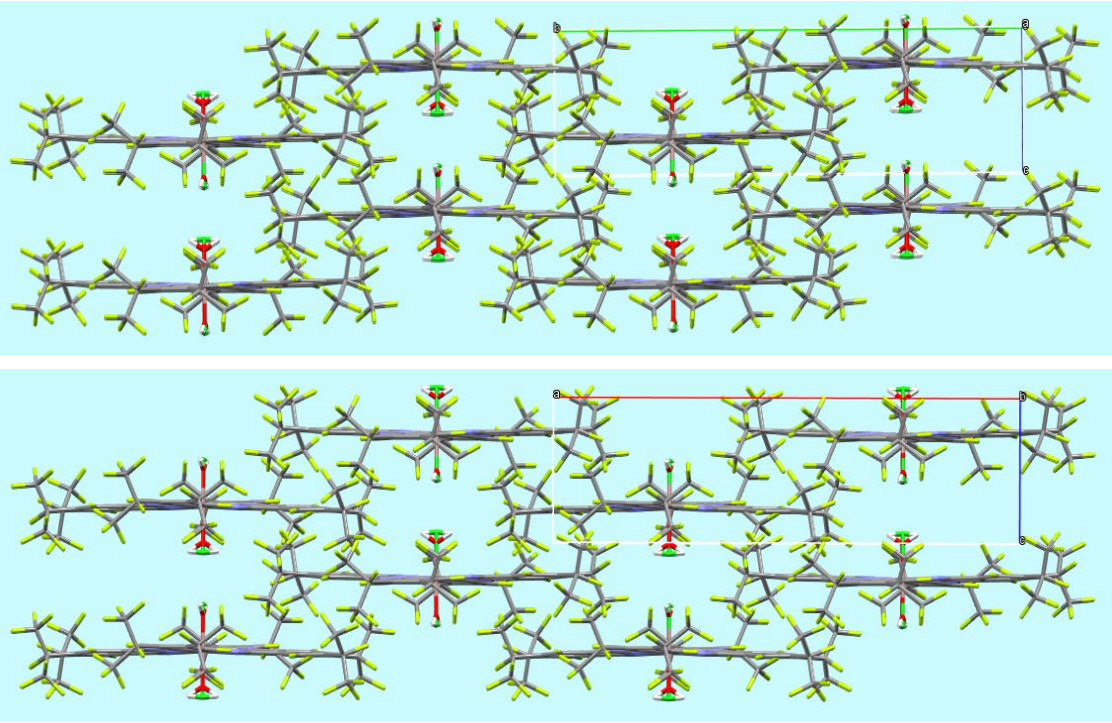

Figure 4.15 Graphic representation of the unit cell of the crystal of **$F_{64}PcGaCl(H_2O)$**, views along **a**-axis (top), and **b**-axis (bottom).

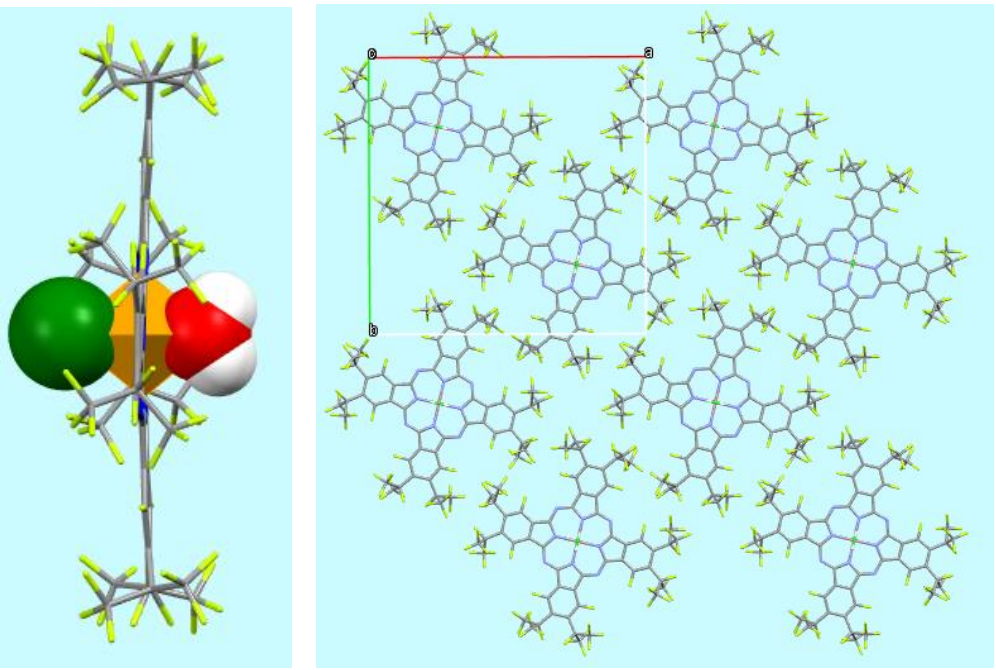

Figure 4.16 Graphic representation of the crystal of **F_{64}PcGaCl(H_2O)** polyhedron view (left) and a view along the **c**-axis of the unit cell (right).

F_{52}PcCu(MeOH·2Acetone): F_{52}PcCu gave signs to crystalize from acetone, but the crystals were very tinny and data were not good. A mixture 1:1 acetone: methanol gave better quality crystals by slow the evaporation in the dark. Crystal data, data collection, and refinement parameters are summarized in Table M.1. The X-ray structure of **F_{52}PcCu(MeOH·2Acetone)** represented as ORTEP is present in Figure M.1 and full data are listed in Tables M.2 to M.5. The views along the axes are shown in Figure 4.17 and 4.18.

Looking closely at the view along **a**- and **b**-axis, of the **F_{52}PcCu(MeOH·2Acetone)** crystal cell, one can see that the Pc molecules arrange as dimers. Isolating one dimer we can see how the non-alkylated benzene ring from one of the Pc molecules interacts with an alkylated benzene ring (neighbor to a non-alkylated ring) from the second Pc. This interaction becomes cleared as we simplify the molecules removing the substituents, revealing a slipped-parallel structure of the dimer with π-π stacking interaction, see Figure 4.19, same as in PAHs (Silva *et al.*, 2016).

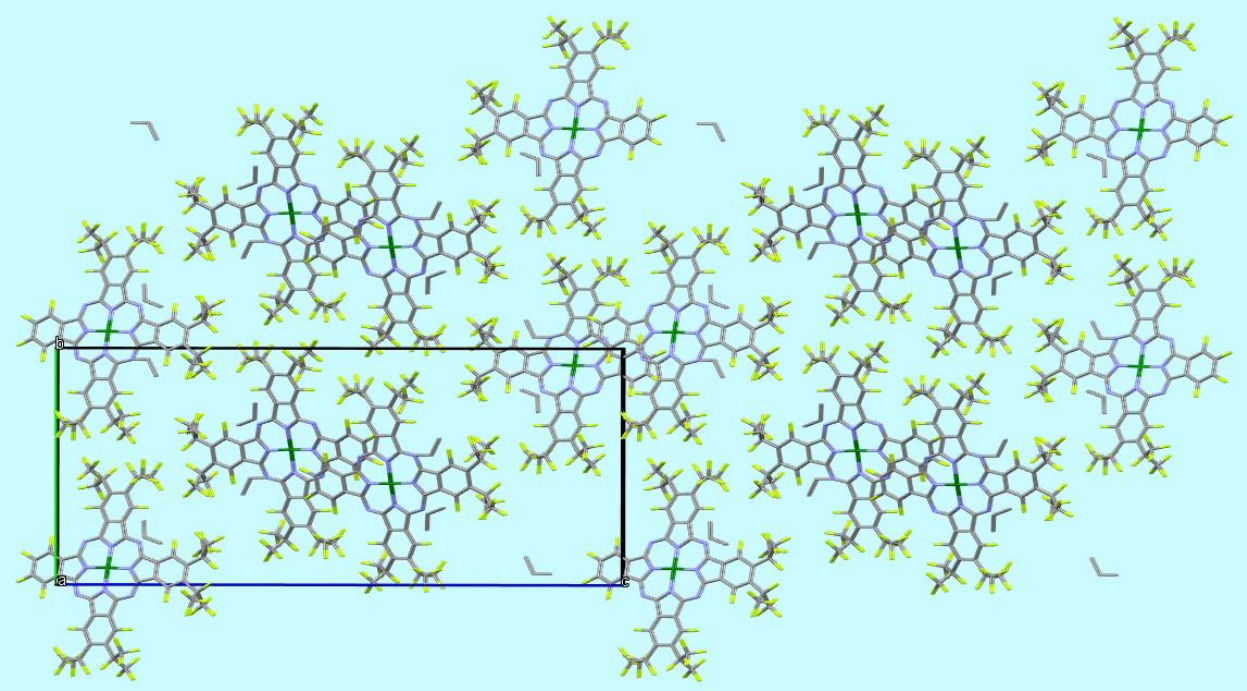

Figure 4.17 Graphic representation of the unit cell of the crystal of **F_{52}PcCu(MeOH·2Acetone)** view along **a**-axis.

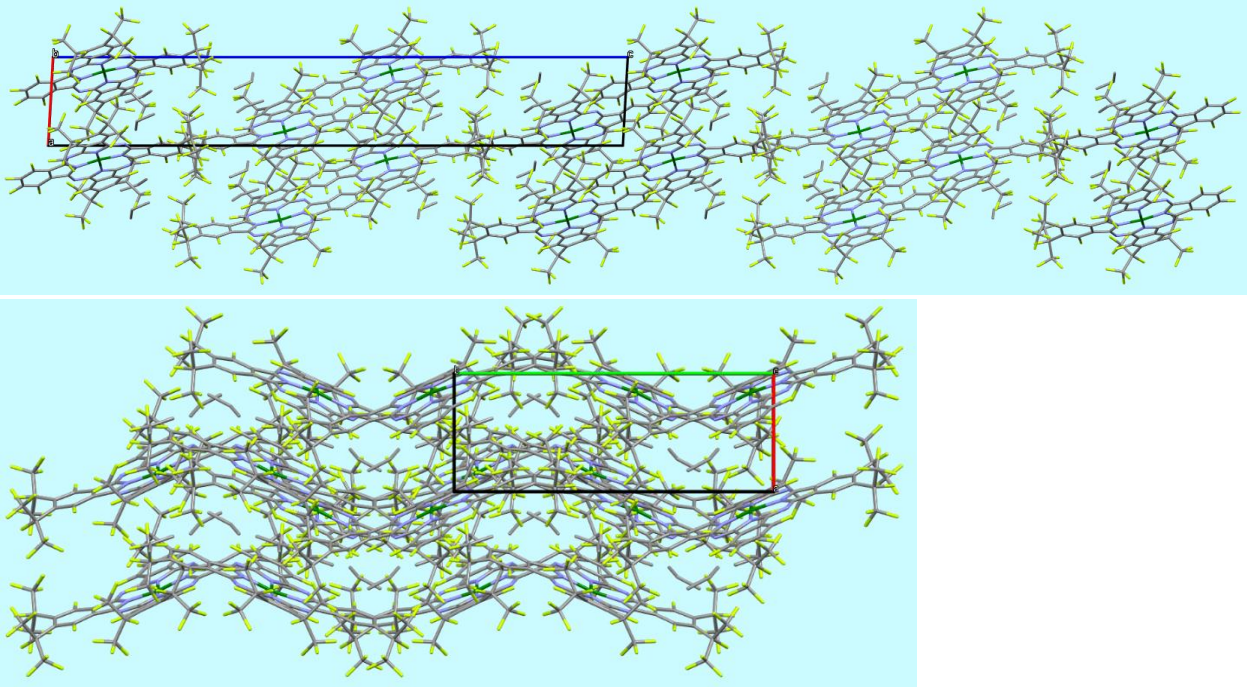

Figure 4.18 Graphic representation of the unit cell of the crystal of **F_{52}PcCu(MeOH·2Acetone)**, views along **b**-axis (top), and **c**-axis (bottom).

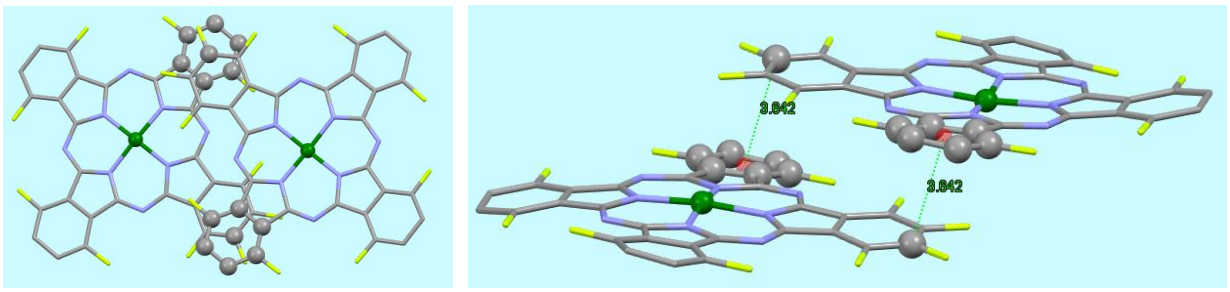

Figure 4.19 Graphic representation of the slipped-parallel structure of the dimer present in the crystal structure of **F_{52}PcCu(MeOH·2Acetone)**, overlap view (left), and distance between Pc molecules (right). The *i*-C_3F_7 groups are not shown.

F_{40}PcCu·2Toluene: F_{40}PcCu gave signs to crystalize from acetone, but the crystals did not diffract. A mixture 1:1 ethyl acetate: toluene gave better-quality crystals by slow the evaporation in the dark. Crystal data, data collection, and refinement parameters are summarized in Table N.1. The X-ray structure of **F_{40}PcCu·2Toluene** represented as ORTEP is present in Figure N.1 and full data are listed in Tables N.2 to N.5. The views along the axes are shown in Figure 4.20 and 4.21.

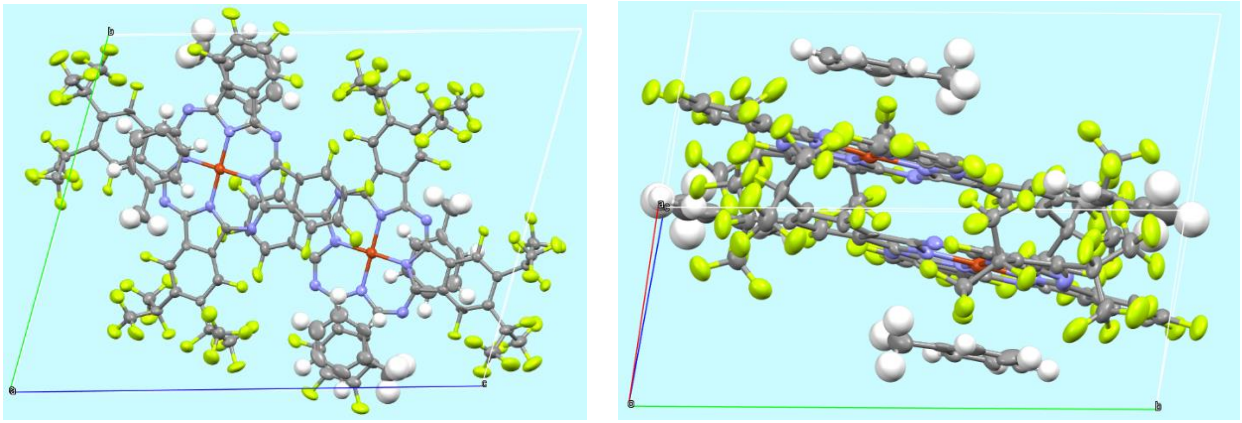

Figure 4.20 Graphic representation of the unit cell of the crystal of **F_{40}PcCu·Toluene**, views along **a**-axis (left), and **c**-axis offset (right).

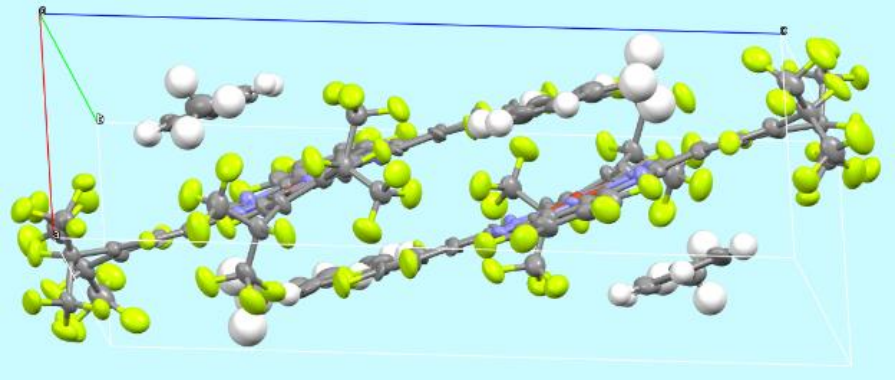

Figure 4.21 Graphic representation of the unit cell of the crystal of **F_{40}PcCu·Toluene**, view along **b**-axis offset.

Looking closely at the view along the axes, of the **F_{40}PcCu·2Toluene** crystal cell, we can see that the 2 Pc molecules are found as a dimer with 4 toluene rings arranged around it, 2 toluene molecules for each Pc. One toluene molecule interacts with one of the non-alkylated benzene rings of the Pc while the second one interacts with the porphyrazine macrocycle, Figure 4.22. By simplifying the Pc structure through the removal of all substituents we can see clearly how the 2 Pc interact and measure the distances, Figure 4.23. A similar arrangement was previously reported for one of the crystalline forms of PcTiO (Hiller *et al.*, 1973). The interactions indicate π stacked systems as slipped-parallel structures.

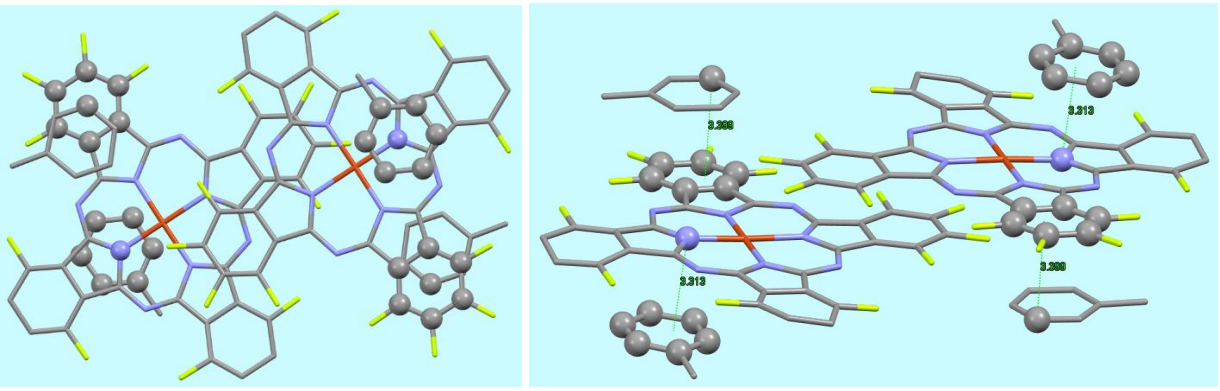

Figure 4.22 Graphic representation of the toluene – Pc interactions in the **F_{40}PcCu·Toluene** crystal: overlap view (left), atom to benzene ring plane distances (right). The *i*-C_3F_7 groups and H atoms were omitted for a better view of the structures.

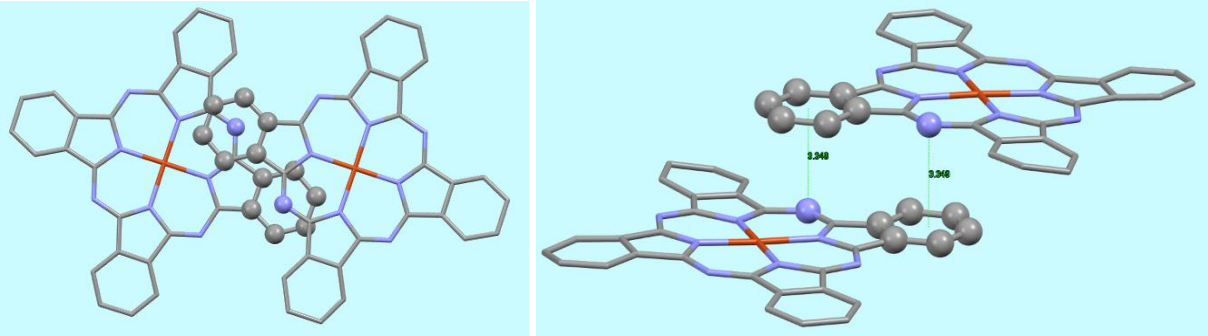

Figure 4.23 Graphic representation of the Pc – Pc interactions in the **F_{40}PcCu·Toluene** crystal, the C_3F_7 groups, F and H atoms were omitted: overlap view (left), atom to benzene ring plane distances (right).

4.4 Conclusions

The present chapter covers the perfluorinated non-functionalized MPcs, hexadecafluoro MPc series, and perfluoro(octakis-*iso*-propyl) MPc series. Microwave synthetic methods are being described for F_{16}PcZn production, three new representatives of the F_{64}PcM series (M = Ni, Ga, and In), and two new low symmetry Pcs, F_{52}- and F_{40}PcCu. The Pcs were characterized through spectroscopic techniques NMR, FT-IR, UV-Vis showing characteristic spectral data. No aggregating properties, linear dependence being registered by UV-Vis spectroscopy for the absorption's variation with the concentration, 10 – 50 µM, proving that the compounds are found in the monomer state in the tested solutions for reactivity studies, 20 µM. Electrochemical characterization for F_{64}PcGaCl and F_{64}PcInCl showed that the compounds suffer only reductions, and the potentials were comparative with data obtained for F_{64}PcZn and F_{64}PcCo. All the reduction processes were reversible or quasi-reversible and through spectroelectrochemical experiments was able to see the spectral changes that accompany the redox process. X-ray quality crystals were obtained by slow evaporation of the Pc solutions. The X-ray analysis offered information about the interactions between the molecules and their arrangement in the solid-state, π stacking was noticed for the F_{52}- and F_{40}PcCu due to the presence of non-alkylated quadrants.

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CHAPTER 5

SYNTHESIS AND CHARACTERIZATION OF THE THIRD GENERATION, FUNCTIONALIZED PERFLUORINATED METAL PHTHALOCYANINES

5.1 Introduction

Functionalization by grafting reactive groups (amino, carboxyl, hydroxyl, thiol, etc.) on an organic ligand is a path for revealing structure-reactivity trends and for expanding the applications of Pcs. Peripheral substitution of an already formed Pc from underivatized precursors and its production from derivatized precursors are the main synthetic routes. The derivatization (with functionalized molecules, biomolecules, and/or surfaces) process can modify some physicochemical properties of Pcs such as solubility, photochemical/catalytical activity, thermal and chemical stability (Leznoff, 1989; Kadish, 2003; Sharman and van Lier, 2003; McKeown, 2003; Rodriguez-Morgade, 2003; Lukyanets and Nemykin, 2010; Sorokin, 2016; Kuzmina *et al*., 2019).

The solubility of Pcs in organic solvents (polar and/or non-polar) and/or water can be changed dramatically through derivatization. The solubility of Pcs in organic solvents can be increased through the introduction of alkyl/aryl (preferably bulky) peripheral substituents, different metal ions, and/or coordinating axial ligands. To dissolve the Pcs in water, derivatization with highly polar functional groups (*anionic*: sulfonate, phosphate, carboxylate; *cationic*: ammonium, quaternized nitrogen-based heterocycles; *zwitterionic*: ammonium/pyridinium and sulfonate; *non-ionic*: polyethoxylated, polyhydroxy, polyamine, polythiols) is the main strategy (Moser, 1963; Linstead, 1950; Moser 1983; Dumoulin *et al*., 2010).

In Dr. Gorun's group, were developed carboxyl (Patel, 2014; Sabatino *et al*., 2014; Patel, 2015; Carrion *et al*., 2017; Carrion, 2018), amino (Patel, 2015; Patel *et al*., 2018), and amido (Pelmuş *et al.*, 2018; Pelmuş *et al.*, 2019; Pelmuş, Colomier *et al.*, 2020) functionalized fluorinated Pcs for bioconjugation and immobilization purposes. The synthetic strategy was mixing 2 different PNs, of which one presents a reactive functional group, while the other one exhibits bulky perfluoroalkyl substituents.

Previously described amido-substituted Pcs were synthesized from amino-substituted Pcs through acylation and used for the production of oligomers and polymers (Ekren *et al*., 2019), folic acid conjugates (Ogbodu *et al*., 2015), water-soluble photosensitizers (Zhang *et al.*, 2012; Pavaskar *et al.*, 2013), aggregating materials (Yuksel *et al.*, 2008).

The present chapter is focused on the synthesis, purification, and characterization of amino and acylated (acetyl, bisacetyl, and perfluoro *n*-butyryl) Pcs. The different acylating groups were introduced to reveal their influence upon the physicochemical properties of the Pcs. The synthetic pathways are shown in Figures 5.1 – 5.5.

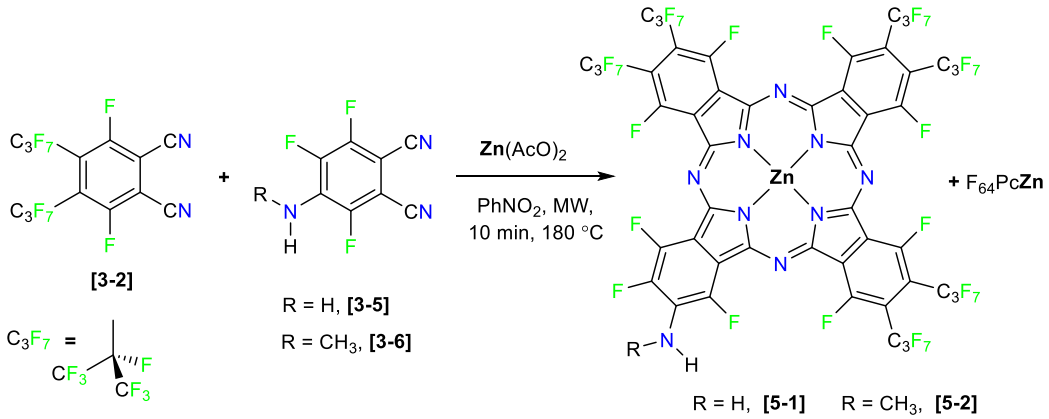


Figure 5.1 Microwave (MW) assisted synthesis of amino-substituted fluorinated Pcs: $NH_2F_{51}PcZn$ **[5-1]** and $NHMeF_{51}PcZn$ **[5-2]**.

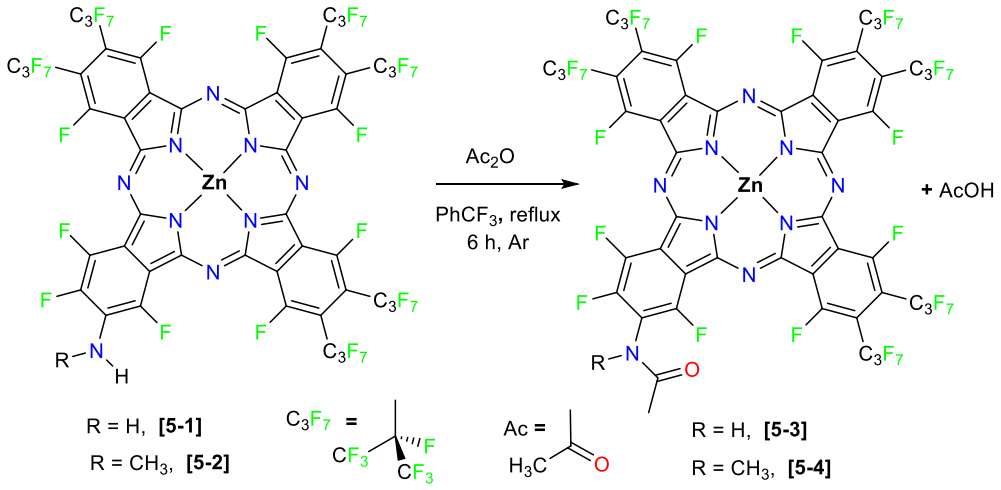


Figure 5.2 Acetylation of amino-substituted fluorinated Pcs to produce acetamido-substituted Pcs: $NHAcF_{51}PcZn$ **[5-3]** and $NMeAcF_{51}PcZn$ **[5-4]**.

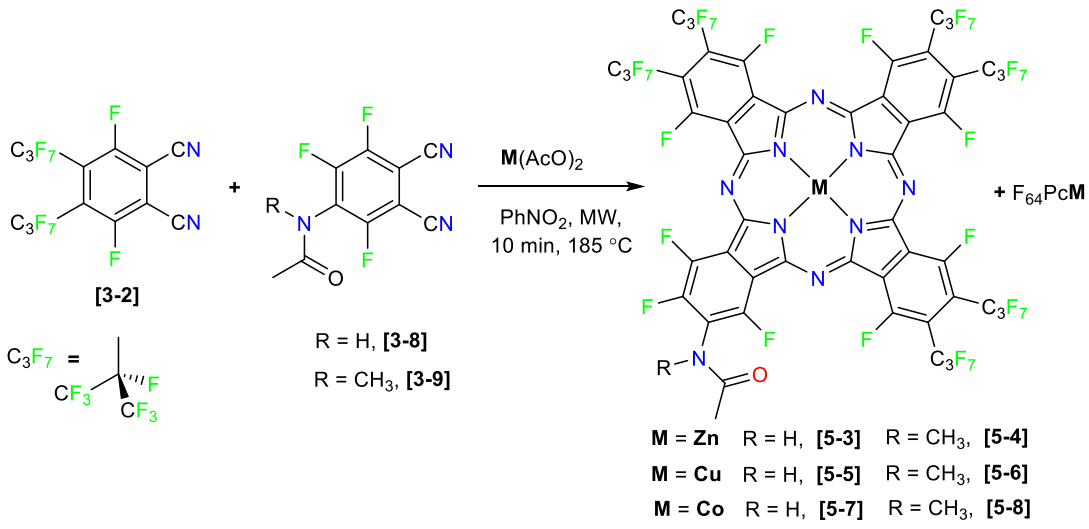


Figure 5.3 MW assisted synthesis of acetamido-substituted Pcs **[5-3]** – **[5-8]**.

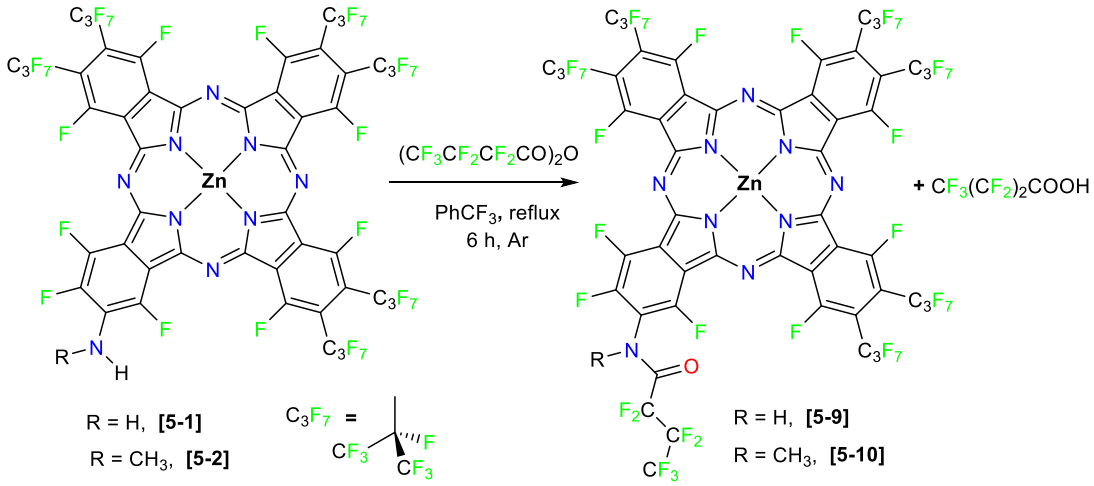


Figure 5.4 Acylation of amino-substituted fluorinated Pcs to produce perfluoro *n*-butyramido-substituted Pcs: $NHF_{58}PcZn$ **[5-9]** and $NMeF_{58}PcZn$ **[5-10]**.

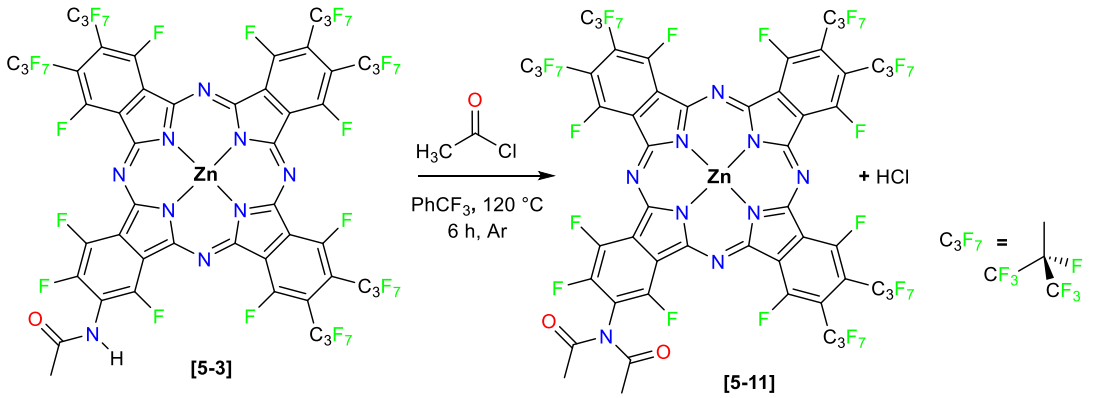


Figure 5.5 Acetylation of acetamido-substituted Pc **[5-3]** to produce imido-substituted Pc, $NAc_2F_{51}PcZn$ **[5-11]**.

5.2 Experimental

5.2.1 Synthesis and purification of functionalized F_nPcM derivatives

The synthesis and purification of functionalized F_nPcM derivatives were performed following the general procedure described in **Chapter 4**, section **4.2.1** unless stated otherwise.

5.2.2 Microwave synthesis and purification of amino-substituted F_{51}PcZn derivatives: NH_2F_{51}PcZn [5-1] and $NHMeF_{51}$PcZn [5-2].

2-amino-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **NH_2F_{51}PcZn [5-1]** and ***2-(N-methylamino)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine***, **$NHMeF_{51}$PcZn [5-2]** were synthesized by mixing two different PNs: a perfluoroalkylated PN and an amino-substituted PN, Figure 5.1 Thus, 100 mg (0.2 mmoles) of **[3-2]** PN were mixed with 0.2 mmoles of the corresponding PN, 39 mg of **[3-5]** PN or 42.2 mg of **[3-6]** PN, 60 mg (0.33 mmoles) of anhydrous zinc acetate and 0.25 mL of nitrobenzene in a microwave (MW) vial. The mixture was stirred for 5 min and heated at 180 °C by microwave irradiation for 10 minutes.

Due to the complexity of the reaction mixture, a series of purification steps were needed. After cooling, the reaction mixture was washed with water and organic solvents (hexane, toluene) until no more changes were visible by UV-Vis in ethanol in the B-bands region (300-450 nm). The material was then dissolved in hot ethyl acetate, filtered, and loaded on silica gel. Gravitational chromatography was performed by equilibrating the column in DCM and washing the loaded Pc mixture with DCM until no more impurities were coming out. The presence of the impurities was checked visually and by UV-Vis spectroscopy in the UV region (200-400 nm). Mixtures of 0.5-1% acetic acid in DCM we added gradually for flushing the amino-substituted F_{51}PcZn from the column. The collected blue fractions were evaporated and loaded on silica for further purification. Gravitational chromatography, with the silica gel column equilibrated in DCM, was performed with 2-5% ACN in DCM. Further, the solid material that resulted after evaporation was washed with ACN on a Teflon membrane (0.45 µm pore size). The purity of the

fractions was tested by TLC (30% acetone in hexane) and UV-Vis measurements in ethanol' Once no more UV active impurities were detected the blue fractions were evaporated. ^{19}F-NMR was performed also to confirm the purity of the material. The solid residue was turned into a powder following the procedure described in **section 4.2.1**. The powder was dried at 100 °C, yielding 5 mg (4% yield) of **[5-1]** and 19 mg (16% yield) of **[5-2]**. Spectroscopic data agreed with the literature (Patel, 2015).

For **[5-1]** Pc new ^{19}F NMR data are reported in 10% acetone-*d*$_6$/THF and ^{1}H NMR data in acetone-*d*$_6$: ^{19}F NMR (376.5 MHz, 10% acetone-*d*$_6$ in THF, $CFCl_3$, 0.00 ppm) δ, ppm: -71.48 (dddd, J = 39.4, 33.5, 16.2, 7.9 Hz, 36F, CF_3), -103.76 (s, 6F, Ar-F), -133.87 (s, 1F, Ar-F), -140.88 (s, 1F, Ar-F), -151.43 (s, 1F, Ar-F), -164.64 (s, 6F, C-F aliphatic); ^{1}H NMR (400 MHz, acetone-*d*$_6$, 2.05 ppm) δ, ppm: 6.63 (s, 2H, NH_2).

5.2.3 Conventional synthesis and purification of amido-substituted F_{51}PcZn derivatives: $NHAcF_{51}$PcZn, [5-3] and $NMeAcF_{51}$PcZn, [5-4]

20 mg (~11.3 μmoles) of the corresponding amino-substituted Pc, NH_2F_{51}PcZn **[5-1]**, or $NHMeF_{51}$PcZn **[5-2]**, was dissolved in 10 mL TFT, and 0.5 mL (5.3 mmoles) of acetic anhydride were added to the Pc solution. The mixture was refluxed for 6 h under Ar. The color of the reaction mixture changed from dark blue to dark green. The solvent, excess anhydride, and resulting acetic acid were removed by vacuum evaporation. The TLC of the reaction mixture using silica gel with 30% acetone in hexane indicated that a brown side product is still present. The acetylated Pc was isolated as a green fraction by chromatography, using silica gel and 20% ACN in DCM. After the solvent removal, the remaining green solid was turned into a powder following the procedure described in **section 4.2.1** and dried at 100 °C for 24 h. Crystallization from ethyl acetate: toluene 1:1 mixture yielded X-ray quality crystals.

2-(acetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **NHAcF$_{51}$PcZn [5-3]**, $C_{52}H_4F_{51}N_9OZn$, 1804.96 g/mol, yield 18 mg (88 %). UV-Vis ($CHCl_3$): λ, nm (log ε) 708 (5.28), 679 (5.28), 647 (3.70), 381 (3.85), 320 (3.61). ^{1}H NMR (400 MHz, acetone-*d*$_6$, 2.05 ppm) δ, ppm: 2.45 (s, 3H, N-Me), 9.78 (s, 1H, N-H). ^{19}F NMR (376.5 MHz, acetone-*d*$_6$ + 1 drop AcOH, $CFCl_3$, 0.00 ppm) δ, ppm: -71.35 (ddt, *J* = 40.6, 19.0, 11.3 Hz, 36F, CF_3), -103.93 (dt, *J* = 58.3, 24.5 Hz, 6F, Ar-F), -119.94 (d, *J* = 18.1 Hz, 1F, Ar-F), -132.45 (d, *J* = 18.9 Hz, 1F, Ar-F), -141.12 (t, *J* = 19.4 Hz, 1F, Ar-F), -161.72 – -170.45 (m, 6F, C-F aliphatic). FT-IR (KBr): 3446.77, 1669.32, 1488.44, 1454.36, 1248.79, 1167.84, 1148.34, 1099.41, 1057.53, 982.28, 968.00, 937.67, 788.99, 754.27, 731.12, 544.80, 458.15 cm^{-1}. HRMS (ESI-): calculated for $[M+Cl]^-$ ($C_{52}H_4F_{51}ON_9ZnCl^-$) 1837.8699, found 1837.8484 $|M_{calcd}-M_{obsd}|/M_{calcd}$ = 12 ppm. The Cl is adventitious.

2-(N-methylacetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **NMeAcF$_{51}$PcZn [5-4]**, appears as a mixture of *cis* and *trans* rotamers (1:1.5 molar ratio by ^{19}F NMR), at the NMR time scale in acetone-*d*$_6$ (an explanation and graphic representation of this phenomena was provided in **Chapter 3**, **section 3.3.2**), $C_{53}H_6F_{51}N_9OZn$, 1818.99 g/mol yield 19 mg (93%). UV-Vis ($CHCl_3$): λ, nm (log ε) 705 (5.20), 669 (5.20), 646 (4.58), 618 (4.49), 384 (4.79), 320 (4.53). ^{1}H NMR (400 MHz, acetone-*d*$_6$, 2.05 ppm) δ, ppm: 2.18 (s, 3H, CO-Me), 2.36 (s, 3H, CO-Me), 3.57 (s, 3H, N-Me), 3.74 (s, 3H, N-Me). ^{19}F NMR (376.5 MHz, acetone-*d*$_6$, $CFCl_3$, 0.00 ppm): δ, ppm -71.31 (tt, *J* = 32.3, 8.3 Hz, 36F, CF_3), -103.75 (dddd, *J* = 68.6, 54.1, 31.0, 16.6 Hz, 6F, Ar-F), -119.64 (d, *J* = 18.3 Hz, 1F, Ar-F), -121.88 (d, *J* = 19.0 Hz, 1F, Ar-F), -133.11 (d, *J* = 20.7 Hz, 1F, Ar-F), -134.59 (s, 1F, Ar -F), -139.39 (t, *J* = 20.3 Hz, 1F, Ar-F), -140.86 (t, *J* = 20.4 Hz, 1F, Ar-F), -162.10 – -165.75 (m, 6F, CF). FT-IR (KBr): 1642.76, 1486.38, 1454.39, 1392.80, 1335.80, 1282.46, 1251.04,

1169.56, 1148.71, 1100.37, 1058.99, 983.12, 967.60, 936.75, 853.24, 787.96, 754.84, 731.19, 722.48, 644.80, 542.45, 458.94, 449.47, 440.45, 431.26, 421.66, 413.07 cm^{-1}. HRMS (-ve ESI): calcd for $[M+Cl^-]$ ($C_{53}H_6F_{51}ON_9ZnCl^-$) 1851.8855, found 1851.8463 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 21 ppm. The Cl is adventitious.

5.2.4 Microwave-assisted synthesis of amido-substituted $F_{51}PcM$ complexes: $NHAcF_{51}PcM$ and $NMeAcF_{51}PcM$, (M = Zn, Cu, Co)

$NHAcF_{51}PcM$ (M = Zn [5-3], Cu [5-5], Co [5-7]) and $NMeAcF_{51}PcM$ (M = Zn [5-4], Cu [5-6], Co [5-8]) were synthesized by reacting a perfluoroalkylated PN, an amido-substituted PN and a metal salt. 100 mg (0.2 mmoles) of **[3-2]** PN were mixed with 0.2 mmoles of the corresponding PN, 47.8 mg of **[3-8]** PN or 50.6 mg of **[3-9]** PN, 0.33 mmoles of the corresponding metal (II) acetate, and 0.25 mL of nitrobenzene in microwave (MW) vials. The mixtures were stirred for 5 min and heated from room temperature to 100 °C in maximum 4 minutes, and holding the temperature constant for 2 min, followed by ramping in 20 °C steps, while the last step increase was 25 °C, and hold every time for 2 min, until the 185 °C was reached and holding at this temperature for 10 minutes.

After cooling, the reaction mixtures were washed with water and organic solvents (hexane, toluene) until no more changes were observed by UV-Vis in ethanol in the B-bands region (300-450 nm). The purified materials were dissolved in ethyl acetate, filtered, and loaded on silica gel. Gravity chromatography was performed by equilibrating the column in hexane and gradually increasing the percentage of ethyl acetate until 30%. The presence of the impurities was checked visually and by UV-Vis spectroscopy in the UV region (200-400 nm). The collected fractions were evaporated and loaded on silica for further purification from UV active impurities.

The Pc mixtures, loaded on silica gel, were placed on fritted funnels and washed with water, followed by 10-40% ACN in water, and kept on 40% I in water until no more changes were visible when analyzing the collected washings by UV-Vis. After drying under vacuum and in the oven at 100 °C for 2 hours, the Pc mixtures loaded on silica were cooled and purified by column chromatography using a 5-30% ethyl acetate gradient in hexane. The purity of the fractions was tested by TLC (30% ethyl acetate in hexane) and UV-Vis measurements in ethanol and once no more UV active impurities were detected the solvent was evaporated. ^{19}F-NMR was performed also to confirm the purity of the zinc derivatives. The solid residues were turned into powders following the procedure described in **section 4.2.1**. The Pc powders were dried in the oven at 100 °C. The yields, 12 mg (10% yield) of **[5-3]** and 19 mg (16% yield) of **[5-4]**, were comparable with those obtained via conventional procedures, **section 5.2.3**.

2-(acetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) copper(II) phthalocyanine, **NHAcF$_{51}$PcCu [5-5]**, $C_{52}H_4F_{51}N_9Ocu$, 1803.13 g/mol, yield 13 mg (11%). UV-Vis ($CHCl_3$): λ, nm (log ε) 710 (5.13), 681 (5.13), 648 (4.56), 615 (4.46), 363 (4.74). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -67.09 – -74.05 (m, CF_3), -101.60 (s, Ar-F), -162.04 (s, C-F aliphatic). FT-IR (KBr): 3440.47, 2921.21, 1709.11, 1462.40, 1249.89, 1170.20, 1102.19, 1058.62, 963.96, 787.12, 755.18, 729.76 cm^{-1}. HRMS (ESI-): calculated for $[M+Cl]^-$ ($C_{52}H_4F_{51}ON_9CuCl^-$) 1836.8703, found 1836.8692, $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 0.6 ppm. The Cl is adventitious.

2-(N-methylacetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) copper(II) phthalocyanine, **NMeAcF$_{51}$PcCu [5-6]**, $C_{53}H_6F_{51}N_9OCu$, 1817.16 g/mol, yield 10 mg (8%). UV-Vis ($CHCl_3$): λ, nm (log ε706 (5.16), 681 (5.15), 646 (4.54), 616 (4.48), 363 (4.75). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -

71.77 (m, CF3), -101.25 (s, Ar-F), -162.33 (s, C-F aliphatic). FT-IR (KBr): 2924.31, 2853.63, 1663.26, 1596.30, 1513.86, 1458.57, 1251.06, 1168.50, 1102.93, 961.26, 787.61, 755.25, 729.37 cm^{-1}. HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{53}H_6F_{51}ON_9CuCl^-$) 1850.8860, found 1850.8928, $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 3.7 ppm. The Cl is adventitious.

2-(acetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) cobalt(II) phthalocyanine, **$NHAcF_{51}PcCo$ [5-7]**, $C_{52}H_4F_{51}N_9OCo$, 1798.52 g/mol, yield 40 mg (33%). UV-Vis ($CHCl_3$): λ, nm (log ε) 696 (4.96), 668 (5.00), 631 (4.56), 606 (4.44), 353 (4.70), 325 (4.68). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -67.94 – -72.77 (m, CF_3), -98.37 – -110.77 (m, Ar-F), -123.34 (s, Ar-F), -139.45 (s, Ar-F), -145.31 (s, Ar-F), -164.83 – -166.82 (m, Ar-F). FT-IR (KBr): 3440.91, 1688.70, 1600.47, 1524.08, 1285.52, 1249.76, 1101.33, 1060.55, 984.19, 731.08 cm^{-1}. HRMS (ESI-): calculated for [M+Cl]$^-$ ($C_{52}H_4F_{51}ON_9CoCl^-$) 1832.8739, found 1832.8879 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 7.6 ppm. The Cl is adventitious.

2-(N-methylacetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) cobalt(II) phthalocyanine, **$NMeAcF_{51}PcCo$ [5-8]**, appears as a mixture of *cis* and *trans* rotamers in 1:1.5 molar ratio at troom temperature, $C_{53}H_6F_{51}N_9OCo$, 1812.54 g/mol, yield 35 mg (29%). UV-Vis ($CHCl_3$): λ, nm (log ε) 693 (4.97), 669 (5.00), 631 (4.46), 609 (5.38), 353 (4.69), 317 (4.66). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -71.27- -71.39 (m, CF_3), -100.61 – -109.89 (m, Ar-F), -123.53 (s, Ar-F), -125.35 (s, Ar-F), -140.36 (s, Ar-F), -141.83 (s, Ar-F), -143.59 (s, Ar-F), -145.15 (s, Ar-F), -165.81 (s, C-F aliphatic). FT-IR (KBr): 1649.81, 1523.81, 1448.50, 1286.29, 1250.76, 1169.31, 1103.97, 1060.81, 984.28, 731.51cm^{-1}. HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{53}H_6F_{51}ON_9CoCl^-$) 1846.8896, found 1846.9026 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 7 ppm. The Cl is adventitious.

5.2.5 Conventional synthesis and purification of perfluoro *n*-butyramido-substituted Pcs: $NHF_{58}PcZn$ [5-9] and $NMeF_{58}PcZn$ [5-10]

The corresponding amino-substituted Pc, $NH_2F_{51}PcZn$ **[5-1]** (3 mg, 1.7 μmoles) or $NHMeF_{51}PcZn$ **[5-2]** (10 mg, 5.6 μmoles), were dissolved in a 5 mL round bottom flask with 2 mL TFT and 0.2 mL (~0.8 mmoles) of heptafluorobutyric anhydride were added to the Pc solution. The mixture was refluxed for 6 h under Ar. The color of the reaction mixture changed from dark blue to dark green. The solvent, excess anhydride, and resulting heptafluorobutyric acid were removed by distillation under vacuum. The TLC of the reaction mixtures, using silica gel and 30% acetone in hexane, showed brown side products remaining at the starting point. The acylated Pcs were isolated as green fractions by silica gel chromatography with 0-30% ethyl acetate/hexane. The solution was filtered through a 0.2 μm Teflon membrane and the solvent evaporated under a stream of nitrogen. The green Pcs were dried at 100 °C.

2-(perfluoro-n-butyramido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **$NHF_{58}PcZn$ [5-9]**, $C_{54}HF_{58}N_9OZn$, 1958.95 g/mol, yield 3 mg (90 %). UV-Vis ($CHCl_3$): λ, nm (log ε) 704 (5.21), 680 (5.19), 644 (4.57), 616 (4.48), 384 (4.77), 320 (4.54). ^{1}H NMR (400 MHz, acetone-d_6, 2.05 ppm) δ, ppm: 11.14 (s, 1H, N-H). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -71.39 (ddq, J = 31.7, 14.6, 9.4, 7.7 Hz, 36F, CF_3), -80.25 (t, J = 8.7 Hz, 3F, CF_3), -104.05 (q, J = 71.1, 54.4 Hz, 6F, Ar-F), -119.30 (q, J = 9.0 Hz, 2F, CF_2), -120.43 (s, 1F, Ar-F), -126.45 (s, 2F, CF_2), -133.27 (s, 1F, Ar-F), -140.90 (s, 1F, Ar-F), -164.65 (tq, J = 16.2, 8.4, 7.5 Hz, 6F, C-F aliphatic). HRMS (ESI-): calculated for $[M+Cl]^-$ ($C_{54}HF_{58}N_9OZnCl^-$) 1991.8352, found 1991.8613 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 13 ppm. The Cl is adventitious.

2-(N-methyl-perfluoro-n-butyramido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **$NMeF_{58}PcZn$ [5-10]**, appears as a mixture of *cis* and *trans* rotamers (1:3.2 molar ratio by ^{19}F NMR), at the NMR time scale, $C_{55}H_3F_{58}N_9OZn$, 1972.98 g/mol yield 10 mg (90%). UV-Vis ($CHCl_3$): λ, nm (log ε) 702 (5.19), 680 (5.16), 644 (4.51), 618 (4.47), 384 (4.74), 318 (4.52). ^1H NMR (400 MHz, acetone-d_6, 2.05 ppm) δ, ppm: 3.83 (s, 3H, N-Me), 4.07 (s, 3H, N-Me). ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -71.30 (ddq, J = 32.7, 24.8, 8.4 Hz, 36F, CF_3), -79.41 (t, J = 9.3 Hz, 3F, CF_3), -79.64 (t, J = 9.4 Hz, 3F, CF_3), -99.44 – -106.47 (m, 6F, Ar-F), -112.36 (dd, J = 34.7, 10.0 Hz, 2F, CF_2), -112.54 – -113.34 (m, 2F, CF_2), -121.24 (s, 1F, Ar-F), -122.13 (s, 1F, Ar-F), -124.97 (d, J = 4.6 Hz, 2F, CF_2), -125.07 (s, 2F, CF_2), -134.30 (s, 1F, Ar-F), -134.67 (s, 1F, Ar-F), -139.86 (s, 1F, Ar-F), -140.14 (s, 1F, Ar-F), -164.59 (tq, J = 16.2, 8.4, 7.9 Hz, 6F, C-F aliphatic). HRMS (-ve ESI): calcd for [M+Cl^-] ($C_{55}H_3F_{58}N_9OZnCl^-$) 2005.8509, found 2005.8516 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6$ = 0.3 ppm. The Cl is adventitious.

5.2.6 Conventional synthesis and purification of imido-substituted Pc $NAc_2F_{51}PcZn$ [5-10]

5 mg (2.7 μmoles) of the acetamido-substituted Pc, $NHAcF_{51}PcZn$ **[5-3]**, were dissolved in 2 mL TFT in a 5 mL round bottom flask with and 0.2 mL (~2.8 mmoles) of acetyl chloride were added to the Pc solution. The mixture was refluxed and stirred for 6 h under Ar. The reaction was quenched with 2 mL of 5% sodium bicarbonate aq. solution. The organic layer was extracted with ethyl acetate and washed with brine. TLC of the reaction mixture using silica gel with 30% ethyl acetate in hexane showed the presence of a small amount of unreacted starting material. The imido-substituted Pc was isolated as the first green fraction by silica gel chromatography using 0-30% ethyl acetate/hexane. The solution was filtered through a 0.2 μm Teflon membrane and the solvent was evaporated under a stream of nitrogen. The green Pc was dried in the oven at

100 °C. The material was analyzed by HRMS and ^{19}F NMR but was unstable in solution and further characterization was not performed.

2-(N-acetyl-acetamido)-1,3,4,8,11,15,18,22,25-hepta-fluoro-9,10,16,17,23,24-hexakis-perfluoroisopropyl) zinc(II) phthalocyanine, **$NAc_2F_{51}PcZn$ [5-11]**, $C_{54}H_6F_{51}N_9O_2Zn$, 1847.00 g/mol. ^{19}F NMR (376.5 MHz, acetone-d_6, $CFCl_3$, 0.00 ppm) δ, ppm: -71.33 (36F, CF_3), -103.85 (6F, Ar-F), -121.19 (1F, Ar-F), -134.03 (1F, Ar-F), -139.88 (1F, Ar-F), -164.61 (6F, C-F aliphatic). HRMS (ESI-): calculated for $[M+Cl]^-$ ($C_{54}H_6F_{51}N_9O_2ZnCl^-$) 1879.8805, found 1879.8803 $|M_{calcd}-M_{obsd}|/M_{calcd}*10^6 = 0.1$ ppm. The Cl is adventitious.

5.2.7 Complexation of CoPcs, [5-7] and [5-8], with HO^- or H_2O ligands

In the silica column purification processes of the blue CoPcs, **[5-7]** and **[5-8]** using a 0 – 30% ethyl acetate in hexane gradient, green polar compounds did not elute until the mobile phase' polarity was increased by using up to 70% ethyl acetate in hexane. The fractions were analyzed by UV-Vis spectroscopy and single-crystal X-ray crystallography. Differences in the UV-Vis spectra of the green compounds vs. the blue CoPcs, **[5-7]** and **[5-8]**, were noticed and the hypothesis that an axial ligand (OH^- or H_2O) might be responsible was taken into consideration. Father X-ray data did reveal the presence of an oxygen atom being coordinated to one CoPc in the dimer structure. In the case of an OH^- ligand the metal center will be Co(III) for the overall neutral charge of the complex.

5.3 Results and discussion

5.3.1 Synthesis

The synthesis of acylated MPcs **[5-3]** – **[5-11]** followed two methods: **A** – acylation of amino-substituted MPcs, and **B** – direct production from acylated precursors. The Pcs **[5-3]**, **[5-4]** were

synthesized following both methods, the **[5-9]** – **[5-11]** ones only by method **A**, while the **[5-5]** – **[5-8]** ones only by method **B**.

*Method **A***: The amino-substituted Pcs **[5-1]** and **[5-2]** precursors were synthesized and purified following a modified version of the reported procedure (Patel, 2015). The changes include MW heating and normal phase chromatographic separation with the acidified mobile phase. The acylation of the amino-substituted Pcs with acid anhydrides took place readily, an indication of the increased nucleophilicity of the amino group connected to the Pc macrocycle vs. the PN ring. In other words, in the amino PNs case, the two CN groups have a stronger influence on decreasing the pK_a of the amino group vs. the Pc macrocycle. The yields are almost quantitative for the acylated Pcs **[5-3]**, **[5-4]**, **[5-10]**, and **[5-11]**. Small amounts of degradation by-products are easily separated by column chromatography. The imino-substituted Pc **[5-9]** was unstable and hydrolyzed to the starting material.

*Method **B***: Using a 1:1 mixture of PNs, perfluoroalkylated PN **[3-2]** and the acetylated PN **[3-8]** or **[3-9]**, a series of acetamido-substituted MPcs was synthesized using the following metals: Zn(II): **[5-3]** and **[5-4]**, Cu(II): **[5-5]** and **[5-6]**, and Co(II): **[5-7]** and **[5-8]**. The isolated products were only the F_{64}PcM (A_4 type Pcs), **[4-2]** – **[4-4]**, and the acetamido-substituted MPcs, NHAc- or NMeAc-F_{51}PcM (A_3B type Pcs), **[5-3]** – **[5-8]**. The yields of acetylated Pcs were low to fair and the metal ion had a great influence: Co(II)Pcs, **[5-5]** and **[5-6]**, was obtained in the highest yield *vs*. Zn(II), **[5-3]** and **[5-4]**, and Cu(II)Pcs **[5-7]** and **[5-8]**. The same order was noticed in the case of amino-substituted Co(II)Pcs (Patel, 2015).

5.3.2 NMR spectroscopy

Multinuclear NMR spectroscopy, along with HRMS (Figures C.12 to C.20) played a major role in the structural identification of functionalized MPcs. The ^{1}H and ^{19}F NMR results for MPcs **[5-**

1] – **[5-11]** are shown in Figures A.28 to A.44. Due to the paramagnetism of the Cu(II) and Co(II) ions, the ^{1}H signals were not detected for the MPcs **[5-4]** – **[5-8]**, while, in the case of ^{19}F the signals are broad and some are not even detected. Similar to the *N*-methyl acylated PNs, **[3-9]** and **[3-11],** the corresponding *N*-methyl acylated Pcs **[5-4]** and **[5-10]**, respectively, are seen as a mixture of rotamers in ~1:3 and 1:4.2 ratios at 25 °C, as evidenced by the doubling of their number of signals. A discussion on the amido-substituted rotamers is present in **section 3.3.2**. The NMR assignments for the PNs **[3-5] – [3-12]**, Tables 3.2 and 3.3, were used for the MPcs' spectra interpretation.

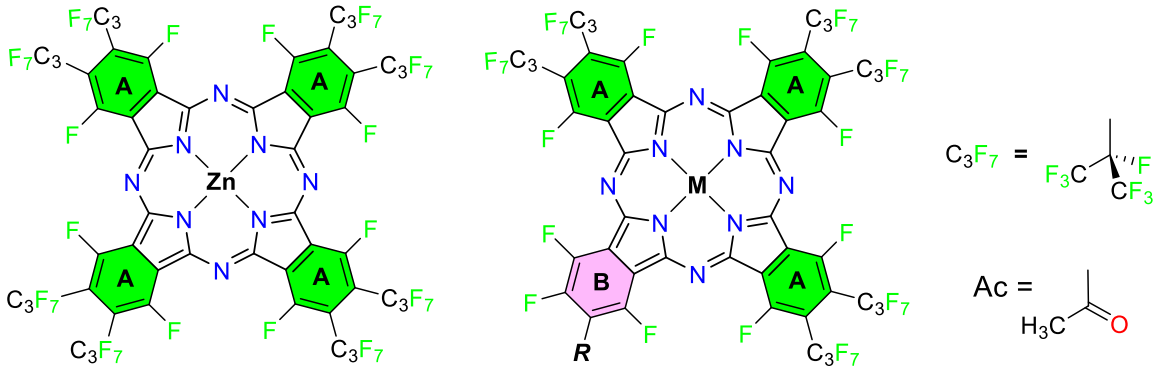
^{1}H signals were detected for the ZnPcs, **[5-1]**, **[5-3]**, **[5-4]**, **[5-9]**, and **[5-10]**, corresponding to the N-H, N-CH_3, and CO-CH_3 protons, see Table 5.1. The different types of ^{19}F NMR signals are represented graphically in Figure 5.6 and their assignment is shown in Table 5.2 for all Zn(II) complexes, and in Table 5.3, as a comparison between the acetylated PcM complexes, M = Zn, Cu, Co.

Table 5.1 Assignments of the ^{1}H NMR chemical shifts for the substituted F_{51}PcZn series

Assignment / **Pc**:	**[5-1]**	**[5-3]**	**[5-4]***	**[5-9]**	**[5-10]****
			δ, ppm		
N-H	6.63	9.78	-	11.14	-
N-CH_3	-	-	3.74	-	4.07
N-CH_3'			3.57		3.83
CO-CH_3	-	2.34	2.36	-	-
CO-CH_3'			2.18		

* rotamer mixture, molar ratio N-CH_3 : N-CH_3' and CO-CH_3 : CO-CH_3' ~1: 3

** rotamer mixture, molar ratio N-CH_3 : N-CH_3' 1: 4.2



Pc (type): **[4-2] (A_4)** **[5-1] - [5-11] (A_3B)**

M	*R*	Pc
Zn	-NH_2	**[5-1]**
Zn, Cu, Co	-NHAc	**[5-3], [5-5], [5-7]**
Zn, Cu, Co	-NMeAc	**[5-4], [5-6], [5-8]**
Zn	-NH-CO(CF_2)$_2$$CF_3$	**[5-9]**
Zn	-NMe-CO(CF_2)$_2$$CF_3$	**[5-10]**
Zn	-NAc_2	**[5-11]**

^{19}F signals

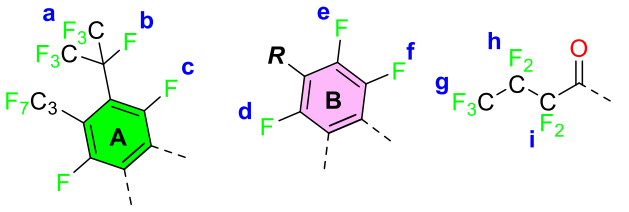


Figure 5.6 Chemical structures of the functionalized Pcs and legend for ^{19}F NMR assignments.

By comparing the ^{1}H chemical shifts assigned to the MPcs, Table 5.1, with the values obtained for the corresponding PNs, Table 3.3, one can see similarities in the chemical shift with variations <0.5 ppm for the N-CH_3 and CO-CH_3 signals. The ratios between the PN vs. ZnPc rotamers and their structures depend on the aromatic substituent. The rotamer ratios of 1:1, for PN **[3-9]**, and 1:1.5, for PN **[3-11]**, increase to 1:3 for Pc **[5-4]**, and to 1:4.2 for Pc **[5-4]**, due to the change of the aromatic fragment.

The ^{19}F signals are divided into 3 main categories:

- 3 *quadrants type A*, perfluoroisopropyl and aromatic F atoms from the PN **[3-2]**, signals: ***a***, ***b***, ***c***;

- 1 *quadrant type B*, the aromatic F atoms of the amino/amido functionalized quarter, signals: ***d***, ***e***, ***f***;

- *perfluorbutyryl* radical, perfluoropropyl tail, signals: ***g***, ***h***, ***i***.

Table 5.2 ^{19}F NMR assignments for the F_{51}PcZn series (legend from Figure 5.6)

			Pc:	**[4-2]***	**[5-1]**	**[5-3]**	**[5-4]****	**[5-9]**	**[5-10]*****	**[5-11]**
Assignment							δ, ppm			
Quadrant A	**a**	$CF(CF_3)_2$		-71.3	-71.48	-71.35	-71.31	-71.39	-71.30	-71.33
	b	$CF(CF_3)_2$		-164.6	-164.64	-164.68	-164.61	-164.65	-164.59	-164.61
	c	Ar-**F**		- 103.9	-103.76	-103.93	-103.75	-104.05	-103.76	-103.85
Quadrant B	**d**	Ar-**F**		-	-133.87	-119.94	-119.64	-120.43	-121.24	-121.19
	d'						-121.88		-122.13	
	e	Ar-**F**		-	-151.43	-141.12	-140.86	-140.90	-140.14	-139.88
	e'						-139.39		-139.86	
	f	Ar-**F**		-	-140.88	-132.45	-133.11	-133.27	-134.30	-134.03
	f'						-134.59		-134.67	
Perfluorobutyryl	**g**	CF_2-CF_3		-	-	-	-	-80.25	-79.41	-
	g'								-79.64	
	h	CF_2-CF_3		-	-	-	-	-126.45	-124.97	-
	h'								-125.07	
	i	CO-CF_2		-	-	-	-	-119.30	-112.32	-
	i'								-112.67	

* data from Bench *et al*. 2002

** rotamer mixture, molar ratio d-f : d'-f' ~1: 2

*** rotamer mixture, molar ratio d-I : d'-I' 1: 3.2

For the F_{51}PcZn series, the ^{19}F chemical shifts for:

- *quadrants type A* have variations <0.5 ppm, *quadrant B* does not have a noticeable influence on them;

- *quadrant type B* show a downfield shift of ~10 ppm as the amino-substituents are acylated, and maximum 2 ppm variations by changing the acylating agent from acetylto perfluobutyryl;
- *perfluorbutyryl* radical exhibit variations <2 ppm for the C**F**$_3$-CF$_2$ and CF$_3$-C**F**$_2$ groups and ~7 ppm for C**F**$_2$-CO going from *N*-H to *N*-methyl; similar values were observed for the PNs **[3-10]** and **[3-11]**.

Table 5.3 ^{19}F NMR assignments for NHAc-, NMeAc-F$_{51}$PcM series (M = Zn, Cu and Co)

			Pc:	**[5-3]**	**[5-4]***	**[5-5]**	**[5-6]***	**[5-7]**	**[5-8]***
Assignment				δ (width at half height), ppm					
Quadrant A	**a**	CF(C**F**$_3$)$_2$		-71.35	-71.31	-71.53	-71.77	-71.25	-71.27
				(0.20)		(0.29)		(0.23)	
	b	C**F**(CF$_3$)$_2$		-164.68	-164.61	-162.04	-162.33	-165.83	-165.81
				(0.12)		(1.17)		(0.21)	
	c	Ar-**F**		-103.93	-103.75	-101.60	-101.25	-105.74	-105.69
				(0.50)		(1.44)		(1.23)	
Quadrant B	**d**	Ar-**F**		-119.94	-119.64	n.d.	n.d.	-123.34	-123.53
	d'				-121.88				-125.35
	e	Ar-**F**		-141.12	-140.86	n.d.	n.d.	-145.31	-145.15
	e'				-139.39				-143.59
	f	Ar-**F**		-132.45	-133.11	n.d.	n.d.	-139.45	-140.36
	f'				-134.59				-141.83

*mixture of rotamers
n.d. – not detected

The ^{19}F NMR chemical shifts, of the MPcs **[5-3] – [5-8]**, and width at half height, for the 3 *quadrants type A* of the NHAcF$_{51}$PcM complexes were compared to highlight the metal ion influence, Table 5.3. Variations in the width at half height values show the following broadening trend PcCu > PcCo > PcZn due to the paramagnetic nature of Cu(II) and Co(II). For chemical shifts comparisons, the diamagnetic Zn(II) complexes data were considered the standard. A

curious fact noticed was that for the tested MPcs, Cu(II) shifted the ^{19}F NMR peak values upfield while Co(II) shifted them downfield, even though both Co(II) and Cu(II) have similar electronegativity and are more electronegative ions vs. the Zn(II) one. Chemical shift variations of 1-2 ppm in 3 *quadrants type A* are seen for the aromatic (Ar-**F**) and aliphatic (C**F**$(CF_3)_2$) type fluorine atoms due to their proximity to the aromatic Pc macrocycle. Higher chemical shift variations, 3 – 7 ppm, were registered for *quadrant type B*, for the Co(II) *vs*. Zn(II) complexes.

5.3.3 FT-IR spectroscopy

The infrared spectra obtained for Pcs **[5-3]** – **[5-8]**, Figures B.15 to B.20, present strong vibrations that overlap in the 1300 – 1100 cm^{-1} region, confirming the presence of the C-F aliphatic and C-F aromatic bonds. The vibrations present around 1450 cm^{-1} correspond to C=C bonds. The C=O amide is present between 1660 – 1700 cm^{-1}. The C-H aliphatic is present around 2900 - 2950 cm^{-1} and N-H amido stretch is present around 3400 - 3450 cm^{-1}.

5.3.4 UV-Vis spectroscopy

The UV-Vis data for Pcs **[5-3]** – **[5-10]**, in a non-coordinating, non-polar solvent ($CHCl_3$) and in coordinating, polar solvents (EtOH or THF), have the characteristic features of asymmetric Pcs, Figures D.12 to D.38. The Q-band of the functionalized Pcs is split in 2 because of the loss in symmetry (Ishii, 2003; Ishii, 2014), very similar to the data obtained for F_{52}PcCu (see chapter 4) and other low symmetry Pcs (Laos, 2012; Patel, 2015), phenomena explained in **Chapter 4**, **section 4.3.4**. Linear dependencies absorbance *vs*. concentration were obtained for all 8 Pcs in both types of solvent, for Pc concentrations 10-50 µM, Figures D.13, D.15, D.17, D.19, D.21, D.23, D.34, D.36. The slopes were extracted from the Lambert-Beer plots and the molar extinction coefficients (as logarithmic values) for each distinct band are shown in Table 5.4.

Several overlayed plots were generated to highlight the influence of *N*-methylation, chelated metal ion, and solvent on the UV-Vis spectra on the acetylated Pc derivatives **[5-3]** – **[5-8]**, Figures D.24 to D.32. The hypsochromic/bathochromic (blue/red-shifting), hyperchromic/hypochromic (increase/decrease in molar absorptivity), and broadening features are discussed vs. the ZnPcs **[5-3]** and **[5-4]**, considered as standards.

Table 5.4 UV-Vis absorption maxima and the molar extinction coefficients of functional F_nPcM

Pc	Solvent	λ_{max} (log ε) nm (L mol^{-1} cm^{-1})
[5-3]	$CHCl_3$	708 (5.28), 679 (5.28), 647 (3.70), 381 (3.85), 320 (3.61)
	EtOH	702 (5.20), 670 (5.20), 645 (4.75), 608 (4.52), 383 (4.85), 320 (4.58)
[5-4]	$CHCl_3$	705 (5.20), 669 (5.20), 646 (4.58), 618 (4.49), 384 (4.79), 320 (4.53)
	EtOH	697 (5.12), 670 (5.13), 642 (4.61), 610 (4.45), 385 (4.77), 320 (4.50)
[5-5]	$CHCl_3$	710 (5.13), 681 (5.13), 648 (4.56), 615 (4.46), 363 (4.74)
	EtOH	700 (5.06), 669 (5.08), 644 (4.62), 605 (4.41), 376 (4.71), 320 (4.56)
[5-6]	$CHCl_3$	706 (5.16), 681 (5.15), 646 (4.54), 616 (4.48), 363 (4.75)
	EtOH	696 (5.07), 669 (5.10), 641 (4.57), 607 (4.40), 377 (4.68), 320 (4.47)
[5-7]	$CHCl_3$	696 (4.96), 668 (5.00), 631 (4.56), 606 (4.44), 353 (4.70), 325 (4.68)
	THF	683 (4.85), 659 (4.91), 602 (4.46), 362 (4.75), 325 (4.68), 292 (4.64)
[5-8]	$CHCl_3$	693 (4.97), 669 (5.00), 631 (4.46), 609 (5.38), 353 (4.69), 317 (4.66)
	THF	680 (4.89), 660 (4.94), 602 (4.49), 363 (4.77), 323 (4.69), 292 (4.64)
[5-9]	$CHCl_3$	704 (5.21), 680 (5.19), 644 (4.57), 616 (4.48), 384 (4.77), 320 (4.54)
	EtOH	698 (5.10), 670 (5.09), 642 (4.60), 610 (4.42), 386 (4.74), 318 (4.48)
[5-10]	$CHCl_3$	702 (5.19), 680 (5.16), 644 (4.51), 618 (4.47), 384 (4.74), 318 (4.52)
	EtOH	694 (5.10), 672 (5.08), 640 (4.53), 612 (4.42), 388 (4.72), 318 (4.48)

The influence of *N*-methylation (*N*-Me Pcs **[5-4]**, **[5-6]**, and **[5-8]** vs. *N*-H Pcs **[5-3]**, **[5-5]**, and **[5-7]**) upon the UV-Vis spectra can be seen in Figures D.26, for $CHCl_3$, and D.29, for the coordinative solvents. Both figures show an overlap in the B-bands region (300 – 450 nm), while

for the split Q-bands a smaller gap for the *N*-methyl analogs is noticed. The shorter Q-band wavelength is not influenced by methylation, remaining practically constant. While the longer Q-band wavelength shows a 4-5 nm hypsochromic shift, the HOMO-LUMO gap decreases in the *N*-Me vs. the *N*-H Pcs. The methyl group has an inductive effect *+I* increasing the electron donor capacity of the amidyl radical. The hypsochromic shift, due to methylation, is responsible for the higher degree of overlapping in the split Q-bands that results in a smaller gap.

The following metal ions Zn(II), Cu(II), and Co(II) were used in the synthesis of functionalized MPcs. The overlayed UV-Vis spectra, shown in Figures D.24, D.25, D.27, and D.28, highlight the influence of the metal ions. Two selected graphs are shown below in Figure 5.7 for the Pcs **[5-3]**, **[5-5]**, and **[5-7]** in $CHCl_3$.

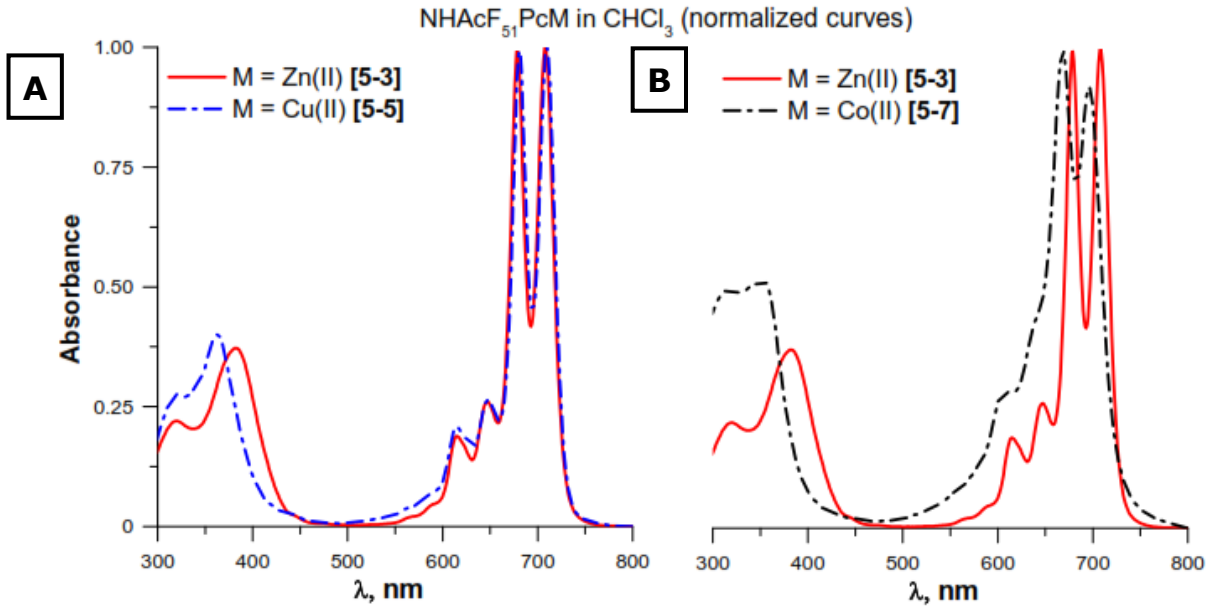


Figure 5.7 UV-Vis spectra of $NHAcF_{51}PcM$ series, M = Zn(II), Cu(II), and Co(II), in $CHCl_3$, normalized curves for Zn(II) vs. Cu(II) complexes (**A**), and Zn(II) vs. Co(II) complexes (**B**).

The influence of the open-shell ions Cu(II) and Co(II) on the electronic absorption is presented separately for the B bands and Q band domains. In the B bands domain, hypsochromic

shifting was registered for the main B band (the band with the highest absorbance and lowest wavelength). The hypsochromic shifting is more accentuated for the Co(II) vs. Cu(II) complexes and it is highly influenced by the solvent type. In chloroform, the difference is ~30 nm for Co(II) Pcs and ~20 nm for Cu(II) Pcs, while in coordinative solvents the values drop to ~20 nm for Co(II) Pcs and ~5 nm for Cu(II) Pcs, Table 5.4.

In the Q-band region, the Cu(II) and Zn(II) complexes overlap very well, while Co(II) complexes are shifted hypsochromic and are broader, Figure 5.7, similar behavior was seen for previously reported fluorinated CoPcs (Bench, 2000; Loas 2012; Patel 2015). A small hypochromic shift (lower extinction coefficients) is registered for the Cu(II) complexes, while the difference increases significantly for the Co(II) complexes, Table 5.4.

The influence of the solvent type is highlighted in Figures D.30, D31, and D32 for Zn(II), Cu(II), and Co(II) complexes. In non-coordinating (chloroform) vs. coordinating solvents, all the complexes are less aggregated, the bands are well defined, and higher extinction coefficients were obtained. The coordinating solvents (ethanol for Zn(II) and Cu(II), and tetrahydrofuran for Co(II) complexes) have a big influence on the Cu(II) and Co(II) complexes. Bathochromic shifts in the B bands region and hypsochromic shifts in the Q band region are seen for the spectra obtained in coordinating solvents by comparison to the data obtained in chloroform. In the case of perfluoro *n*-butyramido-substituted ZnPcs, **[5-9]** and **[5-10]**, the same observations are noticed as for the acetylated ZnPc derivatives **[5-3]** and **[5-4]** regarding the influence of *N*-methylation and solvent type on the UV-Vis spectra, Figures D.37 and D.38.

The UV-Vis data for the Q-band of the Pcs can be correlated with the HOMO-LUMO gap the smaller the gap the longer the wavelength. Theoretical DFT calculations of the HOMO-LUMO energies and their gap showed lower values for the F_{64}PcM representatives vs. the F_{16}PcM and

PcM, M = V=O(IV), due to the complete substitution of the Pc macrocycle with eight fluorine atoms and eight *i*-C_3F_7 groups (Moons *et al*. 2017). The *i*-C_3F_7 groups induce a redshift in the Q-band of the F_{64}PcM. A similar trend for the decrease of the HOMO-LUMO gap was seen also in a series of PNs (Pc precursors) that ranged from tetrafluoro-substituted PN to perfluoisopropyl-substituted PNs (*i*-C_3F_7 = electron-withdrawing group, EWG) and amino-substituted PNs (NH_2 = electron-donating group, EDG) (Pelmuş, Raab *et al.*, 2020). The introduction of amino groups in the Pc structure, done for the ZnPcs **[5-1]** and **[5-2]**, is expected to have effects paralleling those of the amino-substituted PNs, including a decrease of the HOMO-LUMO gap compared to the fluorinated parent complex F_{52}PcZn (Patel, 2015). As seen for the PNs series, nucleophilic substitutions have a major influence on the spectroscopic and electrochemical properties of the resulted derivatives; the fine tunning effects are expected to extend also to the corresponding Pcs.

5.3.5 Crystal structures

X-ray quality single crystals were grown by slow evaporation of MPc solutions. Solvent mixtures (1:1 ethyl acetate or acetone in toluene) were used to dissolve the compounds **[5-3]** – **[5-8],** and the two OH or H_2O complexes of **[5-7]** and **[5-8]**. The solvent mixtures included a medium polarity, coordinating, low boiling point solvent (ethyl acetate or acetone), and a low polarity, non-coordinating, high boiling point solvent (toluene). The medium polarity solvents were chosen primarily for their ability to completely dissolve the MPc, at least ~1 mg MPc/mL solvent. Toluene was used as (*i*) co-crystallization compound, favoring π-π interactions with the Pc macrocycle, (*ii*) miscible co-solvent, and (*iii*) non-solubilizing agent towards the resulted crystals, storage media.

The crystals show similar packing of the MPcs in the lattice, exhibiting the following similar structural features:

- same organic Pc macrocycle, $NRAcF_{51}Pc$ with R = H or Me

- complexation with bivalent metal ions, Zn(II), Cu(II) and Co(II), first-row transition metals

- dimer formation by coordinative interactions, coordinative dimerization, through double coordination: the acetamide oxygen of a Pc molecule coordinates to the metal center of a second Pc while its acetamide oxygen coordinates to the metal center of the first Pc

- negligible influence of *N*-methylation or OH/H_2O coordination, not bulky enough.

Toluene is present in all crystals as a cocrystallization compound and some crystals contain also molecules of the medium polarity solvents, Table 5.5.

Table 5.5 Crystals formed by the **[5-3]** – **[5-8]** Pcs

Pc	Cocrystal formulas	Distance[a] (Å)	Angle[b] (°)	Appendix
[5-3]	**$[NHAcF_{51}PcZn]_2$·7(toluene)**	6.647	40.21	**O**
[5-4]	**$[NMeAcF_{51}PcZn]_2$·3(toluene)·0.75(acetone)**	6.610	40.51	**P**
[5-5]	**$NHAcF_{51}PcCu$·3(toluene)·EtOAc**	6.620	41.82	**Q**
[5-6]	**[$NMeAcF_{51}PcCu]_2$·2.75(toluene)·0.5(acetone)**	6.717	42.95	**R**
[5-7]	**$[NHAcF_{51}PcCo]_2$·7(toluene)**	6.667	39.00	**S**
	$[(NHAcF_{51}PcCo)_2OH]$·7(toluene)*	6.712	38.97	**T**
	$[(NHAcF_{51}PcCo)_2H_2O]$·7(toluene)*	6.712	38.97	**U**
[5-8]	**$[NMeAcF_{51}PcCo]_2$·7(toluene)**	6.769	39.95	**V**
	$[(NMeAcF_{51}PcCo)_2OH]$·7(toluene)*	6.751	39.12	**W**
	$[(NMeAcF_{51}PcCo)_2H_2O]$·7(toluene)*	6.751	39.12	**X**

a – distance between the MPc macrocycle planes from 2 different coordinative dimers
b – the angle between MPc macrocycle planes in the coordinative dimer
* - proposed formulas, undetermined if the actual ligand is OH^- or H_2O, as the H atoms are not detected by XRD

Simplified views of the pentacoordinate MPc and coordinative dimer structures, common for all crystals presented in Table 5.5, are shown in Figure 5.8. Looking further for the views along the axes, especially along the a-axis, one can see how the toluene molecules are arranged in the open space inside of the coordinative dimer and outside of Pc molecules, Figure 5.9.

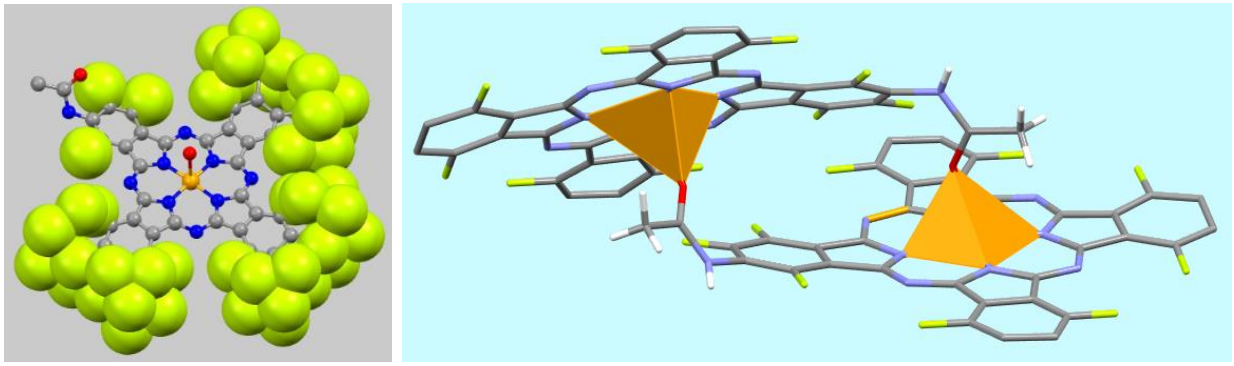


Figure 5.8 Structural representations for **NHAcF$_{51}$PcM**: pentacoordinate metal ion and space-fill fluorine atoms (left), coordinative dimer (right), the *i*-C_3F_7 groups were omitted for a clearer view.

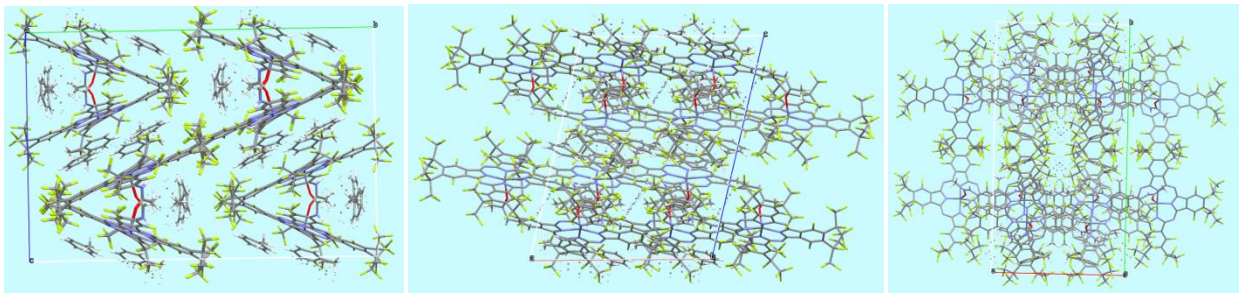


Figure 5.9 Graphic representation of **[NHAcF$_{51}$PcZn]$_2$·7(toluene)** crystal unit cell; views along **a**-axis (left), **b**-axis (middle), and **c**-axis (right).

The coordinative dimers formed by the **NHAcF$_{51}$PcZn** have a "laundry tongs" appearance, especially when viewed along **a**-axis of the crystal unit cell, the 2 MPcs making a ~40° angle. The distance between the sheets of dimers is ~6.65 Å as a layer of toluene molecules gets intercalated in between, Figure 5.10. Stong π-π stacking interactions are established between the 4 toluene molecules and the benzene rings of only one of the MPcs, an analysis performed using the Aromatic Analyzer feature of the Mercury 4.0 software (Macrae *et al*., 2020).

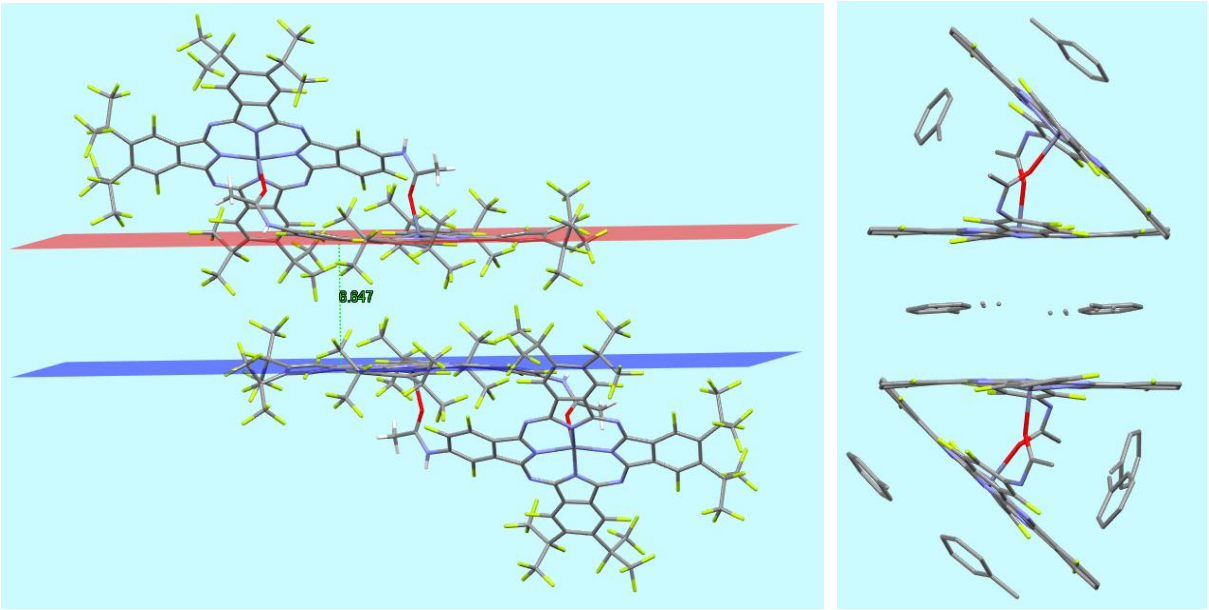


Figure 5.10 Interactions between dimers and toluene in **[NHAcF$_{51}$PcZn]$_2$·7(toluene)** crystal, the distance between dimers is ~6.65 Å (left), and toluene molecules are arranged between the dimers (right).

All MPcs **[5-3]** – **[5-8]** have crystalized as coordinative dimers and they respect the arrangements described for **[NHAcF$_{51}$PcZn]$_2$·7(toluene)** crystal structure. The single-crystal X-ray data bring valuable structural information for the identity of the MPcs especially for the paramagnetic ones, M = Co(II) or Cu(II). The identity of the paramagnetic complexes cannot be completely elucidated by NMR spectroscopy and the X-ray comes as structural proof in the assignment of the chemical structure proposed after the high-resolution mass spectroscopy analysis.

More structural information regarding the formation of coordinative dimers can be connected with the electron-withdrawing nature of the Pc macrocycle. Due to the presence of 6 perfluoroalkyl groups on the Pc ligand, the metal behaves as a Lewis acid and is coordinating electron donor atoms/groups, in this case, the amide group is found in equilibrium with its resonance state. Connecting the observations seen for the solid-state form of the acetylated MPcs with their UV-Vis data in the solution we can say that the coordinative dimers are only stable in

the solid-state as no monomer-dimer equilibria are noticed for the tested concentrations, 10-50 μM, in both coordinative and non-coordinative solvents.

5.4 Conclusions

A new class of acylated Pcs was produced at mg scale, see **sections 5.2.3 – 5.2.6**, but the overall yields are low due to the byproduct Pcs, especially F_{64}PcM. The proposed chemical structures were confirmed using spectroscopic techniques (UV-Vis, FT-IR, NMR, and single-crystal X-ray diffraction). The stable compounds showed no visible aggregation for the tested concentration domain, 10-50 μM, in both coordinating and noncoordinating solvents.

The ^{19}F and ^{1}H NMR data from the acylated Pcs align with the ones for the corresponding acylated PNs and this similarity helped in the assignment. For the *N*-methyl rotamers is observed, by NMR, a change in the ratio as the aromatic fragment changes from PN to Pc. The paramagnetic ions, introduced in the acetylated MPc series, have a strong influence on the ^{19}F NMR signals (broaden the signals and decrease their intensity), especially in the case Cu^{2+}.

Coordinative dimers were observed for all the acetylated MPcs (M = Zn, Cu, and Co) in the solid-state by X-ray single-crystal crystallography, this being the first report of the acetylated Pcs crystal structures to the best of our knowledge. The crystal unit cells are similar for all compounds with small differences regarding the angle formed between the monomers and the distances between the dimers. The toluene molecules interact with the dimers through π-π stacking interactions aromatic ring – Pc macrocycle acting as bridges between the coordinative dimers.

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Appendix A: NMR spectra

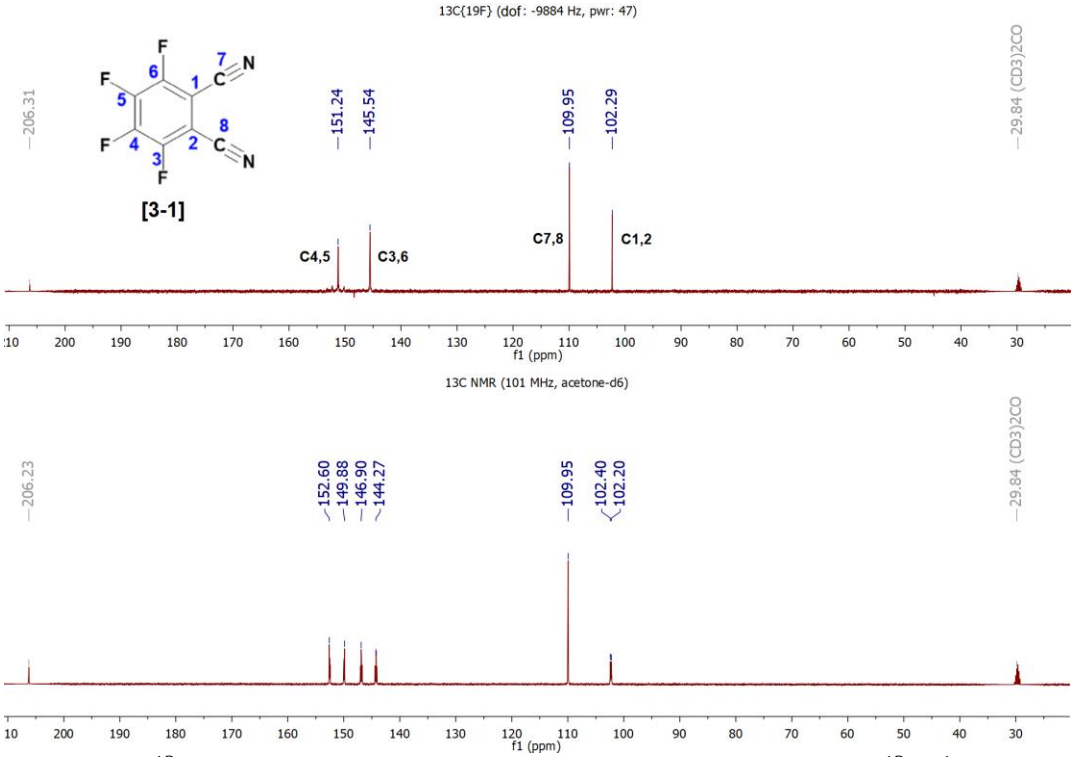


Figure A.1 ^{13}C NMR (101 MHz) spectra of **[3-1]** in acetone-d_6, top: $^{13}C\{^{1}H\}$, bottom: $^{13}C\{^{19}F\}$.

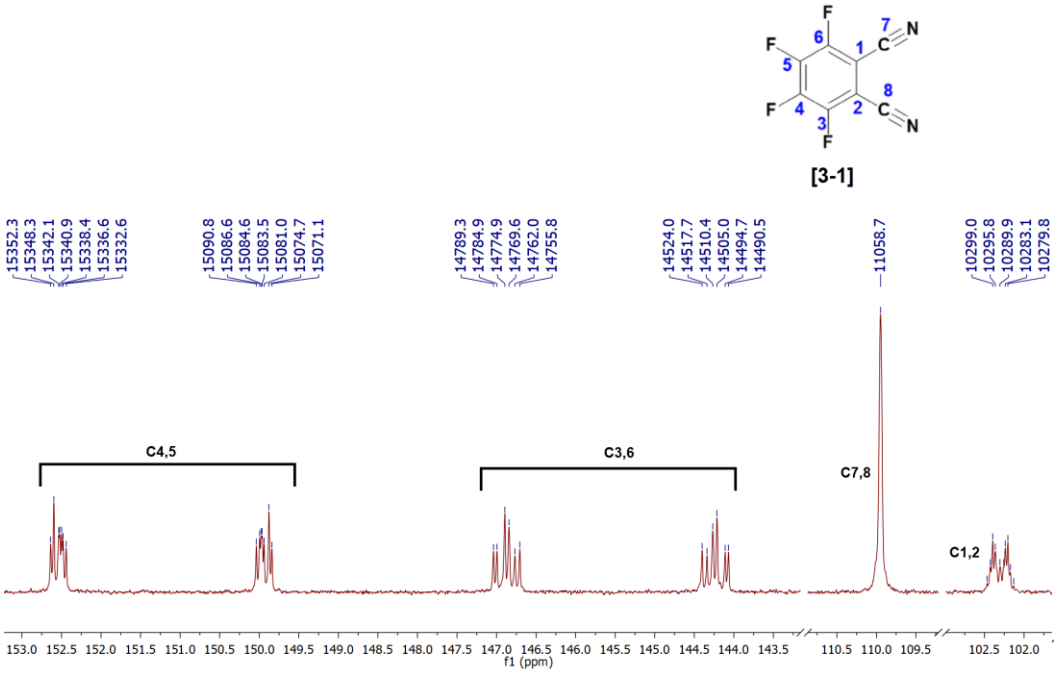


Figure A.2 $^{13}C\{^{1}H\}$ NMR (101 MHz) spectrum of **[3-1]** in acetone-d_6, expanded signal domains. The peak values are in Hz.

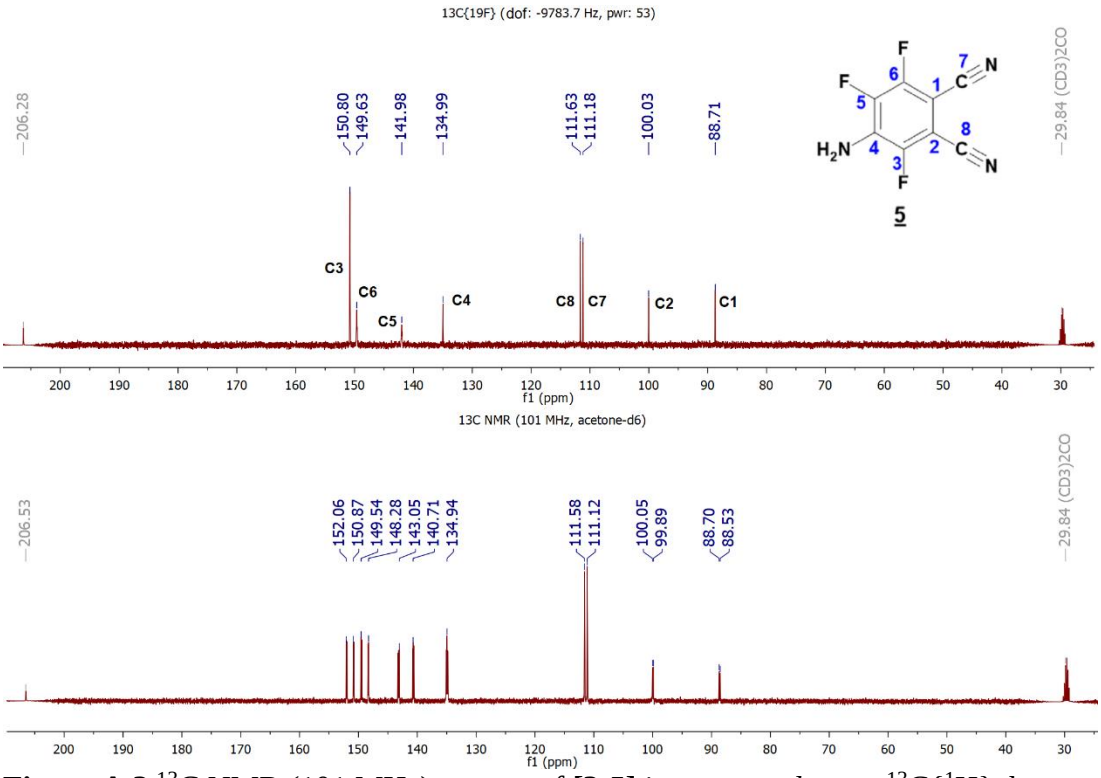


Figure A.3 ^{13}C NMR (101 MHz) spectra of **[3-5]** in acetone-d_6, top: $^{13}C\{^{1}H\}$, bottom: $^{13}C\{^{19}F\}$.

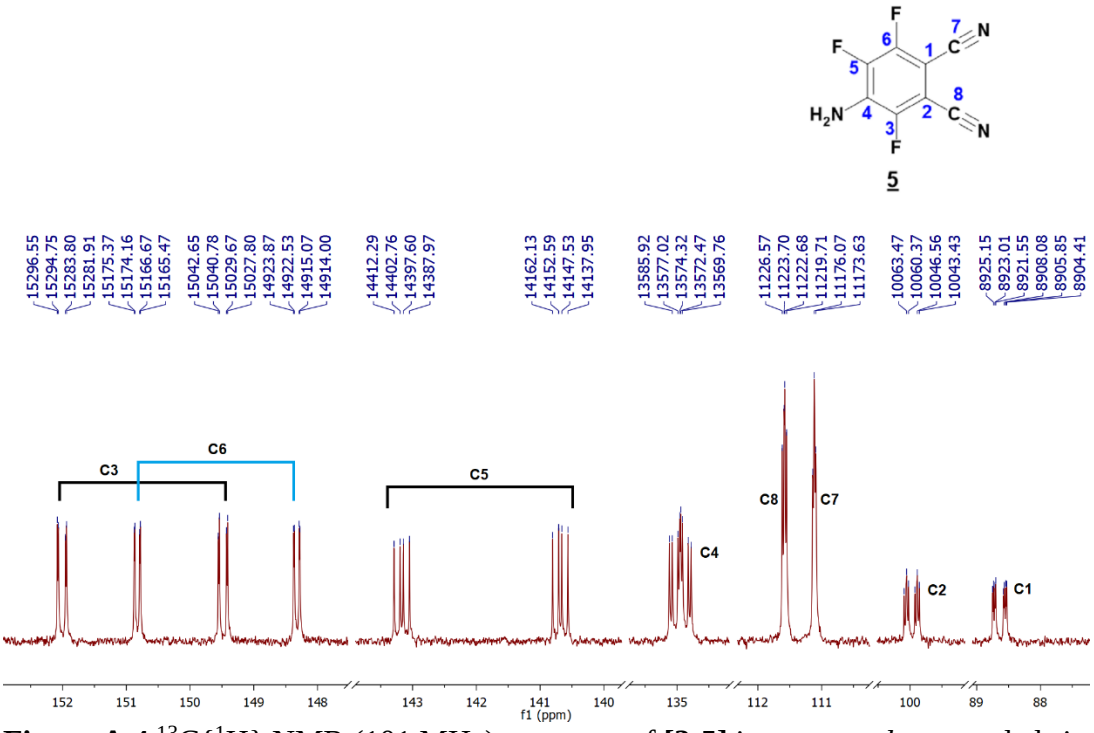


Figure A.4 $^{13}C\{^{1}H\}$ NMR (101 MHz) spectrum of **[3-5]** in acetone-d_6, expanded signal domains. The peak values are in Hz.

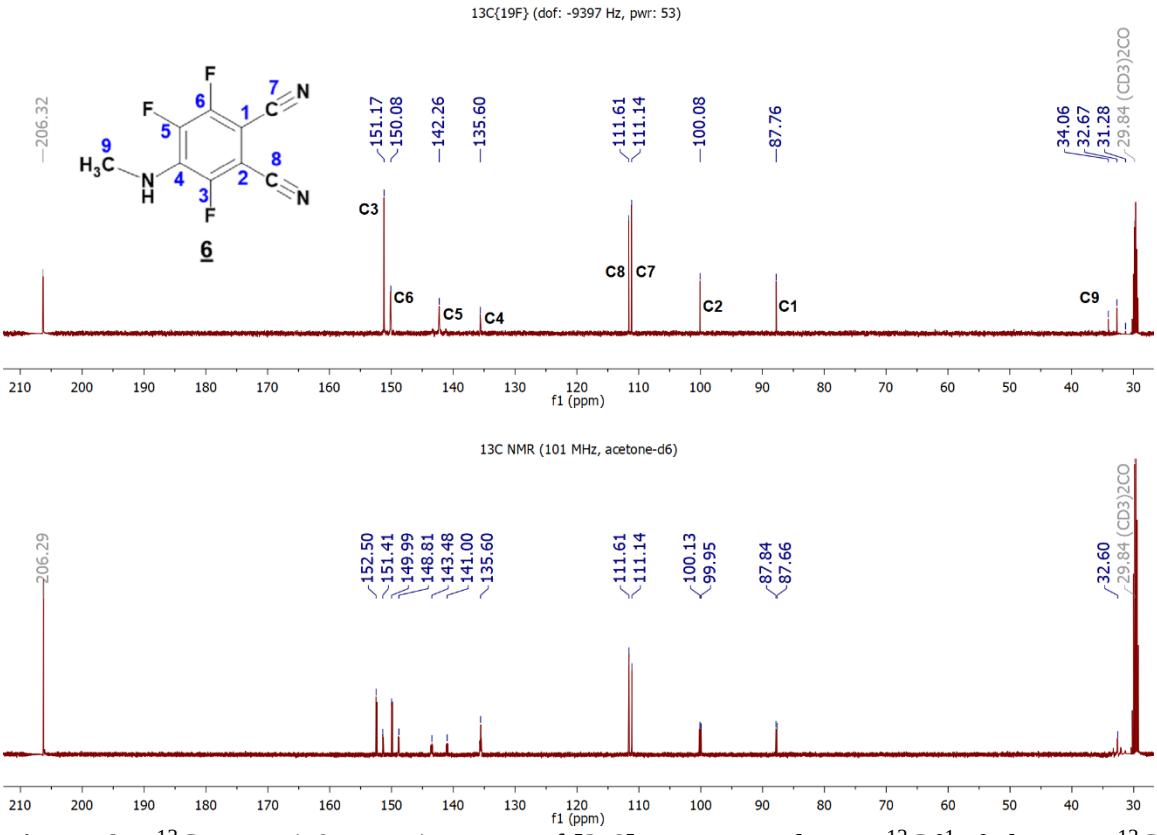


Figure A.5 ^{13}C NMR (101 MHz) spectra of **[3-6]** in acetone-d_6, top: $^{13}C\{^{1}H\}$, bottom: $^{13}C\{^{19}F\}$.

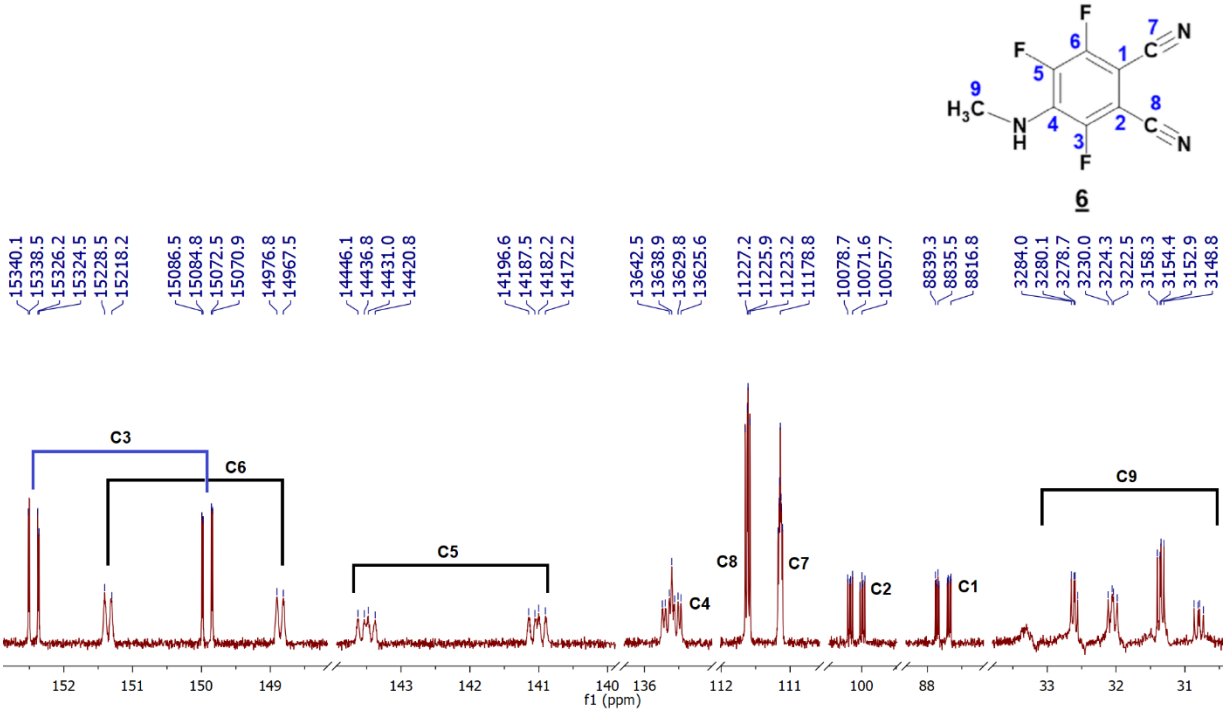


Figure A.6 $^{13}C\{^{1}H\}$ NMR (101 MHz) spectrum of **[3-6]** in acetone-d_6, expanded signal domains. The peak values are in Hz.

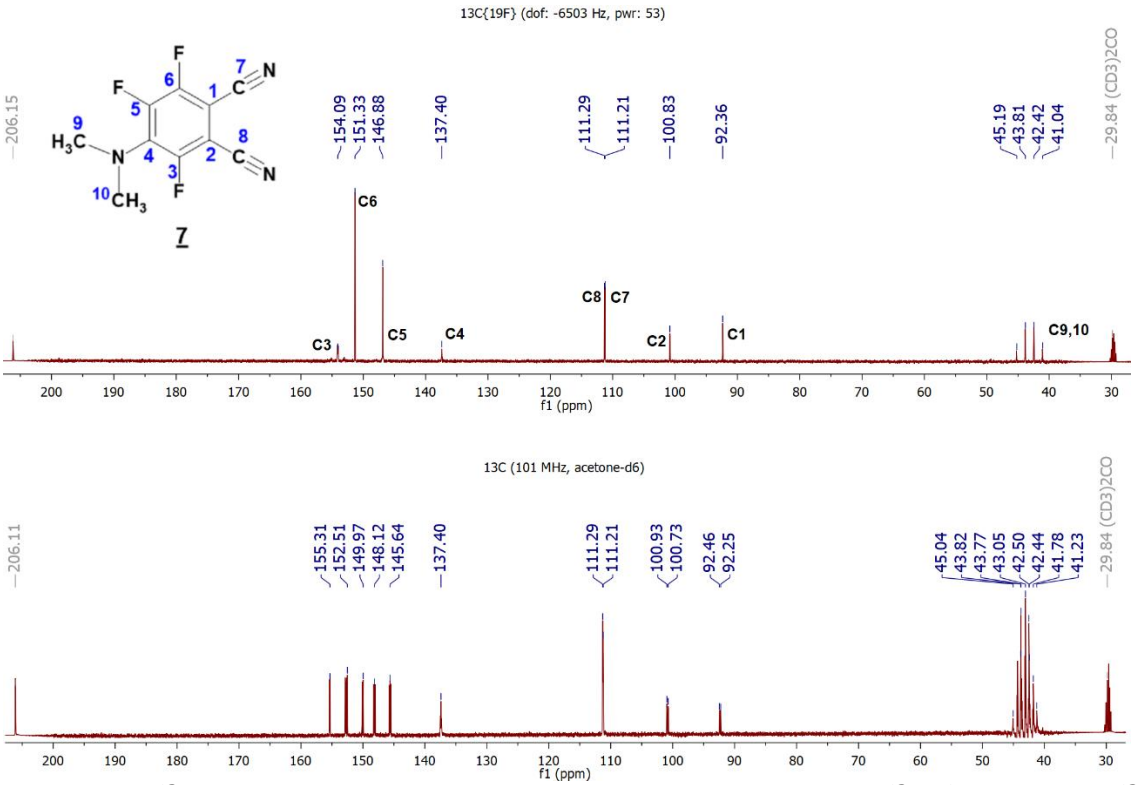


Figure A.7 ^{13}C NMR (101 MHz) spectra of **[3-7]** in acetone-d_6, top: $^{13}C\{^{1}H\}$, bottom: $^{13}C\{^{19}F\}$.

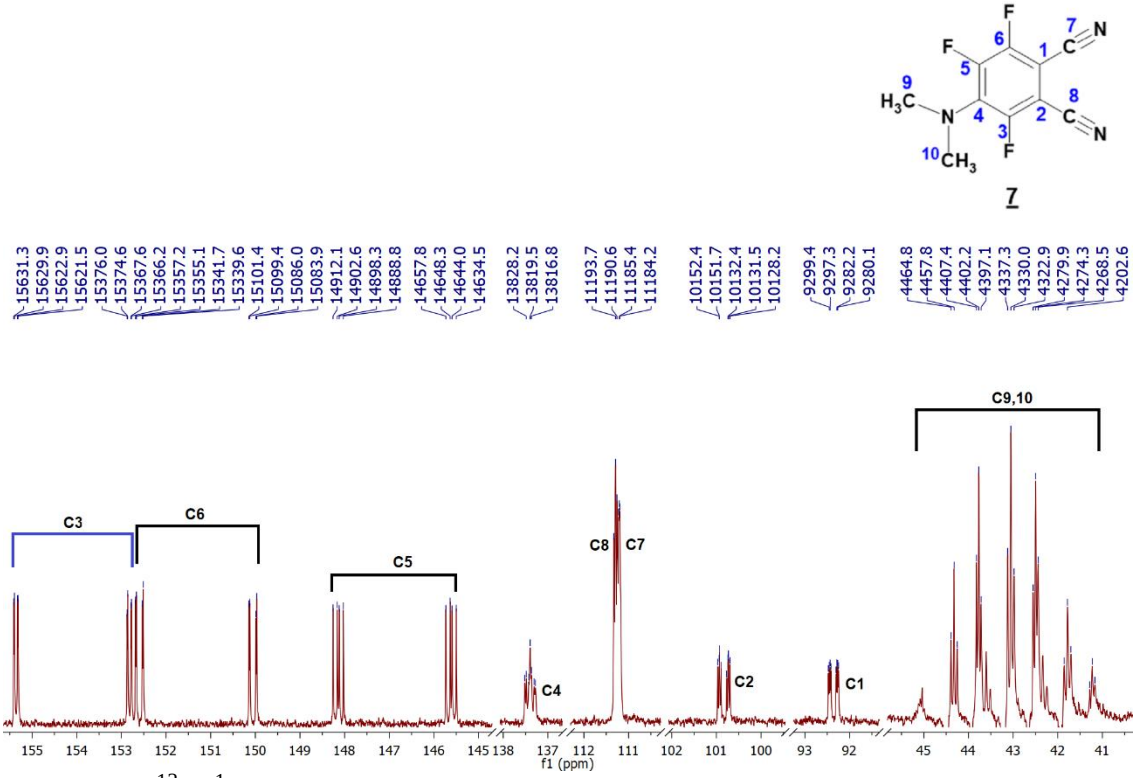


Figure A.8 $^{13}C\{^{1}H\}$ NMR (101 MHz) spectrum of **[3-8]** in acetone-d_6, expanded signal domains. The peak values are in Hz.

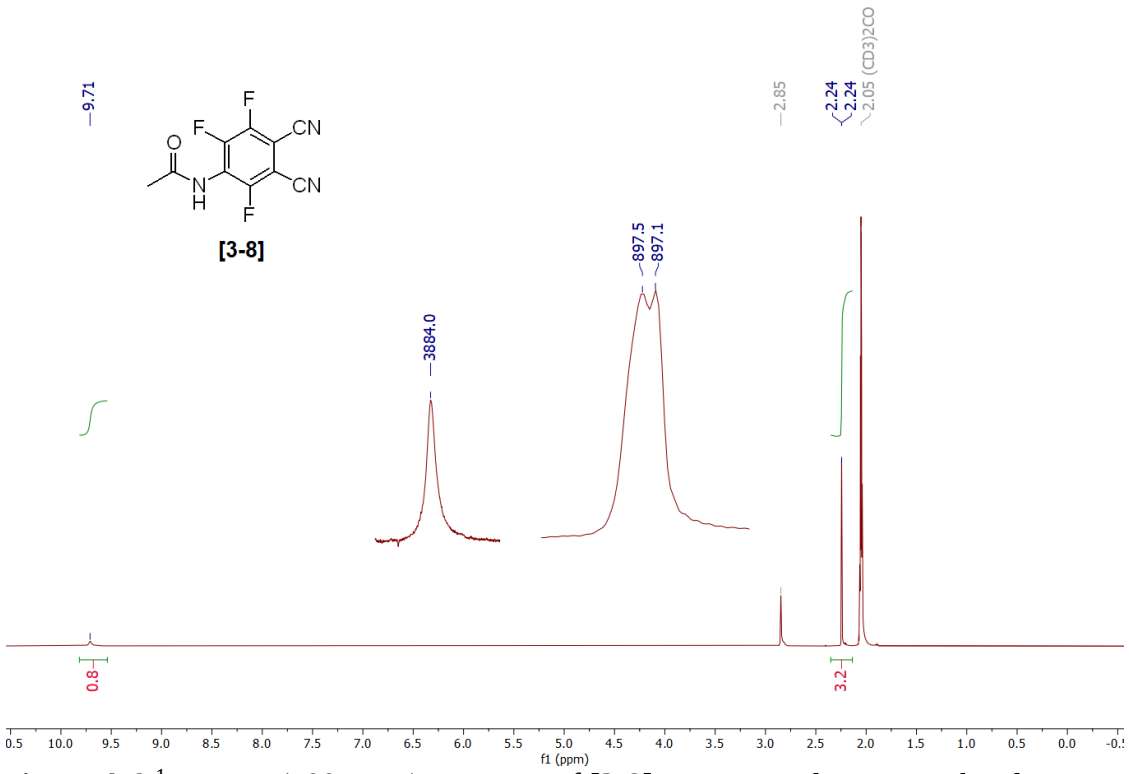


Figure A.9 ^{1}H NMR (400 MHz) spectrum of **[3-8]** in acetone-d_6. Inset peak values are in Hz.

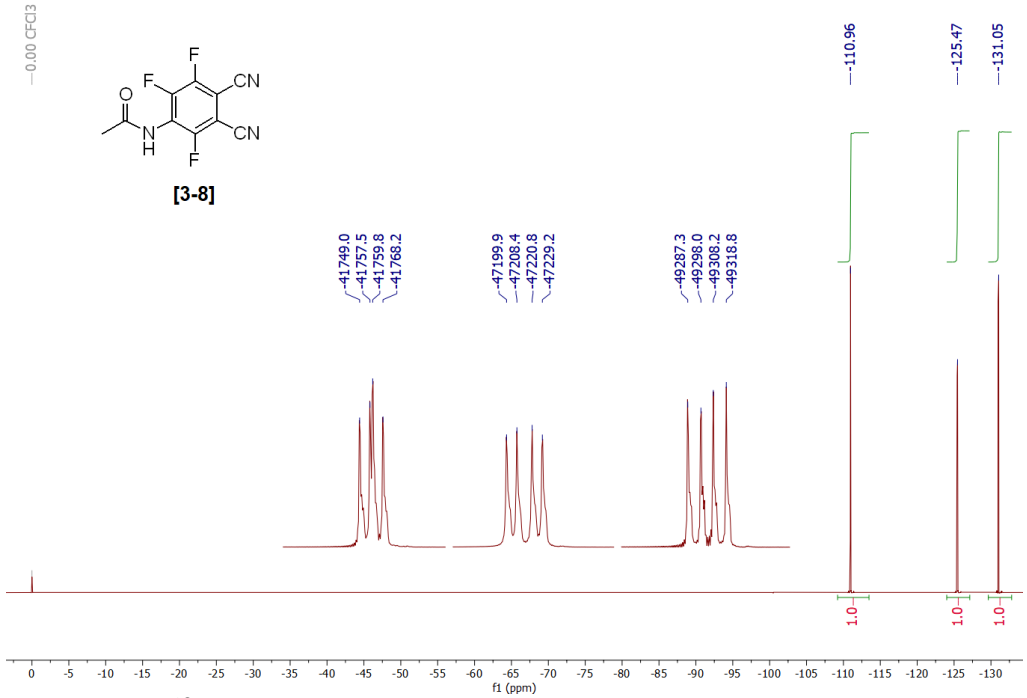


Figure A.10 ^{19}F NMR (376.5 MHz) spectrum of **[3-8]** in acetone-d_6. Inset peak values are in Hz.

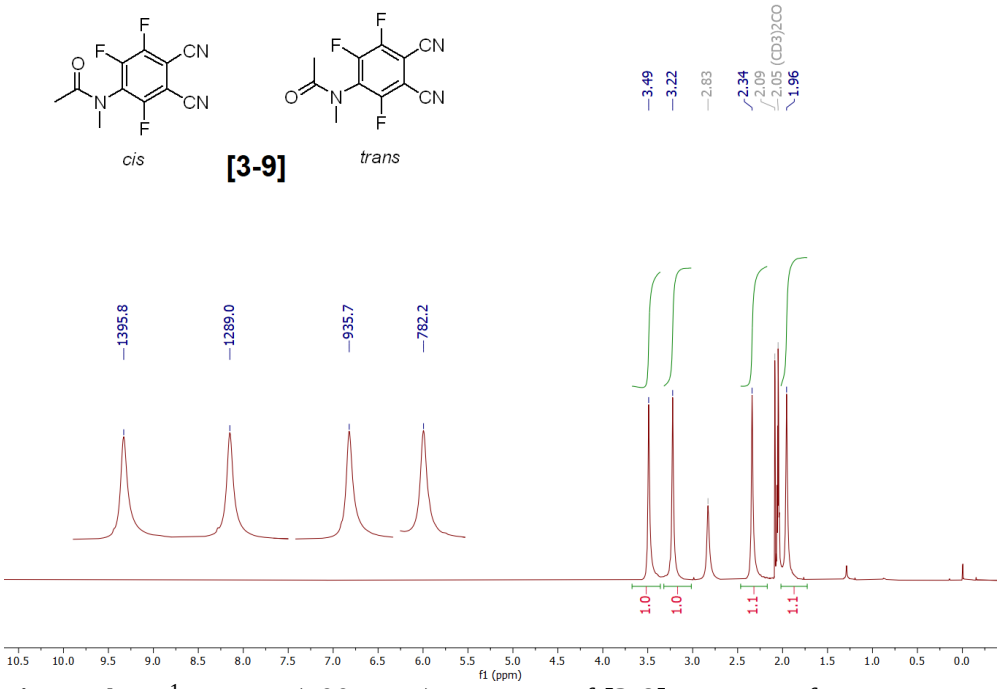


Figure A.11 ^{1}H NMR (400 MHz) spectrum of **[3-9]**, mixture of rotamers, in acetone-d_6. Inset peak values are in Hz.

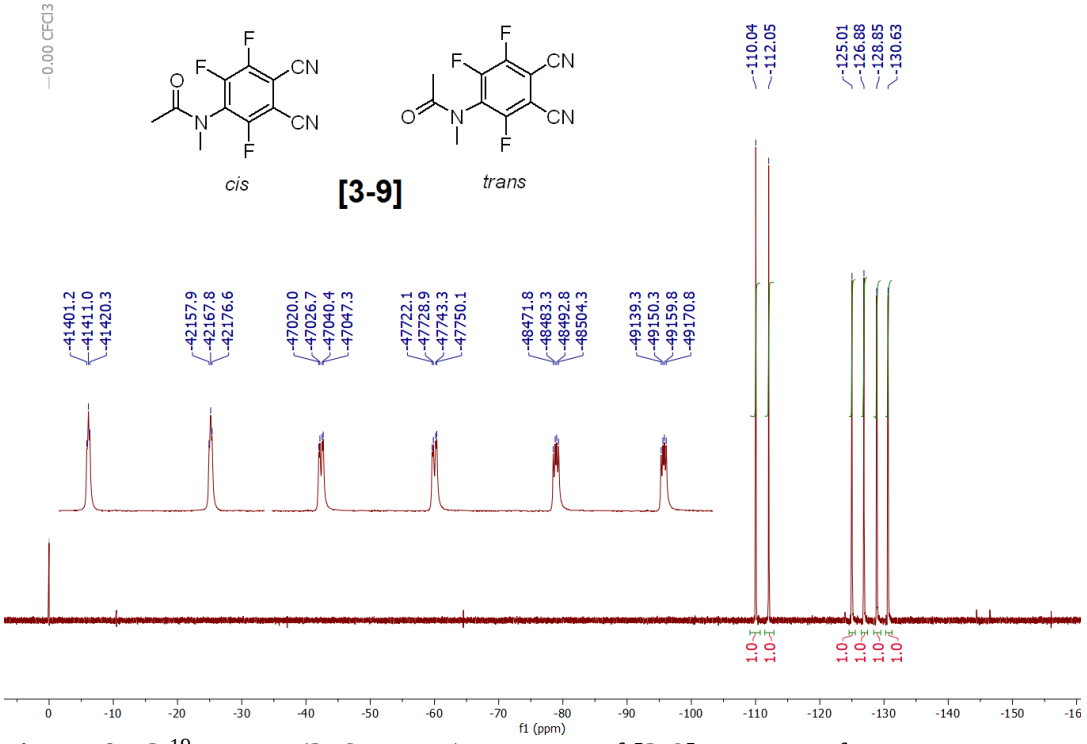


Figure A.12 ^{19}F NMR (376.5 MHz) spectrum of **[3-9]**, mixture of rotamers, in acetone-d_6. Inset peak values are in Hz.

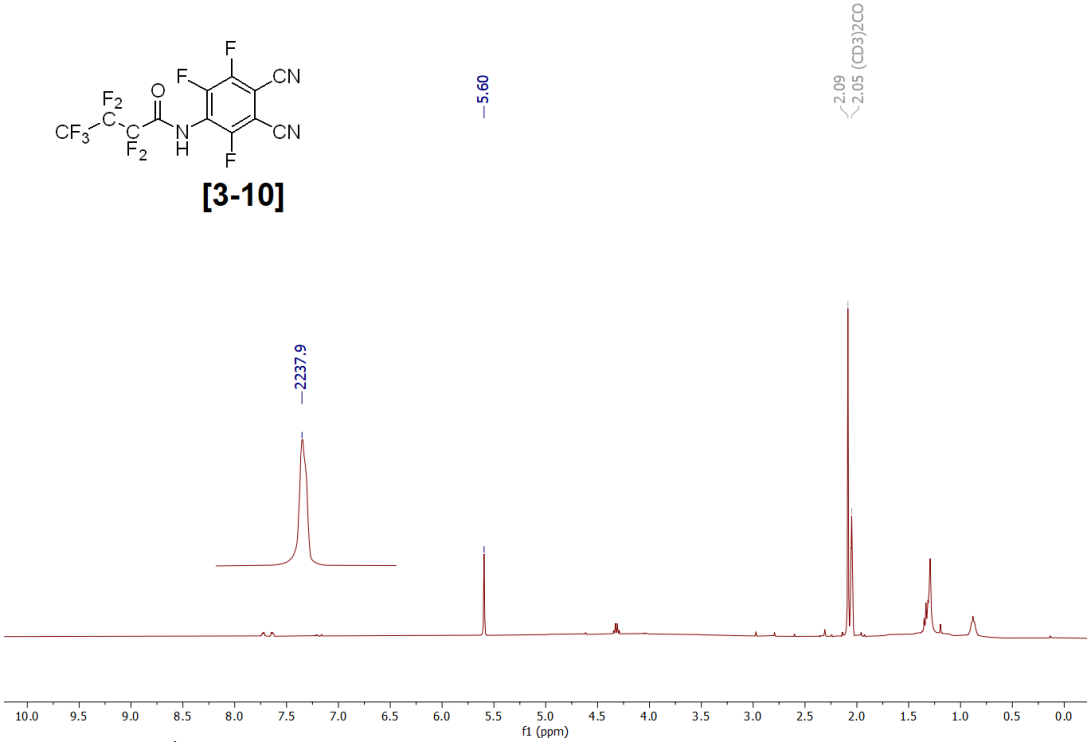


Figure A.13 ^{1}H NMR (400 MHz) spectrum of **[3-10]** in acetone-d_6. Inset peak values are in Hz.

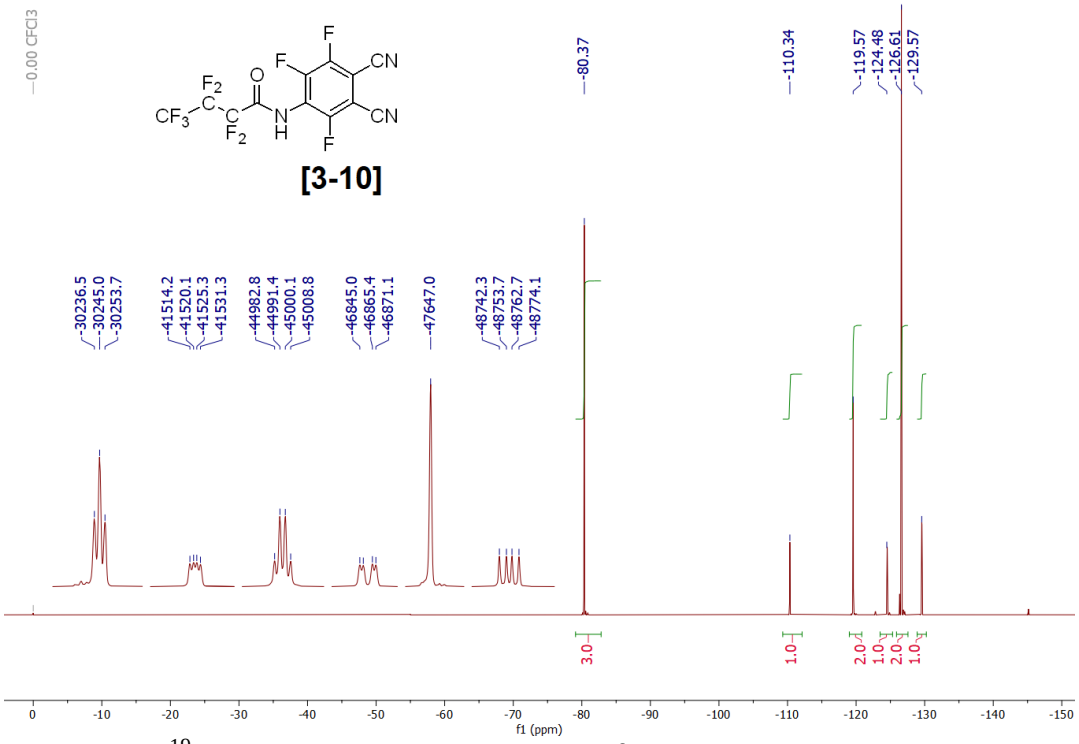


Figure A.14 ^{19}F NMR (376.5 MHz) spectrum of **[3-10]** in acetone-d_6. Inset peak values are in Hz.

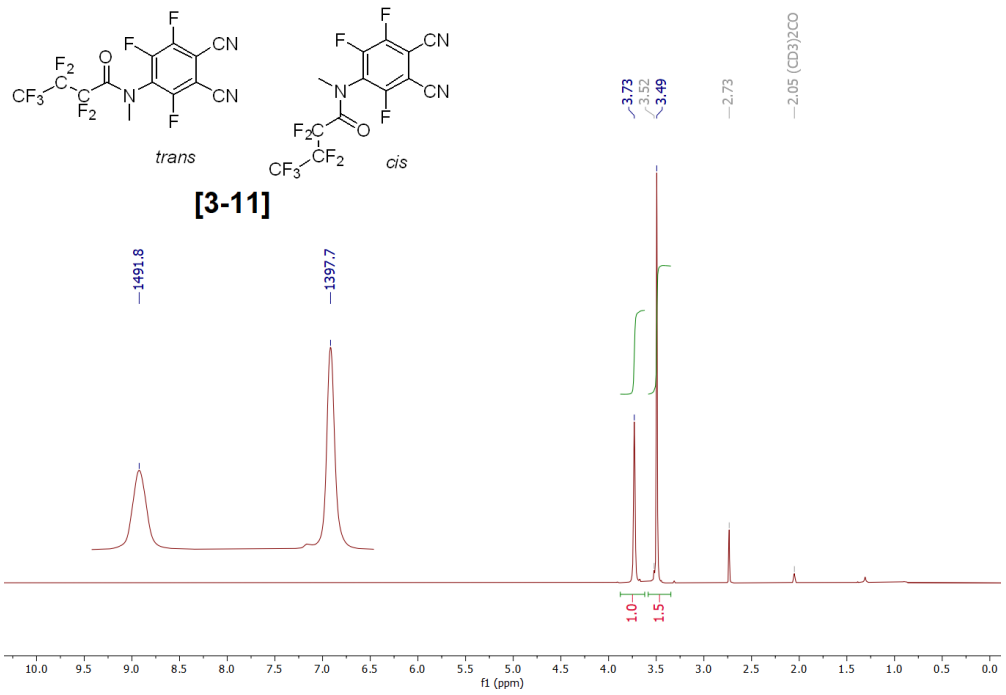


Figure A.15 ^{1}H NMR (400 MHz) spectrum of **[3-11]** isomer mixture in acetone-d_6. Inset peak values are in Hz.

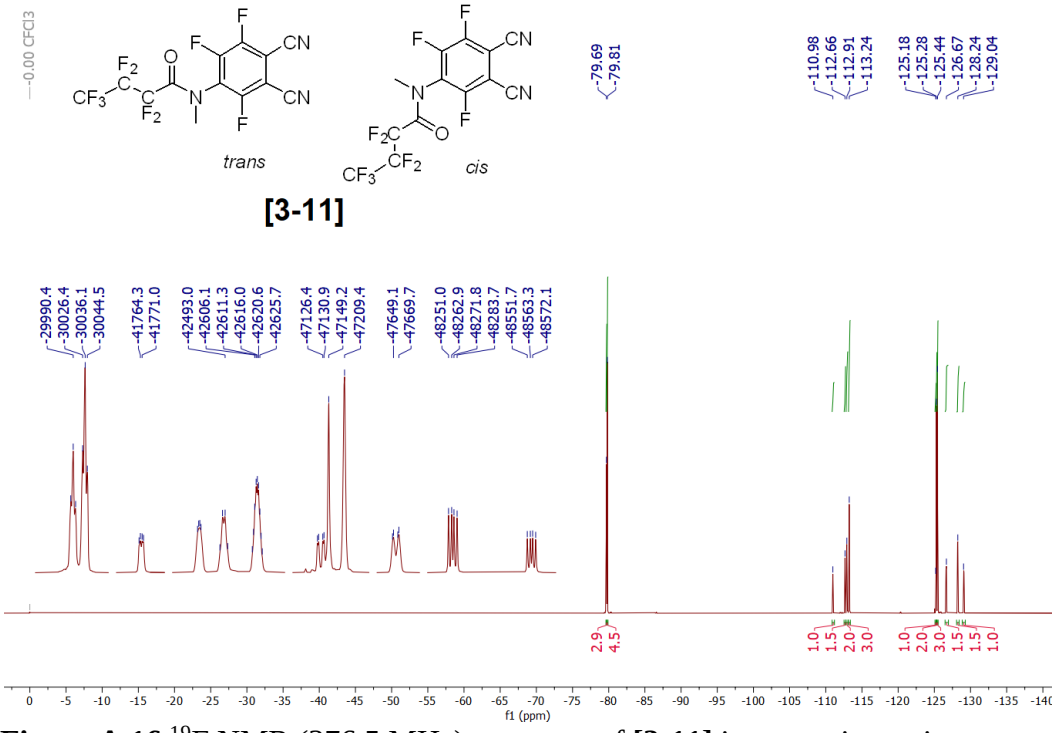


Figure A.16 ^{19}F NMR (376.5 MHz) spectrum of **[3-11]** isomer mixture in acetone-d_6. Inset peak values are in Hz.

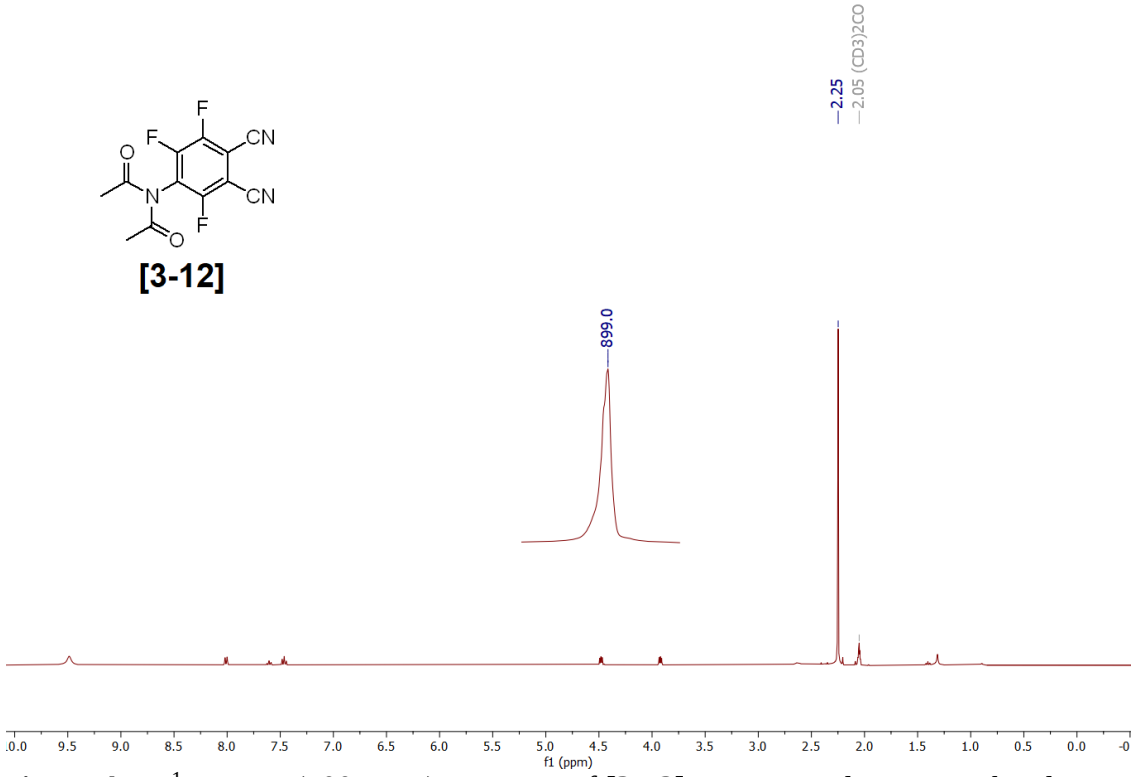


Figure A.17 ^{1}H NMR (400 MHz) spectrum of **[3-12]** in acetone-d_6. Inset peak values are in Hz.

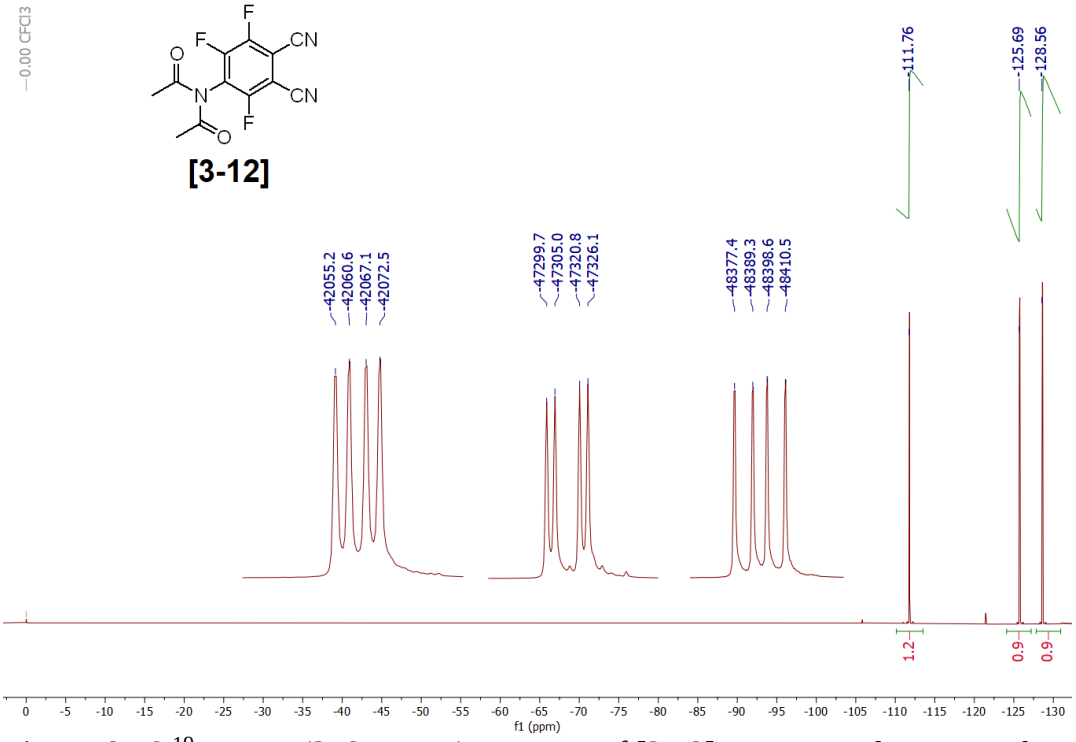


Figure A.18 ^{19}F NMR (376.5 MHz) spectrum of **[3-12]** in acetone-d_6. Inset peak values are in Hz.

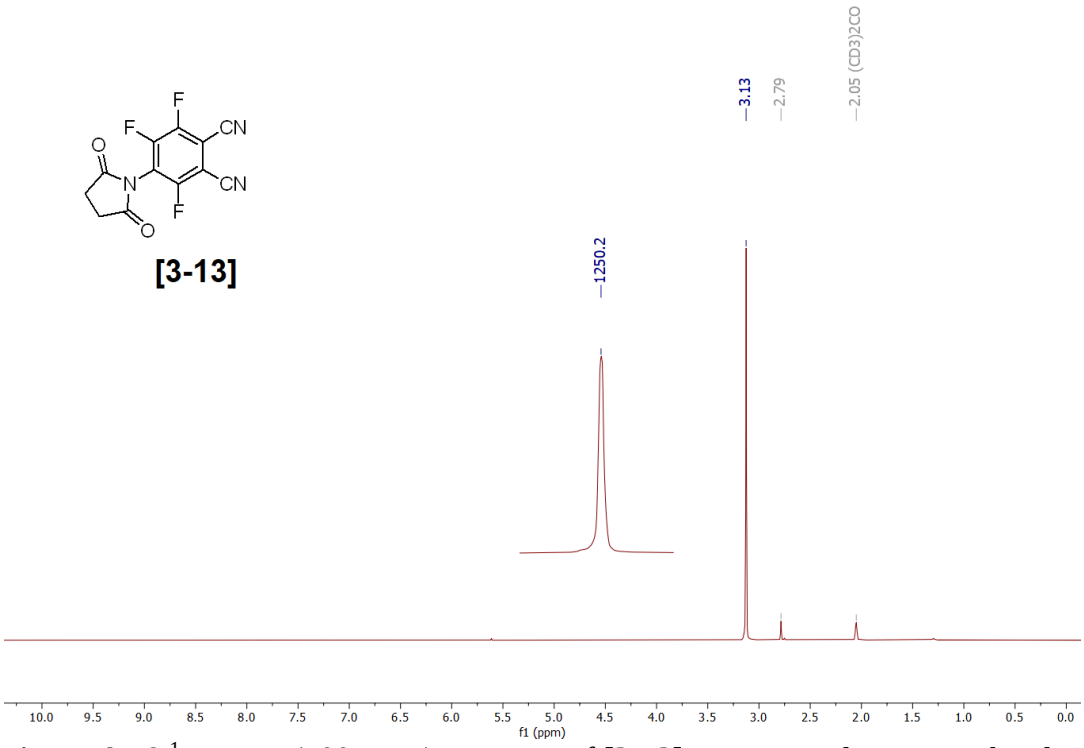


Figure A.19 ^{1}H NMR (400 MHz) spectrum of **[3-13]** in acetone-d_6. Inset peak values are in Hz.

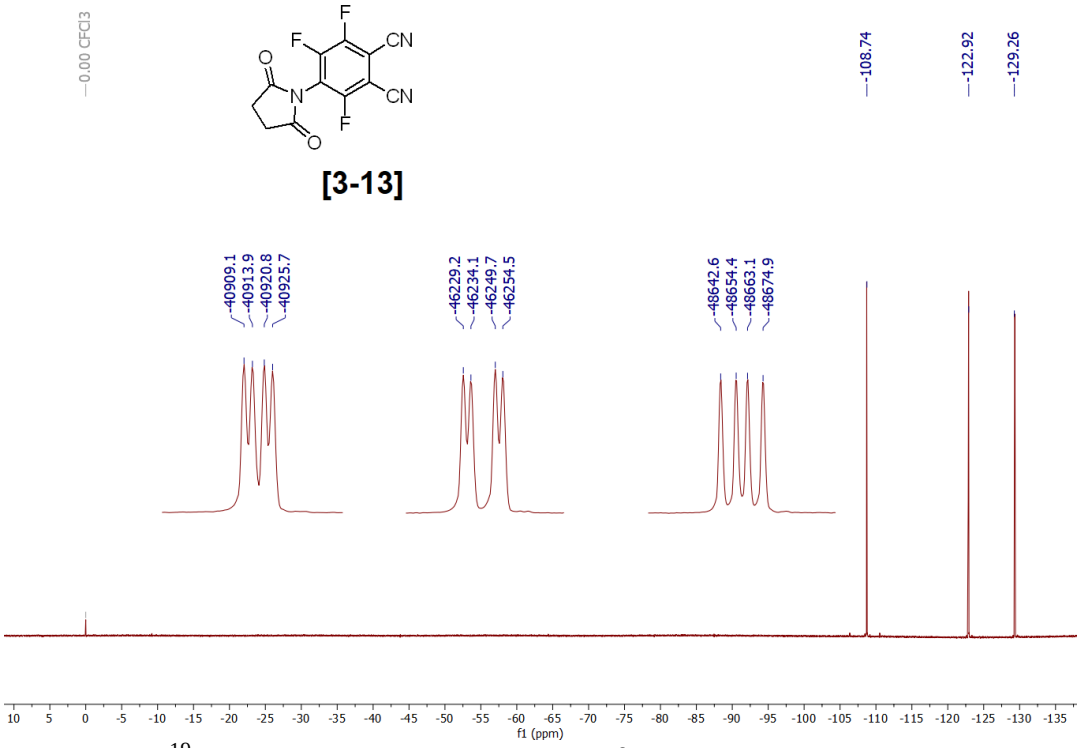


Figure A.20 ^{19}F NMR (376.5 MHz) spectrum of **[3-13]** in acetone-d_6. Inset peak values are in Hz.

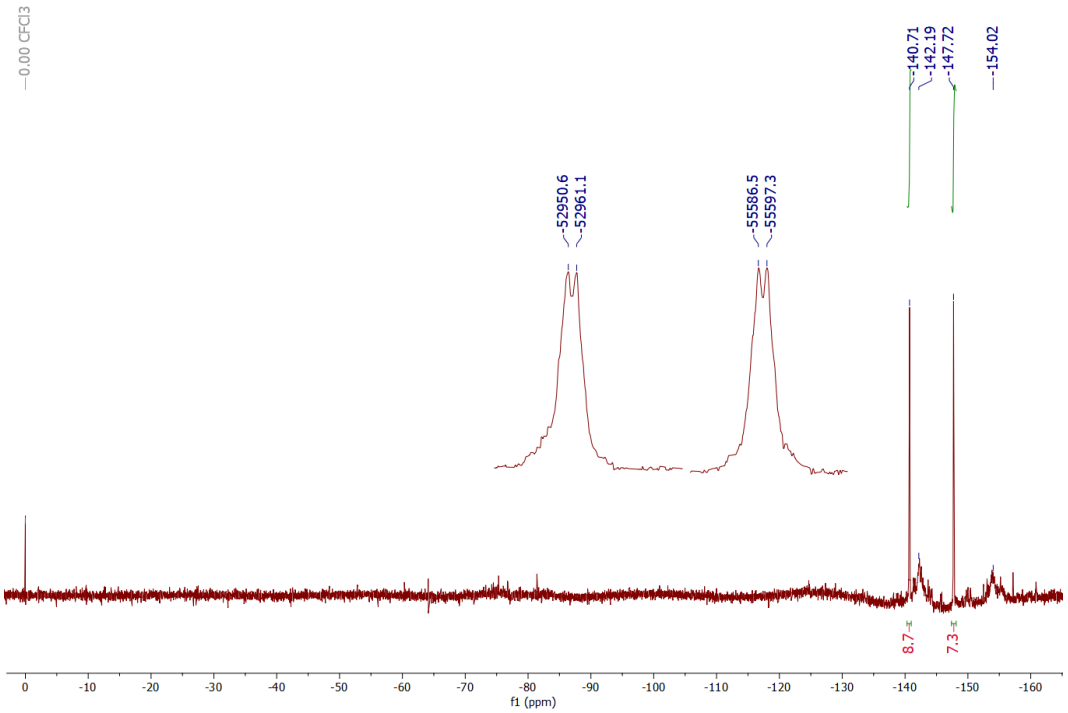


Figure A.21 ^{19}F NMR (376.5 MHz) spectrum of F_{16}PcZn **[4-1]** in methanol-d_4. Inset peak values are in Hz.

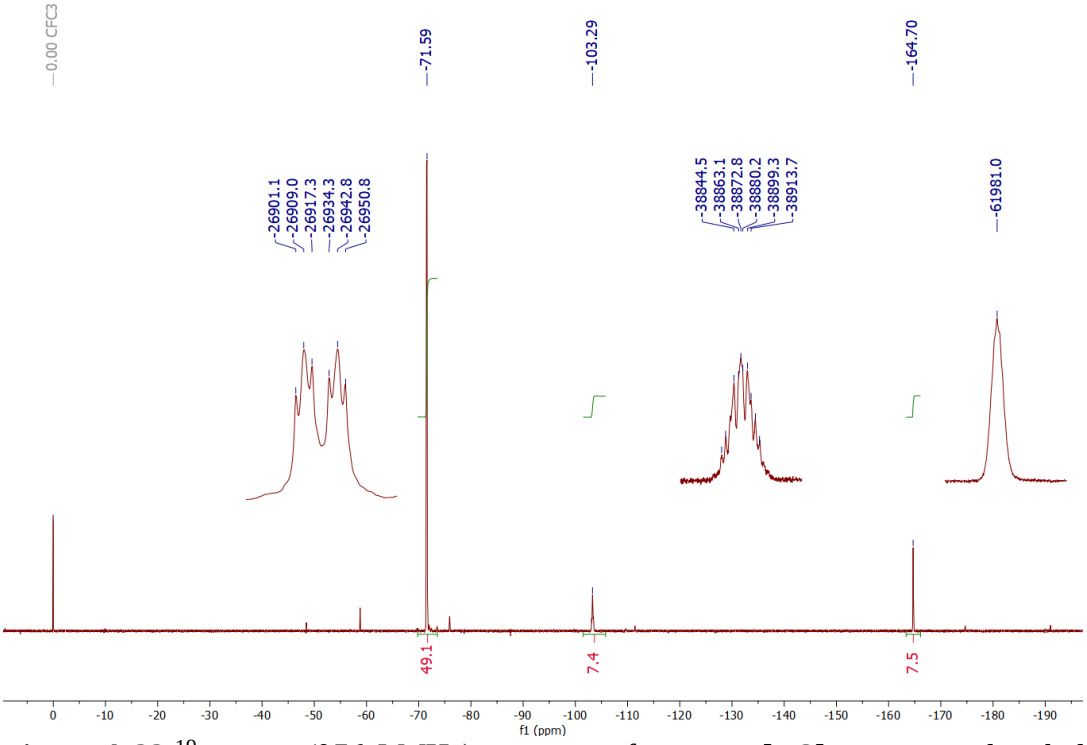


Figure A.22 ^{19}F NMR (376.5 MHz) spectrum of F_{64}PcZn **[4-2]** in acetone-d_6: ethyl acetate 1: 9. Inset peak values are in Hz.

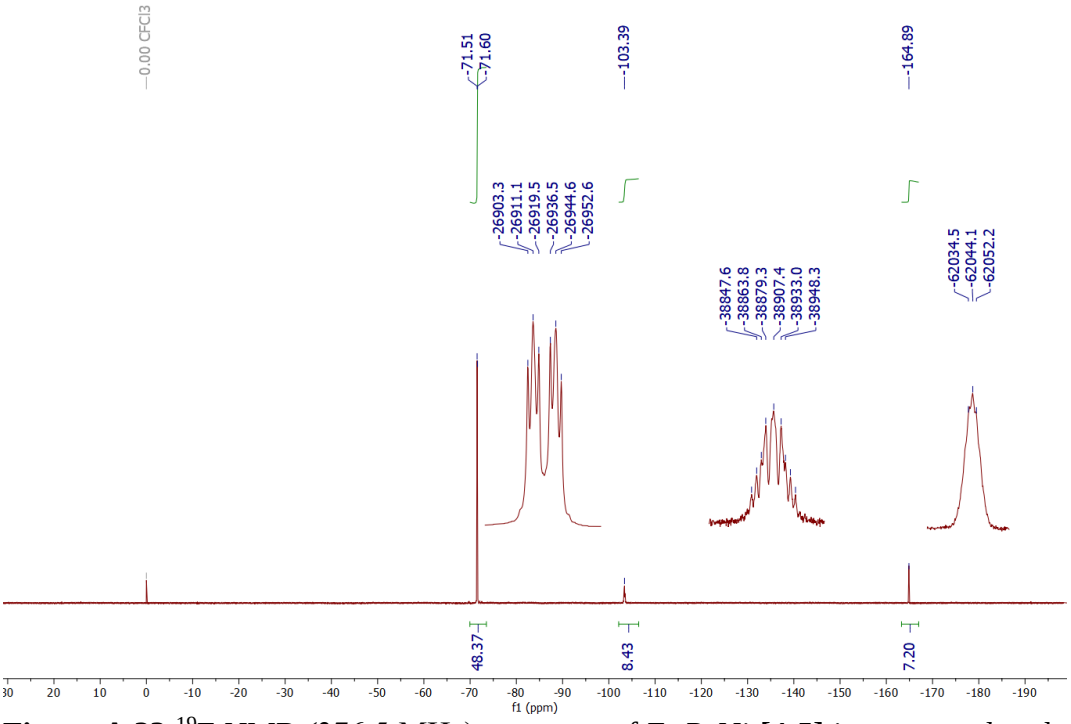


Figure A.23 ^{19}F NMR (376.5 MHz) spectrum of F_{64}PcNi **[4-5]** in acetone-d_6: ethyl acetate 1: 9. Inset peak values are in Hz.

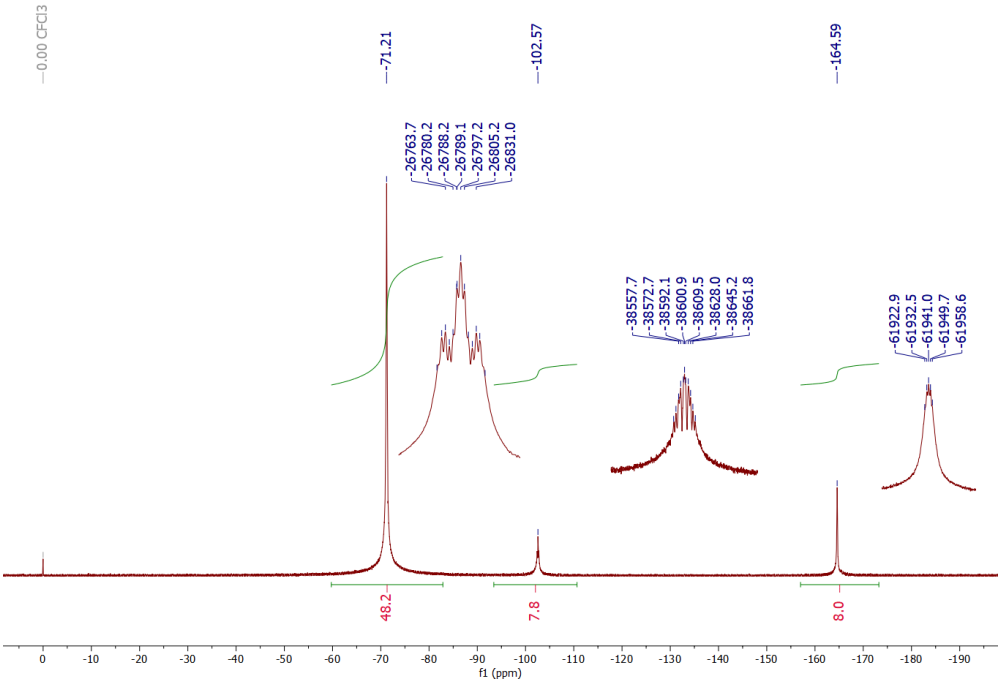


Figure A.24 ^{19}F NMR (376.5 MHz) spectrum of F_{64}PcGaCl **[4-6]** in acetone-d_6. Inset peak values are in Hz. The spectrum was processed using phase correction.

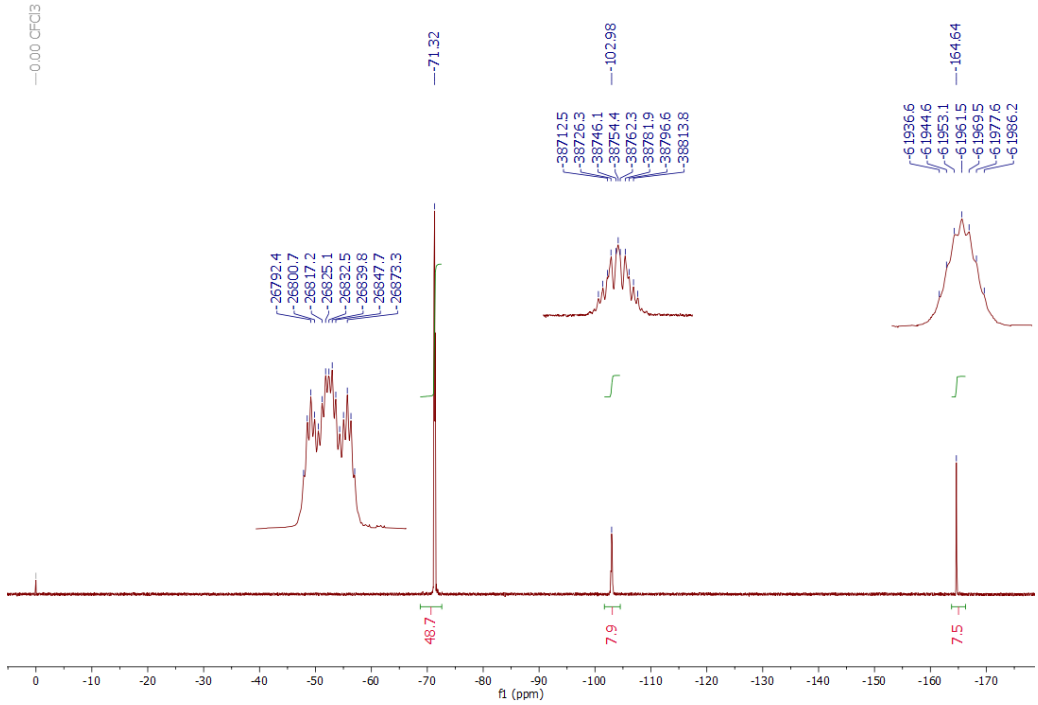


Figure A.25 ^{19}FNMR (375 MHz) spectrum of F_{64}PcInCl **[4-7]** in acetone-d_6. Inset peak values are in Hz.

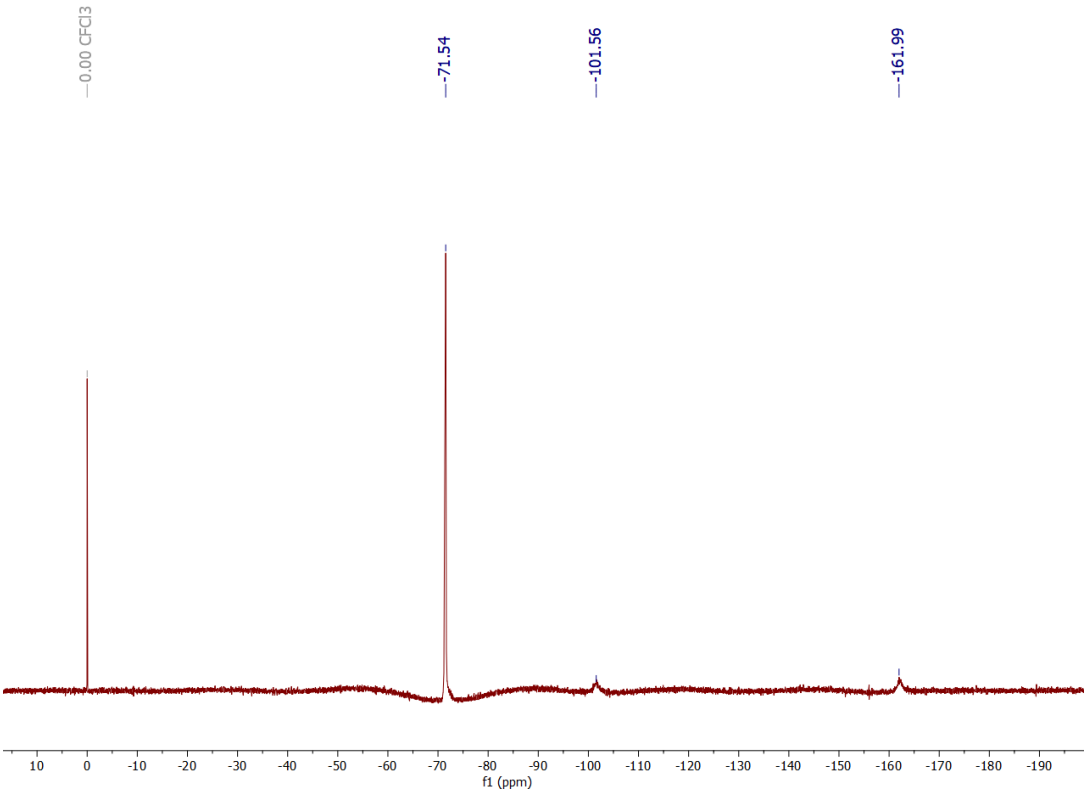


Figure A.26 ^{19}F NMR (376.5 MHz) spectrum of F_{52}PcCu **[4-8]** in acetone-d_6.

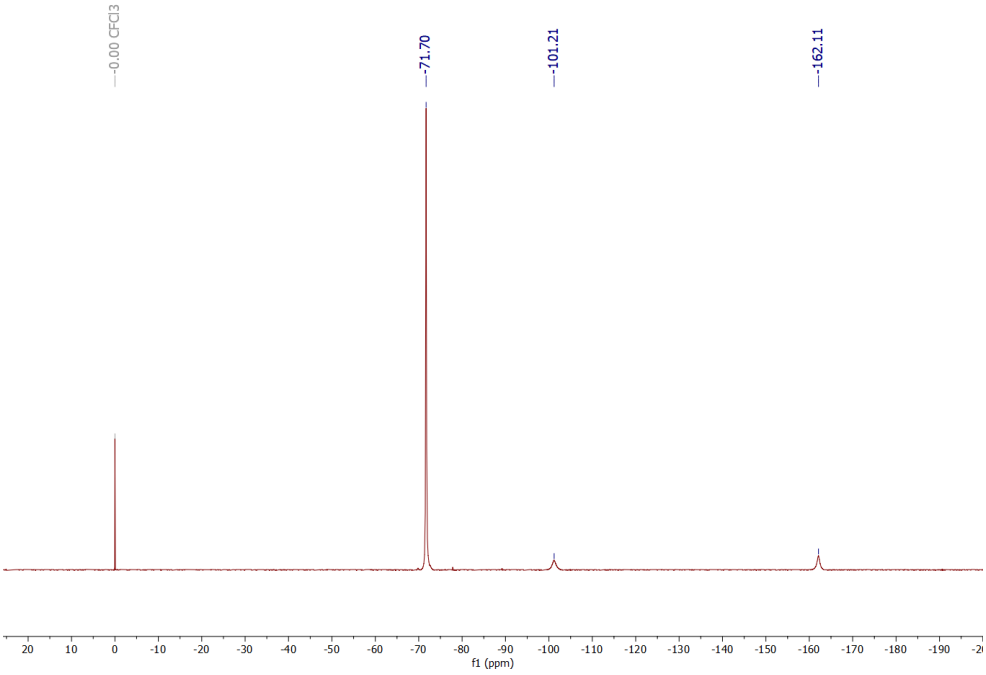


Figure A.27 ^{19}F NMR (376.5 MHz) spectrum of F_{40}PcCu **[4-9]** in 10% acetone-d_6/EtOAc.

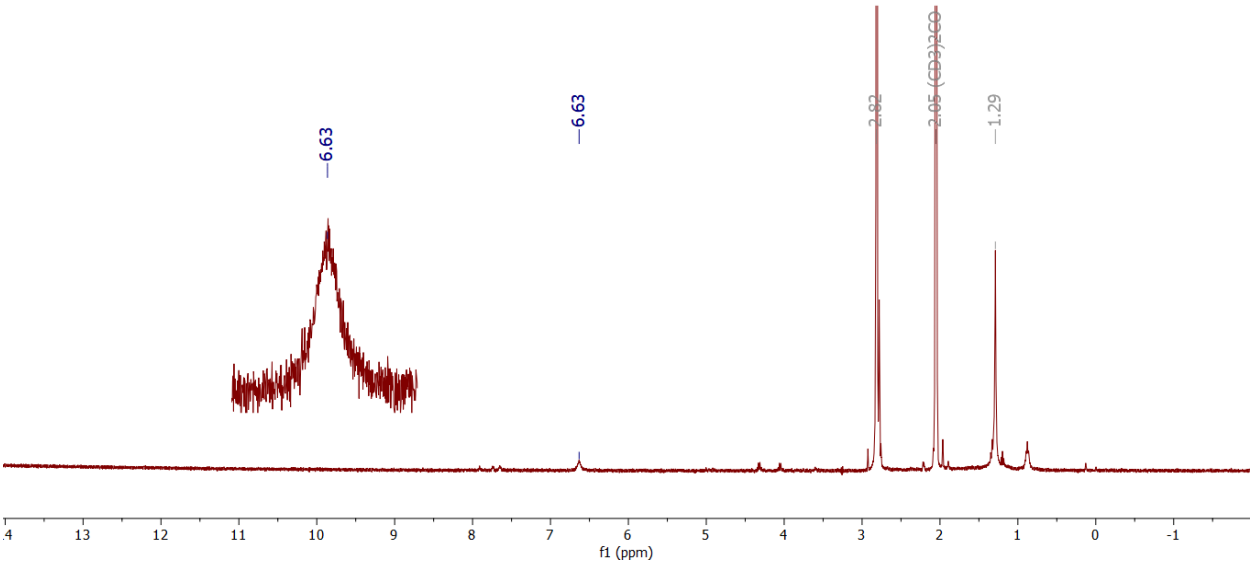


Figure A.28 ^{1}H NMR (400 MHz) spectrum of $NH_2F_{51}PcZn$ **[5-1]** in 10% acetone-d_6/THF.

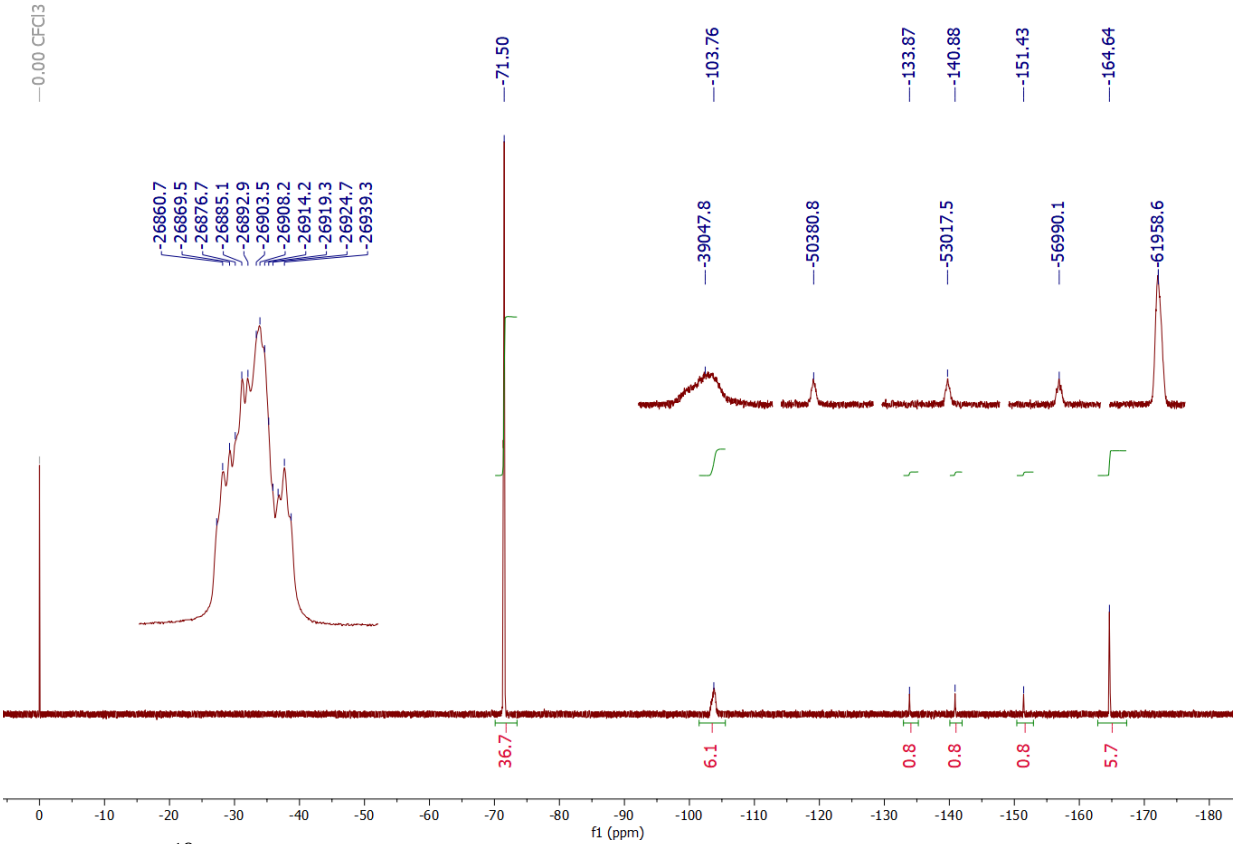


Figure A.29 ^{19}F NMR (376.5 MHz) spectrum of $NH_2F_{51}PcZn$ **[5-1]** in 10% acetone-d_6/THF. Inset peak values are in Hz.

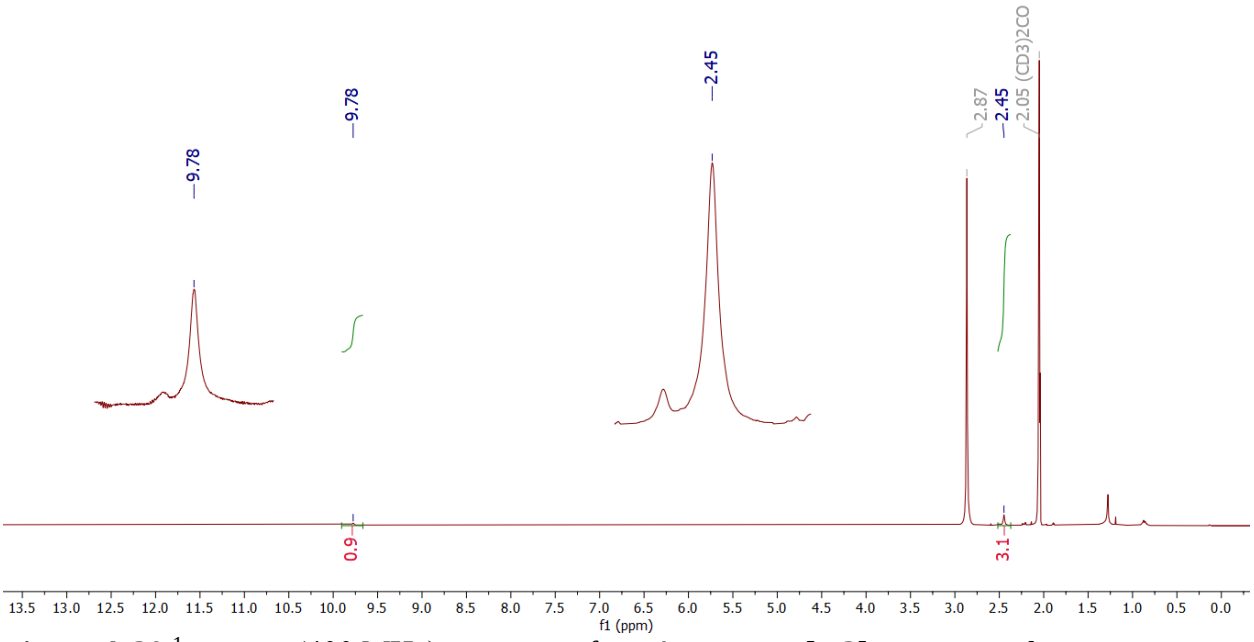


Figure A.30 ^{1}H NMR (400 MHz) spectrum of NHAcF_{51}PcZn **[5-3]** in acetone-d_6.

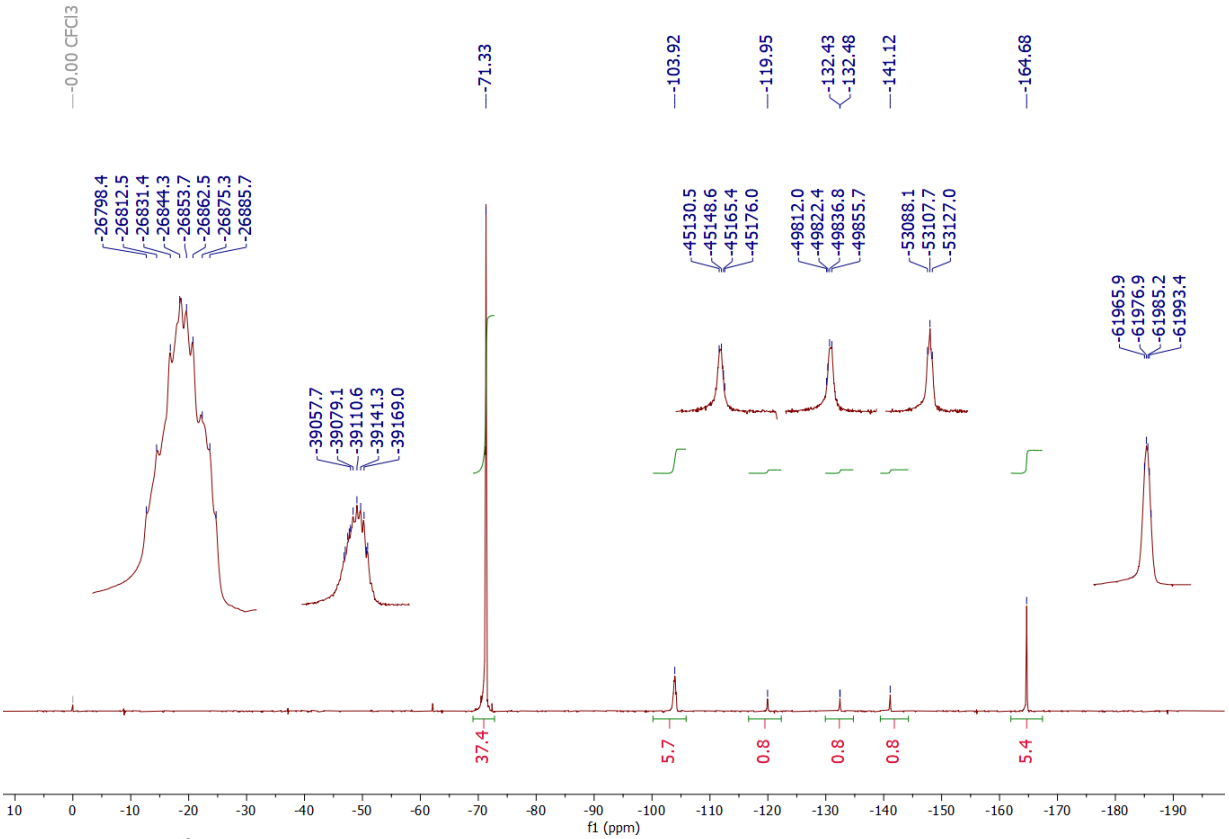


Figure A.31 ^{19}F NMR (376.5 MHz) spectrum of NHAcF_{51}PcZn **[5-3]** in acetone-d_6 spiked with AcOH. Inset peak values are in Hz.

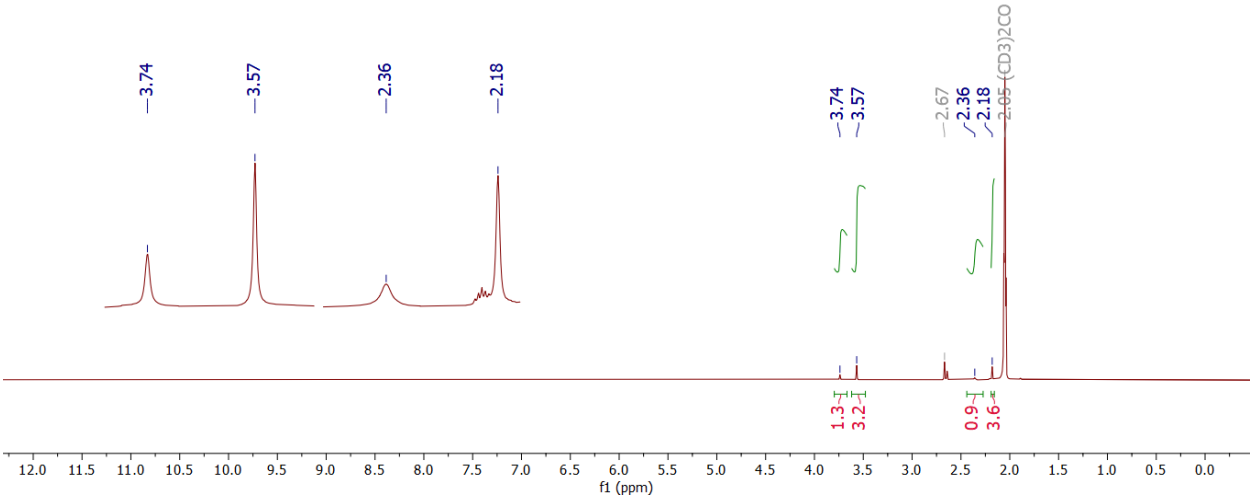


Figure A.32 ^{1}H NMR (400 MHz) spectrum of NMeAcF$_{51}$PcZn **[5-4]**, mixture of rotamers, in acetone-d_6.

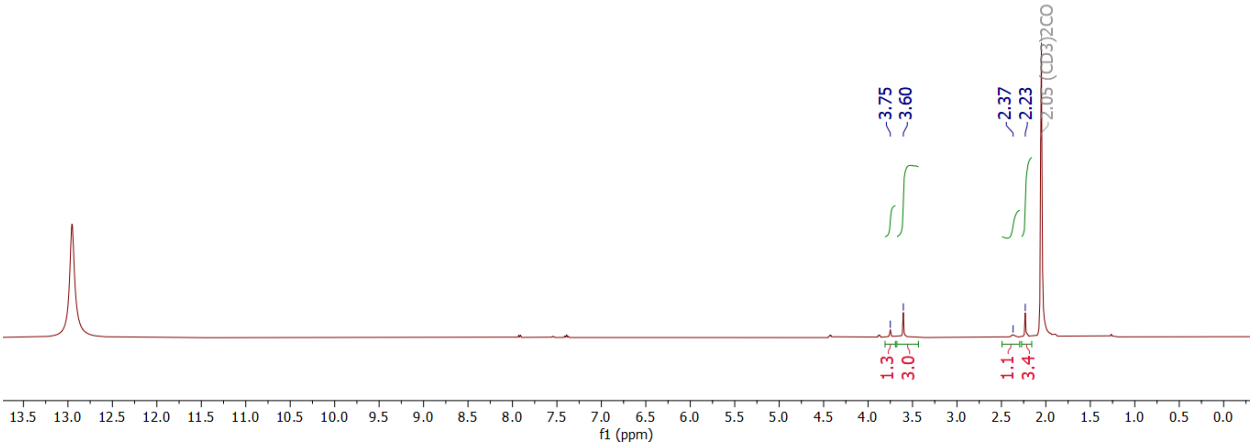


Figure A.33 ^{1}H NMR (400 MHz) spectrum of NMeAcF$_{51}$PcZn **[5-4]**, mixture of rotamers, in acetone-d_6 spiked with TFA.

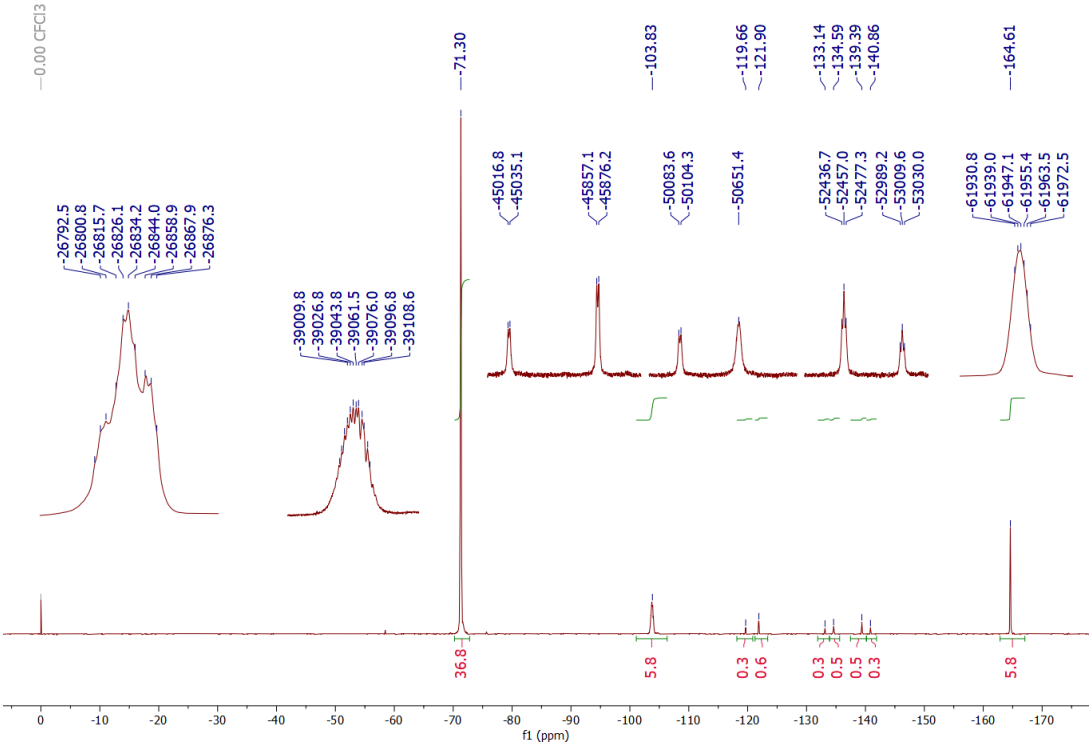


Figure A.34 ^{19}F NMR (376.5 MHz) spectrum of NMeAcF$_{51}$PcZn **[5-4]**, mixture of rotamers, in acetone-d_6. Inset peak values are in Hz.

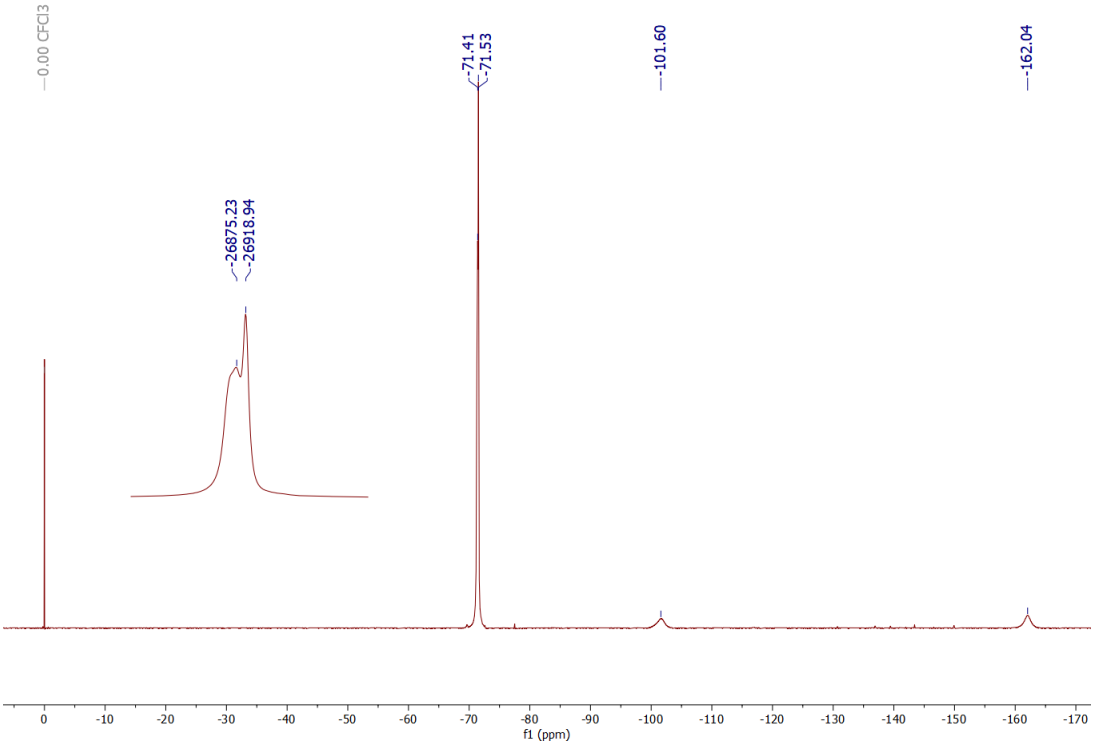


Figure A.35 ^{19}F NMR (376.5 MHz) spectrum of NHAcF$_{51}$PcCu **[5-5]** in acetone-d_6. Inset: magnification for the ~71 ppm signal, peak values are in Hz.

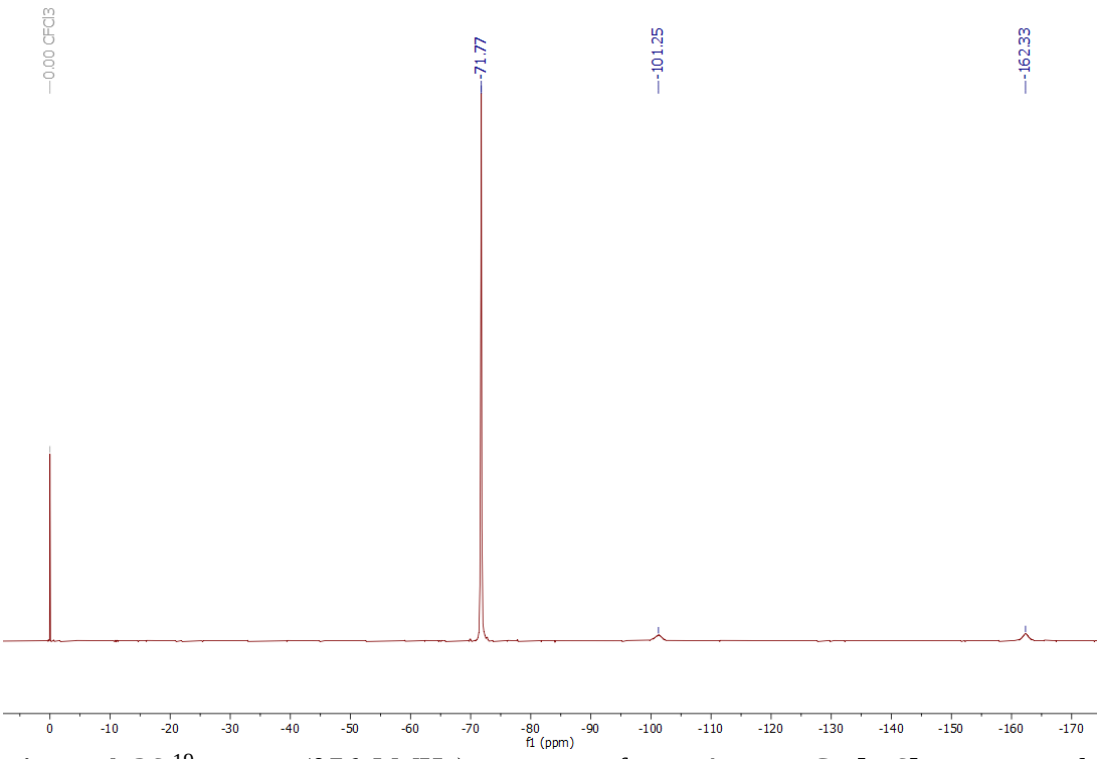


Figure A.36 ^{19}F NMR (376.5 MHz) spectrum of NMeAcF$_{51}$PcCu **[5-6]** in acetone-d_6.

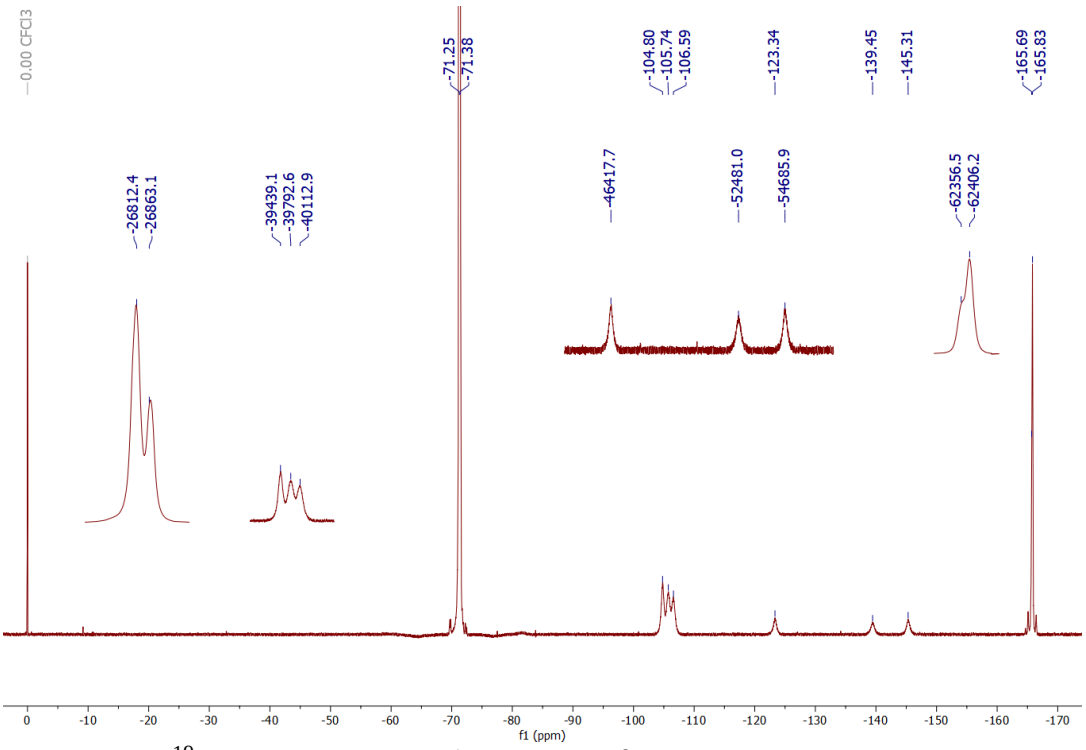


Figure A.37 ^{19}F NMR (376.5 MHz) spectrum of NHAcF$_{51}$PcCo **[5-7]** in 10% acetone-d_6 in ethyl acetate. Inset peak values are in Hz.

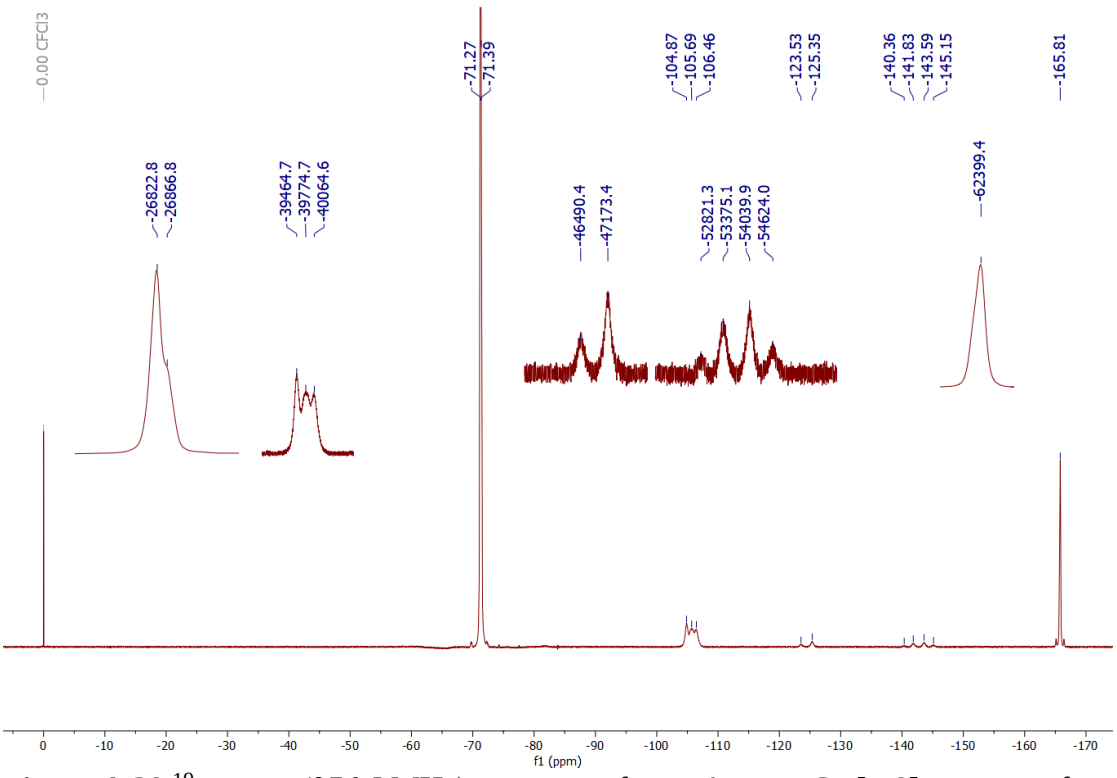


Figure A.38 ^{19}F NMR (376.5 MHz) spectrum of NMeAcF$_{51}$PcCo **[5-8]**, mixture of rotamers, in 10% acetone-*d*$_6$ in ethyl acetate. Inset peak values are in Hz.

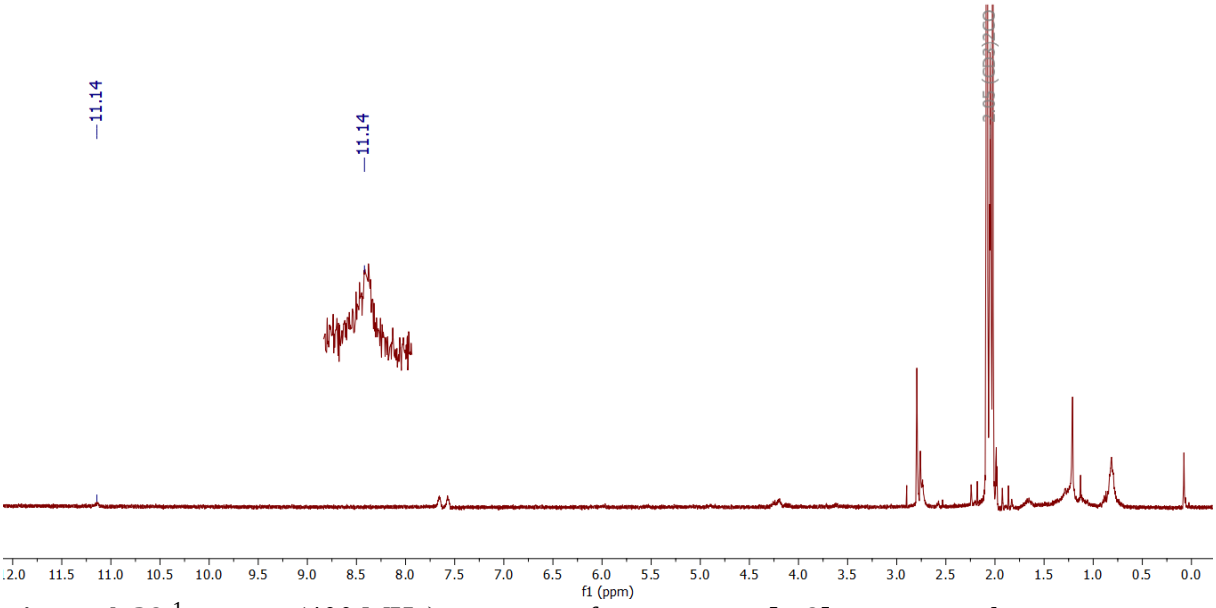


Figure A.39 ^{1}H NMR (400 MHz) spectrum of NHF$_{58}$PcZn **[5-9]** in acetone-*d*$_6$.

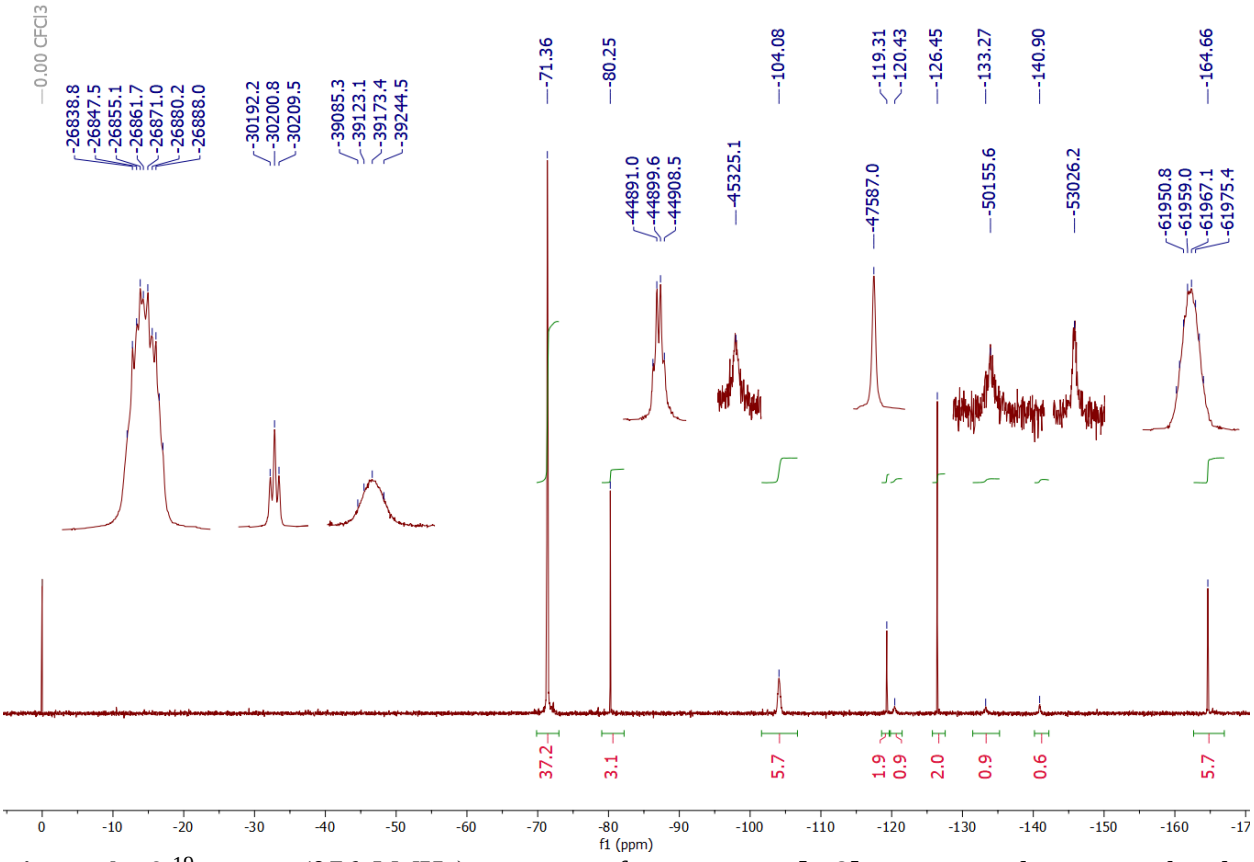


Figure A.40 ^{19}F NMR (376.5 MHz) spectrum of NHF$_{58}$PcZn **[5-9]** in acetone-*d*$_6$. Inset peak values are in Hz.

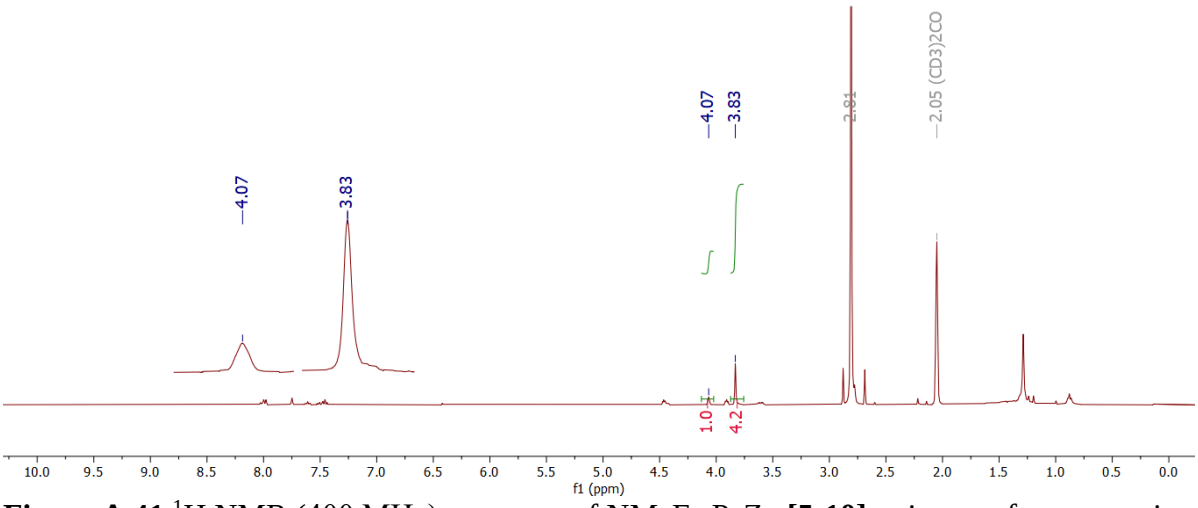


Figure A.41 ^{1}H NMR (400 MHz) spectrum of NMeF$_{58}$PcZn **[5-10]**, mixture of rotamers, in acetone-*d*$_6$.

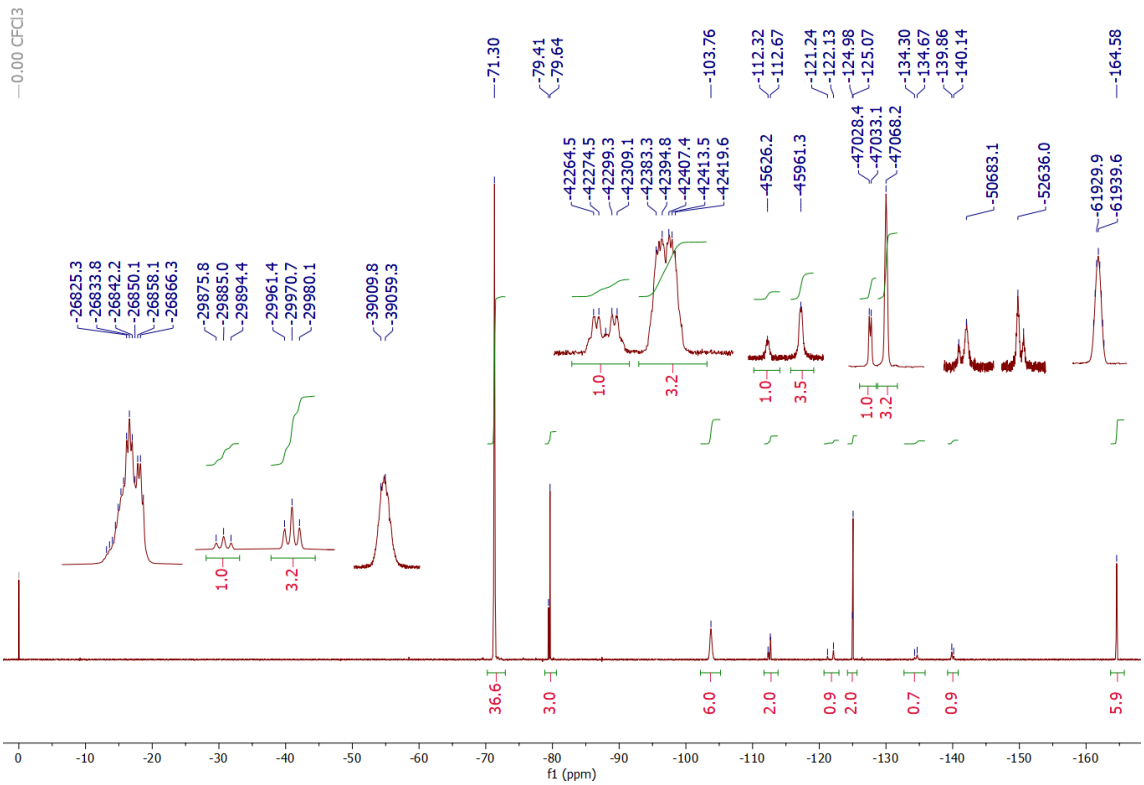


Figure A.42 ^{19}F NMR (376.5 MHz) spectrum of NMeF$_{58}$PcZn **[5-10]**, mixture of rotamers, in acetone-*d*$_6$. Inset peak values are in Hz.

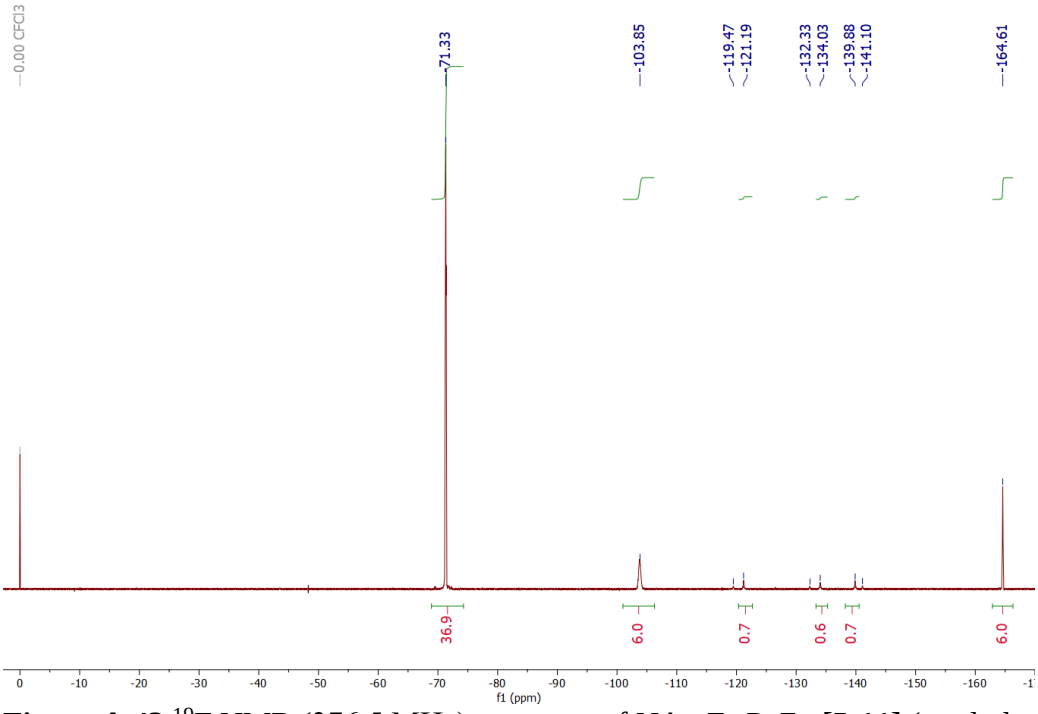


Figure A.43 ^{19}F NMR (376.5 MHz) spectrum of NAc$_2$F$_{51}$PcZn **[5-11]** (partly hydrolyzed) in acetone-*d*$_6$. The signals appearing at -119.47, -132.33, and -141.10 ppm belong to the hydrolysis product NHAcF$_{51}$PcZn **[5-3]**, see figure **A.44**.

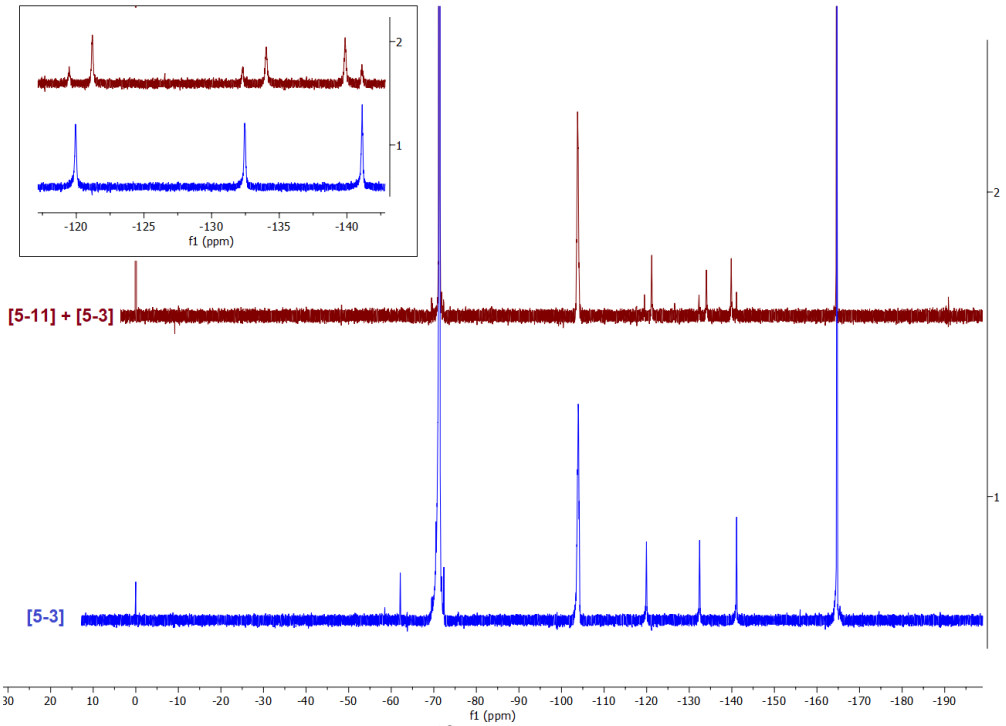


Figure A.44 Comparison of the ^{19}F NMR (376.5 MHz) spectra of $NAc_2F_{51}PcZn$ **[5-11],** partly hydrolyzed, present as a mixture (brown color) vs. $NHAcF_{51}PcZn$ **[5-3],** hydrolysis product (blue color). Inset: magnification of the aromatic ^{19}F neighboring the N substituent.

Appendix B: FT-IR spectra

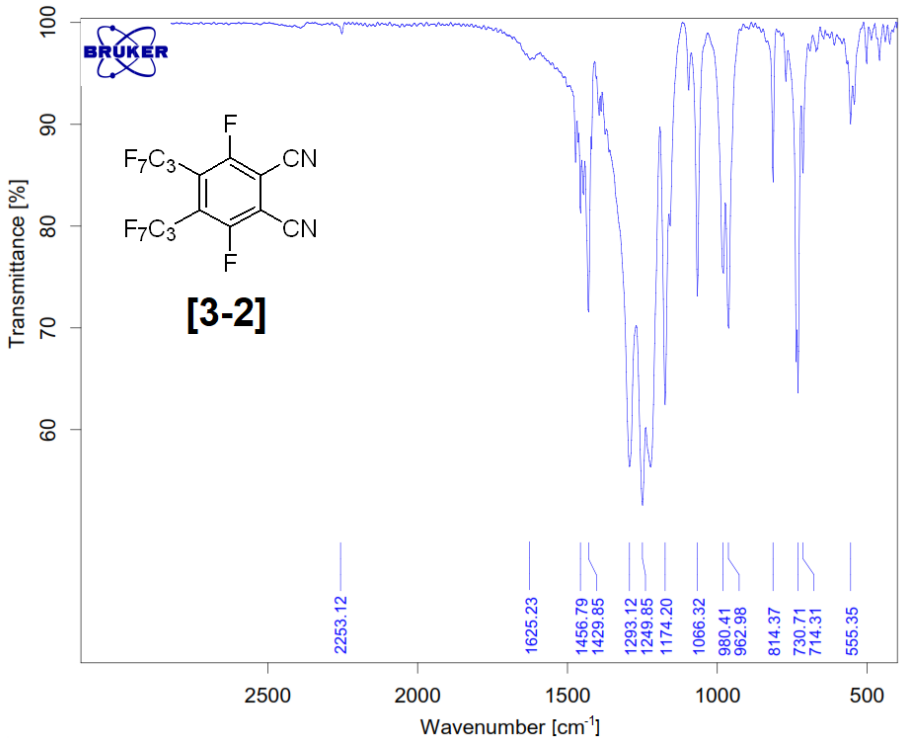


Figure B.1 FT-IR spectrum of **[3-2]** (KBr disk).

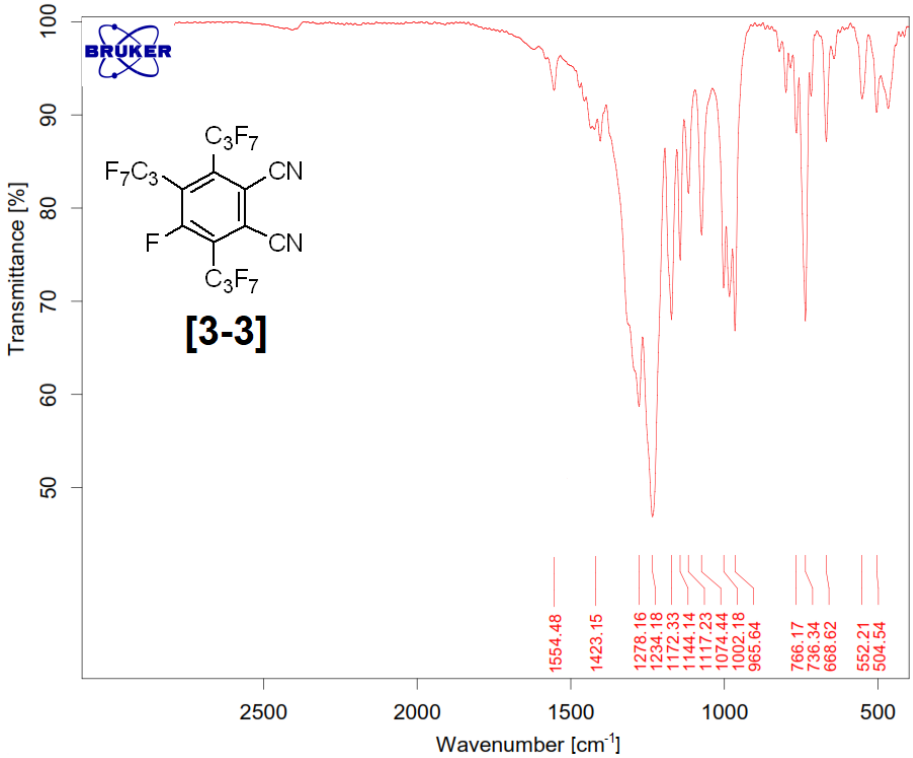


Figure B.2 FT-IR spectrum of **[3-3]** (KBr disk).

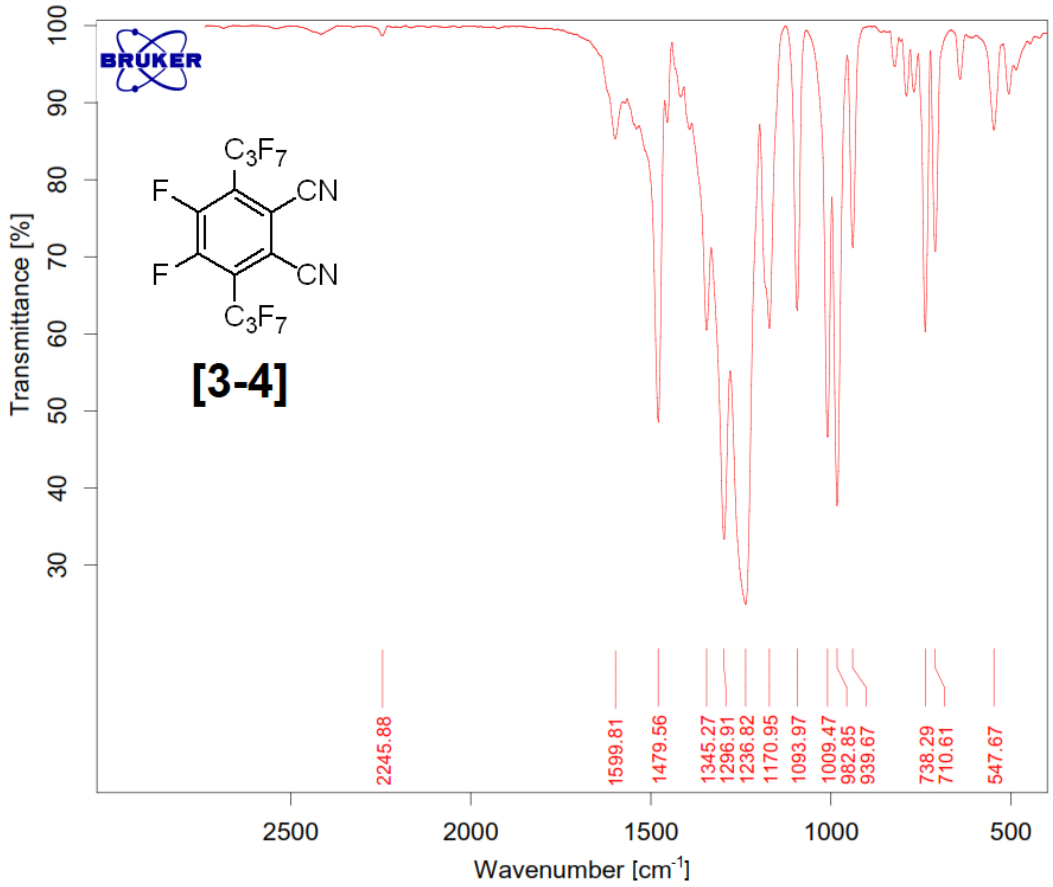


Figure B.3 FT-IR spectrum of **[3-4]** (KBr disk).

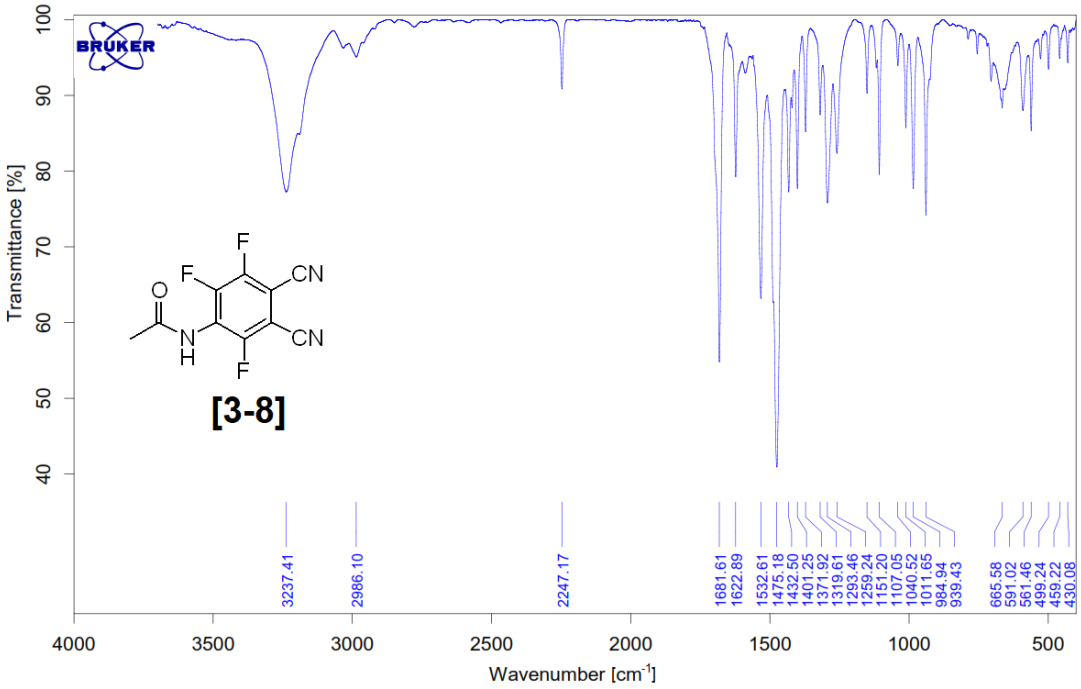


Figure B.4 FT-IR spectrum of **[3-8]** (KBr disk).

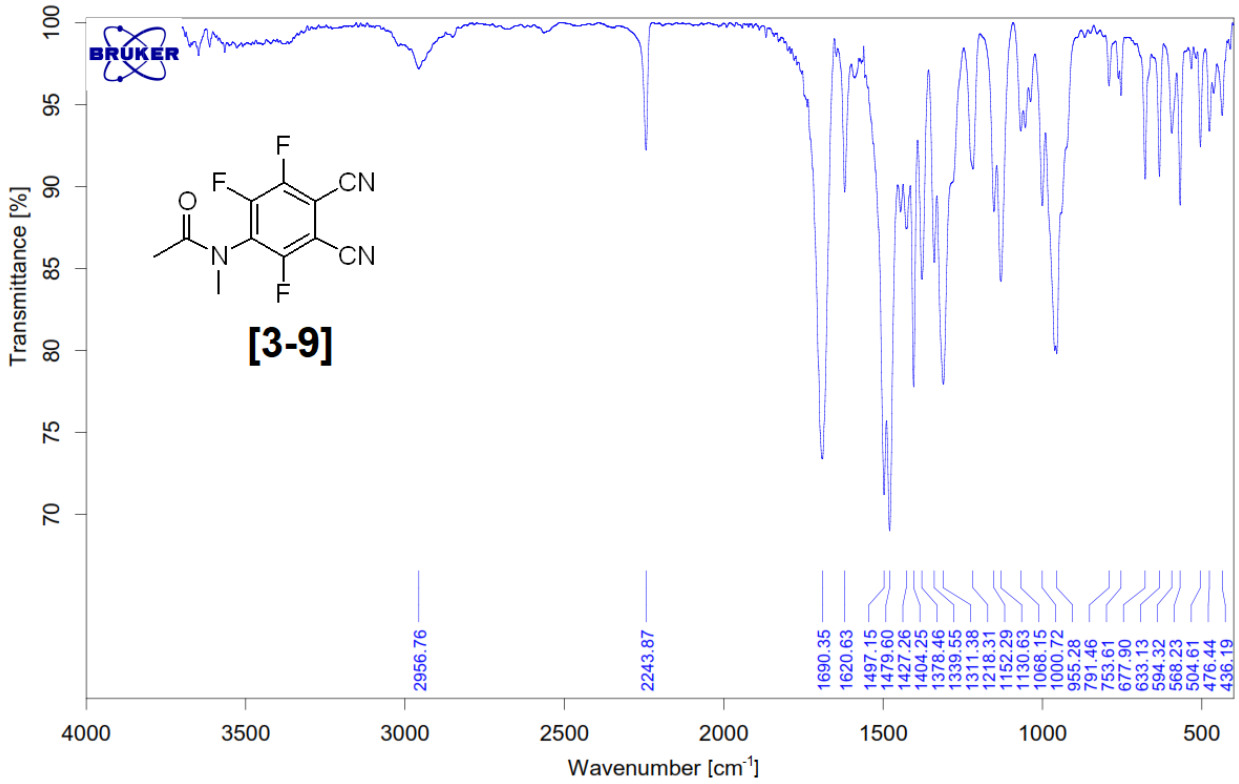


Figure B.5 FT-IR spectrum of **[3-9]** (KBr disk).

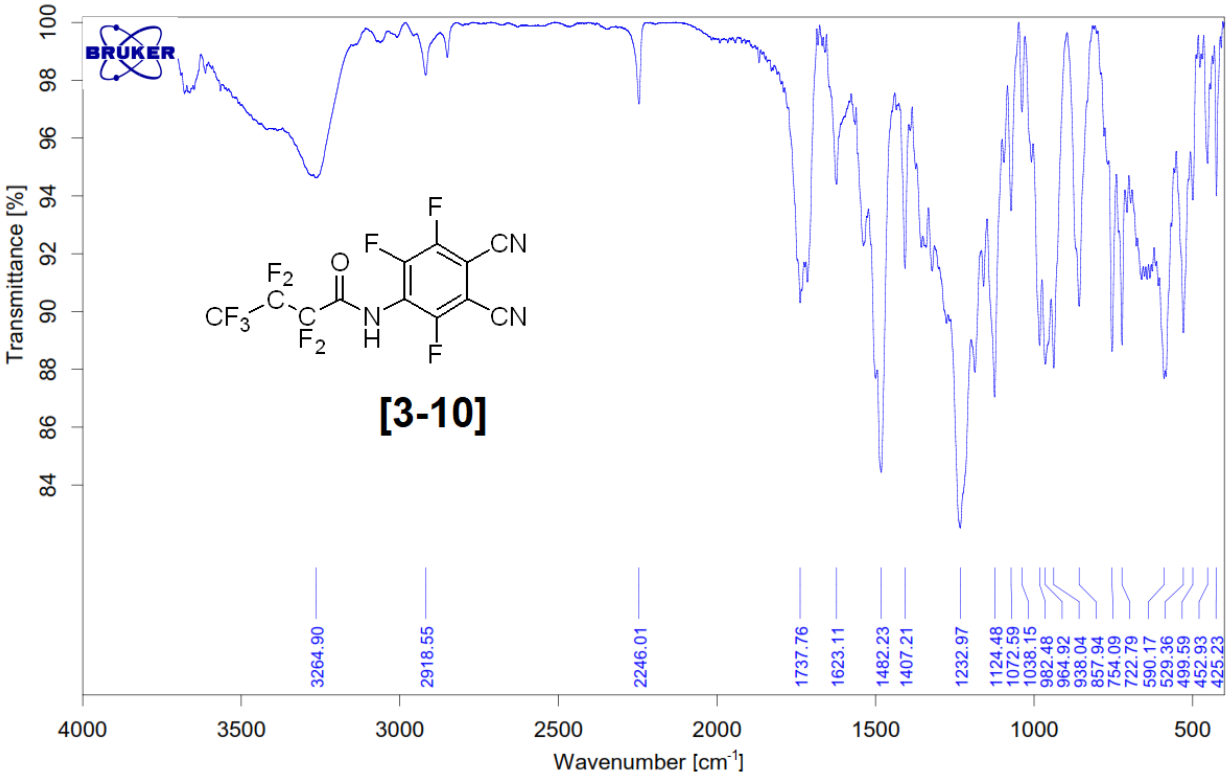


Figure B.6 FT-IR spectrum of **[3-10]** (KBr disk).

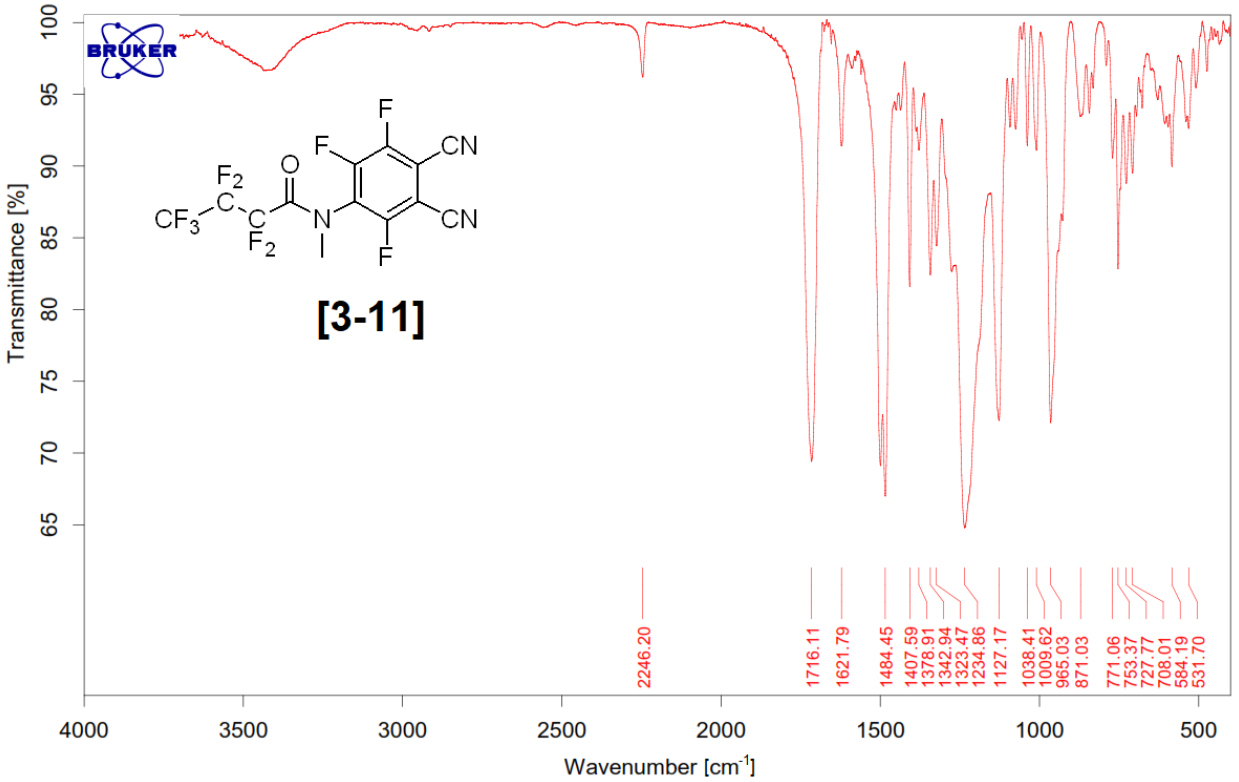


Figure B.7 FT-IR spectrum of **[3-11]** (KBr disk).

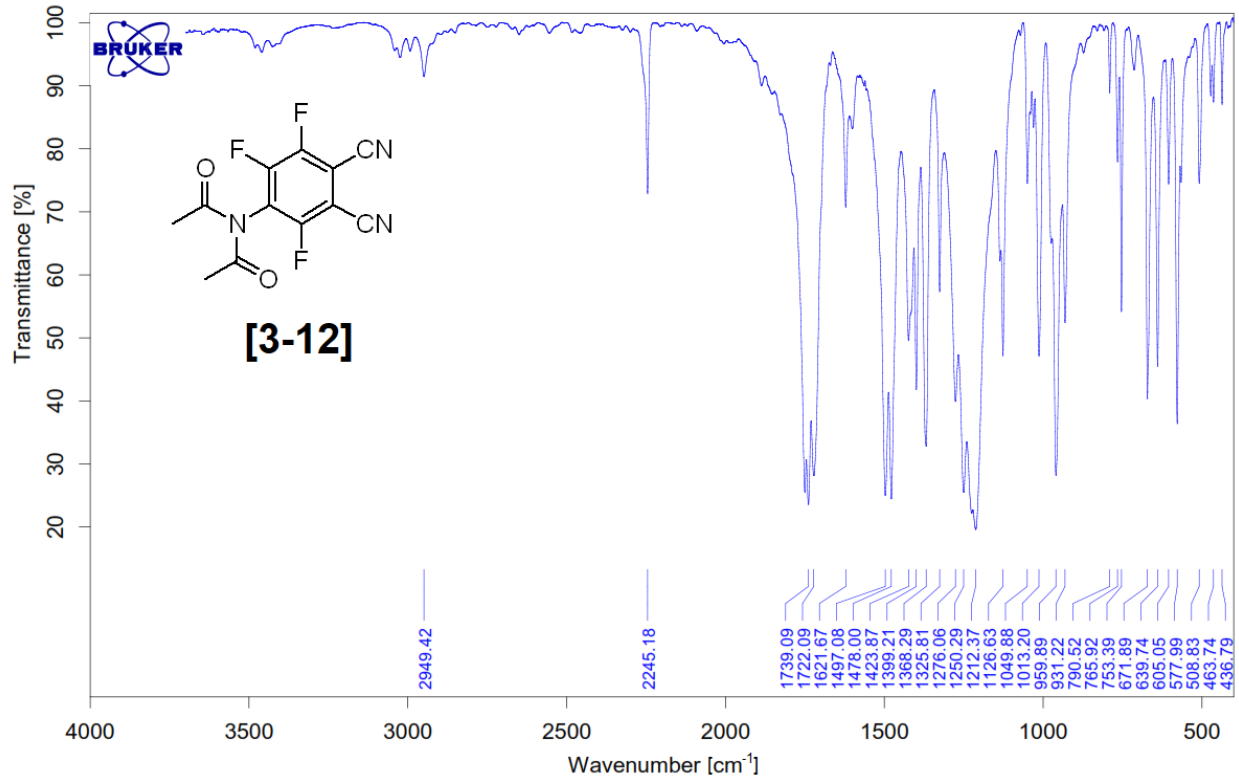


Figure B.8 FT-IR spectrum of **[3-12]** (KBr disk).

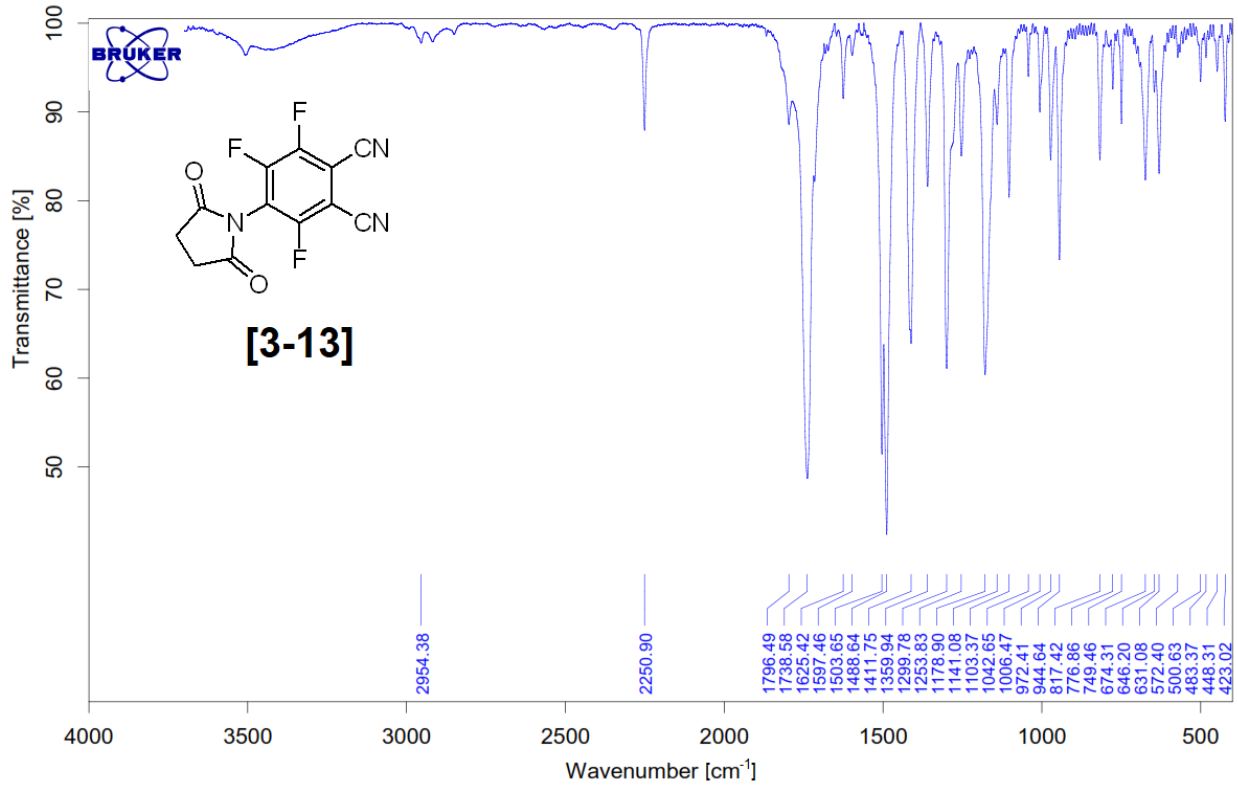


Figure B.9 FT-IR spectrum of **[3-13]** (KBr disk).

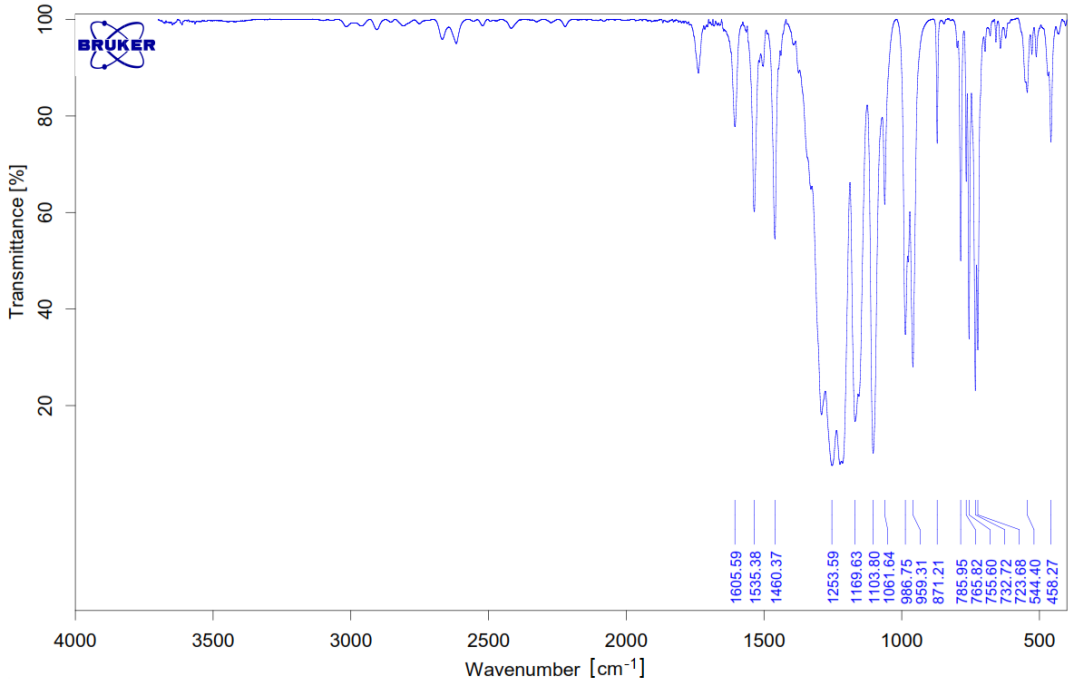


Figure B.10 FT-IR spectrum of F_{64}PcNi **[4-5]** (KBr disk).

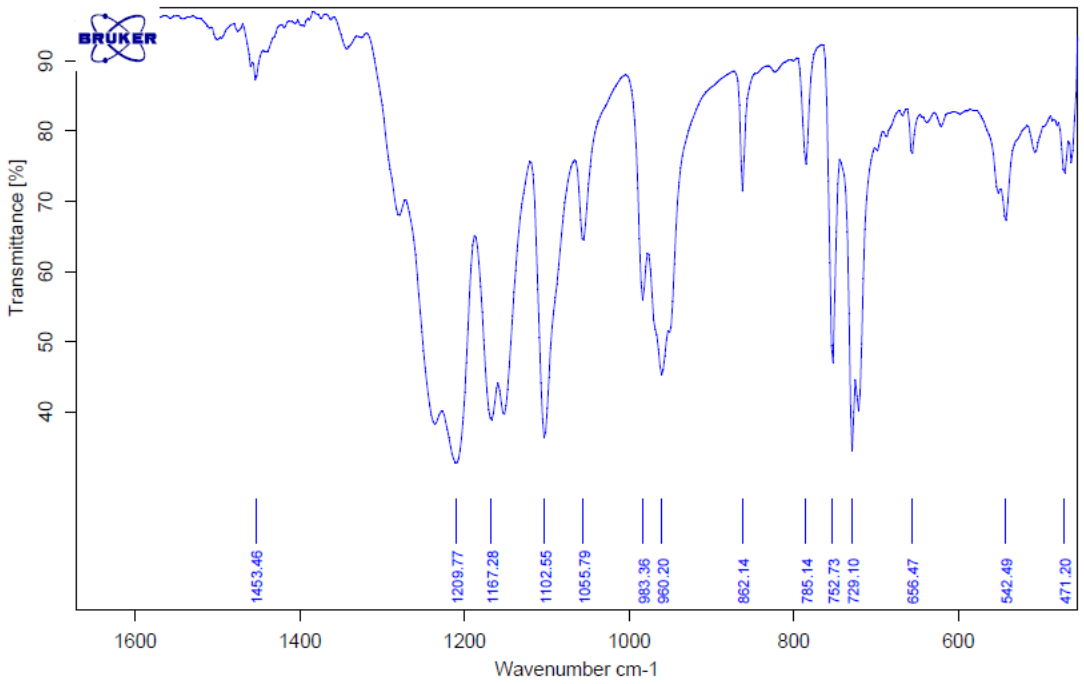


Figure B.11 FT-IR spectrum of F_{64}PcGaCl **[4-6]** (KBr disk). Reproduced with permission from Pelmuş *et al.*, 2016.

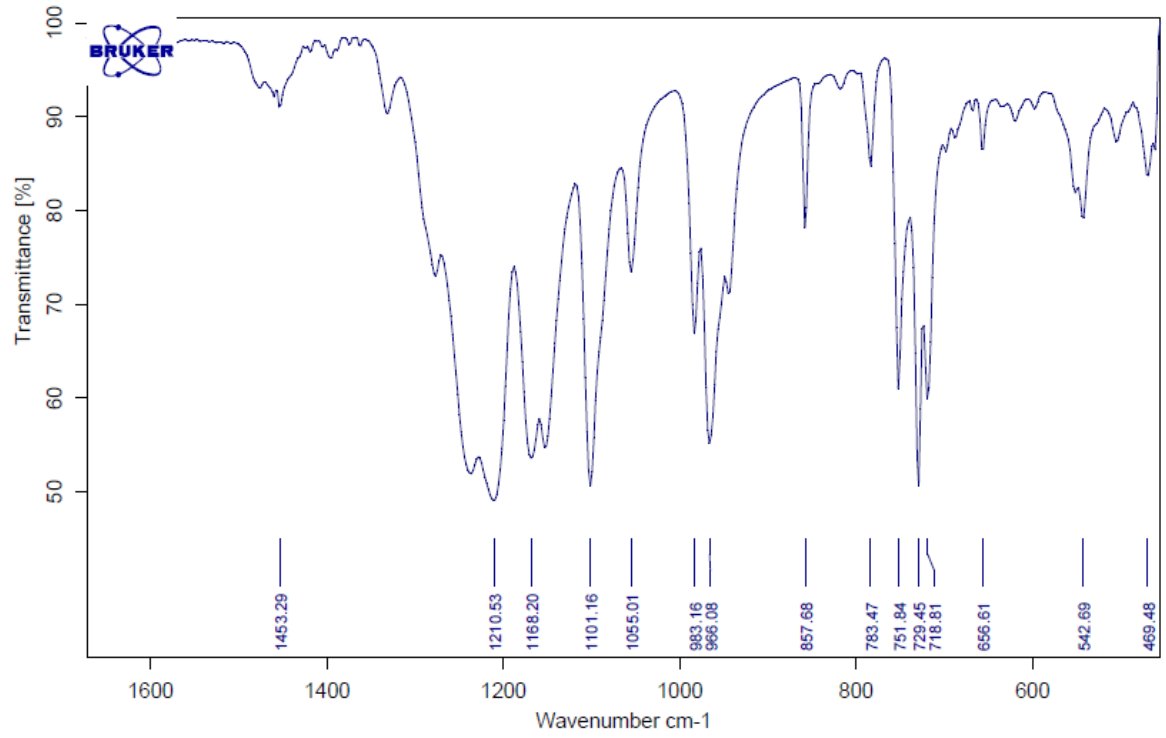


Figure B.12 FT-IR spectrum of F_{64}PcInCl **[4-7]** (KBr disk). Reproduced with permission from Pelmuş *et al.*, 2016.

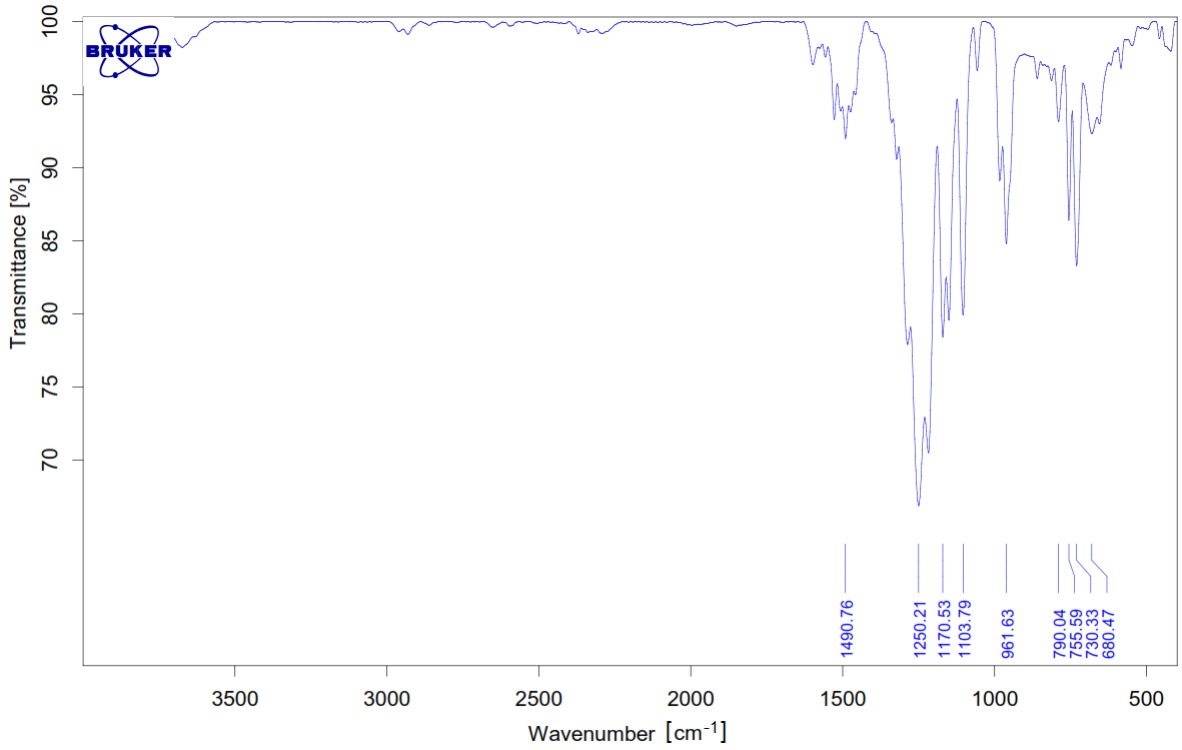


Figure B.13 FT-IR spectrum of F_{52}PcCu **[4-8]** (KBr disk).

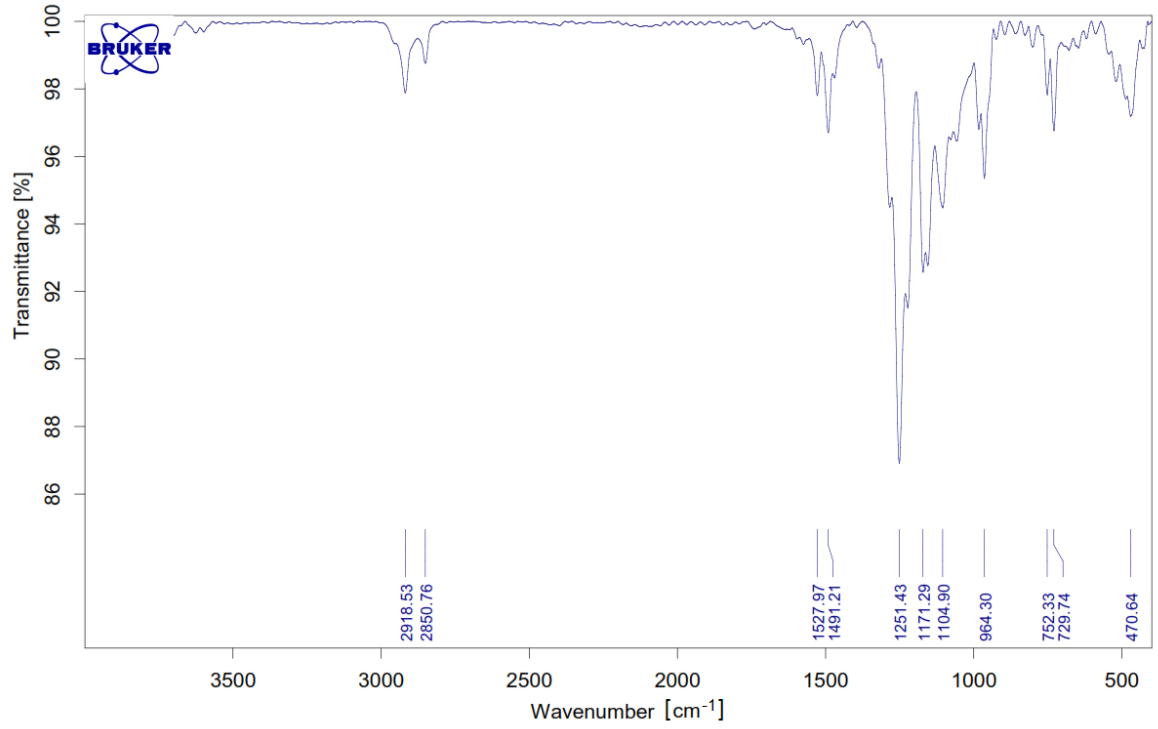


Figure B.14 FT-IR spectrum of F_{40}PcCu **[4-9]** (KBr disk). Reproduced from Nguyen *et al*. 2020 with permission from the PCCP Owner Societies.

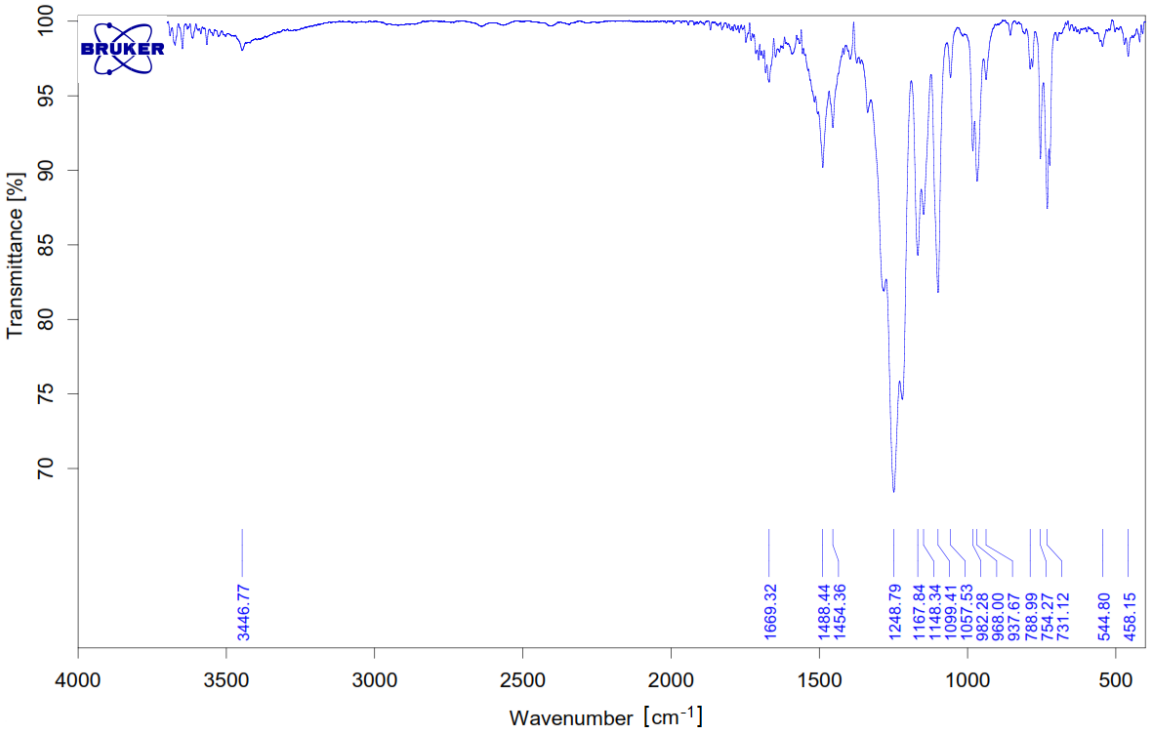


Figure B.15 FT-IR spectrum of NHAcF_{51}PcZn **[5-3]** (KBr disk).

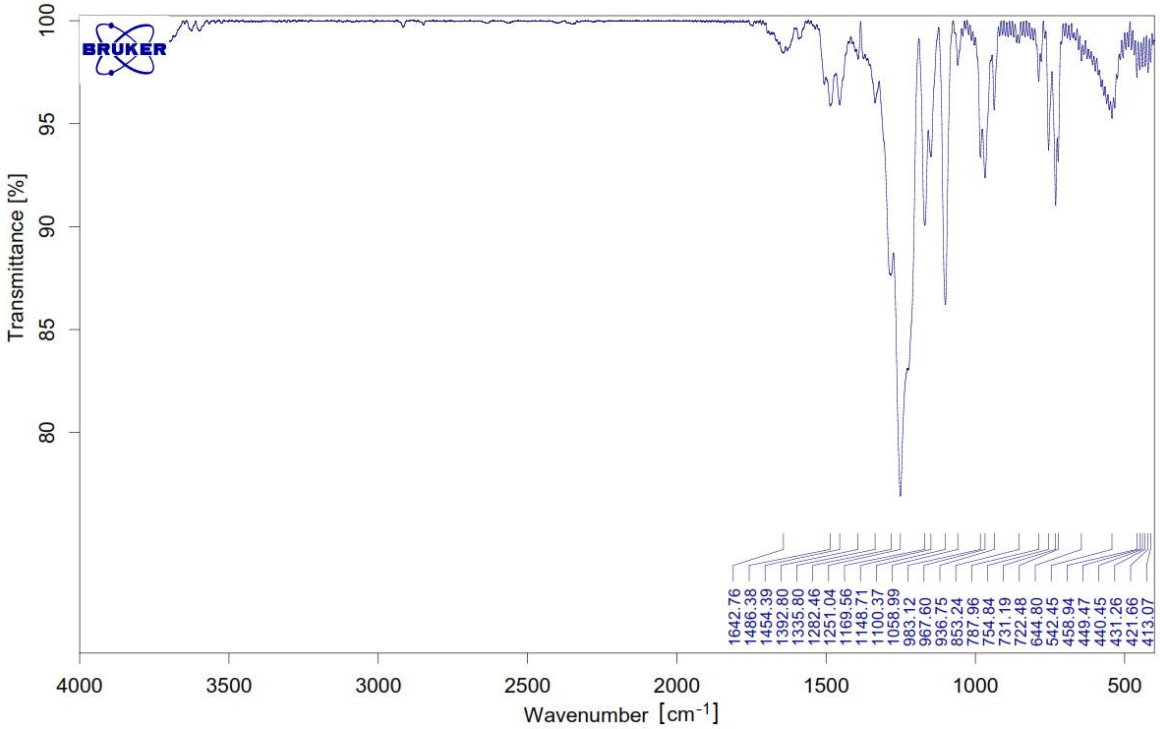


Figure B.16 FT-IR spectrum of NMeAcF_{51}PcZn **[5-4]** (KBr disk).

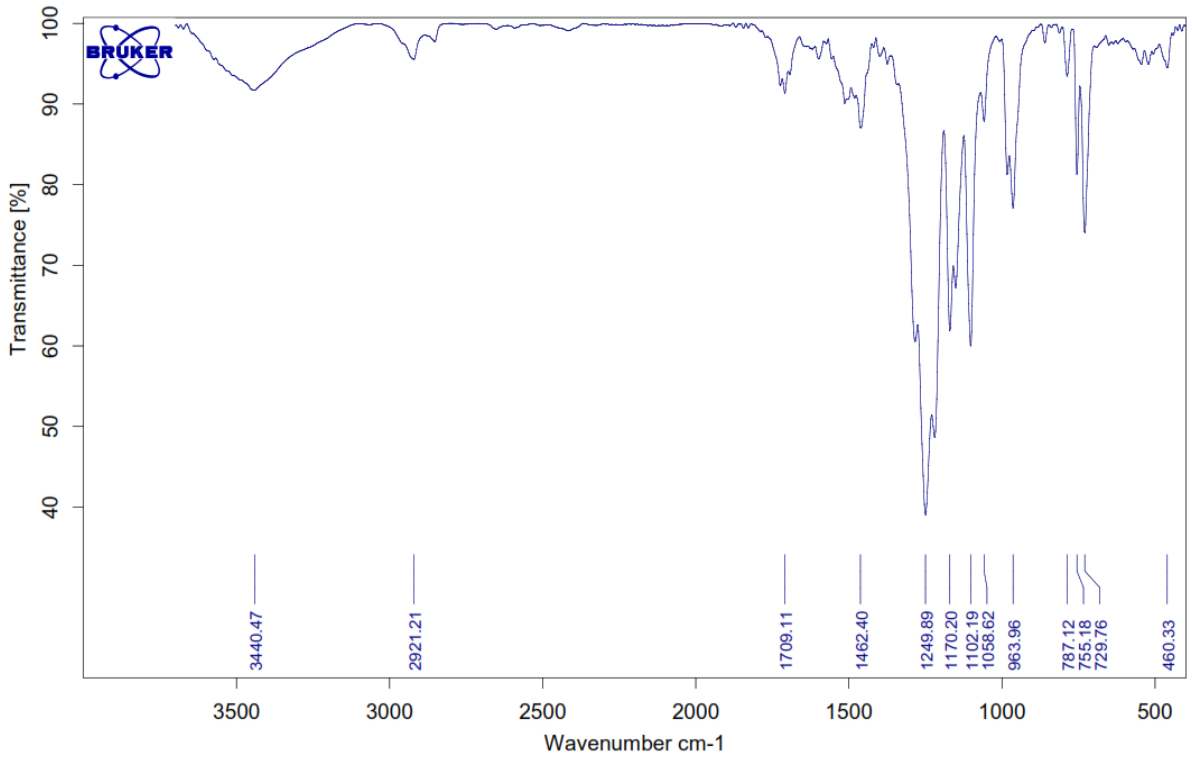


Figure B.17 FT-IR spectrum of NHAcF_{51}PcCu **[5-5]** (KBr disk).

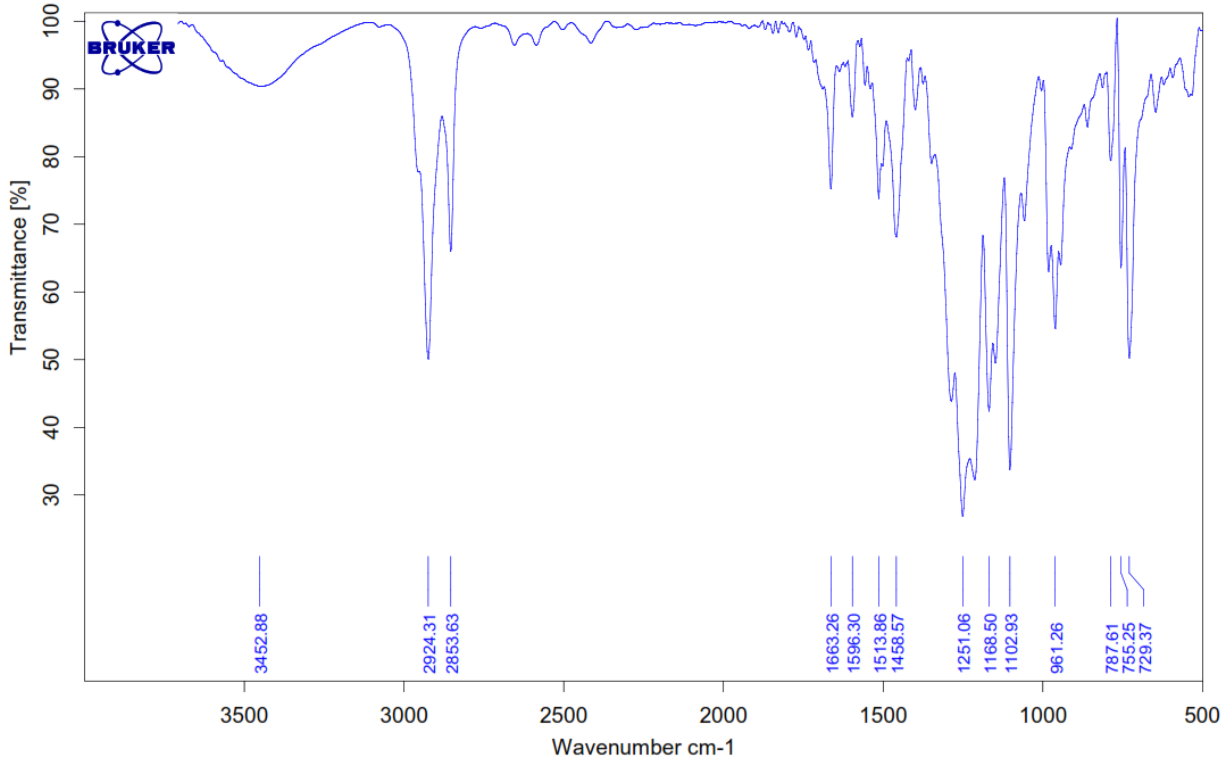


Figure B.18 FT-IR spectrum of NMeAcF_{51}PcCu **[5-6]** (KBr disk).

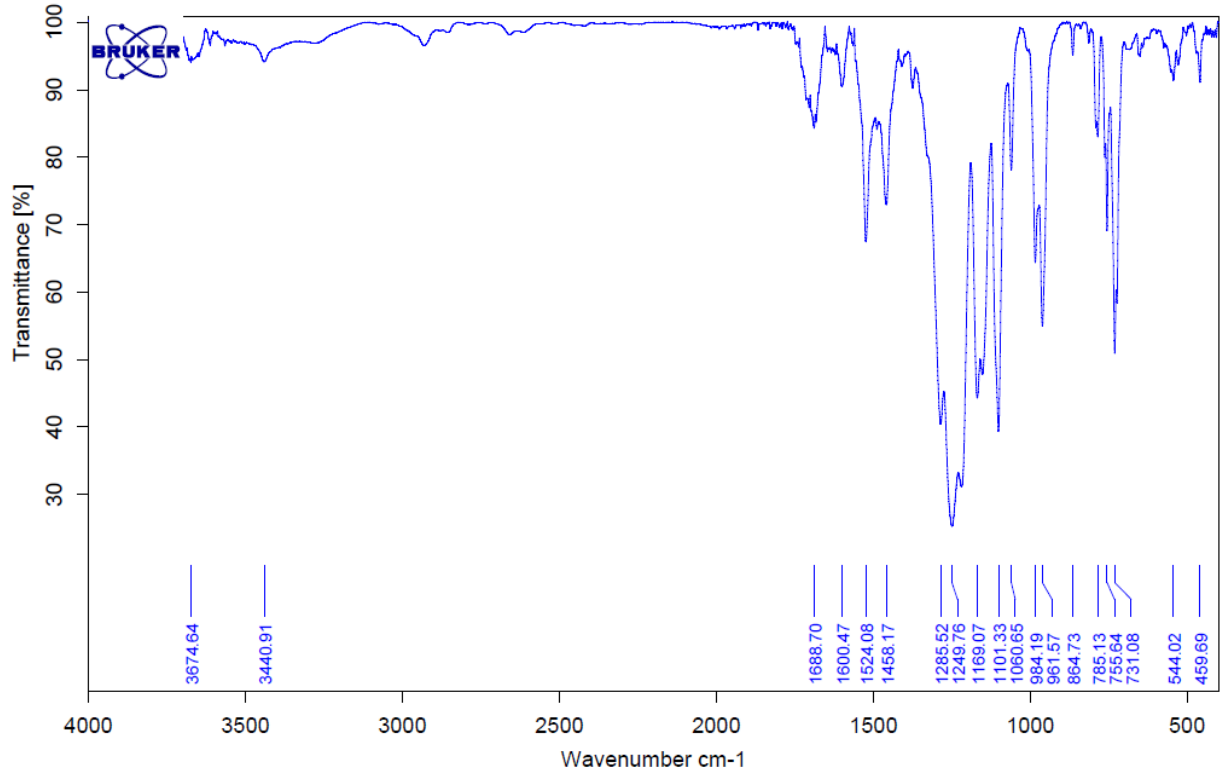


Figure B.19 FT-IR spectrum of NHAcF_{51}PcCo **[5-7]** (KBr disk).

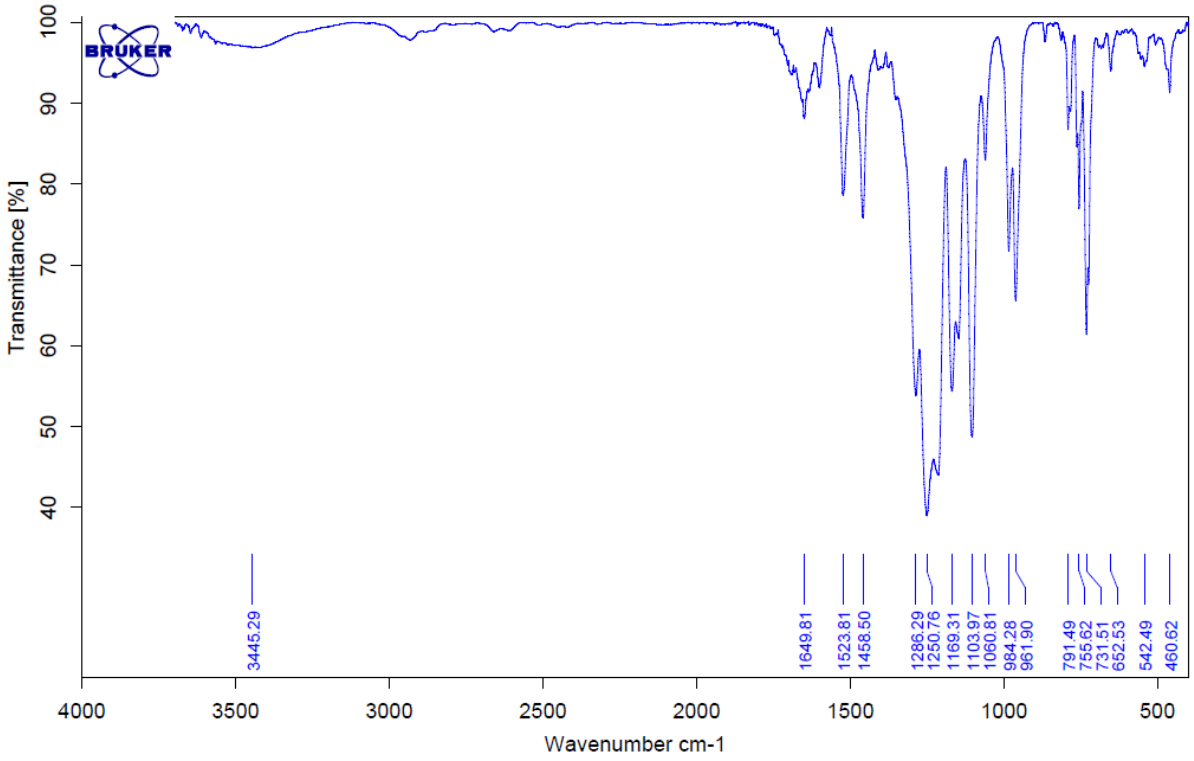


Figure B.20 FT-IR spectrum of NMeAcF_{51}PcCo **[5-8]** (KBr disk).

Appendix C: MS spectra

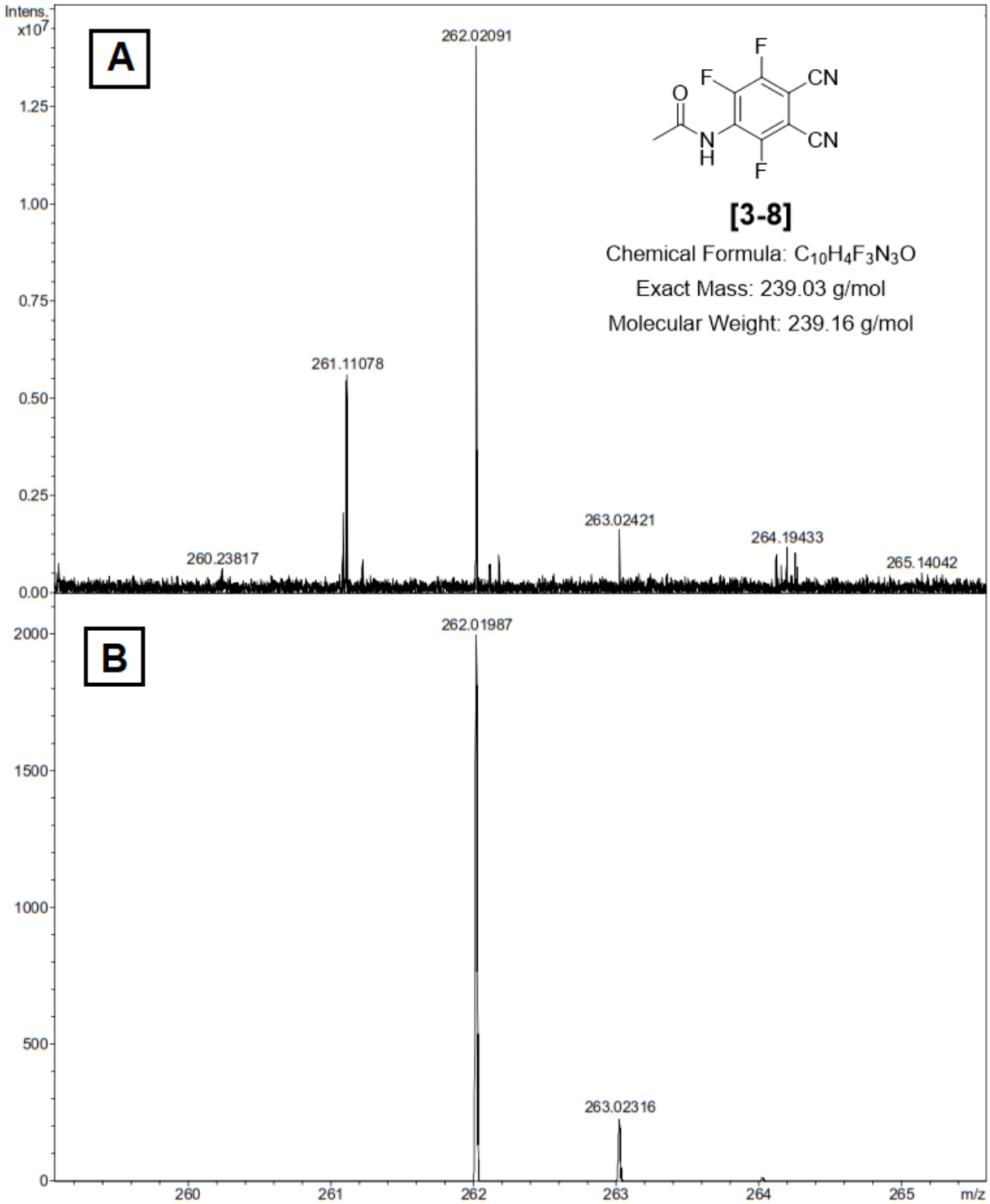


Figure C.1 HRMS spectra of **[3-8]**. A – observed (ESI, positive mode) and B – calculated isotopic pattern for $C_{10}H_4F_3N_3ONa^+$ [M+Na^+], δ = 3.97 ppm.
δ = (|Observed mass - Calculated mass|/Calculated mass) $x10^6$.

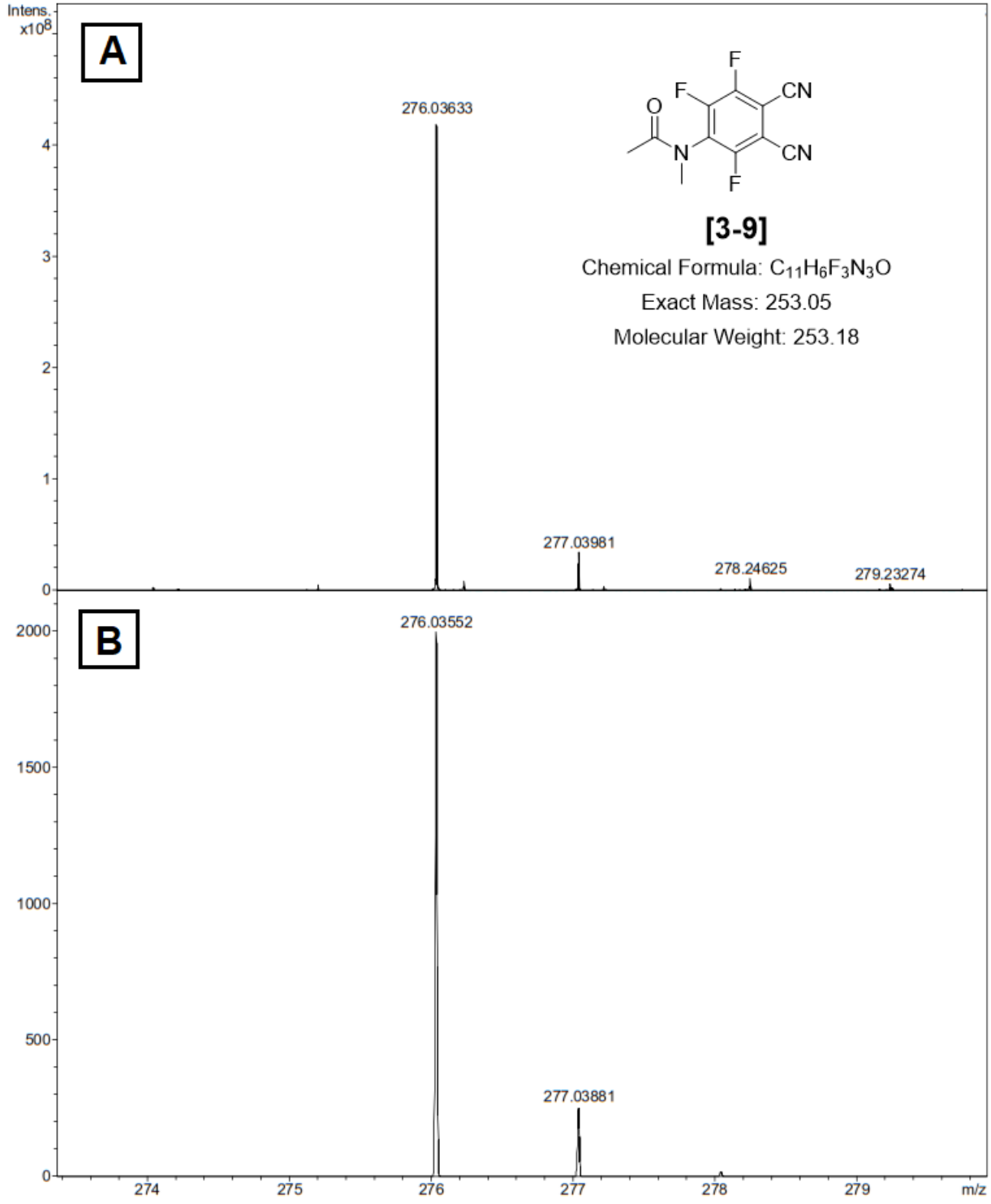


Figure C.2 HRMS spectra of **[3-9]**. A – observed (ESI, positive mode) and B – calculated isotopic pattern for $C_{11}H_6F_3N_3ONa^+$ [M+Na^+], δ = 2.93 ppm.

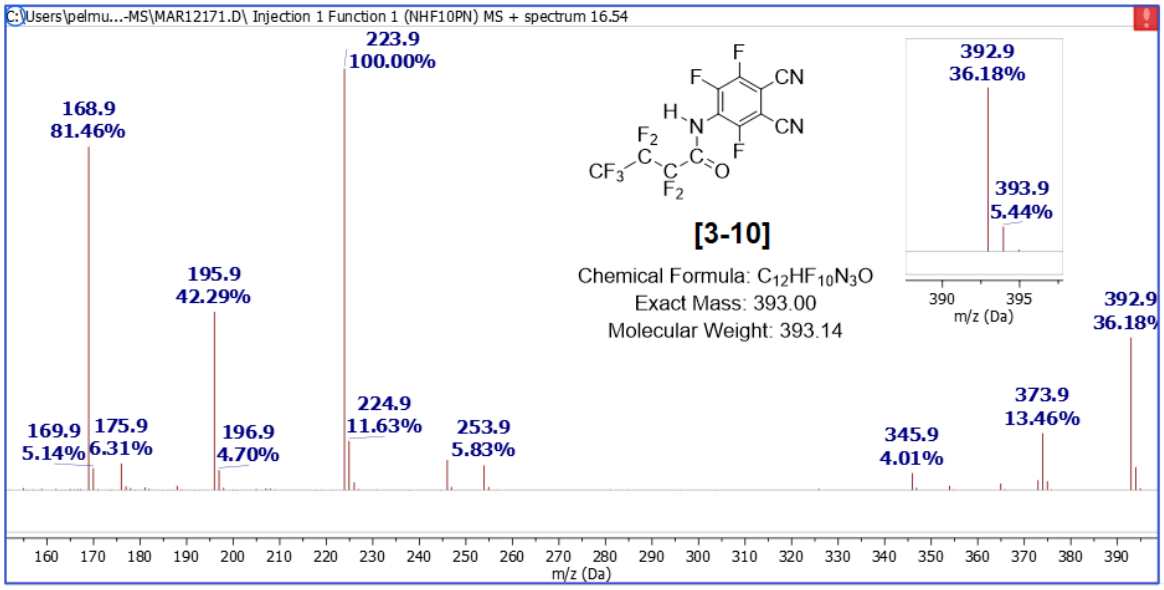


Figure C.3 MS spectrum of **[3-10]**.

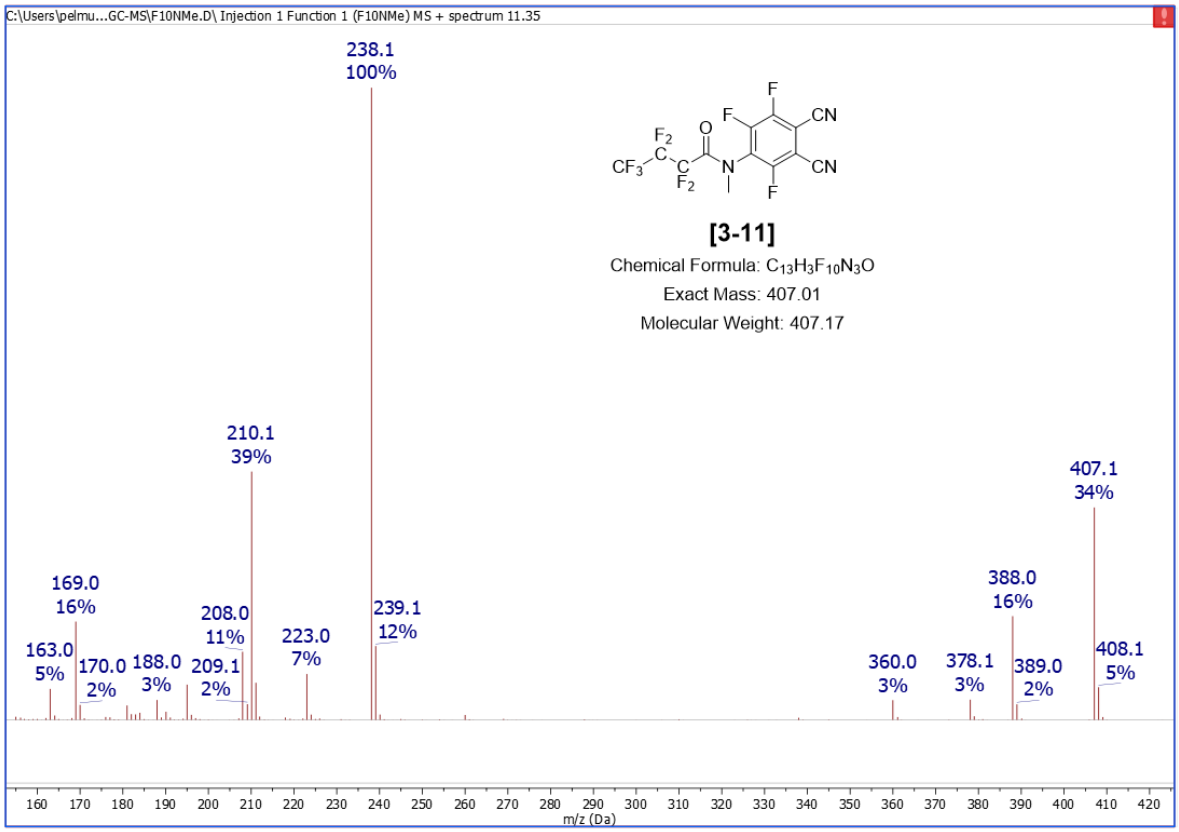


Figure C.4 MS spectrum of **[3-11]**.

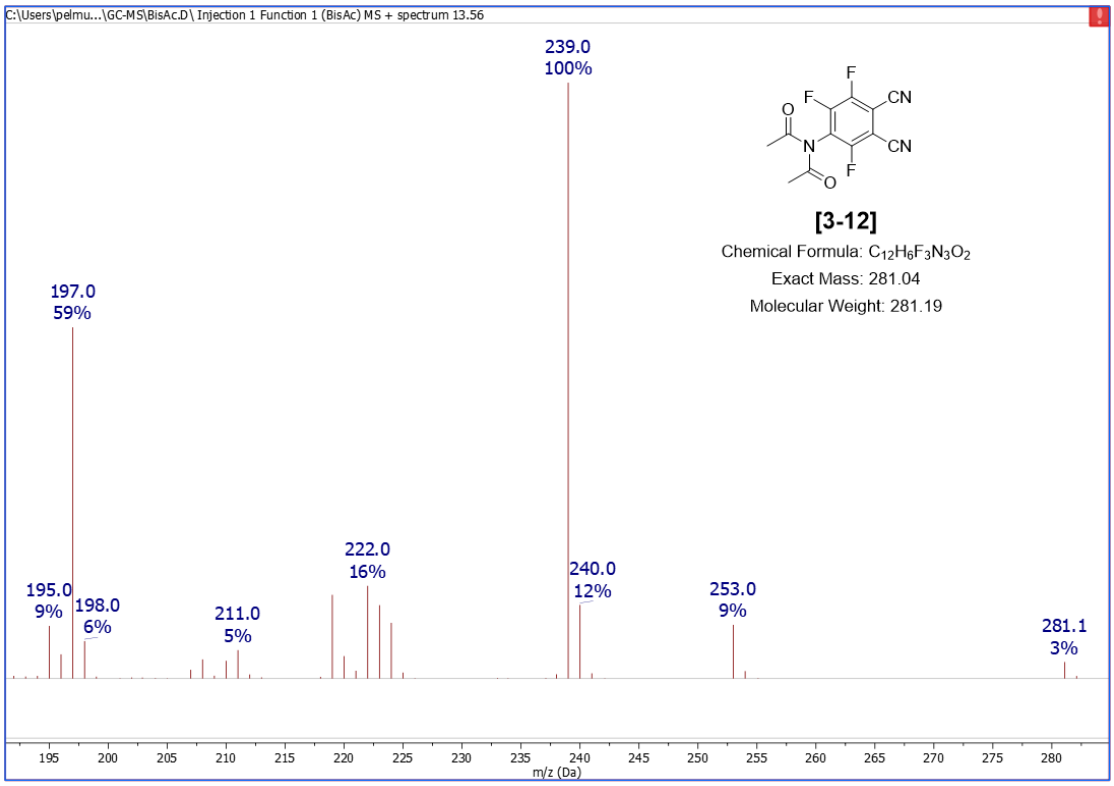


Figure C.5 MS spectrum of **[3-12]**.

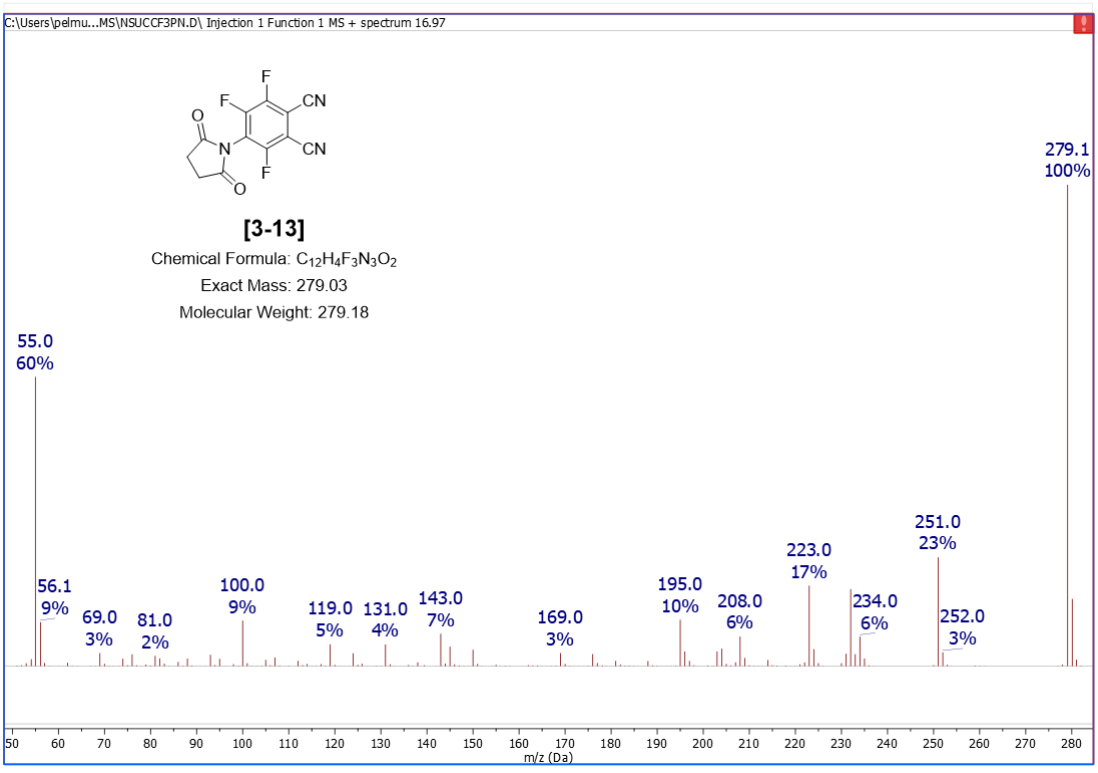


Figure C.6 MS spectrum of **[3-13]**.

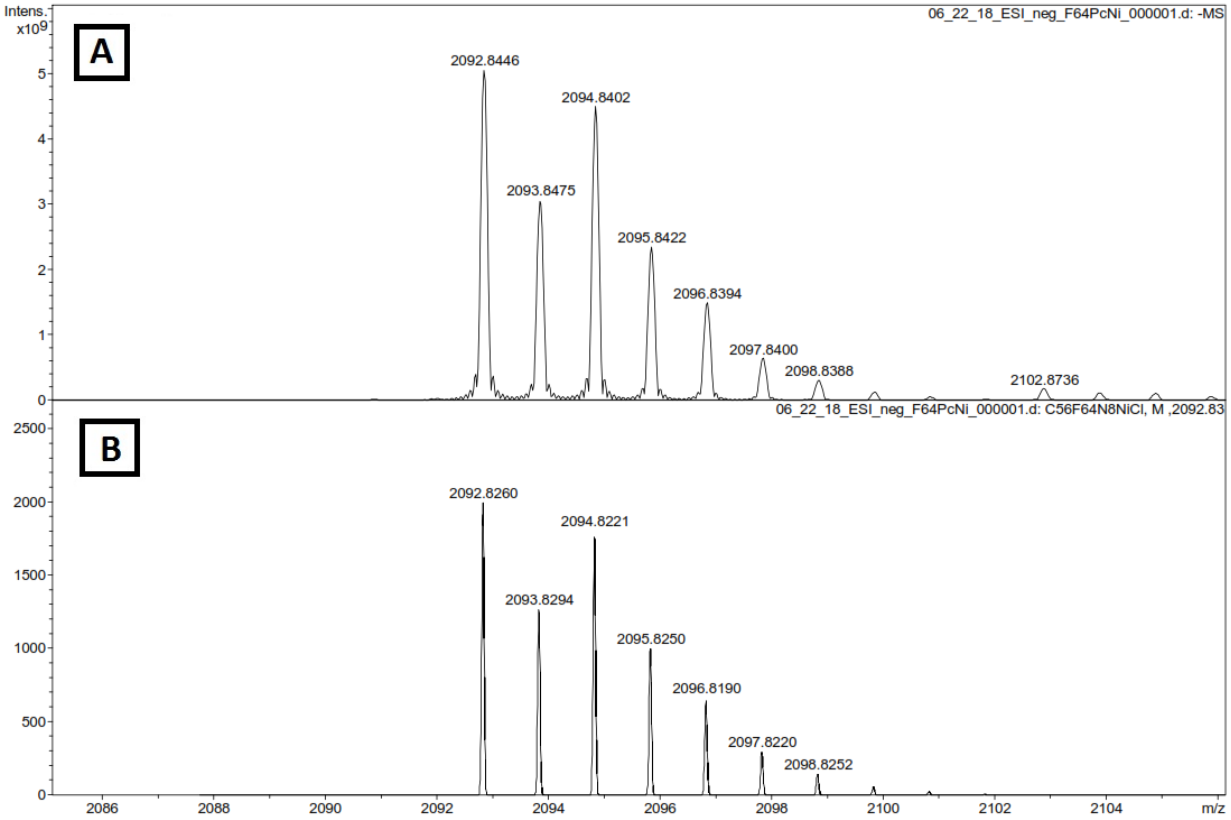


Figure C.7 HRMS of $F_{64}PcNiCl^-$, **[4-5]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern, δ = 9.0 ppm.

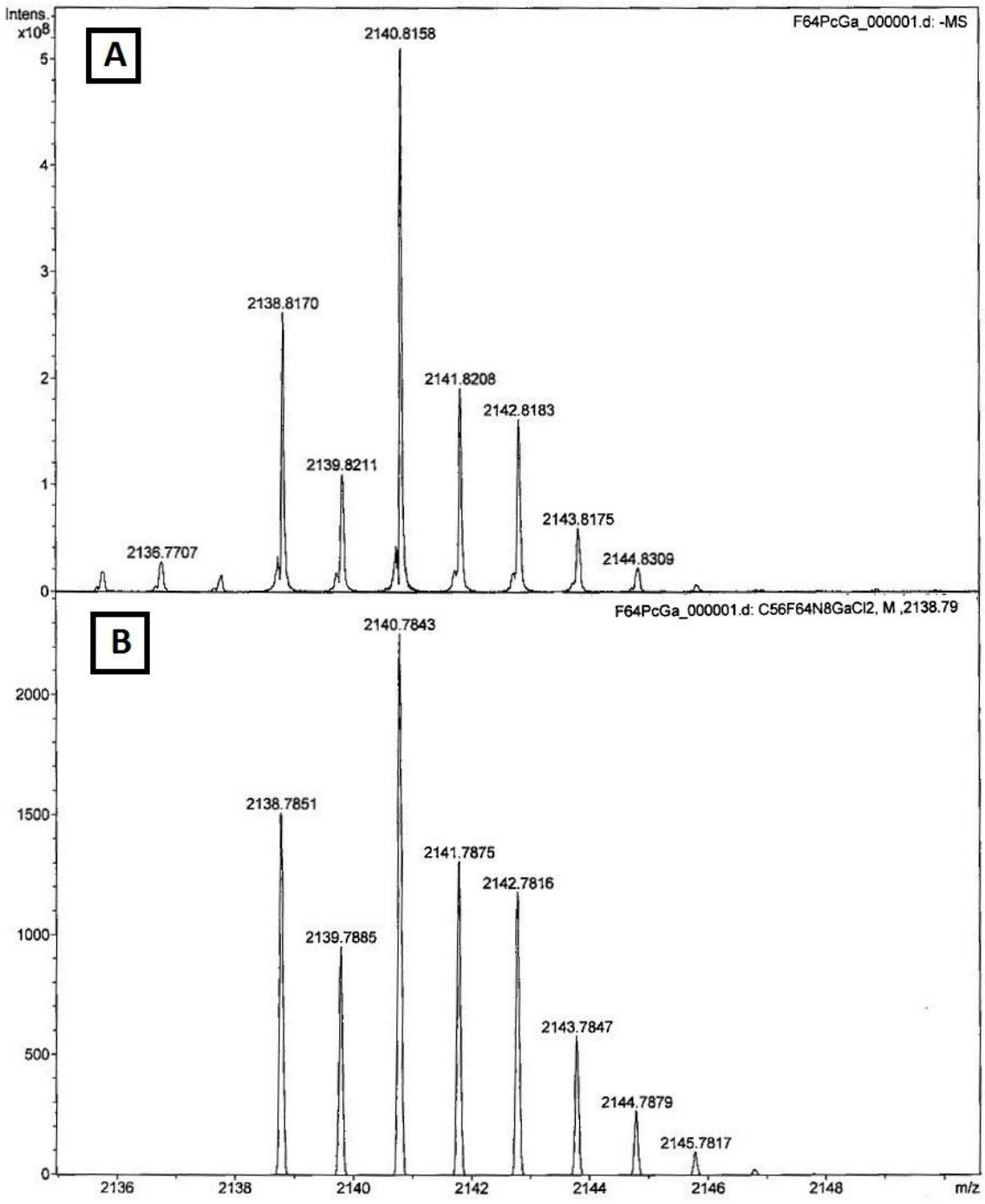


Figure C.8 HRMS of $F_{64}PcGaCl_2^-$, **[4-6]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 14.9 ppm). Figure reproduced with permission from Pelmuş *et al*., 2016.

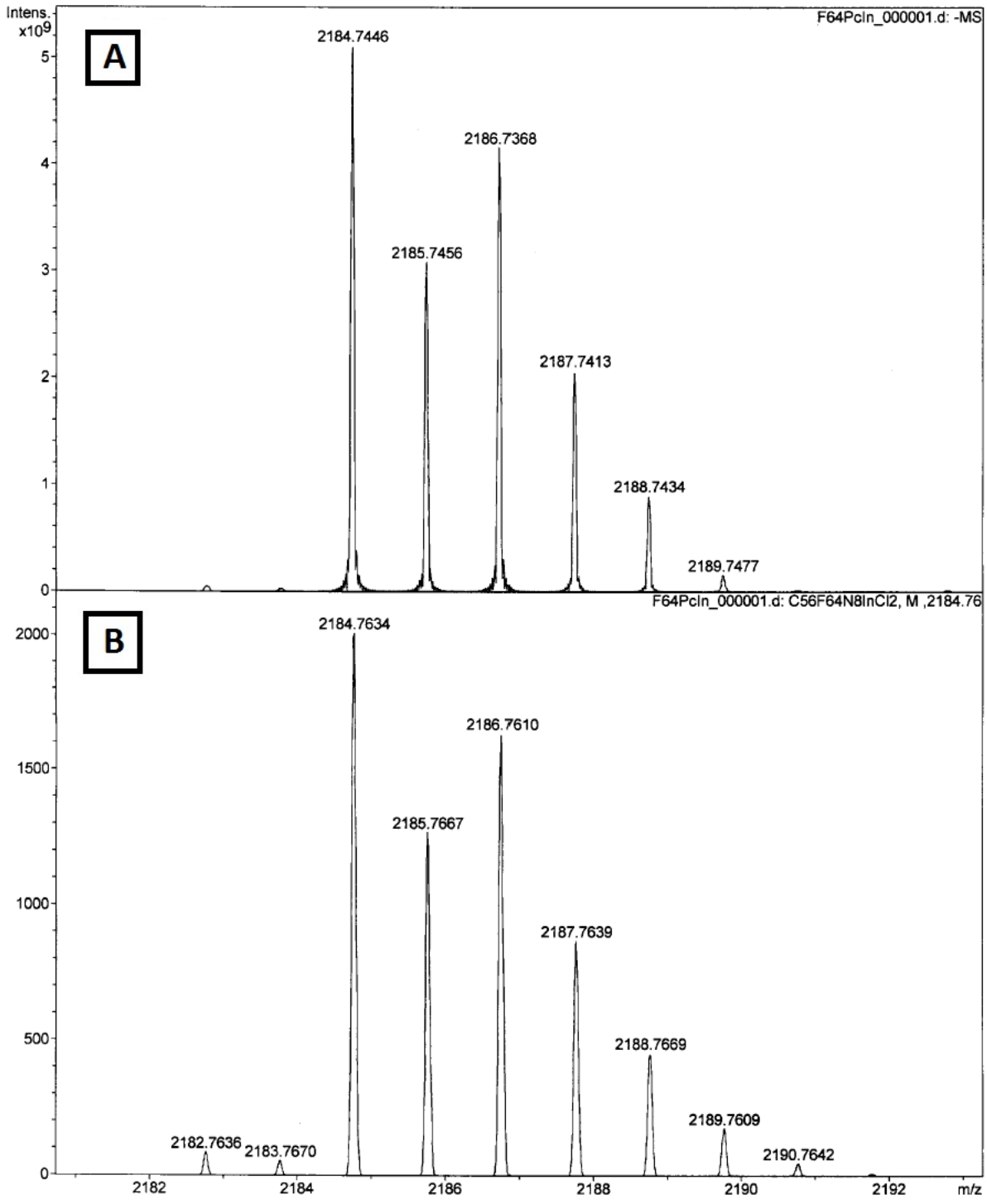


Figure C.9 HRMS of $F_{64}PcInCl_2^-$, **[4-7]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 8.6 ppm). Figure reproduced with permission from Pelmuş *et al*., 2016.

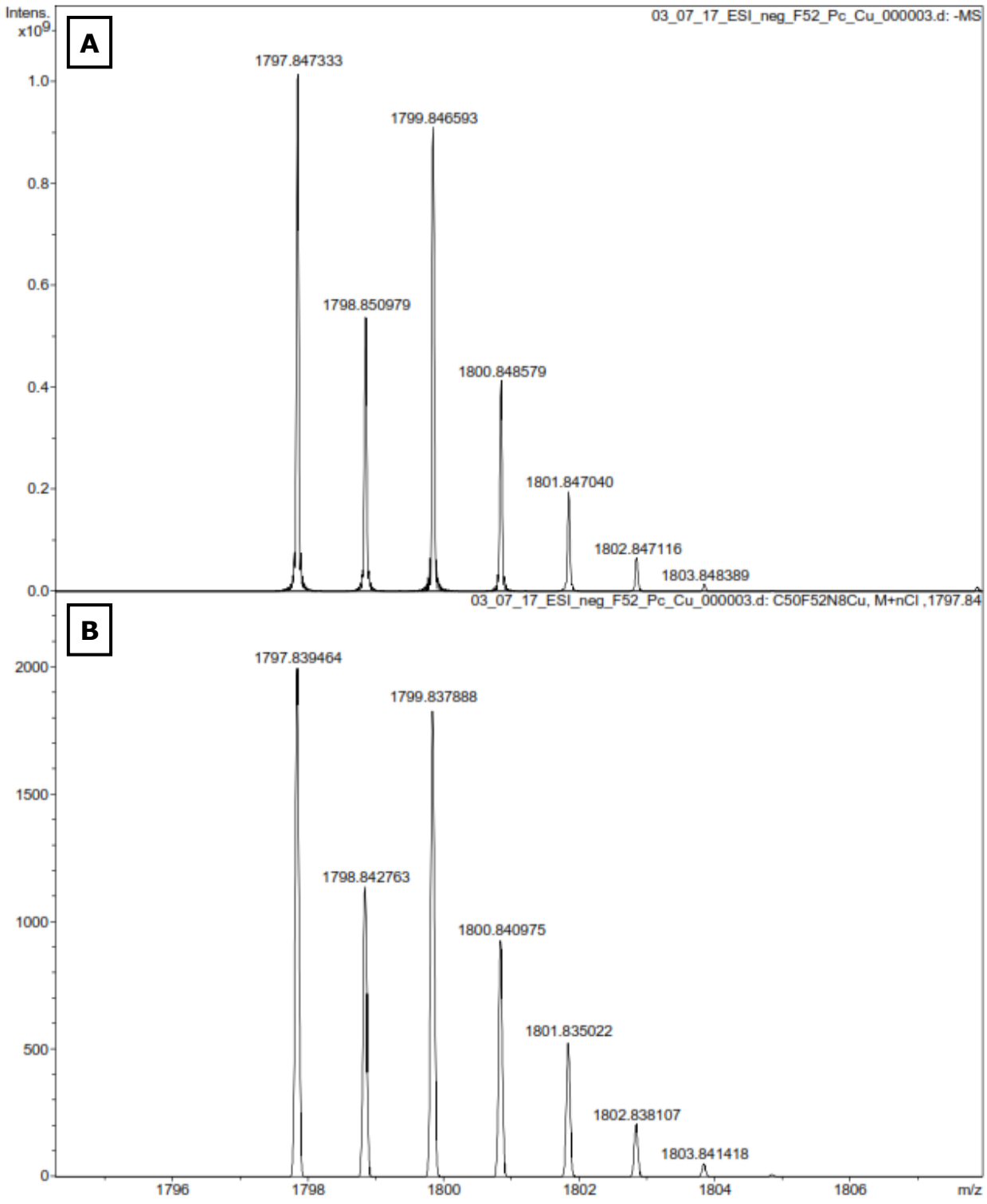


Figure C.10 HRMS of $F_{52}PcCuCl^-$, **[4-8]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 4.4 ppm).

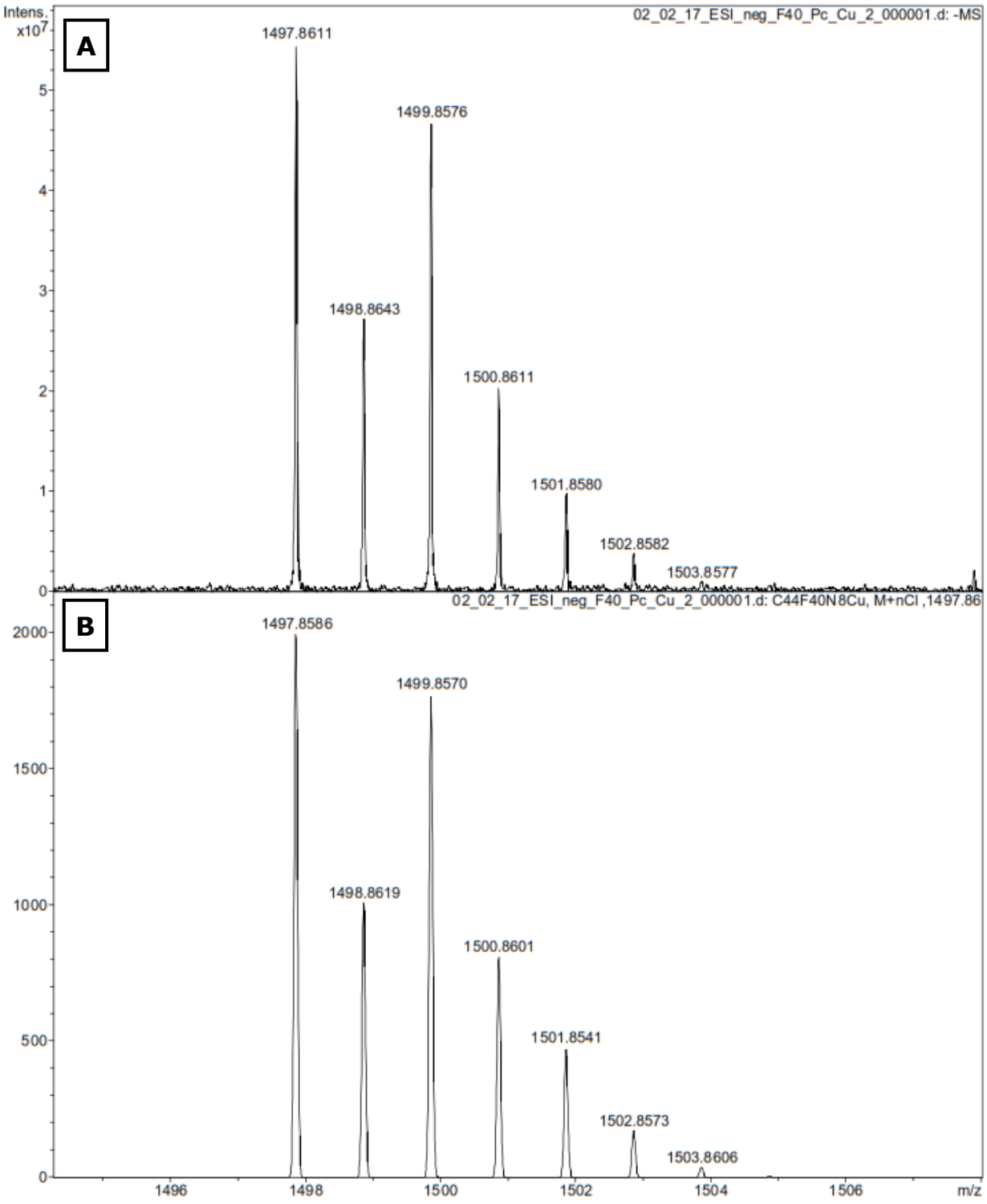


Figure C.11 HRMS of $F_{40}PcCuCl^-$, **[4-9]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 1.7 ppm). Reproduced from Nguyen *et al.* 2020 with permission from the PCCP Owner Societies.

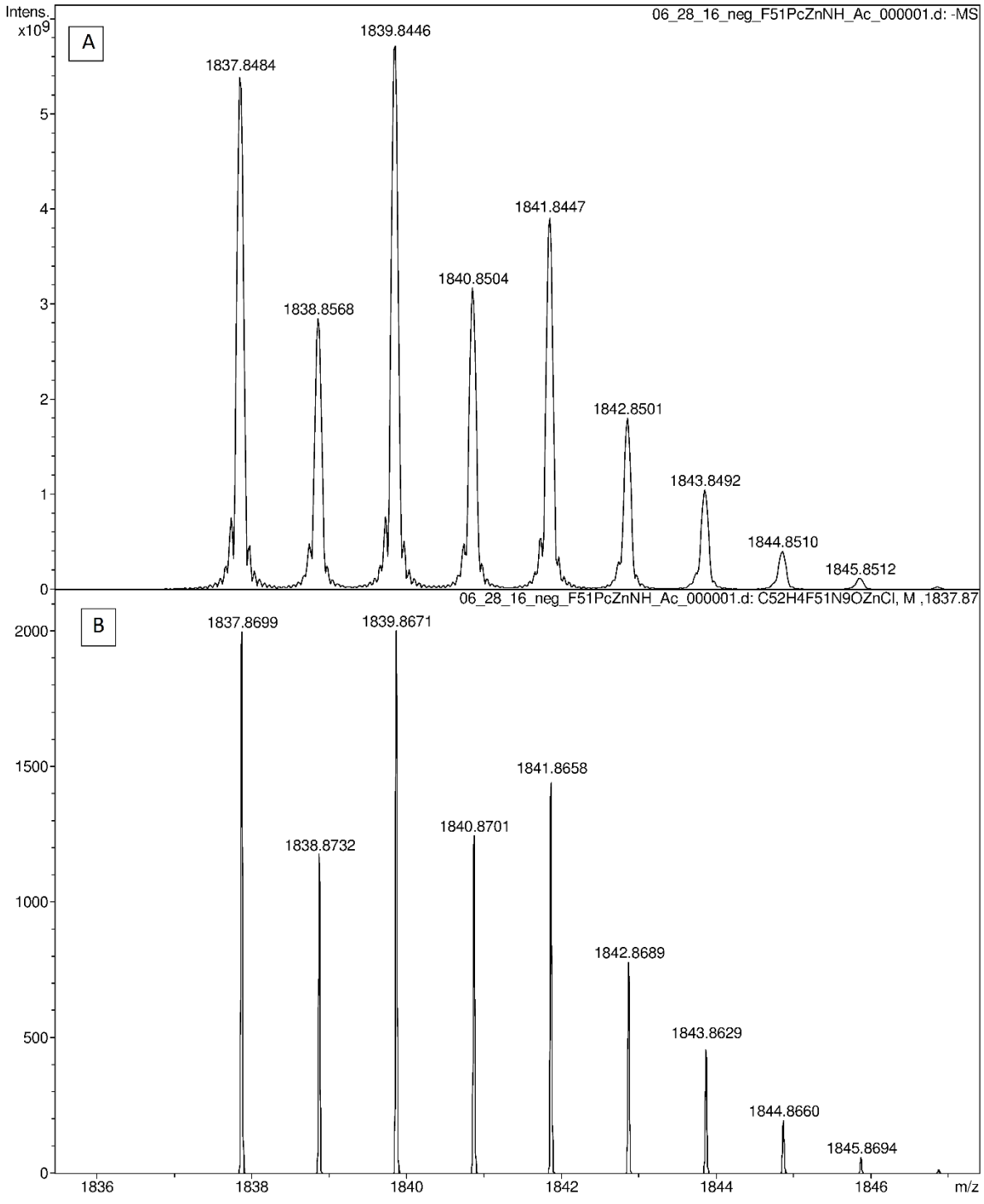


Figure C.12 HRMS of $NHAcF_{51}PcZnCl^-$, **[5-3]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 12 ppm).

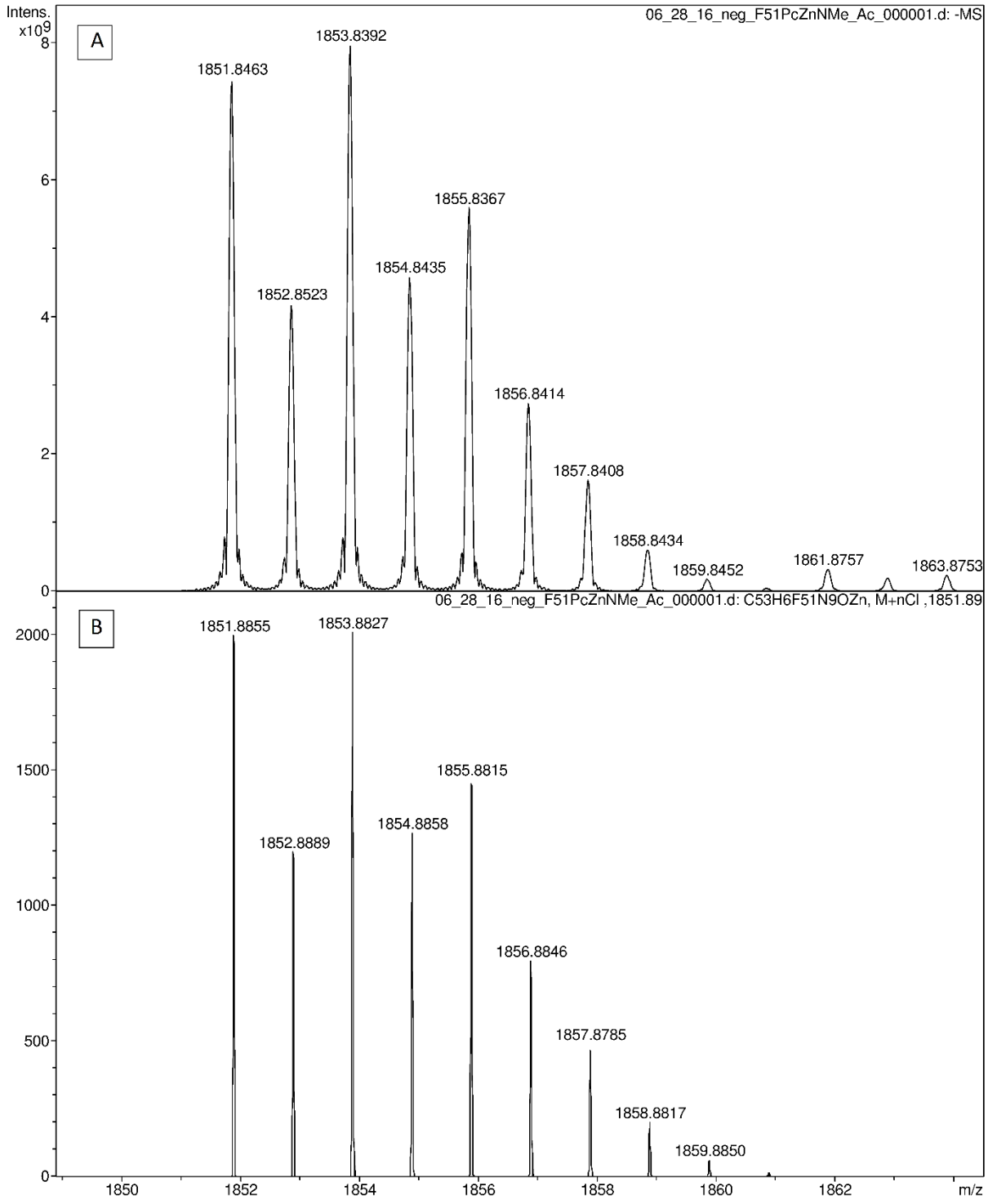


Figure C.13 HRMS of $NMeAcF_{51}PcZnCl^-$, **[5-4]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 21 ppm).

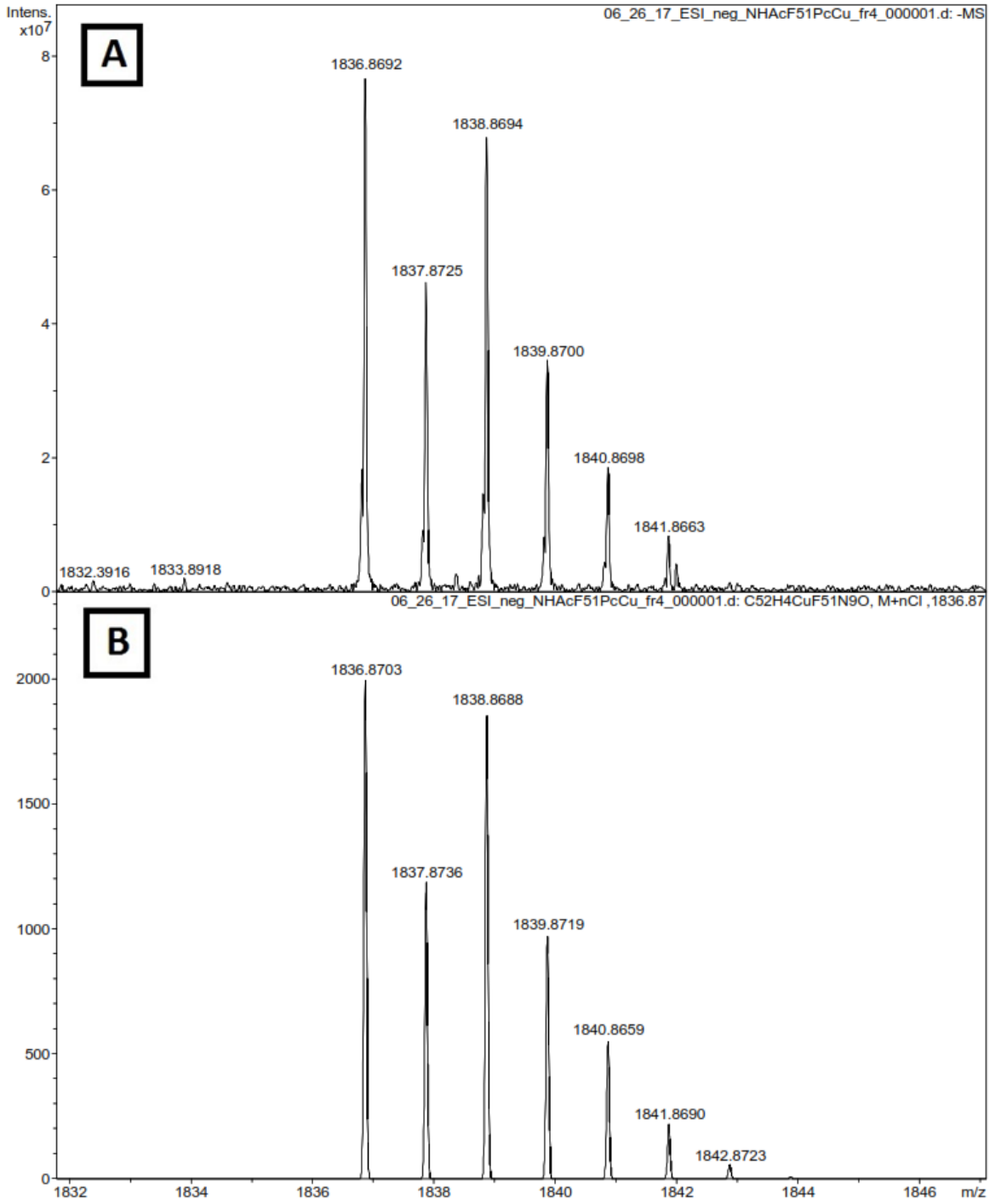


Figure C.14 HRMS of $NHAcF_{51}PcCuCl^-$, **[5-5]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 0.6 ppm).

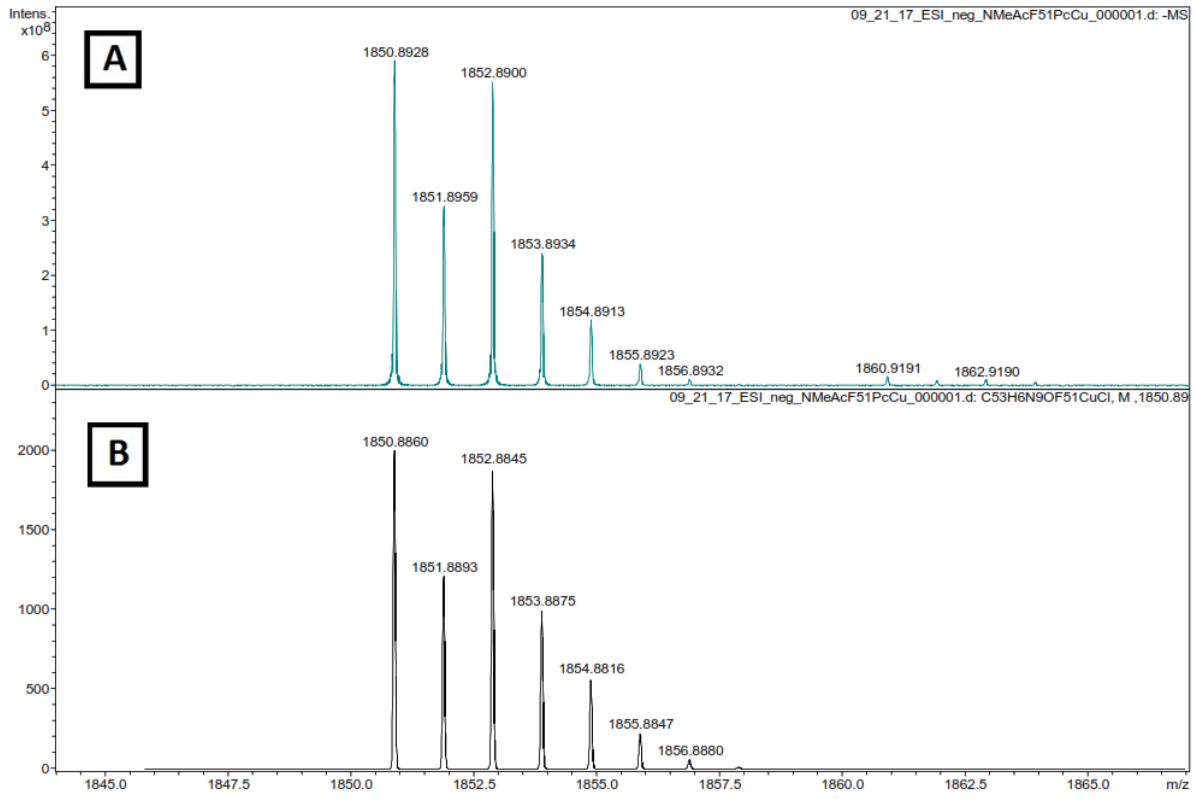


Figure C.15 HRMS of $NMeAcF_{51}PcCuCl^-$, **[5-6]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 3.7 ppm).

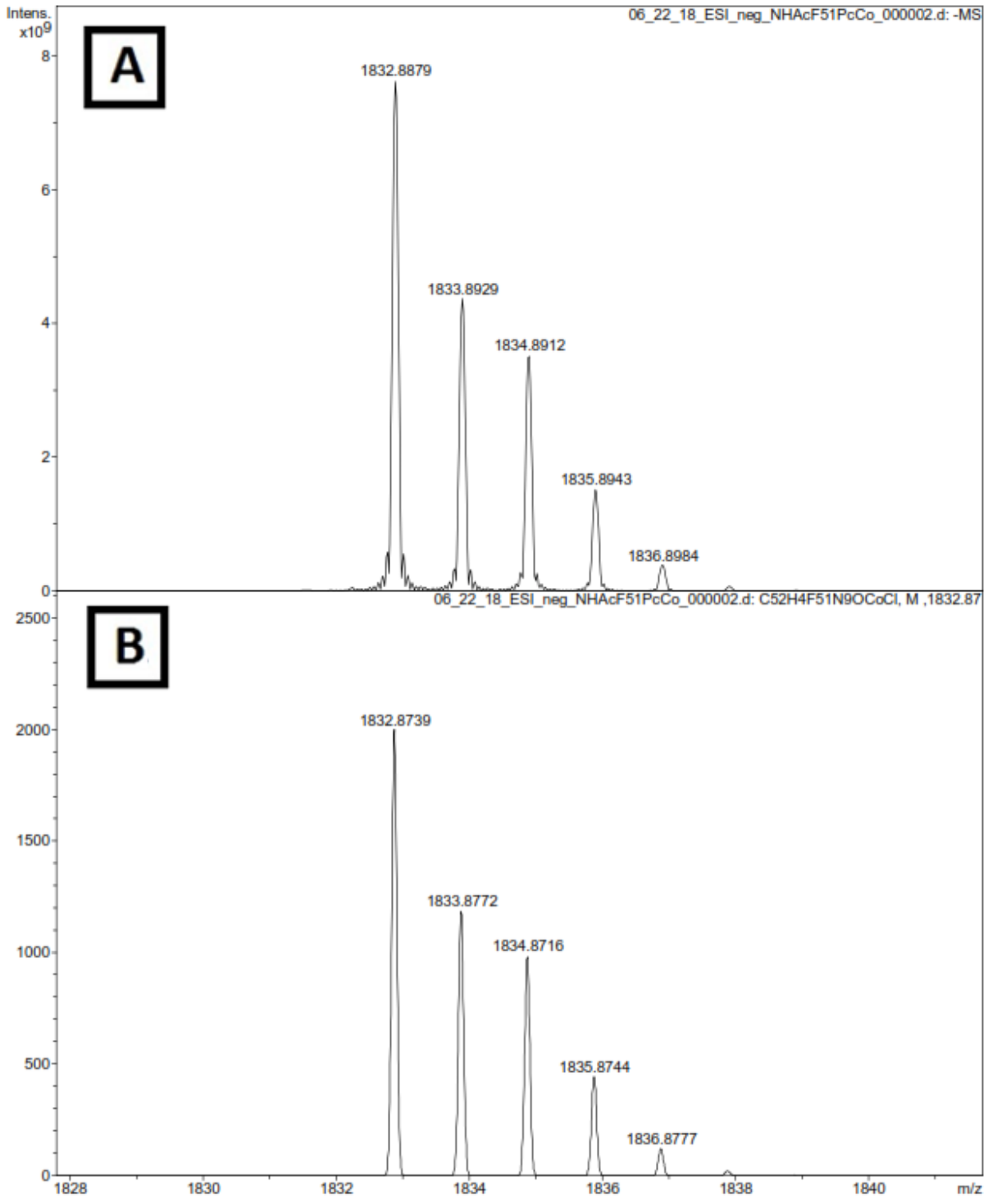


Figure C.16 HRMS of $NHAcF_{51}PcCoCl^-$, **[5-7]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 7.6 ppm).

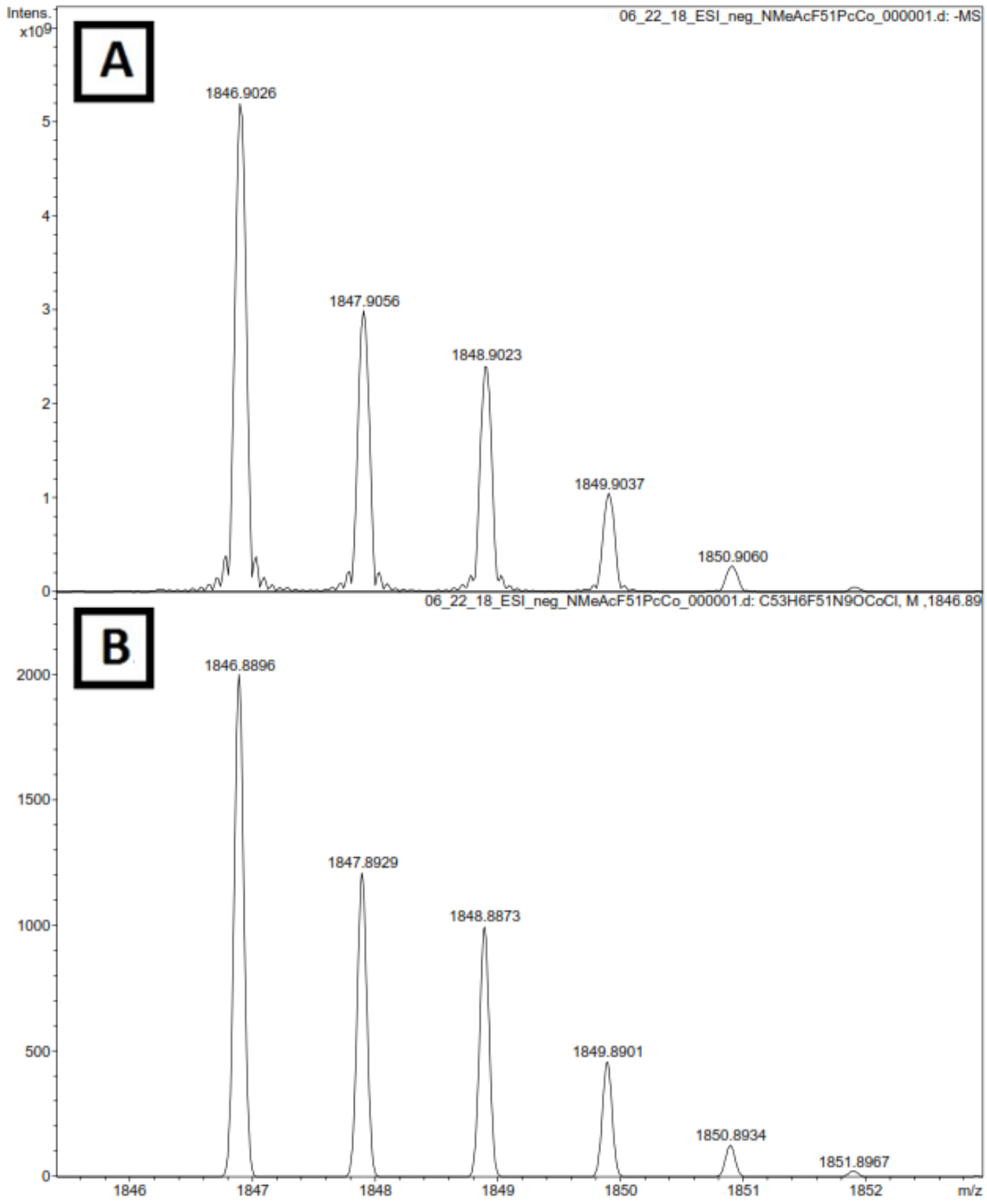


Figure C.17 HRMS of $NMeAcF_{51}PcCoCl^-$, **[5-8]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 7 ppm).

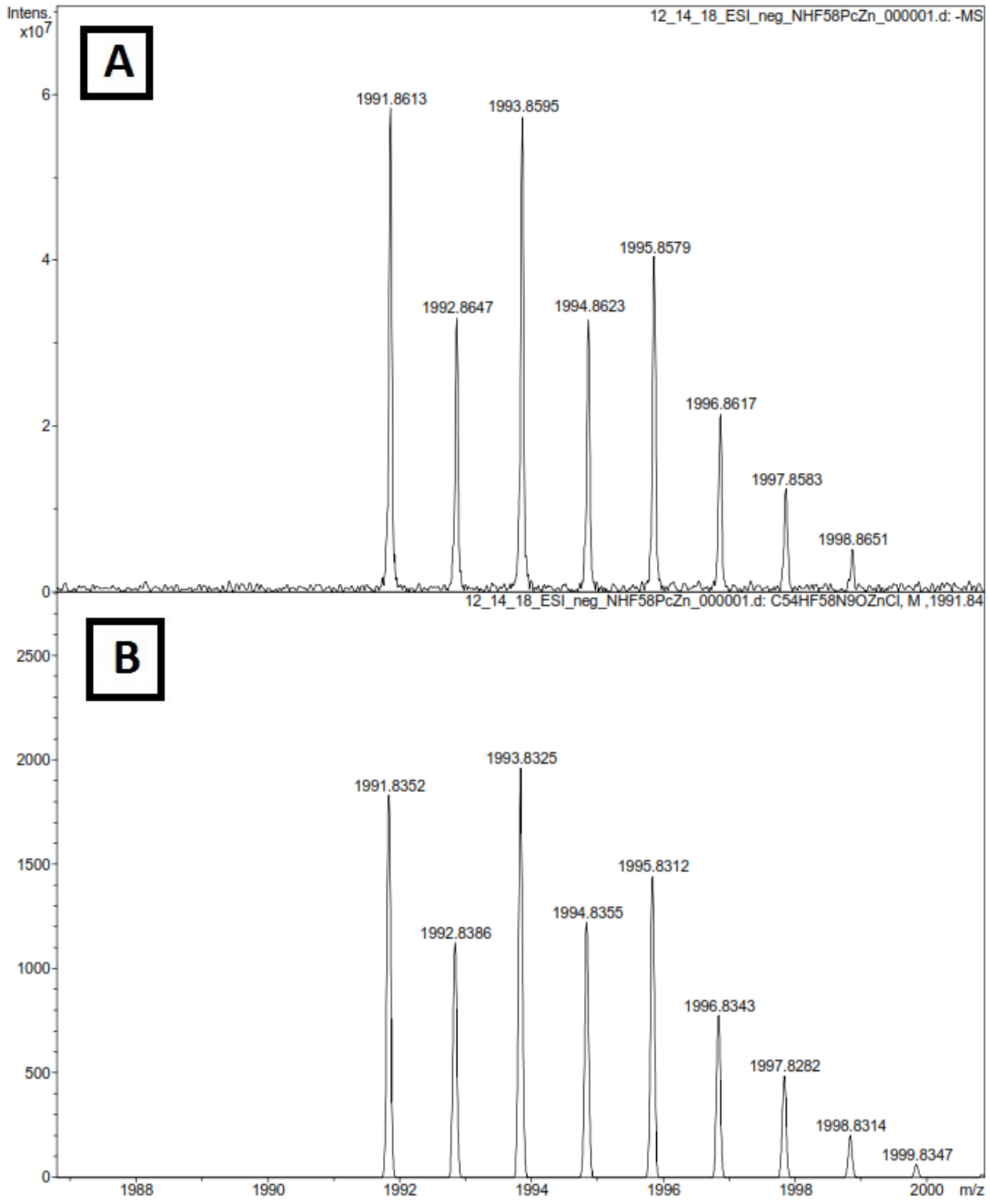


Figure C.18 HRMS of $NHF_{58}PcZnCl^-$, **[5-9]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 13 ppm).

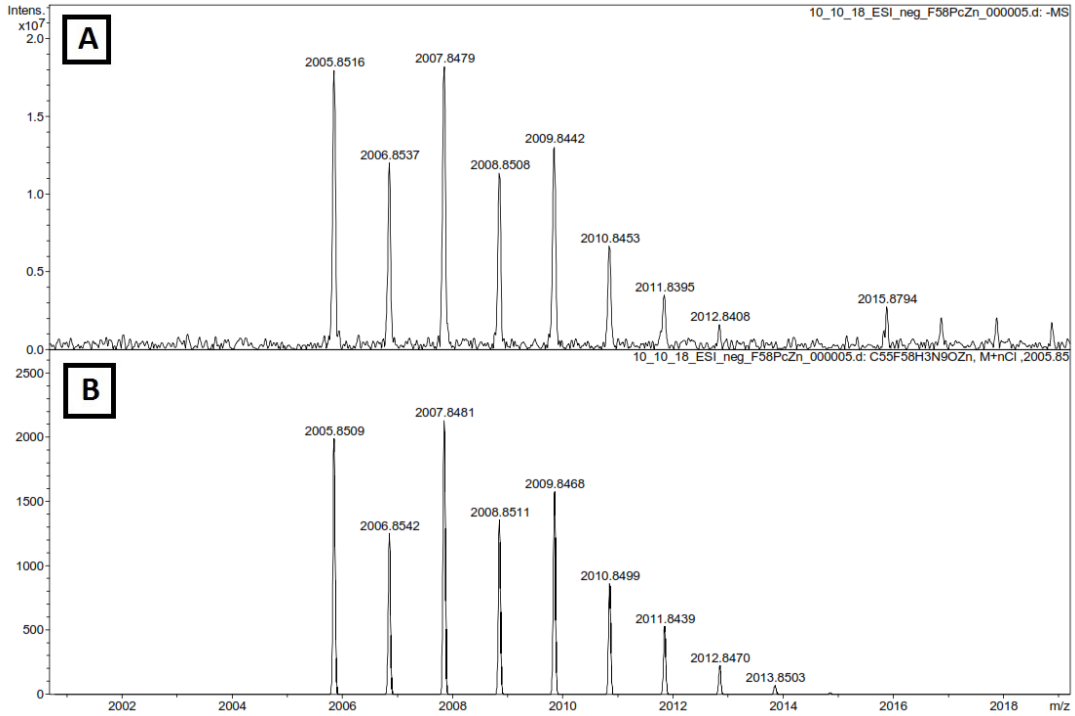


Figure C.19 HRMS of $NMeF_{58}PcZnCl^-$, **[5-10]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 0.3 ppm).

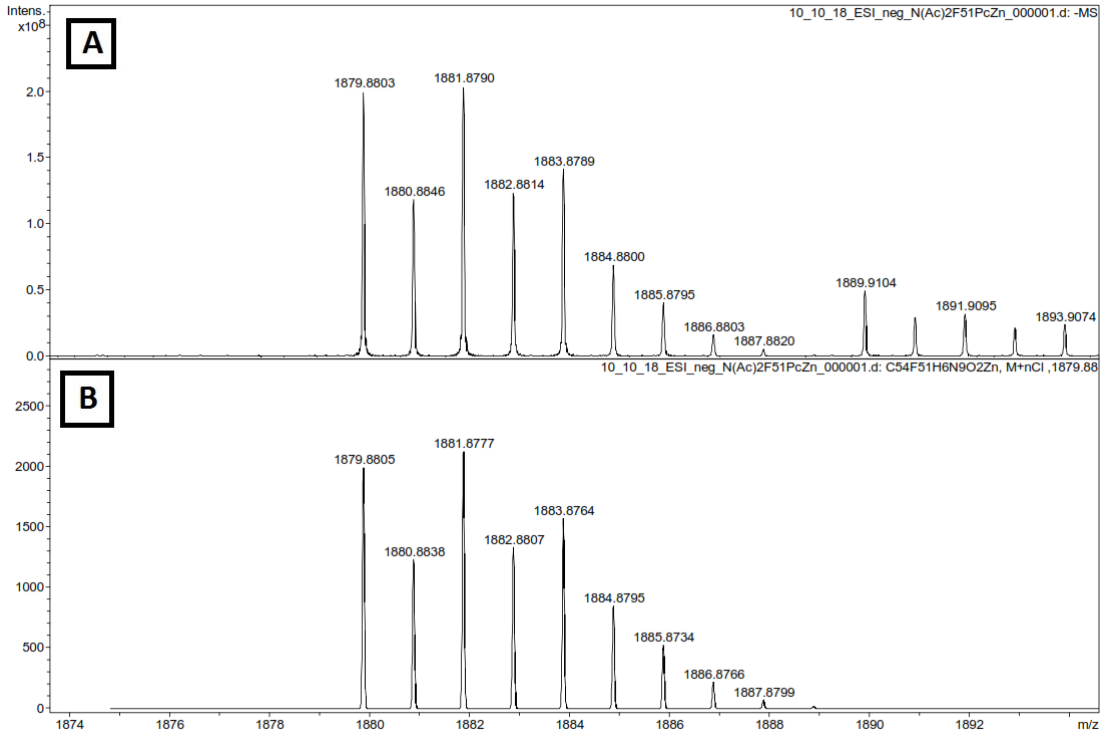


Figure C.20 HRMS of $NAc_2F_{51}PcZnCl^-$, **[5-11]** + Cl^-, A – observed isotopic pattern, B – calculated isotopic pattern (δ = 0.1 ppm).

Appendix D: UV-Vis spectra

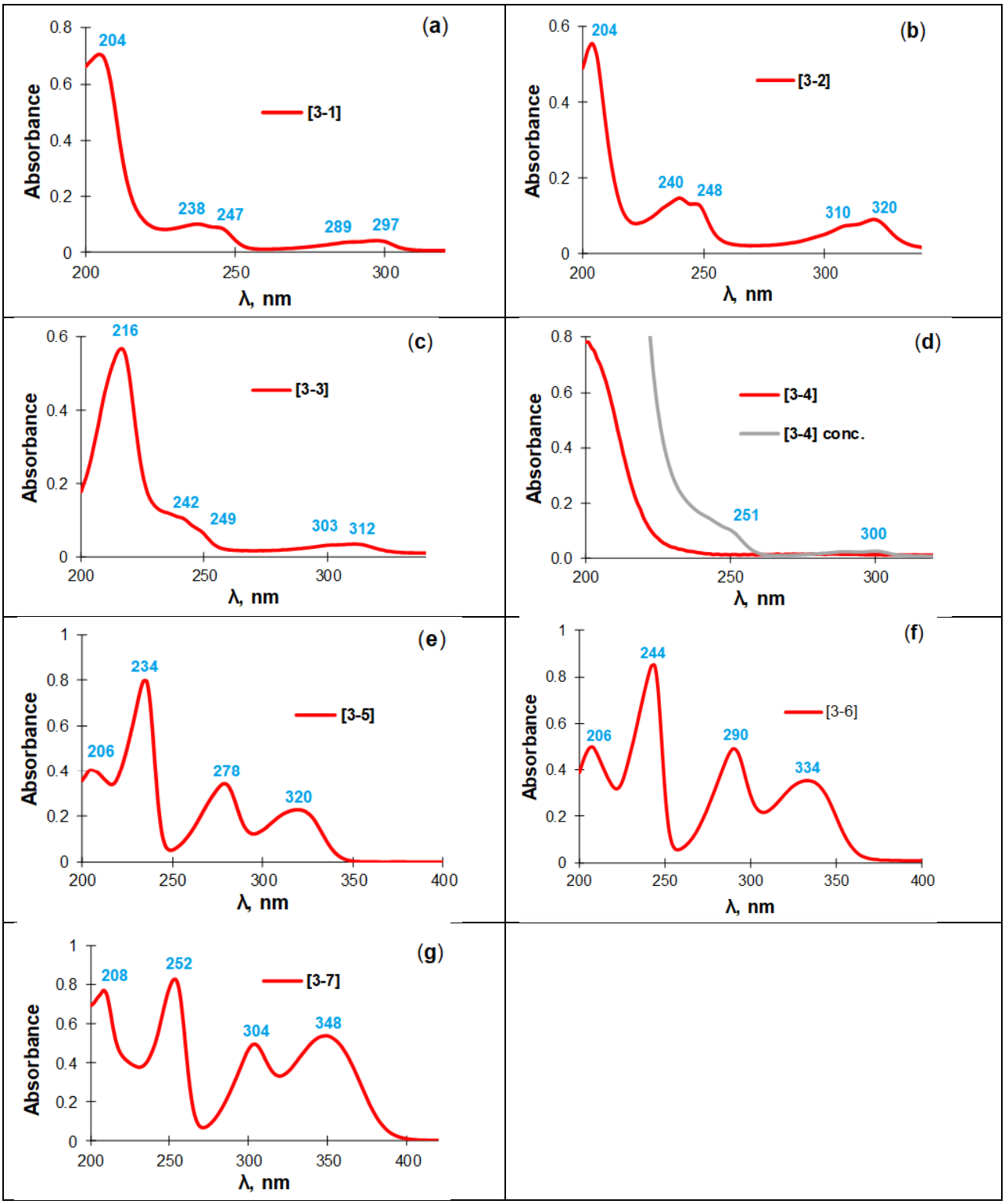


Figure D.1 UV-Vis spectra of the PNs **[3-1] – [3-7]** in acetonitrile.

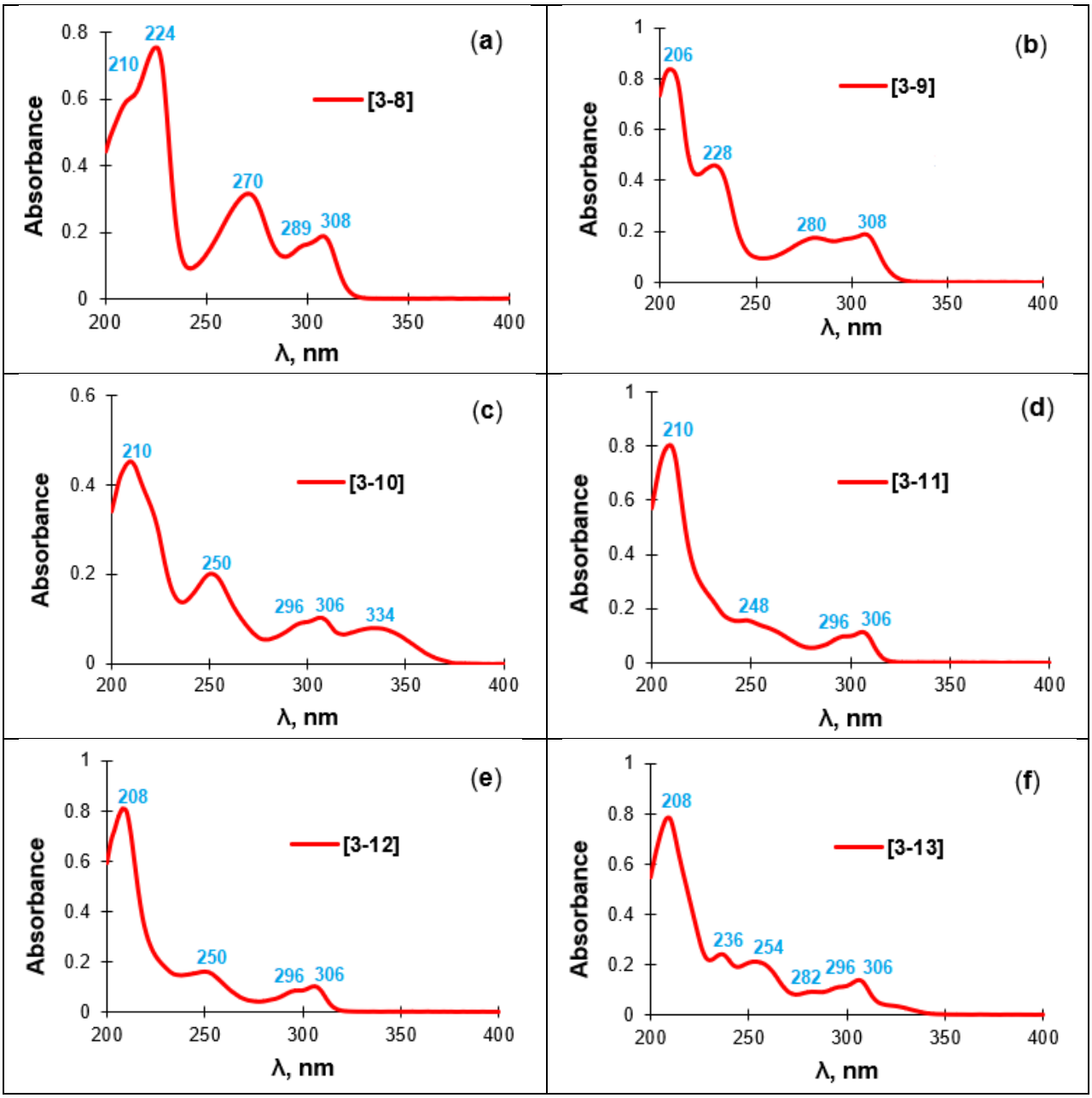


Figure D.2 UV-Vis spectra of the acylated PNs **[3-8] – [3-13]** in acetonitrile.

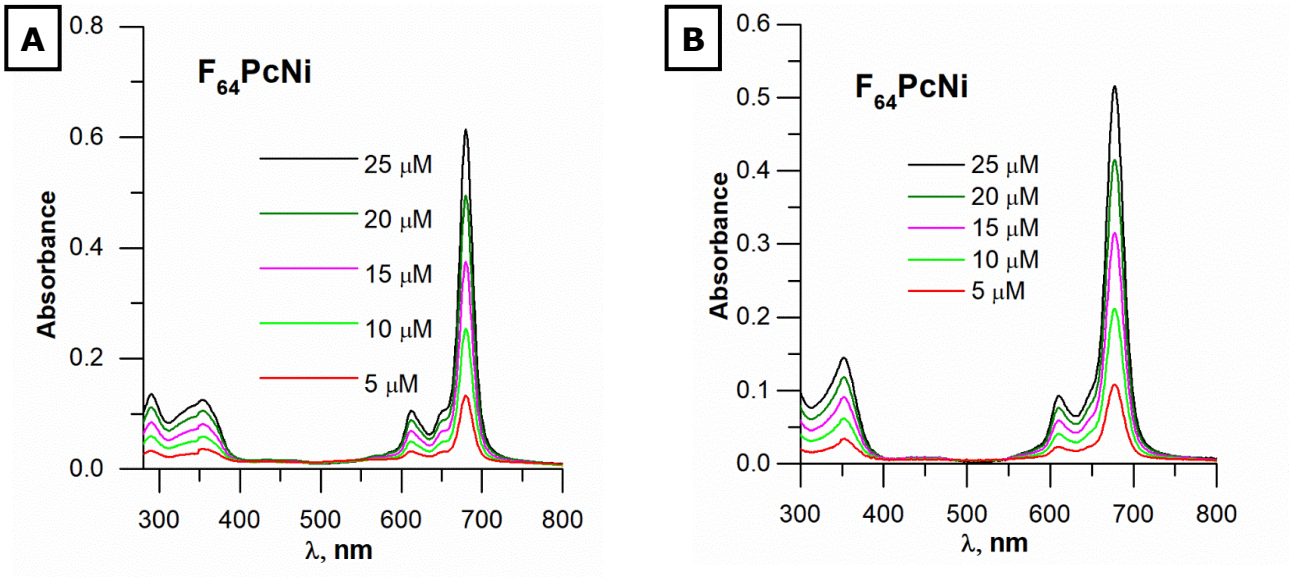
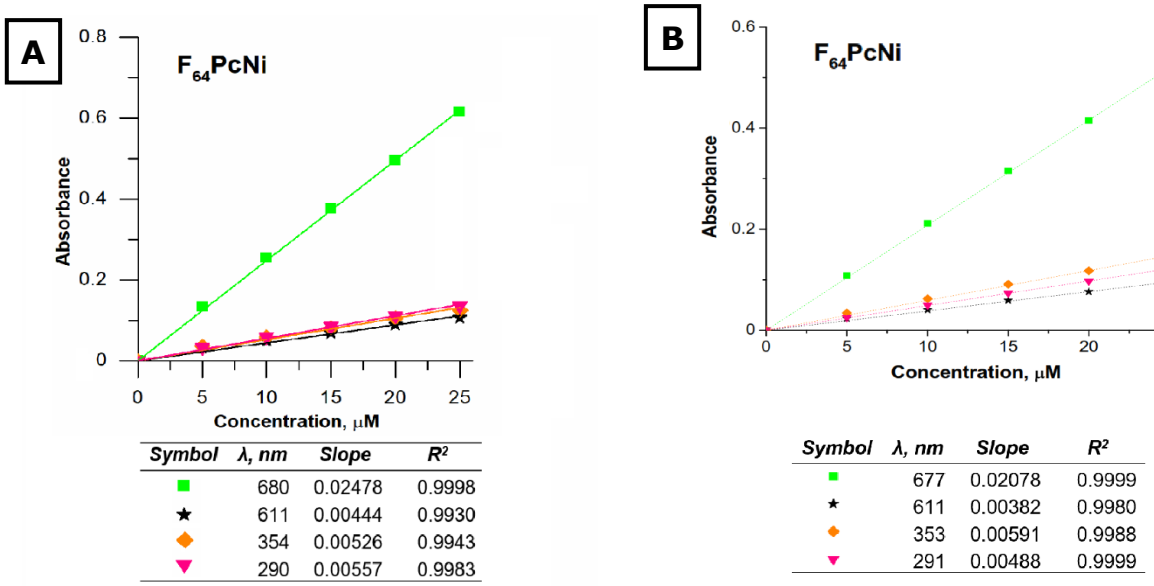


Figure D.3 Concentration dependent UV-Vis spectra of **F64PcNi** in TFT (**A**) and in ethyl acetate (**B**).



Symbol	λ, nm	Slope	R^2
■	680	0.02478	0.9998
★	611	0.00444	0.9930
◆	354	0.00526	0.9943
▼	290	0.00557	0.9983

Symbol	λ, nm	Slope	R^2
■	677	0.02078	0.9999
★	611	0.00382	0.9980
◆	353	0.00591	0.9988
▼	291	0.00488	0.9999

Figure D.4 Beer-Lambert plots of **F64PcNi** in TFT (**A**) and in ethyl acetate (**B**), 1 mm light path-length.

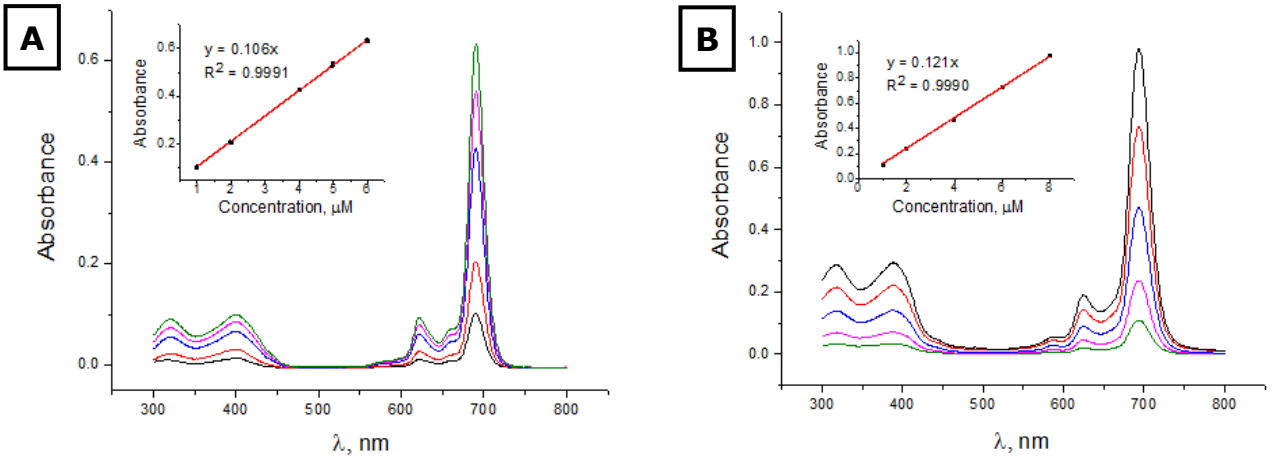


Figure D.5 Concentration dependent UV-Vis spectra of **F_{64}PcGaCl** in TFT (**A**) and in ethanol (**B**). Inset: absorbance at λ_{max} (Q-band) vs. concentration. Figure reproduced with permission from Pelmuş *et al.*, 2016.

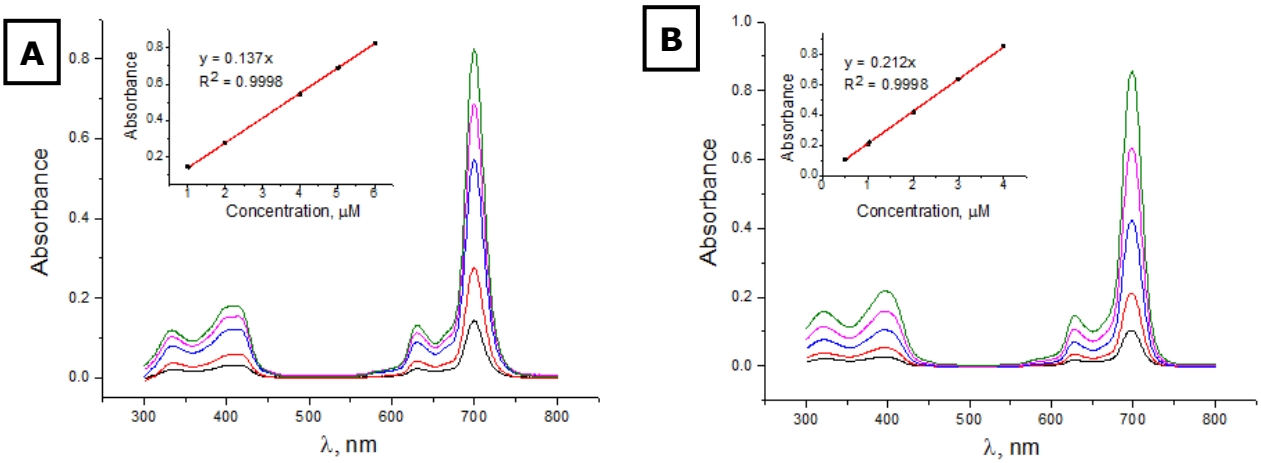


Figure D.6 Concentration dependent UV-Vis spectra of **F_{64}PcInCl** in TFT (**A**) and in ethanol (**B**). Inset: absorbance at λ_{max} (Q-band) vs. concentration. Figure reproduced with permission from Pelmuş *et al.*, 2016.

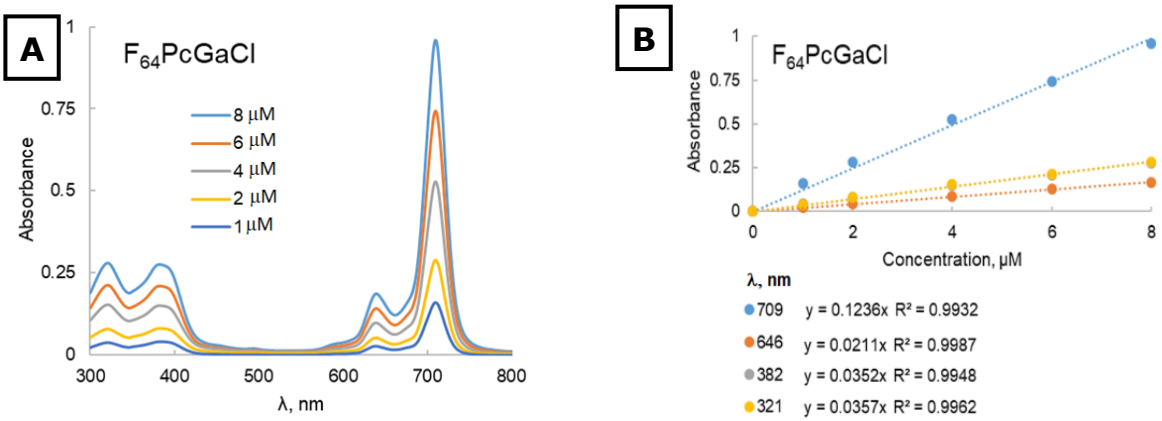


Figure D.7 Concentration dependent UV-Vis spectra of **F_{64}PcGaCl** in $CHCl_3$ (**A**), Beer-Lambert plot (**B**).

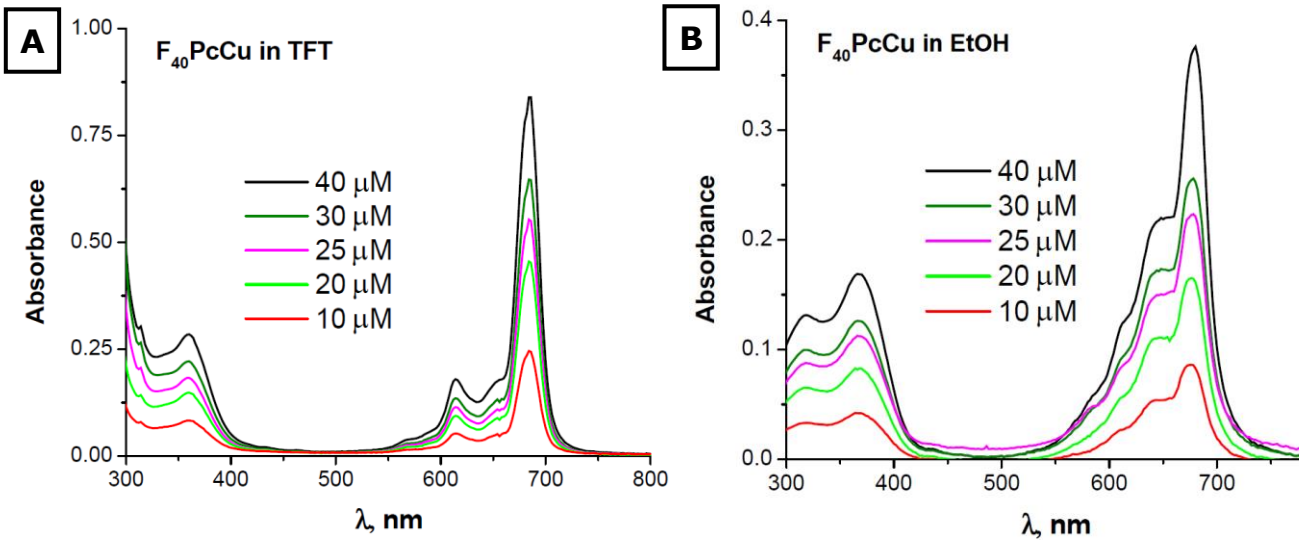
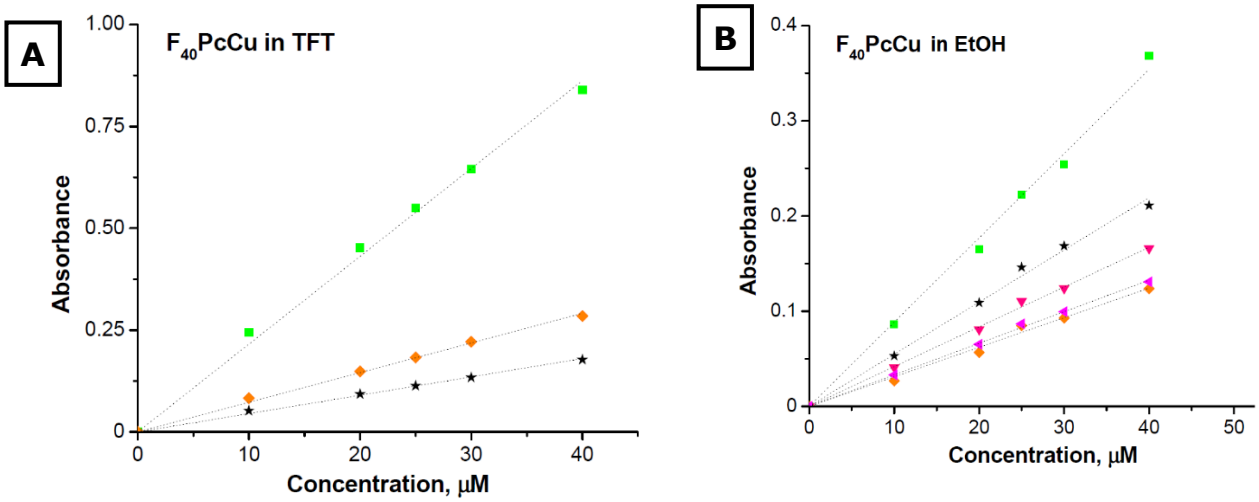


Figure D.8 Concentration dependent UV-Vis spectra of **F_{40}PcCu** in TFT (**A**) and in ethanol (**B**). Reproduced from Nguyen *et al.*, 2020 with permission from the PCCP Owner Societies.



Symbol	*λ, nm*	*Slope*	R^2
■	686	0.02156	0.99867
★	616	0.0045	0.99889
◆	360	0.00728	0.99895

Symbol	*λ, nm*	*Slope*	R^2
■	676	0.00885	0.99796
★	640	0.00548	0.99813
◆	612	0.00311	0.99659
▼	372	0.00418	0.9991
◀	316	0.00332	0.99943

Figure D.9 Beer-Lambert plots of **F_{40}PcCu** in TFT (**A**) and in ethanol (**B**), 1 mm light pathlength. Reproduced from Nguyen *et al.* 2020 with permission from the PCCP Owner Societies.

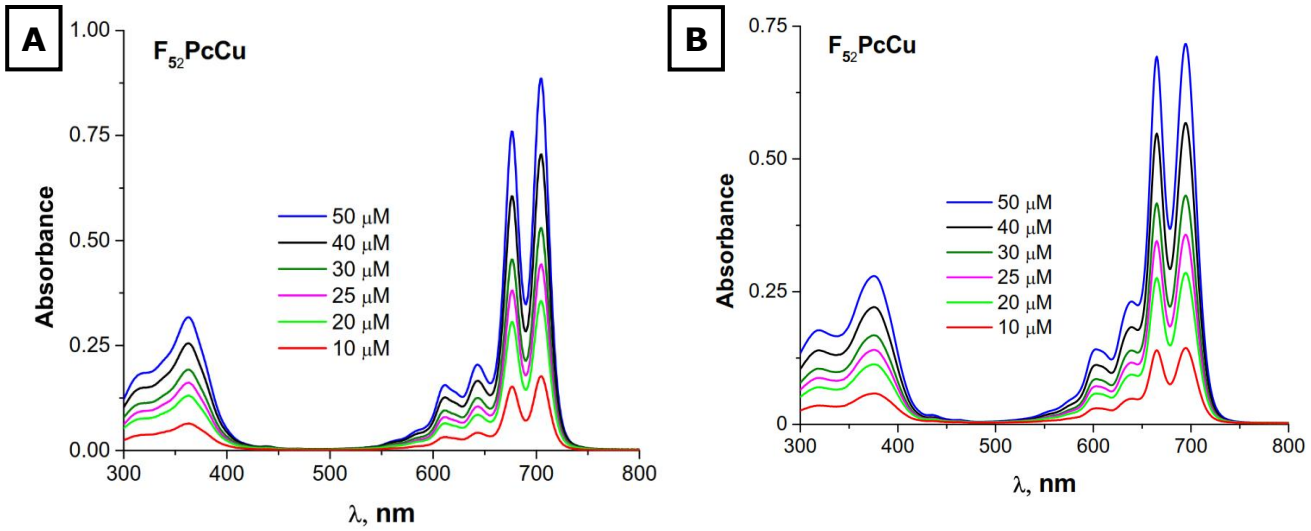
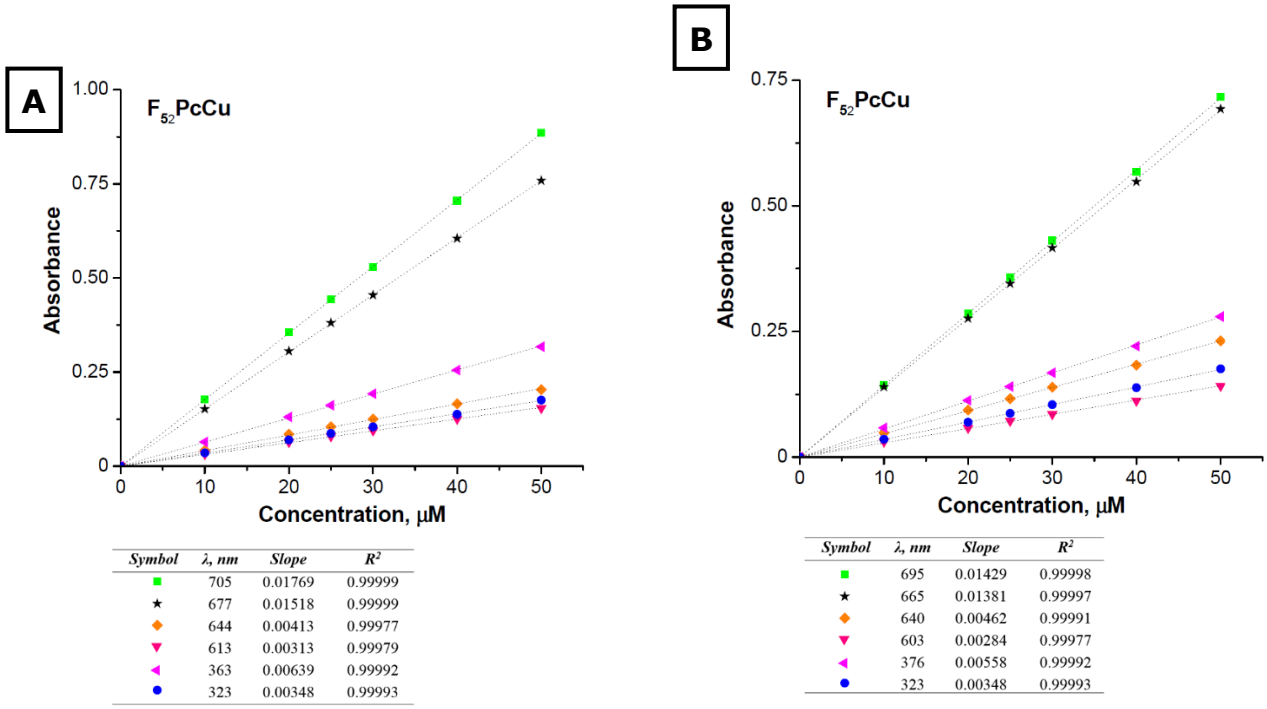


Figure D.10 Concentration dependent UV-Vis spectra of **F52PcCu** in $CHCl_3$ (**A**) and in ethanol (**B**).



Symbol	*λ, nm*	*Slope*	*R^2*
■	705	0.01769	0.99999
★	677	0.01518	0.99999
◆	644	0.00413	0.99977
▼	613	0.00313	0.99979
◀	363	0.00639	0.99992
●	323	0.00348	0.99993

Symbol	*λ, nm*	*Slope*	*R^2*
■	695	0.01429	0.99998
★	665	0.01381	0.99997
◆	640	0.00462	0.99991
▼	603	0.00284	0.99977
◀	376	0.00558	0.99992
●	323	0.00348	0.99993

Figure D.11 Beer-Lambert plots of **F52PcCu** in $CHCl_3$ (**A**) and in ethanol (**B**), 1 mm light path-length.

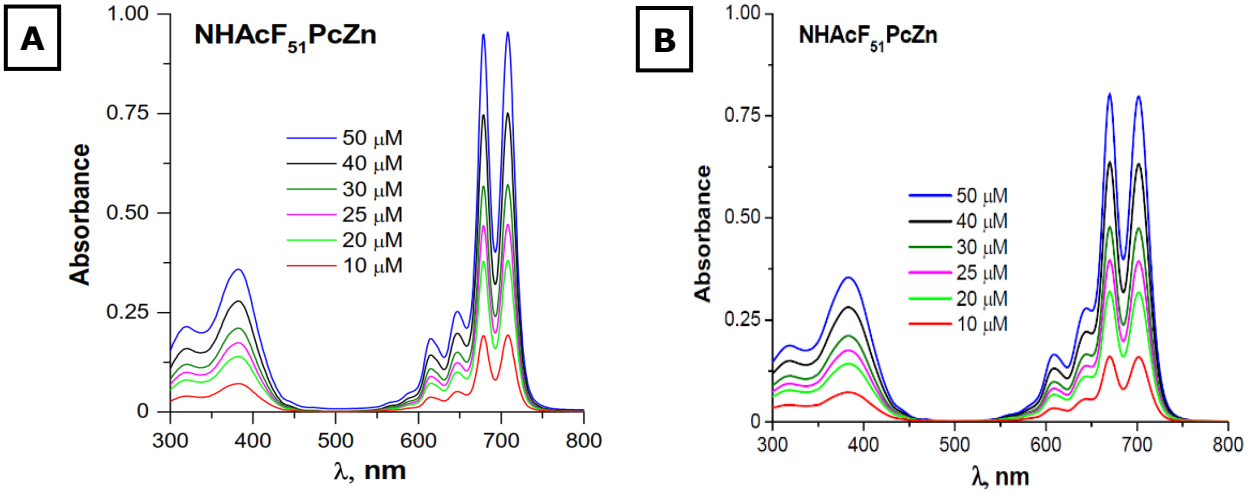
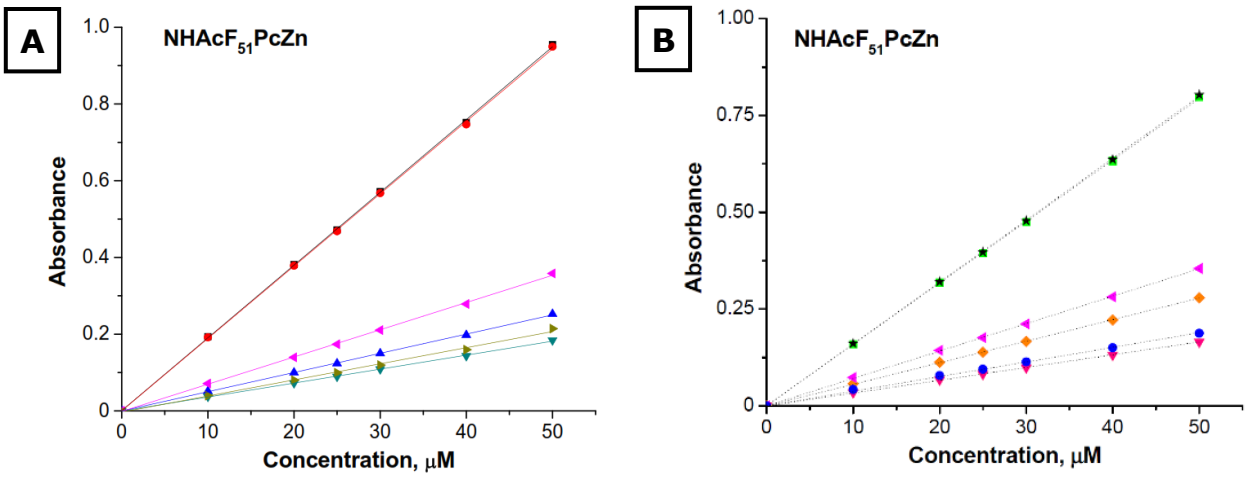


Figure D.12 Concentration dependent UV-Vis spectra of $NHAcF_{51}PcZn$ **[5-4]** in (**A**) $CHCl_3$ and (**B**) ethanol.



Symbol	*λ, nm*	*Slope*	R^2
■	708	0.01897	0.99978
●	679	0.01886	0.99976
▲	647	0.00501	0.99961
▼	615	0.00364	0.99927
◀	381	0.0071	0.99929
▶	320	0.0042	0.99561

Symbol	*λ, nm*	*slope*	R^2
■	702	0.01587	0.99997
★	670	0.01598	0.99997
◆	645	0.00557	0.99996
▼	608	0.00330	0.99992
◀	383	0.00708	0.99994
●	320	0.00378	0.99959

Figure D.13 Beer-Lambert plots of $NHAcF_{51}PcZn$ **[5-4]** in (**A**) $CHCl_3$ and (**B**) ethanol, 1 mm light pathlength.

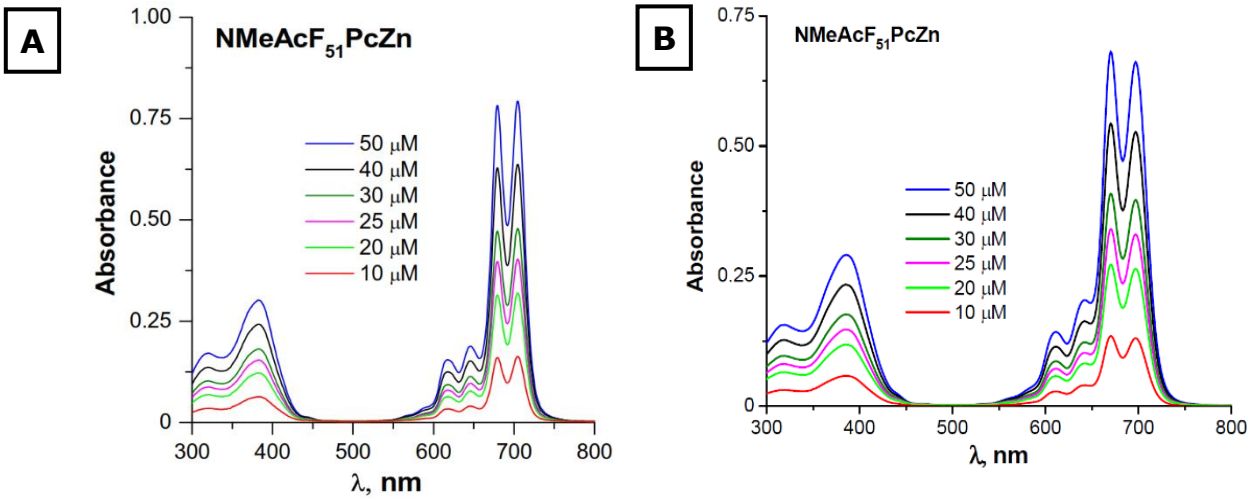
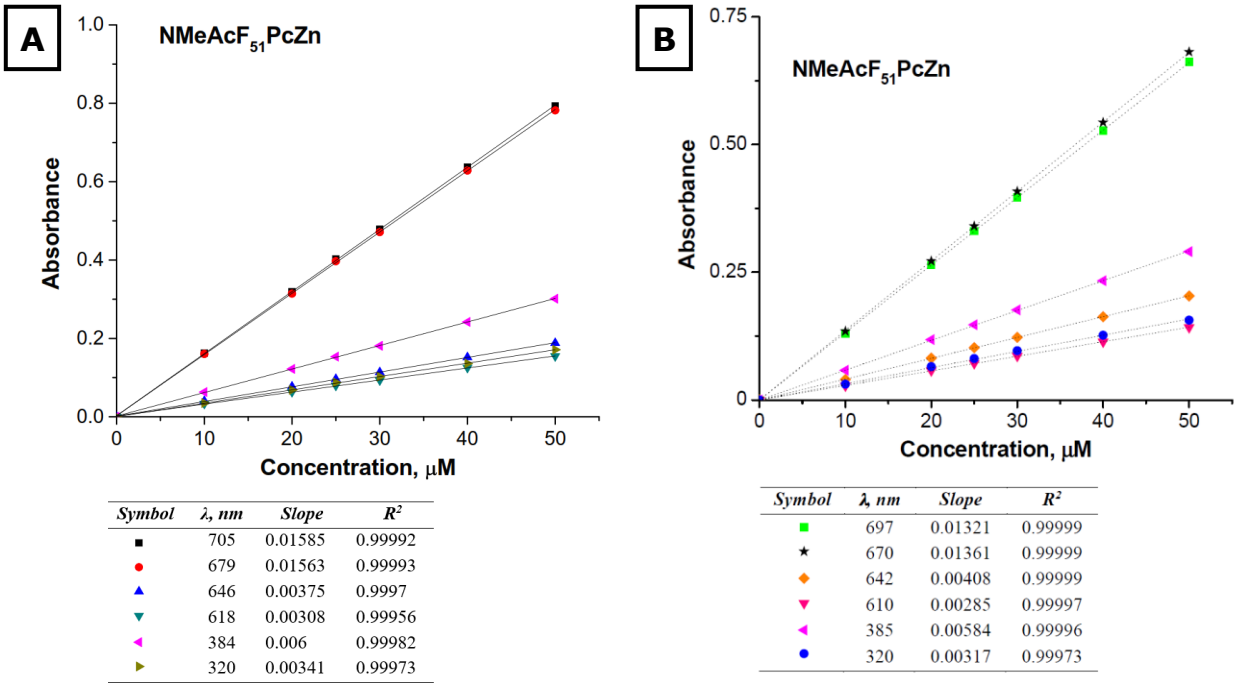


Figure D.14 Variation with the concentration for the UV-Vis spectra of $NMeAcF_{51}PcZn$ **[5-4]** in (**A**) $CHCl_3$ and (**B**) ethanol.



Symbol	*λ, nm*	*Slope*	*R^2*
■	705	0.01585	0.99992
●	679	0.01563	0.99993
▲	646	0.00375	0.9997
▼	618	0.00308	0.99956
◀	384	0.006	0.99982
▶	320	0.00341	0.99973

Symbol	*λ, nm*	*Slope*	*R^2*
■	697	0.01321	0.99999
★	670	0.01361	0.99999
◆	642	0.00408	0.99999
▼	610	0.00285	0.99997
◀	385	0.00584	0.99996
●	320	0.00317	0.99973

Figure D.15 Beer-Lambert plots of $NMeAcF_{51}PcZn$ **[5-4]** in (**A**) $CHCl_3$ and (**B**) ethanol, 1 mm light pathlength.

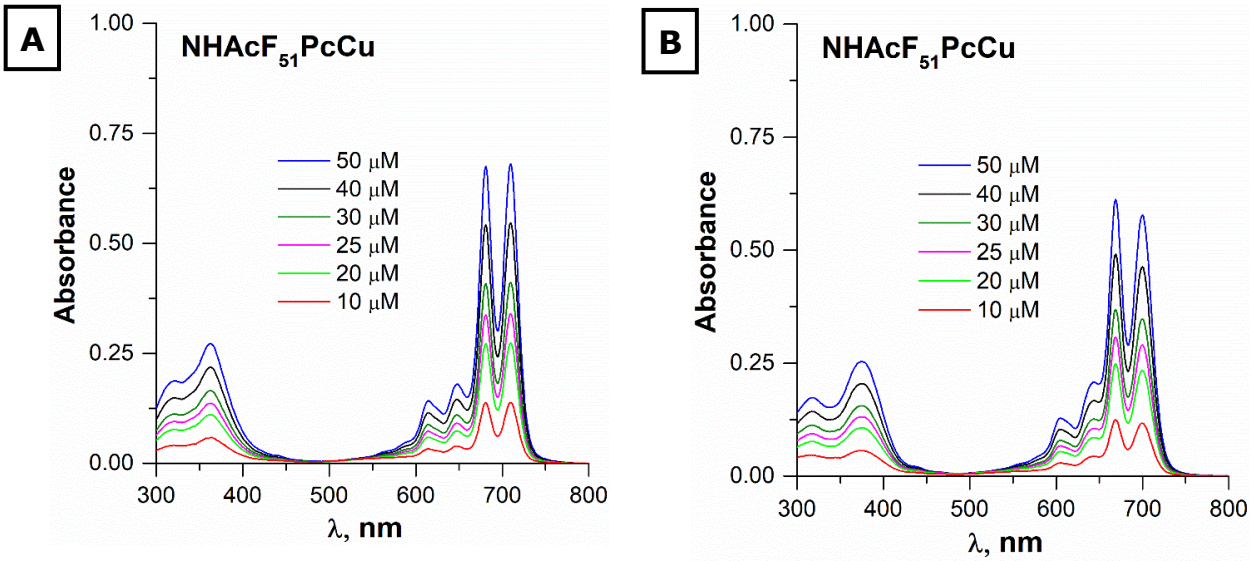
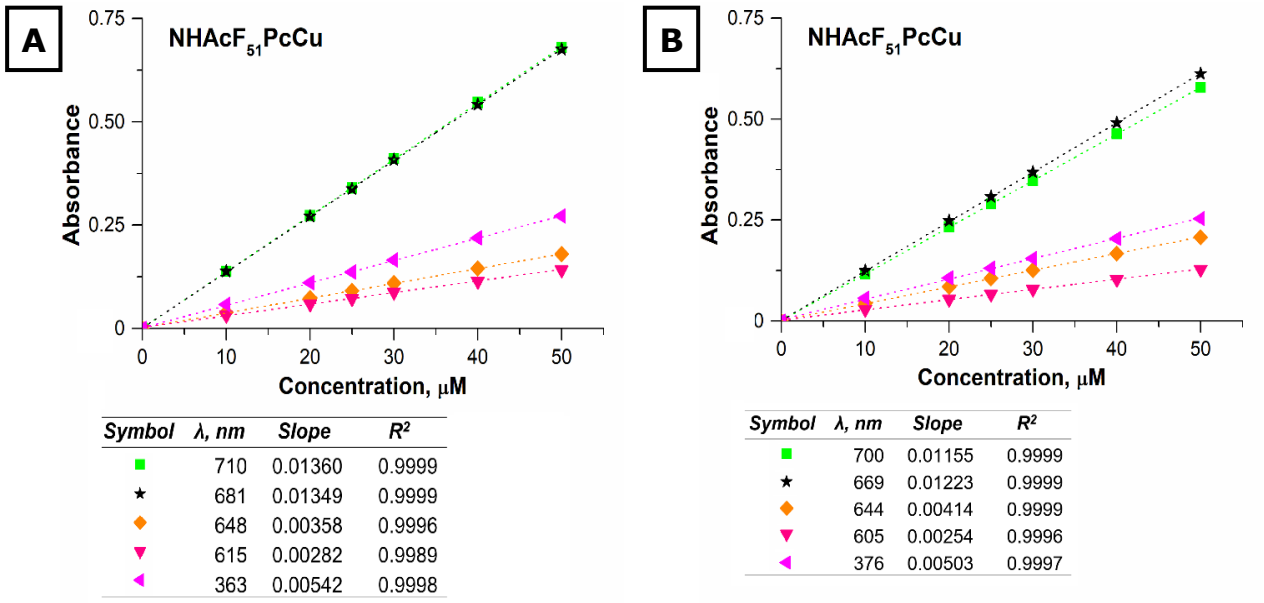


Figure D.16 Variation with the concentration for the UV-Vis spectra of $NHAcF_{51}PcCu$ **[5-5]** in (**A**) $CHCl_3$ and (**B**) ethanol.



Symbol	*λ, nm*	*Slope*	*R^2*
■	710	0.01360	0.9999
★	681	0.01349	0.9999
◆	648	0.00358	0.9996
▼	615	0.00282	0.9989
◀	363	0.00542	0.9998

Symbol	*λ, nm*	*Slope*	*R^2*
■	700	0.01155	0.9999
★	669	0.01223	0.9999
◆	644	0.00414	0.9999
▼	605	0.00254	0.9996
◀	376	0.00503	0.9997

Figure D.17 Beer-Lambert plots of $NHAcF_{51}PcCu$ **[5-5]** in (**A**) $CHCl_3$ and (**B**) ethanol, 1 mm light pathlength.

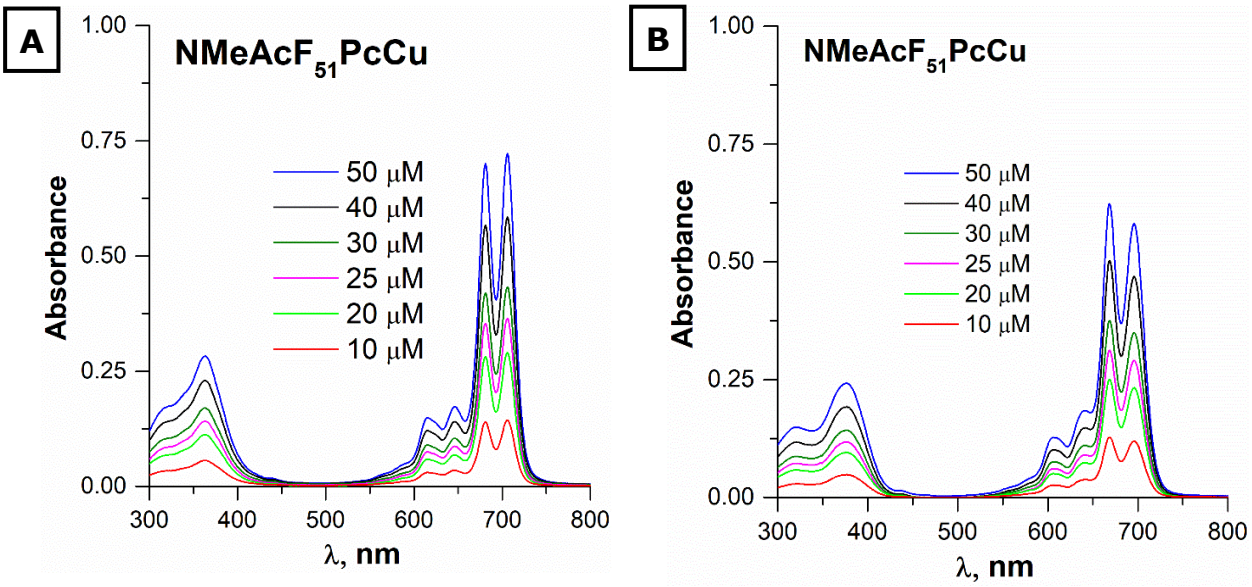
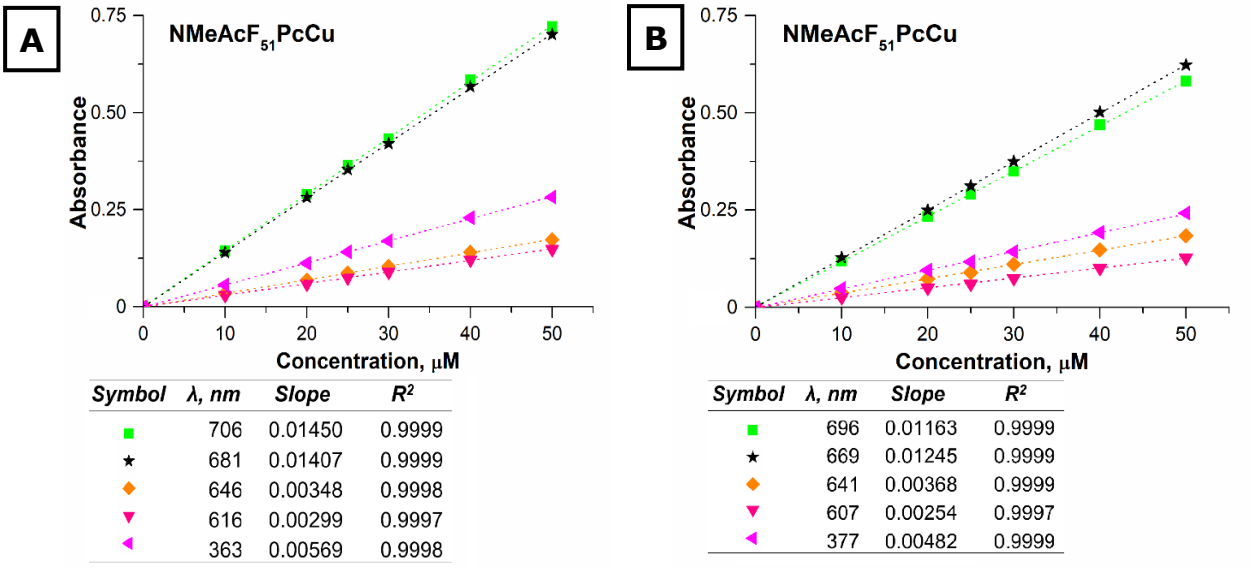


Figure D.18 Variation with the concentration for the UV-Vis spectra of $NMeAcF_{51}PcCu$ **[5-6]** in (**A**) $CHCl_3$ and (**B**) ethanol.



Symbol	λ, nm	Slope	R^2
■	706	0.01450	0.9999
★	681	0.01407	0.9999
◆	646	0.00348	0.9998
▼	616	0.00299	0.9997
◀	363	0.00569	0.9998

Symbol	λ, nm	Slope	R^2
■	696	0.01163	0.9999
★	669	0.01245	0.9999
◆	641	0.00368	0.9999
▼	607	0.00254	0.9997
◀	377	0.00482	0.9999

Figure D.19 Beer-Lambert plot of $NMeAcF_{51}PcCu$ **[5-6]** in (**A**) $CHCl_3$ and (**B**) ethanol, 1 mm light pathlength.

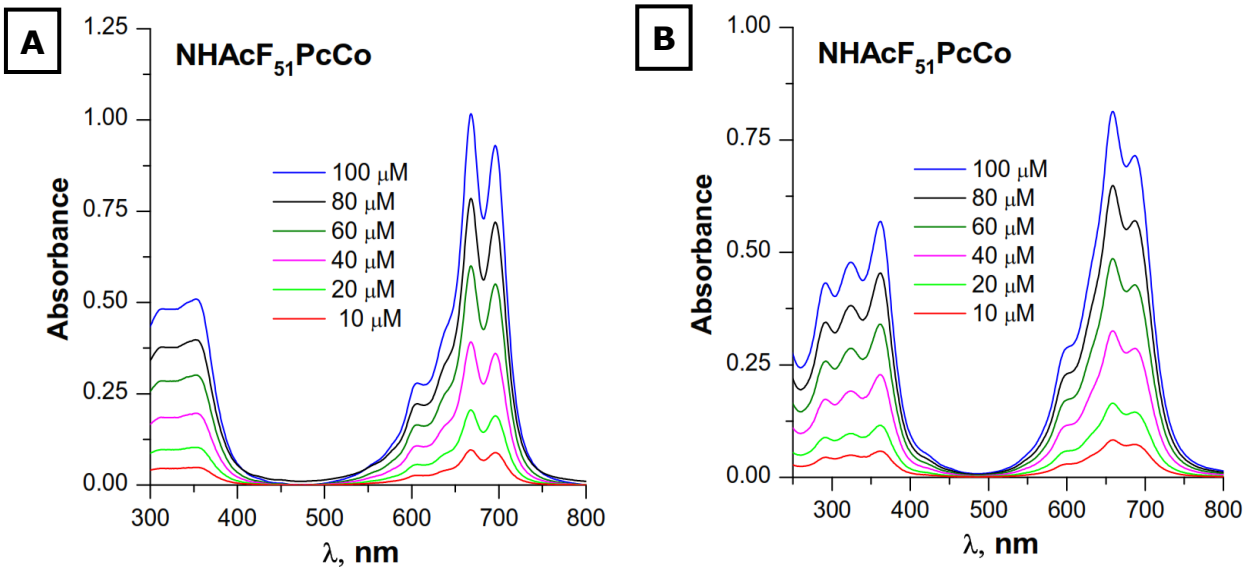
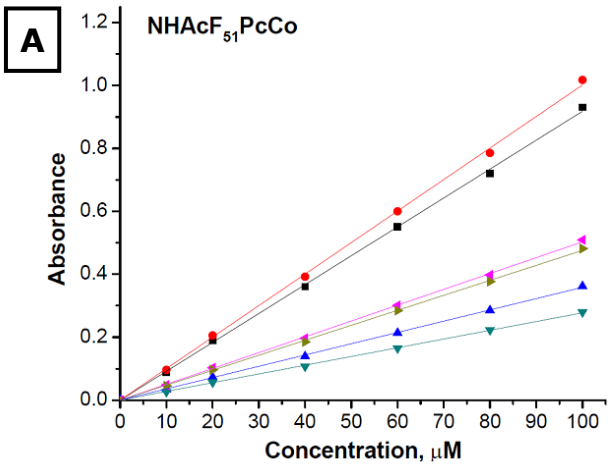
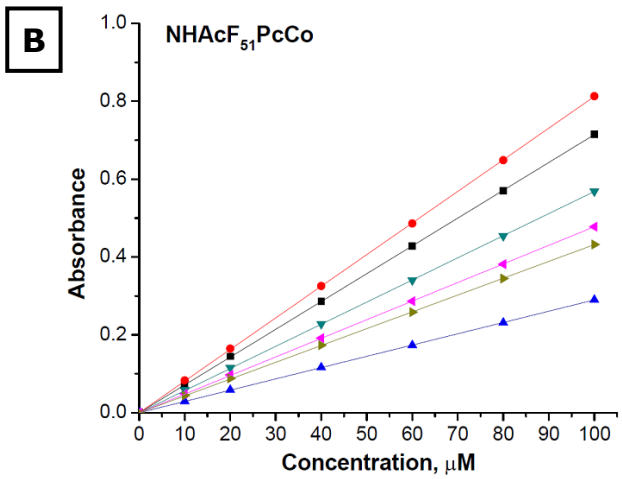


Figure D.20 Variation with the concentration for the UV-Vis spectra of $NHAcF_{51}PcCo$ **[5-7]** in (**A**) $CHCl_3$ and (**B**) THF.



Symbol	*λ, nm*	*Slope*	*R^2*
■	696	0.00918	0.9997
●	668	0.01002	0.9997
▲	631	0.00359	0.9999
▼	606	0.00278	0.9998
◀	353	0.00503	0.9998
▶	325	0.00476	0.9998



Symbol	*λ, nm*	*Slope*	*R^2*
■	683	0.00714	0.9999
●	659	0.00812	0.9999
▲	602	0.00290	0.9999
▼	362	0.00568	0.9999
◀	325	0.00478	0.9999
▶	292	0.00432	0.9998

Figure D.21 Beer-Lambert plot of $NHAcF_{51}PcCo$ **[5-7]** in (**A**) $CHCl_3$ and (**B**) THF, 1 mm light pathlength.

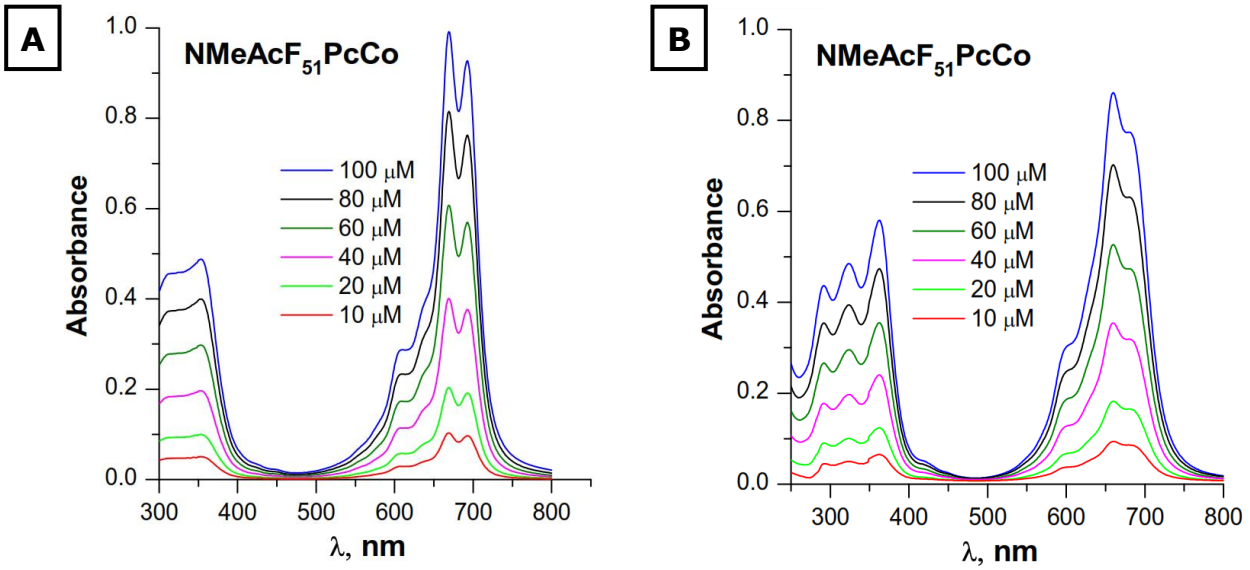
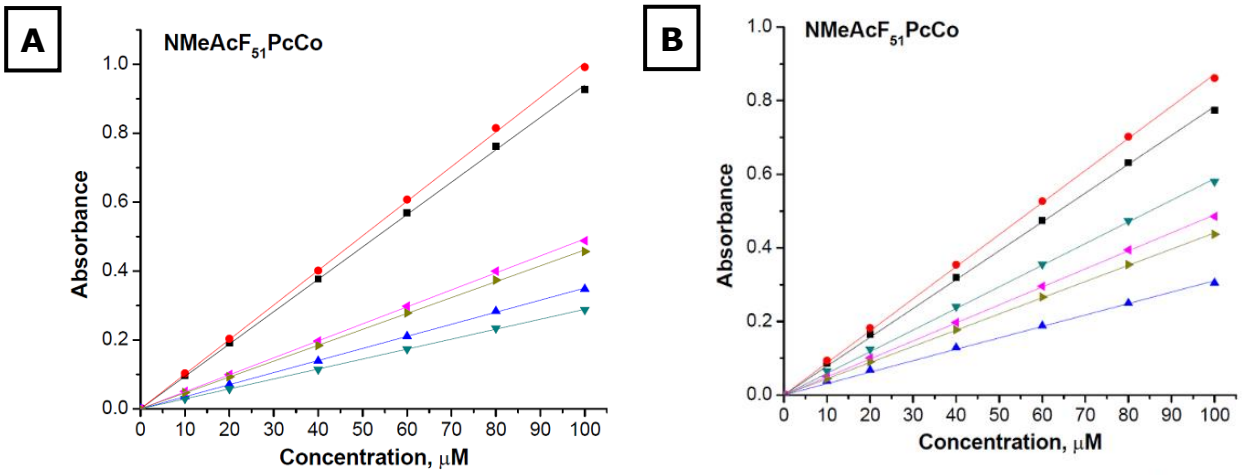


Figure D.22 Variation with the concentration for the UV-Vis spectra of $NMeAcF_{51}PcCo$ **[5-8]** in (**A**) $CHCl_3$ and (**B**) THF.



Symbol	*λ, nm*	*Slope*	*R^2*
■	693	0.00940	0.9998
●	669	0.01004	0.9998
▲	631	0.00350	0.9999
▼	609	0.00289	0.9999
◀	353	0.00493	0.9999
▶	317	0.00461	0.9999

Symbol	*λ, nm*	*Slope*	*R^2*
■	680	0.00784	0.9998
●	660	0.00872	0.9998
▲	602	0.00311	0.9993
▼	363	0.00588	0.9997
◀	323	0.00490	0.9999
▶	292	0.00440	0.9998

Figure D.23 Beer-Lambert plot of $NMeAcF_{51}PcCo$ **[5-8]** in (**A**) $CHCl_3$ and (**B**) THF, 1 mm light pathlength.

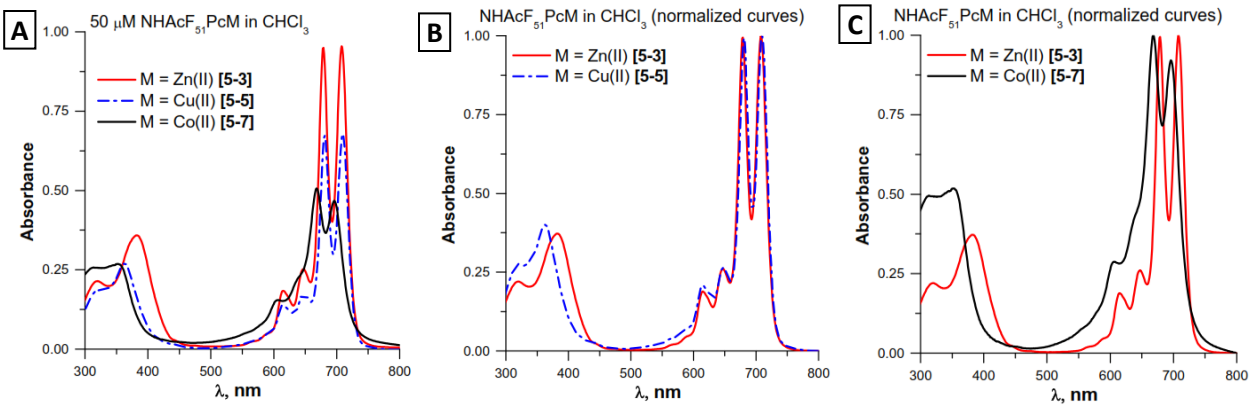


Figure D.24 UV-Vis spectra of NHAcF_{51}PcM series, M = Zn(II), Cu(II), or Co(II), in $CHCl_3$ at (**A**) 50 μM concentration (1 mm path length), (**B**) normalized curves for Zn(II) *vs.* Cu(II) complexes, and (**C**) Zn(II) *vs.* Co(II) complexes.

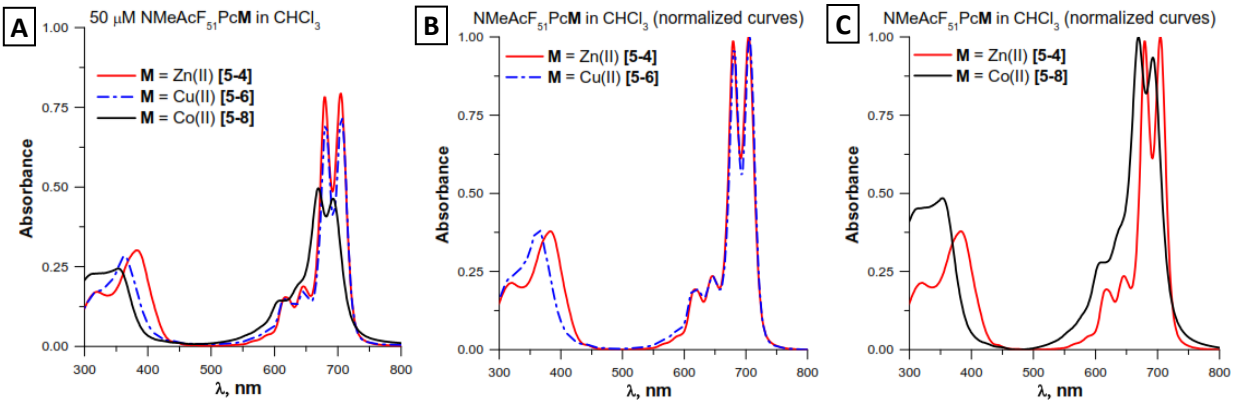


Figure D.25 UV-Vis spectra of NMeAcF_{51}PcM series, M = Zn(II), Cu(II) and Co(II), in $CHCl_3$ (**A**) at 50 μM concentration (1 mm path length). (**B**) normalized curves for Zn(II) *vs.* Cu(II) complexes, and (**C**) Zn(II) *vs.* Co(II) complexes.

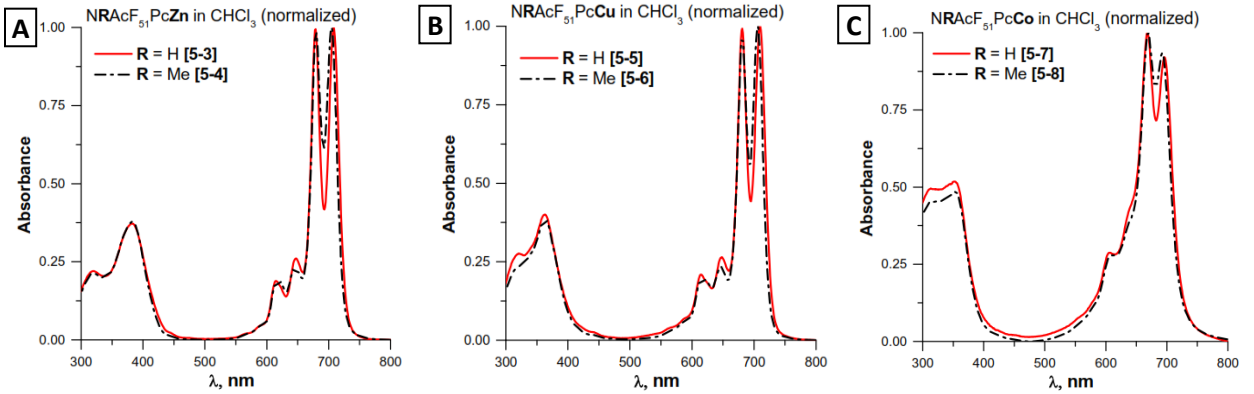


Figure D.26 UV-Vis spectra of NHAc- vs. NMeAc-F_{51}PcM, in $CHCl_3$, normalized curves for (**A**) M = Zn(II) complexes, (**B**) M = Cu(II) complexes, and (**C**) M = Co(II) complexes.

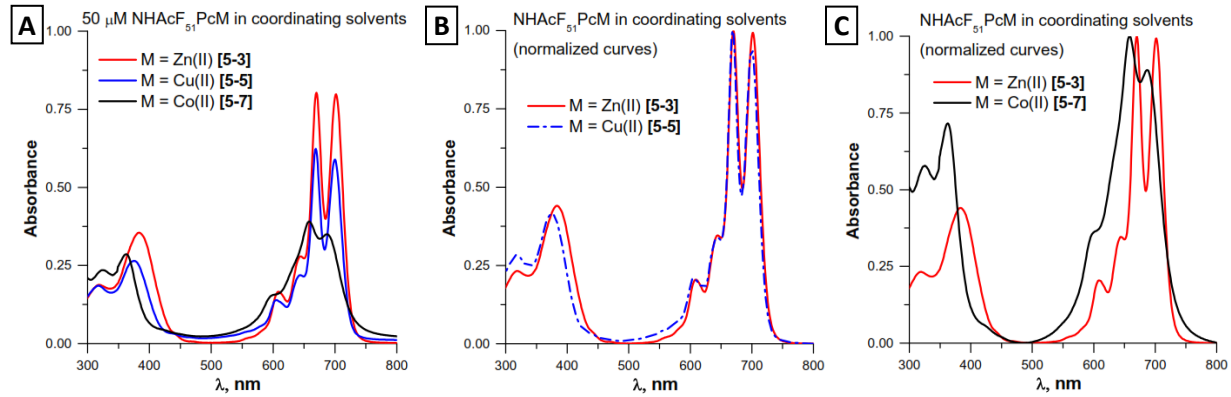


Figure D.27 UV-Vis spectra of NHAcF$_{51}$PcM series, M = Zn(II), Cu(II) or Co(II), in coordinating solvents (**[5-3]** and **[5-5]** MPcs in EtOH, **[5-7]** CoPc in THF) at (**A**) 50 μM concentration (1 mm path length), normalized curves for (**B**) Zn(II) *vs.* Cu(II) complexes, and (**C**) Zn(II) *vs.* Co(II) complexes.

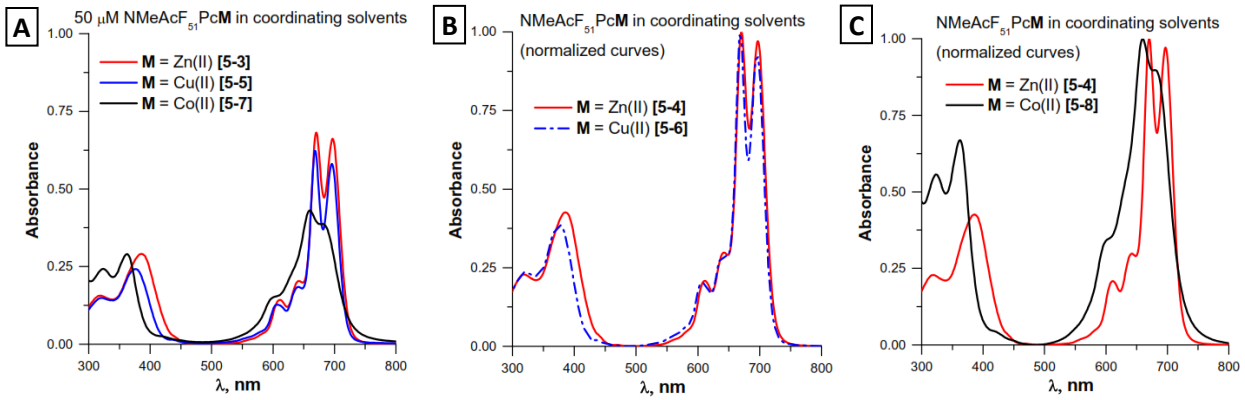


Figure D.28 UV-Vis spectra of NMeAcF$_{51}$PcM series, M = Zn(II), Cu(II) or Co(II), in coordinating solvents (**[5-4]** and **[5-6]** MPcs in EtOH, **[5-8]** CoPc in THF) (**A**) at 50 μM concentration (1 mm path length), normalized curves for (**B**) Zn(II) *vs.* Cu(II) complexes, and (**C**) Zn(II) *vs.* Co(II) complexes.

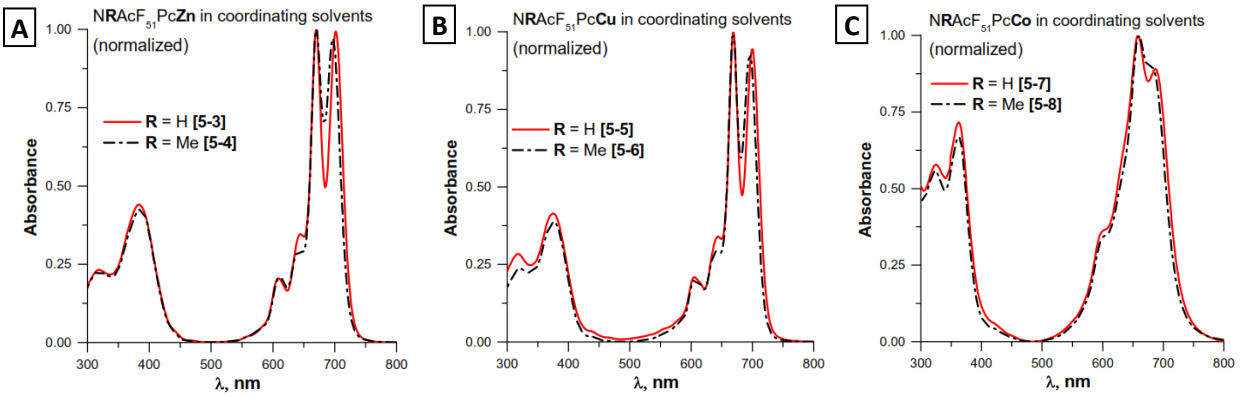


Figure D.29 UV-Vis spectra of NHAc-F$_{51}$PcM vs. NMeAc-F$_{51}$PcM, in coordinating solvents (ZnPcs and CuPcs in EtOH, CoPcs in THF), normalized curves for (**A**) M = Zn(II) complexes, (**B**) M = Cu(II) complexes, and (**C**) M = Co(II) complexes.

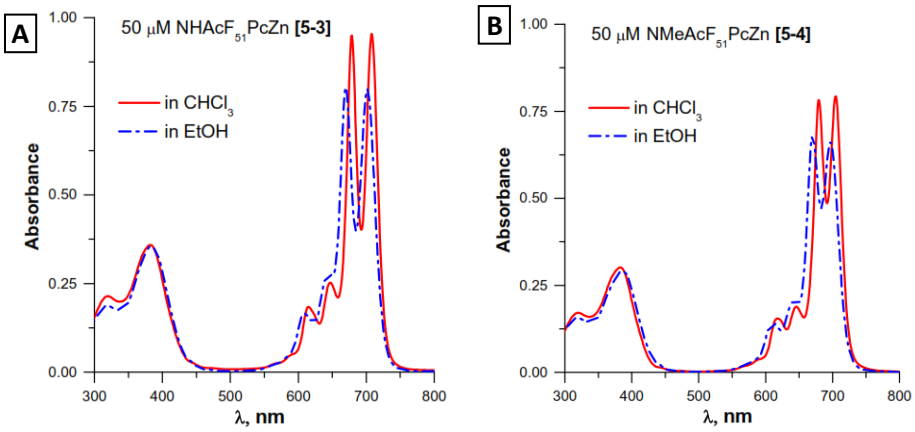


Figure D.30 UV-Vis spectra of $NRAcF_{51}PcZn$ in $CHCl_3$ vs. EtOH at 50 μM concentration (1 mm path length), (**A**) R = H for Pc **[5-3]**, (**B**) R = Me for Pc **[5-4]**.

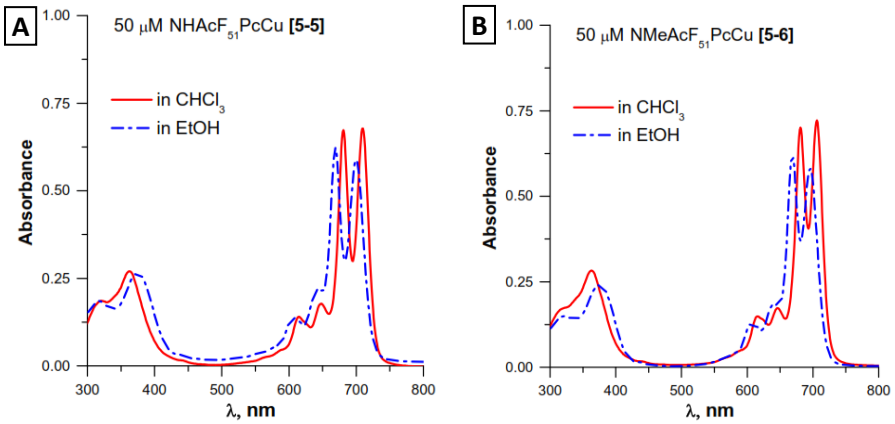


Figure D.31 UV-Vis spectra of $NRAcF_{51}PcCu$ in $CHCl_3$ vs. EtOH at 50 μM concentration (1 mm path length), (**A**) R = H for Pc **[5-5]**, (**B**) R = Me for Pc **[5-6]**.

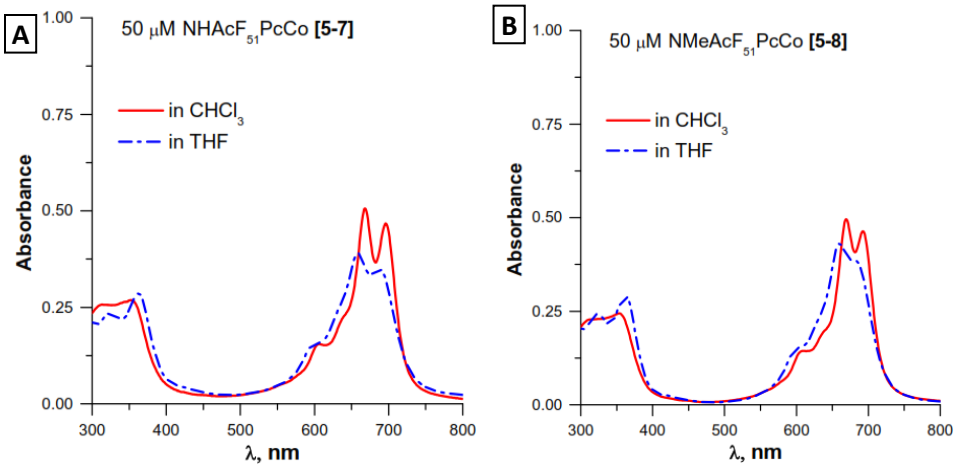


Figure D.32 UV-Vis spectra of $NRAcF_{51}PcCo$ in $CHCl_3$ vs. THF at 50 μM concentration (1 mm path length), (**A**) R = H for Pc **[5-7]**, (**B**) R = Me for Pc **[5-8]**.

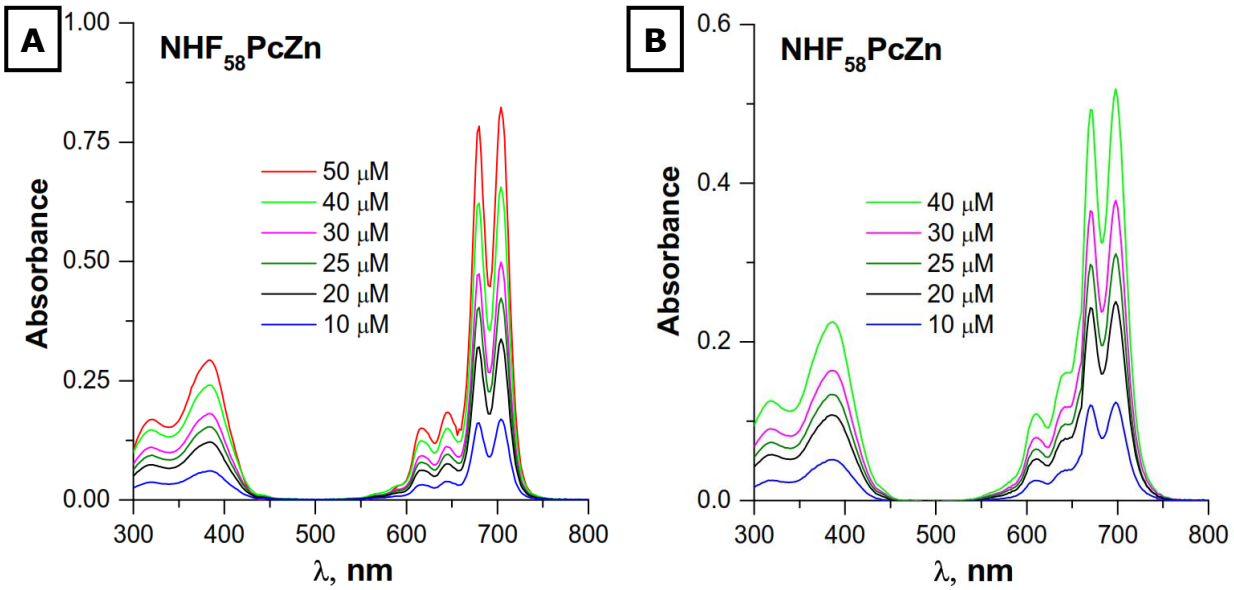
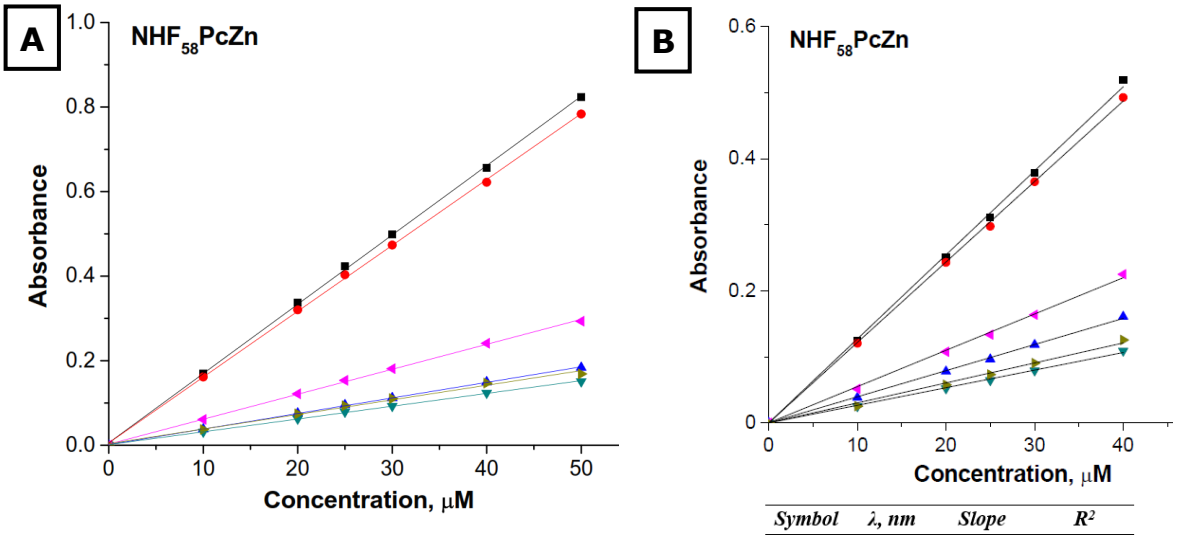


Figure D.33 Concentration dependent UV-Vis spectra of $NHF_{58}PcZn$ **[5-9]** in (**A**) $CHCl_3$ and (**B**) in ethanol.



Symbol	*λ, nm*	*Slope*	*R^2*
■	704	0.0164	0.9996
●	680	0.01558	0.9996
▲	644	0.00368	0.9995
▼	616	0.00303	0.9991
◀	384	0.00591	0.9991
▶	320	0.00346	0.9930

Symbol	*λ, nm*	*Slope*	*R^2*
■	698	0.01272	0.9996
●	670	0.01218	0.9998
▲	642	0.00396	0.9997
▼	610	0.00266	0.9993
◀	386	0.00549	0.9993
▶	318	0.00303	0.9979

Figure D.34 Beer-Lambert plots of $NHF_{58}PcZn$ **[5-9]** in (**A**) $CHCl_3$ and (**B**) ethanol, 1 mm light pathlength.

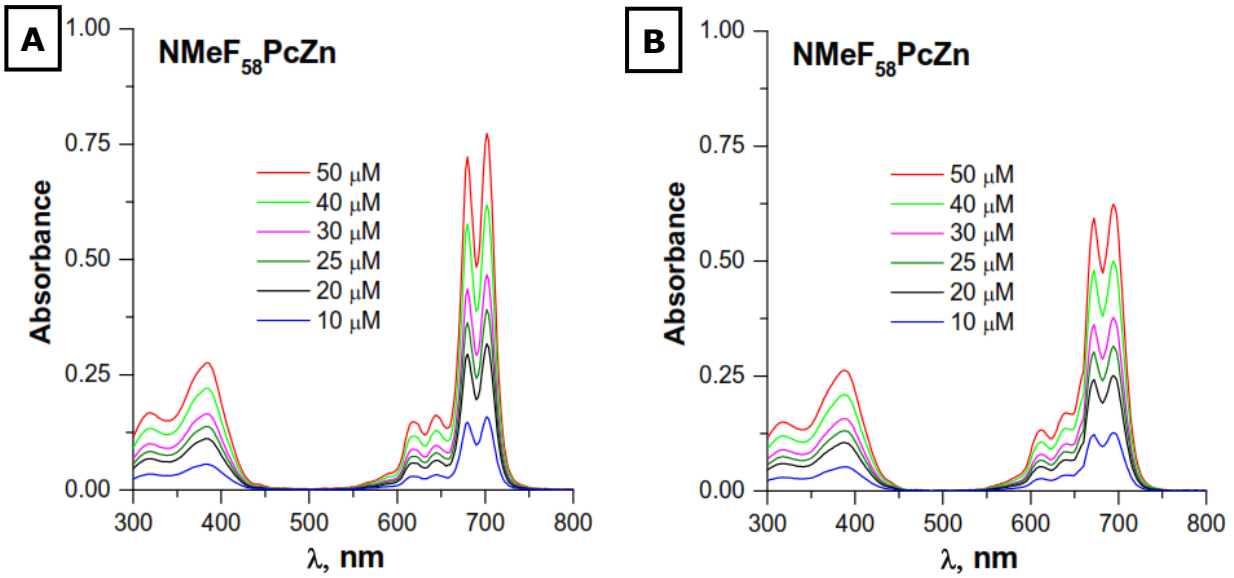
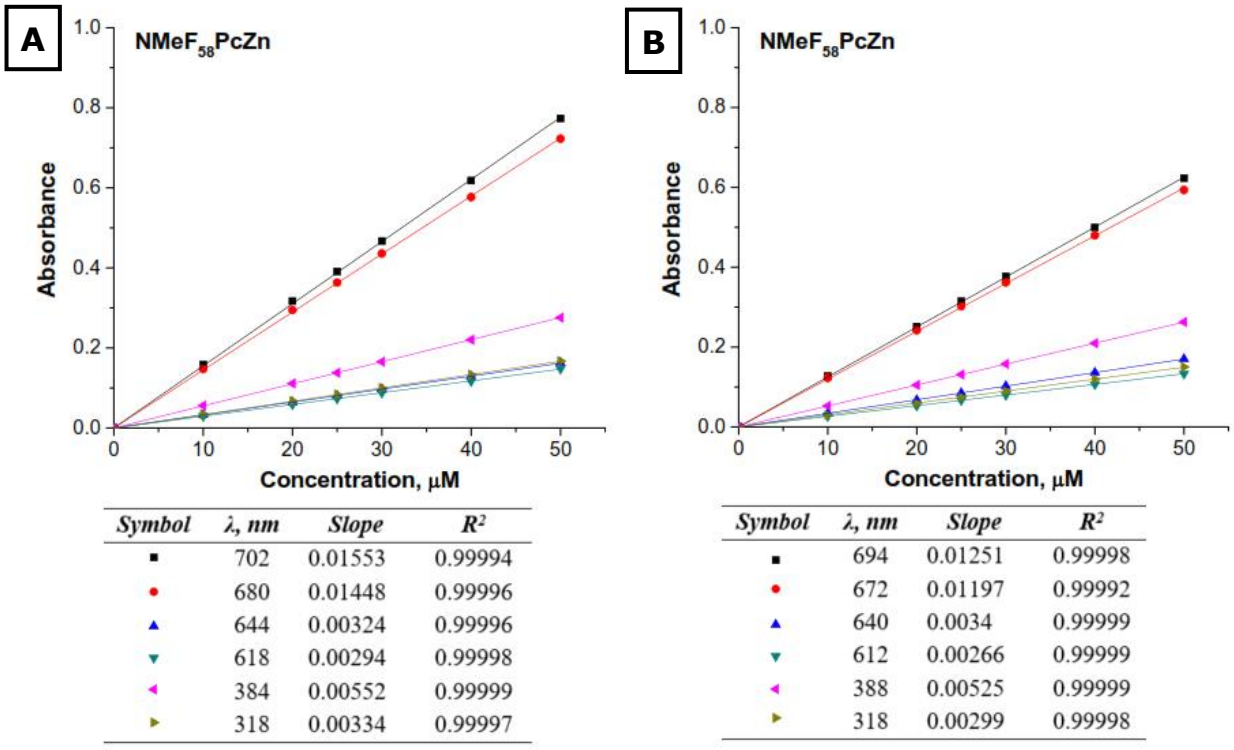


Figure D.35 Concentration dependent UV-Vis spectra of $NMeF_{58}PcZn$ **[5-10]** in (**A**) $CHCl_3$ and (**B**) ethanol.



Symbol	*λ, nm*	*Slope*	*R^2*
■	702	0.01553	0.99994
●	680	0.01448	0.99996
▲	644	0.00324	0.99996
▼	618	0.00294	0.99998
◀	384	0.00552	0.99999
▶	318	0.00334	0.99997

Symbol	*λ, nm*	*Slope*	*R^2*
■	694	0.01251	0.99998
●	672	0.01197	0.99992
▲	640	0.0034	0.99999
▼	612	0.00266	0.99999
◀	388	0.00525	0.99999
▶	318	0.00299	0.99998

Figure D.36 Beer-Lambert plots of $NMeF_{58}PcZn$ **[5-10]** in (**A**) $CHCl_3$ and (**B**) in ethanol, 1 mm light pathlength.

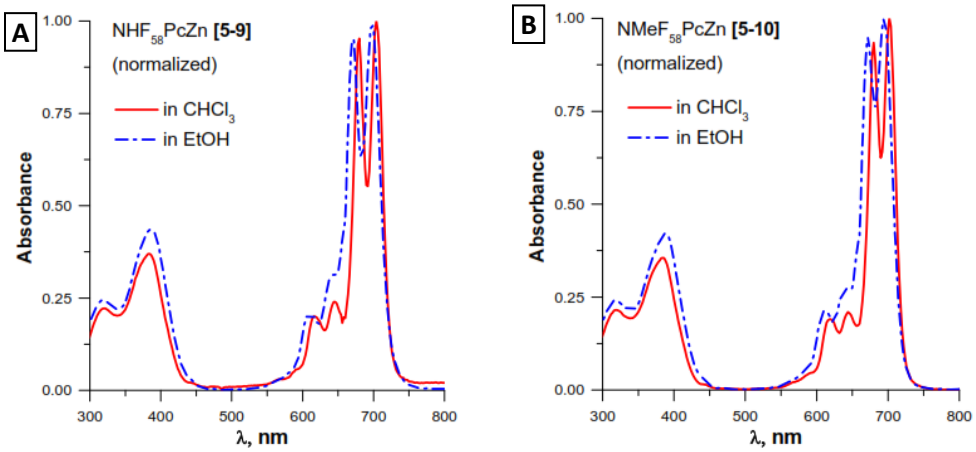


Figure D.37 Normalized UV-Vis spectra of $NRF_{58}PcZn$ in $CHCl_3$ vs. EtOH, (**A**) R = H for Pc **[5-9]**, (**B**) R = Me for Pc **[5-10]**.

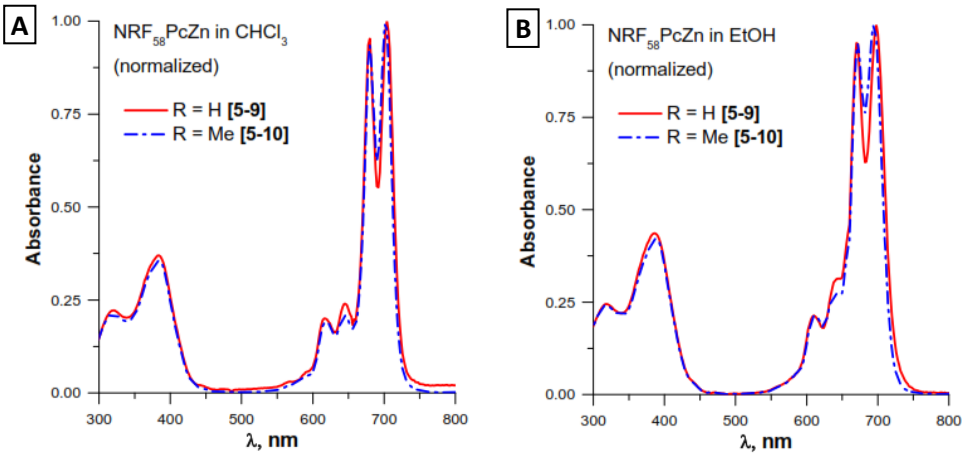


Figure D.38 Normalized UV-Vis spectra of NH- vs. NMe-$F_{58}PcZn$ in (**A**) $CHCl_3$ and (**B**) EtOH.

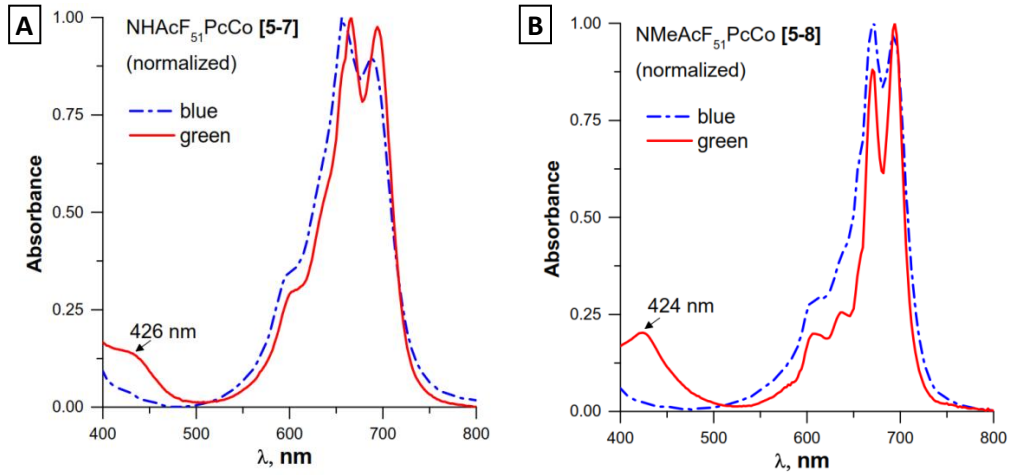


Figure D.39 Normalized UV-Vis spectra of green vs. blue fractions of (**A**) $NHAcF_{51}PcCo$ and (**B**) $NMeAcF_{51}PcCo$, in ethyl acetate.

Appendix E: CV and DPV voltammograms

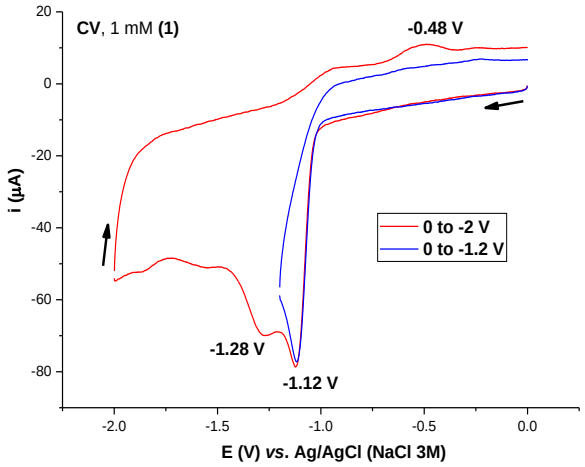


Figure E.1 Cathodic CV of **[3-1]**.

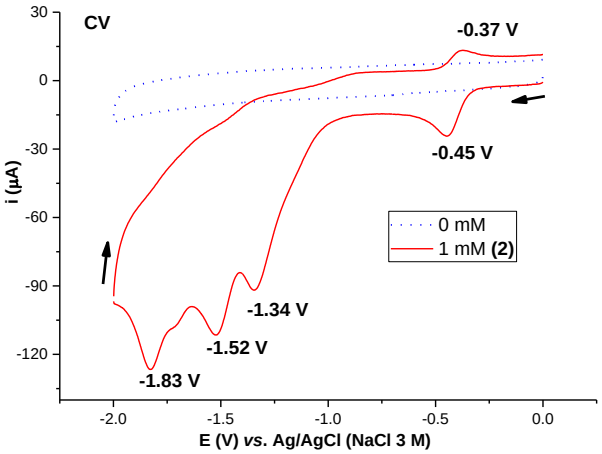


Figure E.2 Cathodic CV of **[3-2]**.

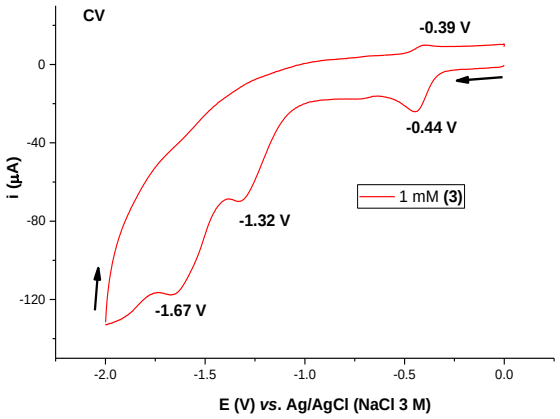


Figure E.3 Cathodic CV of **[3-3]**.

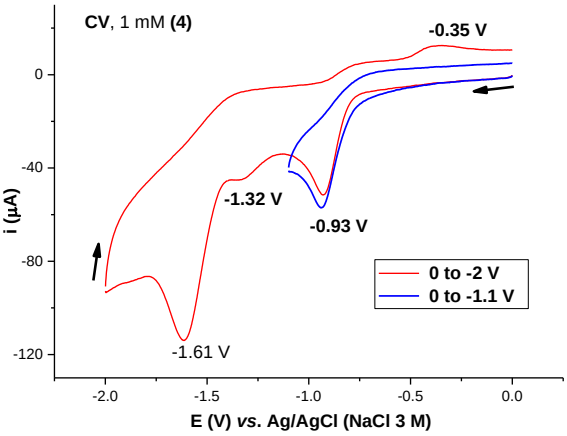


Figure E.4 Cathodic CV of **[3-4]**.

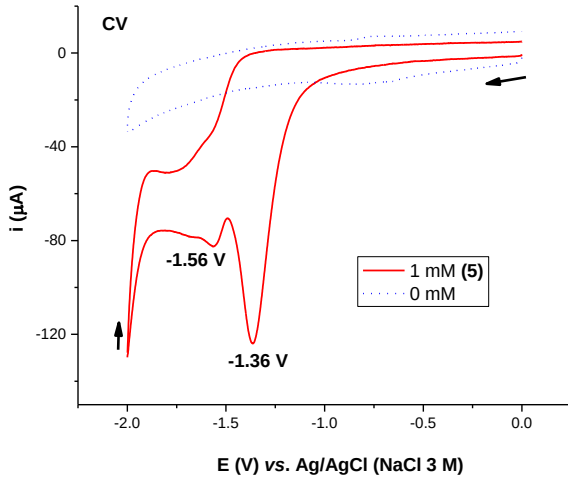


Figure E.5 Cathodic CV of **[3-5]**.

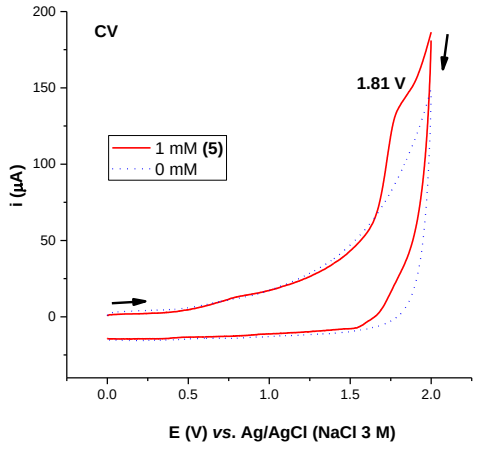


Figure E.6 Anodic CV of **[3-5]**.

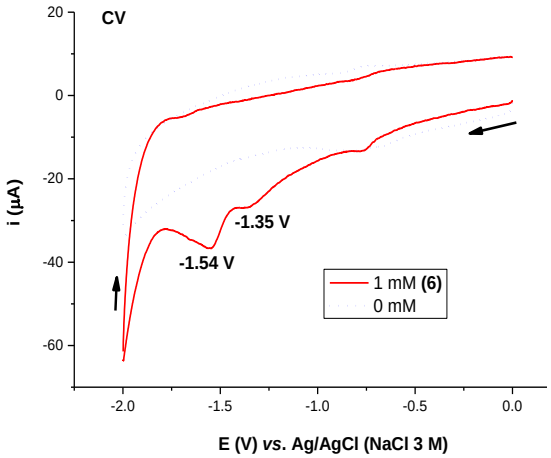


Figure E.7 Cathodic CV of **[3-6]**.

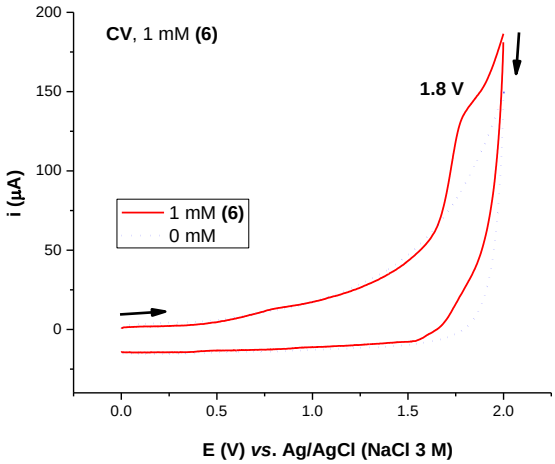


Figure E.8 Anodic CV of **[3-6]**.

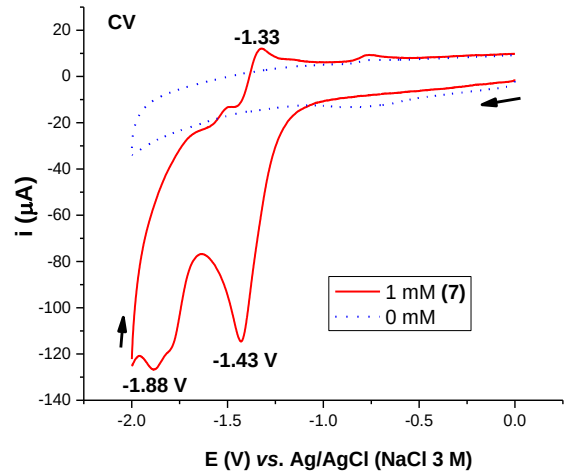


Figure E.9 Cathodic CV of **[3-7]**.

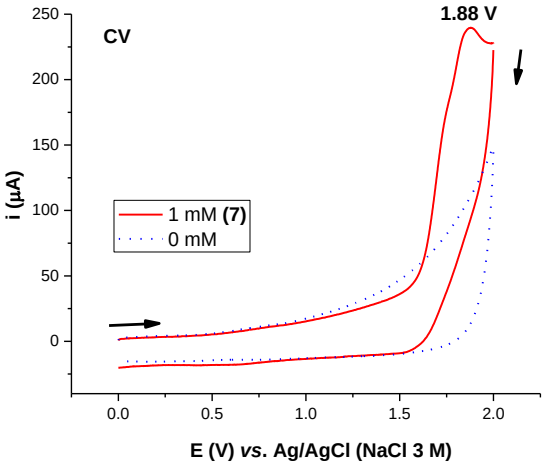


Figure E.10 Anodic CV of **[3-7]**.

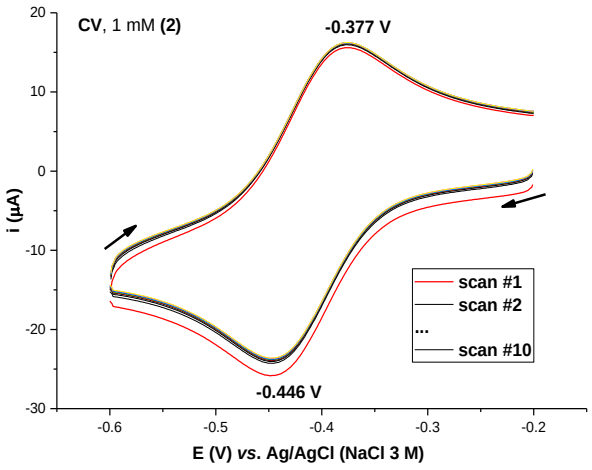


Figure E.11 CV of **[3-2]**, successive scans.

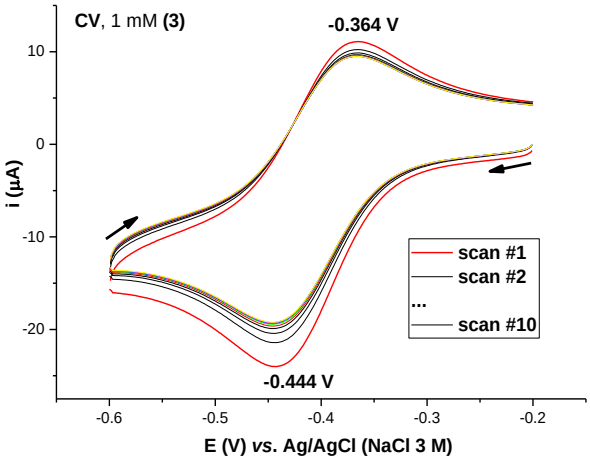


Figure E.12 CV of **[3-3]**, successive scans.

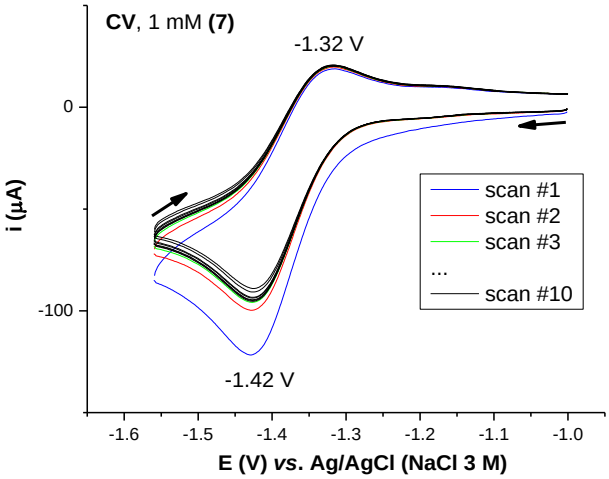


Figure E.13 CV of **[3-7]**, successive scans.

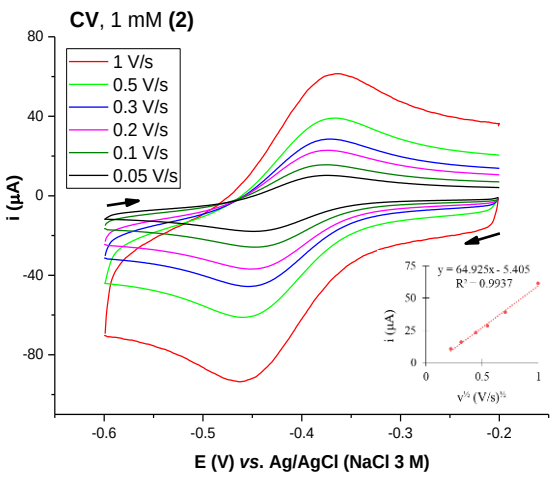


Figure E.14 CV of **[3-2]**, various scan rates.

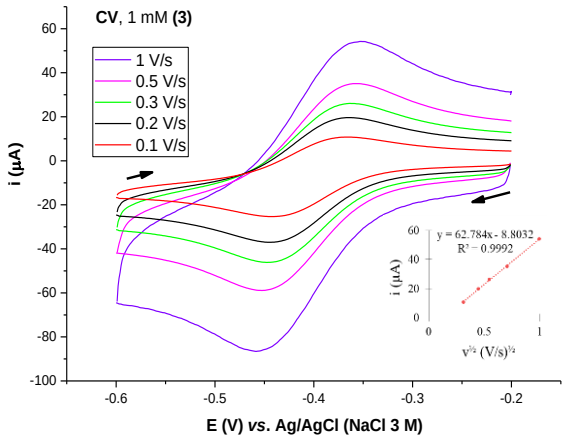


Figure E.15 CV of **[3-3]**, various scan rates.

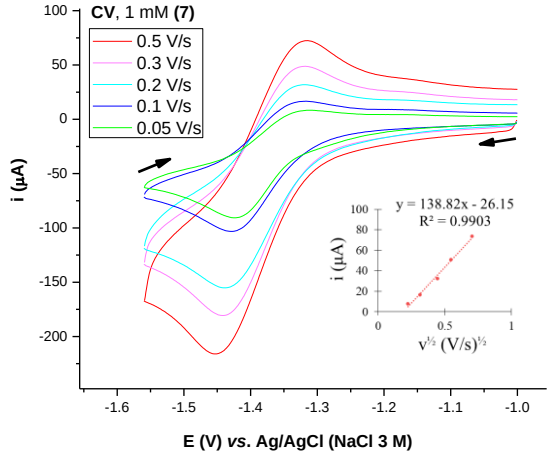


Figure E.16 CV of **[3-7]**, various scan rates.

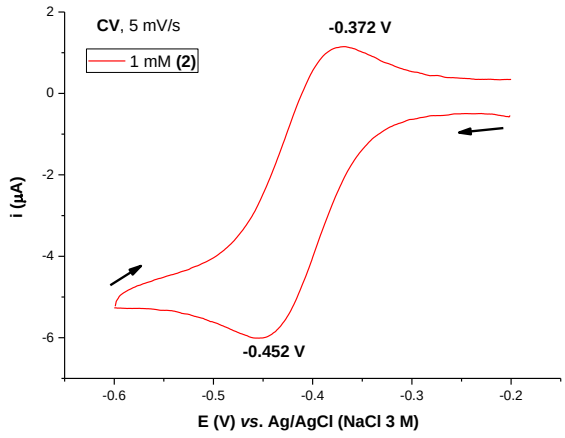


Figure E.17 CV for **[3-2]**, 5 mV/s scan rate.

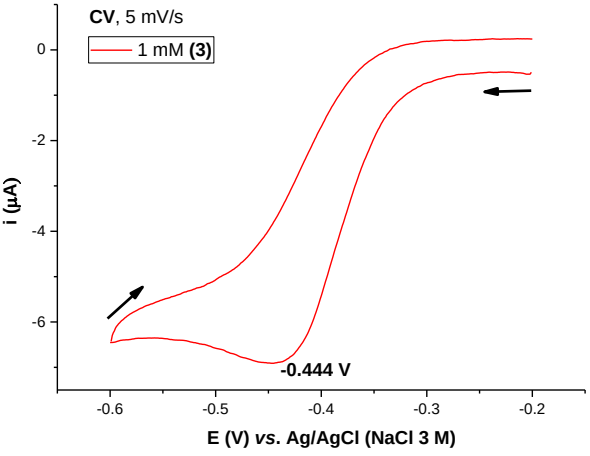


Figure E.18 CV for **[3-3]**, 5 mV/s scan rate.

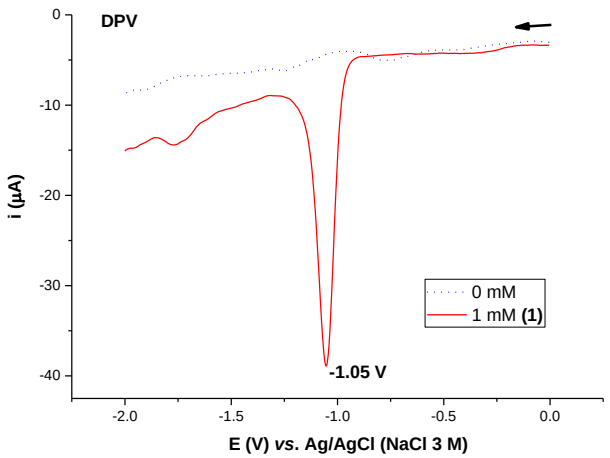


Figure E.19 Cathodic DPV of **[3-1]**.

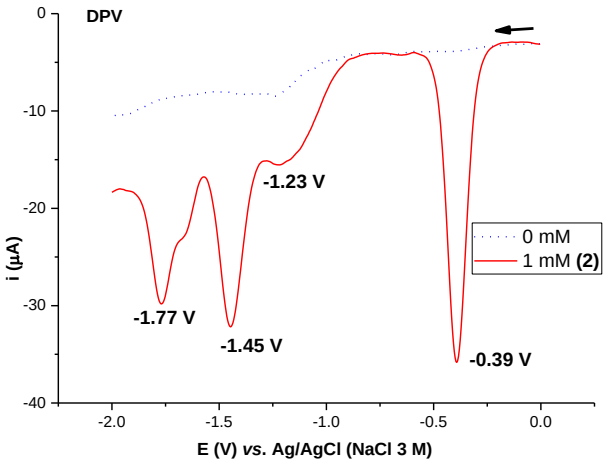


Figure E.20 Cathodic DPV of **[3-2]**.

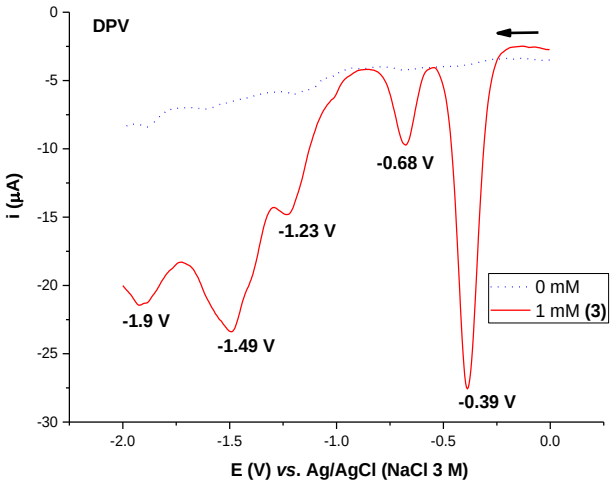


Figure E.21 Cathodic DPV of **[3-3]**.

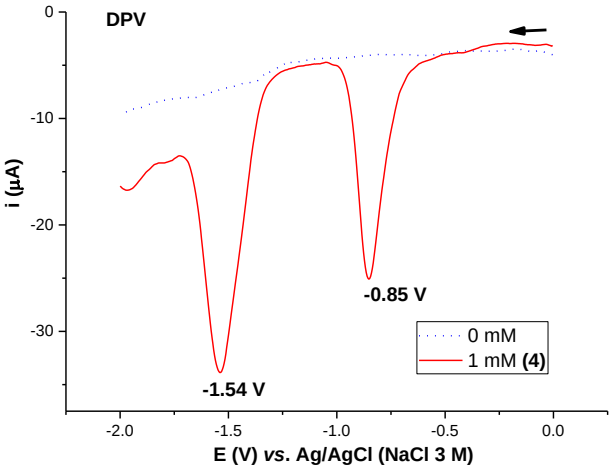


Figure E.22 Cathodic DPV of **[3-4]**.

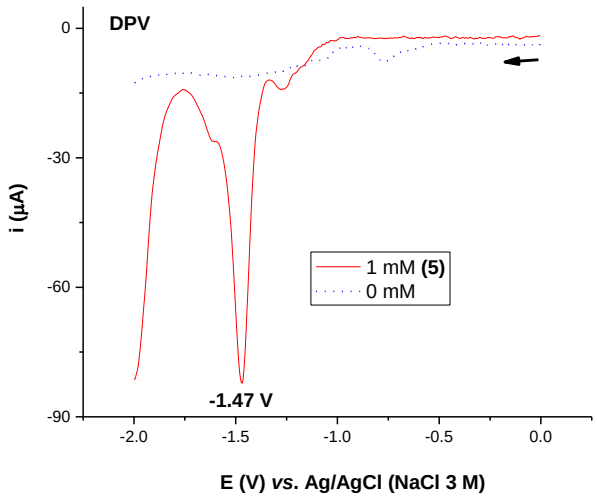


Figure E.23 Cathodic DPV of **[3-5]**.

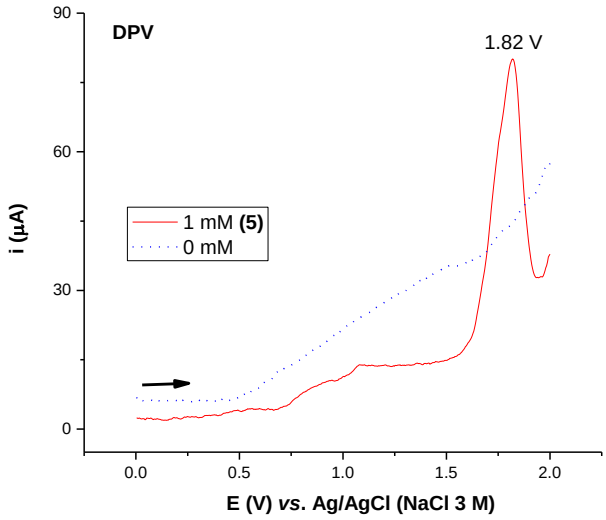


Figure E.24 Anodic DPV of **[3-5]**.

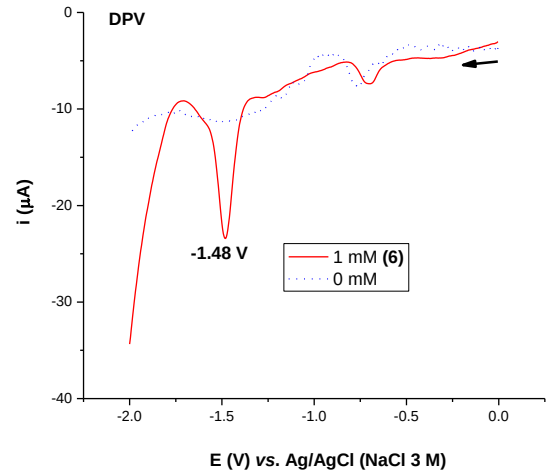


Figure E.25 Cathodic DPV of **[3-6]**.

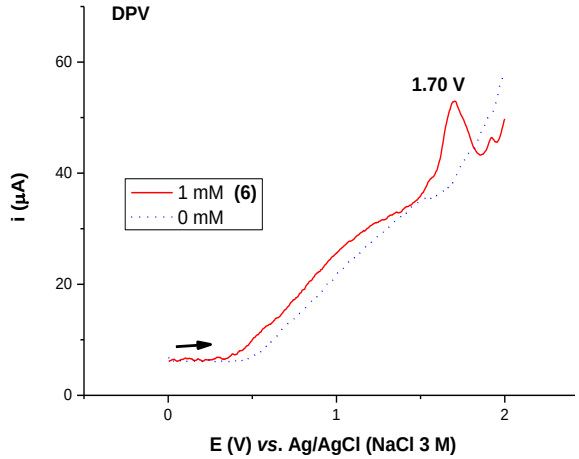


Figure E.26 Anodic DPV of **[3-6]**.

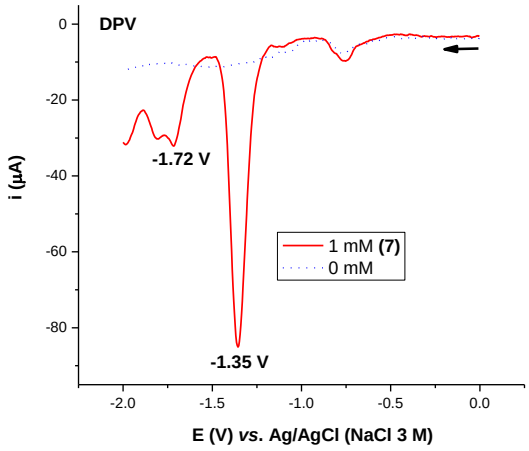


Figure E.27 Cathodic DPV of **[3-7]**.

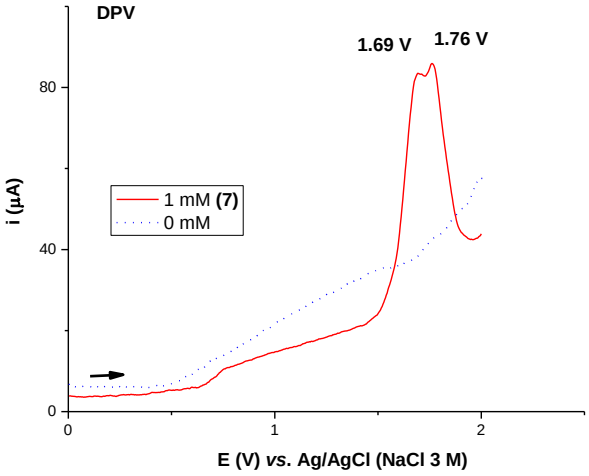


Figure E.28 Anodic DPV of **[3-7]**.

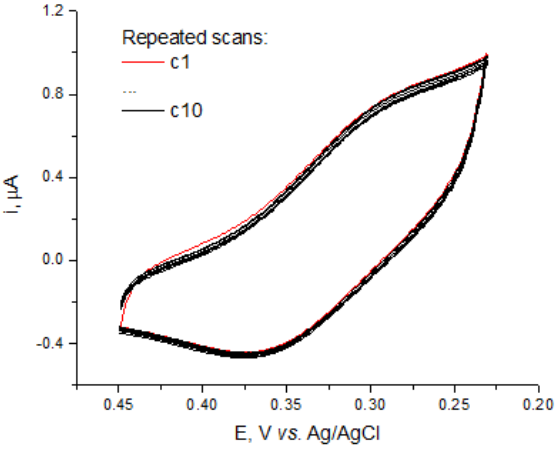


Figure E.29 Repeated CV scans for $F_{64}PcGaCl$. Reproduced with permission from Pelmus *et al.*, 2016.

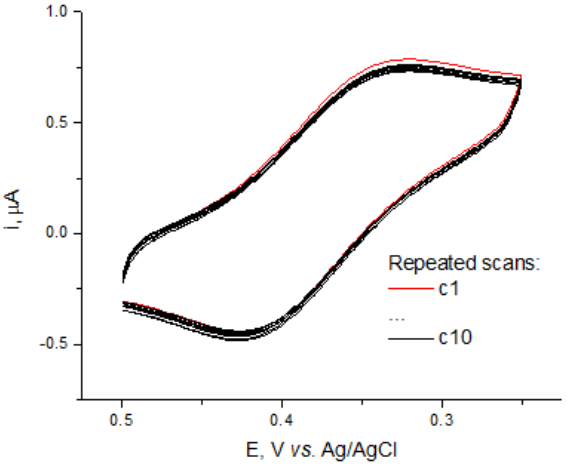


Figure E.30 Repeated CV scans for $F_{64}PcInCl$. Reproduced with permission from Pelmus *et al.*, 2016.

Appendix F: Crystal structure of [3-8]

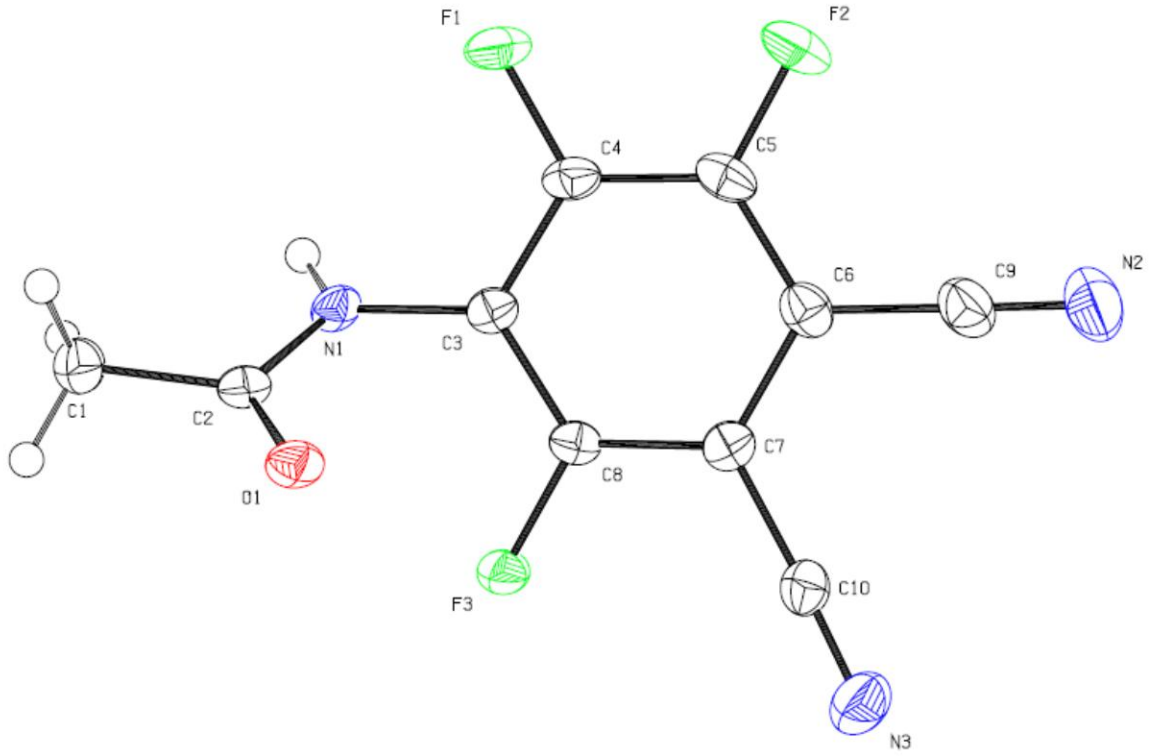


Figure F.1 ORTEP representation for the X-ray crystal structure of **[3-8]**, at 50% probability.

Table F.1 Crystal data and structure refinement for **[3-8]**.

Empirical formula	C10 H4 F3 N3 O
Formula weight	239.16
Temperature	130(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.2417(16) Å alpha = 90 deg. b = 9.5695(13) Å beta = 94.663(2) deg. c = 8.4329(12) Å gamma = 90 deg.
Volume	984.6(2) $Å^3$
Z, Calculated density	4, 1.613 g/cm^3
Absorption coefficient	0.148 mm^{-1}

F(000)	480
Crystal size	0.350 x 0.200 x 0.040 mm
Theta range for data collection	3.339 to 30.516 deg.
Limiting indices	-17<=h<=17, 0<=k<=13, 0<=l<=11
Reflections collected / unique	2824 / 2824 [R(int) = 0.0358
Completeness to theta = 25.000	99.0 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.91676
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2824 / 0 / 160
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.0877
R indices (all data)	R1 = 0.0539, wR2 = 0.0948
Extinction coefficient	n/a
Largest diff. peak and hole	0.301 and -0.239 e.$Å^{-3}$

Table F.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[3-8]**. U(eq) is defined as one-third of the trace of the orthogonalized Uij tensor.

	x	**y**	**z**	**U(eq)**
C(1)	-1386(1)	10873(2)	3146(2)	25(1)
C(2)	-258(1)	10302(2)	2981(2)	19(1)
O(1)	-16(1)	9072(1)	3206(1)	23(1)
N(1)	507(1)	11263(1)	2621(2)	19(1)
C(3)	1610(1)	10888(1)	2530(2)	18(1)
C(4)	2434(1)	11553(2)	3463(2)	22(1)
F(1)	2173(1)	12555(1)	4472(1)	34(1)
C(5)	3530(1)	11200(2)	3396(2)	25(1)
F(2)	4286(1)	11847(1)	4358(1)	38(1)
C(6)	3833(1)	10166(2)	2379(2)	23(1)
C(7)	3012(1)	9473(2)	1411(2)	20(1)

C(8)	1930(1)	9857(2)	1497(2)	18(1)
F(3)	1160(1)	9233(1)	527(1)	24(1)
C(9)	4972(1)	9792(2)	2342(2)	30(1)
N(2)	5877(1)	9507(2)	2321(2)	44(1)
C(10)	3268(1)	8355(2)	369(2)	24(1)
N(3)	3432(1)	7452(2)	-468(2)	38(1)

Table F.3 Bond lengths [Å] and angles [deg] for **[3-8]**.

C(1)-C(2)	1.502(2)	C(4)-C(5)	1.389(2)
C(1)-H(1A)	0.9800	C(5)-F(2)	1.3323(17)
C(1)-H(1B)	0.9800	C(5)-C(6)	1.380(2)
C(1)-H(1C)	0.9800	C(6)-C(7)	1.409(2)
C(2)-O(1)	1.2252(17)	C(6)-C(9)	1.442(2)
C(2)-N(1)	1.3638(19)	C(7)-C(8)	1.3818(19)
N(1)-C(3)	1.4047(18)	C(7)-C(10)	1.436(2)
N(1)-H(1D)	0.810(19)	C(8)-F(3)	1.3377(16)
C(3)-C(4)	1.384(2)	C(9)-N(2)	1.143(2)
C(3)-C(8)	1.394(2)	C(10)-N(3)	1.143(2)
C(4)-F(1)	1.3379(17)		
C(2)-C(1)-H(1A)	109.5	F(1)-C(4)-C(5)	118.83(13)
C(2)-C(1)-H(1B)	109.5	C(3)-C(4)-C(5)	121.83(14)
H(1A)-C(1)-H(1B)	109.5	F(2)-C(5)-C(6)	120.17(14)
C(2)-C(1)-H(1C)	109.5	F(2)-C(5)-C(4)	119.17(14)
H(1A)-C(1)-H(1C)	109.5	C(6)-C(5)-C(4)	120.63(13)
H(1B)-C(1)-H(1C)	109.5	C(5)-C(6)-C(7)	118.85(14)
O(1)-C(2)-N(1)	121.39(13)	C(5)-C(6)-C(9)	120.05(14)
O(1)-C(2)-C(1)	123.18(14)	C(7)-C(6)-C(9)	121.09(15)
N(1)-C(2)-C(1)	115.38(13)	C(8)-C(7)-C(6)	119.09(14)
C(2)-N(1)-C(3)	121.33(12)	C(8)-C(7)-C(10)	119.24(13)
C(2)-N(1)-H(1D)	121.3(13)	C(6)-C(7)-C(10)	121.65(14)
C(3)-N(1)-H(1D)	117.3(13)	F(3)-C(8)-C(7)	118.66(13)
C(4)-C(3)-C(8)	116.83(13)	F(3)-C(8)-C(3)	118.56(12)
C(4)-C(3)-N(1)	120.77(13)	C(7)-C(8)-C(3)	122.76(13)
C(8)-C(3)-N(1)	122.39(13)	N(2)-C(9)-C(6)	179.4(2)
F(1)-C(4)-C(3)	119.34(13)	N(3)-C(10)-C(7)	177.47(17)

Symmetry transformations used to generate equivalent atoms:

Table F.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[3-8]**. 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)	22(1)	26(1)	26(1)	-1(1)	0(1)	3(1)
C(2)	24(1)	17(1)	16(1)	-2(1)	0(1)	0(1)
O(1)	29(1)	13(1)	28(1)	-1(1)	1(1)	-1(1)
N(1)	22(1)	12(1)	24(1)	0(1)	3(1)	3(1)
C(3)	22(1)	13(1)	19(1)	2(1)	3(1)	-1(1)
C(4)	30(1)	16(1)	23(1)	-3(1)	4(1)	-4(1)
F(1)	39(1)	27(1)	36(1)	-17(1)	6(1)	-6(1)
C(5)	26(1)	22(1)	26(1)	1(1)	-1(1)	-10(1)
F(2)	32(1)	38(1)	44(1)	-10(1)	-6(1)	-15(1)
C(6)	22(1)	20(1)	28(1)	4(1)	1(1)	-3(1)
C(7)	24(1)	17(1)	20(1)	2(1)	2(1)	1(1)
C(8)	21(1)	14(1)	17(1)	1(1)	-2(1)	-1(1)
F(3)	22(1)	26(1)	22(1)	-7(1)	-4(1)	2(1)
C(9)	24(1)	27(1)	39(1)	0(1)	0(1)	-5(1)
N(2)	26(1)	44(1)	63(1)	-4(1)	3(1)	-3(1)
C(10)	20(1)	24(1)	28(1)	0(1)	0(1)	4(1)
N(3)	34(1)	38(1)	40(1)	-10(1)	0(1)	12(1)

Table F.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **[3-8]**.

	x	y	z	U(eq)
H(1A)	-1934	10177	2766	38
H(1B)	-1490	11728	2513	38
H(1C)	-1469	11085	4267	38
H(1D)	351(14)	1208(2)	250(2)	24(5)

Table F.6 Torsion angles [deg] for **[3-8]**.

O(1)-C(2)-N(1)-C(3)	-1.6(2)
C(1)-C(2)-N(1)-C(3)	175.98(13)
C(2)-N(1)-C(3)-C(4)	-122.95(15)
C(2)-N(1)-C(3)-C(8)	57.9(2)
C(8)-C(3)-C(4)-F(1)	179.81(13)
N(1)-C(3)-C(4)-F(1)	0.6(2)
C(8)-C(3)-C(4)-C(5)	-0.9(2)
N(1)-C(3)-C(4)-C(5)	179.93(14)
F(1)-C(4)-C(5)-F(2)	1.4(2)
C(3)-C(4)-C(5)-F(2)	-177.98(14)
F(1)-C(4)-C(5)-C(6)	179.54(14)
C(3)-C(4)-C(5)-C(6)	0.2(2)
F(2)-C(5)-C(6)-C(7)	178.13(14)
C(4)-C(5)-C(6)-C(7)	0.0(2)
F(2)-C(5)-C(6)-C(9)	-0.7(2)
C(4)-C(5)-C(6)-C(9)	-178.86(15)
C(5)-C(6)-C(7)-C(8)	0.5(2)
C(9)-C(6)-C(7)-C(8)	179.37(14)
C(5)-C(6)-C(7)-C(10)	-177.78(14)
C(9)-C(6)-C(7)-C(10)	1.0(2)
C(6)-C(7)-C(8)-F(3)	177.31(13)
C(10)-C(7)-C(8)-F(3)	-4.3(2)
C(6)-C(7)-C(8)-C(3)	-1.3(2)
C(10)-C(7)-C(8)-C(3)	177.09(14)
C(4)-C(3)-C(8)-F(3)	-177.17(12)
N(1)-C(3)-C(8)-F(3)	2.0(2)
C(4)-C(3)-C(8)-C(7)	1.4(2)
N(1)-C(3)-C(8)-C(7)	-179.39(13)

Symmetry transformations used to generate equivalent atoms:

Table F.7 Hydrogen bonds for **[3-8]** [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1D)...O(1)#1	0.810(19)	2.029(19)	2.8290(16)	169.6(19)

Symmetry transformations used to generate equivalent atoms: #1 -x,y+1/2,-z+1/2

Appendix G: Crystal structure of [3-10]

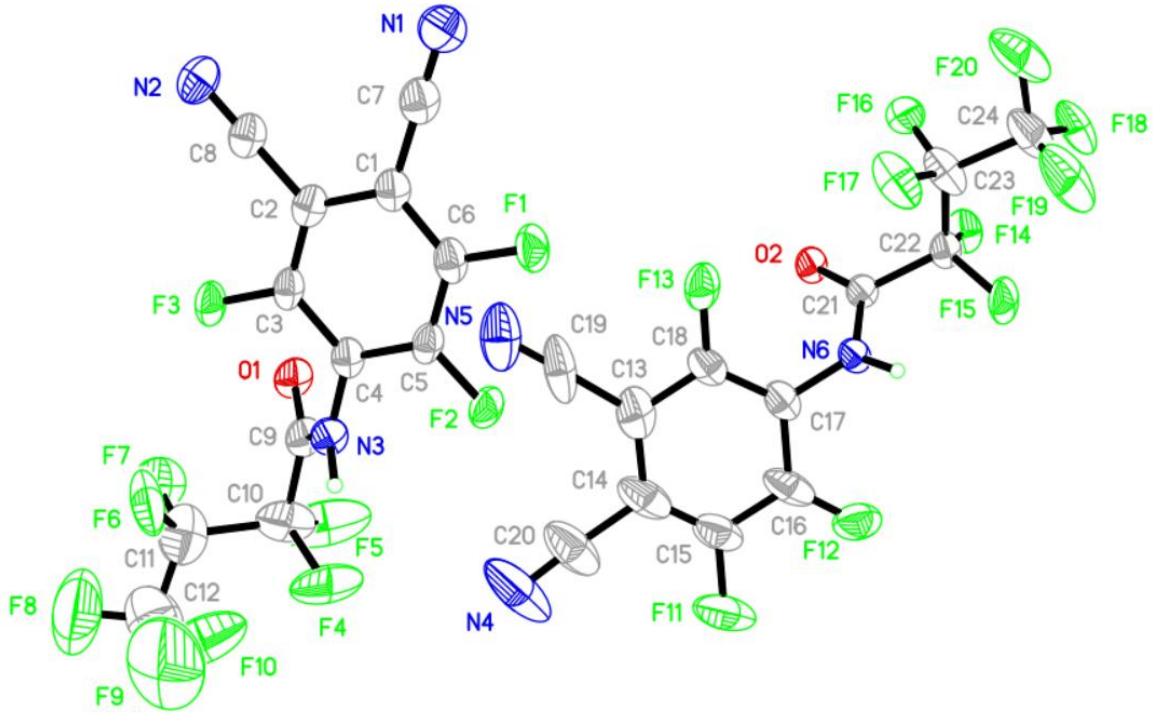


Figure G.1 ORTEP representation for the X-ray crystal structure of **[3-10]**, at 50% probability.

Table G.1 Crystal data and structure refinement for **[3-10]**.

Empirical formula	C12 H F10 N3 O	
Formula weight	393.16	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 17.2483(3) Å	alpha= 90°.
	b = 16.8574(3) Å	beta = 95.296(1)°.
	c = 9.8846(1) Å	gamma = 90°.
Volume	2861.79(8) $Å^3$	
Z	8	
Density (calculated)	1.825 g/cm^3	
Absorption coefficient	1.924 mm^{-1}	
F(000)	1536	

Crystal size	0.069 x 0.150 x 0.254 mm^3
Theta range for data collection	2.573 to 66.635°.
Index ranges	-20<=h<=20, -19<=k<=20, -11<=l<=11
Reflections collected	31509
Independent reflections	5002 [R(int) = 0.0352]
Completeness to theta = 66.635°	98.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5002 / 41 / 513
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0872, wR2 = 0.2345
R indices (all data)	R1 = 0.0932, wR2 = 0.2411
Extinction coefficient	0.0005(2)
Largest diff. peak and hole	1.397 and -0.660 e.$Å^{-3}$

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

	x	y	z	U(eq)
C(1)	3342(2)	-36(3)	6128(4)	34(1)
C(2)	2668(2)	189(2)	6728(4)	33(1)
C(3)	2318(2)	898(3)	6379(3)	32(1)
C(4)	2638(2)	1435(3)	5498(3)	32(1)
C(5)	3287(2)	1193(3)	4888(4)	33(1)
C(6)	3632(2)	465(3)	5188(4)	37(1)
C(7)	3734(3)	-775(3)	6464(4)	41(1)
C(8)	2340(2)	-317(3)	7707(4)	37(1)
C(9)	2200(2)	2667(3)	6312(4)	38(1)
C(10)	1844(4)	3473(3)	5926(4)	62(2)
C(11)	891(6)	3421(5)	6134(9)	75(2)
C(11')	1198(12)	3843(13)	6220(16)	33(4)
C(12)	408(6)	4089(6)	5528(12)	112(3)
C(13)	5265(3)	2964(4)	5481(4)	54(1)
C(14)	5124(3)	3642(4)	4657(5)	61(2)
C(15)	5689(4)	3974(4)	4001(5)	60(2)
C(16)	6452(3)	3683(3)	4121(4)	52(1)
C(17)	6610(2)	2991(3)	4952(4)	40(1)
C(18)	6021(3)	2648(3)	5580(4)	43(1)
C(19)	4704(3)	2564(5)	6242(5)	70(2)
C(20)	4339(4)	3985(5)	4517(6)	83(2)
C(21)	7771(2)	2501(2)	6216(4)	31(1)
C(22)	8590(2)	2164(3)	6074(4)	33(1)
C(23)	8603(3)	1262(3)	6218(5)	51(1)

C(24)	9300(3)	824(3)	5723(5)	64(2)
F(1)	4265(1)	264(2)	4593(2)	47(1)
F(2)	3608(1)	1672(2)	4036(2)	41(1)
F(3)	1651(1)	1086(2)	6878(2)	38(1)
F(4)	1988(5)	3699(4)	4642(8)	80(2)
F(4')	1798(10)	3556(14)	4610(30)	28(4)
F(5)	2279(6)	4035(4)	6668(6)	123(4)
F(5')	2096(7)	3987(9)	6838(15)	21(3)
F(6)	621(2)	2692(2)	5712(7)	91(2)
F(6')	672(18)	3340(20)	5400(30)	129(11)
F(7)	846(4)	3411(4)	7479(5)	102(2)
F(7')	1277(11)	3832(11)	7658(16)	67(4)
F(8)	-252(4)	4002(5)	5995(9)	177(3)
F(9)	357(4)	3932(6)	4198(6)	194(4)
F(10)	834(4)	4721(3)	5848(5)	131(2)
F(11)	5537(2)	4607(2)	3203(3)	84(1)
F(12)	6973(2)	4014(2)	3491(3)	59(1)
F(13)	6163(1)	1983(2)	6276(2)	49(1)
F(14)	9090(1)	2469(2)	7055(2)	44(1)
F(15)	8836(2)	2365(2)	4867(2)	57(1)
F(16)	8583(3)	1090(3)	7573(4)	51(1)
F(16')	8316(19)	940(20)	7290(20)	114(14)
F(17)	7937(2)	948(2)	5613(5)	63(1)
F(17')	8131(12)	1146(13)	4979(17)	74(6)
F(18)	9948(2)	1120(3)	6253(5)	68(1)
F(18')	9864(10)	833(13)	6706(17)	125(14)
F(19)	9245(3)	821(4)	4396(4)	91(2)
F(19')	9572(10)	1152(10)	4651(17)	82(6)
F(20)	9274(3)	62(3)	6116(6)	88(2)
F(20')	9174(11)	90(8)	5411(18)	88(8)
N(1)	4048(3)	-1358(3)	6729(4)	51(1)
N(2)	2082(2)	-716(2)	8482(4)	49(1)
N(3)	2323(2)	2190(2)	5255(3)	35(1)
N(4)	3746(4)	4285(6)	4388(6)	122(3)
N(5)	4264(3)	2284(4)	6842(5)	75(2)
N(6)	7366(2)	2680(2)	5025(3)	34(1)
O(1)	2322(2)	2493(2)	7494(3)	40(1)
O(2)	7542(2)	2566(2)	7329(2)	36(1)

Table G.3 Bond lengths [Å] and angles [°] for **[3-10]**.

C(1)-C(6)	1.383(6)	C(13)-C(18)	1.404(7)
C(1)-C(2)	1.405(5)	C(13)-C(14)	1.412(8)
C(1)-C(7)	1.442(6)	C(13)-C(19)	1.445(8)
C(2)-C(3)	1.370(6)	C(14)-C(15)	1.341(9)
C(2)-C(8)	1.444(6)	C(14)-C(20)	1.467(8)
C(3)-F(3)	1.332(4)	C(15)-F(11)	1.339(6)
C(3)-C(4)	1.403(6)	C(15)-C(16)	1.399(7)
C(4)-C(5)	1.382(5)	C(16)-F(12)	1.269(7)
C(4)-N(3)	1.396(5)	C(16)-C(17)	1.439(7)
C(5)-F(2)	1.324(4)	C(17)-C(18)	1.365(7)
C(5)-C(6)	1.383(6)	C(17)-N(6)	1.401(5)
C(6)-F(1)	1.331(4)	C(18)-F(13)	1.326(5)
C(7)-N(1)	1.140(6)	C(19)-N(5)	1.110(8)
C(8)-N(2)	1.141(6)	C(20)-N(4)	1.138(8)
C(9)-O(1)	1.204(5)	C(21)-O(2)	1.207(5)
C(9)-N(3)	1.351(5)	C(21)-N(6)	1.347(5)
C(9)-C(10)	1.525(7)	C(21)-C(22)	1.541(5)
C(10)-F(5')	1.297(14)	C(22)-F(14)	1.339(4)
C(10)-F(4')	1.31(3)	C(22)-F(15)	1.346(4)
C(10)-C(11')	1.33(2)	C(22)-C(23)	1.526(7)
C(10)-F(4)	1.370(9)	C(23)-F(16')	1.327(16)
C(10)-F(5)	1.378(9)	C(23)-F(17)	1.352(6)
C(10)-C(11)	1.677(11)	C(23)-F(16)	1.374(6)
C(11)-F(7)	1.339(9)	C(23)-F(17')	1.420(14)
C(11)-F(6)	1.366(9)	C(23)-C(24)	1.529(7)
C(11)-C(12)	1.492(14)	C(24)-F(20')	1.289(13)
C(11')-F(7')	1.416(15)	C(24)-F(18)	1.290(7)
C(11')-F(6')	1.436(18)	C(24)-F(18')	1.311(14)
C(11')-C(12)	1.53(2)	C(24)-F(19)	1.306(6)
C(12)-F(8)	1.275(11)	C(24)-F(19')	1.319(13)
C(12)-F(10)	1.316(12)	C(24)-F(20)	1.344(7)
C(12)-F(9)	1.336(12)		

C(6)-C(1)-C(2)	118.9(4)	F(2)-C(5)-C(4)	120.0(4)
C(6)-C(1)-C(7)	119.5(4)	F(2)-C(5)-C(6)	118.8(3)
C(2)-C(1)-C(7)	121.6(4)	C(4)-C(5)-C(6)	121.2(4)
C(3)-C(2)-C(1)	119.5(4)	F(1)-C(6)-C(5)	119.0(4)
C(3)-C(2)-C(8)	119.5(4)	F(1)-C(6)-C(1)	120.3(4)
C(1)-C(2)-C(8)	121.0(4)	C(5)-C(6)-C(1)	120.7(4)
F(3)-C(3)-C(2)	119.3(3)	N(1)-C(7)-C(1)	179.6(5)
F(3)-C(3)-C(4)	118.7(4)	N(2)-C(8)-C(2)	179.9(5)
C(2)-C(3)-C(4)	122.0(4)	O(1)-C(9)-N(3)	125.5(4)
C(5)-C(4)-N(3)	120.8(4)	O(1)-C(9)-C(10)	119.3(4)
C(5)-C(4)-C(3)	117.5(4)	N(3)-C(9)-C(10)	115.2(3)
N(3)-C(4)-C(3)	121.7(3)	F(5')-C(10)-F(4')	127.4(13)

F(5')-C(10)-C(11')	76.6(11)	F(9)-C(12)-C(11')	111.2(9)
F(4')-C(10)-C(11')	101.1(13)	C(11)-C(12)-C(11')	34.2(8)
F(5')-C(10)-F(4)	112.3(9)	C(18)-C(13)-C(14)	117.1(5)
F(4')-C(10)-F(4)	17.2(8)	C(18)-C(13)-C(19)	116.7(5)
C(11')-C(10)-F(4)	107.4(9)	C(14)-C(13)-C(19)	126.1(5)
F(5')-C(10)-F(5)	16.0(7)	C(15)-C(14)-C(13)	121.6(5)
F(4')-C(10)-F(5)	115.9(9)	C(15)-C(14)-C(20)	119.6(6)
C(11')-C(10)-F(5)	89.2(10)	C(13)-C(14)-C(20)	118.8(6)
F(4)-C(10)-F(5)	99.4(6)	F(11)-C(15)-C(14)	120.4(5)
F(5')-C(10)-C(9)	108.7(8)	F(11)-C(15)-C(16)	117.4(6)
F(4')-C(10)-C(9)	109.4(11)	C(14)-C(15)-C(16)	122.2(5)
C(11')-C(10)-C(9)	133.6(10)	F(12)-C(16)-C(15)	120.6(5)
F(4)-C(10)-C(9)	112.1(5)	F(12)-C(16)-C(17)	122.1(4)
F(5)-C(10)-C(9)	107.0(5)	C(15)-C(16)-C(17)	117.3(5)
F(5')-C(10)-C(11)	102.7(7)	C(18)-C(17)-N(6)	123.1(4)
F(4')-C(10)-C(11)	99.1(9)	C(18)-C(17)-C(16)	119.6(4)
C(11')-C(10)-C(11)	31.7(10)	N(6)-C(17)-C(16)	117.3(4)
F(4)-C(10)-C(11)	113.1(6)	F(13)-C(18)-C(17)	119.0(4)
F(5)-C(10)-C(11)	117.6(6)	F(13)-C(18)-C(13)	118.8(4)
C(9)-C(10)-C(11)	107.5(5)	C(17)-C(18)-C(13)	122.2(4)
F(7)-C(11)-F(6)	104.0(8)	N(5)-C(19)-C(13)	177.4(7)
F(7)-C(11)-C(12)	109.1(7)	N(4)-C(20)-C(14)	176.7(10)
F(6)-C(11)-C(12)	113.2(8)	O(2)-C(21)-N(6)	126.1(4)
F(7)-C(11)-C(10)	105.6(7)	O(2)-C(21)-C(22)	119.7(3)
F(6)-C(11)-C(10)	108.6(5)	N(6)-C(21)-C(22)	114.2(3)
C(12)-C(11)-C(10)	115.4(7)	F(14)-C(22)-F(15)	108.1(3)
C(10)-C(11')-F(7')	102.0(14)	F(14)-C(22)-C(23)	108.2(3)
C(10)-C(11')-F(6')	95.6(19)	F(15)-C(22)-C(23)	109.3(3)
F(7')-C(11')-F(6')	124(2)	F(14)-C(22)-C(21)	109.0(3)
C(10)-C(11')-C(12)	139.5(13)	F(15)-C(22)-C(21)	110.7(3)
F(7')-C(11')-C(12)	116.9(15)	C(23)-C(22)-C(21)	111.4(3)
F(6')-C(11')-C(12)	54.3(17)	F(16')-C(23)-F(17)	80.2(15)
F(8)-C(12)-F(10)	120.2(9)	F(16')-C(23)-F(16)	24.5(14)
F(8)-C(12)-F(9)	110.7(10)	F(17)-C(23)-F(16)	104.6(5)
F(10)-C(12)-F(9)	112.4(10)	F(16')-C(23)-F(17')	114.0(18)
F(8)-C(12)-C(11)	104.6(9)	F(17)-C(23)-F(17')	33.8(8)
F(10)-C(12)-C(11)	103.6(8)	F(16)-C(23)-F(17')	138.4(10)
F(9)-C(12)-C(11)	103.3(8)	F(16')-C(23)-C(22)	118.6(17)
F(8)-C(12)-C(11')	126.7(12)	F(17)-C(23)-C(22)	110.2(4)
F(10)-C(12)-C(11')	69.8(10)	F(16)-C(23)-C(22)	107.4(4)

F(17')-C(23)-C(22)	93.2(9)	F(19)-C(24)-F(19')	36.2(7)
F(16')-C(23)-C(24)	114.8(17)	F(20')-C(24)-F(20)	30.9(8)
F(17)-C(23)-C(24)	109.3(4)	F(18)-C(24)-F(20)	107.6(5)
F(16)-C(23)-C(24)	107.5(4)	F(18')-C(24)-F(20)	80.7(9)
F(17')-C(23)-C(24)	93.6(10)	F(19)-C(24)-F(20)	106.6(5)
C(22)-C(23)-C(24)	117.1(5)	F(19')-C(24)-F(20)	130.9(9)
F(20')-C(24)-F(18)	126.1(10)	F(20')-C(24)-C(23)	114.8(10)
F(20')-C(24)-F(18')	106.6(10)	F(18)-C(24)-C(23)	111.2(4)
F(18)-C(24)-F(18')	30.5(8)	F(18')-C(24)-C(23)	108.1(10)
F(20')-C(24)-F(19)	76.2(9)	F(19)-C(24)-C(23)	109.7(4)
F(18)-C(24)-F(19)	112.9(6)	F(19')-C(24)-C(23)	113.8(9)
F(18')-C(24)-F(19)	136.4(10)	F(20)-C(24)-C(23)	108.8(5)
F(20')-C(24)-F(19')	105.9(9)	C(9)-N(3)-C(4)	119.7(3)
F(18)-C(24)-F(19')	78.7(9)	C(21)-N(6)-C(17)	122.3(3)
F(18')-C(24)-F(19')	107.2(9)		

Symmetry transformations used to generate equivalent atoms:

Table G.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[3-10]**. 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)	31(2)	49(2)	22(2)	-3(2)	2(2)	-2(2)
C(2)	33(2)	46(2)	21(2)	-5(2)	2(2)	-9(2)
C(3)	26(2)	51(2)	17(2)	-4(2)	4(1)	-6(2)
C(4)	27(2)	52(2)	17(2)	-4(2)	1(1)	-3(2)
C(5)	28(2)	52(2)	19(2)	1(2)	4(1)	-6(2)
C(6)	27(2)	59(3)	24(2)	-5(2)	4(2)	0(2)
C(7)	40(2)	60(3)	24(2)	-1(2)	6(2)	0(2)
C(8)	39(2)	48(2)	26(2)	-5(2)	7(2)	-5(2)
C(9)	40(2)	55(3)	20(2)	-3(2)	9(2)	0(2)
C(10)	100(4)	67(3)	21(2)	-6(2)	9(2)	30(3)
C(11)	75(5)	73(6)	80(6)	-23(5)	25(5)	-1(5)
C(12)	88(6)	114(7)	134(9)	-7(6)	14(6)	24(5)
C(13)	48(3)	86(4)	28(2)	-21(2)	7(2)	6(2)
C(14)	69(3)	80(4)	32(2)	-12(2)	-16(2)	36(3)
C(15)	71(4)	75(4)	34(2)	4(2)	-1(2)	37(3)
C(16)	65(3)	57(3)	29(2)	-13(2)	-15(2)	32(2)
C(17)	39(2)	62(3)	21(2)	-7(2)	1(2)	17(2)
C(18)	42(2)	67(3)	19(2)	-1(2)	-3(2)	19(2)
C(19)	28(2)	143(6)	38(3)	-40(3)	3(2)	0(3)
C(20)	72(4)	132(6)	43(3)	-19(3)	-10(3)	54(4)

C(21)	33(2)	40(2)	19(2)	-2(1)	4(1)	6(2)
C(22)	31(2)	51(2)	17(2)	-3(2)	2(1)	3(2)
C(23)	38(2)	57(3)	56(3)	-18(2)	-7(2)	15(2)
C(24)	58(3)	75(4)	58(3)	-14(3)	0(3)	35(3)
F(1)	33(1)	71(2)	40(1)	5(1)	17(1)	10(1)
F(2)	36(1)	60(2)	28(1)	7(1)	12(1)	-2(1)
F(3)	28(1)	57(2)	30(1)	-2(1)	11(1)	-4(1)
F(4)	156(7)	62(4)	26(2)	5(3)	19(4)	24(4)
F(5)	268(11)	61(3)	41(3)	-8(2)	12(4)	15(5)
F(6)	28(2)	45(2)	202(6)	-2(3)	18(2)	-2(2)
F(7)	102(4)	126(5)	90(4)	29(3)	64(3)	49(4)
F(8)	97(4)	178(6)	269(9)	32(6)	78(5)	-17(4)
F(9)	146(6)	340(12)	87(4)	-22(5)	-33(4)	-37(6)
F(10)	240(7)	71(3)	83(3)	8(2)	17(4)	-37(4)
F(11)	109(3)	84(2)	56(2)	17(2)	-4(2)	51(2)
F(12)	79(2)	61(2)	38(1)	12(1)	9(1)	15(2)
F(13)	41(1)	75(2)	31(1)	-3(1)	10(1)	-2(1)
F(14)	34(1)	63(2)	33(1)	-9(1)	-2(1)	0(1)
F(15)	38(1)	110(2)	26(1)	11(1)	14(1)	17(1)
F(16)	57(3)	47(2)	53(2)	10(2)	19(2)	13(2)
F(17)	42(2)	53(2)	92(3)	-31(2)	-10(2)	4(2)
F(18)	30(2)	86(3)	85(3)	-8(3)	-3(2)	24(2)
F(19)	87(3)	133(4)	51(2)	-42(3)	-2(2)	64(3)
F(20)	96(4)	68(3)	99(4)	-18(3)	2(3)	50(3)
N(1)	58(2)	62(3)	34(2)	3(2)	12(2)	11(2)
N(2)	53(2)	54(2)	42(2)	1(2)	16(2)	-6(2)
N(3)	37(2)	51(2)	18(2)	1(1)	4(1)	3(2)
N(4)	94(5)	202(8)	66(4)	-24(4)	-20(3)	94(5)
N(5)	50(3)	118(4)	59(3)	-35(3)	13(2)	-15(3)
N(6)	36(2)	50(2)	19(2)	0(1)	6(1)	14(2)
O(1)	45(2)	57(2)	17(1)	-2(1)	6(1)	-2(1)
O(2)	35(1)	56(2)	16(1)	-1(1)	5(1)	9(1)

Table G.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **[3-10]**.

	x	**y**	**z**	**U(eq)**
H(3)	2205	2354	4416	42
H(6)	7583	2599	4266	41

Appendix H: Crystal structure of [3-12]

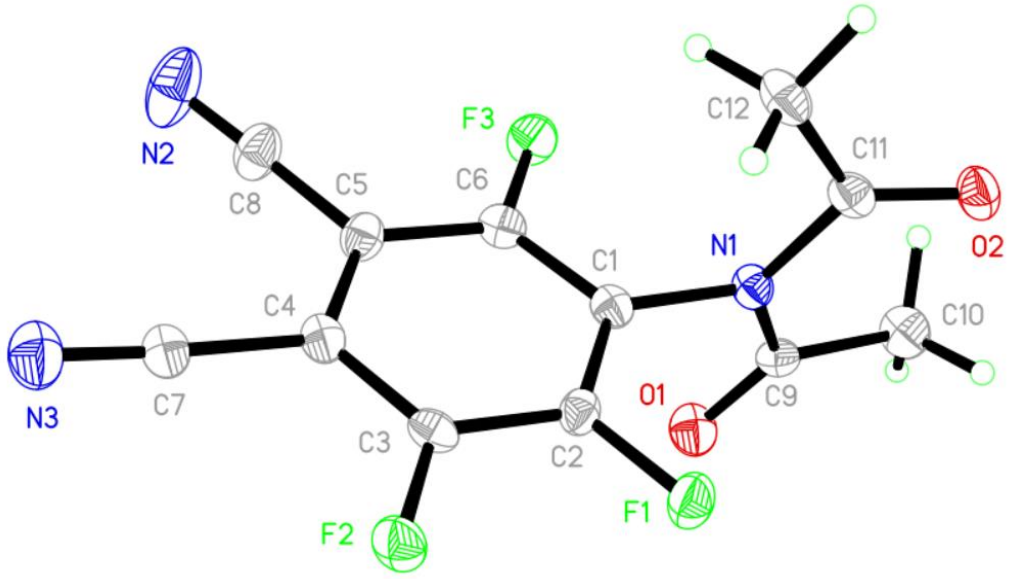


Figure H.1 ORTEP representation for the X-ray crystal structure of **[3-12]**, at 50% probability.

Table H.1 Crystal data and structure refinement for **[3-12]**.

Empirical formula	C12 H6 F3 N3 O2	
Formula weight	281.20	
Temperature	100(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 10.2160(2) Å	alpha = 90°.
	b = 22.6116(4) Å	beta = 90.367(1)°.
	c = 10.2459(2) Å	gamma = 90°.
Volume	2366.76(8) $Å^3$	
Z	8	
Density (calculated)	1.578 g/cm^3	
Absorption coefficient	1.252 mm^{-1}	
F(000)	1136	
Crystal size	0.37 x 0.23 x 0.11 mm^3	
Theta range for data collection	3.91 to 69.15°.	
Index ranges	-11<=h<=12, -26<=k<=27, -12<=l<=11	
Reflections collected	21701	

Independent reflections	4200 [R(int) = 0.0273]
Completeness to theta = 69.15°	95.1 %
Max. and min. transmission	0.8767 and 0.6565
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4200 / 0 / 366
Goodness-of-fit on F^2	1.108
Final R indices [I>2sigma(I)]	R1 = 0.0569, wR2 = 0.1420
R indices (all data)	R1 = 0.0597, wR2 = 0.1442
Extinction coefficient	0.00082(19)
Largest diff. peak and hole	0.652 and -0.260 e.$Å^{-3}$

Table H.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[3-12]**. U(eq) is defined as one-third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8019(2)	3871(1)	8777(2)	16(1)
C(2)	6952(2)	4256(1)	8721(2)	17(1)
C(3)	5709(2)	4069(1)	9051(2)	17(1)
C(4)	5492(2)	3492(1)	9434(2)	18(1)
C(5)	6558(3)	3098(1)	9528(2)	19(1)
C(6)	7798(2)	3299(1)	9207(2)	18(1)
C(7)	4188(3)	3291(1)	9715(2)	20(1)
C(8)	6355(3)	2500(1)	9941(3)	25(1)
C(9)	10126(3)	4245(1)	9399(2)	18(1)
C(10)	11522(3)	4391(1)	9090(3)	26(1)
C(11)	9579(2)	4051(1)	7008(2)	18(1)
C(12)	8609(3)	3724(1)	6184(2)	23(1)
C(13)	7001(2)	6116(1)	6433(2)	15(1)
C(14)	8086(2)	5753(1)	6307(2)	16(1)
C(15)	9327(2)	5943(1)	6667(2)	15(1)
C(16)	9512(2)	6506(1)	7152(2)	17(1)
C(17)	8430(3)	6884(1)	7300(3)	20(1)
C(18)	7202(2)	6678(1)	6940(2)	18(1)
C(19)	10805(2)	6709(1)	7487(2)	18(1)
C(20)	8612(3)	7468(1)	7806(3)	29(1)
C(21)	5426(2)	5887(1)	4691(2)	18(1)
C(22)	6360(3)	6213(1)	3830(3)	25(1)
C(23)	4878(2)	5780(1)	7095(2)	17(1)
C(24)	3498(3)	5609(1)	6799(3)	23(1)
F(1)	7139(2)	4809(1)	8325(2)	23(1)
F(2)	4716(1)	4453(1)	8964(2)	23(1)
F(3)	8818(2)	2929(1)	9293(2)	25(1)
F(4)	7943(1)	5213(1)	5815(1)	20(1)
F(5)	10339(1)	5579(1)	6530(2)	21(1)

F(6)	6158(1)	7033(1)	7086(2)	24(1)
N(1)	9283(2)	4061(1)	8370(2)	17(1)
N(2)	6134(3)	2027(1)	10249(3)	42(1)
N(3)	3158(2)	3112(1)	9901(3)	30(1)
N(4)	8808(3)	7928(1)	8220(4)	50(1)
N(5)	11829(2)	6892(1)	7722(2)	28(1)
N(6)	5733(2)	5916(1)	6041(2)	16(1)
O(1)	9686(2)	4265(1)	10486(2)	25(1)
O(2)	10540(2)	4293(1)	6583(2)	22(1)
O(3)	4478(2)	5621(1)	4290(2)	22(1)
O(4)	5314(2)	5827(1)	8190(2)	22(1)

Table H.3 Bond lengths [Å] and angles [°] for **[3-12]**.

C(1)-C(6)	1.387(4)	C(13)-C(14)	1.386(3)
C(1)-C(2)	1.395(4)	C(13)-C(18)	1.389(4)
C(1)-N(1)	1.425(3)	C(13)-N(6)	1.428(3)
C(2)-F(1)	1.329(3)	C(14)-F(4)	1.329(3)
C(2)-C(3)	1.382(4)	C(14)-C(15)	1.386(4)
C(3)-F(2)	1.337(3)	C(15)-F(5)	1.331(3)
C(3)-C(4)	1.380(4)	C(15)-C(16)	1.378(4)
C(4)-C(5)	1.410(4)	C(16)-C(17)	1.405(4)
C(4)-C(7)	1.438(4)	C(16)-C(19)	1.438(3)
C(5)-C(6)	1.387(4)	C(17)-C(18)	1.386(4)
C(5)-C(8)	1.433(4)	C(17)-C(20)	1.431(4)
C(6)-F(3)	1.339(3)	C(18)-F(6)	1.343(3)
C(7)-N(3)	1.145(4)	C(19)-N(5)	1.149(4)
C(8)-N(2)	1.138(4)	C(20)-N(4)	1.141(4)
C(9)-O(1)	1.204(3)	C(21)-O(3)	1.210(3)
C(9)-N(1)	1.420(3)	C(21)-N(6)	1.418(3)
C(9)-C(10)	1.500(4)	C(21)-C(22)	1.497(4)
C(10)-H(10A)	0.9800	C(22)-H(22A)	0.9800
C(10)-H(10B)	0.9800	C(22)-H(22B)	0.9800
C(10)-H(10C)	0.9800	C(22)-H(22C)	0.9800
C(11)-O(2)	1.208(3)	C(23)-O(4)	1.209(3)
C(11)-N(1)	1.430(3)	C(23)-N(6)	1.427(3)
C(11)-C(12)	1.493(4)	C(23)-C(24)	1.490(4)
C(12)-H(12A)	0.9800	C(24)-H(24A)	0.9800
C(12)-H(12B)	0.9800	C(24)-H(24B)	0.9800
C(12)-H(12C)	0.9800	C(24)-H(24C)	0.9800
C(6)-C(1)-C(2)	117.8(2)	F(1)-C(2)-C(1)	119.0(2)
C(6)-C(1)-N(1)	121.6(2)	C(3)-C(2)-C(1)	121.3(2)
C(2)-C(1)-N(1)	120.6(2)	F(2)-C(3)-C(4)	120.6(2)
F(1)-C(2)-C(3)	119.7(2)	F(2)-C(3)-C(2)	119.0(2)

C(4)-C(3)-C(2)	120.5(2)	F(5)-C(15)-C(16)	120.3(2)
C(3)-C(4)-C(5)	119.4(2)	F(5)-C(15)-C(14)	119.3(2)
C(3)-C(4)-C(7)	120.4(2)	C(16)-C(15)-C(14)	120.4(2)
C(5)-C(4)-C(7)	120.1(2)	C(15)-C(16)-C(17)	119.6(2)
C(6)-C(5)-C(4)	118.9(2)	C(15)-C(16)-C(19)	120.3(2)
C(6)-C(5)-C(8)	120.9(2)	C(17)-C(16)-C(19)	120.1(2)
C(4)-C(5)-C(8)	120.2(2)	C(18)-C(17)-C(16)	118.6(2)
F(3)-C(6)-C(1)	118.4(2)	C(18)-C(17)-C(20)	121.4(2)
F(3)-C(6)-C(5)	119.4(2)	C(16)-C(17)-C(20)	120.0(2)
C(1)-C(6)-C(5)	122.1(2)	F(6)-C(18)-C(17)	119.3(2)
N(3)-C(7)-C(4)	177.1(3)	F(6)-C(18)-C(13)	118.2(2)
N(2)-C(8)-C(5)	176.7(3)	C(17)-C(18)-C(13)	122.5(2)
O(1)-C(9)-N(1)	118.0(2)	N(5)-C(19)-C(16)	177.0(3)
O(1)-C(9)-C(10)	123.3(2)	N(4)-C(20)-C(17)	177.3(3)
N(1)-C(9)-C(10)	118.7(2)	O(3)-C(21)-N(6)	121.7(2)
C(9)-C(10)-H(10A)	109.5	O(3)-C(21)-C(22)	123.8(2)
C(9)-C(10)-H(10B)	109.5	N(6)-C(21)-C(22)	114.5(2)
H(10A)-C(10)-H(10B)	109.5	C(21)-C(22)-H(22A)	109.5
C(9)-C(10)-H(10C)	109.5	C(21)-C(22)-H(22B)	109.5
H(10A)-C(10)-H(10C)	109.5	H(22A)-C(22)-H(22B)	109.5
H(10B)-C(10)-H(10C)	109.5	C(21)-C(22)-H(22C)	109.5
O(2)-C(11)-N(1)	121.5(2)	H(22A)-C(22)-H(22C)	109.5
O(2)-C(11)-C(12)	123.9(2)	H(22B)-C(22)-H(22C)	109.5
N(1)-C(11)-C(12)	114.6(2)	O(4)-C(23)-N(6)	117.3(2)
C(11)-C(12)-H(12A)	109.5	O(4)-C(23)-C(24)	123.7(2)
C(11)-C(12)-H(12B)	109.5	N(6)-C(23)-C(24)	119.0(2)
H(12A)-C(12)-H(12B)	109.5	C(23)-C(24)-H(24A)	109.5
C(11)-C(12)-H(12C)	109.5	C(23)-C(24)-H(24B)	109.5
H(12A)-C(12)-H(12C)	109.5	H(24A)-C(24)-H(24B)	109.5
H(12B)-C(12)-H(12C)	109.5	C(23)-C(24)-H(24C)	109.5
C(14)-C(13)-C(18)	117.5(2)	H(24A)-C(24)-H(24C)	109.5
C(14)-C(13)-N(6)	120.7(2)	H(24B)-C(24)-H(24C)	109.5
C(18)-C(13)-N(6)	121.8(2)	C(9)-N(1)-C(1)	114.6(2)
F(4)-C(14)-C(13)	119.6(2)	C(9)-N(1)-C(11)	126.8(2)
F(4)-C(14)-C(15)	119.0(2)	C(1)-N(1)-C(11)	118.6(2)
C(13)-C(14)-C(15)	121.4(2)		
C(21)-N(6)-C(23)	126.6(2)		
C(21)-N(6)-C(13)	118.9(2)		
C(23)-N(6)-C(13)	114.5(2)		

Table H.4 Anisotropic displacement parameters ($Å^2 \times 10^3$) for **[3-12]**. 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)	15(1)	21(1)	12(1)	-2(1)	-2(1)	-1(1)
C(2)	20(1)	17(1)	13(1)	1(1)	0(1)	-4(1)
C(3)	17(1)	21(1)	13(1)	-2(1)	0(1)	4(1)
C(4)	16(1)	23(1)	13(1)	-1(1)	-1(1)	-2(1)
C(5)	19(1)	19(1)	19(1)	1(1)	-2(1)	-2(1)
C(6)	16(1)	21(1)	18(1)	-1(1)	-3(1)	3(1)
C(7)	18(1)	24(1)	17(1)	1(1)	-1(1)	-1(1)
C(8)	18(1)	22(2)	36(2)	4(1)	-4(1)	-1(1)
C(9)	19(1)	17(1)	18(1)	-3(1)	-1(1)	0(1)
C(10)	17(1)	34(2)	26(1)	-4(1)	-5(1)	-4(1)
C(11)	18(1)	19(1)	19(1)	2(1)	1(1)	6(1)
C(12)	19(1)	35(2)	15(1)	-1(1)	1(1)	0(1)
C(13)	14(1)	20(1)	11(1)	2(1)	-1(1)	-3(1)
C(14)	18(1)	16(1)	13(1)	2(1)	1(1)	-1(1)
C(15)	14(1)	19(1)	14(1)	0(1)	-1(1)	2(1)
C(16)	17(1)	20(1)	14(1)	1(1)	1(1)	-2(1)
C(17)	21(1)	17(1)	21(1)	0(1)	2(1)	0(1)
C(18)	15(1)	18(1)	20(1)	2(1)	1(1)	4(1)
C(19)	16(1)	19(1)	18(1)	-1(1)	0(1)	0(1)
C(20)	15(1)	22(2)	50(2)	-8(1)	3(1)	-2(1)
C(21)	15(1)	20(1)	17(1)	-2(1)	-2(1)	4(1)
C(22)	18(1)	42(2)	15(1)	4(1)	0(1)	-1(1)
C(23)	18(1)	14(1)	19(1)	-1(1)	4(1)	2(1)
C(24)	14(1)	28(1)	26(1)	0(1)	4(1)	-2(1)
F(1)	21(1)	19(1)	29(1)	6(1)	2(1)	-1(1)
F(2)	17(1)	24(1)	28(1)	3(1)	2(1)	5(1)
F(3)	18(1)	22(1)	35(1)	1(1)	-1(1)	4(1)
F(4)	20(1)	17(1)	23(1)	-5(1)	-1(1)	-1(1)
F(5)	15(1)	21(1)	26(1)	-2(1)	-3(1)	5(1)
F(6)	16(1)	21(1)	36(1)	-3(1)	1(1)	3(1)
N(1)	13(1)	20(1)	17(1)	-1(1)	-1(1)	-2(1)
N(2)	26(1)	31(2)	70(2)	16(1)	-11(1)	-4(1)
N(3)	25(1)	36(1)	31(1)	0(1)	1(1)	-5(1)
N(4)	24(1)	31(2)	96(3)	-26(2)	6(2)	-4(1)
N(5)	22(1)	31(1)	31(1)	-1(1)	-2(1)	-3(1)
N(6)	13(1)	21(1)	16(1)	1(1)	1(1)	-1(1)
O(1)	25(1)	32(1)	18(1)	-1(1)	-2(1)	-4(1)
O(2)	17(1)	25(1)	24(1)	4(1)	5(1)	1(1)
O(3)	17(1)	27(1)	22(1)	-5(1)	-4(1)	-2(1)
O(4)	23(1)	28(1)	16(1)	-1(1)	1(1)	-2(1)

Table H.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **[3-12]**.

	x	y	z	U(eq)
H(10A)	11554	4760	8588	39
H(10B)	11904	4070	8575	39
H(10C)	12020	4439	9904	39
H(12A)	7783	3945	6154	34
H(12B)	8455	3332	6559	34
H(12C)	8951	3681	5297	34
H(22A)	7211	6013	3843	37
H(22B)	6465	6619	4148	37
H(22C)	6016	6220	2935	37
H(24A)	3482	5213	6408	34
H(24B)	3115	5894	6187	34
H(24C)	2992	5606	7608	34

Appendix I: Crystal structure of [3-13]

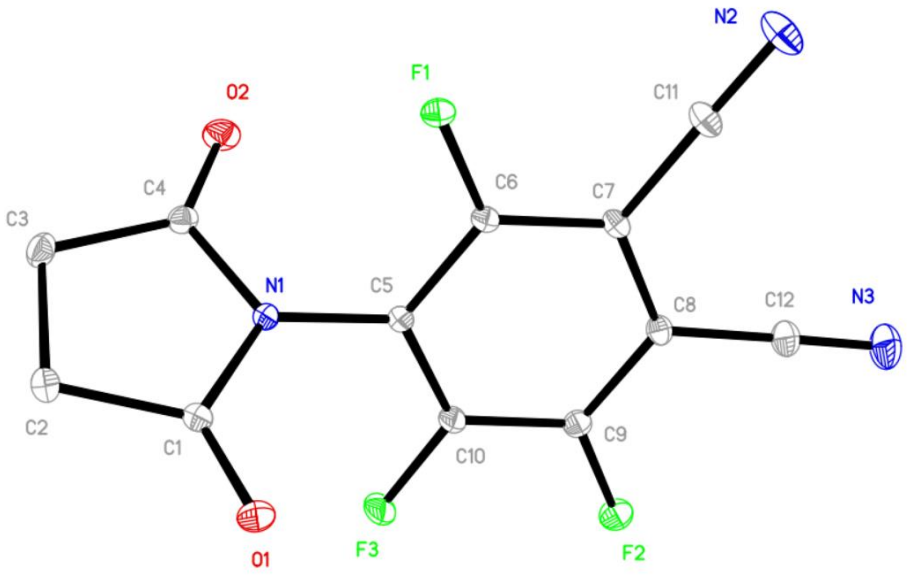


Figure I.1 ORTEP representation for the X-ray crystal structure of **[3-13]**, at 50% probability.

Table I.1 Crystal data and structure refinement for **[3-13]**.

Empirical formula	C12 H4 F3 N3 O2	
Formula weight	279.18	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Orthorhombic, Pbca	
Unit cell dimensions	a = 8.5746(4) Å b = 15.8113(7) Å c = 17.0796(8) Å	alpha = 90 deg. beta = 90 deg. gamma = 90 deg.
Volume	2315.58(18) $Å^3$	
Z, Calculated density	8, 1.602 g/cm^3	
Absorption coefficient	0.145 mm^{-1}	
F(000)	1120	
Crystal size	0.960 x 0.290 x 0.130 mm	
Theta range for data collection	2.954 to 38.772 deg.	
Limiting indices	-15<=h<=15, -27<=k<=27, -29<=l<=29	

Reflections collected / unique	109598 / 6551 [R(int) = 0.0380]
Completeness to theta = 25.000	99.8 %
Absorption correction	Empirical
Max. and min. transmission	0.7476 and 0.7167
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6551 / 0 / 181
Goodness-of-fit on F^2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.1069
R indices (all data)	R1 = 0.0518, wR2 = 0.1178
Extinction coefficient	n/a
Largest diff. peak and hole	0.647 and -0.261 e.$Å^{-3}$

Table I.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[3-13]**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4067(1)	3658(1)	3745(1)	14(1)
N(2)	10732(1)	4374(1)	4302(1)	29(1)
N(3)	9600(1)	6722(1)	3562(1)	32(1)
O(1)	3611(1)	3657(1)	2421(1)	24(1)
O(2)	4094(1)	3371(1)	5063(1)	23(1)
F(1)	7115(1)	3350(1)	4190(1)	19(1)
F(2)	5619(1)	6494(1)	3192(1)	24(1)
F(3)	3417(1)	5302(1)	3268(1)	25(1)
C(1)	3310(1)	3387(1)	3065(1)	16(1)
C(2)	2127(1)	2732(1)	3298(1)	19(1)
C(3)	2349(1)	2600(1)	4176(1)	19(1)
C(4)	3575(1)	3230(1)	4421(1)	16(1)
C(5)	5211(1)	4294(1)	3739(1)	13(1)
C(6)	6740(1)	4126(1)	3964(1)	14(1)
C(7)	7892(1)	4740(1)	3938(1)	14(1)
C(8)	7511(1)	5554(1)	3671(1)	15(1)
C(9)	6000(1)	5726(1)	3444(1)	16(1)
C(10)	4864(1)	5105(1)	3481(1)	16(1)
C(11)	9460(1)	4529(1)	4140(1)	19(1)
C(12)	8665(1)	6205(1)	3621(1)	21(1)

Table I.3 Bond lengths [Å] and angles [deg] for **[3-13]**.

N(1)-C(1)	1.3980(8)	C(2)-H(2B)	0.99
N(1)-C(4)	1.4033(8)	C(3)-C(4)	1.5072(10)
N(1)-C(5)	1.4042(8)	C(3)-H(3A)	0.99
N(2)-C(11)	1.1517(9)	C(3)-H(3B)	0.99
N(3)-C(12)	1.1494(10)	C(5)-C(10)	1.3897(9)
O(1)-C(1)	1.2077(8)	C(5)-C(6)	1.3917(9)
O(2)-C(4)	1.2049(9)	C(6)-C(7)	1.3855(9)
F(1)-C(6)	1.3254(7)	C(7)-C(8)	1.4041(9)
F(2)-C(9)	1.3281(8)	C(7)-C(11)	1.4277(9)
F(3)-C(10)	1.3295(8)	C(8)-C(9)	1.3797(9)
C(1)-C(2)	1.5021(10)	C(8)-C(12)	1.4296(10)
C(2)-C(3)	1.5263(11)	C(9)-C(10)	1.3852(9)
C(2)-H(2A)	0.99		
N(1)-C(1)-C(2)	107.78(5)	C(6)-C(5)-N(1)	121.38(6)
C(1)-C(2)-C(3)	105.68(6)	F(1)-C(6)-C(7)	119.03(5)
C(1)-C(2)-H(2A)	110.6	F(1)-C(6)-C(5)	118.96(6)
C(3)-C(2)-H(2A)	110.6	C(7)-C(6)-C(5)	121.98(6)
C(1)-C(2)-H(2B)	110.6	C(6)-C(7)-C(8)	119.15(6)
C(3)-C(2)-H(2B)	110.6	C(6)-C(7)-C(11)	119.99(6)
H(2A)-C(2)-H(2B)	108.7	C(8)-C(7)-C(11)	120.78(6)
C(4)-C(3)-C(2)	105.61(5)	C(9)-C(8)-C(7)	119.38(6)
C(4)-C(3)-H(3A)	110.6	C(9)-C(8)-C(12)	119.40(6)
C(2)-C(3)-H(3A)	110.6	C(7)-C(8)-C(12)	121.21(6)
C(4)-C(3)-H(3B)	110.6	F(2)-C(9)-C(8)	120.18(6)
C(2)-C(3)-H(3B)	110.6	F(2)-C(9)-C(10)	119.29(6)
H(3A)-C(3)-H(3B)	108.7	C(8)-C(9)-C(10)	120.53(6)
O(2)-C(4)-N(1)	123.21(6)	F(3)-C(10)-C(9)	118.59(6)
O(2)-C(4)-C(3)	129.31(6)	F(3)-C(10)-C(5)	120.17(6)
N(1)-C(4)-C(3)	107.48(5)	C(9)-C(10)-C(5)	121.24(6)
C(10)-C(5)-C(6)	117.72(6)	N(2)-C(11)-C(7)	178.77(9)
C(10)-C(5)-N(1)	120.86(6)	N(3)-C(12)-C(8)	178.39(9)

Symmetry transformations used to generate equivalent atoms:

Table I.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[3-13]**. 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}
N(1)	13(1)	16(1)	13(1)	2(1)	0(1)	-2(1)
N(2)	16(1)	32(1)	37(1)	-9(1)	-5(1)	6(1)
N(3)	27(1)	27(1)	42(1)	-2(1)	1(1)	-10(1)
O(1)	27(1)	31(1)	14(1)	6(1)	-3(1)	-6(1)
O(2)	25(1)	31(1)	13(1)	2(1)	0(1)	1(1)
F(1)	18(1)	15(1)	22(1)	4(1)	-2(1)	3(1)
F(2)	26(1)	15(1)	33(1)	7(1)	-4(1)	1(1)
F(3)	15(1)	22(1)	37(1)	7(1)	-7(1)	2(1)
C(1)	15(1)	18(1)	15(1)	2(1)	-2(1)	-1(1)
C(2)	17(1)	19(1)	22(1)	1(1)	-1(1)	-4(1)
C(3)	18(1)	19(1)	22(1)	4(1)	4(1)	-3(1)
C(4)	14(1)	19(1)	14(1)	3(1)	2(1)	2(1)
C(5)	12(1)	15(1)	14(1)	1(1)	-1(1)	0(1)
C(6)	13(1)	14(1)	14(1)	0(1)	-1(1)	1(1)
C(7)	11(1)	16(1)	15(1)	-3(1)	-1(1)	1(1)
C(8)	14(1)	15(1)	16(1)	-2(1)	0(1)	-1(1)
C(9)	17(1)	14(1)	19(1)	2(1)	-1(1)	1(1)
C(10)	13(1)	16(1)	19(1)	2(1)	-2(1)	1(1)
C(11)	14(1)	21(1)	22(1)	-6(1)	-2(1)	2(1)
C(12)	19(1)	19(1)	24(1)	-2(1)	1(1)	-3(1)

Table I.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **[3-13]**.

	x	y	z	U(eq)
H(2A)	2306	2198	3009	23
H(2B)	1058	2934	3184	23
H(3A)	1361	2703	4460	23
H(3B)	2701	2015	4285	23

Table I.6 Torsion angles [deg] for **[3-13]**.

C(4)-N(1)-C(1)-O(1)	-177.29(7)	F(1)-C(6)-C(7)-C(8)	177.55(6)
C(5)-N(1)-C(1)-O(1)	2.22(11)	C(5)-C(6)-C(7)-C(8)	-0.49(10)
C(4)-N(1)-C(1)-C(2)	2.74(8)	F(1)-C(6)-C(7)-C(11)	0.98(9)
C(5)-N(1)-C(1)-C(2)	-177.75(6)	C(5)-C(6)-C(7)-C(11)	-177.07(6)
O(1)-C(1)-C(2)-C(3)	175.94(8)	C(6)-C(7)-C(8)-C(9)	0.24(9)
N(1)-C(1)-C(2)-C(3)	-4.09(8)	C(11)-C(7)-C(8)-C(9)	176.79(6)
C(1)-C(2)-C(3)-C(4)	3.92(7)	C(6)-C(7)-C(8)-C(12)	-178.87(6)
C(1)-N(1)-C(4)-O(2)	179.68(7)	C(11)-C(7)-C(8)-C(12)	-2.32(10)
C(5)-N(1)-C(4)-O(2)	0.18(10)	C(7)-C(8)-C(9)-F(2)	179.82(6)
C(1)-N(1)-C(4)-C(3)	-0.15(8)	C(12)-C(8)-C(9)-F(2)	-1.05(10)
C(5)-N(1)-C(4)-C(3)	-179.65(6)	C(7)-C(8)-C(9)-C(10)	0.33(10)
C(2)-C(3)-C(4)-O(2)	177.75(7)	C(12)-C(8)-C(9)-C(10)	179.46(7)
C(2)-C(3)-C(4)-N(1)	-2.43(7)	F(2)-C(9)-C(10)-F(3)	-0.53(10)
C(1)-N(1)-C(5)-C(10)	60.56(9)	C(8)-C(9)-C(10)-F(3)	178.96(6)
C(4)-N(1)-C(5)-C(10)	-119.98(7)	F(2)-C(9)-C(10)-C(5)	179.84(6)
C(1)-N(1)-C(5)-C(6)	-117.14(7)	C(8)-C(9)-C(10)-C(5)	-0.67(11)
C(4)-N(1)-C(5)-C(6)	62.32(9)	C(6)-C(5)-C(10)-F(3)	-179.21(6)
C(10)-C(5)-C(6)-F(1)	-177.88(6)	N(1)-C(5)-C(10)-F(3)	3.01(10)
N(1)-C(5)-C(6)-F(1)	-0.11(9)	C(6)-C(5)-C(10)-C(9)	0.42(10)
C(10)-C(5)-C(6)-C(7)	0.17(9)	N(1)-C(5)-C(10)-C(9)	-177.37(6)
N(1)-C(5)-C(6)-C(7)	177.94(6)		

Symmetry transformations used to generate equivalent atoms:

Appendix J: Crystal structure of $F_{64}PcNi \cdot 2(acetone)$

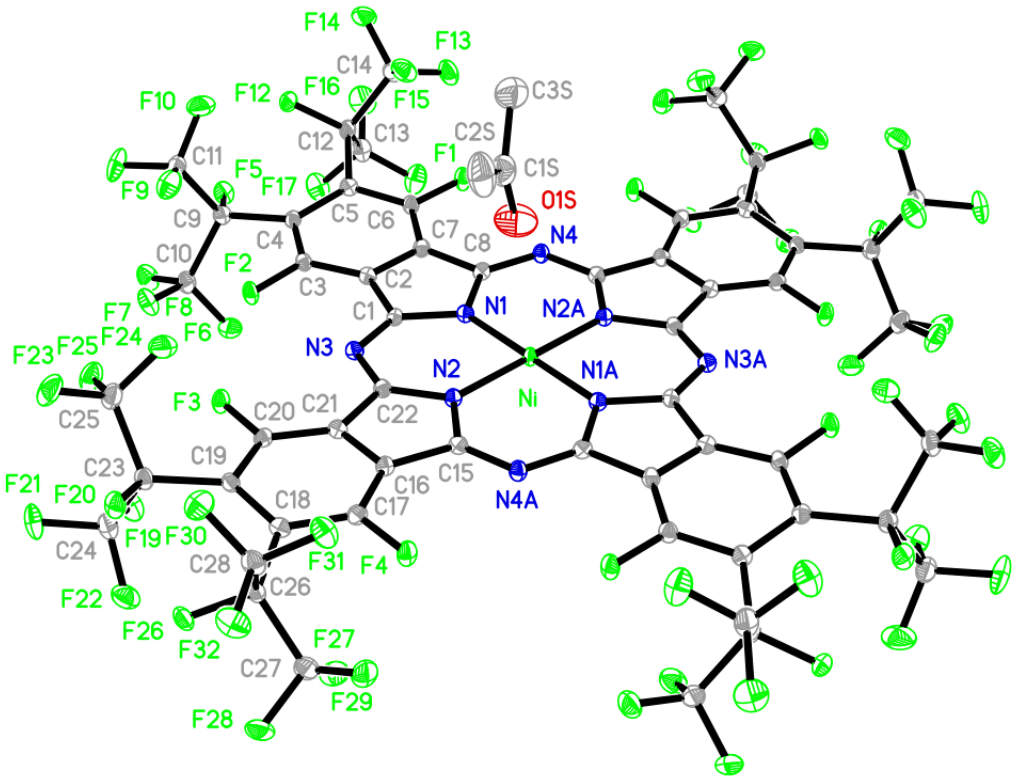


Figure J.1 ORTEP representation for the X-ray crystal structure of **$F_{64}PcNi \cdot 2(acetone)$**, at 50% probability. The symmetric atoms are not numbered; the second acetone molecule is not shown.

Table J.1 Crystal data and structure refinement for **$F_{64}PcNi \cdot 2(acetone)$**

Empirical formula	C62 H12 F64 N8 Ni O2	
Formula weight	2175.51	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 15.3925(7) Å	α= 90°
	b = 20.6745(10) Å	β= 101.609(3)°
	c = 11.9250(6) Å	γ = 90°
Volume	3717.3(3) $Å^3$	
Z	2	
Density (calculated)	1.944 g/cm^3	
Absorption coefficient	2.378 mm^{-1}	
F(000)	2120	

Crystal size	0.702 x 0.497 x 0.080 mm^3
Theta range for data collection	4.277 to 66.772°.
Index ranges	-18<=h<=18, -24<=k<=24, -12<=l<=13
Reflections collected	51778
Independent reflections	6389 [R(int) = 0.0303]
Completeness to theta = 66.772°	96.7 %
Absorption correction	Numerical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6389 / 7 / 652
Goodness-of-fit on F^2	1.060
Final R indices [I>2sigma(I)]	R1 = 0.0261, wR2 = 0.0641
R indices (all data)	R1 = 0.0276, wR2 = 0.0649
Extinction coefficient	0.00022(3)
Largest diff. peak and hole	0.324 and -0.260 e.$Å^{-3}$

Table J.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **F_{64}PcNi·2(acetone)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ni	5000	0	5000	10(1)
N(1)	4154(1)	395(1)	5756(1)	11(1)
N(2)	5500(1)	833(1)	4843(1)	11(1)
N(3)	4553(1)	1528(1)	5714(1)	12(1)
N(4)	3293(1)	-542(1)	6085(1)	12(1)
C(1)	4070(1)	1043(1)	5970(1)	11(1)
C(2)	3317(1)	1145(1)	6514(1)	12(1)
C(3)	2940(1)	1682(1)	6928(1)	12(1)
C(4)	2176(1)	1649(1)	7380(1)	12(1)
C(5)	1743(1)	1024(1)	7365(1)	13(1)
C(6)	2177(1)	491(1)	7030(1)	13(1)
C(7)	2948(1)	544(1)	6605(1)	12(1)
C(8)	3480(1)	79(1)	6128(1)	11(1)
C(9)	1890(1)	2276(1)	7909(1)	14(1)
C(10)	2667(1)	2655(1)	8712(1)	17(1)
C(11)	1364(1)	2743(1)	7003(1)	19(1)
C(12)	797(1)	891(1)	7565(1)	16(1)
C(13)	775(1)	604(1)	8758(2)	21(1)
C(14)	224(1)	456(1)	6586(2)	21(1)
C(15)	6219(1)	955(1)	4361(1)	12(1)
C(16)	6397(1)	1646(1)	4384(1)	12(1)
C(17)	7037(1)	2023(1)	4038(1)	13(1)
C(18)	7075(1)	2693(1)	4168(1)	13(1)
C(19)	6371(1)	3001(1)	4616(1)	12(1)
C(20)	5763(1)	2602(1)	5000(1)	12(1)

C(21)	5764(1)	1935(1)	4891(1)	12(1)
C(22)	5214(1)	1416(1)	5189(1)	12(1)
C(23)	6202(1)	3736(1)	4685(1)	14(1)
C(24)	6557(1)	4010(1)	5899(1)	20(1)
C(25)	5201(1)	3942(1)	4242(1)	19(1)
C(26)	7882(1)	3029(1)	3829(1)	14(1)
C(27)	8806(1)	2674(1)	4248(1)	19(1)
C(28)	7726(1)	3153(1)	2527(1)	17(1)
F(1)	1826(1)	-98(1)	7065(1)	18(1)
F(2)	3344(1)	2254(1)	6895(1)	16(1)
F(3)	5134(1)	2870(1)	5481(1)	16(1)
F(4)	7651(1)	1722(1)	3580(1)	17(1)
F(5)	1346(1)	2132(1)	8650(1)	18(1)
F(6)	3288(1)	2246(1)	9212(1)	25(1)
F(7)	2340(1)	2951(1)	9531(1)	24(1)
F(8)	3042(1)	3116(1)	8191(1)	23(1)
F(9)	1134(1)	3274(1)	7507(1)	33(1)
F(10)	636(1)	2467(1)	6435(1)	34(1)
F(11)	1843(1)	2926(1)	6248(1)	26(1)
F(12)	315(1)	1450(1)	7493(1)	19(1)
F(13)	195(1)	-165(1)	6870(1)	26(1)
F(14)	-608(1)	669(1)	6369(1)	31(1)
F(15)	527(1)	505(1)	5621(1)	25(1)
F(16)	-58(1)	474(1)	8841(1)	32(1)
F(17)	1098(1)	1027(1)	9573(1)	27(1)
F(18)	1248(1)	64(1)	8966(1)	28(1)
F(19)	6625(1)	4077(1)	3971(1)	18(1)
F(20)	6186(1)	3719(1)	6677(1)	24(1)
F(21)	6394(1)	4644(1)	5927(1)	29(1)
F(22)	7426(1)	3924(1)	6188(1)	25(1)
F(23)	5173(1)	4502(1)	3681(1)	29(1)
F(24)	4781(1)	3505(1)	3503(1)	24(1)
F(25)	4749(1)	4028(1)	5065(1)	25(1)
F(26)	8033(1)	3620(1)	4345(1)	18(1)
F(27)	8798(1)	2329(1)	5188(1)	24(1)
F(28)	9434(1)	3122(1)	4507(1)	24(1)
F(29)	9038(1)	2294(1)	3462(1)	24(1)
F(30)	7038(1)	3548(1)	2192(1)	24(1)
F(31)	7552(1)	2606(1)	1933(1)	22(1)
F(32)	8432(1)	3428(1)	2243(1)	26(1)
C(1S)	3331(3)	703(3)	1530(4)	44(1)
C(2S)	3038(1)	328(1)	2438(2)	32(1)
C(3S)	2046(2)	141(2)	2175(4)	42(1)
C(1S')	3949(5)	342(5)	3000(7)	19(2)
C(3S')	2996(11)	634(11)	1306(13)	41(4)
O(1S)	3508(2)	160(1)	3292(2)	60(1)
O(1S')	2373(8)	146(5)	2883(13)	79(4)

Table J.3 Bond lengths [Å] and angles [°] for **F_{64}PcNi·2(acetone)**.

Ni-N(2)#1	1.9098(12)	Ni-N(1)	1.9098(12)
Ni-N(2)	1.9099(12)	Ni-N(1)#1	1.9098(12)
N(1)-C(8)	1.3732(18)	C(15)-N(4)#1	1.3186(19)
N(1)-C(1)	1.3741(18)	C(15)-C(16)	1.454(2)
N(2)-C(15)	1.3702(18)	C(16)-C(21)	1.380(2)
N(2)-C(22)	1.3743(19)	C(16)-C(17)	1.382(2)
N(3)-C(22)	1.3192(19)	C(17)-F(4)	1.3356(16)
N(3)-C(1)	1.3197(19)	C(17)-C(18)	1.395(2)
N(4)-C(8)	1.3144(19)	C(18)-C(19)	1.448(2)
N(4)-C(15)#1	1.3186(19)	C(18)-C(26)	1.5449(19)
C(1)-C(2)	1.4544(19)	C(19)-C(20)	1.393(2)
C(2)-C(7)	1.380(2)	C(19)-C(23)	1.548(2)
C(2)-C(3)	1.388(2)	C(20)-F(3)	1.3398(16)
C(3)-F(2)	1.3398(16)	C(20)-C(21)	1.385(2)
C(3)-C(4)	1.390(2)	C(21)-C(22)	1.455(2)
C(4)-C(5)	1.452(2)	C(23)-F(19)	1.3672(17)
C(4)-C(9)	1.546(2)	C(23)-C(24)	1.548(2)
C(5)-C(6)	1.388(2)	C(23)-C(25)	1.583(2)
C(5)-C(12)	1.5476(19)	C(24)-F(22)	1.3239(19)
C(6)-F(1)	1.3372(17)	C(24)-F(20)	1.3279(19)
C(6)-C(7)	1.384(2)	C(24)-F(21)	1.3364(18)
C(7)-C(8)	1.450(2)	C(25)-F(25)	1.3242(19)
C(9)-F(5)	1.3662(17)	C(25)-F(23)	1.3342(18)
C(9)-C(11)	1.550(2)	C(25)-F(24)	1.3340(19)
C(9)-C(10)	1.582(2)	C(26)-F(26)	1.3673(17)
C(10)-F(6)	1.3253(18)	C(26)-C(28)	1.544(2)
C(10)-F(8)	1.3306(18)	C(26)-C(27)	1.590(2)
C(10)-F(7)	1.3334(18)	C(27)-F(29)	1.3262(19)
C(11)-F(10)	1.3166(19)	C(27)-F(28)	1.3299(18)
C(11)-F(11)	1.3279(19)	C(27)-F(27)	1.3307(18)
C(11)-F(9)	1.3326(18)	C(28)-F(32)	1.3285(17)
C(12)-F(12)	1.3652(17)	C(28)-F(31)	1.3331(18)
C(12)-C(13)	1.548(2)	C(28)-F(30)	1.3333(18)
C(12)-C(14)	1.592(2)	C(1S)-C(2S)	1.474(5)
C(13)-F(17)	1.3279(19)	C(2S)-O(1S)	1.177(3)
C(13)-F(18)	1.3279(19)	C(2S)-O(1S')	1.299(10)
C(13)-F(16)	1.3329(18)	C(2S)-C(1S')	1.428(7)
C(14)-F(14)	1.3287(18)	C(2S)-C(3S')	1.481(14)
C(14)-F(15)	1.3301(19)	C(2S)-C(3S)	1.545(4)
C(14)-F(13)	1.3307(19)		
N(2)#1-Ni-N(2)	180.0	N(2)#1-Ni-N(1)#1	89.27(5)
N(2)#1-Ni-N(1)	90.73(5)	N(2)-Ni-N(1)#1	90.73(5)
N(2)-Ni-N(1)	89.27(5)	N(1)-Ni-N(1)#1	180.0
C(8)-N(1)-C(1)	107.34(12)	C(1)-N(1)-Ni	127.07(9)
C(8)-N(1)-Ni	125.50(10)	(15)-N(2)-C(22)	107.29(12)

C(15)-N(2)-Ni	125.70(10)	C(5)-C(12)-C(14)	112.76(12)
C(22)-N(2)-Ni	127.00(10)	C(13)-C(12)-C(14)	110.24(12)
C(22)-N(3)-C(1)	120.05(12)	F(17)-C(13)-F(18)	107.87(14)
C(8)-N(4)-C(15)#1	120.75(12)	F(17)-C(13)-F(16)	107.59(13)
N(3)-C(1)-N(1)	128.26(13)	F(18)-C(13)-F(16)	108.35(13)
N(3)-C(1)-C(2)	121.96(13)	F(17)-C(13)-C(12)	110.26(12)
N(1)-C(1)-C(2)	109.75(12)	F(18)-C(13)-C(12)	112.46(12)
C(7)-C(2)-C(3)	119.03(13)	F(16)-C(13)-C(12)	110.14(14)
C(7)-C(2)-C(1)	106.35(12)	F(14)-C(14)-F(15)	107.32(14)
C(3)-C(2)-C(1)	134.62(13)	F(14)-C(14)-F(13)	106.83(12)
F(2)-C(3)-C(2)	117.81(12)	F(15)-C(14)-F(13)	109.16(12)
F(2)-C(3)-C(4)	119.25(12)	F(14)-C(14)-C(12)	108.99(12)
C(2)-C(3)-C(4)	122.94(13)	F(15)-C(14)-C(12)	110.68(12)
C(3)-C(4)-C(5)	117.50(13)	F(13)-C(14)-C(12)	113.62(14)
C(3)-C(4)-C(9)	116.71(12)	N(4)#1-C(15)-N(2)	128.54(13)
C(5)-C(4)-C(9)	125.71(12)	N(4)#1-C(15)-C(16)	121.65(13)
C(6)-C(5)-C(4)	117.57(13)	N(2)-C(15)-C(16)	109.81(12)
C(6)-C(5)-C(12)	115.25(12)	C(21)-C(16)-C(17)	119.71(13)
C(4)-C(5)-C(12)	126.87(13)	C(21)-C(16)-C(15)	106.64(12)
F(1)-C(6)-C(7)	117.61(13)	C(17)-C(16)-C(15)	133.63(13)
F(1)-C(6)-C(5)	119.57(12)	F(4)-C(17)-C(16)	117.75(13)
C(7)-C(6)-C(5)	122.75(13)	F(4)-C(17)-C(18)	119.36(12)
C(2)-C(7)-C(6)	119.67(13)	C(16)-C(17)-C(18)	122.88(13)
C(2)-C(7)-C(8)	106.98(12)	C(17)-C(18)-C(19)	117.33(13)
C(6)-C(7)-C(8)	133.23(13)	C(17)-C(18)-C(26)	115.83(12)
N(4)-C(8)-N(1)	128.71(13)	C(19)-C(18)-C(26)	126.83(13)
N(4)-C(8)-C(7)	121.70(13)	C(20)-C(19)-C(18)	117.67(13)
N(1)-C(8)-C(7)	109.58(12)	C(20)-C(19)-C(23)	115.60(12)
F(5)-C(9)-C(4)	110.03(12)	C(18)-C(19)-C(23)	126.70(12)
F(5)-C(9)-C(11)	106.55(12)	F(3)-C(20)-C(21)	117.83(12)
C(4)-C(9)-C(11)	112.98(12)	F(3)-C(20)-C(19)	119.18(12)
F(5)-C(9)-C(10)	101.80(11)	C(21)-C(20)-C(19)	122.98(13)
C(4)-C(9)-C(10)	114.82(12)	C(16)-C(21)-C(20)	119.07(13)
C(11)-C(9)-C(10)	109.78(12)	C(16)-C(21)-C(22)	106.51(12)
F(6)-C(10)-F(8)	109.05(12)	C(20)-C(21)-C(22)	134.41(13)
F(6)-C(10)-F(7)	107.88(13)	N(3)-C(22)-N(2)	128.33(13)
F(8)-C(10)-F(7)	106.06(12)	N(3)-C(22)-C(21)	121.95(13)
F(6)-C(10)-C(9)	110.19(12)	N(2)-C(22)-C(21)	109.72(12)
F(8)-C(10)-C(9)	114.75(13)	F(19)-C(23)-C(19)	111.46(12)
F(7)-C(10)-C(9)	108.64(12)	F(19)-C(23)-C(24)	105.75(12)
F(10)-C(11)-F(11)	107.77(13)	C(19)-C(23)-C(24)	112.19(12)
F(10)-C(11)-F(9)	108.32(13)	F(19)-C(23)-C(25)	101.96(11)
F(11)-C(11)-F(9)	107.78(13)	C(19)-C(23)-C(25)	114.15(12)
F(10)-C(11)-C(9)	111.02(13)	C(24)-C(23)-C(25)	110.56(12)
F(11)-C(11)-C(9)	111.48(12)	F(22)-C(24)-F(20)	108.10(13)
F(9)-C(11)-C(9)	110.34(13)	F(22)-C(24)-F(21)	108.05(13)
F(12)-C(12)-C(5)	110.87(12)	F(20)-C(24)-F(21)	108.49(13)
F(12)-C(12)-C(13)	105.68(12)	F(22)-C(24)-C(23)	110.08(12)
C(5)-C(12)-C(13)	113.87(13)	F(20)-C(24)-C(23)	111.56(12)
F(12)-C(12)-C(14)	102.61(12)	F(21)-C(24)-C(23)	110.47(13)

F(25)-C(25)-F(23)	106.63(12)	F(29)-C(27)-F(28)	106.94(12)
F(25)-C(25)-F(24)	108.85(12)	F(29)-C(27)-F(27)	109.05(13)
F(23)-C(25)-F(24)	107.17(13)	F(28)-C(27)-F(27)	107.85(13)
F(25)-C(25)-C(23)	114.17(13)	F(29)-C(27)-C(26)	113.81(13)
F(23)-C(25)-C(23)	109.36(12)	F(28)-C(27)-C(26)	108.34(12)
F(24)-C(25)-C(23)	110.39(12)	F(27)-C(27)-C(26)	110.62(12)
F(26)-C(26)-C(28)	106.41(12)	F(32)-C(28)-F(31)	108.38(12)
F(26)-C(26)-C(18)	110.95(12)	F(32)-C(28)-F(30)	107.55(12)
C(28)-C(26)-C(18)	111.55(12)	F(31)-C(28)-F(30)	107.34(12)
F(26)-C(26)-C(27)	102.14(11)	F(32)-C(28)-C(26)	110.99(12)
C(28)-C(26)-C(27)	109.87(12)	F(31)-C(28)-C(26)	111.61(12)
C(18)-C(26)-C(27)	115.20(12)	F(30)-C(28)-C(26)	110.81(12)
O(1S)-C(2S)-O(1S')	87.6(7)	C(1S')-C(2S)-C(3S')	106.1(7)
O(1S)-C(2S)-C(1S')	39.2(3)	C(1S)-C(2S)-C(3S')	21.4(6)
O(1S')-C(2S)-C(1S')	126.4(7)	O(1S)-C(2S)-C(3S)	120.8(3)
O(1S)-C(2S)-C(1S)	124.4(3)	O(1S')-C(2S)-C(3S)	35.3(6)
O(1S')-C(2S)-C(1S)	146.6(6)	C(1S')-C(2S)-C(3S)	159.7(4)
C(1S')-C(2S)-C(1S)	85.2(4)	C(1S)-C(2S)-C(3S)	114.7(3)
O(1S)-C(2S)-C(3S')	145.2(6)	C(3S')-C(2S)-C(3S)	93.5(6)
O(1S')-C(2S)-C(3S')	127.1(8)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1

Table J.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **F_{64}PcNi·2(acetone)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a\cdot^2 U^{11} + ... + 2 h k a\cdot b\cdot U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	11(1)	8(1)	13(1)	0(1)	6(1)	-1(1)
N(1)	12(1)	11(1)	12(1)	0(1)	4(1)	-1(1)
N(2)	12(1)	10(1)	12(1)	0(1)	4(1)	0(1)
N(3)	12(1)	12(1)	12(1)	0(1)	4(1)	-1(1)
N(4)	14(1)	10(1)	14(1)	0(1)	5(1)	0(1)
C(1)	12(1)	10(1)	11(1)	0(1)	3(1)	1(1)
C(2)	12(1)	12(1)	10(1)	1(1)	2(1)	-1(1)
C(3)	15(1)	9(1)	12(1)	1(1)	3(1)	-1(1)
C(4)	14(1)	12(1)	11(1)	0(1)	2(1)	1(1)
C(5)	14(1)	14(1)	12(1)	0(1)	4(1)	-1(1)
C(6)	14(1)	10(1)	15(1)	1(1)	4(1)	-1(1)
C(7)	14(1)	11(1)	11(1)	1(1)	3(1)	0(1)
C(8)	12(1)	13(1)	10(1)	1(1)	4(1)	1(1)
C(9)	15(1)	14(1)	14(1)	-1(1)	6(1)	0(1)
C(10)	21(1)	16(1)	17(1)	-5(1)	6(1)	0(1)
C(11)	21(1)	16(1)	21(1)	-1(1)	4(1)	4(1)
C(12)	14(1)	14(1)	22(1)	-5(1)	8(1)	1(1)
C(13)	22(1)	18(1)	26(1)	-2(1)	14(1)	-3(1)
C(14)	14(1)	21(1)	30(1)	-8(1)	8(1)	-2(1)

C(15)	12(1)	12(1)	12(1)	1(1)	3(1)	-1(1)
C(16)	13(1)	12(1)	11(1)	0(1)	3(1)	0(1)
C(17)	12(1)	14(1)	14(1)	-1(1)	5(1)	1(1)
C(18)	13(1)	14(1)	11(1)	1(1)	3(1)	-2(1)
C(19)	12(1)	11(1)	12(1)	-1(1)	2(1)	-1(1)
C(20)	12(1)	13(1)	11(1)	-1(1)	3(1)	2(1)
C(21)	12(1)	12(1)	11(1)	0(1)	3(1)	0(1)
C(22)	13(1)	11(1)	11(1)	1(1)	2(1)	0(1)
C(23)	16(1)	11(1)	17(1)	1(1)	6(1)	-2(1)
C(24)	24(1)	13(1)	22(1)	-3(1)	7(1)	-3(1)
C(25)	20(1)	14(1)	26(1)	3(1)	7(1)	2(1)
C(26)	14(1)	11(1)	17(1)	-2(1)	5(1)	-3(1)
C(27)	15(1)	17(1)	26(1)	3(1)	7(1)	-3(1)
C(28)	17(1)	16(1)	20(1)	1(1)	7(1)	-4(1)
F(1)	18(1)	10(1)	29(1)	-1(1)	13(1)	-3(1)
F(2)	19(1)	9(1)	22(1)	-1(1)	10(1)	-3(1)
F(3)	16(1)	12(1)	22(1)	-2(1)	12(1)	1(1)
F(4)	17(1)	13(1)	26(1)	-2(1)	14(1)	0(1)
F(5)	19(1)	19(1)	19(1)	-5(1)	11(1)	-1(1)
F(6)	22(1)	26(1)	24(1)	-4(1)	-4(1)	2(1)
F(7)	30(1)	24(1)	19(1)	-11(1)	10(1)	-4(1)
F(8)	28(1)	17(1)	26(1)	-7(1)	12(1)	-8(1)
F(9)	44(1)	20(1)	36(1)	0(1)	13(1)	18(1)
F(10)	25(1)	31(1)	38(1)	9(1)	-11(1)	-1(1)
F(11)	32(1)	24(1)	22(1)	8(1)	8(1)	6(1)
F(12)	14(1)	16(1)	29(1)	-6(1)	6(1)	3(1)
F(13)	22(1)	19(1)	41(1)	-9(1)	13(1)	-7(1)
F(14)	12(1)	33(1)	45(1)	-15(1)	2(1)	0(1)
F(15)	23(1)	30(1)	22(1)	-10(1)	6(1)	-4(1)
F(16)	27(1)	35(1)	40(1)	-2(1)	24(1)	-7(1)
F(17)	38(1)	26(1)	19(1)	-4(1)	12(1)	-5(1)
F(18)	37(1)	22(1)	29(1)	6(1)	17(1)	4(1)
F(19)	21(1)	12(1)	22(1)	4(1)	10(1)	-1(1)
F(20)	34(1)	24(1)	16(1)	-4(1)	9(1)	-7(1)
F(21)	43(1)	12(1)	33(1)	-8(1)	11(1)	-2(1)
F(22)	22(1)	28(1)	23(1)	-7(1)	0(1)	-5(1)
F(23)	27(1)	20(1)	43(1)	16(1)	10(1)	8(1)
F(24)	19(1)	26(1)	25(1)	2(1)	-1(1)	0(1)
F(25)	24(1)	20(1)	36(1)	2(1)	16(1)	6(1)
F(26)	18(1)	12(1)	23(1)	-4(1)	5(1)	-5(1)
F(27)	19(1)	25(1)	27(1)	11(1)	3(1)	0(1)
F(28)	13(1)	24(1)	35(1)	3(1)	3(1)	-6(1)
F(29)	18(1)	21(1)	36(1)	-1(1)	14(1)	1(1)
F(30)	26(1)	25(1)	19(1)	5(1)	3(1)	4(1)
F(31)	29(1)	22(1)	17(1)	-4(1)	8(1)	-5(1)
F(32)	25(1)	31(1)	25(1)	5(1)	13(1)	-10(1)
C(1S)	57(3)	31(2)	54(3)	-10(2)	34(2)	-4(2)
C(2S)	40(1)	26(1)	27(1)	-7(1)	4(1)	7(1)
C(3S)	33(2)	39(2)	53(2)	1(2)	7(1)	0(1)
C(1S')	4(4)	42(5)	11(4)	5(3)	4(3)	-3(3)

C(3S')	35(9)	50(10)	37(7)	-1(6)	6(6)	9(7)
O(1S)	63(2)	70(2)	32(1)	-3(1)	-24(1)	7(1)
O(1S')	73(8)	64(6)	103(11)	8(6)	24(7)	-9(5)

Table J.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **F_{64}PcNi·2(acetone)**.

	x	y	z	U(eq)
H(1S1)	3944	846	1801	66
H(1S2)	2946	1080	1334	66
H(1S3)	3298	430	850	66
H(3S1)	1908	-109	2815	63
H(3S2)	1917	-120	1475	63
H(3S3)	1683	534	2067	63
H(1S4)	3994	460	3805	28
H(1S5)	4267	661	2626	28
H(1S6)	4211	-87	2953	28
H(3S4)	3576	601	1092	62
H(3S5)	2833	1090	1344	62
H(3S6)	2550	412	732	62

Appendix K: Crystal structure of $F_{64}PcNi(THF)_2$

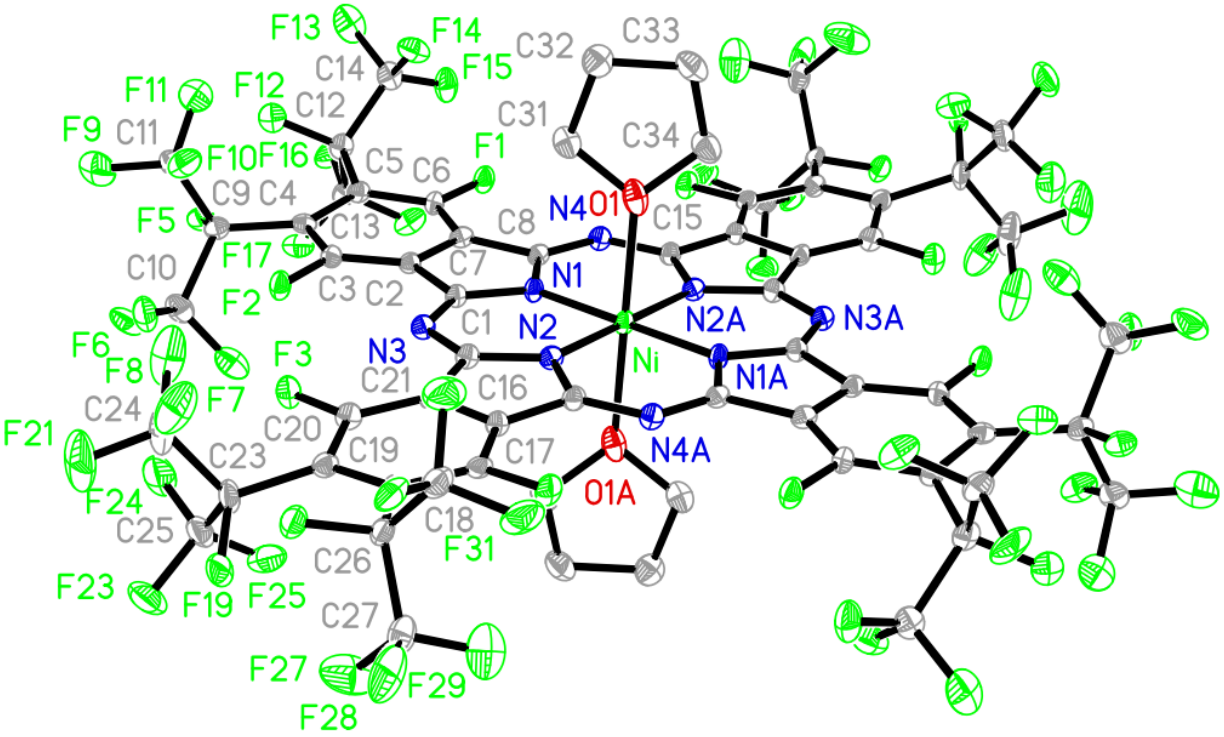


Figure K.1 ORTEP representation for the X-ray crystal structure of **$F_{64}PcNi(THF)_2$**, at 50% probability. The symmetric atoms are not numbered, the second acetone molecule is not showed.

Table K.1 Crystal data and structure refinement for **$F_{64}PcNi(THF)_2$**.

Empirical formula	C64 H16 F64 N8 Ni O2
Formula weight	2203.56
Temperature	130(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 15.1219(11) Å alpha = 90 deg.
	b = 20.9127(15) Å beta = 102.076(2) deg.
	c = 12.0539(9) Å gamma = 90 deg.
Volume	3727.6(5) $Å^3$
Z, Calculated density	2, 1.963 g/cm^3
Absorption coefficient	0.474 mm^{-1}
F(000)	2152
Crystal size	0.220 x 0.130 x 0.020 mm
Theta range for data collection	1.983 to 26.370 deg.
Limiting indices	-18<=h<=18, -26<=k<=26, -15<=l<=15
Reflections collected /unique	85248 / 7608 [R(int) = 0.1437]

Completeness to theta = 25.000	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.5573
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7608 / 222 / 668
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1058
R indices (all data)	R1 = 0.0935, wR2 = 0.1285
Extinction coefficient	n/a
Largest diff. peak and hole	0.838 and -0.758 e.$Å^{-3}$

Table K.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **F_{64}PcNi(THF)$_2$**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ni	5000	5000	5000	14(1)
N(1)	4473(2)	5841(1)	5128(2)	14(1)
N(2)	4153(2)	4620(1)	5833(2)	15(1)
N(3)	3293(2)	5558(1)	6124(2)	15(1)
N(4)	5438(2)	6499(1)	4226(2)	16(1)
C(1)	3770(2)	5966(1)	5644(3)	13(1)
C(2)	3599(2)	6653(1)	5604(3)	14(1)
C(3)	2963(2)	7036(2)	5950(3)	16(1)
C(4)	2937(2)	7696(1)	5810(3)	15(1)
C(5)	3644(2)	7988(1)	5342(3)	15(1)
C(6)	4239(2)	7584(2)	4945(3)	14(1)
C(7)	4229(2)	6925(1)	5075(3)	14(1)
C(8)	4771(2)	6404(1)	4764(3)	14(1)
C(9)	2123(2)	8036(1)	6147(3)	18(1)
C(10)	1179(2)	7697(2)	5721(3)	24(1)
C(11)	2296(2)	8161(2)	7433(3)	21(1)
C(12)	3830(2)	8710(2)	5259(3)	18(1)
C(13)	3440(2)	8976(2)	4060(3)	23(1)
C(14)	4858(2)	8899(2)	5656(3)	21(1)
C(15)	5934(2)	6021(2)	3964(3)	15(1)
C(16)	3300(2)	3886(1)	6578(3)	14(1)
C(17)	2909(2)	3359(1)	6988(3)	14(1)
C(18)	2149(2)	3393(2)	7454(3)	15(1)
C(19)	1713(2)	4013(2)	7442(3)	17(1)
C(20)	2161(2)	4534(2)	7105(3)	16(1)

C(21)	2932(2)	4483(1)	6672(3)	14(1)
C(22)	3474(2)	4940(2)	6192(3)	15(1)
C(23)	765(2)	4154(2)	7671(3)	25(1)
C(24)	769(3)	4418(2)	8856(4)	39(1)
C(25)	165(2)	4592(2)	6729(4)	40(1)
C(26)	1856(2)	2775(2)	7980(3)	17(1)
C(27)	1316(2)	2314(2)	7085(3)	27(1)
C(28)	2648(2)	2408(2)	8787(3)	24(1)
F(1)	4868(1)	7832(1)	4442(2)	20(1)
F(2)	2342(1)	6752(1)	6425(2)	21(1)
F(3)	1808(1)	5120(1)	7144(2)	23(1)
F(4)	3313(1)	2792(1)	6946(2)	21(1)
F(5)	1985(1)	8625(1)	5645(2)	22(1)
F(6)	546(1)	8141(1)	5431(2)	32(1)
F(7)	1188(1)	7345(1)	4805(2)	30(1)
F(8)	928(1)	7332(1)	6498(2)	31(1)
F(9)	1592(1)	8442(1)	7714(2)	37(1)
F(10)	2466(1)	7623(1)	8027(2)	29(1)
F(11)	3010(1)	8538(1)	7765(2)	31(1)
F(12)	3434(1)	9050(1)	5986(2)	22(1)
F(13)	4913(1)	9463(1)	6181(2)	35(1)
F(14)	5288(1)	8478(1)	6398(2)	28(1)
F(15)	5300(1)	8965(1)	4822(2)	29(1)
F(16)	3616(2)	9600(1)	4021(2)	36(1)
F(17)	2553(1)	8899(1)	3791(2)	32(1)
F(18)	3798(1)	8683(1)	3281(2)	29(1)
F(19)	267(1)	3603(1)	7582(2)	30(1)
F(20)	1124(2)	4004(1)	9658(2)	46(1)
F(21)	-68(2)	4549(1)	8966(3)	63(1)
F(22)	1258(2)	4953(1)	9063(2)	49(1)
F(23)	-691(2)	4398(1)	6561(3)	66(1)
F(24)	172(2)	5206(1)	7007(3)	54(1)
F(25)	427(2)	4531(1)	5748(2)	45(1)
F(26)	1305(1)	2916(1)	8710(2)	23(1)
F(27)	588(2)	2595(1)	6504(2)	52(1)
F(28)	1060(2)	1804(1)	7580(2)	47(1)
F(29)	1795(2)	2122(1)	6351(2)	43(1)
F(30)	3263(2)	2808(1)	9304(2)	42(1)
F(31)	3044(2)	1961(1)	8269(2)	40(1)
F(32)	2317(1)	2094(1)	9566(2)	30(1)
O(1)	6026(6)	5170(3)	6607(6)	24(2)
C(31)	5871(7)	5627(4)	7439(7)	22(2)
C(32)	6713(8)	5619(5)	8376(9)	26(2)
C(33)	7443(7)	5305(4)	7845(8)	30(2)

C(34)	6994(7)	5207(4)	6616(8)	27(2)
O(1A)	6350(20)	5190(13)	6840(20)	47(5)
C(31A)	6200(20)	5631(14)	7700(30)	26(4)
C(32A)	7031(18)	5654(17)	8580(30)	25(5)
C(33A)	7761(19)	5320(14)	8070(30)	30(2)
C(34A)	7280(20)	5227(17)	6910(30)	37(5)

Table K.3 Bond lengths [Å] and angles [deg] for **F_{64}PcNi(THF)$_2$**.

Ni-N(1)#1	1.951(3)	C(10)-F(7)	1.329(4)
Ni-N(1)	1.951(3)	C(11)-F(9)	1.321(4)
Ni-N(2)	1.955(3)	C(11)-F(11)	1.329(4)
Ni-N(2)#1	1.955(3)	C(11)-F(10)	1.331(4)
Ni-O(1)#1	2.242(9)	C(12)-F(12)	1.361(4)
Ni-O(1)	2.242(9)	C(12)-C(13)	1.545(5)
Ni-O(1A)	2.71(3)	C(12)-C(14)	1.578(5)
		C(13)-F(17)	1.323(4)
N(1)-C(1)	1.363(4)	C(13)-F(18)	1.327(4)
N(1)-C(8)	1.365(4)	C(13)-F(16)	1.336(4)
N(2)-C(22)	1.370(4)	C(14)-F(15)	1.325(4)
N(2)-C(15)#1	1.372(4)	C(14)-F(14)	1.326(4)
N(3)-C(22)	1.319(4)	C(14)-F(13)	1.332(4)
N(3)-C(1)	1.325(4)	C(15)-C(16)#1	1.457(4)
N(4)-C(8)	1.324(4)	C(16)-C(21)	1.381(4)
N(4)-C(15)	1.327(4)	C(16)-C(17)	1.390(4)
C(1)-C(2)	1.460(4)	C(17)-F(4)	1.340(3)
C(2)-C(7)	1.376(4)	C(17)-C(18)	1.383(4)
C(2)-C(3)	1.381(4)	C(18)-C(19)	1.452(4)
C(3)-F(2)	1.337(3)	C(18)-C(26)	1.546(4)
C(3)-C(4)	1.389(4)	C(19)-C(20)	1.389(4)
C(4)-C(5)	1.445(4)	C(19)-C(23)	1.545(5)
C(4)-C(9)	1.549(4)	C(20)-F(3)	1.340(3)
C(5)-C(6)	1.390(4)	C(20)-C(21)	1.377(4)
C(5)-C(12)	1.542(4)	C(21)-C(22)	1.457(4)
C(6)-F(1)	1.336(3)	C(23)-F(19)	1.369(4)
C(6)-C(7)	1.387(4)	C(23)-C(24)	1.530(6)
C(7)-C(8)	1.459(4)	C(23)-C(25)	1.587(5)
C(9)-F(5)	1.368(3)	C(24)-F(20)	1.326(5)
C(9)-C(11)	1.539(5)	C(24)-F(21)	1.329(5)
C(9)-C(10)	1.580(5)	C(24)-F(22)	1.335(4)
C(10)-F(8)	1.323(4)	C(25)-F(24)	1.327(5)
C(10)-F(6)	1.327(4)	C(25)-F(25)	1.330(5)

C(25)-F(23)	1.330(4)
C(26)-F(26)	1.365(4)
C(26)-C(27)	1.546(5)
C(26)-C(28)	1.576(5)
C(27)-F(27)	1.313(4)
C(27)-F(29)	1.318(4)
C(27)-F(28)	1.319(4)
C(28)-F(30)	1.308(4)
C(28)-F(32)	1.327(4)
C(28)-F(31)	1.333(4)
O(1)-C(31)	1.441(8)
O(1)-C(34)	1.464(7)
C(31)-C(32)	1.515(8)
C(31)-H(31A)	0.99
C(31)-H(31B)	0.99
C(32)-C(33)	1.534(10)
C(32)-H(32A)	0.99
C(32)-H(32B)	0.99
C(33)-C(34)	1.509(8)
C(33)-H(33A)	0.99
C(33)-H(33B)	0.99
C(34)-H(34A)	0.99
C(34)-H(34B)	0.99
O(1A)-C(34A)	1.40(3)
O(1A)-C(31A)	1.44(3)
C(31A)-C(32A)	1.47(2)
C(31A)-H(31C)	0.99
C(31A)-H(31D)	0.99
C(32A)-C(33A)	1.54(4)
C(32A)-H(32C)	0.99
C(32A)-H(32D)	0.99
C(33A)-C(34A)	1.44(3)
C(33A)-H(33C)	0.99
C(33A)-H(33D)	0.99
C(34A)-H(34C)	0.99
C(34A)-H(34D)	0.99

N(1)#1-Ni-N(1)	180.00(14)
N(1)#1-Ni-N(2)	89.80(10)
N(1)-Ni-N(2)	90.20(10)
N(1)#1-Ni-N(2)#1	90.20(10)
N(1)-Ni-N(2)#1	89.80(10)
N(2)-Ni-N(2)#1	180
N(1)#1-Ni-O(1)#1	90.54(17)
N(1)-Ni-O(1)#1	89.46(17)
N(2)-Ni-O(1)#1	88.29(17)
N(2)#1-Ni-O(1)#1	91.71(17)
N(1)#1-Ni-O(1)	89.46(17)
N(1)-Ni-O(1)	90.54(17)
N(2)-Ni-O(1)	91.71(17)
N(2)#1-Ni-O(1)	88.29(17)
O(1)#1-Ni-O(1)	180.0(3)
N(1)#1-Ni-O(1A)	87.0(6)
N(1)-Ni-O(1A)	93.0(6)
N(2)-Ni-O(1A)	95.7(6)
N(2)#1-Ni-O(1A)	84.3(6)

C(1)-N(1)-C(8)	108.8(2)
C(1)-N(1)-Ni	125.4(2)
C(8)-N(1)-Ni	125.7(2)
C(22)-N(2)-C(15)#1	108.4(3)
C(22)-N(2)-Ni	125.3(2)
C(15)#1-N(2)-Ni	125.9(2)
C(22)-N(3)-C(1)	122.2(3)
C(8)-N(4)-C(15)	122.0(3)
N(3)-C(1)-N(1)	128.6(3)
N(3)-C(1)-C(2)	122.6(3)
N(1)-C(1)-C(2)	108.8(3)
C(7)-C(2)-C(3)	119.6(3)
C(7)-C(2)-C(1)	106.7(3)
C(3)-C(2)-C(1)	133.7(3)
F(2)-C(3)-C(2)	117.9(3)
F(2)-C(3)-C(4)	119.3(3)
C(2)-C(3)-C(4)	122.9(3)
C(3)-C(4)-C(5)	117.6(3)
C(3)-C(4)-C(9)	115.4(3)
C(5)-C(4)-C(9)	127.0(3)
C(6)-C(5)-C(4)	117.6(3)
C(6)-C(5)-C(12)	115.6(3)
C(4)-C(5)-C(12)	126.8(3)
F(1)-C(6)-C(7)	117.5(3)
F(1)-C(6)-C(5)	119.7(3)
C(7)-C(6)-C(5)	122.8(3)
C(2)-C(7)-C(6)	119.2(3)
C(2)-C(7)-C(8)	106.9(3)
C(6)-C(7)-C(8)	133.9(3)
N(4)-C(8)-N(1)	128.6(3)
N(4)-C(8)-C(7)	122.7(3)

N(1)-C(8)-C(7)	108.7(3)	F(4)-C(17)-C(16)	117.3(3)
F(5)-C(9)-C(11)	105.7(2)	C(18)-C(17)-C(16)	123.7(3)
F(5)-C(9)-C(4)	110.7(3)	C(17)-C(18)-C(19)	117.2(3)
C(11)-C(9)-C(4)	111.4(3)	C(17)-C(18)-C(26)	117.2(3)
F(5)-C(9)-C(10)	102.5(2)	C(19)-C(18)-C(26)	125.6(3)
C(11)-C(9)-C(10)	110.9(3)	C(20)-C(19)-C(18)	117.1(3)
C(4)-C(9)-C(10)	114.9(3)	C(20)-C(19)-C(23)	115.4(3)
F(8)-C(10)-F(6)	106.9(3)	C(18)-C(19)-C(23)	127.3(3)
F(8)-C(10)-F(7)	108.9(3)	F(3)-C(20)-C(21)	117.4(3)
F(6)-C(10)-F(7)	107.5(3)	F(3)-C(20)-C(19)	119.0(3)
F(8)-C(10)-C(9)	113.7(3)	C(21)-C(20)-C(19)	123.5(3)
F(6)-C(10)-C(9)	108.9(3)	C(20)-C(21)-C(16)	119.3(3)
F(7)-C(10)-C(9)	110.7(3)	C(20)-C(21)-C(22)	133.7(3)
F(9)-C(11)-F(11)	107.8(3)	C(16)-C(21)-C(22)	106.9(3)
F(9)-C(11)-F(10)	108.3(3)	N(3)-C(22)-N(2)	128.2(3)
F(11)-C(11)-F(10)	106.6(3)	N(3)-C(22)-C(21)	122.8(3)
F(9)-C(11)-C(9)	111.0(3)	N(2)-C(22)-C(21)	109.0(3)
F(11)-C(11)-C(9)	111.1(3)	F(19)-C(23)-C(24)	105.8(3)
F(10)-C(11)-C(9)	111.8(3)	F(19)-C(23)-C(19)	109.9(3)
F(12)-C(12)-C(5)	111.1(3)	C(24)-C(23)-C(19)	114.4(3)
F(12)-C(12)-C(13)	106.3(3)	F(19)-C(23)-C(25)	101.9(3)
C(5)-C(12)-C(13)	112.0(3)	C(24)-C(23)-C(25)	110.5(3)
F(12)-C(12)-C(14)	102.2(2)	C(19)-C(23)-C(25)	113.3(3)
C(5)-C(12)-C(14)	114.0(3)	F(20)-C(24)-F(21)	108.1(3)
C(13)-C(12)-C(14)	110.6(3)	F(20)-C(24)-F(22)	106.8(4)
F(17)-C(13)-F(18)	108.3(3)	F(21)-C(24)-F(22)	108.1(3)
F(17)-C(13)-F(16)	108.0(3)	F(20)-C(24)-C(23)	111.5(3)
F(18)-C(13)-F(16)	108.1(3)	F(21)-C(24)-C(23)	110.4(4)
F(17)-C(13)-C(12)	110.8(3)	F(22)-C(24)-C(23)	111.7(3)
F(18)-C(13)-C(12)	111.3(3)	F(24)-C(25)-F(25)	109.2(3)
F(16)-C(13)-C(12)	110.2(3)	F(24)-C(25)-F(23)	106.8(3)
F(15)-C(14)-F(14)	109.1(3)	F(25)-C(25)-F(23)	107.2(4)
F(15)-C(14)-F(13)	106.1(3)	F(24)-C(25)-C(23)	113.8(4)
F(14)-C(14)-F(13)	107.1(3)	F(25)-C(25)-C(23)	110.5(3)
F(15)-C(14)-C(12)	114.6(3)	F(23)-C(25)-C(23)	109.1(3)
F(14)-C(14)-C(12)	110.5(3)	F(26)-C(26)-C(18)	110.4(3)
F(13)-C(14)-C(12)	109.1(3)	F(26)-C(26)-C(27)	106.3(3)
N(4)-C(15)-N(2)#1	127.8(3)	C(18)-C(26)-C(27)	113.0(3)
N(4)-C(15)-C(16)#1	123.2(3)	F(26)-C(26)-C(28)	101.3(2)
N(2)#1-C(15)-C(16)#1	109.0(3)	C(18)-C(26)-C(28)	114.5(3)
C(21)-C(16)-C(17)	118.6(3)	C(27)-C(26)-C(28)	110.5(3)
C(21)-C(16)-C(15)#1	106.7(3)	F(27)-C(27)-F(29)	107.2(3)
C(17)-C(16)-C(15)#1	134.6(3)	F(27)-C(27)-F(28)	108.1(3)
F(4)-C(17)-C(18)	119.1(3)	F(29)-C(27)-F(28)	108.2(3)

F(27)-C(27)-C(26)	110.8(3)	C(33)-C(34)-H(34A)	110.8
F(29)-C(27)-C(26)	111.9(3)	O(1)-C(34)-H(34B)	110.8
F(28)-C(27)-C(26)	110.5(3)	C(33)-C(34)-H(34B)	110.8
F(30)-C(28)-F(32)	108.4(3)	H(34A)-C(34)-H(34B)	108.8
F(30)-C(28)-F(31)	109.1(3)	C(34A)-O(1A)-C(31A)	103.4(19)
F(32)-C(28)-F(31)	104.9(3)	C(34A)-O(1A)-Ni	129.4(18)
F(30)-C(28)-C(26)	110.9(3)	C(31A)-O(1A)-Ni	118.4(15)
F(32)-C(28)-C(26)	109.1(3)	O(1A)-C(31A)-C(32A)	107(2)
F(31)-C(28)-C(26)	114.2(3)	O(1A)-C(31A)-H(31C)	110.3
C(31)-O(1)-C(34)	105.5(5)	C(32A)-C(31A)-H(31C)	110.3
C(31)-O(1)-Ni	121.5(4)	O(1A)-C(31A)-H(31D)	110.3
C(34)-O(1)-Ni	121.7(4)	C(32A)-C(31A)-H(31D)	110.3
O(1)-C(31)-C(32)	106.1(5)	H(31C)-C(31A)-H(31D)	108.5
O(1)-C(31)-H(31A)	110.5	C(31A)-C(32A)-C(33A)	106(2)
C(32)-C(31)-H(31A)	110.5	C(31A)-C(32A)-H(32C)	110.5
O(1)-C(31)-H(31B)	110.5	C(33A)-C(32A)-H(32C)	110.5
C(32)-C(31)-H(31B)	110.5	C(31A)-C(32A)-H(32D)	110.5
H(31A)-C(31)-H(31B)	108.7	C(33A)-C(32A)-H(32D)	110.5
C(31)-C(32)-C(33)	105.1(5)	H(32C)-C(32A)-H(32D)	108.7
C(31)-C(32)-H(32A)	110.7	C(34A)-C(33A)-C(32A)	100.9(19)
C(33)-C(32)-H(32A)	110.7	C(34A)-C(33A)-H(33C)	111.6
C(31)-C(32)-H(32B)	110.7	C(32A)-C(33A)-H(33C)	111.6
C(33)-C(32)-H(32B)	110.7	C(34A)-C(33A)-H(33D)	111.6
H(32A)-C(32)-H(32B)	108.8	C(32A)-C(33A)-H(33D)	111.6
C(34)-C(33)-C(32)	104.6(5)	H(33C)-C(33A)-H(33D)	109.4
C(34)-C(33)-H(33A)	110.8	O(1A)-C(34A)-C(33A)	111(2)
C(32)-C(33)-H(33A)	110.8	O(1A)-C(34A)-H(34C)	109.4
C(34)-C(33)-H(33B)	110.8	C(33A)-C(34A)-H(34C)	109.4
C(32)-C(33)-H(33B)	110.8	O(1A)-C(34A)-H(34D)	109.4
H(33A)-C(33)-H(33B)	108.9	C(33A)-C(34A)-H(34D)	109.4
O(1)-C(34)-C(33)	105.0(5)	H(34C)-C(34A)-H(34D)	108
O(1)-C(34)-H(34A)	110.8		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Table K.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **F_{64}PcNi(THF)$_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{\cdot 2} U^{11}$ + ... + 2 h k a· b· U^{12}].

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ni	16(1)	8(1)	19(1)	1(1)	7(1)	1(1)
N(1)	15(1)	11(1)	18(1)	0(1)	6(1)	-3(1)
N(2)	16(1)	7(1)	22(1)	1(1)	5(1)	1(1)
N(3)	16(1)	10(1)	19(1)	-1(1)	4(1)	0(1)
N(4)	17(1)	12(1)	18(1)	-1(1)	6(1)	1(1)
C(1)	15(2)	9(2)	15(2)	-2(1)	4(1)	-1(1)
C(2)	15(2)	10(2)	16(2)	1(1)	4(1)	1(1)
C(3)	14(2)	14(2)	19(2)	2(1)	4(1)	-1(1)
C(4)	16(2)	12(2)	16(2)	-1(1)	1(1)	3(1)
C(5)	17(2)	10(2)	17(2)	0(1)	2(1)	-1(1)
C(6)	16(2)	13(2)	14(2)	0(1)	5(1)	-2(1)
C(7)	17(2)	12(2)	14(2)	-1(1)	2(1)	1(1)
C(8)	16(2)	11(2)	14(2)	0(1)	3(1)	-1(1)
C(9)	20(2)	10(2)	23(2)	2(1)	5(1)	3(1)
C(10)	21(2)	21(2)	32(2)	-4(2)	7(2)	5(2)
C(11)	19(2)	18(2)	27(2)	-3(1)	7(2)	6(1)
C(12)	23(2)	9(2)	23(2)	-2(1)	8(1)	1(1)
C(13)	28(2)	12(2)	30(2)	4(1)	5(2)	0(1)
C(14)	23(2)	13(2)	28(2)	-6(1)	6(2)	-2(1)
C(15)	16(2)	13(2)	17(2)	0(1)	2(1)	-2(1)
C(16)	15(2)	11(2)	15(2)	-2(1)	3(1)	-2(1)
C(17)	16(2)	8(2)	18(2)	2(1)	2(1)	1(1)
C(18)	18(2)	10(2)	18(2)	-1(1)	4(1)	-2(1)
C(19)	18(2)	14(2)	18(2)	2(1)	5(1)	2(1)
C(20)	20(2)	10(2)	20(2)	-3(1)	7(1)	2(1)
C(21)	16(2)	11(2)	15(2)	2(1)	4(1)	-1(1)
C(22)	17(2)	12(2)	16(2)	-1(1)	4(1)	-1(1)
C(23)	18(2)	17(2)	44(2)	7(2)	16(2)	-2(1)
C(24)	44(3)	22(2)	62(3)	-1(2)	39(2)	-2(2)
C(25)	16(2)	26(2)	81(3)	26(2)	14(2)	3(2)
C(26)	19(2)	15(2)	19(2)	4(1)	8(1)	0(1)
C(27)	29(2)	20(2)	32(2)	1(2)	9(2)	-10(2)
C(28)	28(2)	20(2)	27(2)	7(2)	10(2)	2(2)
F(1)	22(1)	13(1)	28(1)	3(1)	12(1)	-1(1)
F(2)	21(1)	14(1)	33(1)	4(1)	15(1)	1(1)
F(3)	22(1)	10(1)	41(1)	2(1)	16(1)	3(1)
F(4)	23(1)	9(1)	32(1)	2(1)	13(1)	2(1)
F(5)	22(1)	13(1)	32(1)	4(1)	5(1)	7(1)

F(6)	18(1)	26(1)	49(1)	-2(1)	1(1)	7(1)
F(7)	22(1)	28(1)	37(1)	-12(1)	1(1)	1(1)
F(8)	24(1)	26(1)	46(1)	2(1)	18(1)	-1(1)
F(9)	34(1)	44(1)	35(1)	-9(1)	13(1)	16(1)
F(10)	38(1)	28(1)	23(1)	5(1)	9(1)	7(1)
F(11)	33(1)	31(1)	26(1)	-7(1)	1(1)	-5(1)
F(12)	27(1)	12(1)	30(1)	-5(1)	10(1)	2(1)
F(13)	33(1)	20(1)	52(1)	-17(1)	9(1)	-10(1)
F(14)	22(1)	27(1)	31(1)	-1(1)	-3(1)	2(1)
F(15)	29(1)	20(1)	42(1)	-3(1)	16(1)	-7(1)
F(16)	52(1)	12(1)	45(1)	11(1)	7(1)	0(1)
F(17)	27(1)	33(1)	32(1)	9(1)	-1(1)	6(1)
F(18)	42(1)	25(1)	22(1)	4(1)	8(1)	4(1)
F(19)	18(1)	18(1)	54(1)	11(1)	10(1)	-3(1)
F(20)	74(2)	35(1)	37(1)	-1(1)	29(1)	-3(1)
F(21)	61(2)	43(2)	106(2)	2(2)	67(2)	8(1)
F(22)	72(2)	28(1)	61(2)	-14(1)	45(1)	-12(1)
F(23)	16(1)	48(2)	132(3)	49(2)	7(1)	2(1)
F(24)	33(1)	26(1)	111(2)	27(1)	33(1)	13(1)
F(25)	34(1)	44(2)	52(2)	28(1)	-4(1)	0(1)
F(26)	25(1)	19(1)	28(1)	6(1)	13(1)	2(1)
F(27)	43(2)	41(2)	57(2)	-12(1)	-22(1)	-3(1)
F(28)	63(2)	31(1)	50(2)	-1(1)	16(1)	-30(1)
F(29)	50(2)	39(1)	43(1)	-19(1)	18(1)	-19(1)
F(30)	33(1)	38(1)	46(1)	16(1)	-14(1)	-11(1)
F(31)	48(1)	32(1)	46(1)	19(1)	23(1)	23(1)
F(32)	35(1)	28(1)	29(1)	16(1)	12(1)	4(1)
O(1)	21(3)	20(2)	32(3)	-9(2)	12(2)	-6(2)
C(31)	21(4)	26(3)	20(4)	-8(2)	5(3)	-4(3)
C(32)	30(5)	22(3)	26(4)	-3(3)	4(4)	-5(4)
C(33)	18(4)	35(2)	33(4)	-1(3)	0(3)	-3(3)
C(34)	20(5)	38(3)	24(4)	-3(3)	6(3)	-1(3)
O(1A)	31(9)	58(9)	47(9)	-30(7)	-5(7)	-8(8)
C(31A)	19(9)	28(8)	27(10)	-1(7)	-4(8)	-3(9)
C(32A)	15(9)	25(9)	30(8)	-4(7)	-6(7)	-6(8)
C(33A)	18(4)	35(2)	33(4)	-1(3)	0(3)	-3(3)
C(34A)	24(9)	48(11)	34(8)	-6(9)	-4(7)	6(9)

Table K.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **F_{64}PcNi(THF)$_2$**.

	x	y	z	U(eq)
H(31A)	5334	5506	7741	26
H(31B)	5772	6059	7099	26
H(32A)	6610	5368	9033	32
H(32B)	6892	6059	8632	32
H(33A)	7978	5588	7915	35
H(33B)	7637	4892	8218	35
H(34A)	7124	5569	6147	33
H(34B)	7209	4807	6321	33
H(31C)	5685	5485	8030	31
H(31D)	6051	6061	7366	31
H(32C)	6947	5430	9270	30
H(32D)	7205	6103	8772	30
H(33C)	8300	5594	8110	35
H(33D)	7946	4907	8450	35
H(34C)	7418	5587	6442	44
H(34D)	7497	4828	6614	44

Table K.6 Torsion angles [deg] for **F_{64}PcNi(THF)$_2$**.

C(22)-N(3)-C(1)-N(1)	2.2(5)	C(9)-C(4)-C(5)-C(6)	-170.8(3)
C(22)-N(3)-C(1)-C(2)	-177.6(3)	C(3)-C(4)-C(5)-C(12)	-171.2(3)
C(8)-N(1)-C(1)-N(3)	-179.3(3)	C(9)-C(4)-C(5)-C(12)	10.7(5)
Ni-N(1)-C(1)-N(3)	-2.1(5)	C(4)-C(5)-C(6)-F(1)	175.8(3)
C(8)-N(1)-C(1)-C(2)	0.5(3)	C(12)-C(5)-C(6)-F(1)	-5.5(4)
Ni-N(1)-C(1)-C(2)	177.7(2)	C(4)-C(5)-C(6)-C(7)	-6.0(5)
N(3)-C(1)-C(2)-C(7)	178.6(3)	C(12)-C(5)-C(6)-C(7)	172.6(3)
N(1)-C(1)-C(2)-C(7)	-1.2(3)	C(3)-C(2)-C(7)-C(6)	2.9(5)
N(3)-C(1)-C(2)-C(3)	-2.9(6)	C(1)-C(2)-C(7)-C(6)	-178.4(3)
N(1)-C(1)-C(2)-C(3)	177.3(3)	C(3)-C(2)-C(7)-C(8)	-177.3(3)
C(7)-C(2)-C(3)-F(2)	177.7(3)	C(1)-C(2)-C(7)-C(8)	1.5(3)
C(1)-C(2)-C(3)-F(2)	-0.7(5)	F(1)-C(6)-C(7)-C(2)	179.1(3)
C(7)-C(2)-C(3)-C(4)	-1.3(5)	C(5)-C(6)-C(7)-C(2)	0.9(5)
C(1)-C(2)-C(3)-C(4)	-179.7(3)	F(1)-C(6)-C(7)-C(8)	-0.7(5)
F(2)-C(3)-C(4)-C(5)	177.2(3)	C(5)-C(6)-C(7)-C(8)	-178.8(3)
C(2)-C(3)-C(4)-C(5)	-3.8(5)	C(15)-N(4)-C(8)-N(1)	-0.4(5)
F(2)-C(3)-C(4)-C(9)	-4.5(4)	C(15)-N(4)-C(8)-C(7)	179.0(3)
C(2)-C(3)-C(4)-C(9)	174.5(3)	C(1)-N(1)-C(8)-N(4)	179.9(3)
C(3)-C(4)-C(5)-C(6)	7.3(4)	Ni-N(1)-C(8)-N(4)	2.7(5)

C(1)-N(1)-C(8)-C(7)	0.5(3)	C(14)-C(12)-C(13)-F(16)	-51.4(4)
Ni-N(1)-C(8)-C(7)	-176.8(2)	F(12)-C(12)-C(14)-F(15)	-142.5(3)
C(2)-C(7)-C(8)-N(4)	179.3(3)	C(5)-C(12)-C(14)-F(15)	97.5(3)
C(6)-C(7)-C(8)-N(4)	-1.0(6)	C(13)-C(12)-C(14)-F(15)	-29.7(4)
C(2)-C(7)-C(8)-N(1)	-1.2(3)	F(12)-C(12)-C(14)-F(14)	93.7(3)
C(6)-C(7)-C(8)-N(1)	178.5(3)	C(5)-C(12)-C(14)-F(14)	-26.2(4)
C(3)-C(4)-C(9)-F(5)	-159.8(3)	C(13)-C(12)-C(14)-F(14)	-153.5(3)
C(5)-C(4)-C(9)-F(5)	18.3(4)	F(12)-C(12)-C(14)-F(13)	-23.8(3)
C(3)-C(4)-C(9)-C(11)	82.8(3)	C(5)-C(12)-C(14)-F(13)	-143.8(3)
C(5)-C(4)-C(9)-C(11)	-99.0(4)	C(13)-C(12)-C(14)-F(13)	89.0(3)
C(3)-C(4)-C(9)-C(10)	-44.3(4)	C(8)-N(4)-C(15)-N(2)#1	1.2(5)
C(5)-C(4)-C(9)-C(10)	133.8(3)	C(8)-N(4)-C(15)-C(16)#1	-176.9(3)
F(5)-C(9)-C(10)-F(8)	-142.0(3)	C(21)-C(16)-C(17)-F(4)	-176.2(3)
C(11)-C(9)-C(10)-F(8)	-29.5(4)	C(15)#1-C(16)-C(17)-F(4)	3.2(5)
C(4)-C(9)-C(10)-F(8)	97.9(3)	C(21)-C(16)-C(17)-C(18)	2.3(5)
F(5)-C(9)-C(10)-F(6)	-22.9(3)	C(15)#1-C(16)-C(17)-C(18)	-178.3(3)
C(11)-C(9)-C(10)-F(6)	89.5(3)	F(4)-C(17)-C(18)-C(19)	-177.7(3)
C(4)-C(9)-C(10)-F(6)	-143.1(3)	C(16)-C(17)-C(18)-C(19)	3.9(5)
F(5)-C(9)-C(10)-F(7)	95.0(3)	F(4)-C(17)-C(18)-C(26)	4.4(4)
C(11)-C(9)-C(10)-F(7)	-152.5(3)	C(16)-C(17)-C(18)-C(26)	-174.0(3)
C(4)-C(9)-C(10)-F(7)	-25.1(4)	C(17)-C(18)-C(19)-C(20)	-8.4(4)
F(5)-C(9)-C(11)-F(9)	60.7(3)	C(26)-C(18)-C(19)-C(20)	169.3(3)
C(4)-C(9)-C(11)-F(9)	-179.0(3)	C(17)-C(18)-C(19)-C(23)	166.3(3)
C(10)-C(9)-C(11)-F(9)	-49.7(4)	C(26)-C(18)-C(19)-C(23)	-16.0(5)
F(5)-C(9)-C(11)-F(11)	-59.3(3)	C(18)-C(19)-C(20)-F(3)	-176.3(3)
C(4)-C(9)-C(11)-F(11)	61.1(3)	C(23)-C(19)-C(20)-F(3)	8.4(4)
C(10)-C(9)-C(11)-F(11)	-169.6(3)	C(18)-C(19)-C(20)-C(21)	7.3(5)
F(5)-C(9)-C(11)-F(10)	-178.3(2)	C(23)-C(19)-C(20)-C(21)	-168.0(3)
C(4)-C(9)-C(11)-F(10)	-58.0(4)	F(3)-C(20)-C(21)-C(16)	-177.6(3)
C(10)-C(9)-C(11)-F(10)	71.3(3)	C(19)-C(20)-C(21)-C(16)	-1.2(5)
C(6)-C(5)-C(12)-F(12)	-159.4(3)	F(3)-C(20)-C(21)-C(22)	-1.8(5)
C(4)-C(5)-C(12)-F(12)	19.1(4)	C(19)-C(20)-C(21)-C(22)	174.6(3)
C(6)-C(5)-C(12)-C(13)	81.9(3)	C(17)-C(16)-C(21)-C(20)	-3.8(5)
C(4)-C(5)-C(12)-C(13)	-99.6(4)	C(15)#1-C(16)-C(21)-C(20)	176.6(3)
C(6)-C(5)-C(12)-C(14)	-44.6(4)	C(17)-C(16)-C(21)-C(22)	179.4(3)
C(4)-C(5)-C(12)-C(14)	133.9(3)	C(15)#1-C(16)-C(21)-C(22)	-0.2(3)
F(12)-C(12)-C(13)-F(17)	-60.8(3)	C(1)-N(3)-C(22)-N(2)	1.6(5)
C(5)-C(12)-C(13)-F(17)	60.7(4)	C(1)-N(3)-C(22)-C(21)	-177.3(3)
C(14)-C(12)-C(13)-F(17)	-170.9(3)	C(15)#1-N(2)-C(22)-N(3)	-177.9(3)
F(12)-C(12)-C(13)-F(18)	178.7(2)	Ni-N(2)-C(22)-N(3)	-5.0(5)
C(5)-C(12)-C(13)-F(18)	-59.9(4)	C(15)#1-N(2)-C(22)-C(21)	1.2(3)
C(14)-C(12)-C(13)-F(18)	68.5(3)	Ni-N(2)-C(22)-C(21)	174.0(2)
F(12)-C(12)-C(13)-F(16)	58.7(3)	C(20)-C(21)-C(22)-N(3)	2.3(6)
C(5)-C(12)-C(13)-F(16)	-179.8(3)	C(16)-C(21)-C(22)-N(3)	178.5(3)

C(20)-C(21)-C(22)-N(2)	-176.8(3)	F(26)-C(26)-C(27)-F(27)	62.8(3)
C(16)-C(21)-C(22)-N(2)	-0.6(3)	C(18)-C(26)-C(27)-F(27)	-58.4(4)
C(20)-C(19)-C(23)-F(19)	157.8(3)	C(28)-C(26)-C(27)-F(27)	171.9(3)
C(18)-C(19)-C(23)-F(19)	-16.9(5)	F(26)-C(26)-C(27)-F(29)	-177.6(3)
C(20)-C(19)-C(23)-C(24)	-83.4(4)	C(18)-C(26)-C(27)-F(29)	61.2(4)
C(18)-C(19)-C(23)-C(24)	101.9(4)	C(28)-C(26)-C(27)-F(29)	-68.5(3)
C(20)-C(19)-C(23)-C(25)	44.5(4)	F(26)-C(26)-C(27)-F(28)	-56.9(4)
C(18)-C(19)-C(23)-C(25)	-130.2(4)	C(18)-C(26)-C(27)-F(28)	-178.2(3)
F(19)-C(23)-C(24)-F(20)	59.0(4)	C(28)-C(26)-C(27)-F(28)	52.2(4)
C(19)-C(23)-C(24)-F(20)	-62.1(4)	F(26)-C(26)-C(28)-F(30)	-87.1(3)
C(25)-C(23)-C(24)-F(20)	168.5(3)	C(18)-C(26)-C(28)-F(30)	31.7(4)
F(19)-C(23)-C(24)-F(21)	-61.2(4)	C(27)-C(26)-C(28)-F(30)	160.6(3)
C(19)-C(23)-C(24)-F(21)	177.7(3)	F(26)-C(26)-C(28)-F(32)	32.2(3)
C(25)-C(23)-C(24)-F(21)	48.3(4)	C(18)-C(26)-C(28)-F(32)	151.0(3)
F(19)-C(23)-C(24)-F(22)	178.4(3)	C(27)-C(26)-C(28)-F(32)	-80.2(3)
C(19)-C(23)-C(24)-F(22)	57.3(4)	F(26)-C(26)-C(28)-F(31)	149.2(3)
C(25)-C(23)-C(24)-F(22)	-72.1(4)	C(18)-C(26)-C(28)-F(31)	-92.1(3)
F(19)-C(23)-C(25)-F(24)	144.3(3)	C(27)-C(26)-C(28)-F(31)	36.8(4)
C(24)-C(23)-C(25)-F(24)	32.2(4)	C(34)-O(1)-C(31)-C(32)	-34.5(7)
C(19)-C(23)-C(25)-F(24)	-97.7(4)	Ni-O(1)-C(31)-C(32)	-178.6(5)
F(19)-C(23)-C(25)-F(25)	-92.4(3)	O(1)-C(31)-C(32)-C(33)	17.9(8)
C(24)-C(23)-C(25)-F(25)	155.5(3)	C(31)-C(32)-C(33)-C(34)	4.7(8)
C(19)-C(23)-C(25)-F(25)	25.6(4)	C(31)-O(1)-C(34)-C(33)	37.5(7)
F(19)-C(23)-C(25)-F(23)	25.2(4)	Ni-O(1)-C(34)-C(33)	-178.5(5)
C(24)-C(23)-C(25)-F(23)	-86.9(4)	C(32)-C(33)-C(34)-O(1)	-25.3(8)
C(19)-C(23)-C(25)-F(23)	143.2(4)	C(34A)-O(1A)-C(31A)-C(32A)	-28(3)
C(17)-C(18)-C(26)-F(26)	160.3(3)	Ni-O(1A)-C(31A)-C(32A)	-178.7(18)
C(19)-C(18)-C(26)-F(26)	-17.4(4)	O(1A)-C(31A)-C(32A)-C(33A)	12(3)
C(17)-C(18)-C(26)-C(27)	-80.8(4)	C(31A)-C(32A)-C(33A)-C(34A)	8(3)
C(19)-C(18)-C(26)-C(27)	101.5(4)	C(31A)-O(1A)-C(34A)-C(33A)	35(3)
C(17)-C(18)-C(26)-C(28)	46.9(4)	Ni-O(1A)-C(34A)-C(33A)	-179(2)
C(19)-C(18)-C(26)-C(28)	-130.8(3)	C(32A)-C(33A)-C(34A)-O(1A)	-27(3)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

Appendix L: Crystal structure of $F_{64}PcGaCl(H_2O)$

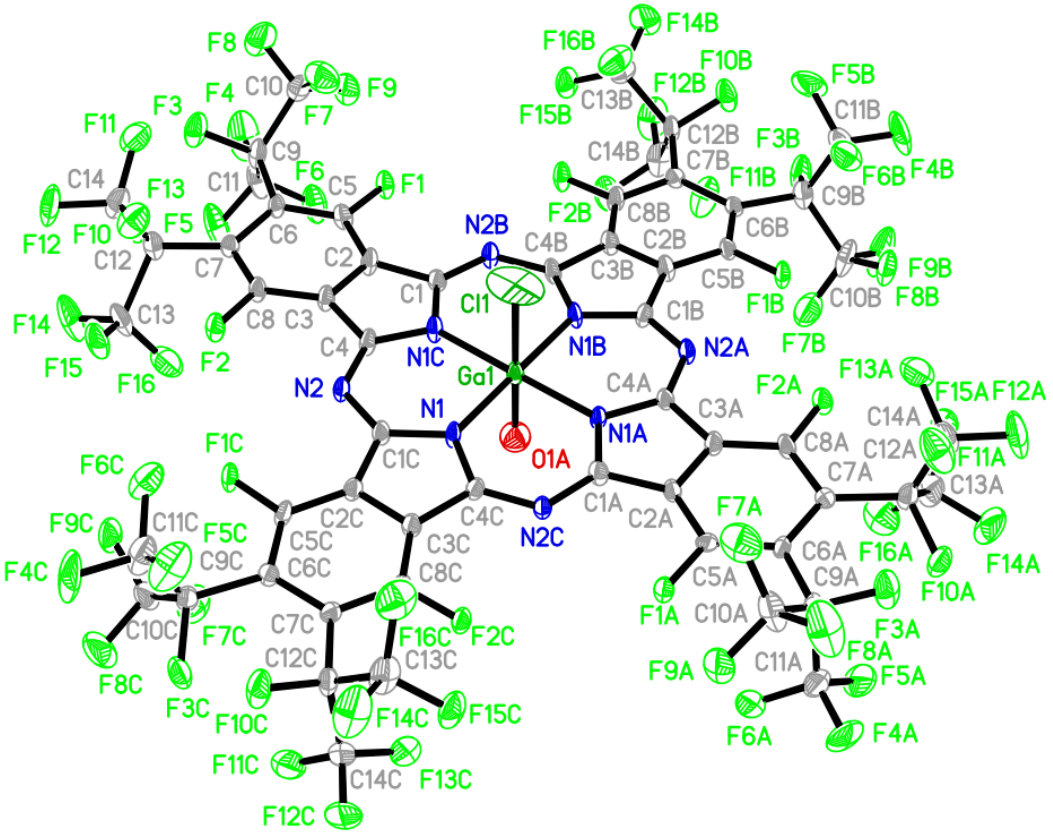


Figure L.1 ORTEP representation of **$F_{64}PcGaCl(H_2O)$** X-ray crystal structure, at 50% probability.

Table L.1 Crystal data and structure refinement for **$F_{64}PcGaCl(H_2O)$**.

Empirical formula	C56 H2 Cl F64 Ga N8 O	
Formula weight	2122.82	
Temperature	102(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	P4(2)/n	
Unit cell dimensions	a = 23.9929(15) Å	α= 90°.
	b = 23.9929(15) Å	β= 90°.
	c = 7.4247(6) Å	γ = 90°.
Volume	4274.1(5) $Å^3$	
Z	2	
Density (calculated)	1.649 g/cm^3	
Absorption coefficient	2.434 mm^{-1}	
F(000)	2050	
Crystal size	0.2 x 0.2 x 0.01 mm^3	
Theta range for data collection	5.21 to 68.89°.	
Index ranges	-27<=h<=28, -27<=k<=27, -7<=l<=8	
Reflections collected	24274	
Independent reflections	3717 [R(int) = 0.0539]	

Completeness to theta = 68.89°	93.8 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3717 / 2 / 298
Goodness-of-fit on F^2	1.098
Final R indices [I>2sigma(I)]	R1 = 0.0749, wR2 = 0.1852
R indices (all data)	R1 = 0.1156, wR2 = 0.1978
Largest diff. peak and hole	0.591 and -0.345 e.Å^{-3}

Table L.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **F_{64}PcGaCl(H_2O)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ga(1)	7500	7500	7500	23(1)
Cl(1)	7500	7500	10717(7)	97(3)
N(1)	6698(1)	7312(1)	7517(5)	26(1)
N(2)	6763(1)	6300(1)	7614(5)	25(1)
C(1)	6269(2)	7685(2)	7482(6)	25(1)
C(2)	5748(2)	7381(2)	7556(6)	27(1)
C(3)	5882(2)	6822(2)	7660(6)	26(1)
C(4)	6487(2)	6784(2)	7612(6)	25(1)
C(5)	5187(2)	7536(2)	7584(6)	24(1)
C(6)	4758(2)	7158(2)	7739(6)	22(1)
C(7)	4898(2)	6565(2)	7744(5)	21(1)
C(8)	5466(2)	6429(2)	7776(6)	26(1)
C(9)	4164(2)	7399(2)	7879(7)	34(1)
C(10)	4109(2)	7917(2)	9222(9)	48(2)
C(11)	3918(2)	7548(2)	6049(9)	51(2)
C(12)	4492(2)	6071(2)	7778(7)	32(1)
C(13)	4653(2)	5582(2)	6365(9)	46(2)
C(14)	4406(2)	5835(2)	9648(8)	45(2)
F(1)	5074(1)	8079(1)	7477(3)	31(1)
F(2)	5616(1)	5894(1)	7858(3)	33(1)
F(3)	3807(1)	7027(1)	8669(5)	55(1)
F(4)	3414(1)	7758(1)	6197(6)	87(1)
F(5)	3883(1)	7089(1)	5006(5)	71(1)
F(6)	4242(1)	7907(1)	5134(4)	53(1)
F(7)	4500(1)	7895(1)	10500(5)	61(1)
F(8)	3620(1)	7890(1)	10029(6)	84(1)
F(9)	4135(1)	8402(1)	8363(4)	50(1)
F(10)	3981(1)	6216(1)	7126(4)	52(1)
F(11)	4171(1)	6216(1)	10717(4)	63(1)
F(12)	4078(1)	5394(1)	9642(5)	71(1)
F(13)	4885(1)	5687(1)	10413(4)	51(1)
F(14)	4195(1)	5357(1)	5749(5)	74(1)
F(15)	4939(1)	5172(1)	7160(4)	49(1)
F(16)	4941(1)	5793(1)	5006(4)	58(1)
O(1)	7500	7500	9972(19)	48(4)

Table L.3 Bond lengths [Å] and angles [°] for **F_{64}PcGaCl(H_2O)**.

Ga(1)-O(1)	1.835(14)	Ga(1)-N(1)#1	1.976(3)
Ga(1)-O(1))#1	1.835(14)	Ga(1)-N(1)	1.976(3)
Ga(1)-N(1)#2	1.976(3)	Ga(1)-Cl(1)	2.389(6)
Ga(1)-N(1)#3	1.976(3)	Ga(1)-Cl(1)#1	2.389(6)
N(1)-C(4)	1.365(5)	C(9)-C(10)	1.600(7)
N(1)-C(1)	1.365(5)	C(10)-F(8)	1.318(5)
N(2)-C(1)#3	1.328(5)	C(10)-F(9)	1.328(5)
N(2)-C(4)	1.338(5)	C(10)-F(7)	1.335(6)
C(1)-N(2)#1	1.328(5)	C(11)-F(4)	1.314(5)
C(1)-C(2)	1.449(6)	C(11)-F(6)	1.343(6)
C(2)-C(3)	1.380(6)	C(11)-F(5)	1.349(6)
C(2)-C(5)	1.398(6)	C(12)-F(10)	1.363(5)
C(3)-C(8)	1.375(5)	C(12)-C(14)	1.514(7)
C(3)-C(4)	1.454(5)	C(12)-C(13)	1.621(7)
C(5)-F(1)	1.332(4)	C(13)-F(14)	1.306(5)
C(5)-C(6)	1.376(6)	C(13)-F(16)	1.324(6)
C(6)-C(7)	1.463(5)	C(13)-F(15)	1.336(6)
C(6)-C(9)	1.540(6)	C(14)-F(12)	1.318(5)
C(7)-C(8)	1.402(6)	C(14)-F(13)	1.331(5)
C(7)-C(12)	1.534(6)	C(14)-F(11)	1.337(6)
C(8)-F(2)	1.335(4)	O(1)-H(2)	0.8829
C(9)-F(3)	1.369(5)	O(1)-H(1)	0.8829
C(9)-C(11)	1.524(7)		
O(1)#1-Ga(1)-O(1)	180.000(13)	N(1)#3-Ga(1)-Cl(1)#1	89.62(10)
O(1)#1-Ga(1)-N(1)#2	90.38(10)	N(1)#1-Ga(1)-Cl(1)#1	89.63(10)
O(1)-Ga(1)-N(1)#2	89.63(10)	N(1)-Ga(1)-Cl(1)#1	90.37(10)
O(1)#1-Ga(1)-N(1)#3	89.62(10)	Cl(1)-Ga(1)-Cl(1)#1	180.000(1)
O(1)-Ga(1)-N(1)#3	90.37(10)	O(1)-Cl(1)-Ga(1)	0.000(19)
N(1)#2-Ga(1)-N(1)#3	90.002(3)	C(4)-N(1)-C(1)	109.2(3)
O(1)#1-Ga(1)-N(1)#1	89.63(10)	C(4)-N(1)-Ga(1)	125.0(3)
O(1)-Ga(1)-N(1)#1	90.37(10)	C(1)-N(1)-Ga(1)	125.7(3)
N(1)#2-Ga(1)-N(1)#1	90.002(3)	C(1)#3-N(2)-C(4)	122.8(4)
N(1)#3-Ga(1)-N(1)#1	179.3(2)	N(2)#1-C(1)-N(1)	127.9(4)
O(1)#1-Ga(1)-N(1)	90.37(10)	N(2)#1-C(1)-C(2)	123.5(4)
O(1)-Ga(1)-N(1)	89.63(10)	N(1)-C(1)-C(2)	108.6(3)
N(1)#2-Ga(1)-N(1)	179.3(2)	C(3)-C(2)-C(5)	118.8(4)
N(1)#3-Ga(1)-N(1)	90.005(4)	C(3)-C(2)-C(1)	106.9(4)
N(1)#1-Ga(1)-N(1)	90.000(4)	C(5)-C(2)-C(1)	134.2(4)
O(1)#1-Ga(1)-Cl(1)	180.000(4)	C(8)-C(3)-C(2)	120.0(4)
O(1)-Ga(1)-Cl(1)	0.000(6)	C(8)-C(3)-C(4)	133.1(4)
N(1)#2-Ga(1)-Cl(1)	89.63(10)	C(2)-C(3)-C(4)	106.9(4)
N(1)#3-Ga(1)-Cl(1)	90.37(10)	N(2)-C(4)-N(1)	128.4(4)
N(1)#1-Ga(1)-Cl(1)	90.37(10)	N(2)-C(4)-C(3)	123.2(4)
N(1)-Ga(1)-Cl(1)	89.63(10)	N(1)-C(4)-C(3)	108.3(4)
O(1)#1-Ga(1)-Cl(1)#1	0.000(4)	F(1)-C(5)-C(6)	119.8(4)
O(1)-Ga(1)-Cl(1)#1	180.000(5)	F(1)-C(5)-C(2)	117.1(4)
N(1)#2-Ga(1)-Cl(1)#1	90.38(10)	C(6)-C(5)-C(2)	123.1(4)

C(5)-C(6)-C(7)	118.0(4)	F(5)-C(11)-C(9)	110.1(4)
C(5)-C(6)-C(9)	116.8(4)	F(10)-C(12)-C(14)	107.4(4)
C(7)-C(6)-C(9)	125.3(3)	F(10)-C(12)-C(7)	111.6(3)
C(8)-C(7)-C(6)	116.7(4)	C(14)-C(12)-C(7)	113.0(4)
C(8)-C(7)-C(12)	116.0(4)	F(10)-C(12)-C(13)	99.8(4)
C(6)-C(7)-C(12)	127.3(4)	C(14)-C(12)-C(13)	110.8(4)
F(2)-C(8)-C(3)	117.8(4)	C(7)-C(12)-C(13)	113.4(4)
F(2)-C(8)-C(7)	119.1(4)	F(14)-C(13)-F(16)	109.3(5)
C(3)-C(8)-C(7)	123.1(4)	F(14)-C(13)-F(15)	106.5(4)
F(3)-C(9)-C(11)	107.0(4)	F(16)-C(13)-F(15)	110.4(4)
F(3)-C(9)-C(6)	111.3(3)	F(14)-C(13)-C(12)	109.0(4)
C(11)-C(9)-C(6)	112.7(4)	F(16)-C(13)-C(12)	109.9(4)
F(3)-C(9)-C(10)	100.8(4)	F(15)-C(13)-C(12)	111.7(5)
C(11)-C(9)-C(10)	109.9(4)	F(12)-C(14)-F(13)	107.7(4)
C(6)-C(9)-C(10)	114.2(4)	F(12)-C(14)-F(11)	107.5(4)
F(8)-C(10)-F(9)	107.7(4)	F(13)-C(14)-F(11)	107.0(5)
F(8)-C(10)-F(7)	107.5(5)	F(12)-C(14)-C(12)	112.3(5)
F(9)-C(10)-F(7)	110.1(4)	F(13)-C(14)-C(12)	111.9(4)
F(8)-C(10)-C(9)	108.6(4)	F(11)-C(14)-C(12)	110.2(4)
F(9)-C(10)-C(9)	112.1(5)	Cl(1)-O(1)-H(2)	56.5
F(7)-C(10)-C(9)	110.7(4)	Cl(1)-O(1)-H(1)	56.5
F(4)-C(11)-F(6)	109.2(4)	H(2)-O(1)-H(1)	113.0
F(4)-C(11)-F(5)	107.7(4)	Cl(1)-O(1)-Ga(1)	180.000(7)
F(6)-C(11)-F(5)	105.6(5)	H(2)-O(1)-Ga(1)	123.5
F(4)-C(11)-C(9)	111.8(5)	H(1)-O(1)-Ga(1)	123.5
F(6)-C(11)-C(9)	112.2(4)		

Symmetry transformations used to generate equivalent atoms:
#1 y,-x+3/2,-z+3/2 #2 -x+3/2,-y+3/2,z #3 -y+3/2,x,-z+3/2

Table L.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F_{64}PcGaCl(H_2O)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{\cdot 2} U^{11} + ... + 2\ h\ k\ a\cdot\ b\cdot\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ga(1)	13(1)	13(1)	43(1)	0	0	0
Cl(1)	178(6)	111(5)	1(3)	0	0	16(4)
N(1)	10(2)	12(2)	56(3)	4(2)	-4(2)	1(1)
N(2)	13(2)	13(2)	49(3)	3(2)	4(2)	-1(1)
C(1)	19(2)	14(2)	42(3)	-2(2)	3(2)	2(2)
C(2)	15(2)	16(2)	49(4)	8(2)	-2(2)	-1(2)
C(3)	14(2)	17(2)	47(4)	4(2)	-1(2)	-2(2)
C(4)	13(2)	16(2)	46(4)	8(2)	-2(2)	-1(2)
C(5)	20(2)	15(2)	38(3)	3(2)	-9(2)	4(2)
C(6)	14(2)	18(2)	33(3)	1(2)	-5(2)	-3(2)
C(7)	20(2)	19(2)	25(3)	4(2)	-1(2)	-1(2)
C(8)	20(2)	12(2)	46(3)	5(2)	2(2)	0(2)
C(9)	19(2)	20(2)	62(4)	10(2)	0(2)	-2(2)

C(10)	35(3)	21(3)	86(5)	1(3)	28(3)	7(2)
C(11)	37(3)	32(3)	85(5)	4(3)	-29(3)	-5(2)
C(12)	17(2)	18(2)	61(4)	1(2)	-4(2)	3(2)
C(13)	44(3)	21(3)	72(5)	-12(3)	-12(3)	-4(2)
C(14)	34(3)	32(3)	67(5)	17(3)	15(3)	1(2)
F(1)	15(1)	13(1)	65(2)	1(1)	-4(1)	3(1)
F(2)	19(1)	16(1)	64(2)	8(1)	2(1)	2(1)
F(3)	21(1)	32(2)	114(3)	10(2)	15(2)	3(1)
F(4)	31(2)	55(2)	173(4)	16(2)	-43(2)	9(2)
F(5)	76(2)	39(2)	99(3)	-1(2)	-54(2)	-17(2)
F(6)	55(2)	35(2)	67(2)	12(2)	-26(2)	-8(1)
F(7)	72(2)	41(2)	70(3)	-6(2)	2(2)	12(2)
F(8)	58(2)	43(2)	151(4)	2(2)	57(2)	12(2)
F(9)	36(2)	23(2)	91(2)	2(2)	5(2)	10(1)
F(10)	24(1)	26(2)	107(3)	5(2)	-20(1)	-2(1)
F(11)	60(2)	44(2)	84(3)	11(2)	36(2)	5(2)
F(12)	48(2)	34(2)	132(3)	20(2)	27(2)	-14(1)
F(13)	46(2)	50(2)	58(2)	21(2)	5(2)	6(1)
F(14)	57(2)	34(2)	130(3)	-14(2)	-43(2)	-10(2)
F(15)	42(2)	18(1)	86(3)	1(1)	-10(2)	3(1)
F(16)	81(2)	39(2)	54(2)	-11(2)	2(2)	1(2)

Table L.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **F_{64}PcGaCl(H_2O)**

	x	**y**	**z**	**U(eq)**
H(1)	7201	7431	10628	57
H(2)	7799	7569	10628	57

Appendix M: Crystal structure of F_{52}PcCu(MeOH·2Acetone)

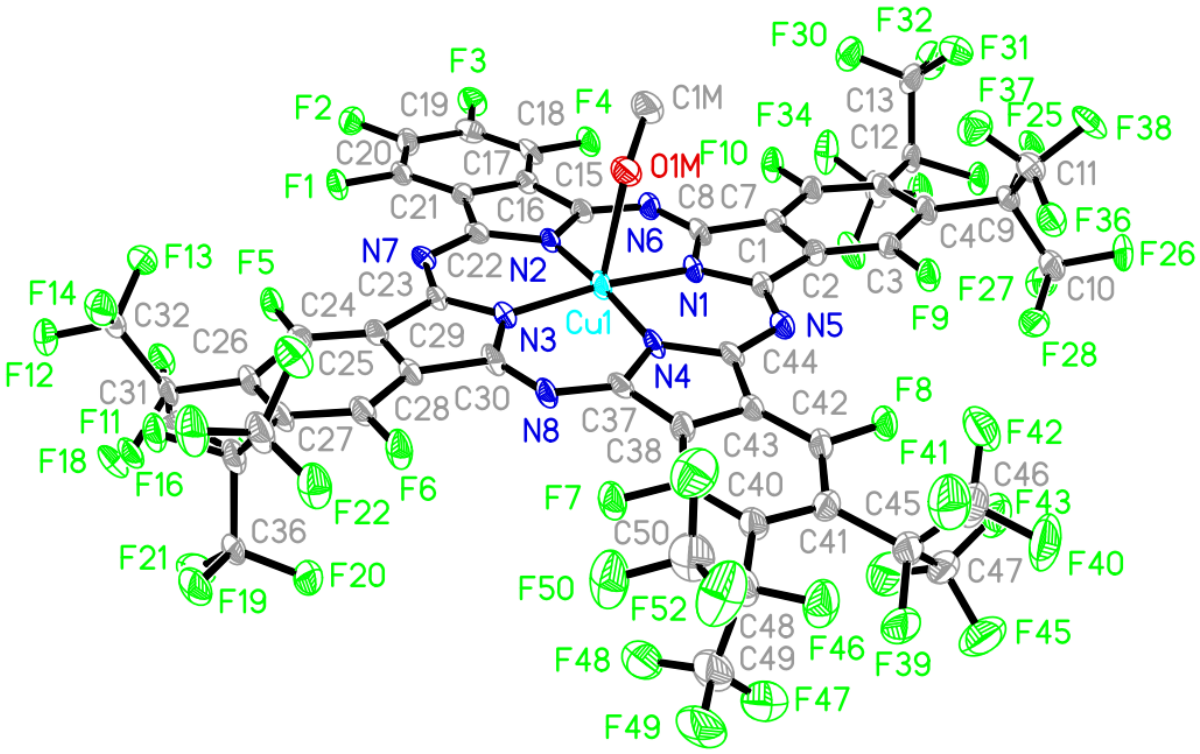


Figure M.1 ORTEP representation of **F_{52}PcCu(MeOH·2Acetone)** X-ray crystal structure, at 50% probability.

Table M.1 Crystal data and structure refinement for **F_{52}PcCu(MeOH·2Acetone)**

Empirical formula	C57 H16 Cu F52 N8 O3	
Formula weight	1912.32	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 7.1912(3) Å	α = 90°.
	b = 19.4876(8) Å	β = 93.188(3)°.
	c = 46.9035(19) Å	γ = 90°.
Volume	6562.8(5) $Å^3$	
Z	4	
Density (calculated)	1.935 g/cm^3	
Absorption coefficient	2.365 mm^{-1}	
F(000)	3740	

Crystal size	0.39 x 0.27 x 0.08 mm^3
Theta range for data collection	1.89 to 69.15°.
Index ranges	-8<=h<=8, -23<=k<=23, -56<=l<=55
Reflections collected	51052
Independent reflections	11742 [R(int) = 0.0583]
Completeness to theta = 69.15°	95.8 %
Max. and min. transmission	0.8407 and 0.4583
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11742 / 0 / 1096
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0865, wR2 = 0.1657
R indices (all data)	R1 = 0.1276, wR2 = 0.1901
Extinction coefficient	0.00025(2)
Largest diff. peak and hole	0.874 and -1.356 e.$Å^{-3}$

Table M.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **F_{52}PcCu(MeOH·2Acetone)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1591(1)	714(1)	897(1)	23(1)
N(1)	2809(8)	1607(2)	958(1)	24(1)
N(2)	2422(7)	709(2)	507(1)	21(1)
N(3)	738(8)	-234(2)	847(1)	23(1)
N(4)	1047(8)	669(2)	1300(1)	25(1)
N(5)	2139(8)	1799(2)	1455(1)	26(1)
N(6)	3894(8)	1824(2)	489(1)	25(1)
N(7)	1367(7)	-422(2)	351(1)	22(1)
N(8)	-190(8)	-481(2)	1327(1)	23(1)
O(1M)	-1189(7)	1331(2)	791(1)	31(1)
C(1M)	-1194(12)	1895(3)	595(2)	42(2)
C(1)	2737(9)	1991(3)	1202(1)	22(1)
C(2)	3468(9)	2669(3)	1151(1)	23(1)
C(3)	3585(10)	3270(3)	1306(1)	24(1)
C(4)	4286(10)	3882(3)	1206(1)	27(2)
C(5)	5081(10)	3864(3)	927(1)	25(2)
C(6)	4844(10)	3261(3)	771(1)	25(2)
C(7)	4011(9)	2673(3)	873(1)	22(1)
C(8)	3605(9)	1991(3)	756(1)	24(1)
C(9)	4040(10)	4522(3)	1396(1)	25(2)
C(10)	5529(11)	4570(3)	1645(2)	32(2)
F(26)	5208(6)	5123(2)	1804(1)	42(1)
F(27)	7223(6)	4620(2)	1552(1)	37(1)
F(28)	5481(6)	4022(2)	1816(1)	33(1)
C(11)	2018(11)	4597(3)	1505(2)	31(2)
F(36)	1814(6)	4336(2)	1764(1)	35(1)

F(37)	770(6)	4298(2)	1323(1)	41(1)
F(38)	1572(6)	5259(2)	1521(1)	42(1)
C(12)	6202(10)	4438(3)	792(1)	25(2)
C(13)	5027(12)	4866(3)	572(1)	37(2)
F(30)	4221(7)	4472(2)	371(1)	48(1)
F(31)	6096(7)	5324(2)	446(1)	49(1)
F(32)	3712(7)	5209(2)	700(1)	46(1)
C(14)	8062(11)	4187(3)	657(2)	37(2)
F(33)	9361(6)	4667(2)	694(1)	44(1)
F(34)	7874(7)	4062(2)	378(1)	47(1)
F(35)	8714(6)	3619(2)	788(1)	42(1)
C(15)	3348(9)	1229(3)	380(1)	22(1)
C(16)	3620(9)	1042(3)	82(1)	19(1)
C(17)	4533(9)	1364(3)	-136(1)	24(1)
C(18)	4525(9)	1041(3)	-398(1)	26(2)
C(19)	3722(10)	399(3)	-438(1)	26(2)
C(20)	2858(9)	71(3)	-223(1)	20(1)
C(21)	2818(8)	397(3)	38(1)	19(1)
C(22)	2102(9)	191(3)	312(1)	20(1)
C(23)	776(9)	-613(3)	603(1)	23(1)
C(24)	82(9)	-1303(3)	653(1)	23(1)
C(25)	-61(9)	-1895(3)	494(1)	22(1)
C(26)	-703(10)	-2518(3)	597(1)	26(2)
C(27)	-1393(10)	-2516(3)	880(1)	28(2)
C(28)	-1166(10)	-1916(3)	1039(1)	26(2)
C(29)	-398(9)	-1316(3)	937(1)	23(1)
C(30)	10(9)	-639(3)	1057(1)	23(1)
C(31)	-410(9)	-3151(3)	405(1)	22(1)
C(32)	-1893(10)	-3224(3)	161(2)	27(2)
F(12)	-1551(6)	-3780(2)	3(1)	37(1)
F(13)	-1934(6)	-2680(2)	-16(1)	31(1)
F(14)	-3590(5)	-3293(2)	257(1)	34(1)
C(33)	1603(10)	-3206(3)	294(1)	28(2)
F(15)	1750(6)	-2948(2)	31(1)	31(1)
F(16)	2113(6)	-3863(2)	278(1)	35(1)
F(17)	2855(5)	-2891(2)	472(1)	33(1)
C(34)	-2459(10)	-3100(3)	1022(1)	29(2)
C(35)	-4270(12)	-2871(3)	1174(2)	37(2)
F(22)	-3979(6)	-2768(2)	1456(1)	41(1)
F(23)	-5559(6)	-3357(2)	1142(1)	45(1)
F(24)	-4977(6)	-2297(2)	1057(1)	41(1)
C(36)	-1183(11)	-3529(3)	1230(1)	32(2)
F(19)	-2177(7)	-3997(2)	1363(1)	43(1)
F(20)	-318(6)	-3136(2)	1428(1)	42(1)
F(21)	113(6)	-3861(2)	1092(1)	43(1)
C(37)	308(9)	118(3)	1436(1)	23(1)
C(38)	224(10)	284(3)	1739(1)	26(2)
C(39)	-308(11)	-82(3)	1974(1)	31(2)
C(40)	-95(11)	168(3)	2255(1)	32(2)
C(41)	765(11)	836(3)	2297(1)	32(2)

C(42)	1158(10)	1205(3)	2051(1)	29(2)
C(43)	928(10)	940(3)	1776(1)	25(2)
C(44)	1427(9)	1182(3)	1498(1)	23(1)
C(45)	1380(13)	1180(4)	2582(2)	42(2)
C(46)	-27(14)	1708(4)	2678(2)	51(2)
F(40)	565(9)	2017(3)	2920(1)	72(2)
F(41)	-1638(8)	1396(3)	2729(1)	64(1)
F(42)	-400(8)	2185(2)	2482(1)	60(1)
C(47)	3427(13)	1514(4)	2588(2)	45(2)
F(43)	3410(8)	2183(2)	2537(1)	58(1)
F(44)	4499(7)	1203(3)	2411(1)	59(1)
F(45)	4213(8)	1439(3)	2855(1)	70(2)
C(48)	-787(12)	-308(3)	2488(2)	38(2)
C(49)	665(15)	-854(4)	2583(2)	55(3)
F(47)	2215(8)	-574(3)	2692(1)	71(2)
F(48)	1099(8)	-1239(2)	2361(1)	59(1)
F(49)	8(9)	-1277(2)	2775(1)	72(2)
C(50)	-2735(14)	-637(4)	2420(2)	55(2)
F(50)	-2667(8)	-1272(2)	2306(1)	65(2)
F(51)	-3780(7)	-257(3)	2242(1)	58(1)
F(52)	-3623(7)	-715(3)	2660(1)	70(2)
F(1)	2108(5)	-551(2)	-270(1)	28(1)
F(2)	3762(5)	107(2)	-700(1)	30(1)
F(3)	5354(6)	1342(2)	-615(1)	32(1)
F(4)	5359(5)	1971(2)	-102(1)	30(1)
F(5)	533(5)	-1868(2)	226(1)	28(1)
F(6)	-1682(6)	-1901(2)	1311(1)	36(1)
F(7)	-1018(6)	-711(2)	1928(1)	37(1)
F(8)	1843(6)	1842(2)	2078(1)	35(1)
F(9)	2922(5)	3254(2)	1571(1)	29(1)
F(10)	5460(6)	3232(2)	505(1)	33(1)
F(11)	-522(5)	-3745(2)	561(1)	28(1)
F(18)	-3178(6)	-3541(2)	817(1)	32(1)
F(25)	4206(6)	5111(2)	1240(1)	30(1)
F(29)	6896(5)	4882(2)	998(1)	30(1)
F(39)	1609(7)	703(2)	2796(1)	55(1)
F(46)	-1101(7)	66(2)	2729(1)	53(1)
C(1S)	6439(15)	1746(7)	1806(2)	86(4)
C(2S)	7238(13)	2000(6)	1520(2)	69(3)
C(3S)	8199(15)	2672(5)	1508(3)	95(4)
O(1S)	7176(10)	1647(4)	1306(2)	86(3)
C(4S)	3810(20)	8822(6)	1739(3)	104(4)
C(5S)	4443(15)	9510(8)	1597(2)	83(4)
C(6S)	5065(17)	9527(8)	1309(2)	113(5)
O(2S)	4411(12)	10056(4)	1718(2)	104(3)

Table M.3 Bond lengths [Å] and angles [°] for **F_{52}PcCu(MeOH·2Acetone)**.

Cu(1)-N(2)	1.955(5)	Cu(1)-N(1)	1.963(5)
Cu(1)-N(3)	1.956(5)	Cu(1)-O(1M)	2.361(5)
Cu(1)-N(4)	1.956(5)		
N(1)-C(8)	1.359(8)	C(14)-F(33)	1.326(8)
N(1)-C(1)	1.371(7)	C(14)-F(34)	1.333(8)
N(2)-C(15)	1.367(8)	C(14)-F(35)	1.339(8)
N(2)-C(22)	1.371(7)	C(15)-C(16)	1.469(8)
N(3)-C(23)	1.366(8)	C(16)-C(17)	1.393(8)
N(3)-C(30)	1.386(7)	C(16)-C(21)	1.393(8)
N(4)-C(37)	1.371(7)	C(17)-F(4)	1.330(7)
N(4)-C(44)	1.380(8)	C(17)-C(18)	1.380(9)
N(5)-C(44)	1.328(8)	C(18)-F(3)	1.345(7)
N(5)-C(1)	1.336(8)	C(18)-C(19)	1.386(9)
N(6)-C(15)	1.318(8)	C(19)-F(2)	1.352(7)
N(6)-C(8)	1.321(8)	C(19)-C(20)	1.372(8)
N(7)-C(22)	1.323(7)	C(20)-F(1)	1.339(7)
N(7)-C(23)	1.331(8)	C(20)-C(21)	1.381(8)
N(8)-C(37)	1.316(7)	C(21)-C(22)	1.471(8)
N(8)-C(30)	1.318(8)	C(23)-C(24)	1.458(8)
O(1M)-C(1M)	1.434(8)	C(24)-C(25)	1.376(8)
C(1)-C(2)	1.448(8)	C(24)-C(29)	1.392(8)
C(2)-C(3)	1.380(8)	C(25)-F(5)	1.349(7)
C(2)-C(7)	1.380(8)	C(25)-C(26)	1.395(8)
C(3)-F(9)	1.354(7)	C(26)-C(27)	1.445(9)
C(3)-C(4)	1.386(8)	C(26)-C(31)	1.547(8)
C(4)-C(5)	1.459(8)	C(27)-C(28)	1.390(8)
C(4)-C(9)	1.547(8)	C(27)-C(34)	1.541(8)
C(5)-C(6)	1.390(8)	C(28)-F(6)	1.352(7)
C(5)-C(12)	1.536(8)	C(28)-C(29)	1.389(8)
C(6)-F(10)	1.349(7)	C(29)-C(30)	1.458(8)
C(6)-C(7)	1.391(8)	C(31)-F(11)	1.374(7)
C(7)-C(8)	1.462(8)	C(31)-C(32)	1.527(9)
C(9)-F(25)	1.367(7)	C(31)-C(33)	1.570(9)
C(9)-C(10)	1.545(10)	C(32)-F(14)	1.330(8)
C(9)-C(11)	1.575(10)	C(32)-F(13)	1.346(7)
C(10)-F(27)	1.322(8)	C(32)-F(12)	1.346(7)
C(10)-F(28)	1.336(7)	C(33)-F(16)	1.335(7)
C(10)-F(26)	1.337(7)	C(33)-F(15)	1.342(7)
C(11)-F(38)	1.333(7)	C(33)-F(17)	1.342(7)
C(11)-F(36)	1.333(7)	C(34)-F(18)	1.367(7)
C(11)-F(37)	1.337(8)	C(34)-C(36)	1.549(10)
C(12)-F(29)	1.371(7)	C(34)-C(35)	1.585(10)
C(12)-C(13)	1.544(10)	C(35)-F(23)	1.328(8)
C(12)-C(14)	1.587(10)	C(35)-F(24)	1.336(8)
C(13)-F(30)	1.322(7)	C(35)-F(22)	1.341(8)
C(13)-F(32)	1.328(9)	C(36)-F(20)	1.328(7)
C(13)-F(31)	1.336(8)	C(36)-F(21)	1.331(8)

C(36)-F(19)	1.335(7)	C(47)-F(44)	1.309(9)
C(37)-C(38)	1.464(8)	C(47)-F(43)	1.326(9)
C(38)-C(43)	1.383(8)	C(47)-F(45)	1.354(8)
C(38)-C(39)	1.383(9)	C(48)-F(46)	1.375(8)
C(39)-F(7)	1.340(7)	C(48)-C(49)	1.540(12)
C(39)-C(40)	1.405(9)	C(48)-C(50)	1.558(12)
C(40)-C(41)	1.451(9)	C(49)-F(47)	1.318(11)
C(40)-C(48)	1.536(9)	C(49)-F(49)	1.327(9)
C(41)-C(42)	1.401(9)	C(49)-F(48)	1.337(9)
C(41)-C(45)	1.539(9)	C(50)-F(51)	1.319(10)
C(42)-F(8)	1.339(7)	C(50)-F(52)	1.337(9)
C(42)-C(43)	1.391(8)	C(50)-F(50)	1.347(10)
C(43)-C(44)	1.449(8)	C(1S)-C(2S)	1.567(14)
C(45)-F(39)	1.371(8)	C(2S)-O(1S)	1.215(12)
C(45)-C(46)	1.528(12)	C(2S)-C(3S)	1.483(14)
C(45)-C(47)	1.608(12)	C(4S)-C(5S)	1.575(17)
C(46)-F(42)	1.322(9)	C(5S)-O(2S)	1.207(14)
C(46)-F(40)	1.334(9)	C(5S)-C(6S)	1.450(14)
C(46)-F(41)	1.341(10)		

N(2)-Cu(1)-N(3)	89.7(2)	N(4)-Cu(1)-N(1)	90.5(2)
N(2)-Cu(1)-N(4)	173.2(2)	N(2)-Cu(1)-O(1M)	96.02(19)
N(3)-Cu(1)-N(4)	89.7(2)	N(3)-Cu(1)-O(1M)	101.50(19)
N(2)-Cu(1)-N(1)	89.1(2)	N(4)-Cu(1)-O(1M)	90.78(19)
N(3)-Cu(1)-N(1)	171.6(2)	N(1)-Cu(1)-O(1M)	86.86(19)

C(8)-N(1)-C(1)	108.7(5)	F(9)-C(3)-C(4)	118.8(5)
C(8)-N(1)-Cu(1)	125.9(4)	C(2)-C(3)-C(4)	124.3(6)
C(1)-N(1)-Cu(1)	124.7(4)	C(3)-C(4)-C(5)	116.8(5)
C(15)-N(2)-C(22)	108.9(5)	C(3)-C(4)-C(9)	116.4(5)
C(15)-N(2)-Cu(1)	125.8(4)	C(5)-C(4)-C(9)	126.6(5)
C(22)-N(2)-Cu(1)	125.2(4)	C(6)-C(5)-C(4)	116.8(5)
C(23)-N(3)-C(30)	108.2(5)	C(6)-C(5)-C(12)	116.7(5)
C(23)-N(3)-Cu(1)	126.1(4)	C(4)-C(5)-C(12)	126.5(5)
C(30)-N(3)-Cu(1)	125.6(4)	F(10)-C(6)-C(5)	119.1(5)
C(37)-N(4)-C(44)	108.8(5)	F(10)-C(6)-C(7)	117.0(5)
C(37)-N(4)-Cu(1)	126.0(4)	C(5)-C(6)-C(7)	123.9(6)
C(44)-N(4)-Cu(1)	125.2(4)	C(2)-C(7)-C(6)	118.6(6)
C(44)-N(5)-C(1)	122.3(5)	C(2)-C(7)-C(8)	106.9(5)
C(15)-N(6)-C(8)	121.7(5)	C(6)-C(7)-C(8)	134.4(6)
C(22)-N(7)-C(23)	121.6(5)	N(6)-C(8)-N(1)	128.4(5)
C(37)-N(8)-C(30)	122.6(5)	N(6)-C(8)-C(7)	122.8(5)
C(1M)-O(1M)-Cu(1)	119.8(4)	N(1)-C(8)-C(7)	108.6(5)
N(5)-C(1)-N(1)	128.2(5)	F(25)-C(9)-C(10)	106.0(5)
N(5)-C(1)-C(2)	122.7(5)	F(25)-C(9)-C(4)	110.8(5)
N(1)-C(1)-C(2)	109.1(5)	C(10)-C(9)-C(4)	112.7(5)
C(3)-C(2)-C(7)	118.9(5)	F(25)-C(9)-C(11)	101.9(5)
C(3)-C(2)-C(1)	134.3(6)	C(10)-C(9)-C(11)	111.2(5)
C(7)-C(2)-C(1)	106.6(5)	C(4)-C(9)-C(11)	113.4(5)
F(9)-C(3)-C(2)	116.8(5)	F(27)-C(10)-F(28)	108.2(6)

F(27)-C(10)-F(26)	108.4(6)	N(7)-C(22)-N(2)	128.9(6)
F(28)-C(10)-F(26)	107.5(5)	N(7)-C(22)-C(21)	121.9(5)
F(27)-C(10)-C(9)	111.4(6)	N(2)-C(22)-C(21)	109.1(5)
F(28)-C(10)-C(9)	111.5(5)	N(7)-C(23)-N(3)	128.0(5)
F(26)-C(10)-C(9)	109.6(6)	N(7)-C(23)-C(24)	122.1(5)
F(38)-C(11)-F(36)	106.1(5)	N(3)-C(23)-C(24)	109.9(5)
F(38)-C(11)-F(37)	107.7(6)	C(25)-C(24)-C(29)	119.3(5)
F(36)-C(11)-F(37)	108.2(5)	C(25)-C(24)-C(23)	134.5(6)
F(38)-C(11)-C(9)	109.7(5)	C(29)-C(24)-C(23)	106.1(5)
F(36)-C(11)-C(9)	114.3(6)	F(5)-C(25)-C(24)	117.1(5)
F(37)-C(11)-C(9)	110.6(5)	F(5)-C(25)-C(26)	119.0(5)
F(29)-C(12)-C(5)	110.4(5)	C(24)-C(25)-C(26)	123.8(6)
F(29)-C(12)-C(13)	107.1(5)	C(25)-C(26)-C(27)	117.0(5)
C(5)-C(12)-C(13)	112.9(6)	C(25)-C(26)-C(31)	115.7(6)
F(29)-C(12)-C(14)	101.1(5)	C(27)-C(26)-C(31)	126.9(5)
C(5)-C(12)-C(14)	114.4(5)	C(28)-C(27)-C(26)	117.2(6)
C(13)-C(12)-C(14)	110.0(6)	C(28)-C(27)-C(34)	116.0(5)
F(30)-C(13)-F(32)	108.6(7)	C(26)-C(27)-C(34)	126.7(5)
F(30)-C(13)-F(31)	108.4(6)	F(6)-C(28)-C(29)	116.3(5)
F(32)-C(13)-F(31)	107.8(5)	F(6)-C(28)-C(27)	119.5(5)
F(30)-C(13)-C(12)	111.3(5)	C(29)-C(28)-C(27)	124.2(6)
F(32)-C(13)-C(12)	110.2(6)	C(28)-C(29)-C(24)	117.9(6)
F(31)-C(13)-C(12)	110.5(6)	C(28)-C(29)-C(30)	134.7(6)
F(33)-C(14)-F(34)	106.8(6)	C(24)-C(29)-C(30)	107.3(5)
F(33)-C(14)-F(35)	107.3(6)	N(8)-C(30)-N(3)	127.8(5)
F(34)-C(14)-F(35)	108.3(5)	N(8)-C(30)-C(29)	123.6(5)
F(33)-C(14)-C(12)	109.5(5)	N(3)-C(30)-C(29)	108.5(5)
F(34)-C(14)-C(12)	113.9(6)	F(11)-C(31)-C(32)	105.1(5)
F(35)-C(14)-C(12)	110.7(5)	F(11)-C(31)-C(26)	110.5(5)
N(6)-C(15)-N(2)	128.7(6)	C(32)-C(31)-C(26)	113.4(5)
N(6)-C(15)-C(16)	122.3(5)	F(11)-C(31)-C(33)	101.6(5)
N(2)-C(15)-C(16)	109.0(5)	C(32)-C(31)-C(33)	111.2(5)
C(17)-C(16)-C(21)	120.4(5)	C(26)-C(31)-C(33)	114.0(5)
C(17)-C(16)-C(15)	132.7(6)	F(14)-C(32)-F(13)	107.5(5)
C(21)-C(16)-C(15)	106.8(5)	F(14)-C(32)-F(12)	107.7(5)
F(4)-C(17)-C(18)	119.6(5)	F(13)-C(32)-F(12)	106.9(5)
F(4)-C(17)-C(16)	122.5(6)	F(14)-C(32)-C(31)	111.8(6)
C(18)-C(17)-C(16)	117.9(6)	F(13)-C(32)-C(31)	112.4(5)
F(3)-C(18)-C(17)	119.8(6)	F(12)-C(32)-C(31)	110.3(5)
F(3)-C(18)-C(19)	119.2(6)	F(16)-C(33)-F(15)	105.9(5)
C(17)-C(18)-C(19)	121.1(6)	F(16)-C(33)-F(17)	107.2(5)
F(2)-C(19)-C(20)	120.2(6)	F(15)-C(33)-F(17)	108.4(5)
F(2)-C(19)-C(18)	118.4(6)	F(16)-C(33)-C(31)	110.2(5)
C(20)-C(19)-C(18)	121.4(6)	F(15)-C(33)-C(31)	113.7(6)
F(1)-C(20)-C(19)	119.8(5)	F(17)-C(33)-C(31)	111.1(5)
F(1)-C(20)-C(21)	122.2(5)	F(18)-C(34)-C(27)	110.0(5)
C(19)-C(20)-C(21)	118.0(6)	F(18)-C(34)-C(36)	106.9(5)
C(20)-C(21)-C(16)	121.2(6)	C(27)-C(34)-C(36)	112.2(6)
C(20)-C(21)-C(22)	132.6(6)	F(18)-C(34)-C(35)	101.8(5)
C(16)-C(21)-C(22)	106.1(5)	C(27)-C(34)-C(35)	115.3(5)

C(36)-C(34)-C(35)	109.8(6)	F(39)-C(45)-C(47)	100.9(6)
F(23)-C(35)-F(24)	107.7(7)	C(46)-C(45)-C(47)	110.1(6)
F(23)-C(35)-F(22)	106.8(5)	C(41)-C(45)-C(47)	114.1(6)
F(24)-C(35)-F(22)	108.3(5)	F(42)-C(46)-F(40)	108.4(7)
F(23)-C(35)-C(34)	109.6(5)	F(42)-C(46)-F(41)	107.3(8)
F(24)-C(35)-C(34)	110.6(5)	F(40)-C(46)-F(41)	106.9(7)
F(22)-C(35)-C(34)	113.6(7)	F(42)-C(46)-C(45)	112.5(7)
F(20)-C(36)-F(21)	107.7(6)	F(40)-C(46)-C(45)	111.7(8)
F(20)-C(36)-F(19)	108.1(5)	F(41)-C(46)-C(45)	109.9(7)
F(21)-C(36)-F(19)	107.5(5)	F(44)-C(47)-F(43)	109.9(7)
F(20)-C(36)-C(34)	111.6(5)	F(44)-C(47)-F(45)	107.8(7)
F(21)-C(36)-C(34)	111.2(5)	F(43)-C(47)-F(45)	105.7(6)
F(19)-C(36)-C(34)	110.5(6)	F(44)-C(47)-C(45)	111.9(6)
N(8)-C(37)-N(4)	128.2(6)	F(43)-C(47)-C(45)	113.3(7)
N(8)-C(37)-C(38)	123.2(5)	F(45)-C(47)-C(45)	107.9(7)
N(4)-C(37)-C(38)	108.5(5)	F(46)-C(48)-C(40)	109.9(5)
C(43)-C(38)-C(39)	119.6(6)	F(46)-C(48)-C(49)	105.4(6)
C(43)-C(38)-C(37)	106.8(5)	C(40)-C(48)-C(49)	112.6(7)
C(39)-C(38)-C(37)	133.5(6)	F(46)-C(48)-C(50)	101.5(6)
F(7)-C(39)-C(38)	117.5(6)	C(40)-C(48)-C(50)	115.3(6)
F(7)-C(39)-C(40)	119.3(6)	C(49)-C(48)-C(50)	111.2(7)
C(38)-C(39)-C(40)	123.1(6)	F(47)-C(49)-F(49)	108.6(8)
C(39)-C(40)-C(41)	117.5(6)	F(47)-C(49)-F(48)	107.8(8)
C(39)-C(40)-C(48)	115.7(6)	F(49)-C(49)-F(48)	106.8(6)
C(41)-C(40)-C(48)	126.7(6)	F(47)-C(49)-C(48)	111.8(7)
C(42)-C(41)-C(40)	116.9(6)	F(49)-C(49)-C(48)	111.5(8)
C(42)-C(41)-C(45)	115.5(6)	F(48)-C(49)-C(48)	110.1(7)
C(40)-C(41)-C(45)	127.5(6)	F(51)-C(50)-F(52)	108.4(8)
F(8)-C(42)-C(43)	117.1(6)	F(51)-C(50)-F(50)	107.4(7)
F(8)-C(42)-C(41)	119.3(6)	F(52)-C(50)-F(50)	105.0(6)
C(43)-C(42)-C(41)	123.6(6)	F(51)-C(50)-C(48)	111.8(6)
C(38)-C(43)-C(42)	118.9(6)	F(52)-C(50)-C(48)	109.9(7)
C(38)-C(43)-C(44)	107.3(5)	F(50)-C(50)-C(48)	114.0(8)
C(42)-C(43)-C(44)	133.6(6)	O(1S)-C(2S)-C(3S)	117.7(11)
N(5)-C(44)-N(4)	128.1(6)	O(1S)-C(2S)-C(1S)	121.9(11)
N(5)-C(44)-C(43)	123.3(6)	C(3S)-C(2S)-C(1S)	120.3(11)
N(4)-C(44)-C(43)	108.7(5)	O(2S)-C(5S)-C(6S)	115.6(14)
F(39)-C(45)-C(46)	107.2(6)	O(2S)-C(5S)-C(4S)	122.6(11)
F(39)-C(45)-C(41)	110.9(6)	C(6S)-C(5S)-C(4S)	121.8(13)
C(46)-C(45)-C(41)	112.7(7)		

Symmetry transformations used to generate equivalent atoms:

Table M.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **F_{52}PcCu(MeOH·2Acetone)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{\cdot 2} U^{11} + ...\ + 2\ h\ k\ a\cdot\ b\cdot\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	34(1)	11(1)	26(1)	0(1)	1(1)	-5(1)
N(1)	33(3)	11(2)	27(3)	-3(2)	-1(2)	-3(2)
N(2)	22(3)	10(2)	31(3)	-2(2)	-5(2)	-1(2)
N(3)	29(3)	13(2)	27(3)	-1(2)	-1(2)	2(2)
N(4)	33(3)	7(2)	34(3)	-1(2)	0(3)	-1(2)
N(5)	35(3)	14(2)	27(3)	1(2)	0(3)	-2(2)
N(6)	34(3)	14(3)	26(3)	-1(2)	-1(2)	-4(2)
N(7)	28(3)	12(2)	25(3)	4(2)	-1(2)	-1(2)
N(8)	35(3)	10(2)	25(3)	0(2)	4(2)	-4(2)
O(1M)	28(3)	25(2)	39(3)	2(2)	2(2)	0(2)
C(1M)	47(5)	22(4)	56(5)	3(3)	-12(4)	-3(4)
C(1)	29(4)	15(3)	23(3)	-1(2)	-2(3)	-1(3)
C(2)	26(4)	15(3)	27(3)	1(3)	-2(3)	-4(3)
C(3)	34(4)	17(3)	19(3)	1(2)	1(3)	-2(3)
C(4)	41(4)	12(3)	27(3)	-1(3)	1(3)	-4(3)
C(5)	36(4)	13(3)	25(3)	3(3)	0(3)	1(3)
C(6)	36(4)	17(3)	22(3)	0(3)	1(3)	-5(3)
C(7)	30(4)	13(3)	24(3)	1(2)	-4(3)	-1(3)
C(8)	30(4)	9(3)	32(3)	3(3)	3(3)	-4(3)
C(9)	38(4)	11(3)	26(3)	2(3)	-1(3)	-2(3)
C(10)	42(5)	17(3)	36(4)	-1(3)	1(3)	-2(3)
F(26)	63(3)	23(2)	39(2)	-16(2)	-5(2)	0(2)
F(27)	36(2)	34(2)	41(2)	1(2)	-4(2)	-9(2)
F(28)	42(3)	26(2)	31(2)	4(2)	-5(2)	-4(2)
C(11)	38(4)	20(3)	35(4)	1(3)	1(3)	0(3)
F(36)	50(3)	25(2)	31(2)	1(2)	9(2)	3(2)
F(37)	34(2)	46(2)	41(2)	-4(2)	-2(2)	-2(2)
F(38)	50(3)	23(2)	53(3)	4(2)	9(2)	18(2)
C(12)	36(4)	13(3)	26(3)	-4(2)	0(3)	-10(3)
C(13)	62(6)	18(3)	28(4)	1(3)	-13(4)	-16(4)
F(30)	81(4)	23(2)	37(2)	3(2)	-15(2)	-18(2)
F(31)	85(4)	23(2)	38(2)	8(2)	0(2)	-24(2)
F(32)	64(3)	32(2)	43(2)	6(2)	-6(2)	10(2)
C(14)	50(5)	17(3)	43(4)	-7(3)	10(4)	-16(3)
F(33)	50(3)	30(2)	54(3)	-14(2)	20(2)	-24(2)
F(34)	70(3)	36(2)	35(2)	-14(2)	20(2)	-23(2)
F(35)	44(3)	20(2)	62(3)	-7(2)	10(2)	-3(2)
C(15)	24(4)	13(3)	29(3)	3(3)	-2(3)	-3(3)
C(16)	21(3)	15(3)	20(3)	1(2)	5(3)	0(3)
C(17)	25(4)	13(3)	33(4)	2(3)	7(3)	4(3)
C(18)	27(4)	23(3)	29(3)	11(3)	7(3)	-1(3)
C(19)	35(4)	20(3)	24(3)	-3(3)	3(3)	1(3)
C(20)	18(3)	14(3)	28(3)	-1(2)	0(3)	0(3)
C(21)	16(3)	15(3)	25(3)	1(2)	-3(3)	-1(3)
C(22)	17(3)	14(3)	30(3)	3(3)	-2(3)	0(3)

C(23)	29(4)	9(3)	29(3)	-1(2)	-4(3)	0(3)
C(24)	24(4)	14(3)	31(3)	3(3)	-5(3)	-5(3)
C(25)	23(4)	18(3)	26(3)	0(3)	1(3)	1(3)
C(26)	36(4)	12(3)	31(3)	0(3)	-1(3)	-4(3)
C(27)	44(5)	10(3)	29(3)	2(3)	6(3)	-2(3)
C(28)	40(4)	16(3)	23(3)	2(3)	5(3)	0(3)
C(29)	31(4)	12(3)	26(3)	0(2)	1(3)	2(3)
C(30)	32(4)	9(3)	29(3)	3(2)	10(3)	-8(3)
C(31)	26(4)	9(3)	31(3)	-2(3)	1(3)	-4(3)
C(32)	29(4)	13(3)	39(4)	2(3)	-4(3)	-6(3)
F(12)	45(3)	23(2)	41(2)	-13(2)	-4(2)	-1(2)
F(13)	40(2)	22(2)	32(2)	5(2)	-3(2)	-3(2)
F(14)	30(2)	26(2)	46(2)	4(2)	2(2)	-10(2)
C(33)	40(4)	11(3)	33(4)	2(3)	-6(3)	-4(3)
F(15)	44(3)	18(2)	31(2)	0(2)	6(2)	-2(2)
F(16)	45(3)	14(2)	48(2)	2(2)	7(2)	8(2)
F(17)	32(2)	26(2)	40(2)	-3(2)	-1(2)	-4(2)
C(34)	43(4)	14(3)	30(3)	-2(3)	5(3)	-7(3)
C(35)	57(5)	20(3)	36(4)	0(3)	10(4)	-10(4)
F(22)	62(3)	30(2)	33(2)	-1(2)	16(2)	-13(2)
F(23)	54(3)	32(2)	50(3)	-5(2)	16(2)	-21(2)
F(24)	50(3)	28(2)	47(2)	4(2)	13(2)	0(2)
C(36)	51(5)	13(3)	31(4)	5(3)	-6(3)	-13(3)
F(19)	71(3)	20(2)	38(2)	9(2)	3(2)	-14(2)
F(20)	64(3)	25(2)	37(2)	2(2)	-12(2)	-14(2)
F(21)	58(3)	34(2)	37(2)	7(2)	3(2)	11(2)
C(37)	29(4)	11(3)	28(3)	5(2)	1(3)	0(3)
C(38)	42(4)	16(3)	21(3)	0(3)	5(3)	-3(3)
C(39)	47(5)	13(3)	34(4)	1(3)	4(3)	-6(3)
C(40)	53(5)	20(3)	22(3)	3(3)	6(3)	-2(3)
C(41)	51(5)	25(4)	21(3)	-1(3)	-2(3)	-3(3)
C(42)	44(5)	17(3)	26(3)	-4(3)	1(3)	-1(3)
C(43)	38(4)	13(3)	23(3)	1(2)	-1(3)	0(3)
C(44)	28(4)	12(3)	27(3)	2(3)	2(3)	4(3)
C(45)	74(6)	27(4)	24(4)	1(3)	-1(4)	1(4)
C(46)	76(7)	44(5)	34(4)	-11(4)	2(4)	-9(5)
F(40)	121(5)	58(3)	38(3)	-23(2)	13(3)	-11(3)
F(41)	75(4)	62(3)	57(3)	-13(3)	17(3)	-2(3)
F(42)	98(4)	33(2)	49(3)	-2(2)	17(3)	19(3)
C(47)	59(6)	35(4)	37(4)	-2(4)	-19(4)	-6(4)
F(43)	91(4)	39(3)	43(3)	-4(2)	-7(3)	-22(3)
F(44)	56(3)	60(3)	60(3)	-3(3)	-6(3)	-6(3)
F(45)	90(4)	70(3)	46(3)	7(3)	-29(3)	-17(3)
C(48)	68(6)	21(3)	27(4)	0(3)	9(4)	-7(4)
C(49)	89(8)	31(4)	46(5)	11(4)	9(5)	-7(5)
F(47)	84(4)	55(3)	70(4)	4(3)	-24(3)	6(3)
F(48)	92(4)	40(3)	43(3)	1(2)	2(3)	17(3)
F(49)	132(5)	40(3)	47(3)	22(2)	17(3)	5(3)
C(50)	74(7)	46(5)	46(5)	9(4)	17(5)	-15(5)
F(50)	102(4)	47(3)	47(3)	-4(2)	19(3)	-39(3)

F(51)	50(3)	70(3)	55(3)	-7(3)	3(3)	-3(3)
F(52)	73(4)	92(4)	47(3)	-12(3)	26(3)	-35(3)
F(1)	35(2)	15(2)	34(2)	-5(2)	2(2)	-4(2)
F(2)	36(2)	28(2)	24(2)	-2(2)	0(2)	-1(2)
F(3)	40(2)	26(2)	29(2)	6(2)	9(2)	0(2)
F(4)	39(2)	14(2)	38(2)	1(2)	2(2)	-6(2)
F(5)	45(2)	15(2)	25(2)	-1(1)	7(2)	-8(2)
F(6)	63(3)	20(2)	25(2)	-1(2)	11(2)	-15(2)
F(7)	63(3)	19(2)	30(2)	1(2)	6(2)	-11(2)
F(8)	56(3)	17(2)	31(2)	-2(2)	-1(2)	-9(2)
F(9)	45(3)	17(2)	24(2)	-2(2)	6(2)	-6(2)
F(10)	56(3)	20(2)	24(2)	-4(2)	9(2)	-13(2)
F(11)	42(2)	11(2)	32(2)	4(2)	4(2)	-3(2)
F(18)	45(3)	18(2)	34(2)	-4(2)	4(2)	-12(2)
F(25)	47(3)	11(2)	34(2)	3(2)	5(2)	-1(2)
F(29)	43(3)	17(2)	31(2)	-6(2)	2(2)	-12(2)
F(39)	94(4)	41(2)	29(2)	8(2)	-7(2)	-8(3)
F(46)	88(4)	41(3)	30(2)	-3(2)	13(2)	-16(3)
C(1S)	56(7)	132(11)	71(7)	8(7)	1(6)	21(7)
C(2S)	40(6)	88(8)	79(7)	-1(6)	9(5)	24(6)
C(3S)	52(7)	54(6)	179(14)	9(8)	0(8)	7(6)
O(1S)	68(5)	127(7)	62(4)	-35(5)	-1(4)	39(5)
C(4S)	132(12)	82(9)	95(9)	22(7)	-4(9)	15(8)
C(5S)	54(7)	123(11)	72(7)	-6(7)	-1(6)	31(7)
C(6S)	80(9)	203(16)	59(7)	22(9)	25(6)	42(10)
O(2S)	106(7)	84(6)	117(7)	-25(5)	-36(6)	43(5)

Table M.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **F_{52}PcCu(MeOH·2Acetone)**.

	x	y	z	U(eq)
H(1M)	-2301	1205	878	37
H(1M1)	-635	2298	691	63
H(1M2)	-2479	2001	528	63
H(1M3)	-473	1773	431	63
H(1S1)	5250	1976	1833	129
H(1S2)	7323	1856	1966	129
H(1S3)	6245	1249	1796	129
H(3S1)	9410	2643	1614	143
H(3S2)	7438	3026	1594	143
H(3S3)	8385	2791	1309	143
H(4S1)	4858	8501	1755	155
H(4S2)	2785	8618	1621	155
H(4S3)	3386	8920	1930	155
H(6S1)	5275	10004	1253	169
H(6S2)	4111	9321	1178	169
H(6S3)	6228	9268	1301	169

Appendix N: Crystal structure of $F_{40}PcCu$

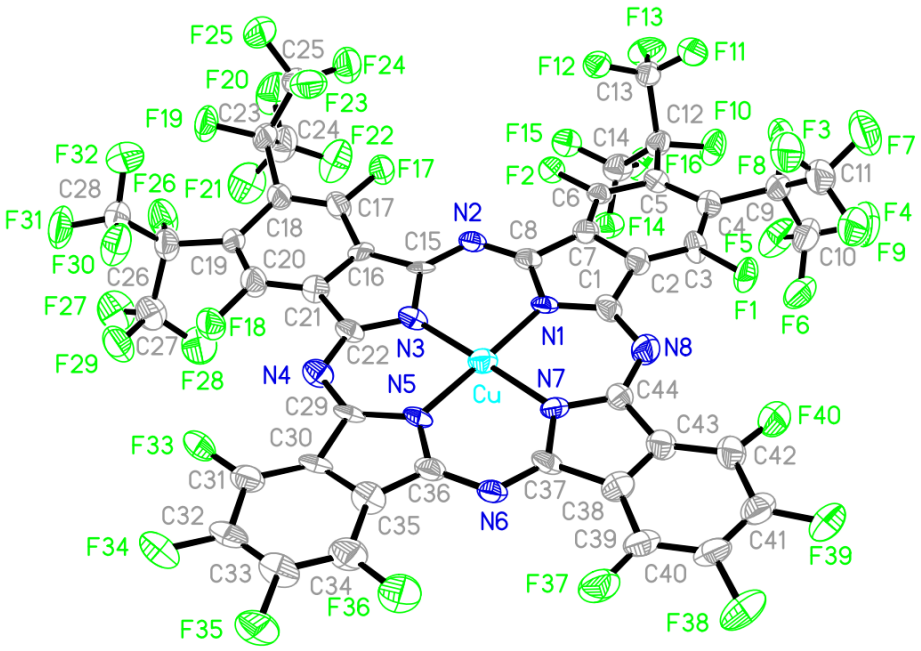


Figure N.1 ORTEP representation of **$F_{40}PcCu$** X-ray crystal structure, at 50% probability.

Table N.1 Crystal data and structure refinement for **$F_{40}PcCu \cdot 2Toluene$**

Empirical formula	C58 H16 Cu F40 N8	
Formula weight	1648.33	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.9803(17) Å	α = 73.516(9)°
	b = 18.422(5) Å	β = 86.242(7)°
	c = 23.424(6) Å	γ = 85.458(7)°
Volume	2876.3(12) $Å^3$	
Z	2	
Density (calculated)	1.903 g/cm^3	
Absorption coefficient	0.561 mm^{-1}	
F(000)	1618	
Crystal size	0.250 x 0.080 x 0.020 mm^3	
Theta range for data collection	1.253 to 25.027°.	
Index ranges	-8<=h<=8, -21<=k<=21, -27<=l<=27	
Reflections collected	65588	
Independent reflections	10172 [R(int) = 0.8325]	

Completeness to theta = 25.000°	100.0 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6267
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10172 / 1680 / 962
Goodness-of-fit on F^2	1.007
Final R indices [I>2sigma(I)]	R1 = 0.1251, wR2 = 0.2312
R indices (all data)	R1 = 0.3935, wR2 = 0.3429
Extinction coefficient	0.0042(8)
Largest diff. peak and hole	0.513 and -0.601 e.$Å^{-3}$

Table N.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **F_{40}PcCu·2Toluene**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu	5892(3)	3798(1)	6857(1)	33(1)
N(1)	4870(18)	3458(7)	7673(6)	25(3)
N(2)	3860(19)	4686(8)	7840(6)	30(2)
N(3)	5281(19)	4850(8)	6841(6)	30(3)
N(4)	6210(20)	5493(8)	5822(6)	35(4)
N(5)	6805(18)	4131(8)	6025(6)	27(3)
N(6)	7839(19)	2916(8)	5846(6)	30(2)
N(7)	6580(19)	2750(8)	6866(6)	32(3)
N(8)	5590(20)	2117(8)	7871(7)	43(4)
C(1)	4920(30)	2751(10)	8022(8)	33(4)
C(2)	4070(30)	2704(10)	8606(8)	31(4)
C(3)	3850(30)	2165(9)	9117(8)	32(4)
C(4)	3120(30)	2279(10)	9655(8)	39(4)
C(5)	2870(20)	3075(9)	9676(7)	30(4)
C(6)	3040(20)	3621(9)	9135(8)	26(4)
C(7)	3600(20)	3477(9)	8603(8)	30(4)
C(8)	4130(20)	3946(10)	8007(8)	27(4)
C(9)	2700(30)	1573(10)	10194(9)	49(3)
C(10)	4550(40)	1247(12)	10516(11)	63(4)
C(11)	1750(40)	949(13)	10026(11)	63(4)
C(12)	2380(30)	3380(10)	10229(8)	35(3)
C(13)	160(30)	3639(11)	10292(9)	39(3)
C(14)	3670(30)	3990(11)	10260(9)	44(4)
C(15)	4370(20)	5095(9)	7309(8)	23(4)
C(16)	4180(20)	5906(9)	7120(7)	24(3)
C(17)	3280(30)	6474(10)	7356(8)	41(5)
C(18)	3130(30)	7228(10)	7077(8)	42(4)
C(19)	4140(30)	7485(9)	6492(7)	31(4)
C(20)	4810(30)	6908(10)	6240(8)	42(5)

C(21)	4860(30)	6145(10)	6526(8)	31(4)
C(22)	5540(20)	5463(10)	6375(8)	29(4)
C(23)	1750(30)	7735(10)	7376(8)	43(3)
C(24)	2650(40)	7915(13)	7895(10)	61(4)
C(25)	-130(30)	7387(12)	7608(9)	49(4)
C(26)	4390(30)	8296(10)	6126(8)	44(3)
C(27)	6630(30)	8412(12)	5908(10)	52(4)
C(28)	3070(30)	8633(12)	5636(10)	50(4)
C(29)	6780(20)	4877(10)	5668(8)	30(4)
C(30)	7540(20)	4887(10)	5080(8)	34(4)
C(31)	7710(30)	5465(12)	4560(9)	42(4)
C(32)	8460(30)	5270(12)	4041(9)	39(4)
C(33)	8910(30)	4540(12)	4063(8)	41(4)
C(34)	8700(30)	3968(12)	4561(9)	50(5)
C(35)	7950(30)	4117(10)	5098(8)	34(4)
C(36)	7570(20)	3685(10)	5686(8)	34(4)
C(37)	7400(20)	2519(10)	6378(8)	31(4)
C(38)	7740(30)	1682(10)	6590(9)	40(4)
C(39)	8580(30)	1169(11)	6295(9)	42(5)
C(40)	8710(30)	438(12)	6624(10)	52(5)
C(41)	8100(30)	188(11)	7228(10)	46(5)
C(42)	7250(30)	714(11)	7516(10)	47(5)
C(43)	7130(30)	1458(10)	7178(9)	39(4)
C(44)	6400(20)	2144(9)	7341(8)	29(4)
F(1)	4251(15)	1438(5)	9114(4)	43(3)
F(2)	2686(13)	4351(5)	9122(4)	31(2)
F(3)	1456(16)	1780(5)	10601(5)	63(4)
F(4)	4230(20)	616(7)	10935(6)	99(5)
F(5)	5296(18)	1745(7)	10758(5)	74(4)
F(6)	5982(16)	1101(6)	10139(5)	63(3)
F(7)	560(20)	597(6)	10488(6)	88(4)
F(8)	594(18)	1237(6)	9569(6)	70(3)
F(9)	2899(17)	403(6)	9917(5)	70(4)
F(10)	2729(16)	2812(5)	10752(4)	51(3)
F(11)	-825(15)	3055(6)	10396(5)	56(3)
F(12)	-345(14)	4155(5)	9818(4)	42(3)
F(13)	-6(15)	3930(6)	10758(4)	57(3)
F(14)	5393(14)	3930(5)	9962(4)	48(3)
F(15)	2984(14)	4704(5)	10047(4)	42(3)
F(16)	4106(16)	3911(6)	10820(5)	55(3)
F(17)	2512(15)	6218(5)	7917(4)	43(3)
F(18)	5665(15)	7112(5)	5688(4)	48(3)
F(19)	1244(16)	8392(5)	6980(4)	58(3)
F(20)	1360(20)	8305(6)	8154(5)	81(4)
F(21)	4133(19)	8372(6)	7678(5)	72(4)
F(22)	3354(18)	7324(6)	8296(5)	75(4)
F(23)	-653(15)	6898(6)	7285(5)	56(3)
F(24)	-359(17)	7010(6)	8164(5)	65(3)
F(25)	-1610(17)	7919(6)	7507(5)	69(4)
F(26)	4297(17)	8765(6)	6514(5)	63(3)

F(27)	7100(17)	9081(6)	5923(5)	69(3)
F(28)	7808(16)	7878(6)	6218(5)	65(3)
F(29)	6927(16)	8403(6)	5341(5)	61(3)
F(30)	3240(17)	8237(6)	5249(5)	63(3)
F(31)	3571(17)	9351(6)	5347(5)	69(4)
F(32)	1331(18)	8669(6)	5843(5)	74(4)
F(33)	7247(15)	6185(6)	4529(4)	48(3)
F(34)	8639(16)	5834(6)	3535(5)	58(3)
F(35)	9651(16)	4399(6)	3553(4)	58(3)
F(36)	9181(17)	3231(6)	4555(4)	62(3)
F(37)	9155(16)	1374(6)	5735(5)	57(3)
F(38)	9528(17)	-107(6)	6365(5)	66(4)
F(39)	8338(17)	-547(6)	7527(5)	67(4)
F(40)	6790(16)	447(6)	8079(5)	59(3)
C(51)	-510(20)	4032(11)	7747(9)	42(5)
C(52)	-140(30)	3277(11)	7739(9)	46(5)
C(53)	-540(30)	2694(11)	8289(9)	52(5)
C(54)	-1360(30)	2927(13)	8781(10)	64(6)
C(55)	-1730(30)	3674(13)	8754(9)	49(5)
C(56)	-1310(30)	4233(12)	8250(9)	44(5)
C(57)	-1570(30)	5053(12)	8247(10)	77(7)
C(61)	12110(30)	1628(11)	7151(10)	50(5)
C(62)	12450(30)	2053(13)	6546(10)	64(6)
C(63)	13210(30)	1639(15)	6163(11)	75(6)
C(64)	13540(30)	866(14)	6356(11)	67(6)
C(65)	13200(30)	465(13)	6928(11)	61(6)
C(66)	12440(30)	834(13)	7349(10)	61(6)
C(67)	12120(40)	433(14)	7974(10)	106(9)

Table N.3 Bond lengths [Å] and angles [°] for **F_{40}PcCu·2Toluene**.

Cu-N(1)	1.939(13)	Cu-N(7)	1.946(13)
Cu-N(3)	1.941(13)	Cu-N(5)	1.951(14)
N(1)-C(1)	1.327(19)	N(8)-C(44)	1.32(2)
N(1)-C(8)	1.400(19)	N(8)-C(1)	1.35(2)
N(2)-C(15)	1.301(19)	C(1)-C(2)	1.44(2)
N(2)-C(8)	1.309(19)	C(2)-C(3)	1.33(2)
N(3)-C(22)	1.344(19)	C(2)-C(7)	1.43(2)
N(3)-C(15)	1.397(19)	C(3)-F(1)	1.349(17)
N(4)-C(29)	1.313(19)	C(3)-C(4)	1.39(2)
N(4)-C(22)	1.335(19)	C(4)-C(5)	1.48(2)
N(5)-C(36)	1.355(19)	C(4)-C(9)	1.57(2)
N(5)-C(29)	1.39(2)	C(5)-C(6)	1.38(2)
N(6)-C(37)	1.285(19)	C(5)-C(12)	1.56(2)
N(6)-C(36)	1.36(2)	C(6)-F(2)	1.340(17)
N(7)-C(44)	1.342(19)	C(6)-C(7)	1.37(2)
N(7)-C(37)	1.403(19)	C(7)-C(8)	1.46(2)

C(9)-F(3)	1.362(19)	C(30)-C(35)	1.42(2)
C(9)-C(11)	1.53(3)	C(31)-F(33)	1.32(2)
C(9)-C(10)	1.53(3)	C(31)-C(32)	1.42(2)
C(10)-F(4)	1.32(2)	C(32)-C(33)	1.34(2)
C(10)-F(6)	1.35(2)	C(32)-F(34)	1.34(2)
C(10)-F(5)	1.36(2)	C(33)-C(34)	1.34(2)
C(11)-F(9)	1.31(2)	C(33)-F(35)	1.355(18)
C(11)-F(8)	1.34(3)	C(34)-F(36)	1.38(2)
C(11)-F(7)	1.36(2)	C(34)-C(35)	1.42(2)
C(12)-F(10)	1.387(18)	C(35)-C(36)	1.40(2)
C(12)-C(14)	1.52(2)	C(37)-C(38)	1.48(2)
C(12)-C(13)	1.59(2)	C(38)-C(43)	1.37(2)
C(13)-F(11)	1.28(2)	C(38)-C(39)	1.39(2)
C(13)-F(12)	1.290(19)	C(39)-F(37)	1.31(2)
C(13)-F(13)	1.340(19)	C(39)-C(40)	1.35(2)
C(14)-F(16)	1.33(2)	C(40)-F(38)	1.38(2)
C(14)-F(15)	1.33(2)	C(40)-C(41)	1.41(3)
C(14)-F(14)	1.36(2)	C(41)-F(39)	1.34(2)
C(15)-C(16)	1.43(2)	C(41)-C(42)	1.41(2)
C(16)-C(21)	1.40(2)	C(42)-F(40)	1.30(2)
C(16)-C(17)	1.41(2)	C(42)-C(43)	1.37(2)
C(17)-F(17)	1.352(18)	C(43)-C(44)	1.46(2)
C(17)-C(18)	1.36(2)	C(51)-C(52)	1.40(2)
C(18)-C(19)	1.47(2)	C(51)-C(56)	1.40(2)
C(18)-C(23)	1.56(2)	C(51)-H(51A)	0.9500
C(19)-C(20)	1.39(2)	C(52)-C(53)	1.45(2)
C(19)-C(26)	1.51(2)	C(52)-H(52A)	0.9500
C(20)-F(18)	1.353(18)	C(53)-C(54)	1.41(3)
C(20)-C(21)	1.37(2)	C(53)-H(53A)	0.9500
C(21)-C(22)	1.44(2)	C(54)-C(55)	1.37(3)
C(23)-F(19)	1.337(18)	C(54)-H(54A)	0.9500
C(23)-C(25)	1.51(3)	C(55)-C(56)	1.36(3)
C(23)-C(24)	1.53(3)	C(55)-H(55A)	0.9500
C(24)-F(22)	1.30(2)	C(56)-C(57)	1.51(3)
C(24)-F(20)	1.33(2)	C(57)-H(57A)	0.9800
C(24)-F(21)	1.36(2)	C(57)-H(57B)	0.9800
C(25)-F(24)	1.30(2)	C(57)-H(57C)	0.9800
C(25)-F(25)	1.35(2)	C(61)-C(66)	1.41(3)
C(25)-F(23)	1.41(2)	C(61)-C(62)	1.43(3)
C(26)-F(26)	1.41(2)	C(61)-H(61A)	0.9500
C(26)-C(28)	1.48(3)	C(62)-C(63)	1.39(3)
C(26)-C(27)	1.63(3)	C(62)-H(62)	0.9500
C(27)-F(28)	1.31(2)	C(63)-C(64)	1.37(3)
C(27)-F(27)	1.31(2)	C(63)-H(63A)	0.9500
C(27)-F(29)	1.33(2)	C(64)-C(65)	1.35(3)
C(28)-F(32)	1.28(2)	C(64)-H(64A)	0.9500
C(28)-F(30)	1.31(2)	C(65)-C(66)	1.41(3)
C(28)-F(31)	1.37(2)	C(65)-H(65A)	0.9500
C(29)-C(30)	1.44(2)	C(66)-C(67)	1.45(3)
C(30)-C(31)	1.38(2)	C(67)-H(67A)	0.9800

C(67)-H(67B)	0.9800	C(67)-H(67C)	0.9800
N(1)-Cu-N(3)	91.0(5)	N(1)-Cu-N(5)	177.3(6)
N(1)-Cu-N(7)	90.0(6)	N(3)-Cu-N(5)	89.3(6)
N(3)-Cu-N(7)	178.4(6)	N(7)-Cu-N(5)	89.7(6)
C(1)-N(1)-C(8)	108.8(14)	C(11)-C(9)-C(4)	114.1(18)
C(1)-N(1)-Cu	126.8(12)	C(10)-C(9)-C(4)	110.3(17)
C(8)-N(1)-Cu	124.1(11)	F(4)-C(10)-F(6)	108.8(17)
C(15)-N(2)-C(8)	122.5(15)	F(4)-C(10)-F(5)	110(2)
C(22)-N(3)-C(15)	108.1(14)	F(6)-C(10)-F(5)	103.7(19)
C(22)-N(3)-Cu	126.7(11)	F(4)-C(10)-C(9)	110(2)
C(15)-N(3)-Cu	125.1(11)	F(6)-C(10)-C(9)	112.1(19)
C(29)-N(4)-C(22)	121.6(15)	F(5)-C(10)-C(9)	112.4(17)
C(36)-N(5)-C(29)	107.2(14)	F(9)-C(11)-F(8)	109(2)
C(36)-N(5)-Cu	126.8(12)	F(9)-C(11)-F(7)	104.8(17)
C(29)-N(5)-Cu	126.0(11)	F(8)-C(11)-F(7)	105(2)
C(37)-N(6)-C(36)	121.1(15)	F(9)-C(11)-C(9)	116(2)
C(44)-N(7)-C(37)	109.7(14)	F(8)-C(11)-C(9)	111.5(18)
C(44)-N(7)-Cu	125.5(12)	F(7)-C(11)-C(9)	109.0(19)
C(37)-N(7)-Cu	124.8(11)	F(10)-C(12)-C(14)	103.1(15)
C(44)-N(8)-C(1)	122.2(16)	F(10)-C(12)-C(5)	110.5(13)
N(1)-C(1)-N(8)	126.9(17)	C(14)-C(12)-C(5)	113.0(15)
N(1)-C(1)-C(2)	112.2(15)	F(10)-C(12)-C(13)	104.7(14)
N(8)-C(1)-C(2)	120.9(16)	C(14)-C(12)-C(13)	111.7(15)
C(3)-C(2)-C(7)	118.4(16)	C(5)-C(12)-C(13)	113.0(15)
C(3)-C(2)-C(1)	136.6(17)	F(11)-C(13)-F(12)	112.1(18)
C(7)-C(2)-C(1)	104.6(15)	F(11)-C(13)-F(13)	110.4(16)
C(2)-C(3)-F(1)	118.0(16)	F(12)-C(13)-F(13)	109.5(15)
C(2)-C(3)-C(4)	125.6(17)	F(11)-C(13)-C(12)	108.6(15)
F(1)-C(3)-C(4)	116.3(15)	F(12)-C(13)-C(12)	110.1(15)
C(3)-C(4)-C(5)	116.3(15)	F(13)-C(13)-C(12)	106.0(16)
C(3)-C(4)-C(9)	118.9(16)	F(16)-C(14)-F(15)	106.4(15)
C(5)-C(4)-C(9)	124.8(16)	F(16)-C(14)-F(14)	105.3(16)
C(6)-C(5)-C(4)	115.9(15)	F(15)-C(14)-F(14)	106.3(16)
C(6)-C(5)-C(12)	115.7(15)	F(16)-C(14)-C(12)	110.7(16)
C(4)-C(5)-C(12)	128.3(15)	F(15)-C(14)-C(12)	116.3(17)
F(2)-C(6)-C(7)	116.6(15)	F(14)-C(14)-C(12)	111.2(15)
F(2)-C(6)-C(5)	118.4(15)	N(2)-C(15)-N(3)	128.1(15)
C(7)-C(6)-C(5)	124.9(16)	N(2)-C(15)-C(16)	123.9(15)
C(6)-C(7)-C(2)	117.9(16)	N(3)-C(15)-C(16)	107.9(15)
C(6)-C(7)-C(8)	134.6(16)	C(21)-C(16)-C(17)	115.9(16)
C(2)-C(7)-C(8)	106.8(15)	C(21)-C(16)-C(15)	107.8(15)
N(2)-C(8)-N(1)	129.1(16)	C(17)-C(16)-C(15)	135.6(16)
N(2)-C(8)-C(7)	123.5(15)	F(17)-C(17)-C(18)	119.3(16)
N(1)-C(8)-C(7)	107.4(14)	F(17)-C(17)-C(16)	114.5(15)
F(3)-C(9)-C(11)	105.3(17)	C(18)-C(17)-C(16)	126.2(17)
F(3)-C(9)-C(10)	106.5(17)	C(17)-C(18)-C(19)	117.2(16)
C(11)-C(9)-C(10)	109.9(18)	C(17)-C(18)-C(23)	117.0(16)
F(3)-C(9)-C(4)	110.2(14)	C(19)-C(18)-C(23)	125.5(15)

C(20)-C(19)-C(18)	114.8(16)	N(5)-C(29)-C(30)	109.3(15)
C(20)-C(19)-C(26)	117.9(16)	C(31)-C(30)-C(35)	122.1(17)
C(18)-C(19)-C(26)	127.2(16)	C(31)-C(30)-C(29)	132.3(18)
F(18)-C(20)-C(21)	116.5(16)	C(35)-C(30)-C(29)	105.3(16)
F(18)-C(20)-C(19)	117.5(16)	F(33)-C(31)-C(30)	122.9(17)
C(21)-C(20)-C(19)	125.6(17)	F(33)-C(31)-C(32)	119.4(18)
C(20)-C(21)-C(16)	119.0(16)	C(30)-C(31)-C(32)	117.7(19)
C(20)-C(21)-C(22)	135.6(17)	C(33)-C(32)-F(34)	122.3(18)
C(16)-C(21)-C(22)	105.4(15)	C(33)-C(32)-C(31)	120(2)
N(4)-C(22)-N(3)	128.7(16)	F(34)-C(32)-C(31)	117.6(18)
N(4)-C(22)-C(21)	120.4(16)	C(34)-C(33)-C(32)	123.2(19)
N(3)-C(22)-C(21)	110.7(15)	C(34)-C(33)-F(35)	120.2(18)
F(19)-C(23)-C(25)	104.4(16)	C(32)-C(33)-F(35)	116.6(18)
F(19)-C(23)-C(24)	108.0(16)	C(33)-C(34)-F(36)	120.4(18)
C(25)-C(23)-C(24)	107.6(17)	C(33)-C(34)-C(35)	120.2(19)
F(19)-C(23)-C(18)	110.7(15)	F(36)-C(34)-C(35)	119.4(17)
C(25)-C(23)-C(18)	113.1(16)	C(36)-C(35)-C(30)	107.1(15)
C(24)-C(23)-C(18)	112.6(17)	C(36)-C(35)-C(34)	136.2(18)
F(22)-C(24)-F(20)	109.6(18)	C(30)-C(35)-C(34)	116.7(17)
F(22)-C(24)-F(21)	107(2)	N(5)-C(36)-N(6)	127.8(16)
F(20)-C(24)-F(21)	106.9(18)	N(5)-C(36)-C(35)	111.0(16)
F(22)-C(24)-C(23)	114.8(18)	N(6)-C(36)-C(35)	121.1(16)
F(20)-C(24)-C(23)	109.4(19)	N(6)-C(37)-N(7)	129.8(16)
F(21)-C(24)-C(23)	109.2(18)	N(6)-C(37)-C(38)	123.7(16)
F(24)-C(25)-F(25)	105.1(15)	N(7)-C(37)-C(38)	106.4(15)
F(24)-C(25)-F(23)	105.2(17)	C(43)-C(38)-C(39)	122.1(18)
F(25)-C(25)-F(23)	101.4(17)	C(43)-C(38)-C(37)	107.4(16)
F(24)-C(25)-C(23)	120.0(19)	C(39)-C(38)-C(37)	130.5(18)
F(25)-C(25)-C(23)	110.9(17)	F(37)-C(39)-C(40)	121.7(18)
F(23)-C(25)-C(23)	112.3(16)	F(37)-C(39)-C(38)	122.7(18)
F(26)-C(26)-C(28)	109.1(16)	C(40)-C(39)-C(38)	116(2)
F(26)-C(26)-C(19)	109.0(15)	C(39)-C(40)-F(38)	119.1(19)
C(28)-C(26)-C(19)	117.9(17)	C(39)-C(40)-C(41)	124(2)
F(26)-C(26)-C(27)	96.2(15)	F(38)-C(40)-C(41)	116.9(18)
C(28)-C(26)-C(27)	112.1(17)	F(39)-C(41)-C(40)	120.1(18)
C(19)-C(26)-C(27)	110.3(16)	F(39)-C(41)-C(42)	120.3(19)
F(28)-C(27)-F(27)	110.5(19)	C(40)-C(41)-C(42)	119.6(19)
F(28)-C(27)-F(29)	106.4(18)	F(40)-C(42)-C(43)	127.7(18)
F(27)-C(27)-F(29)	105.7(17)	F(40)-C(42)-C(41)	116.1(18)
F(28)-C(27)-C(26)	112.9(17)	C(43)-C(42)-C(41)	116(2)
F(27)-C(27)-C(26)	110.0(17)	C(38)-C(43)-C(42)	122.8(18)
F(29)-C(27)-C(26)	111.0(17)	C(38)-C(43)-C(44)	107.0(16)
F(32)-C(28)-F(30)	111(2)	C(42)-C(43)-C(44)	130.2(18)
F(32)-C(28)-F(31)	108.6(17)	N(8)-C(44)-N(7)	128.3(16)
F(30)-C(28)-F(31)	107.6(17)	N(8)-C(44)-C(43)	122.2(16)
F(32)-C(28)-C(26)	110.5(18)	N(7)-C(44)-C(43)	109.4(16)
F(30)-C(28)-C(26)	109.9(17)	C(52)-C(51)-C(56)	122.7(19)
F(31)-C(28)-C(26)	108.9(18)	C(52)-C(51)-H(51A)	118.7
N(4)-C(29)-N(5)	127.5(16)	C(56)-C(51)-H(51A)	118.7
N(4)-C(29)-C(30)	123.2(17)	C(51)-C(52)-C(53)	117.1(18)

C(51)-C(52)-H(52A)	121.4	C(62)-C(61)-H(61A)	118.6
C(53)-C(52)-H(52A)	121.4	C(63)-C(62)-C(61)	116(2)
C(54)-C(53)-C(52)	117.9(19)	C(63)-C(62)-H(62)	122.1
C(54)-C(53)-H(53A)	121.1	C(61)-C(62)-H(62)	122.1
C(52)-C(53)-H(53A)	121.1	C(64)-C(63)-C(62)	122(2)
C(55)-C(54)-C(53)	122(2)	C(64)-C(63)-H(63A)	119.2
C(55)-C(54)-H(54A)	119.0	C(62)-C(63)-H(63A)	119.2
C(53)-C(54)-H(54A)	119.0	C(65)-C(64)-C(63)	122(2)
C(56)-C(55)-C(54)	121(2)	C(65)-C(64)-H(64A)	118.9
C(56)-C(55)-H(55A)	119.4	C(63)-C(64)-H(64A)	118.9
C(54)-C(55)-H(55A)	119.4	C(64)-C(65)-C(66)	120(2)
C(55)-C(56)-C(51)	119(2)	C(64)-C(65)-H(65A)	119.9
C(55)-C(56)-C(57)	120.3(19)	C(66)-C(65)-H(65A)	119.9
C(51)-C(56)-C(57)	121(2)	C(65)-C(66)-C(61)	117(2)
C(56)-C(57)-H(57A)	109.5	C(65)-C(66)-C(67)	122(2)
C(56)-C(57)-H(57B)	109.5	C(61)-C(66)-C(67)	120(2)
H(57A)-C(57)-H(57B)	109.5	C(66)-C(67)-H(67A)	109.5
C(56)-C(57)-H(57C)	109.5	C(66)-C(67)-H(67B)	109.5
H(57A)-C(57)-H(57C)	109.5	H(67A)-C(67)-H(67B)	109.5
H(57B)-C(57)-H(57C)	109.5	C(66)-C(67)-H(67C)	109.5
C(66)-C(61)-C(62)	123(2)	H(67A)-C(67)-H(67C)	109.5
C(66)-C(61)-H(61A)	118.6	H(67B)-C(67)-H(67C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table N.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **F_{40}PcCu·2Toluene**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{\cdot 2} U^{11} + ... + 2 h k a^{\cdot} b^{\cdot} U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu	30(2)	35(1)	35(2)	-14(1)	3(1)	0(1)
N(1)	12(8)	31(6)	34(6)	-13(5)	4(6)	-3(6)
N(2)	21(6)	36(4)	34(5)	-11(3)	6(4)	-3(4)
N(3)	26(9)	37(5)	30(7)	-15(5)	8(6)	-9(6)
N(4)	39(10)	40(7)	29(7)	-17(6)	4(7)	-6(7)
N(5)	13(8)	36(6)	34(6)	-10(5)	6(6)	-11(6)
N(6)	21(6)	36(4)	34(5)	-11(3)	6(4)	-3(4)
N(7)	24(8)	35(5)	33(7)	-9(5)	4(6)	7(6)
N(8)	53(11)	36(7)	37(7)	-7(6)	7(7)	5(7)
C(1)	32(10)	30(6)	39(7)	-11(5)	4(7)	-11(7)
C(2)	34(10)	25(6)	36(7)	-12(5)	1(7)	-8(7)
C(3)	42(11)	19(6)	41(7)	-13(5)	-5(8)	-17(7)
C(4)	41(11)	30(6)	42(7)	-7(5)	5(7)	-1(7)
C(5)	29(10)	33(6)	29(6)	-9(5)	2(7)	-5(7)
C(6)	20(10)	28(6)	32(6)	-10(5)	2(7)	-4(7)
C(7)	27(10)	30(6)	35(6)	-11(5)	1(7)	-2(7)
C(8)	19(10)	32(5)	34(7)	-15(5)	2(7)	-6(6)
C(9)	53(8)	30(7)	54(8)	-4(5)	21(6)	5(6)
C(10)	75(10)	39(10)	63(12)	-1(6)	6(7)	13(7)

C(11)	70(11)	39(9)	76(11)	-12(7)	21(7)	-6(6)
C(12)	41(7)	32(7)	31(7)	-11(5)	0(6)	5(5)
C(13)	43(7)	35(8)	34(8)	-6(6)	9(7)	4(6)
C(14)	44(8)	43(7)	50(8)	-23(7)	0(7)	-2(6)
C(15)	6(9)	35(6)	33(6)	-15(5)	3(6)	0(6)
C(16)	9(9)	36(6)	27(7)	-9(5)	-10(6)	3(6)
C(17)	52(12)	27(6)	41(8)	-9(6)	17(8)	-4(7)
C(18)	48(11)	33(6)	37(8)	-3(6)	14(7)	5(7)
C(19)	33(10)	30(6)	26(8)	-4(5)	2(7)	4(6)
C(20)	57(12)	35(6)	31(8)	-7(6)	8(8)	1(8)
C(21)	39(11)	32(5)	25(7)	-16(5)	-2(7)	-2(7)
C(22)	27(10)	32(6)	33(7)	-16(5)	9(7)	-11(7)
C(23)	53(8)	26(7)	44(8)	-7(5)	9(6)	8(6)
C(24)	84(11)	46(10)	52(9)	-16(6)	-3(7)	7(7)
C(25)	50(8)	47(9)	43(8)	-8(6)	13(7)	8(6)
C(26)	62(7)	29(7)	38(8)	-5(5)	4(6)	-2(7)
C(27)	58(8)	49(9)	49(8)	-14(8)	-1(7)	-10(6)
C(28)	54(8)	39(8)	47(9)	0(6)	4(7)	7(8)
C(29)	17(10)	42(6)	32(7)	-16(5)	13(7)	-8(7)
C(30)	20(10)	48(6)	35(7)	-16(5)	14(7)	-5(7)
C(31)	34(11)	55(7)	36(7)	-12(6)	6(8)	0(8)
C(32)	23(11)	63(7)	36(7)	-19(6)	7(8)	-12(8)
C(33)	45(12)	68(7)	20(7)	-26(6)	-5(8)	-10(9)
C(34)	58(13)	60(7)	34(7)	-21(6)	6(9)	4(9)
C(35)	41(11)	44(6)	27(6)	-21(5)	-5(7)	-9(8)
C(36)	22(10)	39(5)	40(7)	-11(5)	7(8)	-6(7)
C(37)	25(10)	35(6)	37(6)	-17(5)	12(7)	-14(7)
C(38)	42(11)	37(6)	44(8)	-17(5)	1(8)	3(8)
C(39)	30(11)	42(7)	58(8)	-24(6)	2(8)	4(8)
C(40)	40(12)	44(7)	72(9)	-22(6)	7(9)	12(8)
C(41)	33(12)	39(7)	67(9)	-18(6)	-6(9)	4(8)
C(42)	52(13)	30(6)	59(8)	-14(6)	11(9)	-10(8)
C(43)	40(11)	31(6)	49(8)	-16(5)	8(8)	-10(7)
C(44)	26(10)	30(6)	33(7)	-9(5)	-2(7)	-6(7)
F(1)	61(8)	19(5)	50(7)	-11(5)	-3(6)	0(5)
F(2)	37(7)	30(5)	32(6)	-16(4)	2(5)	-5(5)
F(3)	76(8)	31(6)	70(8)	-6(5)	41(6)	1(6)
F(4)	122(12)	64(8)	79(10)	22(7)	13(8)	12(7)
F(5)	94(10)	68(8)	59(8)	-21(6)	-22(7)	34(7)
F(6)	65(8)	48(7)	70(8)	-12(6)	2(6)	21(6)
F(7)	115(11)	51(8)	93(9)	-15(7)	42(8)	-27(7)
F(8)	73(9)	44(7)	92(9)	-18(6)	8(7)	-12(6)
F(9)	80(9)	37(7)	90(9)	-17(6)	15(7)	-6(6)
F(10)	80(8)	40(6)	28(6)	-4(5)	-6(6)	10(5)
F(11)	46(7)	43(6)	75(8)	-13(6)	16(6)	-5(5)
F(12)	43(7)	45(6)	34(6)	-7(5)	4(5)	7(5)
F(13)	57(8)	75(8)	43(6)	-31(6)	3(6)	15(6)
F(14)	35(6)	52(7)	62(7)	-25(6)	-3(5)	-2(5)
F(15)	43(7)	43(6)	45(6)	-21(5)	0(5)	-5(5)
F(16)	66(8)	49(7)	56(6)	-27(5)	-15(6)	6(6)

F(17)	60(8)	28(6)	38(6)	-9(5)	16(5)	2(5)
F(18)	66(8)	39(6)	35(6)	-11(5)	14(5)	2(6)
F(19)	88(9)	30(6)	44(7)	0(5)	11(6)	19(5)
F(20)	125(11)	58(8)	60(8)	-26(6)	5(7)	25(7)
F(21)	92(9)	55(7)	83(9)	-37(6)	-13(7)	-8(6)
F(22)	108(11)	55(7)	62(8)	-19(6)	-24(7)	17(7)
F(23)	42(7)	60(7)	66(7)	-21(6)	5(6)	3(6)
F(24)	90(9)	43(7)	52(6)	-6(5)	22(6)	11(6)
F(25)	66(8)	55(7)	72(8)	-6(6)	17(7)	20(6)
F(26)	101(10)	38(6)	50(7)	-14(5)	15(6)	-7(6)
F(27)	78(9)	61(7)	74(8)	-25(6)	-3(7)	-24(6)
F(28)	61(8)	69(7)	65(8)	-14(6)	-11(6)	-12(6)
F(29)	73(9)	54(7)	49(7)	-6(6)	17(6)	-15(6)
F(30)	87(9)	48(7)	49(7)	-7(6)	-16(6)	14(6)
F(31)	81(9)	36(6)	72(8)	14(5)	-14(7)	-1(6)
F(32)	60(7)	66(8)	84(9)	-13(7)	14(6)	14(6)
F(33)	57(8)	57(6)	24(6)	-8(5)	16(5)	1(6)
F(34)	57(8)	71(7)	44(7)	-13(5)	18(6)	-19(6)
F(35)	71(9)	76(8)	33(6)	-28(6)	12(6)	3(7)
F(36)	87(9)	64(7)	40(7)	-30(6)	8(6)	9(7)
F(37)	64(9)	55(7)	54(7)	-27(6)	6(6)	15(6)
F(38)	73(9)	51(7)	87(9)	-43(6)	-11(7)	20(6)
F(39)	73(9)	38(6)	88(9)	-21(6)	7(7)	13(6)
F(40)	68(9)	40(7)	63(7)	-11(5)	11(7)	6(6)
C(51)	29(11)	49(8)	52(10)	-21(8)	8(9)	-9(9)
C(52)	39(12)	48(9)	60(11)	-29(8)	6(9)	-13(9)
C(53)	29(12)	48(10)	74(12)	-14(8)	13(10)	-3(9)
C(54)	29(12)	89(10)	65(12)	-15(10)	5(10)	11(11)
C(55)	26(12)	99(11)	38(10)	-42(8)	-14(9)	-1(10)
C(56)	17(11)	79(10)	52(10)	-41(8)	-14(9)	1(9)
C(57)	61(17)	86(11)	106(19)	-65(12)	-3(14)	-1(12)
C(61)	35(12)	55(9)	75(11)	-37(8)	-24(10)	0(9)
C(62)	29(12)	73(12)	86(12)	-17(9)	-23(11)	15(11)
C(63)	35(14)	108(13)	83(13)	-31(11)	-14(11)	12(12)
C(64)	29(12)	102(13)	90(12)	-62(11)	-6(12)	13(12)
C(65)	31(12)	61(12)	105(13)	-44(10)	-14(12)	-3(10)
C(66)	48(13)	60(10)	76(11)	-20(8)	-7(11)	-3(10)
C(67)	100(20)	130(20)	79(12)	5(12)	-23(14)	-33(17)

Table N.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **F_{40}PcCu·2Toluene**.

	x	y	z	U(eq)
H(51A)	-207	4424	7398	51
H(52A)	344	3152	7388	55
H(53A)	-252	2172	8317	62
H(54A)	-1669	2552	9141	76
H(55A)	-2295	3807	9094	59
H(57A)	-2828	5147	8432	116
H(57B)	-1489	5377	7836	116
H(57C)	-554	5168	8473	116
H(61A)	11638	1892	7431	60
H(62)	12186	2587	6413	77
H(63A)	13492	1897	5757	90
H(64A)	14042	603	6077	81
H(65A)	13468	-69	7046	73
H(67A)	12403	-112	8032	159
H(67B)	10780	527	8099	159
H(67C)	12973	615	8213	159

Appendix O: Crystal structure of [NHAcF$_{51}$PcZn]·7(toluene)

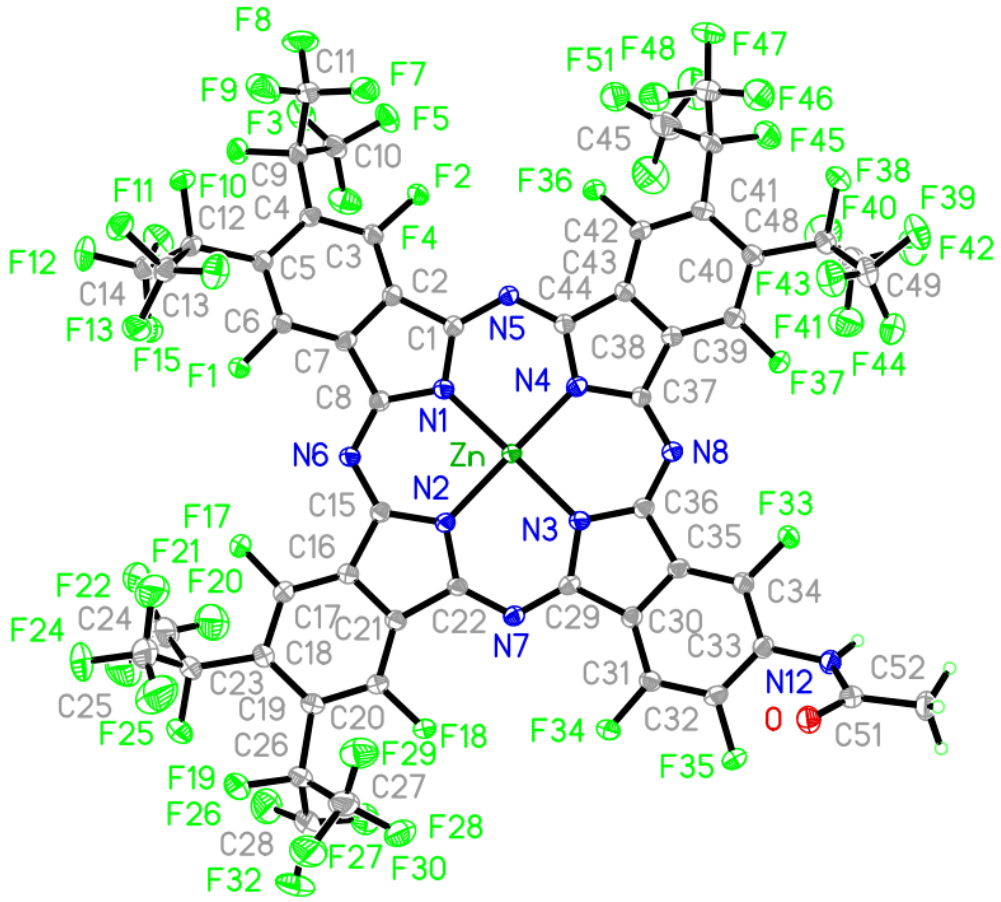


Figure O.1 ORTEP representation of **NHAcF$_{51}$PcZn** X-ray crystal structure, at 50% probability.

Table O.1 Crystal data and structure refinement for **[NHAcF$_{51}$PcZn]$_2$·7(toluene)**.

Empirical formula	C153 H64 F102 N18 O2 Zn2	
Formula weight	4254.96	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 19.2890(7) Å	alpha = 90 deg.
	b = 35.2821(13) Å	beta = 103.8470(10) deg.
	c = 23.7942(9) Å	gamma = 90 deg.
Volume	15722.7(10) Å^3	
Z, Calculated density	4, 1.798 g/cm^3	
Absorption coefficient	0.488 mm^{-1}	

F(000)	8408
Crystal size	0.550 x 0.250 x 0.130 mm
Theta range for data collection	1.354 to 30.685 deg.
Limiting indices	-27<=h<=27, -50<=k<=50, -34<=l<=34
Reflections collected / unique	251172 / 24345 [R(int) = 0.0734]
Completeness to theta = 25.000	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6840
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	24345 / 10 / 1304
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1206
R indices (all data)	R1 = 0.1076, wR2 = 0.1521
Extinction coefficient	n/a
Largest diff. peak and hole	1.312 and -0.705 e.$Å^{-3}$

Table O.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **$[NHAcF_{51}PcZn]_2 \cdot 7$(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn	7599(1)	2940(1)	6383(1)	19(1)
N(1)	6528(1)	2941(1)	6175(1)	19(1)
N(2)	7576(1)	2382(1)	6543(1)	18(1)
N(3)	8620(1)	2881(1)	6325(1)	18(1)
N(4)	7572(1)	3448(1)	5999(1)	20(1)
N(5)	6303(1)	3574(1)	5779(1)	20(1)
N(6)	6319(1)	2313(1)	6521(1)	18(1)
N(7)	8842(1)	2250(1)	6733(1)	18(1)
N(8)	8840(1)	3528(1)	6083(1)	20(1)
N(12)	11719(1)	3283(1)	6842(1)	25(1)
O	12024(1)	3097(1)	7759(1)	26(1)
C(1)	6103(1)	3240(1)	5951(1)	19(1)
C(2)	5368(1)	3142(1)	5939(1)	20(1)
C(3)	4715(1)	3320(1)	5734(1)	21(1)
C(4)	4074(1)	3168(1)	5792(1)	20(1)
C(5)	4103(1)	2821(1)	6125(1)	20(1)
C(6)	4753(1)	2635(1)	6276(1)	19(1)
C(7)	5378(1)	2784(1)	6182(1)	19(1)
C(8)	6116(1)	2655(1)	6311(1)	18(1)
C(9)	3390(1)	3365(1)	5444(1)	24(1)
C(10)	3394(2)	3452(1)	4794(1)	28(1)
C(11)	3187(2)	3729(1)	5731(1)	31(1)
C(12)	3503(1)	2660(1)	6383(1)	21(1)

C(13)	3116(1)	2309(1)	6068(1)	26(1)
C(14)	3744(1)	2576(1)	7054(1)	25(1)
C(15)	6990(1)	2194(1)	6629(1)	18(1)
C(16)	7219(1)	1826(1)	6885(1)	20(1)
C(17)	6862(1)	1522(1)	7048(1)	24(1)
C(18)	7205(1)	1196(1)	7298(1)	29(1)
C(19)	7975(1)	1194(1)	7425(1)	27(1)
C(20)	8314(1)	1495(1)	7222(1)	22(1)
C(21)	7954(1)	1809(1)	6957(1)	19(1)
C(22)	8170(1)	2165(1)	6730(1)	17(1)
C(23)	6709(2)	866(1)	7377(2)	43(1)
C(24)	6075(2)	786(1)	6826(2)	59(1)
C(25)	6414(2)	908(1)	7918(2)	65(1)
C(26)	8473(2)	898(1)	7803(1)	34(1)
C(27)	9099(2)	1076(1)	8274(1)	39(1)
C(28)	8758(2)	602(1)	7437(2)	43(1)
C(29)	9038(1)	2580(1)	6553(1)	18(1)
C(30)	9789(1)	2686(1)	6619(1)	19(1)
C(31)	10423(1)	2494(1)	6814(1)	20(1)
C(32)	11058(1)	2691(1)	6862(1)	21(1)
C(33)	11072(1)	3077(1)	6733(1)	22(1)
C(34)	10427(1)	3258(1)	6511(1)	20(1)
C(35)	9790(1)	3067(1)	6450(1)	19(1)
C(36)	9041(1)	3181(1)	6264(1)	18(1)
C(37)	8163(1)	3642(1)	5947(1)	19(1)
C(38)	7936(1)	4015(1)	5705(1)	20(1)
C(39)	8291(1)	4327(1)	5570(1)	24(1)
C(40)	7951(1)	4661(1)	5348(1)	26(1)
C(41)	7178(1)	4665(1)	5215(1)	25(1)
C(42)	6838(1)	4346(1)	5368(1)	24(1)
C(43)	7200(1)	4027(1)	5613(1)	21(1)
C(44)	6977(1)	3664(1)	5803(1)	20(1)
C(45)	6678(2)	4983(1)	4908(2)	35(1)
C(46)	6412(2)	5238(1)	5338(2)	48(1)
C(47)	6027(2)	4847(1)	4414(2)	52(1)
C(48)	8447(2)	4996(1)	5287(1)	32(1)
C(49)	8705(2)	4966(1)	4725(2)	44(1)
C(50)	9106(2)	5059(1)	5826(2)	39(1)
C(51)	12165(1)	3292(1)	7377(1)	23(1)
C(52)	12803(2)	3547(1)	7476(1)	31(1)
F(1)	4797(1)	2306(1)	6561(1)	26(1)
F(2)	4714(1)	3648(1)	5451(1)	28(1)
F(3)	2818(1)	3126(1)	5385(1)	30(1)
F(4)	3788(1)	3200(1)	4597(1)	41(1)

F(5)	3621(1)	3795(1)	4707(1)	35(1)
F(6)	2730(1)	3426(1)	4470(1)	42(1)
F(7)	3709(1)	3976(1)	5851(1)	40(1)
F(8)	2626(1)	3895(1)	5385(1)	50(1)
F(9)	3005(1)	3644(1)	6219(1)	54(1)
F(10)	2984(1)	2929(1)	6358(1)	27(1)
F(11)	2794(1)	2394(1)	5528(1)	39(1)
F(12)	2621(1)	2193(1)	6334(1)	39(1)
F(13)	3555(1)	2025(1)	6055(1)	34(1)
F(14)	3197(1)	2647(1)	7290(1)	32(1)
F(15)	3935(1)	2221(1)	7182(1)	34(1)
F(16)	4272(1)	2803(1)	7308(1)	35(1)
F(17)	6150(1)	1544(1)	6942(1)	33(1)
F(18)	9022(1)	1487(1)	7298(1)	27(1)
F(19)	7072(1)	531(1)	7436(1)	59(1)
F(20)	6247(1)	901(1)	6343(1)	62(1)
F(21)	5464(1)	947(1)	6851(1)	68(1)
F(22)	5957(1)	415(1)	6776(2)	90(1)
F(23)	6071(1)	1230(1)	7926(1)	68(1)
F(24)	5966(1)	623(1)	7940(2)	102(1)
F(25)	6936(1)	895(1)	8394(1)	87(1)
F(26)	8107(1)	699(1)	8129(1)	50(1)
F(27)	9240(1)	852(1)	8741(1)	58(1)
F(28)	9708(1)	1110(1)	8112(1)	44(1)
F(29)	8916(1)	1413(1)	8441(1)	45(1)
F(30)	9137(1)	757(1)	7104(1)	45(1)
F(31)	8226(1)	414(1)	7091(1)	61(1)
F(32)	9168(1)	351(1)	7781(1)	66(1)
F(33)	10444(1)	3626(1)	6369(1)	29(1)
F(34)	10451(1)	2127(1)	6947(1)	26(1)
F(35)	11674(1)	2500(1)	7028(1)	28(1)
F(36)	6128(1)	4341(1)	5268(1)	34(1)
F(37)	9003(1)	4307(1)	5674(1)	31(1)
F(38)	8097(1)	5333(1)	5270(1)	45(1)
F(39)	9086(1)	5269(1)	4663(1)	64(1)
F(40)	8144(1)	4954(1)	4271(1)	62(1)
F(41)	9087(1)	4661(1)	4709(1)	53(1)
F(42)	9240(1)	5429(1)	5880(1)	58(1)
F(43)	8958(1)	4938(1)	6308(1)	47(1)
F(44)	9704(1)	4897(1)	5768(1)	50(1)
F(45)	7026(1)	5217(1)	4608(1)	50(1)
F(46)	6954(1)	5431(1)	5659(1)	59(1)
F(47)	5933(1)	5483(1)	5065(1)	68(1)
F(48)	6121(1)	5033(1)	5689(1)	55(1)

F(49)	6180(1)	4528(1)	4180(1)	64(1)
F(50)	5887(1)	5108(1)	4001(1)	81(1)
F(51)	5430(1)	4795(1)	4587(1)	62(1)
C(1S)	7013(3)	3157(1)	4611(2)	46(2)
C(2S)	7703(2)	3280(1)	4632(2)	47(2)
C(3S)	7813(2)	3628(1)	4395(2)	48(2)
C(4S)	7233(2)	3853(1)	4136(2)	45(2)
C(5S)	6543(2)	3730(1)	4114(2)	42(1)
C(6S)	6433(2)	3382(1)	4352(2)	37(2)
C(7S)	5685(3)	3260(2)	4337(3)	50(2)
C(8S)	7079(4)	3539(2)	4382(3)	57(3)
C(9S)	7749(3)	3373(2)	4569(3)	51(3)
C(10S)	7813(2)	3014(2)	4816(3)	64(3)
C(11S)	7208(3)	2820(2)	4876(2)	49(2)
C(12S)	6538(3)	2985(2)	4689(3)	41(2)
C(13S)	6474(3)	3344(2)	4442(3)	43(4)
C(14S)	5755(4)	3525(3)	4229(5)	67(3)
C(1T)	1046(2)	3164(1)	5201(2)	61(1)
C(2T)	1001(2)	2792(1)	5361(2)	60(1)
C(3T)	357(3)	2613(1)	5264(2)	58(1)
C(4T)	-242(2)	2804(1)	4995(2)	58(1)
C(5T)	-200(2)	3170(1)	4826(2)	70(1)
C(6T)	439(2)	3361(1)	4931(2)	70(1)
C(7T)	480(4)	3765(2)	4747(4)	159(4)
C(1E)	8008(4)	5516(1)	2205(2)	197(7)
C(2E)	7331(4)	5425(1)	2272(2)	135(3)
C(3E)	7183(2)	5449(1)	2814(3)	107(2)
C(4E)	7711(3)	5563(1)	3290(2)	105(2)
C(5E)	8388(3)	5654(1)	3224(3)	102(2)
C(6E)	8536(3)	5631(1)	2681(3)	146(4)
C(7E)	9215(5)	5708(4)	2502(6)	245(7)
C(1K)	4958(5)	4451(1)	7526(3)	53(2)
C(2K)	5214(4)	4371(1)	7040(3)	54(2)
C(3K)	5324(4)	3997(2)	6899(3)	52(2)
C(4K)	5177(7)	3704(1)	7243(4)	60(3)
C(5K)	4921(6)	3784(1)	7728(4)	49(3)
C(6K)	4812(4)	4158(2)	7870(2)	47(2)
C(7K)	4546(5)	4244(3)	8398(3)	63(2)

Table O.3 Bond lengths [Å] and angles [deg] for **[NHAcF_{51}PcZn]$_2$·7(toluene)**.

Zn-N(4)	2.006(2)	C(10)-F(6)	1.331(3)
Zn-N(1)	2.007(2)	C(11)-F(7)	1.312(3)
Zn-N(2)	2.010(2)	C(11)-F(9)	1.325(4)
Zn-N(3)	2.017(2)	C(11)-F(8)	1.329(3)
Zn-O#1	2.0727(18)	C(12)-F(10)	1.369(3)
N(1)-C(1)	1.365(3)	C(12)-C(13)	1.545(4)
N(1)-C(8)	1.368(3)	C(12)-C(14)	1.582(4)
N(2)-C(22)	1.359(3)	C(13)-F(13)	1.316(3)
N(2)-C(15)	1.367(3)	C(13)-F(11)	1.319(3)
N(3)-C(36)	1.364(3)	C(13)-F(12)	1.332(3)
N(3)-C(29)	1.364(3)	C(14)-F(15)	1.318(3)
N(4)-C(37)	1.360(3)	C(14)-F(16)	1.324(3)
N(4)-C(44)	1.363(3)	C(14)-F(14)	1.333(3)
N(5)-C(44)	1.326(3)	C(15)-C(16)	1.456(3)
N(5)-C(1)	1.335(3)	C(16)-C(17)	1.380(3)
N(6)-C(15)	1.326(3)	C(16)-C(21)	1.388(3)
N(6)-C(8)	1.330(3)	C(17)-F(17)	1.338(3)
N(7)-C(29)	1.327(3)	C(17)-C(18)	1.387(4)
N(7)-C(22)	1.329(3)	C(18)-C(19)	1.443(4)
N(8)-C(36)	1.324(3)	C(18)-C(23)	1.548(4)
N(8)-C(37)	1.330(3)	C(19)-C(20)	1.394(4)
N(12)-C(51)	1.355(3)	C(19)-C(26)	1.552(4)
N(12)-C(33)	1.414(3)	C(20)-F(18)	1.335(3)
N(12)-H(12)	0.85(3)	C(20)-C(21)	1.376(3)
O-C(51)	1.221(3)	C(21)-C(22)	1.467(3)
C(1)-C(2)	1.454(3)	C(23)-F(19)	1.362(3)
C(2)-C(3)	1.386(3)	C(23)-C(25)	1.535(6)
C(2)-C(7)	1.387(3)	C(23)-C(24)	1.589(6)
C(3)-F(2)	1.338(3)	C(24)-F(21)	1.321(4)
C(3)-C(4)	1.386(3)	C(24)-F(22)	1.329(4)
C(4)-C(5)	1.450(3)	C(24)-F(20)	1.332(5)
C(4)-C(9)	1.544(3)	C(25)-F(23)	1.318(5)
C(5)-C(6)	1.384(3)	C(25)-F(25)	1.325(5)
C(5)-C(12)	1.542(3)	C(25)-F(24)	1.332(5)
C(6)-F(1)	1.339(3)	C(26)-F(26)	1.362(3)
C(6)-C(7)	1.383(3)	C(26)-C(28)	1.544(5)
C(7)-C(8)	1.454(3)	C(26)-C(27)	1.568(5)
C(9)-F(3)	1.369(3)	C(27)-F(28)	1.326(4)
C(9)-C(11)	1.548(4)	C(27)-F(29)	1.327(4)
C(9)-C(10)	1.580(4)	C(27)-F(27)	1.336(3)
C(10)-F(5)	1.320(3)	C(28)-F(30)	1.318(4)
C(10)-F(4)	1.325(3)	C(28)-F(31)	1.330(4)

C(28)-F(32)	1.332(4)	C(52)-H(52B)	0.98
C(29)-C(30)	1.466(3)	C(52)-H(52C)	0.98
C(30)-C(31)	1.378(3)	C(1S)-C(2S)	1.39
C(30)-C(35)	1.402(3)	C(1S)-C(6S)	1.39
C(31)-F(34)	1.330(3)	C(1S)-H(1SA)	0.95
C(31)-C(32)	1.388(3)	C(2S)-C(3S)	1.39
C(32)-F(35)	1.341(3)	C(2S)-H(2SA)	0.95
C(32)-C(33)	1.398(4)	C(3S)-C(4S)	1.39
C(33)-C(34)	1.385(3)	C(3S)-H(3SA)	0.95
C(34)-F(33)	1.342(3)	C(4S)-C(5S)	1.39
C(34)-C(35)	1.379(3)	C(4S)-H(4SA)	0.95
C(35)-C(36)	1.464(3)	C(5S)-C(6S)	1.39
C(37)-C(38)	1.462(3)	C(5S)-H(5SA)	0.95
C(38)-C(39)	1.376(3)	C(6S)-C(7S)	1.498(4)
C(38)-C(43)	1.383(3)	C(7S)-H(7SA)	0.98
C(39)-F(37)	1.338(3)	C(7S)-H(7SB)	0.98
C(39)-C(40)	1.389(4)	C(7S)-H(7SC)	0.98
C(40)-C(41)	1.448(4)	C(8S)-C(9S)	1.39
C(40)-C(48)	1.548(4)	C(8S)-C(13S)	1.39
C(41)-C(42)	1.394(4)	C(8S)-H(8SA)	0.95
C(41)-C(45)	1.546(4)	C(9S)-C(10S)	1.39
C(42)-F(36)	1.332(3)	C(9S)-H(9SA)	0.95
C(42)-C(43)	1.379(3)	C(10S)-C(11S)	1.39
C(43)-C(44)	1.458(3)	C(10S)-H(10A)	0.95
C(45)-F(45)	1.368(3)	C(11S)-C(12S)	1.39
C(45)-C(46)	1.538(5)	C(11S)-H(11A)	0.95
C(45)-C(47)	1.576(5)	C(12S)-C(13S)	1.39
C(46)-F(47)	1.318(4)	C(12S)-H(12A)	0.95
C(46)-F(46)	1.325(4)	C(13S)-C(14S)	1.498(4)
C(46)-F(48)	1.328(4)	C(14S)-H(14A)	0.98
C(47)-F(49)	1.319(5)	C(14S)-H(14B)	0.98
C(47)-F(50)	1.326(4)	C(14S)-H(14C)	0.98
C(47)-F(51)	1.326(5)	C(1T)-C(2T)	1.374(6)
C(48)-F(38)	1.364(3)	C(1T)-C(6T)	1.381(6)
C(48)-C(49)	1.538(5)	C(1T)-H(1TA)	0.95
C(48)-C(50)	1.591(5)	C(2T)-C(3T)	1.363(6)
C(49)-F(41)	1.312(4)	C(2T)-H(2TA)	0.95
C(49)-F(39)	1.324(4)	C(3T)-C(4T)	1.357(6)
C(49)-F(40)	1.334(4)	C(3T)-H(3TA)	0.95
C(50)-F(43)	1.316(4)	C(4T)-C(5T)	1.363(6)
C(50)-F(44)	1.324(4)	C(4T)-H(4TA)	0.95
C(50)-F(42)	1.331(3)	C(5T)-C(6T)	1.374(6)
C(51)-C(52)	1.496(4)	C(5T)-H(5TA)	0.95
C(52)-H(52A)	0.98	C(6T)-C(7T)	1.498(4)

C(7T)-H(7TA)	0.98	C(1K)-C(2K)	1.39
C(7T)-H(7TB)	0.98	C(1K)-C(6K)	1.39
C(7T)-H(7TC)	0.98	C(1K)-H(1KA)	0.95
C(1E)-C(2E)	1.39	C(2K)-C(3K)	1.39
C(1E)-C(6E)	1.39	C(2K)-H(2KA)	0.95
C(1E)-H(1EA)	0.95	C(3K)-C(4K)	1.39
C(2E)-C(3E)	1.39	C(3K)-H(3KA)	0.95
C(2E)-H(2EA)	0.95	C(4K)-C(5K)	1.39
C(3E)-C(4E)	1.39	C(4K)-H(4KA)	0.95
C(3E)-H(3EA)	0.95	C(5K)-C(6K)	1.39
C(4E)-C(5E)	1.39	C(5K)-H(5KA)	0.95
C(4E)-H(4EA)	0.95	C(6K)-C(7K)	1.498(4)
C(5E)-C(6E)	1.39	C(7K)-H(7KA)	0.98
C(5E)-H(5EA)	0.95	C(7K)-H(7KB)	0.98
C(6E)-C(7E)	1.496(4)	C(7K)-H(7KC)	0.98
C(7E)-H(7EA)	0.98		
C(7E)-H(7EB)	0.98		
C(7E)-H(7EC)	0.98		

N(4)-Zn-N(1)	88.52(8)	C(29)-N(7)-C(22)	123.3(2)
N(4)-Zn-N(2)	164.31(8)	C(36)-N(8)-C(37)	123.4(2)
N(1)-Zn-N(2)	88.79(8)	C(51)-N(12)-C(33)	121.2(2)
N(4)-Zn-N(3)	88.92(8)	C(51)-N(12)-H(12)	120(2)
N(1)-Zn-N(3)	161.38(8)	C(33)-N(12)-H(12)	117(2)
N(2)-Zn-N(3)	88.71(8)	C(51)-O-Zn#1	142.74(18)
N(4)-Zn-O#1	100.06(8)	N(5)-C(1)-N(1)	127.9(2)
N(1)-Zn-O#1	109.87(8)	N(5)-C(1)-C(2)	123.7(2)
N(2)-Zn-O#1	95.39(8)	N(1)-C(1)-C(2)	108.4(2)
N(3)-Zn-O#1	88.73(8)	C(3)-C(2)-C(7)	118.7(2)
C(1)-N(1)-C(8)	109.5(2)	C(3)-C(2)-C(1)	134.4(2)
C(1)-N(1)-Zn	125.66(16)	C(7)-C(2)-C(1)	106.9(2)
C(8)-N(1)-Zn	124.32(16)	F(2)-C(3)-C(2)	117.4(2)
C(22)-N(2)-C(15)	109.94(19)	F(2)-C(3)-C(4)	119.4(2)
C(22)-N(2)-Zn	123.86(16)	C(2)-C(3)-C(4)	123.2(2)
C(15)-N(2)-Zn	124.09(16)	C(3)-C(4)-C(5)	117.5(2)
C(36)-N(3)-C(29)	109.56(19)	C(3)-C(4)-C(9)	116.1(2)
C(36)-N(3)-Zn	122.85(16)	C(5)-C(4)-C(9)	126.1(2)
C(29)-N(3)-Zn	123.23(16)	C(6)-C(5)-C(4)	117.2(2)
C(37)-N(4)-C(44)	110.1(2)	C(6)-C(5)-C(12)	116.1(2)
C(37)-N(4)-Zn	123.99(16)	C(4)-C(5)-C(12)	126.3(2)
C(44)-N(4)-Zn	125.62(16)	F(1)-C(6)-C(7)	117.4(2)
C(44)-N(5)-C(1)	123.2(2)	F(1)-C(6)-C(5)	119.2(2)
C(15)-N(6)-C(8)	123.2(2)	C(7)-C(6)-C(5)	123.2(2)

C(6)-C(7)-C(2)	119.2(2)	N(2)-C(15)-C(16)	108.3(2)
C(6)-C(7)-C(8)	133.9(2)	C(17)-C(16)-C(21)	119.7(2)
C(2)-C(7)-C(8)	106.8(2)	C(17)-C(16)-C(15)	133.4(2)
N(6)-C(8)-N(1)	128.4(2)	C(21)-C(16)-C(15)	106.9(2)
N(6)-C(8)-C(7)	123.3(2)	F(17)-C(17)-C(16)	117.5(2)
N(1)-C(8)-C(7)	108.3(2)	F(17)-C(17)-C(18)	119.4(2)
F(3)-C(9)-C(4)	109.98(19)	C(16)-C(17)-C(18)	123.1(2)
F(3)-C(9)-C(11)	105.9(2)	C(17)-C(18)-C(19)	117.1(2)
C(4)-C(9)-C(11)	114.2(2)	C(17)-C(18)-C(23)	115.6(2)
F(3)-C(9)-C(10)	102.2(2)	C(19)-C(18)-C(23)	127.2(2)
C(4)-C(9)-C(10)	114.2(2)	C(20)-C(19)-C(18)	117.9(2)
C(11)-C(9)-C(10)	109.4(2)	C(20)-C(19)-C(26)	115.9(2)
F(5)-C(10)-F(4)	108.7(2)	C(18)-C(19)-C(26)	126.1(2)
F(5)-C(10)-F(6)	106.4(2)	F(18)-C(20)-C(21)	117.8(2)
F(4)-C(10)-F(6)	107.7(2)	F(18)-C(20)-C(19)	119.1(2)
F(5)-C(10)-C(9)	114.2(2)	C(21)-C(20)-C(19)	123.0(2)
F(4)-C(10)-C(9)	110.7(2)	C(20)-C(21)-C(16)	118.7(2)
F(6)-C(10)-C(9)	108.8(2)	C(20)-C(21)-C(22)	134.6(2)
F(7)-C(11)-F(9)	108.0(3)	C(16)-C(21)-C(22)	106.7(2)
F(7)-C(11)-F(8)	108.1(2)	N(7)-C(22)-N(2)	128.3(2)
F(9)-C(11)-F(8)	107.1(2)	N(7)-C(22)-C(21)	123.5(2)
F(7)-C(11)-C(9)	112.7(2)	N(2)-C(22)-C(21)	108.1(2)
F(9)-C(11)-C(9)	110.3(2)	F(19)-C(23)-C(25)	106.3(3)
F(8)-C(11)-C(9)	110.4(2)	F(19)-C(23)-C(18)	110.5(2)
F(10)-C(12)-C(5)	109.8(2)	C(25)-C(23)-C(18)	113.2(3)
F(10)-C(12)-C(13)	105.61(19)	F(19)-C(23)-C(24)	101.9(3)
C(5)-C(12)-C(13)	115.1(2)	C(25)-C(23)-C(24)	110.0(3)
F(10)-C(12)-C(14)	102.12(19)	C(18)-C(23)-C(24)	114.1(3)
C(5)-C(12)-C(14)	113.9(2)	F(21)-C(24)-F(22)	106.9(3)
C(13)-C(12)-C(14)	109.3(2)	F(21)-C(24)-F(20)	108.4(3)
F(13)-C(13)-F(11)	107.8(2)	F(22)-C(24)-F(20)	107.1(4)
F(13)-C(13)-F(12)	108.3(2)	F(21)-C(24)-C(23)	114.0(4)
F(11)-C(13)-F(12)	107.9(2)	F(22)-C(24)-C(23)	109.2(3)
F(13)-C(13)-C(12)	112.5(2)	F(20)-C(24)-C(23)	110.9(3)
F(11)-C(13)-C(12)	110.6(2)	F(23)-C(25)-F(25)	107.3(4)
F(12)-C(13)-C(12)	109.6(2)	F(23)-C(25)-F(24)	108.5(3)
F(15)-C(14)-F(16)	109.2(2)	F(25)-C(25)-F(24)	108.0(3)
F(15)-C(14)-F(14)	106.8(2)	F(23)-C(25)-C(23)	112.6(3)
F(16)-C(14)-F(14)	107.0(2)	F(25)-C(25)-C(23)	110.8(3)
F(15)-C(14)-C(12)	114.2(2)	F(24)-C(25)-C(23)	109.6(4)
F(16)-C(14)-C(12)	110.7(2)	F(26)-C(26)-C(28)	105.9(2)
F(14)-C(14)-C(12)	108.6(2)	F(26)-C(26)-C(19)	110.1(2)
N(6)-C(15)-N(2)	128.4(2)	C(28)-C(26)-C(19)	112.5(3)
N(6)-C(15)-C(16)	123.3(2)	F(26)-C(26)-C(27)	102.4(2)

C(28)-C(26)-C(27)	110.9(2)	F(37)-C(39)-C(38)	117.4(2)
C(19)-C(26)-C(27)	114.2(2)	F(37)-C(39)-C(40)	119.0(2)
F(28)-C(27)-F(29)	108.9(3)	C(38)-C(39)-C(40)	123.5(2)
F(28)-C(27)-F(27)	106.1(2)	C(39)-C(40)-C(41)	117.2(2)
F(29)-C(27)-F(27)	107.3(3)	C(39)-C(40)-C(48)	115.8(2)
F(28)-C(27)-C(26)	114.4(3)	C(41)-C(40)-C(48)	126.9(2)
F(29)-C(27)-C(26)	110.9(2)	C(42)-C(41)-C(40)	117.4(2)
F(27)-C(27)-C(26)	109.0(3)	C(42)-C(41)-C(45)	115.5(2)
F(30)-C(28)-F(31)	107.1(3)	C(40)-C(41)-C(45)	127.1(2)
F(30)-C(28)-F(32)	108.3(3)	F(36)-C(42)-C(43)	117.4(2)
F(31)-C(28)-F(32)	107.7(3)	F(36)-C(42)-C(41)	119.5(2)
F(30)-C(28)-C(26)	112.4(2)	C(43)-C(42)-C(41)	123.1(2)
F(31)-C(28)-C(26)	111.2(3)	C(42)-C(43)-C(38)	119.3(2)
F(32)-C(28)-C(26)	110.0(3)	C(42)-C(43)-C(44)	133.7(2)
N(7)-C(29)-N(3)	128.5(2)	C(38)-C(43)-C(44)	107.0(2)
N(7)-C(29)-C(30)	122.6(2)	N(5)-C(44)-N(4)	128.3(2)
N(3)-C(29)-C(30)	108.7(2)	N(5)-C(44)-C(43)	123.7(2)
C(31)-C(30)-C(35)	120.3(2)	N(4)-C(44)-C(43)	108.0(2)
C(31)-C(30)-C(29)	133.3(2)	F(45)-C(45)-C(46)	106.1(2)
C(35)-C(30)-C(29)	106.4(2)	F(45)-C(45)-C(41)	110.9(2)
F(34)-C(31)-C(30)	122.7(2)	C(46)-C(45)-C(41)	112.3(3)
F(34)-C(31)-C(32)	118.8(2)	F(45)-C(45)-C(47)	101.4(3)
C(30)-C(31)-C(32)	118.4(2)	C(46)-C(45)-C(47)	110.0(3)
F(35)-C(32)-C(31)	118.3(2)	C(41)-C(45)-C(47)	115.2(2)
F(35)-C(32)-C(33)	119.5(2)	F(47)-C(46)-F(46)	108.1(3)
C(31)-C(32)-C(33)	122.2(2)	F(47)-C(46)-F(48)	108.4(3)
C(34)-C(33)-C(32)	118.1(2)	F(46)-C(46)-F(48)	108.0(3)
C(34)-C(33)-N(12)	120.4(2)	F(47)-C(46)-C(45)	111.2(3)
C(32)-C(33)-N(12)	121.5(2)	F(46)-C(46)-C(45)	110.0(3)
F(33)-C(34)-C(35)	121.4(2)	F(48)-C(46)-C(45)	111.1(3)
F(33)-C(34)-C(33)	117.9(2)	F(49)-C(47)-F(50)	107.8(4)
C(35)-C(34)-C(33)	120.6(2)	F(49)-C(47)-F(51)	108.3(3)
C(34)-C(35)-C(30)	120.2(2)	F(50)-C(47)-F(51)	106.7(3)
C(34)-C(35)-C(36)	133.4(2)	F(49)-C(47)-C(45)	110.9(3)
C(30)-C(35)-C(36)	106.4(2)	F(50)-C(47)-C(45)	109.0(3)
N(8)-C(36)-N(3)	128.1(2)	F(51)-C(47)-C(45)	114.0(3)
N(8)-C(36)-C(35)	123.0(2)	F(38)-C(48)-C(49)	107.1(2)
N(3)-C(36)-C(35)	108.9(2)	F(38)-C(48)-C(40)	110.8(2)
N(8)-C(37)-N(4)	128.5(2)	C(49)-C(48)-C(40)	111.5(3)
N(8)-C(37)-C(38)	123.5(2)	F(38)-C(48)-C(50)	101.2(2)
N(4)-C(37)-C(38)	108.0(2)	C(49)-C(48)-C(50)	110.4(3)
C(39)-C(38)-C(43)	119.1(2)	C(40)-C(48)-C(50)	115.1(2)
C(39)-C(38)-C(37)	134.0(2)	F(41)-C(49)-F(39)	109.1(3)
C(43)-C(38)-C(37)	106.8(2)	F(41)-C(49)-F(40)	107.6(3)

F(39)-C(49)-F(40)	107.6(3)	C(9S)-C(8S)-H(8SA)	120
F(41)-C(49)-C(48)	112.4(3)	C(13S)-C(8S)-H(8SA)	120
F(39)-C(49)-C(48)	110.2(3)	C(8S)-C(9S)-C(10S)	120
F(40)-C(49)-C(48)	109.7(3)	C(8S)-C(9S)-H(9SA)	120
F(43)-C(50)-F(44)	109.1(3)	C(10S)-C(9S)-H(9SA)	120
F(43)-C(50)-F(42)	108.1(3)	C(9S)-C(10S)-C(11S)	120
F(44)-C(50)-F(42)	106.2(2)	C(9S)-C(10S)-H(10A)	120
F(43)-C(50)-C(48)	111.1(2)	C(11S)-C(10S)-H(10A)	120
F(44)-C(50)-C(48)	113.8(3)	C(12S)-C(11S)-C(10S)	120
F(42)-C(50)-C(48)	108.3(3)	C(12S)-C(11S)-H(11A)	120
O-C(51)-N(12)	118.8(2)	C(10S)-C(11S)-H(11A)	120
O-C(51)-C(52)	122.8(2)	C(11S)-C(12S)-C(13S)	120
N(12)-C(51)-C(52)	118.4(2)	C(11S)-C(12S)-H(12A)	120
C(51)-C(52)-H(52A)	109.5	C(13S)-C(12S)-H(12A)	120
C(51)-C(52)-H(52B)	109.5	C(12S)-C(13S)-C(8S)	120
H(52A)-C(52)-H(52B)	109.5	C(12S)-C(13S)-C(14S)	120.8(6)
C(51)-C(52)-H(52C)	109.5	C(8S)-C(13S)-C(14S)	119.2(6)
H(52A)-C(52)-H(52C)	109.5	C(13S)-C(14S)-H(14A)	109.5
H(52B)-C(52)-H(52C)	109.5	C(13S)-C(14S)-H(14B)	109.5
C(2S)-C(1S)-C(6S)	120	H(14A)-C(14S)-H(14B)	109.5
C(2S)-C(1S)-H(1SA)	120	C(13S)-C(14S)-H(14C)	109.5
C(6S)-C(1S)-H(1SA)	120	H(14A)-C(14S)-H(14C)	109.5
C(3S)-C(2S)-C(1S)	120	H(14B)-C(14S)-H(14C)	109.5
C(3S)-C(2S)-H(2SA)	120	C(2T)-C(1T)-C(6T)	120.5(4)
C(1S)-C(2S)-H(2SA)	120	C(2T)-C(1T)-H(1TA)	119.7
C(2S)-C(3S)-C(4S)	120	C(6T)-C(1T)-H(1TA)	119.7
C(2S)-C(3S)-H(3SA)	120	C(3T)-C(2T)-C(1T)	120.7(4)
C(4S)-C(3S)-H(3SA)	120	C(3T)-C(2T)-H(2TA)	119.6
C(3S)-C(4S)-C(5S)	120	C(1T)-C(2T)-H(2TA)	119.6
C(3S)-C(4S)-H(4SA)	120	C(4T)-C(3T)-C(2T)	119.2(4)
C(5S)-C(4S)-H(4SA)	120	C(4T)-C(3T)-H(3TA)	120.4
C(6S)-C(5S)-C(4S)	120	C(2T)-C(3T)-H(3TA)	120.4
C(6S)-C(5S)-H(5SA)	120	C(3T)-C(4T)-C(5T)	120.4(4)
C(4S)-C(5S)-H(5SA)	120	C(3T)-C(4T)-H(4TA)	119.8
C(5S)-C(6S)-C(1S)	120	C(5T)-C(4T)-H(4TA)	119.8
C(5S)-C(6S)-C(7S)	119.0(4)	C(4T)-C(5T)-C(6T)	121.7(4)
C(1S)-C(6S)-C(7S)	121.0(4)	C(4T)-C(5T)-H(5TA)	119.2
C(6S)-C(7S)-H(7SA)	109.5	C(6T)-C(5T)-H(5TA)	119.2
C(6S)-C(7S)-H(7SB)	109.5	C(5T)-C(6T)-C(1T)	117.4(4)
H(7SA)-C(7S)-H(7SB)	109.5	C(5T)-C(6T)-C(7T)	121.4(4)
C(6S)-C(7S)-H(7SC)	109.5	C(1T)-C(6T)-C(7T)	121.1(5)
H(7SA)-C(7S)-H(7SC)	109.5	C(6T)-C(7T)-H(7TA)	109.5
H(7SB)-C(7S)-H(7SC)	109.5	C(6T)-C(7T)-H(7TB)	109.5
C(9S)-C(8S)-C(13S)	120	H(7TA)-C(7T)-H(7TB)	109.5

C(6T)-C(7T)-H(7TC)	109.5	H(7EB)-C(7E)-H(7EC)	109.5
H(7TA)-C(7T)-H(7TC)	109.5	C(2K)-C(1K)-C(6K)	120
H(7TB)-C(7T)-H(7TC)	109.5	C(2K)-C(1K)-H(1KA)	120
C(2E)-C(1E)-C(6E)	120	C(6K)-C(1K)-H(1KA)	120
C(2E)-C(1E)-H(1EA)	120	C(1K)-C(2K)-C(3K)	120
C(6E)-C(1E)-H(1EA)	120	C(1K)-C(2K)-H(2KA)	120
C(1E)-C(2E)-C(3E)	120	C(3K)-C(2K)-H(2KA)	120
C(1E)-C(2E)-H(2EA)	120	C(4K)-C(3K)-C(2K)	120
C(3E)-C(2E)-H(2EA)	120	C(4K)-C(3K)-H(3KA)	120
C(2E)-C(3E)-C(4E)	120	C(2K)-C(3K)-H(3KA)	120
C(2E)-C(3E)-H(3EA)	120	C(3K)-C(4K)-C(5K)	120
C(4E)-C(3E)-H(3EA)	120	C(3K)-C(4K)-H(4KA)	120
C(3E)-C(4E)-C(5E)	120	C(5K)-C(4K)-H(4KA)	120
C(3E)-C(4E)-H(4EA)	120	C(6K)-C(5K)-C(4K)	120
C(5E)-C(4E)-H(4EA)	120	C(6K)-C(5K)-H(5KA)	120
C(6E)-C(5E)-C(4E)	120	C(4K)-C(5K)-H(5KA)	120
C(6E)-C(5E)-H(5EA)	120	C(5K)-C(6K)-C(1K)	120
C(4E)-C(5E)-H(5EA)	120	C(5K)-C(6K)-C(7K)	119.8(5)
C(5E)-C(6E)-C(1E)	120	C(1K)-C(6K)-C(7K)	120.2(5)
C(5E)-C(6E)-C(7E)	130.0(8)	C(6K)-C(7K)-H(7KA)	109.5
C(1E)-C(6E)-C(7E)	110.0(8)	C(6K)-C(7K)-H(7KB)	109.5
C(6E)-C(7E)-H(7EA)	109.5	H(7KA)-C(7K)-H(7KB)	109.5
C(6E)-C(7E)-H(7EB)	109.5	C(6K)-C(7K)-H(7KC)	109.5
H(7EA)-C(7E)-H(7EB)	109.5	H(7KA)-C(7K)-H(7KC)	109.5
C(6E)-C(7E)-H(7EC)	109.5	H(7KB)-C(7K)-H(7KC)	109.5
H(7EA)-C(7E)-H(7EC)	109.5	H(7KB)-C(7K)-H(7KC)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table O.4 Anisotropic displacement parameters (Å^2 x 10^3) **[NHAcF$_{51}$PcZn]$_2$·7(toluene)**. The anisotropic displacement factor exponent takes the form: -2 π^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	15(1)	16(1)	23(1)	2(1)	2(1)	1(1)
N(1)	17(1)	18(1)	22(1)	2(1)	3(1)	1(1)
N(2)	15(1)	17(1)	22(1)	0(1)	2(1)	0(1)
N(3)	17(1)	17(1)	21(1)	1(1)	3(1)	2(1)
N(4)	16(1)	20(1)	22(1)	2(1)	1(1)	0(1)
N(5)	15(1)	19(1)	25(1)	4(1)	3(1)	1(1)
N(6)	17(1)	17(1)	20(1)	2(1)	2(1)	1(1)
N(7)	16(1)	19(1)	18(1)	-1(1)	3(1)	1(1)
N(8)	16(1)	19(1)	24(1)	2(1)	3(1)	1(1)
N(12)	19(1)	27(1)	26(1)	11(1)	1(1)	-2(1)
O	26(1)	26(1)	23(1)	4(1)	2(1)	-5(1)
C(1)	18(1)	19(1)	22(1)	1(1)	4(1)	0(1)
C(2)	16(1)	20(1)	24(1)	0(1)	2(1)	-2(1)
C(3)	18(1)	19(1)	25(1)	5(1)	2(1)	0(1)
C(4)	15(1)	21(1)	22(1)	2(1)	0(1)	1(1)
C(5)	16(1)	20(1)	22(1)	1(1)	2(1)	-1(1)
C(6)	18(1)	17(1)	22(1)	2(1)	2(1)	0(1)
C(7)	12(1)	22(1)	20(1)	1(1)	0(1)	1(1)
C(8)	16(1)	20(1)	17(1)	0(1)	1(1)	-1(1)
C(9)	16(1)	21(1)	33(1)	4(1)	2(1)	-2(1)
C(10)	27(1)	23(1)	31(1)	6(1)	-2(1)	-1(1)
C(11)	23(1)	26(1)	44(2)	6(1)	9(1)	4(1)
C(12)	14(1)	24(1)	24(1)	3(1)	2(1)	2(1)
C(13)	21(1)	27(1)	28(1)	3(1)	2(1)	-2(1)
C(14)	17(1)	32(1)	23(1)	4(1)	3(1)	1(1)
C(15)	17(1)	18(1)	19(1)	0(1)	2(1)	0(1)
C(16)	19(1)	18(1)	24(1)	1(1)	5(1)	1(1)
C(17)	18(1)	23(1)	31(1)	4(1)	6(1)	1(1)
C(18)	24(1)	24(1)	39(2)	9(1)	11(1)	2(1)
C(19)	24(1)	20(1)	37(2)	6(1)	9(1)	4(1)
C(20)	18(1)	20(1)	28(1)	3(1)	6(1)	2(1)
C(21)	19(1)	17(1)	21(1)	1(1)	4(1)	1(1)
C(22)	17(1)	14(1)	19(1)	-1(1)	4(1)	1(1)
C(23)	28(2)	27(2)	77(2)	23(2)	17(2)	3(1)
C(24)	34(2)	30(2)	107(4)	11(2)	5(2)	-10(1)
C(25)	40(2)	67(3)	95(3)	49(2)	31(2)	13(2)
C(26)	29(1)	27(1)	49(2)	18(1)	16(1)	8(1)
C(27)	34(2)	44(2)	39(2)	18(1)	11(1)	12(1)
C(28)	38(2)	22(1)	72(2)	9(1)	18(2)	4(1)

C(29)	15(1)	21(1)	18(1)	-2(1)	3(1)	1(1)
C(30)	17(1)	21(1)	17(1)	1(1)	3(1)	0(1)
C(31)	21(1)	19(1)	20(1)	2(1)	4(1)	1(1)
C(32)	16(1)	25(1)	21(1)	2(1)	2(1)	4(1)
C(33)	18(1)	25(1)	22(1)	6(1)	3(1)	-1(1)
C(34)	20(1)	20(1)	20(1)	4(1)	3(1)	0(1)
C(35)	17(1)	20(1)	18(1)	3(1)	3(1)	2(1)
C(36)	17(1)	21(1)	17(1)	1(1)	3(1)	1(1)
C(37)	17(1)	18(1)	20(1)	3(1)	3(1)	0(1)
C(38)	18(1)	19(1)	24(1)	2(1)	4(1)	2(1)
C(39)	20(1)	22(1)	29(1)	4(1)	7(1)	1(1)
C(40)	27(1)	18(1)	34(1)	5(1)	12(1)	2(1)
C(41)	23(1)	20(1)	34(1)	5(1)	8(1)	4(1)
C(42)	17(1)	22(1)	33(1)	5(1)	6(1)	4(1)
C(43)	18(1)	18(1)	25(1)	3(1)	4(1)	0(1)
C(44)	17(1)	19(1)	22(1)	2(1)	3(1)	1(1)
C(45)	29(1)	19(1)	55(2)	12(1)	8(1)	4(1)
C(46)	33(2)	25(2)	89(3)	6(2)	19(2)	6(1)
C(47)	45(2)	38(2)	64(2)	21(2)	-2(2)	7(2)
C(48)	27(1)	22(1)	50(2)	11(1)	14(1)	1(1)
C(49)	44(2)	40(2)	53(2)	17(2)	21(2)	-1(2)
C(50)	35(2)	26(1)	58(2)	1(1)	12(2)	-8(1)
C(51)	21(1)	22(1)	26(1)	2(1)	6(1)	2(1)
C(52)	26(1)	30(1)	34(2)	4(1)	3(1)	-8(1)
F(1)	19(1)	21(1)	36(1)	10(1)	5(1)	2(1)
F(2)	21(1)	22(1)	40(1)	13(1)	4(1)	2(1)
F(3)	17(1)	30(1)	38(1)	10(1)	-4(1)	-5(1)
F(4)	56(1)	36(1)	29(1)	4(1)	7(1)	10(1)
F(5)	36(1)	28(1)	36(1)	12(1)	-1(1)	-6(1)
F(6)	36(1)	39(1)	40(1)	13(1)	-15(1)	-7(1)
F(7)	33(1)	29(1)	55(1)	-8(1)	7(1)	0(1)
F(8)	31(1)	38(1)	75(1)	4(1)	-2(1)	17(1)
F(9)	79(2)	34(1)	64(1)	5(1)	44(1)	12(1)
F(10)	17(1)	29(1)	34(1)	6(1)	5(1)	6(1)
F(11)	42(1)	36(1)	30(1)	2(1)	-9(1)	-8(1)
F(12)	29(1)	43(1)	46(1)	-2(1)	13(1)	-17(1)
F(13)	31(1)	26(1)	41(1)	-4(1)	2(1)	-2(1)
F(14)	26(1)	43(1)	29(1)	6(1)	11(1)	4(1)
F(15)	36(1)	36(1)	32(1)	13(1)	10(1)	9(1)
F(16)	28(1)	48(1)	28(1)	-3(1)	0(1)	-10(1)
F(17)	18(1)	28(1)	53(1)	13(1)	9(1)	0(1)
F(18)	18(1)	22(1)	41(1)	7(1)	6(1)	4(1)
F(19)	36(1)	26(1)	117(2)	28(1)	20(1)	3(1)
F(20)	54(1)	44(1)	80(2)	-6(1)	1(1)	-13(1)

F(21)	28(1)	44(1)	127(2)	26(1)	8(1)	-6(1)
F(22)	55(2)	29(1)	175(3)	11(2)	2(2)	-17(1)
F(23)	56(1)	79(2)	84(2)	38(1)	43(1)	23(1)
F(24)	60(2)	89(2)	174(3)	83(2)	61(2)	7(1)
F(25)	58(2)	136(3)	75(2)	59(2)	36(1)	33(2)
F(26)	38(1)	47(1)	70(1)	37(1)	23(1)	10(1)
F(27)	50(1)	73(2)	51(1)	37(1)	11(1)	14(1)
F(28)	28(1)	54(1)	50(1)	16(1)	9(1)	9(1)
F(29)	45(1)	51(1)	37(1)	4(1)	7(1)	12(1)
F(30)	46(1)	29(1)	68(1)	-4(1)	28(1)	1(1)
F(31)	53(1)	29(1)	104(2)	-10(1)	25(1)	-8(1)
F(32)	62(1)	36(1)	102(2)	26(1)	26(1)	30(1)
F(33)	22(1)	22(1)	41(1)	12(1)	1(1)	-2(1)
F(34)	23(1)	19(1)	36(1)	5(1)	3(1)	3(1)
F(35)	17(1)	28(1)	36(1)	5(1)	3(1)	3(1)
F(36)	18(1)	26(1)	56(1)	13(1)	6(1)	4(1)
F(37)	17(1)	26(1)	49(1)	10(1)	10(1)	1(1)
F(38)	36(1)	21(1)	82(1)	12(1)	20(1)	2(1)
F(39)	63(1)	56(1)	88(2)	27(1)	45(1)	-5(1)
F(40)	62(1)	78(2)	46(1)	21(1)	16(1)	6(1)
F(41)	60(1)	50(1)	59(1)	12(1)	34(1)	12(1)
F(42)	52(1)	28(1)	91(2)	-1(1)	11(1)	-15(1)
F(43)	50(1)	41(1)	49(1)	-1(1)	9(1)	-10(1)
F(44)	29(1)	42(1)	78(2)	10(1)	12(1)	-6(1)
F(45)	40(1)	35(1)	73(1)	28(1)	12(1)	3(1)
F(46)	46(1)	39(1)	94(2)	-15(1)	21(1)	-3(1)
F(47)	42(1)	26(1)	134(2)	11(1)	20(1)	15(1)
F(48)	52(1)	34(1)	92(2)	-1(1)	41(1)	4(1)
F(49)	69(2)	59(1)	54(1)	1(1)	-4(1)	-6(1)
F(50)	63(2)	76(2)	86(2)	54(2)	-20(1)	-7(1)
F(51)	30(1)	44(1)	101(2)	28(1)	-4(1)	4(1)
C(1S)	56(4)	52(4)	28(3)	-11(3)	7(3)	5(3)
C(2S)	53(6)	50(4)	36(4)	-13(3)	7(4)	5(4)
C(3S)	45(4)	55(4)	44(3)	-20(3)	12(3)	-1(3)
C(4S)	55(4)	40(3)	39(3)	-13(2)	9(3)	-2(3)
C(5S)	41(3)	46(3)	34(3)	-16(2)	1(2)	2(3)
C(6S)	37(5)	45(5)	26(3)	-12(3)	3(3)	1(4)
C(7S)	48(4)	57(4)	41(3)	-14(3)	5(3)	-7(3)
C(8S)	83(8)	60(6)	28(4)	-14(4)	14(4)	-24(5)
C(9S)	42(7)	72(8)	42(6)	-18(6)	14(5)	-18(6)
C(10S)	54(6)	95(9)	41(5)	-27(5)	8(4)	18(6)
C(11S)	55(5)	46(5)	42(5)	-12(4)	4(4)	12(4)
C(12S)	44(5)	44(4)	36(4)	-9(3)	12(3)	-6(4)
C(13S)	64(10)	47(7)	15(4)	-11(4)	1(4)	-4(7)

C(14S)	84(8)	52(6)	50(6)	5(5)	-12(5)	5(6)
C(1T)	32(2)	93(3)	58(2)	14(2)	12(2)	4(2)
C(2T)	55(2)	77(3)	48(2)	8(2)	13(2)	33(2)
C(3T)	87(3)	42(2)	50(2)	-3(2)	29(2)	14(2)
C(4T)	53(2)	64(3)	55(2)	-14(2)	11(2)	-9(2)
C(5T)	38(2)	77(3)	87(3)	29(3)	-2(2)	11(2)
C(6T)	46(2)	70(3)	90(3)	34(3)	10(2)	-1(2)
C(7T)	101(5)	102(5)	259(11)	112(6)	14(6)	-7(4)
C(1E)	335(17)	95(6)	220(13)	69(7)	180(13)	109(9)
C(2E)	273(12)	53(3)	85(5)	-12(3)	54(6)	0(5)
C(3E)	150(6)	33(2)	128(6)	16(3)	13(5)	-7(3)
C(4E)	166(7)	38(3)	112(5)	29(3)	38(5)	16(3)
C(5E)	116(5)	55(3)	129(6)	22(3)	16(4)	10(3)
C(6E)	160(8)	112(6)	199(10)	55(7)	110(8)	52(6)
C(7E)	270(16)	234(14)	279(17)	-44(12)	160(14)	4(12)
C(1K)	56(4)	35(3)	65(4)	13(8)	13(3)	4(7)
C(2K)	59(5)	42(4)	60(5)	4(4)	10(4)	3(4)
C(3K)	49(4)	45(4)	54(5)	-7(4)	-1(4)	0(4)
C(4K)	61(7)	35(4)	70(8)	9(4)	-12(5)	7(5)
C(5K)	57(6)	30(4)	50(6)	0(4)	-6(5)	-5(4)
C(6K)	42(4)	37(4)	53(5)	7(4)	-3(3)	0(4)
C(7K)	57(5)	69(6)	66(5)	2(5)	16(4)	6(4)

Table O.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **[NHAcF$_{51}$PcZn]$_2$·7(toluene)**.

	x	y	z	U(eq)
H(12)	11760(17)	3446(9)	6591(14)	30
H(52A)	12907	3645	7872	46
H(52B)	12706	3759	7202	46
H(52C)	13215	3403	7417	46
H(1SA)	6938	2919	4773	55
H(2SA)	8100	3126	4809	56
H(3SA)	8285	3713	4409	57
H(4SA)	7308	4092	3974	54
H(5SA)	6146	3884	3937	50
H(7SA)	5406	3250	3934	75
H(7SB)	5466	3441	4554	75
H(7SC)	5693	3008	4512	75
H(8SA)	7035	3784	4213	68
H(9SA)	8163	3506	4528	61
H(10A)	8271	2901	4944	76
H(11A)	7252	2575	5045	59

H(12A)	6124	2853	4730	49
H(14A)	5411	3333	4038	100
H(14B)	5787	3726	3951	100
H(14C)	5598	3633	4556	100
H(1TA)	1498	3286	5276	73
H(2TA)	1423	2659	5542	72
H(3TA)	328	2358	5384	69
H(4TA)	-693	2680	4924	69
H(5TA)	-624	3297	4632	84
H(7TA)	60	3903	4799	239
H(7TB)	495	3773	4338	239
H(7TC)	913	3883	4983	239
H(1EA)	8109	5500	1834	237
H(2EA)	6970	5347	1947	162
H(3EA)	6720	5386	2860	128
H(4EA)	7610	5579	3661	125
H(5EA)	8749	5732	3549	123
H(7EA)	9499	5894	2766	368
H(7EB)	9104	5809	2107	368
H(7EC)	9488	5472	2517	368
H(1KA)	4883	4707	7622	63
H(2KA)	5314	4571	6805	65
H(3KA)	5498	3942	6567	62
H(4KA)	5252	3448	7146	72
H(5KA)	4821	3583	7963	59
H(7KA)	4295	4022	8499	95
H(7KB)	4218	4460	8320	95
H(7KC)	4951	4305	8721	95

Table O.6 Torsion angles [deg] for **[NHAcF_{51}PcZn]$_2$·7(toluene)**.

C(44)-N(5)-C(1)-N(1)	0.4(4)	C(1)-C(2)-C(3)-C(4)	-178.1(3)
C(44)-N(5)-C(1)-C(2)	178.4(2)	F(2)-C(3)-C(4)-C(5)	-177.3(2)
C(8)-N(1)-C(1)-N(5)	178.2(2)	C(2)-C(3)-C(4)-C(5)	5.0(4)
Zn-N(1)-C(1)-N(5)	6.3(4)	F(2)-C(3)-C(4)-C(9)	8.5(3)
C(8)-N(1)-C(1)-C(2)	-0.1(3)	C(2)-C(3)-C(4)-C(9)	-169.2(2)
Zn-N(1)-C(1)-C(2)	-172.00(16)	C(3)-C(4)-C(5)-C(6)	-10.6(3)
N(5)-C(1)-C(2)-C(3)	5.8(5)	C(9)-C(4)-C(5)-C(6)	163.0(2)
N(1)-C(1)-C(2)-C(3)	-175.8(3)	C(3)-C(4)-C(5)-C(12)	162.6(2)
N(5)-C(1)-C(2)-C(7)	-176.3(2)	C(9)-C(4)-C(5)-C(12)	-23.9(4)
N(1)-C(1)-C(2)-C(7)	2.1(3)	C(4)-C(5)-C(6)-F(1)	-177.1(2)
C(7)-C(2)-C(3)-F(2)	-173.5(2)	C(12)-C(5)-C(6)-F(1)	9.1(3)
C(1)-C(2)-C(3)-F(2)	4.2(4)	C(4)-C(5)-C(6)-C(7)	7.4(4)
C(7)-C(2)-C(3)-C(4)	4.2(4)	C(12)-C(5)-C(6)-C(7)	-166.4(2)

F(1)-C(6)-C(7)-C(2)	-173.8(2)	C(6)-C(5)-C(12)-C(13)	-80.2(3)
C(5)-C(6)-C(7)-C(2)	1.8(4)	C(4)-C(5)-C(12)-C(13)	106.6(3)
F(1)-C(6)-C(7)-C(8)	2.5(4)	C(6)-C(5)-C(12)-C(14)	47.0(3)
C(5)-C(6)-C(7)-C(8)	178.0(3)	C(4)-C(5)-C(12)-C(14)	-126.1(3)
C(3)-C(2)-C(7)-C(6)	-7.7(4)	F(10)-C(12)-C(13)-F(13)	179.7(2)
C(1)-C(2)-C(7)-C(6)	174.0(2)	C(5)-C(12)-C(13)-F(13)	58.4(3)
C(3)-C(2)-C(7)-C(8)	175.1(2)	C(14)-C(12)-C(13)-F(13)	-71.1(3)
C(1)-C(2)-C(7)-C(8)	-3.2(3)	F(10)-C(12)-C(13)-F(11)	59.1(3)
C(15)-N(6)-C(8)-N(1)	-0.6(4)	C(5)-C(12)-C(13)-F(11)	-62.2(3)
C(15)-N(6)-C(8)-C(7)	178.8(2)	C(14)-C(12)-C(13)-F(11)	168.3(2)
C(1)-N(1)-C(8)-N(6)	177.6(2)	F(10)-C(12)-C(13)-F(12)	-59.8(3)
Zn-N(1)-C(8)-N(6)	-10.3(4)	C(5)-C(12)-C(13)-F(12)	179.0(2)
C(1)-N(1)-C(8)-C(7)	-1.9(3)	C(14)-C(12)-C(13)-F(12)	49.4(3)
Zn-N(1)-C(8)-C(7)	170.15(16)	F(10)-C(12)-C(14)-F(15)	146.2(2)
C(6)-C(7)-C(8)-N(6)	7.1(4)	C(5)-C(12)-C(14)-F(15)	-95.5(3)
C(2)-C(7)-C(8)-N(6)	-176.3(2)	C(13)-C(12)-C(14)-F(15)	34.7(3)
C(6)-C(7)-C(8)-N(1)	-173.4(3)	F(10)-C(12)-C(14)-F(16)	-90.1(2)
C(2)-C(7)-C(8)-N(1)	3.2(3)	C(5)-C(12)-C(14)-F(16)	28.3(3)
C(3)-C(4)-C(9)-F(3)	160.4(2)	C(13)-C(12)-C(14)-F(16)	158.4(2)
C(5)-C(4)-C(9)-F(3)	-13.3(4)	F(10)-C(12)-C(14)-F(14)	27.2(3)
C(3)-C(4)-C(9)-C(11)	-80.7(3)	C(5)-C(12)-C(14)-F(14)	145.5(2)
C(5)-C(4)-C(9)-C(11)	105.6(3)	C(13)-C(12)-C(14)-F(14)	-84.3(3)
C(3)-C(4)-C(9)-C(10)	46.2(3)	C(8)-N(6)-C(15)-N(2)	-1.2(4)
C(5)-C(4)-C(9)-C(10)	-127.4(3)	C(8)-N(6)-C(15)-C(16)	176.9(2)
F(3)-C(9)-C(10)-F(5)	147.4(2)	C(22)-N(2)-C(15)-N(6)	177.7(2)
C(4)-C(9)-C(10)-F(5)	-93.9(3)	Zn-N(2)-C(15)-N(6)	13.7(4)
C(11)-C(9)-C(10)-F(5)	35.5(3)	C(22)-N(2)-C(15)-C(16)	-0.6(3)
F(3)-C(9)-C(10)-F(4)	-89.4(2)	Zn-N(2)-C(15)-C(16)	-164.60(16)
C(4)-C(9)-C(10)-F(4)	29.3(3)	N(6)-C(15)-C(16)-C(17)	3.3(4)
C(11)-C(9)-C(10)-F(4)	158.7(2)	N(2)-C(15)-C(16)-C(17)	-178.3(3)
F(3)-C(9)-C(10)-F(6)	28.8(3)	N(6)-C(15)-C(16)-C(21)	-177.2(2)
C(4)-C(9)-C(10)-F(6)	147.5(2)	N(2)-C(15)-C(16)-C(21)	1.2(3)
C(11)-C(9)-C(10)-F(6)	-83.1(3)	C(21)-C(16)-C(17)-F(17)	-176.6(2)
F(3)-C(9)-C(11)-F(7)	175.7(2)	C(15)-C(16)-C(17)-F(17)	2.9(4)
C(4)-C(9)-C(11)-F(7)	54.5(3)	C(21)-C(16)-C(17)-C(18)	1.6(4)
C(10)-C(9)-C(11)-F(7)	-74.9(3)	C(15)-C(16)-C(17)-C(18)	-179.0(3)
F(3)-C(9)-C(11)-F(9)	54.8(3)	F(17)-C(17)-C(18)-C(19)	-177.4(2)
C(4)-C(9)-C(11)-F(9)	-66.4(3)	C(16)-C(17)-C(18)-C(19)	4.5(4)
C(10)-C(9)-C(11)-F(9)	164.3(2)	F(17)-C(17)-C(18)-C(23)	5.8(4)
F(3)-C(9)-C(11)-F(8)	-63.4(3)	C(16)-C(17)-C(18)-C(23)	-172.3(3)
C(4)-C(9)-C(11)-F(8)	175.4(2)	C(17)-C(18)-C(19)-C(20)	-8.2(4)
C(10)-C(9)-C(11)-F(8)	46.1(3)	C(23)-C(18)-C(19)-C(20)	168.1(3)
C(6)-C(5)-C(12)-F(10)	160.8(2)	C(17)-C(18)-C(19)-C(26)	167.7(3)
C(4)-C(5)-C(12)-F(10)	-12.3(3)	C(23)-C(18)-C(19)-C(26)	-16.0(5)

C(18)-C(19)-C(20)-F(18)	-175.4(2)	C(18)-C(23)-C(25)-F(24)	176.9(3)
C(26)-C(19)-C(20)-F(18)	8.3(4)	C(24)-C(23)-C(25)-F(24)	48.0(4)
C(18)-C(19)-C(20)-C(21)	6.4(4)	C(20)-C(19)-C(26)-F(26)	159.5(3)
C(26)-C(19)-C(20)-C(21)	-169.9(3)	C(18)-C(19)-C(26)-F(26)	-16.5(4)
F(18)-C(20)-C(21)-C(16)	-178.6(2)	C(20)-C(19)-C(26)-C(28)	-82.6(3)
C(19)-C(20)-C(21)-C(16)	-0.4(4)	C(18)-C(19)-C(26)-C(28)	101.4(3)
F(18)-C(20)-C(21)-C(22)	-1.3(4)	C(20)-C(19)-C(26)-C(27)	44.9(4)
C(19)-C(20)-C(21)-C(22)	176.9(3)	C(18)-C(19)-C(26)-C(27)	-131.1(3)
C(17)-C(16)-C(21)-C(20)	-3.7(4)	F(26)-C(26)-C(27)-F(28)	146.1(2)
C(15)-C(16)-C(21)-C(20)	176.7(2)	C(28)-C(26)-C(27)-F(28)	33.5(3)
C(17)-C(16)-C(21)-C(22)	178.3(2)	C(19)-C(26)-C(27)-F(28)	-94.9(3)
C(15)-C(16)-C(21)-C(22)	-1.3(3)	F(26)-C(26)-C(27)-F(29)	-90.3(3)
C(29)-N(7)-C(22)-N(2)	1.3(4)	C(28)-C(26)-C(27)-F(29)	157.1(2)
C(29)-N(7)-C(22)-C(21)	-176.6(2)	C(19)-C(26)-C(27)-F(29)	28.7(3)
C(15)-N(2)-C(22)-N(7)	-178.4(2)	F(26)-C(26)-C(27)-F(27)	27.6(3)
Zn-N(2)-C(22)-N(7)	-14.3(3)	C(28)-C(26)-C(27)-F(27)	-85.1(3)
C(15)-N(2)-C(22)-C(21)	-0.2(3)	C(19)-C(26)-C(27)-F(27)	146.6(3)
Zn-N(2)-C(22)-C(21)	163.82(16)	F(26)-C(26)-C(28)-F(30)	-178.9(3)
C(20)-C(21)-C(22)-N(7)	1.7(4)	C(19)-C(26)-C(28)-F(30)	60.7(4)
C(16)-C(21)-C(22)-N(7)	179.3(2)	C(27)-C(26)-C(28)-F(30)	-68.5(3)
C(20)-C(21)-C(22)-N(2)	-176.5(3)	F(26)-C(26)-C(28)-F(31)	61.0(3)
C(16)-C(21)-C(22)-N(2)	1.0(3)	C(19)-C(26)-C(28)-F(31)	-59.3(3)
C(17)-C(18)-C(23)-F(19)	159.6(3)	C(27)-C(26)-C(28)-F(31)	171.4(3)
C(19)-C(18)-C(23)-F(19)	-16.8(5)	F(26)-C(26)-C(28)-F(32)	-58.2(3)
C(17)-C(18)-C(23)-C(25)	-81.3(4)	C(19)-C(26)-C(28)-F(32)	-178.5(2)
C(19)-C(18)-C(23)-C(25)	102.3(4)	C(27)-C(26)-C(28)-F(32)	52.2(3)
C(17)-C(18)-C(23)-C(24)	45.5(4)	C(22)-N(7)-C(29)-N(3)	-1.9(4)
C(19)-C(18)-C(23)-C(24)	-130.9(3)	C(22)-N(7)-C(29)-C(30)	172.9(2)
F(19)-C(23)-C(24)-F(21)	144.1(3)	C(36)-N(3)-C(29)-N(7)	172.5(2)
C(25)-C(23)-C(24)-F(21)	31.6(4)	Zn-N(3)-C(29)-N(7)	15.4(3)
C(18)-C(23)-C(24)-F(21)	-96.8(4)	C(36)-N(3)-C(29)-C(30)	-3.0(3)
F(19)-C(23)-C(24)-F(22)	24.6(4)	Zn-N(3)-C(29)-C(30)	-160.06(15)
C(25)-C(23)-C(24)-F(22)	-87.9(4)	N(7)-C(29)-C(30)-C(31)	5.7(4)
C(18)-C(23)-C(24)-F(22)	143.7(3)	N(3)-C(29)-C(30)-C(31)	-178.5(3)
F(19)-C(23)-C(24)-F(20)	-93.2(3)	N(7)-C(29)-C(30)-C(35)	-172.6(2)
C(25)-C(23)-C(24)-F(20)	154.3(3)	N(3)-C(29)-C(30)-C(35)	3.1(3)
C(18)-C(23)-C(24)-F(20)	25.9(4)	C(35)-C(30)-C(31)-F(34)	-175.9(2)
F(19)-C(23)-C(25)-F(23)	177.6(3)	C(29)-C(30)-C(31)-F(34)	5.9(4)
C(18)-C(23)-C(25)-F(23)	56.1(4)	C(35)-C(30)-C(31)-C(32)	3.0(4)
C(24)-C(23)-C(25)-F(23)	-72.8(4)	C(29)-C(30)-C(31)-C(32)	-175.2(2)
F(19)-C(23)-C(25)-F(25)	57.4(4)	F(34)-C(31)-C(32)-F(35)	1.7(3)
C(18)-C(23)-C(25)-F(25)	-64.0(4)	C(30)-C(31)-C(32)-F(35)	-177.2(2)
C(24)-C(23)-C(25)-F(25)	167.0(3)	F(34)-C(31)-C(32)-C(33)	-179.7(2)
F(19)-C(23)-C(25)-F(24)	-61.6(4)	C(30)-C(31)-C(32)-C(33)	1.4(4)

F(35)-C(32)-C(33)-C(34)	173.9(2)	F(37)-C(39)-C(40)-C(48)	-4.8(4)
C(31)-C(32)-C(33)-C(34)	-4.7(4)	C(38)-C(39)-C(40)-C(48)	173.5(3)
F(35)-C(32)-C(33)-N(12)	-8.1(4)	C(39)-C(40)-C(41)-C(42)	5.5(4)
C(31)-C(32)-C(33)-N(12)	173.3(2)	C(48)-C(40)-C(41)-C(42)	-172.4(3)
C(51)-N(12)-C(33)-C(34)	122.4(3)	C(39)-C(40)-C(41)-C(45)	-173.1(3)
C(51)-N(12)-C(33)-C(32)	-55.5(4)	C(48)-C(40)-C(41)-C(45)	9.0(5)
C(32)-C(33)-C(34)-F(33)	-177.8(2)	C(40)-C(41)-C(42)-F(36)	178.2(2)
N(12)-C(33)-C(34)-F(33)	4.2(4)	C(45)-C(41)-C(42)-F(36)	-3.0(4)
C(32)-C(33)-C(34)-C(35)	3.6(4)	C(40)-C(41)-C(42)-C(43)	-2.8(4)
N(12)-C(33)-C(34)-C(35)	-174.4(2)	C(45)-C(41)-C(42)-C(43)	176.0(3)
F(33)-C(34)-C(35)-C(30)	-177.9(2)	F(36)-C(42)-C(43)-C(38)	177.8(2)
C(33)-C(34)-C(35)-C(30)	0.7(4)	C(41)-C(42)-C(43)-C(38)	-1.2(4)
F(33)-C(34)-C(35)-C(36)	-2.4(4)	F(36)-C(42)-C(43)-C(44)	-0.4(5)
C(33)-C(34)-C(35)-C(36)	176.2(3)	C(41)-C(42)-C(43)-C(44)	-179.4(3)
C(31)-C(30)-C(35)-C(34)	-4.0(4)	C(39)-C(38)-C(43)-C(42)	2.4(4)
C(29)-C(30)-C(35)-C(34)	174.6(2)	C(37)-C(38)-C(43)-C(42)	-178.0(2)
C(31)-C(30)-C(35)-C(36)	179.4(2)	C(39)-C(38)-C(43)-C(44)	-178.9(2)
C(29)-C(30)-C(35)-C(36)	-2.0(3)	C(37)-C(38)-C(43)-C(44)	0.6(3)
C(37)-N(8)-C(36)-N(3)	2.5(4)	C(1)-N(5)-C(44)-N(4)	-0.4(4)
C(37)-N(8)-C(36)-C(35)	-175.7(2)	C(1)-N(5)-C(44)-C(43)	179.5(2)
C(29)-N(3)-C(36)-N(8)	-176.7(2)	C(37)-N(4)-C(44)-N(5)	179.5(2)
Zn-N(3)-C(36)-N(8)	-19.5(3)	Zn-N(4)-C(44)-N(5)	-6.2(4)
C(29)-N(3)-C(36)-C(35)	1.7(3)	C(37)-N(4)-C(44)-C(43)	-0.4(3)
Zn-N(3)-C(36)-C(35)	158.88(16)	Zn-N(4)-C(44)-C(43)	173.87(16)
C(34)-C(35)-C(36)-N(8)	2.8(4)	C(42)-C(43)-C(44)-N(5)	-1.7(5)
C(30)-C(35)-C(36)-N(8)	178.8(2)	C(38)-C(43)-C(44)-N(5)	179.9(2)
C(34)-C(35)-C(36)-N(3)	-175.6(3)	C(42)-C(43)-C(44)-N(4)	178.2(3)
C(30)-C(35)-C(36)-N(3)	0.3(3)	C(38)-C(43)-C(44)-N(4)	-0.2(3)
C(36)-N(8)-C(37)-N(4)	4.9(4)	C(42)-C(41)-C(45)-F(45)	-159.6(3)
C(36)-N(8)-C(37)-C(38)	-175.1(2)	C(40)-C(41)-C(45)-F(45)	19.1(4)
C(44)-N(4)-C(37)-N(8)	-179.2(2)	C(42)-C(41)-C(45)-C(46)	82.0(3)
Zn-N(4)-C(37)-N(8)	6.4(4)	C(40)-C(41)-C(45)-C(46)	-99.4(3)
C(44)-N(4)-C(37)-C(38)	0.8(3)	C(42)-C(41)-C(45)-C(47)	-45.0(4)
Zn-N(4)-C(37)-C(38)	-173.61(16)	C(40)-C(41)-C(45)-C(47)	133.6(3)
N(8)-C(37)-C(38)-C(39)	-1.4(5)	F(45)-C(45)-C(46)-F(47)	65.0(3)
N(4)-C(37)-C(38)-C(39)	178.6(3)	C(41)-C(45)-C(46)-F(47)	-173.7(2)
N(8)-C(37)-C(38)-C(43)	179.1(2)	C(47)-C(45)-C(46)-F(47)	-44.0(3)
N(4)-C(37)-C(38)-C(43)	-0.9(3)	F(45)-C(45)-C(46)-F(46)	-54.7(3)
C(43)-C(38)-C(39)-F(37)	179.0(2)	C(41)-C(45)-C(46)-F(46)	66.6(3)
C(37)-C(38)-C(39)-F(37)	-0.4(4)	C(47)-C(45)-C(46)-F(46)	-163.7(3)
C(43)-C(38)-C(39)-C(40)	0.6(4)	F(45)-C(45)-C(46)-F(48)	-174.3(3)
C(37)-C(38)-C(39)-C(40)	-178.8(3)	C(41)-C(45)-C(46)-F(48)	-53.0(4)
F(37)-C(39)-C(40)-C(41)	177.0(2)	C(47)-C(45)-C(46)-F(48)	76.8(3)
C(38)-C(39)-C(40)-C(41)	-4.6(4)	F(45)-C(45)-C(47)-F(49)	92.3(3)

C(46)-C(45)-C(47)-F(49)	-155.7(3)	C(2S)-C(3S)-C(4S)-C(5S)	0
C(41)-C(45)-C(47)-F(49)	-27.6(4)	C(3S)-C(4S)-C(5S)-C(6S)	0
F(45)-C(45)-C(47)-F(50)	-26.2(4)	C(4S)-C(5S)-C(6S)-C(1S)	0
C(46)-C(45)-C(47)-F(50)	85.8(4)	C(4S)-C(5S)-C(6S)-C(7S)	178.5(4)
C(41)-C(45)-C(47)-F(50)	-146.1(3)	C(2S)-C(1S)-C(6S)-C(5S)	0
F(45)-C(45)-C(47)-F(51)	-145.3(3)	C(2S)-C(1S)-C(6S)-C(7S)	-178.4(5)
C(46)-C(45)-C(47)-F(51)	-33.3(4)	C(13S)-C(8S)-C(9S)-C(10S)	0
C(41)-C(45)-C(47)-F(51)	94.9(3)	C(8S)-C(9S)-C(10S)-C(11S)	0
C(39)-C(40)-C(48)-F(38)	-158.1(3)	C(9S)-C(10S)-C(11S)-C(12S)	0
C(41)-C(40)-C(48)-F(38)	19.8(4)	C(10S)-C(11S)-C(12S)-C(13S)	0
C(39)-C(40)-C(48)-C(49)	82.7(3)	C(11S)-C(12S)-C(13S)-C(8S)	0
C(41)-C(40)-C(48)-C(49)	-99.4(3)	C(11S)-C(12S)-C(13S)-C(14S)	179.0(7)
C(39)-C(40)-C(48)-C(50)	-44.0(4)	C(9S)-C(8S)-C(13S)-C(12S)	0
C(41)-C(40)-C(48)-C(50)	133.9(3)	C(9S)-C(8S)-C(13S)-C(14S)	-179.0(7)
F(38)-C(48)-C(49)-F(41)	176.2(3)	C(6T)-C(1T)-C(2T)-C(3T)	-0.8(7)
C(40)-C(48)-C(49)-F(41)	-62.4(4)	C(1T)-C(2T)-C(3T)-C(4T)	1.3(6)
C(50)-C(48)-C(49)-F(41)	66.8(3)	C(2T)-C(3T)-C(4T)-C(5T)	-0.3(6)
F(38)-C(48)-C(49)-F(39)	54.3(3)	C(3T)-C(4T)-C(5T)-C(6T)	-1.2(8)
C(40)-C(48)-C(49)-F(39)	175.6(3)	C(4T)-C(5T)-C(6T)-C(1T)	1.7(8)
C(50)-C(48)-C(49)-F(39)	-55.1(3)	C(4T)-C(5T)-C(6T)-C(7T)	-179.7(6)
F(38)-C(48)-C(49)-F(40)	-64.1(3)	C(2T)-C(1T)-C(6T)-C(5T)	-0.7(7)
C(40)-C(48)-C(49)-F(40)	57.3(3)	C(2T)-C(1T)-C(6T)-C(7T)	-179.3(6)
C(50)-C(48)-C(49)-F(40)	-173.5(2)	C(6E)-C(1E)-C(2E)-C(3E)	0
F(38)-C(48)-C(50)-F(43)	91.8(3)	C(1E)-C(2E)-C(3E)-C(4E)	0
C(49)-C(48)-C(50)-F(43)	-155.0(3)	C(2E)-C(3E)-C(4E)-C(5E)	0
C(40)-C(48)-C(50)-F(43)	-27.7(4)	C(3E)-C(4E)-C(5E)-C(6E)	0
F(38)-C(48)-C(50)-F(44)	-144.7(2)	C(4E)-C(5E)-C(6E)-C(1E)	0
C(49)-C(48)-C(50)-F(44)	-31.5(3)	C(4E)-C(5E)-C(6E)-C(7E)	-179.2(8)
C(40)-C(48)-C(50)-F(44)	95.8(3)	C(2E)-C(1E)-C(6E)-C(5E)	0
F(38)-C(48)-C(50)-F(42)	-26.8(3)	C(2E)-C(1E)-C(6E)-C(7E)	179.4(7)
C(49)-C(48)-C(50)-F(42)	86.4(3)	C(6K)-C(1K)-C(2K)-C(3K)	0
C(40)-C(48)-C(50)-F(42)	-146.3(3)	C(1K)-C(2K)-C(3K)-C(4K)	0
Zn#1-O-C(51)-N(12)	177.1(2)	C(2K)-C(3K)-C(4K)-C(5K)	0
Zn#1-O-C(51)-C(52)	-3.9(5)	C(3K)-C(4K)-C(5K)-C(6K)	0
C(33)-N(12)-C(51)-O	5.1(4)	C(4K)-C(5K)-C(6K)-C(1K)	0
C(33)-N(12)-C(51)-C(52)	-173.9(2)	C(4K)-C(5K)-C(6K)-C(7K)	-179.1(6)
C(6S)-C(1S)-C(2S)-C(3S)	0	C(2K)-C(1K)-C(6K)-C(5K)	0
C(1S)-C(2S)-C(3S)-C(4S)	0	C(2K)-C(1K)-C(6K)-C(7K)	179.1(6)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Appendix P: Crystal structure of [NMeAcF$_{51}$PcZn]$_2$·3(toluene)·0.75(acetone)

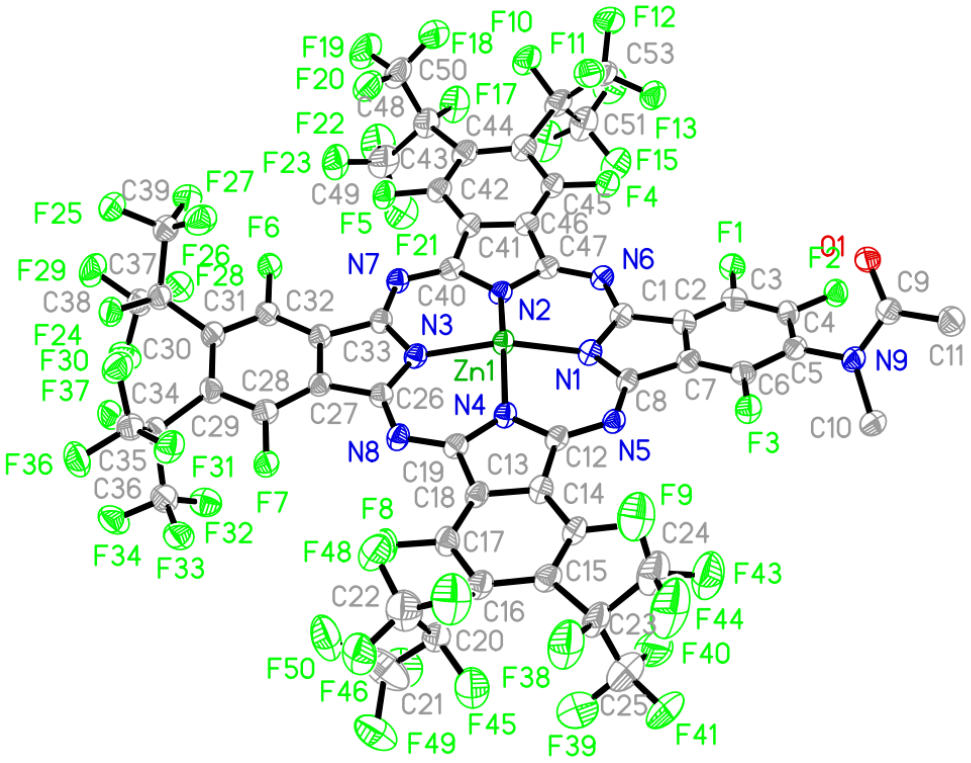


Figure P.1 ORTEP representation of **NMeAcF$_{51}$PcZn** X-ray crystal structure, at 50% probability.

Table P.1 Crystal data and structure refinement for **[NMeAcF$_{51}$PcZn]$_2$·3(toluene)·0.75(acetone)**.

Empirical formula	C152.50 H69 F102 N18 O3.50 Zn2	
Formula weight	4277.99	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c (No. 15)	
Unit cell dimensions	a = 19.6290(4) Å	α = 90°.
	b = 35.0085(7) Å	β = 105.590(1)°.
	c = 23.9878(5) Å	γ = 90°.
Volume	15877.5(6) Å^3	
Z	4	
Density (calculated)	1.790 g/cm^3	
Absorption coefficient	2.048 mm^{-1}	
F(000)	8464	
Crystal size	0.265 x 0.215 x 0.192 mm^3	

Theta range for data collection	2.524 to 69.826°.
Index ranges	-22<=h<=21, -41<=k<=40, -28<=l<=27
Reflections collected	74855
Independent reflections	14278 [R(int) = 0.0385]
Completeness to theta = 67.679°	98.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14263 / 1456 / 1172
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0743
R indices (all data)	R1 = 0.0950, wR2 = 0.22139
Extinction coefficient	n/a
Largest diff. peak and hole	1.60, -1.28 e.Å^{-3}

Table P.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters U(eq) (Å^2) for **[NMeAcF$_{51}$PcZn]$_2$·3(toluene)·0.75(acetone)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Zn	0.25877(3)	0.20602(1)	0.14184(2)	0.0271(2)
F1	0.54287(13)	0.28813(7)	0.19358(11)	0.0352(8)
F2	0.66165(12)	0.24969(7)	0.19930(11)	0.0371(8)
F3	0.53414(13)	0.13592(7)	0.14373(11)	0.0365(8)
F4	0.40374(13)	0.35226(7)	0.23470(11)	0.0354(8)
F5	0.12146(13)	0.34552(7)	0.20283(12)	0.0394(8)
F6	-0.01738(12)	0.26917(7)	0.15864(11)	0.0369(8)
F7	-0.02903(13)	0.13766(7)	0.03858(12)	0.0392(8)
F8	0.10783(13)	0.06769(7)	0.01971(13)	0.0445(9)
F9	0.39137(12)	0.07104(7)	0.06312(12)	0.0367(8)
F10	0.32170(16)	0.42931(9)	0.32302(15)	0.0589(11)
F11	0.40482(10)	0.35718(7)	0.35011(9)	0.0511(10)
F12	0.43658(11)	0.41300(7)	0.38309(9)	0.0647(12)
F13	0.47616(10)	0.38971(7)	0.31557(9)	0.0525(10)
F14	0.42057(16)	0.46612(6)	0.28540(12)	0.0782(15)
F15	0.32378(14)	0.45944(6)	0.21898(13)	0.0729(13)
F16	0.41385(13)	0.42542(6)	0.21762(11)	0.0545(10)
F17	0.21462(17)	0.44655(8)	0.25724(17)	0.0657(13)
F18	0.21249(15)	0.40571(9)	0.35201(10)	0.0723(14)
F19	0.12316(14)	0.37366(8)	0.30482(10)	0.0642(12)
F20	0.11455(16)	0.43388(8)	0.31453(11)	0.0844(16)
F21	0.12307(12)	0.41128(7)	0.14737(11)	0.0614(11)
F22	0.09825(12)	0.45921(7)	0.19331(12)	0.0839(16)
F23	0.05474(12)	0.40444(7)	0.20247(10)	0.0625(13)

F25	-0.17372(12)	0.23386(7)	0.23025(7)	0.0513(10)
F26	-0.10036(12)	0.27588(7)	0.21730(7)	0.0518(10)
F27	-0.06778(12)	0.21767(7)	0.23307(7)	0.0542(10)
F28	-0.14478(11)	0.29634(5)	0.10984(10)	0.0468(9)
F29	-0.23736(11)	0.27633(6)	0.13178(10)	0.0545(11)
F30	-0.21654(11)	0.25851(5)	0.05257(9)	0.0526(10)
F31	-0.21689(13)	0.18331(8)	0.04084(12)	0.0446(9)
F32	-0.12918(13)	0.17959(7)	-0.04328(7)	0.0510(10)
F33	-0.23268(12)	0.15673(7)	-0.05301(7)	0.0538(10)
F34	-0.14261(12)	0.11987(7)	-0.03107(7)	0.0486(9)
F35	-0.11784(12)	0.09944(5)	0.07555(9)	0.0465(9)
F36	-0.23017(12)	0.10804(5)	0.04859(10)	0.0551(10)
F37	-0.16898(12)	0.13105(5)	0.12948(10)	0.0490(10)
*F38	0.30350(19)	-0.03225(9)	0.02042(19)	0.0523(13)
*F38'	0.2904(6)	-0.0136(4)	-0.0429(5)	0.035(3)
*F39	0.29566(18)	0.00659(10)	-0.08097(12)	0.0606(17)
*F39'	0.4545(5)	0.0279(3)	0.0141(4)	0.047(4)
*F40	0.39376(19)	-0.02310(11)	-0.04336(12)	0.0638(17)
*F40'	0.3657(6)	0.0553(4)	-0.0441(5)	0.067(5)
*F41	0.38955(19)	0.03846(11)	-0.03854(13)	0.0563(17)
*F41'	0.3956(6)	-0.0013(4)	-0.0622(5)	0.061(4)
*F42	0.39569(13)	0.00740(9)	0.12201(13)	0.0506(14)
*F42'	0.3146(7)	-0.0411(3)	0.0712(5)	0.063(4)
*F43	0.46217(13)	0.01350(8)	0.06513(12)	0.0535(14)
*F43'	0.4036(8)	-0.0044(4)	0.1022(6)	0.065(6)
*F44'	0.4030(7)	-0.0450(4)	0.0356(5)	0.063(4)
*F45	0.19274(19)	-0.02166(10)	-0.0423(2)	0.0484(14)
*F45'	0.1943(8)	-0.0302(4)	-0.0099(7)	0.042(4)
*F46	0.0920(2)	-0.04833(11)	0.00876(16)	0.0524(18)
*F46'	0.1145(9)	0.0044(7)	0.0669(9)	0.059(9)
*F47	0.1158(2)	-0.00184(12)	0.06850(17)	0.0478(17)
*F47'	0.0410(14)	0.0159(8)	-0.0194(12)	0.184(14)
*F48	0.19677(17)	-0.04142(9)	0.06352(14)	0.0540(14)
*F48'	0.0804(10)	-0.0429(6)	0.0040(9)	0.048(7)
*F49	0.0737(2)	-0.01286(12)	-0.10318(15)	0.0678(17)
*F49'	0.0967(10)	0.0392(7)	-0.0941(5)	0.075(9)
*F50	0.10130(18)	0.04693(13)	-0.08789(16)	0.0626(19)
*F50'	0.0879(11)	-0.0165(6)	-0.1056(5)	0.061(6)
*F51	0.03690(16)	0.01897(9)	-0.03935(16)	0.0605(16)
*F51'	0.1760(7)	0.0096(4)	-0.1079(5)	0.062(4)
O1	0.69750(15)	0.18872(9)	0.27381(13)	0.0355(10)
N1	0.35800(18)	0.21256(9)	0.13519(15)	0.0286(10)
N2	0.25749(18)	0.26246(9)	0.15809(15)	0.0282(10)
N3	0.15188(18)	0.20701(10)	0.11804(15)	0.0286(11)

N4	0.25323(17)	0.15622(9)	0.09954(15)	0.0280(10)
N5	0.37816(18)	0.14766(10)	0.10989(15)	0.0282(10)
N6	0.38252(18)	0.27589(10)	0.17626(15)	0.0276(10)
N7	0.13438(18)	0.26919(10)	0.15605(15)	0.0287(11)
N8	0.12743(18)	0.14442(10)	0.07447(15)	0.0304(11)
N9	0.66388(18)	0.17082(11)	0.18119(16)	0.0336(11)
C1	0.4005(2)	0.24298(11)	0.15784(18)	0.0276(12)
C2	0.4747(2)	0.23178(12)	0.16382(18)	0.0296(12)
C3	0.5388(2)	0.25097(12)	0.18202(18)	0.0309(12)
C4	0.6000(2)	0.23074(13)	0.18502(19)	0.0320(12)
C5	0.6000(2)	0.19189(13)	0.17359(18)	0.0315(12)
C6	0.5351(2)	0.17337(12)	0.15474(18)	0.0309(12)
C7	0.4733(2)	0.19354(12)	0.14865(18)	0.0295(12)
C8	0.3986(2)	0.18217(12)	0.12948(18)	0.0276(12)
C9	0.7111(2)	0.17039(12)	0.23454(19)	0.0328(12)
C10	0.6742(3)	0.14924(15)	0.1316(2)	0.0424(17)
C11	0.7766(2)	0.14676(14)	0.2446(2)	0.0419(17)
C12	0.3106(2)	0.13669(11)	0.09433(18)	0.0281(12)
C13	0.2872(2)	0.09983(12)	0.06729(19)	0.0302(12)
C14	0.3209(2)	0.06887(12)	0.05220(19)	0.0304(12)
C15	0.2864(2)	0.03577(12)	0.0281(2)	0.0350(14)
C16	0.2107(2)	0.03521(12)	0.0148(2)	0.0358(14)
C17	0.1773(2)	0.06702(12)	0.0302(2)	0.0336(14)
C18	0.2142(2)	0.09890(12)	0.05661(19)	0.0296(12)
C19	0.1934(2)	0.13506(11)	0.07752(18)	0.0282(12)
C20	0.1600(2)	0.00256(12)	-0.0145(2)	0.0377(14)
*C21	0.08998(18)	0.01441(8)	-0.06332(13)	0.052(2)
*C21'	0.1280(7)	0.0092(4)	-0.0854(5)	0.049(6)
*C22	0.14025(14)	-0.02345(8)	0.03378(13)	0.0428(19)
*C22'	0.0973(8)	-0.0052(5)	0.0099(7)	0.045(6)
C23	0.3353(3)	0.00344(14)	0.0176(3)	0.0514(19)
*C24	0.40781(12)	-0.00474(6)	0.07397(11)	0.044(2)
*C24'	0.3641(5)	-0.0217(3)	0.0566(4)	0.046(6)
*C25	0.35404(13)	0.00642(7)	-0.03772(11)	0.051(2)
*C25'	0.3913(5)	0.0225(3)	-0.0210(4)	0.068(9)
C26	0.1093(2)	0.17750(12)	0.09318(18)	0.0291(12)
C27	0.0371(2)	0.18747(12)	0.09167(18)	0.0298(12)
C28	-0.0279(2)	0.16945(13)	0.0697(2)	0.0344(12)
C29	-0.0904(2)	0.18345(13)	0.0776(2)	0.0345(12)
C30	-0.0859(2)	0.21714(13)	0.11319(19)	0.0330(12)
C31	-0.0219(2)	0.23638(12)	0.12883(19)	0.0326(12)
C32	0.0392(2)	0.22236(12)	0.11852(18)	0.0294(12)
C33	0.1125(2)	0.23536(12)	0.13299(18)	0.0290(12)
C34	-0.1582(2)	0.16149(13)	0.0443(2)	0.0374(14)

C35	-0.16925(8)	0.12342(5)	0.07579(7)	0.0443(17)
C36	-0.16604(8)	0.15405(5)	-0.02411(7)	0.0433(17)
C37	-0.1447(2)	0.23182(13)	0.1391(2)	0.0354(16)
C38	-0.18768(8)	0.26726(5)	0.10695(7)	0.0419(16)
C39	-0.12047(8)	0.24022(5)	0.20829(7)	0.0408(16)
C40	0.2006(2)	0.28099(12)	0.16730(18)	0.0286(12)
C41	0.2250(2)	0.31804(12)	0.19423(18)	0.0301(12)
C42	0.1914(2)	0.34794(12)	0.2123(2)	0.0333(12)
C43	0.2269(3)	0.38024(13)	0.2386(2)	0.0384(16)
C44	0.3027(3)	0.38071(13)	0.2503(2)	0.0384(16)
C45	0.3341(2)	0.35117(12)	0.2278(2)	0.0342(12)
C46	0.2971(2)	0.31976(12)	0.20053(18)	0.0297(12)
C47	0.3167(2)	0.28437(11)	0.17669(18)	0.0278(12)
C48	0.1793(3)	0.41284(14)	0.2505(3)	0.0493(19)
C49	0.11023(11)	0.42245(5)	0.19555(10)	0.060(2)
C50	0.15638(10)	0.40624(6)	0.30793(9)	0.0581(19)
C51	0.3545(3)	0.40997(13)	0.2885(2)	0.0445(16)
C52	0.37924(10)	0.44160(5)	0.25101(10)	0.0558(19)
C53	0.42131(9)	0.39156(5)	0.33669(7)	0.0491(17)
C54	0.4646(2)	0.17718(10)	0.52726(18)	0.068(2)
C55	0.40248(16)	0.19594(11)	0.49917(17)	0.0582(19)
C56	0.40531(15)	0.22977(11)	0.46953(16)	0.0561(19)
C57	0.47030(19)	0.24483(9)	0.46799(16)	0.0540(19)
C58	0.53245(15)	0.22607(11)	0.49608(18)	0.061(2)
C59	0.52962(16)	0.19224(11)	0.52571(19)	0.071(2)
C60	0.4614(5)	0.1410(2)	0.5617(4)	0.106(4)
C61	0.8444(4)	0.44484(19)	0.7482(5)	0.160(7)
C62	0.8382(6)	0.4445(2)	0.8046(4)	0.146(6)
C63	0.7726(7)	0.45012(19)	0.8149(3)	0.179(8)
C64	0.7131(5)	0.45600(18)	0.7689(5)	0.180(7)
C65	0.7193(5)	0.45630(17)	0.7125(4)	0.138(6)
C66	0.7849(6)	0.45072(18)	0.7022(3)	0.116(5)
C67	0.9162(12)	0.4380(4)	0.7479(10)	0.258(15)
*O2	0.9512(9)	0.0864(5)	0.3332(8)	0.219(6)
C71	0.34546(15)	0.33932(10)	0.06681(15)	0.0506(17)
C72	0.33528(18)	0.37392(10)	0.09183(15)	0.0556(19)
C73	0.2672(2)	0.38607(9)	0.08983(16)	0.0603(19)
C74	0.20939(16)	0.36362(11)	0.06280(17)	0.063(2)
C75	0.21957(17)	0.32902(11)	0.03777(15)	0.057(2)
C76	0.2876(2)	0.31687(8)	0.03978(15)	0.0578(19)
C77	0.4210(4)	0.3282(2)	0.0697(3)	0.082(2)
*C68	0.9919(11)	0.0590(3)	0.2636(7)	0.117(4)
*C69	0.9750(7)	0.0926(3)	0.2960(5)	0.095(3)
*C70	0.9855(5)	0.1290(2)	0.2751(4)	0.0589(19)

Table P.3 Bond lengths [Å] and angles [°] for **[NMeAcF$_{51}$PcZn]$_2$·3(toluene)·0.75(acetone)**.

Zn-N1	2.010(4)	F38 -C23	1.406(6)
Zn-N2	2.015(3)	F38' -C23	1.597(14)
Zn-N3	2.021(4)	F39 -C25	1.323(4)
Zn-N4	2.006(3)	F40 -C25	1.323(5)
Zn-O1_a	2.065(3)	F41 -C25	1.324(5)
F1-C3	1.328(5)	F42 -C24	1.309(4)
F2-C4	1.341(5)	F43 -C24	1.309(4)
F3-C6	1.337(5)	F44 -C24	1.308(4)
F4-C45	1.333(5)	F45 -C20	1.344(6)
F5-C42	1.333(5)	F45' -C20	1.319(15)
F6 -C31	1.343(5)	F46 -C22	1.308(5)
F7 -C28	1.337(5)	F47 -C22	1.308(5)
F8 -C17	1.319(5)	F48 -C22	1.308(4)
F9 -C14	1.339(5)	F49 -C21	1.328(5)
F10 -C51	1.358(6)	F50 -C21	1.328(5)
F11 -C53	1.309(3)	F51 -C21	1.328(5)
F12 -C53	1.309(3)	N1 -C1	1.372(5)
F13 -C53	1.309(3)	N1 -C8	1.358(5)
F14 -C52	1.310(3)	N2 -C40	1.360(5)
F15 -C52	1.310(3)	N2 -C47	1.364(5)
F16 -C52	1.310(3)	N3 -C26	1.362(5)
F17 -C48	1.356(6)	N3 -C33	1.364(5)
F18 -C50	1.306(3)	N4 -C12	1.352(5)
F19 -C50	1.306(3)	N4 -C19	1.369(5)
F20 -C50	1.306(4)	N5 -C12	1.334(5)
F21 -C49	1.307(3)	N5 -C8	1.319(5)
F22 -C49	1.307(3)	N6 -C1	1.316(5)
F23 -C49	1.307(3)	N6 -C47	1.328(5)
F24 -C37	1.361(5)	N7 -C33	1.329(5)
F25 -C39	1.310(3)	N7 -C40	1.321(5)
F26 -C39	1.310(3)	N8 -C19	1.319(5)
F27 -C39	1.310(3)	N8 -C26	1.325(5)
F28 -C38	1.311(3)	N9 -C10	1.469(6)
F29-C38	1.311(3)	N9 -C5	1.424(6)
F30-C38	1.311(3)	N9 -C9	1.364(6)
F31-C34	1.366(5)	O1 -C9	1.227(5)
F32-C36	1.309(3)	O2 -C69	1.13(2)
F33 -C36	1.309(3)	C1 -C2	1.478(6)
F34 -C36	1.309(3)	C2 -C3	1.389(6)
F35 -C35	1.314(3)	C2 -C7	1.386(6)
F36 -C35	1.314(3)	C3 -C4	1.380(6)
F37 -C35	1.314(3)	C4 -C5	1.387(6)

C5 -C6	1.392(6)	C41 -C46	1.384(6)
C6 -C7	1.377(6)	C42 -C43	1.388(6)
C7 -C8	1.469(6)	C43 -C44	1.438(8)
C9 -C11	1.493(6)	C43 -C48	1.549(8)
C10 -H4	0.96	C44 -C45	1.385(7)
C10 -H5	0.96	C44 -C51	1.556(7)
C10 -H6	0.96	C45 -C46	1.382(6)
C11 -H1	0.96	C46 -C47	1.459(6)
C11 -H2	0.96	C48 -C49	1.652(7)
C11 -H3	0.96	C48 -C50	1.577(7)
C12 -C13	1.462(6)	C51 -C52	1.583(5)
C13 -C14	1.368(6)	C51 -C53	1.630(5)
C13 -C18	1.387(6)	C54 -C55	1.389(5)
C14 -C15	1.388(6)	C54 -C59	1.391(5)
C15 -C16	1.434(6)	C54 -C60	1.523(9)
C15 -C23	1.548(7)	C55 -C56	1.390(5)
C16 -C17	1.392(6)	C55 -H12	0.93
C16 -C20	1.554(6)	C56 -C57	1.390(5)
C17 -C18	1.387(6)	C56 -H8	0.93
C18 -C19	1.460(6)	C57 -C58	1.390(5)
C20 -C21	1.602(5)	C57 -H7	0.93
C20 -C21'	1.663(13)	C58 -C59	1.390(6)
C20 -C22	1.601(5)	C58 -H18	0.93
C20 -C22'	1.523(17)	C59 -H19	0.93
C23 -C24	1.704(7)	C60 -H20	0.96
C23 -C24'	1.298(12)	C60 -H21	0.96
C23 -C25	1.473(7)	C60 -H22	0.96
C23 -C25'	1.749(12)	C61 -C62	1.391(15)
C26 -C27	1.451(6)	C61 -C66	1.390(14)
C27 -C28	1.394(6)	C61 -C67	1.43(3)
C27 -C32	1.376(6)	C62 -C63	1.389(18)
C28 -C29	1.381(6)	C62 -H2T	0.93
C29 -C30	1.445(6)	C63 -C64	1.390(15)
C29 -C34	1.559(6)	C63 -H3T	0.93
C30 -C31	1.385(6)	C64 -C65	1.391(15)
C30 -C37	1.539(6)	C64 -H4T	0.93
C31 -C32	1.378(6)	C65 -C66	1.389(15)
C32 -C33	1.459(6)	C65 -H5T	0.93
C34 -C35	1.575(5)	C66 -H6T	0.93
C34 -C36	1.628(5)	C67 -H7T1	0.96
C37 -C38	1.580(5)	C67 -H7T2	0.96
C37 -C39	1.626(5)	C67 -H7T3	0.96
C40 -C41	1.471(6)	C68 -C69	1.495(18)
C41 -C42	1.368(6)	C68 -H81A	0.96

C68 -H81B	0.96	C73 -C74	1.389(5)
C68 -H81C	0.96	C73 -H73	0.93
C69 -C70	1.405(13)	C74 -C75	1.390(5)
C70 -H80A	0.96	C74 -H74	0.93
C70 -H80B	0.96	C75 -C76	1.390(5)
C70 -H80C	0.96	C75 -H75	0.93
C71 -C72	1.390(5)	C76 -H76	0.93
C71 -C76	1.390(5)	C77 -H77A	0.96
C71 -C77	1.517(9)	C77 -H77B	0.96
C72 -C73	1.391(5)	C77 -H77C	0.96
C72 -H72	0.93		

N1 -Zn -N2	88.08(14)	N4 -C12 -N5	128.2(4)
N1 -Zn -N3	158.48(14)	N4 -C19 -C18	108.2(3)
N1 -Zn -N4	88.90(14)	N4 -C19 -N8	127.9(4)
N2 -Zn -N3	88.39(15)	N5 -C12 -C13	123.3(4)
N2 -Zn -N4	161.51(14)	N5 -C8 -C7	122.8(4)
N3 -Zn -N4	87.76(14)	N6 -C1 -C2	123.1(4)
O1_a -Zn -N1	87.40(13)	N6 -C47 -C46	123.5(4)
O1_a -Zn -N2	96.98(13)	N7 -C33 -C32	124.4(4)
O1_a -Zn -N3	114.10(13)	N7 -C40 -C41	123.5(4)
O1_a -Zn -N4	101.10(13)	N8 -C19 -C18	123.9(4)
Zn -N1 -C1	123.8(3)	N8 -C26 -C27	123.5(4)
Zn -N1 -C8	121.8(3)	N9 -C10 -H4	109
Zn -N2 -C40	123.5(3)	N9 -C10 -H5	110
Zn -N2 -C47	124.1(3)	N9 -C10 -H6	109
Zn -N3 -C26	125.4(3)	N9 -C5 -C4	122.0(4)
Zn -N3 -C33	123.8(3)	N9 -C5 -C6	119.9(4)
Zn -N4 -C12	123.6(3)	N9 -C9 -C11	119.8(4)
Zn -N4 -C19	126.2(3)	O1 -C9 -C11	121.4(4)
Zn_a -O1 -C9	141.9(3)	O1 -C9 -N9	118.8(4)
N1 -C1 -C2	108.1(3)	O2 -C69 -C68	117.0(14)
N1 -C1 -N6	128.6(4)	O2 -C69 -C70	125.8(13)
N1 -C8 -C7	108.6(4)	C1 -C2 -C3	133.5(4)
N1 -C8 -N5	128.5(4)	C1 -C2 -C7	106.3(3)
N2 -C40 -C41	107.9(3)	C2 -C3 -C4	118.1(4)
N2 -C40 -N7	128.6(4)	C2 -C7 -C6	120.9(4)
N2 -C47 -C46	108.3(3)	C2 -C7 -C8	107.0(4)
N2 -C47 -N6	128.1(4)	C3 -C2 -C7	120.1(4)
N3 -C26 -C27	108.0(4)	C3-C4-C5	122.6(4)
N3 -C26 -N8	128.5(4)	C4 -C5 -C6	118.2(4)
N3 -C33 -C32	107.6(4)	C5 -C6 -C7	119.9(4)
N3 -C33 -N7	128.0(4)	C6 -C7 -C8	132.2(4)
N4 -C12 -C13	108.5(3)	C9 -C11 -H1	109

C9 -C11 -H2	109	C38 -C37 -C39	109.1(3)
C9 -C11 -H3	110	C40 -C41 -C42	133.3(4)
C12 -C13 -C14	134.4(4)	C40 -C41 -C46	106.8(4)
C12 -C13 -C18	106.8(4)	C40 -N2 -C47	110.1(3)
C13 -C14 -C15	123.7(4)	C41 -C42 -C43	122.8(4)
C13 -C18 -C17	119.3(4)	C41 -C46 -C45	118.6(4)
C13 -C18 -C19	106.7(4)	C41 -C46 -C47	106.9(4)
C14 -C13 -C18	118.8(4)	C42 -C41 -C46	119.9(4)
C14 -C15 -C16	117.7(4)	C42 -C43 -C44	117.7(4)
C14 -C15 -C23	115.1(4)	C42 -C43 -C48	115.5(5)
C15 -C16 -C17	117.7(4)	C43 -C44 -C45	117.4(4)
C15 -C16 -C20	127.6(4)	C43 -C44 -C51	126.9(4)
C15 -C23 -C24	114.6(4)	C43 -C48 -C49	114.2(4)
C15 -C23 -C24'	123.2(7)	C43 -C48 -C50	112.4(4)
C15 -C23 -C25	114.3(4)	C44 -C43 -C48	126.8(4)
C15 -C23 -C25'	108.2(5)	C44 -C45 -C46	123.1(4)
C16 -C15 -C23	127.2(4)	C44 -C51 -C52	112.2(3)
C16 -C17 -C18	122.7(4)	C44 -C51 -C53	115.5(3)
C16 -C20 -C21	117.4(3)	C45 -C44 -C51	115.6(5)
C16 -C20 -C21'	112.3(6)	C45 -C46 -C47	134.5(4)
C16 -C20 -C22	110.0(3)	C49 -C48 -C50	111.2(4)
C16 -C20 -C22'	116.3(7)	C52 -C51 -C53	111.6(4)
C17 -C16 -C20	114.7(4)	C54 -C55 -C56	120.0(3)
C17 -C18 -C19	134.0(4)	C54 -C55 -H12	120
C26 -C27 -C28	133.6(4)	C54 -C59 -C58	120.0(3)
C26 -C27 -C32	107.2(4)	C54 -C59 -H19	120
C27 -C28 -C29	123.0(4)	C54 -C60 -H20	109
C27 -C32 -C31	118.8(4)	C54 -C60 -H21	109
C27 -C32 -C33	107.0(4)	C54 -C60 -H22	109
C28 -C27 -C32	119.2(4)	C55 -C54 -C59	120.0(3)
C28 -C29 -C30	117.1(4)	C55 -C54 -C60	119.8(5)
C28 -C29 -C34	115.0(4)	C55 -C56 -C57	120.0(3)
C29 -C30 -C31	117.6(4)	C55 -C56 -H8	120
C29 -C30 -C37	125.3(4)	C56 -C55 -H12	120
C29 -C34 -C35	112.4(3)	C56 -C57 -C58	120.0(3)
C29 -C34 -C36	115.6(3)	C56 -C57 -H7	120
C30 -C29 -C34	127.9(4)	C57 -C56 -H8	120
C30 -C31 -C32	123.2(4)	C57 -C58 -C59	120.0(3)
C30 -C37 -C38	115.2(3)	C57 -C58 -H18	120
C30 -C37 -C39	115.3(3)	C58 -C57 -H7	120
C31 -C30 -C37	116.9(4)	C58 -C59 -H19	120
C31 -C32 -C33	134.1(4)	C59 -C54 -C60	120.1(5)
C33 -N7 -C40	123.7(4)	C59 -C58 -H18	120
C35 -C34 -C36	111.1(3)	C61 -C62 -C63	120.0(9)

C61 -C62 -H2T	120	C75 -C74 -H74	120
C61 -C66 -C65	120.1(8)	C75 -C76 -H76	120
C61 -C66 -H6T	120	C76 -C71 -C77	122.9(4)
C61 -C67 -H7T1	110	C76 -C75 -H75	120
C61 -C67 -H7T2	109	C1 -N6 -C47	123.2(4)
C61 -C67 -H7T3	110	C12 -N4 -C19	109.9(3)
C62 -C61 -C66	119.9(9)	C19 -N8 -C26	123.2(4)
C62 -C61 -C67	110.3(13)	C1-N1-C8	109.7(3)
C62 -C63 -C64	120.1(8)	C26 -N3 -C33	110.1(4)
C62 -C63 -H3T	120	C8 -N5 -C12	123.2(4)
C63 -C62 -H2T	120	C5 -N9 -C10	118.1(4)
C63 -C64 -C65	119.9(10)	C5 -N9 -C9	118.6(4)
C63 -C64 -H4T	120	C9 -N9 -C10	123.2(4)
C64 -C63 -H3T	120	F1 -C3 -C2	122.5(4)
C64 -C65 -C66	120.0(9)	F1 -C3 -C4	119.3(4)
C64 -C65 -H5T	120	F2 -C4 -C3	118.2(4)
C65 -C64 -H4T	120	F2 -C4 -C5	119.2(4)
C65 -C66 -H6T	120	F3 -C6 -C5	119.0(4)
C66 -C61 -C67	129.7(13)	F3 -C6 -C7	121.1(4)
C66 -C65 -H5T	120	F4 -C45 -C44	118.6(4)
C68 -C69 -C70	117.0(11)	F4 -C45 -C46	118.2(4)
C69 -C68 -H81A	109	F5 -C42 -C41	117.4(4)
C69 -C68 -H81B	109	F5 -C42 -C43	119.9(4)
C69 -C68 -H81C	110	F6 -C31 -C30	119.0(4)
C69 -C70 -H80A	109	F6 -C31 -C32	117.6(4)
C69 -C70 -H80B	109	F7 -C28 -C27	117.7(4)
C69 -C70 -H80C	110	F7 -C28 -C29	119.4(4)
C71 -C72 -C73	120.0(3)	F8 -C17 -C16	120.0(4)
C71 -C72 -H72	120	F8 -C17 -C18	117.3(4)
C71 -C76 -C75	120.0(3)	F9 -C14 -C13	116.8(4)
C71 -C76 -H76	120	F9 -C14 -C15	119.5(4)
C71 -C77 -H77A	109	F10 -C51 -C44	110.2(5)
C71 -C77 -H77B	109	F10 -C51 -C52	105.4(3)
C71 -C77 -H77C	110	F10 -C51 -C53	100.8(3)
C72 -C71 -C76	120.0(3)	F11 -C53 -C51	109.5(2)
C72 -C71 -C77	117.2(4)	F11 -C53 -F12	109.48(18)
C72 -C73 -C74	120.0(3)	F11 -C53 -F13	109.46(19)
C72 -C73 -H73	120	F12 -C53 -C51	109.5(2)
C73 -C72 -H72	120	F12 -C53 -F13	109.47(19)
C73 -C74 -C75	120.0(3)	F13 -C53 -C51	109.5(2)
C73 -C74 -H74	120	F14 -C52 -C51	109.5(3)
C74 -C73 -H73	120	F14 -C52 -F15	109.5(2)
C74 -C75 -C76	120.0(3)	F14 -C52 -F16	109.5(2)
C74 -C75 -H75	120	F15 -C52 -C51	109.5(3)

F15 -C52 -F16	109.5(2)	F36 -C35 -C34	109.4(2)
F16 -C52 -C51	109.5(2)	F36 -C35 -F37	109.48(19)
F17 -C48 -C43	110.4(5)	F37 -C35 -C34	109.5(2)
F17 -C48 -C49	101.6(4)	F38 -C23 -C15	109.8(5)
F17 -C48 -C50	106.3(4)	F38' -C23 -C15	101.9(6)
F18 -C50 -C48	109.4(3)	F39' -C25'	1.312(14)
F18 -C50 -F19	109.5(2)	F39 -C25 -C23	109.5(3)
F18 -C50 -F20	109.5(2)	F39' -C25' -C23	109.6(8)
F19 -C50 -C48	109.5(3)	F39 -C25 -F40	109.5(3)
F19 -C50 -F20	109.5(2)	F39' -C25' -F40'	109.5(10)
F20 -C50 -C48	109.5(3)	F39 -C25 -F41	109.5(3)
F21 -C49 -C48	109.4(3)	F39' -C25' -F41'	109.5(10)
F21 -C49 -F22	109.5(2)	F40' -C25'	1.315(17)
F21 -C49 -F23	109.5(2)	F40 -C25 -C23	109.5(3)
F22 -C49 -C48	109.5(3)	F40' -C25' -C23	109.5(8)
F22 -C49 -F23	109.5(2)	F40 -C25 -F41	109.5(3)
F23 -C49 -C48	109.5(3)	F40' -C25' -F41'	109.4(10)
F24 -C37 -C30	110.2(4)	F41' -C25'	1.313(16)
F24 -C37 -C38	105.0(3)	F41 -C25 -C23	109.5(3)
F24 -C37 -C39	100.6(3)	F41' -C25' -C23	109.5(9)
F25 -C39 -C37	109.5(2)	F42' -C24'	1.308(17)
F25 -C39 -F26	109.47(19)	F42 -C24 -C23	109.5(3)
F25 -C39 -F27	109.46(18)	F42' -C24' -C23	109.5(9)
F26 -C39 -C37	109.5(2)	F42 -C24 -F43	109.5(2)
F26 -C39 -F27	109.48(18)	F42' -C24' -F43'	109.4(11)
F27 -C39 -C37	109.5(2)	F42 -C24 -F44	109.5(3)
F28 -C38 -C37	109.4(2)	F42' -C24' -F44'	109.4(11)
F28 -C38 -F29	109.48(18)	F43' -C24'	1.307(17)
F28 -C38 -F30	109.49(18)	F43 -C24 -C23	109.5(3)
F29 -C38 -C37	109.5(2)	F43' -C24' -C23	109.5(10)
F29 -C38 -F30	109.47(18)	F43 -C24 -F44	109.5(2)
F30 -C38 -C37	109.5(2)	F43' -C24' -F44'	109.6(11)
F31 -C34 -C29	110.2(4)	F44' -C24'	1.307(17)
F31 -C34 -C35	106.2(3)	F44 -C24 -C23	109.5(3)
F31 -C34 -C36	100.3(3)	F44' -C24' -C23	109.4(9)
F32 -C36 -C34	109.5(2)	F45 -C20 -C16	110.8(4)
F32 -C36 -F33	109.46(18)	F45' -C20 -C16	110.6(8)
F32 -C36 -F34	109.48(19)	F45 -C20 -C22	104.0(3)
F33 -C36 -C34	109.4(2)	F45' -C20 -C22'	105.1(10)
F33 -C36 -F34	109.48(19)	F46' -C22'	1.36(3)
F34 -C36 -C34	109.5(2)	F46 -C22 -C20	109.5(3)
F35 -C35 -C34	109.5(2)	F46' -C22' -C20	109.6(14)
F35 -C35 -F36	109.49(18)	F46 -C22 -F47	109.5(3)
F35 -C35 -F37	109.48(18)	F46' -C22' -F47'	109.5(19)

F46 -C22 -F48	109.5(3)	F51 -C21 -C20	109.5(3)
F46' -C22' -F48'	109.4(18)	F51' -C21' -C20	109.5(11)
F47' -C22'	1.36(3)	H1 -C11 -H2	109
F47 -C22 -C20	109.5(3)	H1 -C11 -H3	109
F47' -C22' -C20	109.5(16)	H2 -C11 -H3	110
F47 -C22 -F48	109.5(3)	H20 -C60 -H21	109
F47' -C22' -F48'	109.4(19)	H20 -C60 -H22	110
F48' -C22'	1.36(3)	H21 -C60 -H22	109
F48 -C22 -C20	109.5(3)	H4 -C10 -H5	109
F48' -C22' -C20	109.5(14)	H4 -C10 -H6	110
F49' -C21'	1.21(3)	H5 -C10 -H6	109
F49 -C21 -C20	109.5(3)	H77A -C77 -H77B	109
F49' -C21' -C20	109.5(10)	H77A -C77 -H77C	110
F49 -C21 -F50	109.5(3)	H77B -C77 -H77C	110
F49' -C21' -F50'	109.4(17)	H7T1 -C67 -H7T2	109
F49 -C21 -F51	109.5(3)	H7T1 -C67 -H7T3	110
F49' -C21' -F51'	109.6(15)	H7T2 -C67 -H7T3	109
F50' -C21'	1.21(2)	H80A -C70 -H80B	109
F50 -C21 -C20	109.5(3)	H80A -C70 -H80C	109
F50' -C21' -C20	109.4(11)	H80B -C70 -H80C	110
F50 -C21 -F51	109.5(3)	H81A -C68 -H81B	110
F50' -C21' -F51'	109.4(15)	H81A -C68 -H81C	109
F51' -C21'	1.205(19)	H81B -C68 -H81C	109

Table P.4 Anisotropic displacement parameters ($Å^2$) for **$[NMeAcF_{51}PcZn]_2$·3(toluene)·0.75(acetone)**. 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	0.0260(3)	0.0200(3)	0.0367(3)	-0.0003(2)	0.0107(2)	0.0018(2)
F1	0.0377(14)	0.0258(13)	0.0426(14)	-0.0041(11)	0.0115(11)	-0.0031(10)
F2	0.0295(13)	0.0350(14)	0.0472(15)	-0.0069(11)	0.0108(11)	-0.0052(10)
F3	0.0328(13)	0.0251(13)	0.0517(15)	-0.0073(11)	0.0118(11)	0.0011(10)
F4	0.0344(13)	0.0256(12)	0.0498(15)	-0.0060(11)	0.0174(11)	-0.0033(10)
F5	0.0335(13)	0.0285(13)	0.0590(17)	-0.0098(12)	0.0174(12)	0.0018(10)
F6	0.0289(13)	0.0288(13)	0.0518(15)	-0.0135(11)	0.0089(11)	0.0039(10)
F7	0.0322(13)	0.0328(14)	0.0536(16)	-0.0155(12)	0.0134(12)	0.0005(10)
F8	0.0299(13)	0.0314(14)	0.0743(19)	-0.0143(13)	0.0174(13)	-0.0016(11)
F9	0.0290(13)	0.0264(13)	0.0584(16)	-0.0062(11)	0.0179(11)	0.0020(10)
F10	0.0583(19)	0.0479(18)	0.080(2)	-0.0336(16)	0.0352(17)	-0.0119(14)
F11	0.0537(17)	0.0516(18)	0.0503(17)	-0.0053(14)	0.0179(14)	-0.0107(14)
F12	0.063(2)	0.071(2)	0.065(2)	-0.0364(18)	0.0256(16)	-0.0201(17)
F13	0.0443(16)	0.0558(18)	0.0628(19)	-0.0174(15)	0.0239(14)	-0.0136(14)

F14	0.087(3)	0.0354(17)	0.124(3)	-0.0305(19)	0.049(2)	-0.0298(17)
F15	0.072(2)	0.0318(16)	0.124(3)	0.0121(19)	0.042(2)	0.0083(15)
F16	0.0630(19)	0.0304(15)	0.080(2)	0.0010(14)	0.0363(17)	-0.0048(13)
F17	0.0613(19)	0.0260(15)	0.117(3)	-0.0225(17)	0.0366(19)	-0.0028(13)
F18	0.059(2)	0.096(3)	0.066(2)	-0.031(2)	0.0239(17)	-0.0116(19)
F19	0.062(2)	0.069(2)	0.073(2)	-0.0227(18)	0.0381(17)	-0.0133(17)
F20	0.071(2)	0.080(3)	0.116(3)	-0.048(2)	0.049(2)	0.003(2)
F21	0.069(2)	0.0435(17)	0.072(2)	0.0084(16)	0.0196(17)	0.0130(15)
F22	0.075(2)	0.0325(17)	0.143(4)	-0.007(2)	0.027(2)	0.0163(16)
F23	0.0490(18)	0.0423(17)	0.099(3)	-0.0181(17)	0.0249(17)	0.0081(14)
F24	0.0323(14)	0.0425(15)	0.0555(16)	-0.0145(13)	0.0165(12)	-0.0030(11)
F25	0.0444(16)	0.0603(19)	0.0557(18)	-0.0158(15)	0.0247(14)	-0.0063(14)
F26	0.0506(17)	0.0515(18)	0.0559(18)	-0.0194(14)	0.0190(14)	-0.0095(14)
F27	0.0511(18)	0.067(2)	0.0441(16)	-0.0019(15)	0.0121(13)	0.0177(15)
F28	0.0413(15)	0.0376(15)	0.0588(18)	-0.0019(13)	0.0087(13)	0.0089(12)
F29	0.0396(16)	0.0563(19)	0.072(2)	-0.0031(16)	0.0226(14)	0.0184(13)
F30	0.0499(17)	0.0516(18)	0.0485(17)	-0.0080(14)	-0.0001(13)	0.0104(14)
F31	0.0275(13)	0.0458(16)	0.0573(17)	-0.0161(13)	0.0061(12)	0.0066(11)
F32	0.0577(18)	0.0479(17)	0.0464(16)	-0.0033(13)	0.0122(14)	-0.0023(14)
F33	0.0386(15)	0.0561(19)	0.0566(18)	-0.0180(15)	-0.0047(13)	0.0099(13)
F34	0.0433(15)	0.0422(16)	0.0562(17)	-0.0158(13)	0.0061(13)	0.0073(12)
F35	0.0460(16)	0.0343(15)	0.0645(18)	-0.0075(13)	0.0240(14)	0.0049(12)
F36	0.0358(15)	0.0500(18)	0.078(2)	-0.0182(16)	0.0127(14)	-0.0126(13)
F37	0.0489(16)	0.0473(17)	0.0571(18)	-0.0102(14)	0.0251(14)	-0.0023(13)
F38	0.047(2)	0.0251(17)	0.092(3)	-0.0158(18)	0.031(2)	-0.0024(14)
F39	0.064(3)	0.068(3)	0.055(3)	-0.017(2)	0.025(2)	-0.002(2)
F40	0.070(3)	0.051(3)	0.087(3)	-0.018(2)	0.050(2)	0.011(2)
F41	0.059(3)	0.058(3)	0.067(3)	-0.011(2)	0.043(2)	-0.010(2)
F42	0.052(2)	0.039(2)	0.065(3)	0.006(2)	0.023(2)	0.0117(17)
F43	0.0381(19)	0.037(2)	0.092(3)	-0.0053(19)	0.0291(19)	0.0053(15)
F44	0.058(2)	0.0299(19)	0.094(3)	0.005(2)	0.029(2)	0.0162(17)
F45	0.050(2)	0.0325(19)	0.067(3)	-0.0190(19)	0.0231(19)	-0.0052(15)
F46	0.044(3)	0.025(2)	0.090(4)	0.000(2)	0.021(2)	-0.0067(18)
F47	0.050(3)	0.038(3)	0.065(3)	-0.0002(19)	0.032(2)	0.0007(17)
F48	0.049(2)	0.040(2)	0.075(3)	0.0171(19)	0.0201(19)	0.0076(16)
F49	0.061(3)	0.062(3)	0.069(3)	-0.021(2)	-0.002(2)	-0.009(2)
F50	0.084(4)	0.037(3)	0.064(3)	0.014(2)	0.015(2)	0.003(2)
F51	0.0277(18)	0.035(2)	0.111(4)	-0.024(2)	0.005(2)	-0.0018(14)
O1	0.0336(16)	0.0338(17)	0.0377(17)	-0.0084(14)	0.0074(13)	0.0007(13)
N1	0.0294(18)	0.0216(17)	0.0377(19)	0.0021(15)	0.0142(15)	0.0001(14)
N2	0.0314(18)	0.0215(17)	0.0338(18)	-0.0046(15)	0.0126(15)	-0.0002(14)
N3	0.0286(18)	0.0236(18)	0.0348(19)	-0.0003(15)	0.0106(15)	0.0041(14)
N4	0.0271(17)	0.0198(17)	0.0386(19)	-0.0003(15)	0.0114(15)	0.0025(13)

N5	0.0266(17)	0.0238(18)	0.0352(19)	-0.0033(15)	0.0102(14)	0.0016(14)
N6	0.0304(18)	0.0232(18)	0.0317(18)	0.0024(14)	0.0126(14)	-0.0027(14)
N7	0.0292(18)	0.0233(18)	0.0342(19)	-0.0001(15)	0.0096(14)	0.0036(14)
N8	0.0279(18)	0.0273(18)	0.038(2)	-0.0014(15)	0.0125(15)	0.0024(14)
N9	0.0289(19)	0.032(2)	0.041(2)	-0.0093(16)	0.0112(16)	0.0005(15)
C1	0.031(2)	0.023(2)	0.031(2)	0.0041(17)	0.0119(17)	-0.0011(16)
C2	0.032(2)	0.027(2)	0.030(2)	0.0037(17)	0.0088(17)	0.0001(17)
C3	0.037(2)	0.027(2)	0.030(2)	0.0021(18)	0.0114(18)	-0.0024(18)
C4	0.027(2)	0.033(2)	0.036(2)	-0.0037(19)	0.0083(17)	-0.0066(17)
C5	0.029(2)	0.034(2)	0.033(2)	-0.0047(19)	0.0108(17)	-0.0007(18)
C6	0.034(2)	0.026(2)	0.033(2)	-0.0029(18)	0.0096(18)	-0.0013(17)
C7	0.029(2)	0.029(2)	0.032(2)	-0.0008(18)	0.0109(17)	0.0019(17)
C8	0.028(2)	0.024(2)	0.032(2)	0.0005(17)	0.0102(17)	0.0024(16)
C9	0.032(2)	0.029(2)	0.039(2)	-0.0046(19)	0.0121(19)	-0.0042(17)
C10	0.036(3)	0.049(3)	0.044(3)	-0.015(2)	0.014(2)	-0.001(2)
C11	0.038(3)	0.036(3)	0.050(3)	-0.008(2)	0.009(2)	0.005(2)
C12	0.029(2)	0.023(2)	0.034(2)	0.0027(17)	0.0114(17)	0.0028(16)
C13	0.031(2)	0.022(2)	0.040(2)	0.0016(18)	0.0135(18)	-0.0001(16)
C14	0.030(2)	0.028(2)	0.038(2)	0.0024(18)	0.0173(18)	0.0018(17)
C15	0.041(2)	0.024(2)	0.045(3)	-0.0048(19)	0.020(2)	0.0010(18)
C16	0.039(2)	0.023(2)	0.050(3)	-0.006(2)	0.020(2)	-0.0018(18)
C17	0.030(2)	0.027(2)	0.047(3)	-0.0015(19)	0.0158(19)	-0.0009(17)
C18	0.029(2)	0.025(2)	0.038(2)	0.0007(18)	0.0147(18)	0.0012(16)
C19	0.032(2)	0.021(2)	0.033(2)	-0.0006(17)	0.0113(17)	0.0014(16)
C20	0.037(2)	0.022(2)	0.056(3)	-0.009(2)	0.016(2)	-0.0027(18)
C21	0.067(5)	0.029(3)	0.053(4)	0.001(3)	0.006(3)	-0.015(3)
C22	0.038(3)	0.030(3)	0.062(4)	-0.003(3)	0.016(3)	-0.001(3)
C23	0.042(3)	0.032(3)	0.088(4)	-0.024(3)	0.031(3)	-0.002(2)
C24	0.045(4)	0.024(3)	0.069(5)	0.003(3)	0.024(3)	0.007(2)
C25	0.054(4)	0.049(4)	0.062(4)	-0.010(3)	0.036(4)	0.004(3)
C26	0.030(2)	0.025(2)	0.033(2)	-0.0023(17)	0.0098(17)	0.0003(16)
C27	0.027(2)	0.029(2)	0.034(2)	-0.0032(18)	0.0095(17)	0.0028(17)
C28	0.033(2)	0.031(2)	0.040(2)	-0.0063(19)	0.0110(19)	0.0038(18)
C29	0.026(2)	0.033(2)	0.043(2)	-0.004(2)	0.0067(18)	0.0018(17)
C30	0.027(2)	0.032(2)	0.040(2)	-0.0024(19)	0.0088(18)	0.0068(17)
C31	0.030(2)	0.028(2)	0.038(2)	-0.0050(19)	0.0058(18)	0.0055(17)
C32	0.028(2)	0.024(2)	0.036(2)	0.0000(18)	0.0082(17)	0.0053(17)
C33	0.028(2)	0.026(2)	0.033(2)	0.0024(18)	0.0083(17)	0.0074(16)
C34	0.025(2)	0.035(2)	0.051(3)	-0.007(2)	0.0080(19)	0.0056(18)
C35	0.038(3)	0.044(3)	0.053(3)	-0.018(2)	0.016(2)	-0.003(2)
C36	0.037(3)	0.038(3)	0.052(3)	-0.007(2)	0.007(2)	0.006(2)
C37	0.028(2)	0.037(3)	0.042(3)	-0.008(2)	0.0106(19)	0.0018(18)
C38	0.034(2)	0.043(3)	0.048(3)	-0.010(2)	0.010(2)	0.004(2)

C39	0.033(2)	0.042(3)	0.049(3)	-0.010(2)	0.014(2)	0.001(2)
C40	0.034(2)	0.021(2)	0.031(2)	0.0023(17)	0.0091(17)	0.0039(16)
C41	0.036(2)	0.022(2)	0.034(2)	0.0026(17)	0.0124(18)	0.0004(17)
C42	0.038(2)	0.024(2)	0.041(2)	-0.0010(19)	0.0162(19)	0.0013(18)
C43	0.044(3)	0.027(2)	0.048(3)	-0.002(2)	0.019(2)	0.0011(19)
C44	0.047(3)	0.024(2)	0.050(3)	-0.003(2)	0.023(2)	-0.0040(19)
C45	0.037(2)	0.027(2)	0.042(2)	-0.0010(19)	0.0164(19)	-0.0024(18)
C46	0.035(2)	0.024(2)	0.033(2)	0.0017(17)	0.0142(18)	-0.0010(17)
C47	0.033(2)	0.020(2)	0.031(2)	0.0021(17)	0.0097(17)	-0.0006(16)
C48	0.046(3)	0.031(3)	0.077(4)	-0.020(3)	0.027(3)	-0.003(2)
C49	0.063(4)	0.030(3)	0.092(5)	-0.011(3)	0.030(3)	0.014(3)
C50	0.055(3)	0.050(3)	0.079(4)	-0.026(3)	0.035(3)	-0.003(3)
C51	0.051(3)	0.028(2)	0.062(3)	-0.017(2)	0.028(2)	-0.006(2)
C52	0.059(3)	0.027(3)	0.089(4)	-0.013(3)	0.033(3)	-0.006(2)
C53	0.050(3)	0.048(3)	0.055(3)	-0.020(3)	0.024(2)	-0.012(2)
C54	0.071(4)	0.064(4)	0.065(4)	0.010(3)	0.011(3)	-0.001(3)
C55	0.048(3)	0.076(4)	0.050(3)	-0.005(3)	0.012(3)	-0.009(3)
C56	0.047(3)	0.070(4)	0.048(3)	-0.005(3)	0.007(2)	0.001(3)
C57	0.065(4)	0.057(3)	0.042(3)	-0.004(3)	0.018(3)	-0.001(3)
C58	0.048(3)	0.065(4)	0.072(4)	-0.015(3)	0.019(3)	-0.005(3)
C59	0.050(3)	0.069(4)	0.090(5)	0.010(4)	0.010(3)	0.007(3)
C60	0.104(7)	0.084(6)	0.125(7)	0.038(5)	0.024(6)	0.001(5)
C61	0.217(15)	0.088(8)	0.181(13)	-0.022(9)	0.063(12)	-0.027(9)
C62	0.223(14)	0.103(8)	0.092(7)	-0.015(6)	0.010(9)	-0.007(9)
C63	0.33(2)	0.061(6)	0.113(9)	-0.034(6)	0.004(11)	0.005(10)
C64	0.323(18)	0.056(6)	0.167(12)	-0.021(7)	0.077(13)	0.046(8)
C65	0.239(13)	0.059(5)	0.138(9)	0.013(6)	0.089(9)	0.044(7)
C66	0.194(11)	0.074(6)	0.077(6)	-0.021(5)	0.031(7)	-0.009(7)
C67	0.32(3)	0.188(18)	0.31(3)	0.048(17)	0.16(2)	0.009(18)
C71	0.059(3)	0.051(3)	0.043(3)	0.015(2)	0.016(2)	0.000(3)
C72	0.069(4)	0.048(3)	0.052(3)	0.013(3)	0.020(3)	-0.007(3)
C73	0.085(4)	0.047(3)	0.052(3)	0.011(3)	0.024(3)	0.002(3)
C74	0.064(4)	0.070(4)	0.058(4)	0.021(3)	0.024(3)	0.005(3)
C75	0.060(4)	0.064(4)	0.051(3)	0.016(3)	0.020(3)	-0.005(3)
C76	0.076(4)	0.048(3)	0.051(3)	0.010(3)	0.020(3)	-0.003(3)

Table P.5 Hydrogen coordinates and isotropic displacement parameters ($Å^2$) for **[NMeAcF$_{51}$PcZn]$_2$·3(toluene)·0.75(acetone)**.

	x	y	z	U(eq)
H1	0.8064	0.1516	0.2828	0.063
H2	0.8015	0.1533	0.2166	0.063
H3	0.7641	0.1202	0.241	0.063
H4	0.7014	0.1643	0.1119	0.064
H5	0.6291	0.1434	0.1055	0.064
H6	0.6989	0.1259	0.1451	0.064
H7	0.4722	0.2675	0.4482	0.065
H8	0.3637	0.2423	0.4507	0.067
H12	0.359	0.1859	0.5002	0.07
H18	0.5759	0.2361	0.495	0.073
H19	0.5712	0.1797	0.5445	0.085
H20	0.4135	0.132	0.5527	0.158
H21	0.4777	0.1465	0.6023	0.158
H22	0.4909	0.1218	0.5518	0.158
H7T1	0.93	0.4562	0.723	0.384
H7T2	0.9204	0.4126	0.734	0.384
H2T	0.878	0.4406	0.8354	0.174
H7T3	0.9465	0.4405	0.7865	0.384
H3T	0.7684	0.4499	0.8526	0.215
H4T	0.6692	0.4597	0.7758	0.216
H5T	0.6795	0.4602	0.6817	0.166
H6T	0.7891	0.4509	0.6644	0.139
H72	0.374	0.3889	0.1099	0.067
H73	0.2604	0.4092	0.1066	0.072
H74	0.1639	0.3717	0.0615	0.075
H75	0.1809	0.314	0.0197	0.069
H76	0.2944	0.2937	0.023	0.069
H77A	0.4408	0.3466	0.0487	0.122
H77B	0.4214	0.3034	0.0527	0.122
H77C	0.4485	0.3276	0.1093	0.122
*H80A	0.9413	0.1426	0.2647	0.088
*H80B	1.0031	0.1264	0.2416	0.088
*H80C	1.0191	0.1429	0.3046	0.088
*H81A	1.0257	0.043	0.2896	0.176
*H81B	1.0113	0.0678	0.2332	0.176
*H81C	0.9495	0.0447	0.2472	0.176

Appendix Q: Crystal structure of NHAcF$_{51}$PcZCu·3(toluene)·EtOAc

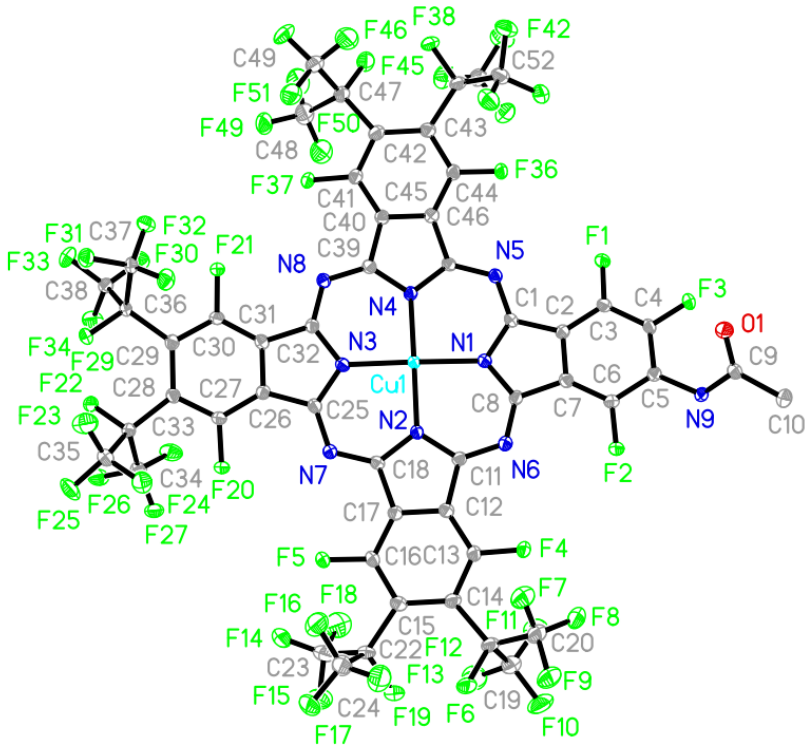


Figure Q.1 ORTEP representation of **NHAcF$_{51}$PcCu·3(toluene)·EtOAc** X-ray crystal structure, at 50% probability.

Table Q.1 Crystal data and structure refinement for **NHAcF$_{51}$PcCu·3(toluene)·EtOAc**.

Empirical formula	C74 H30 Cu F51 N9 O2	
Formula weight	2109.61	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.2172(6) Å	α = 90°.
	b = 35.1891(12) Å	β = 103.419(2)°.
	c = 23.8102(8) Å	γ = 90°.
Volume	15661.7(9) Å^3	
Z	8	
Density (calculated)	1.789 g/cm^3	
Absorption coefficient	2.028 mm^{-1}	
F(000)	8328	
Crystal size	0.536 x 0.430 x 0.234 mm	
Theta range for data collection	2.511 to 69.157°.	
Index ranges	-23<=h<=21, -42<=k<=37, -28<=l<=27	
Reflections collected	73004	

Independent reflections	14040 [R(int) = 0.0298]
Completeness to theta =	67.679° 98.3 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14040 / 31 / 1264
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0544, wR2 = 0.1391
R indices (all data)	R1 = 0.0570, wR2 = 0.1408
Extinction coefficient	0.000030(5)
Largest diff. peak and hole	2.687 and -0.953 e.$Å^{-3}$

Table Q.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **$NHAcF_{51}PcCu·3(toluene)·EtOAc$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2423(1)	7082(1)	3729(1)	13(1)
N(1)	1391(2)	7115(1)	3676(1)	15(1)
N(2)	2434(2)	6565(1)	4031(1)	15(1)
N(3)	3467(2)	7066(1)	3854(1)	15(1)
N(4)	2424(2)	7609(1)	3461(1)	14(1)
N(5)	1155(2)	7744(1)	3261(1)	15(1)
N(6)	1161(2)	6469(1)	3926(1)	17(1)
N(7)	3706(2)	6433(1)	4258(1)	16(1)
N(8)	3685(2)	7684(1)	3485(1)	15(1)
N(9)	-1717(2)	6705(1)	3153(1)	18(1)
O(1)	-2026(1)	6890(1)	2225(1)	23(1)
C(1)	963(2)	7414(1)	3443(1)	14(1)
C(2)	218(2)	7307(1)	3378(1)	15(1)
C(3)	-424(2)	7496(1)	3176(2)	16(1)
C(4)	-1058(2)	7298(1)	3125(2)	17(1)
C(5)	-1072(2)	6911(1)	3256(2)	17(1)
C(6)	-422(2)	6731(1)	3487(2)	18(1)
C(7)	214(2)	6926(1)	3548(1)	16(1)
C(8)	964(2)	6814(1)	3736(2)	16(1)
C(9)	-2162(2)	6696(1)	2610(2)	17(1)
C(10)	-2803(2)	6444(1)	2525(2)	25(1)
C(11)	1840(2)	6362(1)	4069(2)	16(1)
C(12)	2066(2)	5988(1)	4304(2)	17(1)
C(13)	1706(2)	5671(1)	4427(2)	19(1)
C(14)	2048(2)	5336(1)	4649(2)	21(1)
C(15)	2822(2)	5336(1)	4792(2)	22(1)
C(16)	3166(2)	5657(1)	4651(2)	20(1)

C(17)	2804(2)	5978(1)	4406(2)	18(1)
C(18)	3028(2)	6345(1)	4226(2)	16(1)
C(19)	1548(2)	4999(1)	4702(2)	26(1)
C(20)	882(1)	4928(1)	4151(1)	32(1)
F(7)	1045(1)	5062(1)	3682(1)	37(1)
F(8)	311(1)	5103(1)	4235(1)	39(1)
F(9)	754(1)	4562(1)	4089(1)	44(1)
C(21)	1280(1)	5023(1)	5277(1)	35(1)
F(10)	890(1)	4721(1)	5321(1)	50(1)
F(11)	890(1)	5332(1)	5270(1)	41(1)
F(12)	1835(1)	5036(1)	5722(1)	49(1)
C(22)	3321(2)	5015(1)	5099(2)	29(1)
C(24)	3602(1)	4759(1)	4654(1)	40(1)
F(17)	4080(1)	4518(1)	4936(1)	56(1)
F(18)	3898(1)	4976(1)	4324(1)	48(1)
F(19)	3064(1)	4571(1)	4331(1)	47(1)
C(23)	3980(1)	5151(1)	5615(1)	43(1)
F(14)	4553(1)	5202(1)	5410(1)	52(1)
F(15)	4111(1)	4889(1)	6021(1)	72(1)
F(16)	3811(1)	5472(1)	5834(1)	52(1)
C(25)	3896(2)	6766(1)	4082(2)	16(1)
C(26)	4632(2)	6862(1)	4080(2)	16(1)
C(27)	5288(2)	6683(1)	4281(2)	17(1)
C(28)	5930(2)	6833(1)	4214(2)	16(1)
C(29)	5897(2)	7178(1)	3874(2)	16(1)
C(30)	5246(2)	7365(1)	3721(2)	17(1)
C(31)	4620(2)	7217(1)	3827(2)	16(1)
C(32)	3882(2)	7346(1)	3702(1)	15(1)
C(33)	6617(2)	6633(1)	4557(2)	18(1)
C(34)	6627(1)	6548(1)	5227(1)	22(1)
F(26)	7285(1)	6576(1)	5540(1)	31(1)
F(27)	6384(1)	6203(1)	5276(1)	26(1)
F(28)	6219(1)	6796(1)	5410(1)	30(1)
C(35)	6825(1)	6261(1)	4259(1)	24(1)
F(23)	6987(1)	6352(1)	3770(1)	39(1)
F(24)	6281(1)	6025(1)	4157(1)	30(1)
F(25)	7379(1)	6098(1)	4602(1)	37(1)
C(36)	6500(2)	7339(1)	3612(2)	16(1)
C(37)	6268(1)	7424(1)	2925(1)	19(1)
F(30)	5724(1)	7204(1)	2687(1)	26(1)
F(31)	6810(1)	7352(1)	2691(1)	24(1)
F(32)	6080(1)	7782(1)	2840(1)	25(1)
C(38)	6898(1)	7698(1)	3936(1)	20(1)
F(33)	7383(1)	7818(1)	3666(1)	28(1)

F(34)	7212(1)	7605(1)	4470(1)	28(1)
F(35)	6431(1)	7971(1)	3941(1)	25(1)
C(39)	3010(2)	7799(1)	3374(1)	15(1)
C(40)	2782(2)	8166(1)	3112(2)	16(1)
C(41)	3143(2)	8471(1)	2953(2)	20(1)
C(42)	2801(2)	8799(1)	2704(2)	23(1)
C(43)	2030(2)	8801(1)	2576(2)	21(1)
C(44)	1686(2)	8497(1)	2772(2)	18(1)
C(45)	2047(2)	8183(1)	3039(2)	16(1)
C(46)	1832(2)	7828(1)	3268(1)	14(1)
C(47)	3300(2)	9134(1)	2637(2)	34(1)
C(48)	3935(1)	9219(1)	3204(1)	47(1)
F(49)	4526(1)	9049(1)	3149(1)	52(1)
F(50)	3748(1)	9089(1)	3667(1)	47(1)
F(51)	4047(1)	9588(1)	3256(1)	70(1)
C(49)	3616(1)	9098(1)	2081(1)	50(2)
F(46)	3092(1)	9112(1)	1616(1)	65(1)
F(47)	3954(1)	8772(1)	2095(1)	53(1)
F(48)	4064(1)	9378(1)	2071(1)	75(1)
C(50)	1535(2)	9098(1)	2197(2)	26(1)
C(51)	896(1)	8918(1)	1702(1)	30(1)
F(39)	768(1)	9141(1)	1246(1)	42(1)
F(40)	314(1)	8888(1)	1901(1)	33(1)
F(41)	1087(1)	8579(1)	1557(1)	34(1)
C(52)	1233(1)	9403(1)	2569(1)	31(1)
F(42)	827(1)	9647(1)	2222(1)	49(1)
F(43)	1769(1)	9584(1)	2906(1)	44(1)
F(44)	853(1)	9231(1)	2886(1)	33(1)
F(1)	-452(1)	7865(1)	3044(1)	21(1)
F(2)	-437(1)	6364(1)	3632(1)	23(1)
F(3)	-1674(1)	7487(1)	2959(1)	21(1)
F(4)	991(1)	5688(1)	4316(1)	26(1)
F(5)	3880(1)	5665(1)	4757(1)	27(1)
F(6)	1906(1)	4661(1)	4720(1)	35(1)
F(13)	2966(1)	4776(1)	5390(1)	38(1)
F(20)	5289(1)	6356(1)	4573(1)	22(1)
F(21)	5200(1)	7691(1)	3429(1)	20(1)
F(22)	7189(1)	6873(1)	4608(1)	23(1)
F(29)	7026(1)	7072(1)	3636(1)	20(1)
F(36)	974(1)	8504(1)	2692(1)	20(1)
F(37)	3858(1)	8451(1)	3063(1)	26(1)
F(38)	1907(1)	9299(1)	1873(1)	36(1)
F(45)	2931(1)	9469(1)	2574(1)	44(1)
C(1T)	3587(3)	6618(2)	5669(3)	32(3)

C(2T)	3469(2)	6268(2)	5899(2)	33(2)
C(3T)	2774(3)	6146(1)	5874(2)	37(2)
C(4T)	2198(2)	6374(2)	5617(3)	39(2)
C(5T)	2316(3)	6724(2)	5387(3)	35(3)
C(6T)	3011(4)	6846(1)	5412(3)	34(2)
C(7T)	4346(4)	6745(3)	5684(4)	37(2)
C(15T)	9565(3)	6647(2)	5080(3)	56(2)
C(16T)	8957(3)	6837(2)	4796(2)	49(1)
C(17T)	8993(3)	7207(2)	4621(2)	55(2)
C(18T)	9637(4)	7391(2)	4723(2)	54(2)
C(19T)	10247(3)	7206(2)	5007(2)	51(1)
C(20T)	10207(3)	6842(2)	5186(3)	57(2)
C(21T)	9524(5)	6248(3)	5283(6)	135(5)
C(1D)	3498(4)	6654(2)	5582(3)	34(5)
C(2D)	2882(5)	6462(2)	5631(4)	42(3)
C(3D)	2216(4)	6633(3)	5440(4)	44(5)
C(4D)	2166(3)	6995(3)	5201(4)	42(3)
C(5D)	2781(4)	7187(2)	5153(3)	37(3)
C(6D)	3447(3)	7017(2)	5343(3)	27(2)
C(7D)	4216(7)	6474(4)	5802(5)	47(3)
C(1S)	3541(4)	625(2)	2692(5)	190(11)
C(2S)	3384(3)	644(2)	3232(4)	107(3)
C(3S)	2702(4)	552(1)	3294(2)	83(2)
C(4S)	2178(3)	441(1)	2816(3)	93(3)
C(5S)	2335(5)	422(2)	2276(2)	138(5)
C(6S)	3016(6)	514(2)	2213(3)	291(19)
C(7S)	4204(8)	705(4)	2501(8)	212(9)
C(1F)	9872(4)	1259(2)	2754(3)	18(1)
C(2F)	9791(7)	822(4)	2889(5)	55(3)
O(1F)	10000	557(3)	2500	106(3)
O(2F)	9568(11)	833(6)	3317(9)	158(7)
C(1G)	9872(4)	1259(2)	2754(3)	18(1)
C(2G)	9791(7)	822(4)	2889(5)	55(3)
O(1G)	10000	557(3)	2500	106(3)

Table Q.3 Bond lengths [Å] and angles [°] for **NHAcF_{51}PcCu·3(toluene)·EtOAc**.

Cu(1)-N(2)	1.957(3)	Cu(1)-N(4)	1.961(3)
Cu(1)-N(1)	1.960(3)	Cu(1)-O(1)#1	2.322(3)
Cu(1)-N(3)	1.960(3)		
N(1)-C(8)	1.367(4)	N(2)-C(11)	1.365(4)
N(1)-C(1)	1.371(4)	N(2)-C(18)	1.368(4)

N(3)-C(32)	1.367(5)	C(26)-C(31)	1.386(5)
N(3)-C(25)	1.371(4)	C(26)-C(27)	1.390(5)
N(4)-C(46)	1.361(4)	C(27)-C(28)	1.387(5)
N(4)-C(39)	1.366(4)	C(28)-C(29)	1.451(5)
N(5)-C(1)	1.323(5)	C(28)-C(33)	1.551(5)
N(5)-C(46)	1.330(5)	C(29)-C(30)	1.386(5)
N(6)-C(8)	1.321(5)	C(29)-C(36)	1.547(5)
N(6)-C(11)	1.324(5)	C(30)-C(31)	1.386(5)
N(7)-C(18)	1.322(5)	C(31)-C(32)	1.451(5)
N(7)-C(25)	1.327(5)	C(33)-C(35)	1.583(4)
N(8)-C(32)	1.319(5)	C(33)-C(34)	1.619(4)
N(8)-C(39)	1.325(5)	C(36)-C(38)	1.583(4)
N(9)-C(9)	1.374(5)	C(36)-C(37)	1.618(4)
N(9)-C(5)	1.407(5)	C(39)-C(40)	1.456(5)
N(9)-H(9)	0.8800	C(40)-C(41)	1.380(5)
O(1)-C(9)	1.218(4)	C(40)-C(45)	1.383(5)
O(1)-Cu(1)#1	2.322(3)	C(41)-C(42)	1.391(5)
C(1)-C(2)	1.455(5)	C(42)-C(43)	1.440(5)
C(2)-C(3)	1.387(5)	C(42)-C(47)	1.552(5)
C(2)-C(7)	1.400(5)	C(43)-C(44)	1.393(5)
C(3)-C(4)	1.385(5)	C(43)-C(50)	1.554(5)
C(4)-C(5)	1.400(5)	C(44)-C(45)	1.381(5)
C(5)-C(6)	1.394(5)	C(45)-C(46)	1.460(5)
C(6)-C(7)	1.379(5)	C(47)-C(49)	1.586(5)
C(7)-C(8)	1.460(5)	C(47)-C(48)	1.625(5)
C(9)-C(10)	1.494(5)	C(50)-C(52)	1.585(4)
C(10)-H(10A)	0.9800	C(50)-C(51)	1.620(5)
C(10)-H(10B)	0.9800	C(1T)-C(2T)	1.3900
C(10)-H(10C)	0.9800	C(1T)-C(6T)	1.3900
C(11)-C(12)	1.459(5)	C(1T)-C(7T)	1.516(10)
C(12)-C(13)	1.380(5)	C(2T)-C(3T)	1.3900
C(12)-C(17)	1.382(5)	C(2T)-H(2T)	0.9500
C(13)-C(14)	1.393(5)	C(3T)-C(4T)	1.3900
C(14)-C(15)	1.447(5)	C(3T)-H(3T)	0.9500
C(14)-C(19)	1.550(5)	C(4T)-C(5T)	1.3900
C(15)-C(16)	1.388(5)	C(4T)-H(4T)	0.9500
C(15)-C(22)	1.551(5)	C(5T)-C(6T)	1.3900
C(16)-C(17)	1.382(5)	C(5T)-H(5T)	0.9500
C(17)-C(18)	1.460(5)	C(6T)-H(6T)	0.9500
C(19)-C(21)	1.572(4)	C(7T)-H(7T1)	0.9800
C(19)-C(20)	1.626(5)	C(7T)-H(7T2)	0.9800
C(22)-C(24)	1.578(5)	C(7T)-H(7T3)	0.9800
C(22)-C(23)	1.619(5)	C(15T)-C(16T)	1.381(7)
C(25)-C(26)	1.455(5)	C(15T)-C(20T)	1.382(7)

C(15T)-C(21T)	1.494(8)	C(7D)-H(7D3)	0.9800
C(16T)-C(17T)	1.373(8)	C(1S)-C(2S)	1.3900
C(16T)-H(16T)	0.9500	C(1S)-C(6S)	1.3900
C(17T)-C(18T)	1.368(8)	C(1S)-C(7S)	1.476(12)
C(17T)-H(17T)	0.9500	C(2S)-C(3S)	1.3900
C(18T)-C(19T)	1.374(8)	C(2S)-H(2S)	0.9500
C(18T)-H(18T)	0.9500	C(3S)-C(4S)	1.3900
C(19T)-C(20T)	1.360(7)	C(3S)-H(3S)	0.9500
C(19T)-H(19T)	0.9500	C(4S)-C(5S)	1.3900
C(20T)-H(20T)	0.9500	C(4S)-H(4S)	0.9500
C(21T)-H(21A)	0.9800	C(5S)-C(6S)	1.3900
C(21T)-H(21B)	0.9800	C(5S)-H(5S)	0.9500
C(21T)-H(21C)	0.9800	C(6S)-H(6S)	0.9500
C(1D)-C(2D)	1.3900	C(7S)-H(7S1)	0.9800
C(1D)-C(6D)	1.3900	C(7S)-H(7S2)	0.9800
C(1D)-C(7D)	1.499(13)	C(7S)-H(7S3)	0.9800
C(2D)-C(3D)	1.3900	C(1F)-C(1F)#2	1.408(14)
C(2D)-H(2D)	0.9500	C(1F)-C(2F)	1.585(14)
C(3D)-C(4D)	1.3900	C(1F)-H(1F1)	0.9800
C(3D)-H(3D)	0.9500	C(1F)-H(1F2)	0.9800
C(4D)-C(5D)	1.3900	C(1F)-H(1F3)	0.9800
C(4D)-H(4D)	0.9500	C(1F)-H(1G1)	0.9830
C(5D)-C(6D)	1.3900	C(1F)-H(1G2)	1.0984
C(5D)-H(5D)	0.9500	C(1F)-H(1G3)	1.0101
C(6D)-H(6D)	0.9500	C(2F)-O(2F)	1.19(2)
C(7D)-H(7D1)	0.9800	C(2F)-O(1F)	1.435(14)
C(7D)-H(7D2)	0.9800	O(1F)-C(2F)#2	1.435(14)

N(2)-Cu(1)-N(1)	90.15(12)	N(3)-Cu(1)-N(4)	89.91(12)
N(2)-Cu(1)-N(3)	89.66(12)	N(2)-Cu(1)-O(1)#1	93.49(11)
N(1)-Cu(1)-N(3)	174.82(12)	N(1)-Cu(1)-O(1)#1	81.76(11)
N(2)-Cu(1)-N(4)	177.48(12)	N(3)-Cu(1)-O(1)#1	103.42(11)
N(1)-Cu(1)-N(4)	90.06(12)	N(4)-Cu(1)-O(1)#1	89.02(11)

C(8)-N(1)-C(1)	108.5(3)	C(39)-N(4)-Cu(1)	125.1(2)
C(8)-N(1)-Cu(1)	124.8(2)	C(1)-N(5)-C(46)	122.4(3)
C(1)-N(1)-Cu(1)	125.0(2)	C(8)-N(6)-C(11)	122.3(3)
C(11)-N(2)-C(18)	109.2(3)	C(18)-N(7)-C(25)	121.8(3)
C(11)-N(2)-Cu(1)	124.9(2)	C(32)-N(8)-C(39)	122.2(3)
C(18)-N(2)-Cu(1)	126.0(2)	C(9)-N(9)-C(5)	120.4(3)
C(32)-N(3)-C(25)	108.9(3)	C(9)-N(9)-H(9)	119.8
C(32)-N(3)-Cu(1)	125.4(2)	C(5)-N(9)-H(9)	119.8
C(25)-N(3)-Cu(1)	125.6(2)	C(9)-O(1)-Cu(1)#1	145.2(2)
C(46)-N(4)-C(39)	109.1(3)	N(5)-C(1)-N(1)	128.3(3)
C(46)-N(4)-Cu(1)	125.5(2)	N(5)-C(1)-C(2)	122.4(3)

N(1)-C(1)-C(2)	109.1(3)	C(24)-C(22)-C(23)	110.4(3)
C(3)-C(2)-C(7)	119.8(3)	N(7)-C(25)-N(3)	128.4(3)
C(3)-C(2)-C(1)	133.4(3)	N(7)-C(25)-C(26)	123.0(3)
C(7)-C(2)-C(1)	106.7(3)	N(3)-C(25)-C(26)	108.5(3)
C(4)-C(3)-C(2)	118.8(3)	C(31)-C(26)-C(27)	118.8(3)
C(3)-C(4)-C(5)	122.2(3)	C(31)-C(26)-C(25)	106.9(3)
C(6)-C(5)-C(4)	117.8(3)	C(27)-C(26)-C(25)	134.3(3)
C(6)-C(5)-N(9)	120.6(3)	C(28)-C(27)-C(26)	123.2(3)
C(4)-C(5)-N(9)	121.6(3)	C(27)-C(28)-C(29)	117.3(3)
C(7)-C(6)-C(5)	120.6(3)	C(27)-C(28)-C(33)	116.0(3)
C(6)-C(7)-C(2)	120.5(3)	C(29)-C(28)-C(33)	126.5(3)
C(6)-C(7)-C(8)	133.3(3)	C(30)-C(29)-C(28)	117.6(3)
C(2)-C(7)-C(8)	106.0(3)	C(30)-C(29)-C(36)	115.8(3)
N(6)-C(8)-N(1)	128.1(3)	C(28)-C(29)-C(36)	126.3(3)
N(6)-C(8)-C(7)	122.4(3)	C(31)-C(30)-C(29)	122.9(3)
N(1)-C(8)-C(7)	109.5(3)	C(26)-C(31)-C(30)	119.3(3)
O(1)-C(9)-N(9)	120.1(3)	C(26)-C(31)-C(32)	106.8(3)
O(1)-C(9)-C(10)	122.8(3)	C(30)-C(31)-C(32)	133.9(3)
N(9)-C(9)-C(10)	117.1(3)	N(8)-C(32)-N(3)	128.4(3)
N(6)-C(11)-N(2)	128.6(3)	N(8)-C(32)-C(31)	122.7(3)
N(6)-C(11)-C(12)	122.8(3)	N(3)-C(32)-C(31)	108.9(3)
N(2)-C(11)-C(12)	108.5(3)	C(28)-C(33)-C(35)	114.3(3)
C(13)-C(12)-C(17)	119.1(3)	C(28)-C(33)-C(34)	114.6(3)
C(13)-C(12)-C(11)	133.8(3)	C(35)-C(33)-C(34)	110.1(2)
C(17)-C(12)-C(11)	107.0(3)	C(29)-C(36)-C(38)	114.8(3)
C(12)-C(13)-C(14)	123.3(3)	C(29)-C(36)-C(37)	114.7(2)
C(13)-C(14)-C(15)	117.2(3)	C(38)-C(36)-C(37)	109.6(2)
C(13)-C(14)-C(19)	115.6(3)	N(8)-C(39)-N(4)	128.7(3)
C(15)-C(14)-C(19)	127.2(3)	N(8)-C(39)-C(40)	122.6(3)
C(16)-C(15)-C(14)	117.7(3)	N(4)-C(39)-C(40)	108.7(3)
C(16)-C(15)-C(22)	115.5(3)	C(41)-C(40)-C(45)	119.7(3)
C(14)-C(15)-C(22)	126.8(3)	C(41)-C(40)-C(39)	133.4(3)
C(17)-C(16)-C(15)	123.0(3)	C(45)-C(40)-C(39)	106.8(3)
C(16)-C(17)-C(12)	119.4(3)	C(40)-C(41)-C(42)	123.0(3)
C(16)-C(17)-C(18)	133.9(3)	C(41)-C(42)-C(43)	117.1(3)
C(12)-C(17)-C(18)	106.6(3)	C(41)-C(42)-C(47)	115.6(3)
N(7)-C(18)-N(2)	128.5(3)	C(43)-C(42)-C(47)	127.2(3)
N(7)-C(18)-C(17)	122.9(3)	C(44)-C(43)-C(42)	118.1(3)
N(2)-C(18)-C(17)	108.6(3)	C(44)-C(43)-C(50)	115.8(3)
C(14)-C(19)-C(21)	111.4(3)	C(42)-C(43)-C(50)	125.9(3)
C(14)-C(19)-C(20)	115.9(3)	C(45)-C(44)-C(43)	122.8(3)
C(21)-C(19)-C(20)	110.8(2)	C(44)-C(45)-C(40)	118.8(3)
C(15)-C(22)-C(24)	111.7(3)	C(44)-C(45)-C(46)	134.6(3)
C(15)-C(22)-C(23)	115.5(3)	C(40)-C(45)-C(46)	106.6(3)

N(5)-C(46)-N(4)	128.2(3)	C(15T)-C(20T)-H(20T)	119.2
N(5)-C(46)-C(45)	123.0(3)	C(2D)-C(1D)-C(6D)	120.0
N(4)-C(46)-C(45)	108.8(3)	C(2D)-C(1D)-C(7D)	119.9(8)
C(42)-C(47)-C(49)	112.9(4)	C(6D)-C(1D)-C(7D)	120.1(8)
C(42)-C(47)-C(48)	114.7(3)	C(3D)-C(2D)-C(1D)	120.0
C(49)-C(47)-C(48)	110.4(3)	C(3D)-C(2D)-H(2D)	120.0
C(43)-C(50)-C(52)	112.7(3)	C(1D)-C(2D)-H(2D)	120.0
C(43)-C(50)-C(51)	114.7(3)	C(4D)-C(3D)-C(2D)	120.0
C(52)-C(50)-C(51)	110.9(2)	C(4D)-C(3D)-H(3D)	120.0
C(2T)-C(1T)-C(6T)	120.0	C(2D)-C(3D)-H(3D)	120.0
C(2T)-C(1T)-C(7T)	119.7(5)	C(3D)-C(4D)-C(5D)	120.0
C(6T)-C(1T)-C(7T)	120.3(5)	C(3D)-C(4D)-H(4D)	120.0
C(3T)-C(2T)-C(1T)	120.0	C(5D)-C(4D)-H(4D)	120.0
C(3T)-C(2T)-H(2T)	120.0	C(4D)-C(5D)-C(6D)	120.0
C(1T)-C(2T)-H(2T)	120.0	C(4D)-C(5D)-H(5D)	120.0
C(2T)-C(3T)-C(4T)	120.0	C(6D)-C(5D)-H(5D)	120.0
C(2T)-C(3T)-H(3T)	120.0	C(5D)-C(6D)-C(1D)	120.0
C(4T)-C(3T)-H(3T)	120.0	C(5D)-C(6D)-H(6D)	120.0
C(5T)-C(4T)-C(3T)	120.0	C(1D)-C(6D)-H(6D)	120.0
C(5T)-C(4T)-H(4T)	120.0	C(2S)-C(1S)-C(6S)	120.0
C(3T)-C(4T)-H(4T)	120.0	C(2S)-C(1S)-C(7S)	131.6(10)
C(6T)-C(5T)-C(4T)	120.0	C(6S)-C(1S)-C(7S)	108.4(10)
C(6T)-C(5T)-H(5T)	120.0	C(3S)-C(2S)-C(1S)	120.0
C(4T)-C(5T)-H(5T)	120.0	C(3S)-C(2S)-H(2S)	120.0
C(5T)-C(6T)-C(1T)	120.0	C(1S)-C(2S)-H(2S)	120.0
C(5T)-C(6T)-H(6T)	120.0	C(2S)-C(3S)-C(4S)	120.0
C(1T)-C(6T)-H(6T)	120.0	C(2S)-C(3S)-H(3S)	120.0
C(16T)-C(15T)-C(20T)	117.8(5)	C(4S)-C(3S)-H(3S)	120.0
C(16T)-C(15T)-C(21T)	120.9(6)	C(3S)-C(4S)-C(5S)	120.0
C(20T)-C(15T)-C(21T)	121.3(6)	C(3S)-C(4S)-H(4S)	120.0
C(17T)-C(16T)-C(15T)	120.9(5)	C(5S)-C(4S)-H(4S)	120.0
C(17T)-C(16T)-H(16T)	119.6	C(6S)-C(5S)-C(4S)	120.0
C(15T)-C(16T)-H(16T)	119.6	C(6S)-C(5S)-H(5S)	120.0
C(18T)-C(17T)-C(16T)	120.1(5)	C(4S)-C(5S)-H(5S)	120.0
C(18T)-C(17T)-H(17T)	119.9	C(5S)-C(6S)-C(1S)	120.0
C(16T)-C(17T)-H(17T)	119.9	C(5S)-C(6S)-H(6S)	120.0
C(17T)-C(18T)-C(19T)	119.8(5)	C(1S)-C(6S)-H(6S)	120.0
C(17T)-C(18T)-H(18T)	120.1	C(1S)-C(7S)-H(7S1)	109.5
C(19T)-C(18T)-H(18T)	120.1	C(1S)-C(7S)-H(7S2)	109.5
C(20T)-C(19T)-C(18T)	119.8(5)	H(7S1)-C(7S)-H(7S2)	109.5
C(20T)-C(19T)-H(19T)	120.1	C(1S)-C(7S)-H(7S3)	109.5
C(18T)-C(19T)-H(19T)	120.1	H(7S1)-C(7S)-H(7S3)	109.5
C(19T)-C(20T)-C(15T)	121.6(5)	H(7S2)-C(7S)-H(7S3)	109.5
C(19T)-C(20T)-H(20T)	119.2	C(1F)#2-C(1F)-C(2F)	104.1(5)

C(1F)#2-C(1F)-H(1F1)	107.7	C(1F)#2-C(1F)-H(1F2)	4.3
C(2F)-C(1F)-H(1F1)	110.9	C(2F)-C(1F)-H(1F2)	106.7
H(1F1)-C(1F)-H(1F2)	109.5	H(1F3)-C(1F)-H(1G2)	106.2
C(1F)#2-C(1F)-H(1F3)	113.7	H(1G1)-C(1F)-H(1G2)	100.4
C(2F)-C(1F)-H(1F3)	110.8	C(1F)#2-C(1F)-H(1G3)	106.4
H(1F1)-C(1F)-H(1F3)	109.5	C(2F)-C(1F)-H(1G3)	117.7
H(1F2)-C(1F)-H(1F3)	109.5	H(1F1)-C(1F)-H(1G3)	109.4
C(1F)#2-C(1F)-H(1G1)	101.1	H(1F2)-C(1F)-H(1G3)	102.1
C(2F)-C(1F)-H(1G1)	118.6	H(1F3)-C(1F)-H(1G3)	8.4
H(1F1)-C(1F)-H(1G1)	8.7	H(1G1)-C(1F)-H(1G3)	106.8
H(1F2)-C(1F)-H(1G1)	102.5	H(1G2)-C(1F)-H(1G3)	98.7
H(1F3)-C(1F)-H(1G1)	108.2	O(2F)-C(2F)-O(1F)	141.3(15)
C(1F)#2-C(1F)-H(1G2)	8.6	O(2F)-C(2F)-C(1F)	102.3(13)
C(2F)-C(1F)-H(1G2)	111.5	O(1F)-C(2F)-C(1F)	116.4(9)
H(1F1)-C(1F)-H(1G2)	107.7	C(2F)-O(1F)-C(2F)#2	99.0(12)
H(1F2)-C(1F)-H(1G2)	4.9		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2 #2 -x+2,y,-z+1/2

Table Q.4 Anisotropic displacement parameters **NHAcF_{51}PcCu·3(toluene)·EtOAc**. 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}
Cu(1)	11(1)	12(1)	16(1)	2(1)	3(1)	1(1)
N(1)	14(1)	14(1)	16(1)	0(1)	3(1)	0(1)
N(2)	12(1)	14(1)	19(1)	0(1)	3(1)	1(1)
N(3)	15(1)	15(1)	16(1)	1(1)	3(1)	2(1)
N(4)	13(1)	13(1)	16(1)	-1(1)	3(1)	0(1)
N(5)	13(1)	14(1)	16(1)	0(1)	3(1)	1(1)
N(6)	14(1)	16(1)	20(2)	0(1)	4(1)	-1(1)
N(7)	14(1)	15(1)	20(1)	1(1)	4(1)	1(1)
N(8)	14(1)	15(1)	15(1)	-1(1)	3(1)	1(1)
N(9)	14(1)	22(2)	18(1)	6(1)	2(1)	-3(1)
O(1)	23(1)	26(1)	19(1)	5(1)	3(1)	-2(1)
C(1)	14(2)	15(2)	14(2)	0(1)	2(1)	2(1)
C(2)	15(2)	15(2)	14(2)	0(1)	4(1)	0(1)
C(3)	16(2)	15(2)	17(2)	2(1)	3(1)	2(1)
C(4)	13(2)	20(2)	17(2)	2(1)	3(1)	4(1)
C(5)	14(2)	20(2)	16(2)	3(1)	4(1)	0(1)
C(6)	18(2)	15(2)	20(2)	4(1)	5(1)	0(1)
C(7)	15(2)	18(2)	15(2)	0(1)	3(1)	1(1)
C(8)	14(2)	16(2)	17(2)	0(1)	5(1)	-1(1)
C(9)	15(2)	17(2)	20(2)	1(1)	4(1)	2(1)

C(10)	19(2)	25(2)	29(2)	3(2)	0(2)	-6(2)
C(11)	16(2)	14(2)	17(2)	0(1)	4(1)	-1(1)
C(12)	17(2)	15(2)	20(2)	1(1)	5(1)	1(1)
C(13)	15(2)	18(2)	26(2)	1(1)	6(1)	1(1)
C(14)	22(2)	14(2)	29(2)	2(1)	10(2)	0(1)
C(15)	21(2)	15(2)	29(2)	3(2)	7(2)	4(1)
C(16)	16(2)	18(2)	28(2)	2(2)	5(2)	3(1)
C(17)	16(2)	14(2)	22(2)	1(1)	5(1)	1(1)
C(18)	16(2)	14(2)	18(2)	2(1)	4(1)	2(1)
C(19)	23(2)	15(2)	45(2)	7(2)	15(2)	2(2)
C(20)	27(2)	20(2)	48(3)	1(2)	10(2)	-5(2)
F(7)	39(1)	32(1)	42(1)	-1(1)	10(1)	-8(1)
F(8)	24(1)	30(1)	66(2)	5(1)	12(1)	-5(1)
F(9)	39(2)	23(1)	66(2)	-1(1)	9(1)	-11(1)
C(21)	32(2)	31(2)	44(3)	11(2)	14(2)	-1(2)
F(10)	51(2)	37(2)	73(2)	18(1)	36(2)	-6(1)
F(11)	47(2)	33(1)	50(2)	4(1)	28(1)	6(1)
F(12)	48(2)	61(2)	39(2)	14(1)	13(1)	2(1)
C(22)	24(2)	15(2)	47(3)	12(2)	7(2)	2(2)
C(24)	29(2)	20(2)	72(3)	1(2)	17(2)	3(2)
F(17)	32(1)	20(1)	119(3)	9(2)	19(2)	11(1)
F(18)	42(2)	27(1)	86(2)	-1(1)	37(2)	3(1)
F(19)	38(2)	29(1)	79(2)	-13(1)	22(1)	-2(1)
C(23)	35(3)	28(2)	59(3)	19(2)	-2(2)	3(2)
F(14)	23(1)	36(2)	88(2)	25(2)	-3(1)	3(1)
F(15)	48(2)	70(2)	82(2)	52(2)	-19(2)	-11(2)
F(16)	54(2)	55(2)	40(2)	2(1)	-4(1)	-10(2)
C(25)	14(2)	17(2)	17(2)	1(1)	3(1)	2(1)
C(26)	15(2)	16(2)	17(2)	0(1)	4(1)	-1(1)
C(27)	16(2)	14(2)	19(2)	4(1)	3(1)	0(1)
C(28)	14(2)	17(2)	17(2)	0(1)	2(1)	1(1)
C(29)	14(2)	17(2)	17(2)	-1(1)	2(1)	-1(1)
C(30)	16(2)	16(2)	17(2)	3(1)	2(1)	0(1)
C(31)	15(2)	16(2)	16(2)	-1(1)	2(1)	1(1)
C(32)	13(2)	18(2)	14(2)	0(1)	3(1)	0(1)
C(33)	13(2)	17(2)	24(2)	3(1)	2(1)	-1(1)
C(34)	18(2)	21(2)	25(2)	5(2)	-1(2)	-1(2)
F(26)	27(1)	29(1)	29(1)	9(1)	-9(1)	-7(1)
F(27)	26(1)	20(1)	30(1)	9(1)	1(1)	-4(1)
F(28)	43(1)	26(1)	22(1)	3(1)	9(1)	5(1)
C(35)	20(2)	22(2)	30(2)	4(2)	6(2)	4(2)
F(23)	55(2)	28(1)	42(2)	3(1)	29(1)	8(1)
F(24)	27(1)	23(1)	38(1)	-6(1)	6(1)	-1(1)
F(25)	25(1)	27(1)	54(2)	3(1)	0(1)	12(1)

C(36)	11(2)	19(2)	19(2)	3(1)	3(1)	2(1)
C(37)	11(2)	24(2)	22(2)	4(1)	3(1)	0(1)
F(30)	19(1)	35(1)	21(1)	-2(1)	0(1)	-5(1)
F(31)	19(1)	31(1)	22(1)	4(1)	7(1)	3(1)
F(32)	25(1)	25(1)	26(1)	8(1)	7(1)	7(1)
C(38)	17(2)	23(2)	19(2)	4(1)	4(1)	-1(1)
F(33)	21(1)	30(1)	34(1)	-1(1)	10(1)	-10(1)
F(34)	30(1)	28(1)	21(1)	2(1)	-6(1)	-5(1)
F(35)	24(1)	20(1)	30(1)	-2(1)	3(1)	0(1)
C(39)	15(2)	15(2)	15(2)	0(1)	3(1)	1(1)
C(40)	17(2)	16(2)	16(2)	0(1)	5(1)	2(1)
C(41)	16(2)	19(2)	25(2)	3(1)	8(1)	0(1)
C(42)	21(2)	19(2)	30(2)	5(2)	10(2)	0(2)
C(43)	21(2)	17(2)	28(2)	5(2)	9(2)	3(1)
C(44)	15(2)	16(2)	24(2)	0(1)	6(1)	1(1)
C(45)	17(2)	14(2)	17(2)	-2(1)	5(1)	0(1)
C(46)	16(2)	12(2)	14(2)	-1(1)	2(1)	1(1)
C(47)	22(2)	21(2)	62(3)	18(2)	13(2)	2(2)
C(48)	27(2)	21(2)	89(4)	9(2)	3(2)	-8(2)
F(49)	21(1)	33(1)	98(2)	21(2)	7(1)	-4(1)
F(50)	40(2)	36(2)	59(2)	-4(1)	0(1)	-12(1)
F(51)	41(2)	26(2)	132(3)	10(2)	0(2)	-14(1)
C(49)	30(2)	52(3)	75(4)	41(3)	26(3)	13(2)
F(46)	45(2)	100(3)	59(2)	44(2)	30(2)	24(2)
F(47)	41(2)	60(2)	69(2)	30(2)	34(2)	18(1)
F(48)	40(2)	65(2)	129(3)	63(2)	43(2)	6(2)
C(50)	23(2)	21(2)	38(2)	13(2)	15(2)	5(2)
C(51)	26(2)	33(2)	33(2)	14(2)	11(2)	10(2)
F(39)	37(1)	53(2)	36(1)	25(1)	9(1)	12(1)
F(40)	21(1)	40(1)	39(1)	13(1)	8(1)	6(1)
F(41)	33(1)	38(1)	30(1)	3(1)	7(1)	10(1)
C(52)	26(2)	18(2)	54(3)	8(2)	14(2)	4(2)
F(42)	48(2)	26(1)	76(2)	18(1)	22(2)	21(1)
F(43)	38(2)	22(1)	74(2)	-8(1)	18(1)	-7(1)
F(44)	34(1)	21(1)	50(2)	-1(1)	22(1)	1(1)
F(1)	18(1)	13(1)	29(1)	4(1)	3(1)	2(1)
F(2)	18(1)	16(1)	34(1)	8(1)	2(1)	0(1)
F(3)	12(1)	22(1)	28(1)	4(1)	3(1)	3(1)
F(4)	14(1)	19(1)	44(1)	6(1)	9(1)	0(1)
F(5)	15(1)	20(1)	47(1)	9(1)	7(1)	4(1)
F(6)	29(1)	14(1)	65(2)	6(1)	16(1)	1(1)
F(13)	30(1)	27(1)	58(2)	22(1)	9(1)	1(1)
F(20)	18(1)	17(1)	30(1)	10(1)	4(1)	1(1)
F(21)	16(1)	18(1)	26(1)	9(1)	5(1)	1(1)

F(22)	14(1)	24(1)	28(1)	8(1)	-2(1)	-4(1)
F(29)	14(1)	22(1)	25(1)	5(1)	5(1)	5(1)
F(36)	13(1)	17(1)	31(1)	3(1)	6(1)	2(1)
F(37)	14(1)	23(1)	41(1)	10(1)	8(1)	0(1)
F(38)	28(1)	35(1)	51(2)	27(1)	19(1)	7(1)
F(45)	26(1)	20(1)	86(2)	18(1)	14(1)	2(1)
C(1T)	40(7)	33(7)	22(5)	-12(4)	3(4)	4(5)
C(2T)	38(4)	32(4)	27(4)	-8(3)	2(3)	5(3)
C(3T)	43(5)	35(4)	34(4)	-10(3)	9(4)	-3(4)
C(4T)	37(5)	50(6)	36(5)	-14(4)	17(4)	-6(4)
C(5T)	34(5)	46(7)	28(5)	-10(5)	11(4)	6(5)
C(6T)	41(5)	37(4)	23(4)	-5(3)	3(3)	6(4)
C(7T)	35(4)	41(5)	35(4)	-2(4)	5(3)	2(4)
C(15T)	37(3)	56(3)	71(4)	27(3)	7(3)	2(2)
C(16T)	31(3)	75(4)	42(3)	9(3)	12(2)	4(2)
C(17T)	58(4)	71(4)	38(3)	12(3)	18(3)	40(3)
C(18T)	95(5)	35(3)	42(3)	0(2)	34(3)	16(3)
C(19T)	59(3)	53(3)	41(3)	-12(2)	14(3)	-16(3)
C(20T)	34(3)	60(4)	68(4)	23(3)	-4(3)	3(2)
C(21T)	75(6)	88(6)	225(13)	94(8)	2(7)	-18(5)
C(1D)	54(11)	32(9)	15(6)	-6(6)	8(6)	-16(8)
C(2D)	57(8)	45(7)	23(5)	-9(5)	8(5)	-16(6)
C(3D)	52(9)	57(10)	30(7)	-15(7)	21(7)	-26(8)
C(4D)	31(6)	62(8)	33(6)	-17(6)	5(5)	11(6)
C(5D)	44(6)	39(6)	25(5)	-12(4)	6(4)	7(5)
C(6D)	32(5)	28(5)	21(4)	-9(4)	7(4)	-6(4)
C(7D)	48(7)	47(8)	36(6)	1(5)	-13(5)	11(6)
C(1S)	216(17)	114(10)	310(30)	97(13)	210(20)	80(10)
C(2S)	107(7)	56(5)	156(10)	35(5)	29(7)	17(5)
C(3S)	124(7)	41(3)	84(5)	22(3)	27(5)	15(4)
C(4S)	149(8)	33(3)	98(6)	8(4)	31(6)	-9(4)
C(5S)	302(18)	41(4)	78(6)	-16(4)	59(8)	1(7)
C(6S)	510(40)	130(13)	350(30)	140(17)	360(30)	200(20)
C(7S)	190(16)	222(19)	250(20)	-104(16)	113(16)	-33(14)

Table Q.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **$NHAcF_{51}PcCu·3(toluene)·EtOAc$**.

	x	y	z	U(eq)
H(9)	-1836	6581	3438	21
H(10A)	-3187	6576	2655	38
H(10B)	-2678	6210	2748	38
H(10C)	-2966	6381	2114	38

H(2T)	3863	6111	6075	39
H(3T)	2693	5906	6031	45
H(4T)	1723	6291	5600	47
H(5T)	1922	6881	5211	42
H(6T)	3092	7086	5254	41
H(7T1)	4604	6786	6086	56
H(7T2)	4334	6982	5467	56
H(7T3)	4590	6548	5510	56
H(16T)	8508	6711	4720	59
H(17T)	8570	7335	4429	66
H(18T)	9662	7646	4598	65
H(19T)	10696	7333	5077	61
H(20T)	10630	6718	5389	68
H(21A)	9811	6082	5094	202
H(21B)	9025	6162	5186	202
H(21C)	9710	6236	5702	202
H(2D)	2917	6215	5794	50
H(3D)	1796	6501	5473	53
H(4D)	1711	7111	5071	51
H(5D)	2747	7434	4990	44
H(6D)	3868	7148	5310	32
H(7D1)	4172	6261	6056	71
H(7D2)	4549	6663	6017	71
H(7D3)	4397	6381	5475	71
H(2S)	3742	720	3559	128
H(3S)	2595	565	3664	99
H(4S)	1712	378	2859	111
H(5S)	1976	347	1949	165
H(6S)	3124	502	1844	349
H(7S1)	4619	648	2817	318
H(7S2)	4214	974	2395	318
H(7S3)	4220	546	2167	318
H(1F1)	9405	1385	2667	27
H(1F2)	10079	1271	2415	27
H(1F3)	10191	1386	3081	27
H(1G1)	9436	1413	2633	27
H(1G2)	10111	1299	2382	27
H(1G3)	10222	1414	3047	27
H(2G1)	10079	770	3283	66
H(2G2)	9284	773	2890	66

Appendix R: Crystal structure of [NMeAcF$_{51}$PcCu]$_2$·2.75(toluene)·0.5(acetone)

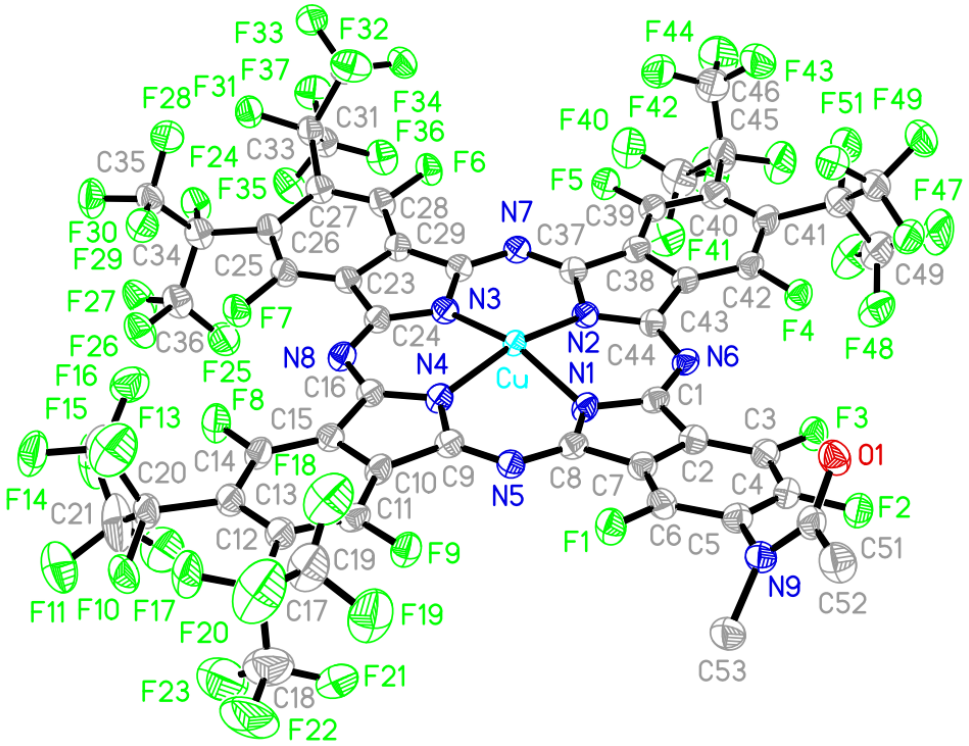


Figure R.1 ORTEP representation of **NMeAcF$_{51}$PcCu** X-ray crystal structure, at 50% probability.

Table R.1. Crystal data and structure refinement for **[NMeAcF$_{51}$PcCu]$_2$·2.75(toluene)·0.5(acetone)**.

Empirical formula	C147.50 H62 Cu2 F102 N18 O3	
Formula weight	4199.23	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	C2/c (No. 15)	
Unit cell dimensions	a = 19.6290(4) Å	α = 90°.
	b = 35.0085(7) Å	β = 105.590(1)°.
	c = 23.9878(5) Å	γ = 90°.
Volume	15877.5(6) Å^3	
Z	4	
Density (calculated)	1.757 g/cm^3	
Absorption coefficient	1.992 mm^{-1}	
F(000)	8292	
Crystal size	0.195 x 0.210 x 0.173 mm^3	

Theta range for data collection	2.524 to 69.826°.
Index ranges	-22<=h<=21, -41<=k<=40, -28<=l<=27
Reflections collected	74587
Independent reflections	14251 [R(int) = 0.0385]
Completeness to theta = 67.679°	98.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14251 / 127 / 1220
Goodness-of-fit on F^2	1.024
Final R indices [I>2sigma(I)]	R1 = 0.0791, wR2 = 0.2225
R indices (all data)	R1 = 0.0994, wR2 = 0.2423
Extinction coefficient	n/a
Largest diff. peak and hole	2.158 and -0.665 e.$Å^{-3}$

Table R.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **$[NMeAcF_{51}PcCu]_2$·2.75(toluene)·0.5(acetone)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu	2588(1)	2060(1)	1418(1)	22(1)
N(1)	3579(2)	2127(1)	1350(2)	29(1)
N(2)	2574(2)	2626(1)	1578(2)	28(1)
N(3)	1518(2)	2070(1)	1178(2)	29(1)
N(4)	2532(2)	1562(1)	995(2)	29(1)
O(1)	6973(2)	1887(1)	2737(1)	36(1)
N(5)	3782(2)	1476(1)	1099(2)	28(1)
N(6)	3823(2)	2758(1)	1761(2)	29(1)
N(7)	1344(2)	2692(1)	1561(2)	29(1)
N(8)	1273(2)	1445(1)	742(2)	31(1)
N(9)	6639(2)	1709(1)	1814(2)	33(1)
C(1)	4007(2)	2430(1)	1579(2)	27(1)
C(2)	4744(2)	2317(1)	1640(2)	30(1)
C(3)	5387(3)	2510(1)	1817(2)	32(1)
C(4)	5999(2)	2309(1)	1850(2)	32(1)
C(5)	6002(2)	1919(1)	1734(2)	32(1)
C(6)	5349(2)	1734(1)	1544(2)	32(1)
C(7)	4732(2)	1934(1)	1487(2)	30(1)
C(8)	3990(2)	1822(1)	1294(2)	28(1)
C(9)	3107(2)	1368(1)	942(2)	29(1)
C(10)	2867(2)	998(1)	672(2)	30(1)
C(11)	3208(2)	688(1)	520(2)	32(1)

C(12)	2862(3)	358(1)	279(2)	36(1)
C(13)	2108(3)	352(1)	153(2)	36(1)
C(14)	1777(2)	670(1)	305(2)	34(1)
C(15)	2144(2)	989(1)	567(2)	29(1)
C(16)	1936(2)	1351(1)	775(2)	29(1)
C(17)	3350(3)	28(2)	181(3)	52(2)
C(18)	3551(4)	65(2)	-355(3)	70(2)
F(21)	3871(2)	397(1)	-392(2)	85(1)
F(22)	3937(2)	-212(2)	-459(2)	99(2)
F(23)	2957(2)	65(1)	-802(2)	86(1)
C(19)	4058(3)	-43(2)	756(3)	59(2)
F(18)	3970(2)	65(1)	1215(2)	69(1)
F(19)	4621(2)	132(1)	642(2)	78(1)
F(20)	4196(2)	-417(1)	742(3)	93(2)
C(20)	1602(3)	26(1)	-138(2)	38(1)
C(21)	928(4)	147(2)	-628(3)	76(2)
F(11)	766(2)	-136(1)	-1028(2)	73(1)
F(12)	1009(2)	457(1)	-890(2)	70(1)
F(13)	358(2)	189(1)	-398(2)	79(1)
C(22)	1400(3)	-228(2)	330(3)	61(2)
F(14)	903(2)	-472(1)	75(2)	57(1)
F(15)	1960(2)	-419(1)	644(2)	73(1)
F(16)	1158(2)	-7(1)	684(1)	52(1)
C(23)	1091(2)	1774(1)	931(2)	29(1)
C(24)	373(2)	1872(1)	920(2)	30(1)
C(25)	-279(2)	1694(1)	697(2)	34(1)
C(26)	-902(2)	1834(1)	777(2)	34(1)
C(27)	-860(2)	2172(1)	1135(2)	33(1)
C(28)	-218(2)	2364(1)	1289(2)	33(1)
C(29)	393(2)	2224(1)	1185(2)	29(1)
C(30)	1124(2)	2355(1)	1329(2)	28(1)
C(31)	-1445(2)	2318(1)	1392(2)	36(1)
C(32)	-1204(3)	2401(2)	2064(2)	42(1)
F(32)	-682(2)	2173(1)	2328(1)	54(1)
F(33)	-1742(2)	2337(1)	2283(1)	51(1)
F(34)	-997(2)	2761(1)	2201(1)	51(1)
C(33)	-1862(3)	2662(2)	1079(2)	40(1)
F(35)	-2170(2)	2587(1)	524(1)	52(1)
F(36)	-1451(2)	2968(1)	1097(1)	48(1)
F(37)	-2371(2)	2761(1)	1321(2)	54(1)
C(34)	-1580(2)	1615(2)	443(2)	38(1)
C(35)	-1682(3)	1245(2)	745(2)	42(1)
F(28)	-1684(2)	1311(1)	1295(1)	50(1)
F(29)	-1182(2)	988(1)	767(1)	46(1)

F(30)	-2307(2)	1087(1)	475(2)	55(1)
C(36)	-1636(3)	1549(2)	-208(2)	43(1)
F(25)	-1293(2)	1799(1)	-429(1)	51(1)
F(26)	-1433(2)	1198(1)	-328(1)	48(1)
F(27)	-2323(2)	1566(1)	-522(1)	55(1)
C(37)	2007(2)	2809(1)	1676(2)	29(1)
C(38)	2252(2)	3178(1)	1941(2)	31(1)
C(39)	1914(3)	3479(1)	2126(2)	34(1)
C(40)	2267(3)	3804(1)	2384(2)	38(1)
C(41)	3026(3)	3809(1)	2503(2)	38(1)
C(42)	3344(3)	3512(1)	2278(2)	34(1)
C(43)	2971(2)	3198(1)	2005(2)	30(1)
C(44)	3167(2)	2842(1)	1766(2)	28(1)
C(45)	1795(3)	4127(2)	2508(3)	49(1)
C(46)	1554(3)	4057(2)	3053(3)	58(2)
F(42)	1228(2)	3736(1)	3054(2)	64(1)
F(43)	2123(2)	4053(1)	3522(2)	74(1)
F(44)	1143(2)	4342(1)	3130(2)	86(1)
C(47)	1112(3)	4217(2)	1974(3)	58(2)
F(39)	1002(2)	4587(1)	1957(2)	82(1)
F(40)	531(2)	4049(1)	2010(2)	62(1)
F(41)	1233(2)	4116(1)	1474(2)	64(1)
C(48)	3542(3)	4102(2)	2883(3)	46(1)
C(49)	3790(3)	4406(2)	2521(3)	57(2)
F(46)	3237(2)	4594(1)	2183(2)	73(1)
F(47)	4210(2)	4657(1)	2864(2)	78(1)
F(48)	4136(2)	4257(1)	2170(2)	56(1)
C(50)	4197(3)	3917(2)	3347(2)	48(1)
F(49)	4367(2)	4131(1)	3821(2)	65(1)
F(50)	4774(2)	3897(1)	3168(1)	53(1)
F(51)	4039(2)	3571(1)	3500(1)	51(1)
C(51)	7112(2)	1703(1)	2345(2)	33(1)
C(52)	7767(3)	1470(2)	2448(2)	42(1)
C(53)	6743(3)	1492(2)	1316(2)	42(1)
F(1)	5340(1)	1359(1)	1438(1)	37(1)
F(2)	6614(1)	2497(1)	1993(1)	38(1)
F(3)	5428(1)	2881(1)	1935(1)	36(1)
F(4)	4036(1)	3522(1)	2347(1)	36(1)
F(5)	1215(1)	3456(1)	2029(1)	40(1)
F(6)	-174(1)	2691(1)	1587(1)	37(1)
F(7)	-293(1)	1377(1)	386(1)	40(1)
F(8)	1077(1)	677(1)	197(1)	46(1)
F(9)	3914(1)	710(1)	632(1)	37(1)
F(10)	1930(2)	-219(1)	-424(2)	49(1)

F(17)	3036(2)	-323(1)	210(2)	59(1)
F(24)	-2169(1)	1834(1)	410(1)	45(1)
F(31)	-1940(1)	2041(1)	1366(1)	44(1)
F(38)	2148(2)	4466(1)	2574(2)	64(1)
F(45)	3216(2)	4296(1)	3228(2)	60(1)
C(1S)	3455(2)	3393(1)	669(2)	50(1)
C(2S)	3352(2)	3739(1)	919(2)	58(2)
C(3S)	2671(2)	3861(1)	897(2)	60(2)
C(4S)	2093(2)	3637(1)	625(2)	64(2)
C(5S)	2196(2)	3291(1)	375(2)	59(2)
C(6S)	2877(2)	3169(1)	397(2)	58(2)
C(7S)	4200(4)	3281(3)	687(3)	79(2)
C(1T)	4644(2)	1773(1)	5274(2)	66(2)
C(2T)	4023(2)	1960(1)	4991(2)	58(2)
C(3T)	4052(2)	2298(1)	4693(2)	57(2)
C(4T)	4702(2)	2448(1)	4678(2)	55(2)
C(5T)	5324(2)	2261(1)	4961(2)	61(2)
C(6T)	5295(2)	1924(1)	5259(2)	71(2)
C(7T)	4607(6)	1405(3)	5608(5)	105(3)
F(17')	2911(7)	-142(4)	-407(6)	35(3)
F(10')	1959(8)	-303(5)	-98(8)	42(4)
C(1F)	3443(4)	555(3)	2501(6)	80(4)
C(2F)	3356(5)	558(4)	3057(4)	74(5)
C(3F)	2690(7)	500(4)	3141(3)	74(4)
C(4F)	2110(5)	440(3)	2668(5)	70(4)
C(5F)	2197(5)	437(4)	2111(4)	75(5)
C(6F)	2864(6)	494(4)	2028(4)	62(4)
C(7F)	4071(12)	617(6)	2476(10)	122(7)
C(1Y)	2478(12)	456(6)	2877(9)	64(7)
C(2Y)	3196(13)	522(7)	3115(7)	61(9)
C(3Y)	3645(8)	550(8)	2757(11)	108(13)
C(4Y)	3377(12)	513(8)	2161(10)	91(10)
C(5Y)	2659(13)	447(8)	1923(6)	66(9)
C(6Y)	2210(8)	419(8)	2281(10)	91(12)
C(7Y)	1920(30)	423(11)	3200(20)	160(20)
C(1B)	9779(11)	1314(5)	2774(8)	19(5)
C(2B)	9668(7)	1008(4)	3092(7)	20(3)
C(3B)	9819(10)	641(5)	2928(8)	31(4)
O(1B)	9450(20)	1020(12)	3497(15)	240(30)
C(1A)	9933(12)	1265(4)	2713(9)	17(4)
C(2A)	9772(7)	893(4)	2896(6)	18(3)
C(3A)	9911(9)	580(3)	2546(7)	14(3)
O(1A)	9523(9)	830(5)	3332(7)	57(4)

Table R.3 Bond lengths [Å] and angles [°] for **[NMeAcF$_{51}$PcCu]$_2$·2.75(toluene)·0.5(acetone)**.

Cu-N(4)	2.005(4)	Cu-N(3)	2.022(4)
Cu-N(1)	2.009(4)	Cu-O(1)#1	2.068(3)
Cu-N(2)	2.018(4)		
N(1)-C(8)	1.366(6)	C(17)-C(18)	1.448(9)
N(1)-C(1)	1.372(6)	C(17)-C(19)	1.693(10)
N(2)-C(44)	1.359(6)	C(20)-C(22)	1.564(9)
N(2)-C(37)	1.360(6)	C(20)-C(21)	1.573(9)
N(3)-C(23)	1.364(6)	C(23)-C(24)	1.444(6)
N(3)-C(30)	1.370(6)	C(24)-C(29)	1.383(6)
N(4)-C(9)	1.354(6)	C(24)-C(25)	1.394(7)
N(4)-C(16)	1.365(6)	C(25)-C(26)	1.378(7)
O(1)-C(51)	1.229(6)	C(26)-C(27)	1.451(7)
O(1)-Cu#1	2.068(3)	C(26)-C(34)	1.558(7)
N(5)-C(8)	1.325(6)	C(27)-C(28)	1.387(7)
N(5)-C(9)	1.333(6)	C(27)-C(31)	1.530(6)
N(6)-C(1)	1.316(6)	C(28)-C(29)	1.378(6)
N(6)-C(44)	1.325(6)	C(29)-C(30)	1.457(6)
N(7)-C(37)	1.322(6)	C(31)-C(33)	1.535(7)
N(7)-C(30)	1.325(6)	C(31)-C(32)	1.579(7)
N(8)-C(23)	1.321(6)	C(34)-C(35)	1.525(8)
N(8)-C(16)	1.324(6)	C(34)-C(36)	1.554(8)
N(9)-C(51)	1.359(6)	C(37)-C(38)	1.464(6)
N(9)-C(5)	1.420(6)	C(38)-C(39)	1.379(7)
N(9)-C(53)	1.474(6)	C(38)-C(43)	1.381(7)
C(1)-C(2)	1.468(6)	C(39)-C(40)	1.387(7)
C(2)-C(7)	1.389(7)	C(40)-C(41)	1.440(7)
C(2)-C(3)	1.391(6)	C(40)-C(45)	1.541(7)
C(3)-C(4)	1.376(7)	C(41)-C(42)	1.393(7)
C(4)-C(5)	1.392(7)	C(41)-C(48)	1.554(7)
C(5)-C(6)	1.399(6)	C(42)-C(43)	1.383(7)
C(6)-C(7)	1.374(6)	C(43)-C(44)	1.465(6)
C(7)-C(8)	1.458(6)	C(45)-C(46)	1.527(9)
C(9)-C(10)	1.465(6)	C(45)-C(47)	1.617(9)
C(10)-C(15)	1.374(6)	C(48)-C(49)	1.530(8)
C(10)-C(11)	1.375(6)	C(48)-C(50)	1.594(9)
C(11)-C(12)	1.385(7)	C(51)-C(52)	1.487(7)
C(12)-C(13)	1.429(7)	C(52)-H(1)	0.9600
C(12)-C(17)	1.558(7)	C(52)-H(2)	0.9600
C(13)-C(14)	1.387(7)	C(52)-H(3)	0.9600
C(13)-C(20)	1.550(7)	C(53)-H(4)	0.9600
C(14)-C(15)	1.385(7)	C(53)-H(5)	0.9600
C(15)-C(16)	1.460(6)	C(53)-H(6)	0.9600

C(1S)-C(2S)	1.3900	C(5F)-C(6F)	1.3900
C(1S)-C(6S)	1.3900	C(5F)-H(5F)	0.9300
C(1S)-C(7S)	1.504(8)	C(6F)-H(6F)	0.9300
C(2S)-C(3S)	1.3900	C(7F)-H(7F1)	0.9600
C(2S)-H(2S)	0.9300	C(7F)-H(7F2)	0.9600
C(3S)-C(4S)	1.3900	C(7F)-H(7F3)	0.9600
C(3S)-H(3S)	0.9300	C(1Y)-C(2Y)	1.3900
C(4S)-C(5S)	1.3900	C(1Y)-C(6Y)	1.3900
C(4S)-H(4S)	0.9300	C(1Y)-C(7Y)	1.52(2)
C(5S)-C(6S)	1.3900	C(2Y)-C(3Y)	1.3900
C(5S)-H(5S)	0.9300	C(2Y)-H(2Y)	0.9300
C(6S)-H(6S)	0.9300	C(3Y)-C(4Y)	1.3900
C(7S)-H(7S1)	0.9600	C(3Y)-H(3Y)	0.9300
C(7S)-H(7S2)	0.9600	C(4Y)-C(5Y)	1.3900
C(7S)-H(7S3)	0.9600	C(4Y)-H(4Y)	0.9300
C(1T)-C(2T)	1.3900	C(5Y)-C(6Y)	1.3900
C(1T)-C(6T)	1.3900	C(5Y)-H(5Y)	0.9300
C(1T)-C(7T)	1.529(9)	C(6Y)-H(6Y)	0.9300
C(2T)-C(3T)	1.3900	C(7Y)-H(7Y1)	0.9600
C(2T)-H(2T)	0.9300	C(7Y)-H(7Y2)	0.9600
C(3T)-C(4T)	1.3900	C(7Y)-H(7Y3)	0.9600
C(3T)-H(3T)	0.9300	C(1B)-C(2B)	1.368(16)
C(4T)-C(5T)	1.3900	C(1B)-H(1B1)	0.9600
C(4T)-H(4T)	0.9300	C(1B)-H(1B2)	0.9600
C(5T)-C(6T)	1.3900	C(1B)-H(1B3)	0.9600
C(5T)-H(5T)	0.9300	C(2B)-O(1B)	1.16(2)
C(6T)-H(6T)	0.9300	C(2B)-C(3B)	1.399(16)
C(7T)-H(7T1)	0.9600	C(3B)-H(3B1)	0.9600
C(7T)-H(7T2)	0.9600	C(3B)-H(3B2)	0.9600
C(7T)-H(7T3)	0.9600	C(3B)-H(3B3)	0.9600
C(1F)-C(7F)	1.27(2)	C(1A)-C(2A)	1.437(15)
C(1F)-C(2F)	1.3900	C(1A)-H(1A1)	0.9600
C(1F)-C(6F)	1.3900	C(1A)-H(1A2)	0.9600
C(2F)-C(3F)	1.3900	C(1A)-H(1A3)	0.9600
C(2F)-H(2F)	0.9300	C(2A)-O(1A)	1.287(15)
C(3F)-C(4F)	1.3900	C(2A)-C(3A)	1.450(15)
C(3F)-H(3F)	0.9300	C(3A)-H(3A1)	0.9600
C(4F)-C(5F)	1.3900	C(3A)-H(3A2)	0.9600
C(4F)-H(4F)	0.9300	C(3A)-H(3A3)	0.9600
N(4)-Cu-N(1)	89.01(15)	N(1)-Cu-N(3)	158.20(16)
N(4)-Cu-N(2)	161.29(16)	N(2)-Cu-N(3)	88.42(15)
N(1)-Cu-N(2)	87.90(15)	N(4)-Cu-O(1)#1	101.10(15)
N(4)-Cu-N(3)	87.63(15)	N(1)-Cu-O(1)#1	87.47(14)

N(2)-Cu-O(1)#1	97.19(14)	N(3)-Cu-O(1)#1	114.32(14)
C(8)-N(1)-C(1)	109.1(4)	C(15)-C(10)-C(9)	107.2(4)
C(8)-N(1)-Cu	121.8(3)	C(11)-C(10)-C(9)	133.8(4)
C(1)-N(1)-Cu	124.1(3)	C(10)-C(11)-C(12)	123.4(4)
C(44)-N(2)-C(37)	110.3(4)	C(11)-C(12)-C(13)	117.7(4)
C(44)-N(2)-Cu	123.8(3)	C(11)-C(12)-C(17)	115.4(4)
C(37)-N(2)-Cu	123.4(3)	C(13)-C(12)-C(17)	126.8(4)
C(23)-N(3)-C(30)	110.1(4)	C(14)-C(13)-C(12)	117.6(4)
C(23)-N(3)-Cu	125.5(3)	C(14)-C(13)-C(20)	114.8(4)
C(30)-N(3)-Cu	123.6(3)	C(12)-C(13)-C(20)	127.6(4)
C(9)-N(4)-C(16)	109.9(4)	C(15)-C(14)-C(13)	123.0(4)
C(9)-N(4)-Cu	123.5(3)	C(10)-C(15)-C(14)	119.2(4)
C(16)-N(4)-Cu	126.3(3)	C(10)-C(15)-C(16)	106.6(4)
C(51)-O(1)-Cu#1	141.5(3)	C(14)-C(15)-C(16)	134.2(4)
C(8)-N(5)-C(9)	123.3(4)	N(8)-C(16)-N(4)	128.0(4)
C(1)-N(6)-C(44)	123.4(4)	N(8)-C(16)-C(15)	123.8(4)
C(37)-N(7)-C(30)	123.8(4)	N(4)-C(16)-C(15)	108.3(4)
C(23)-N(8)-C(16)	123.2(4)	C(18)-C(17)-C(12)	113.2(5)
C(51)-N(9)-C(5)	119.2(4)	C(18)-C(17)-C(19)	112.1(5)
C(51)-N(9)-C(53)	122.9(4)	C(12)-C(17)-C(19)	112.9(5)
C(5)-N(9)-C(53)	117.8(4)	C(13)-C(20)-C(22)	110.6(4)
N(6)-C(1)-N(1)	127.9(4)	C(13)-C(20)-C(21)	116.5(4)
N(6)-C(1)-C(2)	123.5(4)	C(22)-C(20)-C(21)	111.4(5)
N(1)-C(1)-C(2)	108.4(4)	N(8)-C(23)-N(3)	128.3(4)
C(7)-C(2)-C(3)	119.9(4)	N(8)-C(23)-C(24)	123.6(4)
C(7)-C(2)-C(1)	106.6(4)	N(3)-C(23)-C(24)	108.1(4)
C(3)-C(2)-C(1)	133.5(4)	C(29)-C(24)-C(25)	119.0(4)
C(4)-C(3)-C(2)	118.5(4)	C(29)-C(24)-C(23)	107.3(4)
C(3)-C(4)-C(5)	122.6(4)	C(25)-C(24)-C(23)	133.7(4)
C(4)-C(5)-C(6)	117.8(4)	C(26)-C(25)-C(24)	123.0(4)
C(4)-C(5)-N(9)	122.2(4)	C(25)-C(26)-C(27)	117.5(4)
C(6)-C(5)-N(9)	119.9(4)	C(25)-C(26)-C(34)	114.9(4)
C(7)-C(6)-C(5)	120.1(4)	C(27)-C(26)-C(34)	127.6(4)
C(6)-C(7)-C(2)	120.9(4)	C(28)-C(27)-C(26)	117.1(4)
C(6)-C(7)-C(8)	132.4(4)	C(28)-C(27)-C(31)	117.2(4)
C(2)-C(7)-C(8)	106.8(4)	C(26)-C(27)-C(31)	125.6(4)
N(5)-C(8)-N(1)	128.0(4)	C(29)-C(28)-C(27)	123.5(4)
N(5)-C(8)-C(7)	123.0(4)	C(28)-C(29)-C(24)	118.8(4)
N(1)-C(8)-C(7)	109.0(4)	C(28)-C(29)-C(30)	134.0(4)
N(5)-C(9)-N(4)	128.4(4)	C(24)-C(29)-C(30)	107.1(4)
N(5)-C(9)-C(10)	123.6(4)	N(7)-C(30)-N(3)	128.0(4)
N(4)-C(9)-C(10)	108.0(4)	N(7)-C(30)-C(29)	124.6(4)
C(15)-C(10)-C(11)	119.0(4)	N(3)-C(30)-C(29)	107.4(4)

C(27)-C(31)-C(33)	115.2(4)	N(9)-C(53)-H(6)	109.5
C(27)-C(31)-C(32)	114.9(4)	H(4)-C(53)-H(6)	109.5
C(33)-C(31)-C(32)	109.2(4)	H(5)-C(53)-H(6)	109.5
C(35)-C(34)-C(36)	111.6(4)	C(2S)-C(1S)-C(6S)	120.0
C(35)-C(34)-C(26)	112.2(4)	C(2S)-C(1S)-C(7S)	117.8(4)
C(36)-C(34)-C(26)	114.2(4)	C(6S)-C(1S)-C(7S)	122.1(4)
N(7)-C(37)-N(2)	128.5(4)	C(3S)-C(2S)-C(1S)	120.0
N(7)-C(37)-C(38)	123.8(4)	C(3S)-C(2S)-H(2S)	120.0
N(2)-C(37)-C(38)	107.7(4)	C(1S)-C(2S)-H(2S)	120.0
C(39)-C(38)-C(43)	119.6(4)	C(2S)-C(3S)-C(4S)	120.0
C(39)-C(38)-C(37)	133.1(4)	C(2S)-C(3S)-H(3S)	120.0
C(43)-C(38)-C(37)	107.3(4)	C(4S)-C(3S)-H(3S)	120.0
C(38)-C(39)-C(40)	122.9(5)	C(5S)-C(4S)-C(3S)	120.0
C(39)-C(40)-C(41)	117.7(4)	C(5S)-C(4S)-H(4S)	120.0
C(39)-C(40)-C(45)	115.7(4)	C(3S)-C(4S)-H(4S)	120.0
C(41)-C(40)-C(45)	126.6(4)	C(4S)-C(5S)-C(6S)	120.0
C(42)-C(41)-C(40)	117.5(4)	C(4S)-C(5S)-H(5S)	120.0
C(42)-C(41)-C(48)	115.5(4)	C(6S)-C(5S)-H(5S)	120.0
C(40)-C(41)-C(48)	127.0(4)	C(5S)-C(6S)-C(1S)	120.0
C(43)-C(42)-C(41)	122.8(4)	C(5S)-C(6S)-H(6S)	120.0
C(38)-C(43)-C(42)	119.1(4)	C(1S)-C(6S)-H(6S)	120.0
C(38)-C(43)-C(44)	106.4(4)	C(1S)-C(7S)-H(7S1)	109.5
C(42)-C(43)-C(44)	134.4(4)	C(1S)-C(7S)-H(7S2)	109.5
N(6)-C(44)-N(2)	128.5(4)	H(7S1)-C(7S)-H(7S2)	109.5
N(6)-C(44)-C(43)	123.3(4)	C(1S)-C(7S)-H(7S3)	109.5
N(2)-C(44)-C(43)	108.2(4)	H(7S1)-C(7S)-H(7S3)	109.5
C(46)-C(45)-C(40)	112.7(5)	H(7S2)-C(7S)-H(7S3)	109.5
C(46)-C(45)-C(47)	109.1(5)	C(2T)-C(1T)-C(6T)	120.0
C(40)-C(45)-C(47)	113.9(5)	C(2T)-C(1T)-C(7T)	119.6(5)
C(49)-C(48)-C(41)	112.5(5)	C(6T)-C(1T)-C(7T)	120.4(5)
C(49)-C(48)-C(50)	111.0(5)	C(3T)-C(2T)-C(1T)	120.0
C(41)-C(48)-C(50)	114.6(4)	C(3T)-C(2T)-H(2T)	120.0
O(1)-C(51)-N(9)	118.2(4)	C(1T)-C(2T)-H(2T)	120.0
O(1)-C(51)-C(52)	121.4(4)	C(2T)-C(3T)-C(4T)	120.0
N(9)-C(51)-C(52)	120.4(4)	C(2T)-C(3T)-H(3T)	120.0
C(51)-C(52)-H(1)	109.5	C(4T)-C(3T)-H(3T)	120.0
C(51)-C(52)-H(2)	109.5	C(3T)-C(4T)-C(5T)	120.0
H(1)-C(52)-H(2)	109.5	C(3T)-C(4T)-H(4T)	120.0
C(51)-C(52)-H(3)	109.5	C(5T)-C(4T)-H(4T)	120.0
H(1)-C(52)-H(3)	109.5	C(6T)-C(5T)-C(4T)	120.0
H(2)-C(52)-H(3)	109.5	C(6T)-C(5T)-H(5T)	120.0
N(9)-C(53)-H(4)	109.5	C(4T)-C(5T)-H(5T)	120.0
N(9)-C(53)-H(5)	109.5	C(5T)-C(6T)-C(1T)	120.0
H(4)-C(53)-H(5)	109.5	C(5T)-C(6T)-H(6T)	120.0

C(1T)-C(6T)-H(6T)	120.0	C(4Y)-C(5Y)-C(6Y)	120.0
C(1T)-C(7T)-H(7T1)	109.5	C(4Y)-C(5Y)-H(5Y)	120.0
C(1T)-C(7T)-H(7T2)	109.5	C(6Y)-C(5Y)-H(5Y)	120.0
H(7T1)-C(7T)-H(7T2)	109.5	C(5Y)-C(6Y)-C(1Y)	120.0
C(1T)-C(7T)-H(7T3)	109.5	C(5Y)-C(6Y)-H(6Y)	120.0
H(7T1)-C(7T)-H(7T3)	109.5	C(1Y)-C(6Y)-H(6Y)	120.0
H(7T2)-C(7T)-H(7T3)	109.5	C(1Y)-C(7Y)-H(7Y1)	109.5
C(7F)-C(1F)-C(2F)	114.5(14)	C(1Y)-C(7Y)-H(7Y2)	109.5
C(7F)-C(1F)-C(6F)	125.5(14)	H(7Y1)-C(7Y)-H(7Y2)	109.5
C(2F)-C(1F)-C(6F)	120.0	C(1Y)-C(7Y)-H(7Y3)	109.5
C(1F)-C(2F)-C(3F)	120.0	H(7Y1)-C(7Y)-H(7Y3)	109.5
C(1F)-C(2F)-H(2F)	120.0	H(7Y2)-C(7Y)-H(7Y3)	109.5
C(3F)-C(2F)-H(2F)	120.0	C(2B)-C(1B)-H(1B1)	109.5
C(2F)-C(3F)-C(4F)	120.0	C(2B)-C(1B)-H(1B2)	109.5
C(2F)-C(3F)-H(3F)	120.0	H(1B1)-C(1B)-H(1B2)	109.5
C(4F)-C(3F)-H(3F)	120.0	C(2B)-C(1B)-H(1B3)	109.5
C(5F)-C(4F)-C(3F)	120.0	H(1B1)-C(1B)-H(1B3)	109.5
C(5F)-C(4F)-H(4F)	120.0	H(1B2)-C(1B)-H(1B3)	109.5
C(3F)-C(4F)-H(4F)	120.0	O(1B)-C(2B)-C(1B)	126(2)
C(6F)-C(5F)-C(4F)	120.0	O(1B)-C(2B)-C(3B)	115(2)
C(6F)-C(5F)-H(5F)	120.0	C(1B)-C(2B)-C(3B)	119.1(17)
C(4F)-C(5F)-H(5F)	120.0	C(2B)-C(3B)-H(3B1)	109.5
C(5F)-C(6F)-C(1F)	120.0	C(2B)-C(3B)-H(3B2)	109.5
C(5F)-C(6F)-H(6F)	120.0	H(3B1)-C(3B)-H(3B2)	109.5
C(1F)-C(6F)-H(6F)	120.0	C(2B)-C(3B)-H(3B3)	109.5
C(1F)-C(7F)-H(7F1)	109.5	H(3B1)-C(3B)-H(3B3)	109.5
C(1F)-C(7F)-H(7F2)	109.5	H(3B2)-C(3B)-H(3B3)	109.5
H(7F1)-C(7F)-H(7F2)	109.5	C(2A)-C(1A)-H(1A1)	109.5
C(1F)-C(7F)-H(7F3)	109.5	C(2A)-C(1A)-H(1A2)	109.5
H(7F1)-C(7F)-H(7F3)	109.5	H(1A1)-C(1A)-H(1A2)	109.5
H(7F2)-C(7F)-H(7F3)	109.5	C(2A)-C(1A)-H(1A3)	109.5
C(2Y)-C(1Y)-C(6Y)	120.0	H(1A1)-C(1A)-H(1A3)	109.5
C(2Y)-C(1Y)-C(7Y)	127(3)	H(1A2)-C(1A)-H(1A3)	109.5
C(6Y)-C(1Y)-C(7Y)	113(3)	O(1A)-C(2A)-C(1A)	124.5(16)
C(3Y)-C(2Y)-C(1Y)	120.0	O(1A)-C(2A)-C(3A)	121.0(13)
C(3Y)-C(2Y)-H(2Y)	120.0	C(1A)-C(2A)-C(3A)	114.6(13)
C(1Y)-C(2Y)-H(2Y)	120.0	C(2A)-C(3A)-H(3A1)	109.5
C(4Y)-C(3Y)-C(2Y)	120.0	C(2A)-C(3A)-H(3A2)	109.5
C(4Y)-C(3Y)-H(3Y)	120.0	H(3A1)-C(3A)-H(3A2)	109.5
C(2Y)-C(3Y)-H(3Y)	120.0	C(2A)-C(3A)-H(3A3)	109.5
C(3Y)-C(4Y)-C(5Y)	120.0	H(3A1)-C(3A)-H(3A3)	109.5
C(3Y)-C(4Y)-H(4Y)	120.0	H(3A2)-C(3A)-H(3A3)	109.5
C(5Y)-C(4Y)-H(4Y)	120.0		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,y,-z+1/2

Table R.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[NMeAcF$_{51}$PcCu]$_2$·2.75(toluene)·0.5(acetone)**. 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}
Cu	20(1)	15(1)	31(1)	0(1)	9(1)	2(1)
N(1)	31(2)	18(2)	40(2)	2(2)	14(2)	-1(1)
N(2)	32(2)	22(2)	34(2)	-3(2)	13(2)	1(2)
N(3)	30(2)	25(2)	34(2)	-1(2)	12(2)	3(2)
N(4)	28(2)	22(2)	39(2)	1(2)	12(2)	2(2)
O(1)	34(2)	33(2)	39(2)	-8(2)	8(1)	1(1)
N(5)	28(2)	23(2)	34(2)	-4(2)	11(2)	2(1)
N(6)	33(2)	24(2)	31(2)	2(2)	13(2)	-3(2)
N(7)	29(2)	25(2)	35(2)	0(2)	10(2)	4(2)
N(8)	28(2)	27(2)	41(2)	1(2)	13(2)	2(2)
N(9)	30(2)	31(2)	40(2)	-9(2)	12(2)	1(2)
C(1)	31(2)	24(2)	30(2)	5(2)	13(2)	0(2)
C(2)	33(2)	27(2)	31(2)	2(2)	9(2)	1(2)
C(3)	38(3)	28(2)	31(2)	2(2)	11(2)	-4(2)
C(4)	29(2)	34(3)	35(2)	-4(2)	10(2)	-7(2)
C(5)	31(2)	32(2)	35(2)	-2(2)	12(2)	0(2)
C(6)	34(2)	27(2)	33(2)	-4(2)	8(2)	0(2)
C(7)	31(2)	29(2)	32(2)	0(2)	11(2)	1(2)
C(8)	27(2)	26(2)	31(2)	2(2)	11(2)	3(2)
C(9)	31(2)	23(2)	35(2)	2(2)	12(2)	3(2)
C(10)	30(2)	20(2)	42(3)	2(2)	15(2)	0(2)
C(11)	33(2)	26(2)	41(3)	3(2)	19(2)	3(2)
C(12)	38(3)	26(2)	46(3)	-4(2)	18(2)	0(2)
C(13)	36(3)	25(2)	49(3)	-5(2)	18(2)	0(2)
C(14)	31(2)	27(2)	47(3)	0(2)	15(2)	-2(2)
C(15)	29(2)	24(2)	37(2)	-1(2)	14(2)	2(2)
C(16)	32(2)	21(2)	35(2)	0(2)	13(2)	2(2)
C(17)	45(3)	29(3)	90(4)	-23(3)	34(3)	-3(2)
C(18)	71(5)	73(5)	79(5)	-5(4)	40(4)	13(4)
F(21)	77(3)	119(4)	76(3)	-34(3)	51(2)	-42(3)
F(22)	73(3)	122(4)	114(4)	-58(3)	44(3)	19(3)
F(23)	89(3)	97(3)	78(3)	-22(3)	30(3)	1(3)
C(19)	55(4)	28(3)	100(5)	2(3)	31(4)	10(2)
F(18)	62(2)	56(2)	91(3)	20(2)	25(2)	12(2)
F(19)	52(2)	58(2)	132(4)	-14(2)	38(2)	4(2)
F(20)	77(3)	35(2)	181(5)	16(3)	59(3)	22(2)
C(20)	39(3)	23(2)	58(3)	-9(2)	19(2)	-3(2)
C(21)	85(5)	41(4)	80(5)	5(4)	-15(4)	-20(3)

F(11)	73(2)	66(2)	67(2)	-14(2)	-5(2)	-15(2)
F(12)	89(3)	50(2)	68(2)	16(2)	19(2)	7(2)
F(13)	38(2)	50(2)	141(4)	-27(2)	10(2)	-2(2)
C(22)	56(4)	46(4)	81(5)	-3(3)	19(3)	-2(3)
F(14)	54(2)	33(2)	88(2)	-3(2)	27(2)	-13(1)
F(15)	66(2)	58(2)	96(3)	21(2)	23(2)	9(2)
F(16)	52(2)	48(2)	64(2)	-2(2)	30(2)	2(2)
C(23)	30(2)	25(2)	34(2)	-1(2)	10(2)	1(2)
C(24)	27(2)	30(2)	33(2)	-3(2)	9(2)	4(2)
C(25)	34(2)	27(2)	42(3)	-6(2)	13(2)	2(2)
C(26)	27(2)	31(2)	42(3)	-5(2)	7(2)	1(2)
C(27)	29(2)	30(2)	40(3)	-2(2)	8(2)	7(2)
C(28)	30(2)	29(2)	38(3)	-6(2)	5(2)	6(2)
C(29)	27(2)	24(2)	36(2)	-1(2)	8(2)	4(2)
C(30)	26(2)	25(2)	34(2)	1(2)	9(2)	6(2)
C(31)	29(2)	34(3)	45(3)	-9(2)	11(2)	1(2)
C(32)	34(3)	46(3)	48(3)	-8(2)	14(2)	3(2)
F(32)	51(2)	65(2)	45(2)	0(2)	13(1)	17(2)
F(33)	44(2)	61(2)	56(2)	-16(2)	24(2)	-8(2)
F(34)	51(2)	52(2)	53(2)	-21(2)	20(2)	-9(2)
C(33)	33(3)	41(3)	48(3)	-9(2)	11(2)	4(2)
F(35)	49(2)	50(2)	50(2)	-8(2)	-2(1)	10(2)
F(36)	44(2)	37(2)	59(2)	-4(1)	9(1)	10(1)
F(37)	40(2)	56(2)	72(2)	-4(2)	23(2)	17(1)
C(34)	25(2)	38(3)	50(3)	-9(2)	8(2)	7(2)
C(35)	37(3)	41(3)	52(3)	-17(2)	16(2)	-2(2)
F(28)	51(2)	47(2)	60(2)	-10(2)	26(2)	-2(1)
F(29)	47(2)	34(2)	63(2)	-6(1)	24(2)	4(1)
F(30)	37(2)	50(2)	77(2)	-16(2)	13(2)	-12(1)
C(36)	37(3)	39(3)	52(3)	-8(2)	8(2)	8(2)
F(25)	58(2)	46(2)	47(2)	-3(2)	12(2)	-4(2)
F(26)	42(2)	44(2)	54(2)	-15(1)	6(1)	7(1)
F(27)	40(2)	58(2)	57(2)	-20(2)	-5(1)	11(2)
C(37)	34(2)	21(2)	32(2)	4(2)	11(2)	4(2)
C(38)	35(2)	26(2)	35(2)	4(2)	13(2)	1(2)
C(39)	39(3)	24(2)	40(3)	-2(2)	16(2)	2(2)
C(40)	44(3)	29(3)	46(3)	-4(2)	19(2)	3(2)
C(41)	45(3)	25(2)	49(3)	-4(2)	20(2)	-7(2)
C(42)	36(3)	27(2)	42(3)	-2(2)	17(2)	-3(2)
C(43)	35(2)	25(2)	33(2)	1(2)	13(2)	1(2)
C(44)	34(2)	19(2)	31(2)	3(2)	10(2)	0(2)
C(45)	47(3)	29(3)	75(4)	-18(3)	24(3)	-3(2)
C(46)	55(4)	51(4)	78(4)	-23(3)	35(3)	-1(3)
F(42)	64(2)	65(2)	76(2)	-24(2)	40(2)	-14(2)

F(43)	63(2)	96(3)	68(2)	-33(2)	28(2)	-15(2)
F(44)	74(3)	81(3)	119(4)	-50(3)	52(3)	1(2)
C(47)	62(4)	32(3)	84(5)	-9(3)	25(3)	14(3)
F(39)	78(3)	31(2)	136(4)	-4(2)	28(3)	18(2)
F(40)	47(2)	44(2)	98(3)	-17(2)	24(2)	9(2)
F(41)	72(2)	44(2)	74(2)	9(2)	19(2)	12(2)
C(48)	54(3)	30(3)	61(3)	-18(2)	29(3)	-7(2)
C(49)	62(4)	28(3)	91(5)	-11(3)	37(4)	-4(3)
F(46)	75(3)	33(2)	120(3)	12(2)	42(2)	7(2)
F(47)	82(3)	38(2)	122(3)	-30(2)	43(2)	-30(2)
F(48)	65(2)	31(2)	82(2)	2(2)	38(2)	-3(1)
C(50)	48(3)	48(3)	54(3)	-20(3)	23(3)	-11(3)
F(49)	60(2)	73(2)	66(2)	-36(2)	23(2)	-18(2)
F(50)	45(2)	55(2)	63(2)	-16(2)	24(2)	-12(2)
F(51)	55(2)	52(2)	49(2)	-5(2)	18(2)	-10(2)
C(51)	33(2)	26(2)	41(3)	-6(2)	12(2)	-6(2)
C(52)	38(3)	37(3)	49(3)	-7(2)	8(2)	6(2)
C(53)	37(3)	47(3)	44(3)	-13(2)	15(2)	0(2)
F(1)	34(1)	24(1)	53(2)	-7(1)	13(1)	1(1)
F(2)	31(1)	35(2)	47(2)	-7(1)	11(1)	-5(1)
F(3)	37(2)	26(1)	46(2)	-4(1)	12(1)	-4(1)
F(4)	35(1)	27(1)	49(2)	-5(1)	17(1)	-4(1)
F(5)	34(2)	31(2)	59(2)	-9(1)	19(1)	2(1)
F(6)	30(1)	30(1)	50(2)	-14(1)	10(1)	4(1)
F(7)	32(1)	35(2)	54(2)	-16(1)	14(1)	1(1)
F(8)	31(1)	33(2)	76(2)	-15(2)	18(1)	-2(1)
F(9)	28(1)	27(1)	59(2)	-5(1)	19(1)	1(1)
F(10)	50(2)	31(2)	68(3)	-19(2)	21(2)	-4(2)
F(17)	47(2)	23(2)	115(4)	-22(2)	37(2)	-3(2)
F(24)	27(1)	45(2)	59(2)	-15(1)	7(1)	7(1)
F(31)	32(2)	45(2)	59(2)	-15(1)	18(1)	-4(1)
F(38)	62(2)	27(2)	110(3)	-20(2)	34(2)	-2(1)
F(45)	56(2)	51(2)	82(2)	-36(2)	34(2)	-10(2)
C(1S)	61(4)	44(3)	43(3)	12(3)	12(3)	-1(3)
C(2S)	67(4)	57(4)	51(3)	13(3)	18(3)	-9(3)
C(3S)	82(5)	46(4)	55(4)	11(3)	22(3)	2(3)
C(4S)	69(4)	66(4)	62(4)	20(3)	26(3)	3(3)
C(5S)	62(4)	64(4)	53(4)	15(3)	22(3)	-8(3)
C(6S)	76(4)	48(4)	50(3)	11(3)	19(3)	-1(3)
C(7S)	73(5)	92(6)	72(5)	18(4)	20(4)	1(4)
C(1T)	67(4)	63(4)	62(4)	8(3)	11(3)	-2(3)
C(2T)	50(3)	71(4)	52(3)	-7(3)	13(3)	-9(3)
C(3T)	48(3)	70(4)	51(3)	-6(3)	8(3)	0(3)
C(4T)	65(4)	56(4)	46(3)	-6(3)	20(3)	2(3)

C(5T)	45(3)	70(4)	69(4)	-10(3)	15(3)	-3(3)
C(6T)	54(4)	62(4)	93(5)	4(4)	12(4)	8(3)
C(7T)	114(8)	83(6)	116(8)	37(6)	28(6)	-4(5)

Table R.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **[NMeAcF$_{51}$PcCu]$_2$·2.75(toluene)·0.5(acetone)**.

	x	y	z	U(eq)
H(1)	8080	1535	2817	63
H(2)	7996	1520	2149	63
H(3)	7648	1204	2445	63
H(4)	7055	1631	1143	63
H(5)	6295	1456	1037	63
H(6)	6947	1248	1446	63
H(2S)	3739	3889	1101	69
H(3S)	2603	4092	1064	72
H(4S)	1638	3718	610	77
H(5S)	1809	3141	193	70
H(6S)	2945	2938	230	69
H(7S1)	4466	3241	1081	119
H(7S2)	4417	3482	521	119
H(7S3)	4194	3050	471	119
H(2T)	3588	1860	5001	69
H(3T)	3636	2423	4504	68
H(4T)	4722	2674	4479	66
H(5T)	5759	2362	4951	73
H(6T)	5710	1798	5449	86
H(7T1)	4881	1210	5489	157
H(7T2)	4123	1324	5530	157
H(7T3)	4792	1451	6015	157
H(2F)	3744	598	3374	89
H(3F)	2632	502	3513	89
H(4F)	1664	401	2723	84
H(5F)	1809	396	1795	89
H(6F)	2922	492	1656	74
H(7F1)	4393	569	2849	183
H(7F2)	4114	877	2367	183
H(7F3)	4180	450	2195	183
H(2Y)	3375	547	3513	73
H(3Y)	4126	594	2916	129
H(4Y)	3678	532	1922	109

H(5Y)	2480	422	1525	79
H(6Y)	1729	375	2122	109
H(7Y1)	1566	618	3070	247
H(7Y2)	2130	454	3608	247
H(7Y3)	1696	176	3131	247
H(1B1)	9338	1393	2516	29
H(1B2)	10102	1244	2554	29
H(1B3)	9975	1521	3030	29
H(3B1)	9386	500	2789	46
H(3B2)	10119	511	3256	46
H(3B3)	10056	659	2628	46
H(1A1)	9545	1435	2700	25
H(1A2)	10010	1247	2335	25
H(1A3)	10353	1362	2981	25
H(3A1)	10230	402	2787	21
H(3A2)	10119	678	2256	21
H(3A3)	9475	453	2362	21

Appendix S: Crystal structure of [NHAcF$_{51}$PcCo]$_2$·7(toluene)

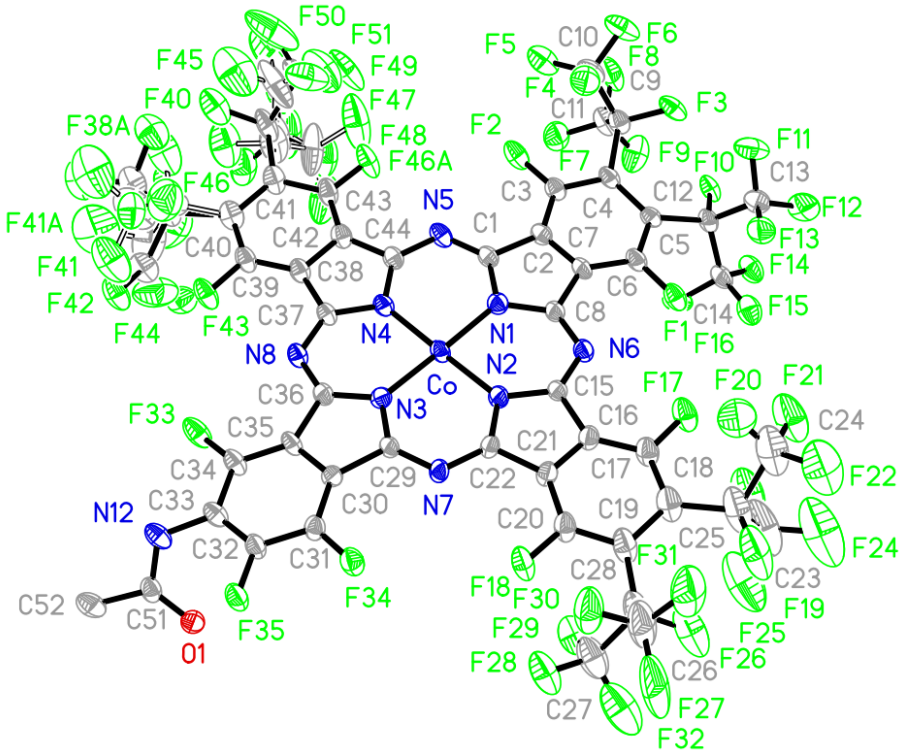


Figure S.1 ORTEP representation of **NHAcF$_{51}$PcCo** X-ray crystal structure, at 50% probability.

Table S.1 Crystal data and structure refinement for **[NHAcF$_{51}$PcCo]$_2$·7(toluene)**.

Empirical formula	C153 H64 Co2 F102 N18 O2	
Formula weight	4242.08	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 19.2390(12) Å	alpha = 90 deg.
	b = 35.295(2) Å	beta = 104.0908(13) deg.
	c = 23.6688(15) Å	gamma = 90 deg.
Volume	15588.3(17) Å^3	
Z, Calculated density	4, 1.808 g/cm^3	
Absorption coefficient	0.397 mm^{-1}	
F(000)	8384	
Crystal size	0.610 x 0.380 x 0.120 mm	
Theta range for data collection	1.356 to 33.389 deg.	
Limiting indices	-29<=h<=28, -53<=k<=54, -36<=l<=36	
Reflections collected / unique	238645 / 29305 [R(int) = 0.0402]	
Completeness to theta = 25.000	99.90%	

Absorption correction	Empirical
Max. and min. transmission	0.7466 and 0.7085
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	29305 / 10 / 1304
Goodness-of-fit on F2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0512, wR2 = 0.1229
R indices (all data)	R1 = 0.0865, wR2 = 0.1450
Extinction coefficient	n/a
Largest diff. peak and hole	1.382 and -0.788 $e.A^{-3}$

Table S.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **$[NHAcF_{51}PcCo]_2 \cdot 7$(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7592(1)	2918(1)	6302(1)	14(1)
N(1)	6567(1)	2938(1)	6179(1)	16(1)
N(2)	7588(1)	2397(1)	6544(1)	15(1)
N(3)	8605(1)	2886(1)	6366(1)	15(1)
N(4)	7586(1)	3428(1)	6021(1)	16(1)
N(5)	6315(1)	3570(1)	5781(1)	18(1)
N(6)	6330(1)	2314(1)	6519(1)	16(1)
N(7)	8852(1)	2249(1)	6742(1)	16(1)
N(8)	8858(1)	3530(1)	6130(1)	17(1)
N(12)	11728(1)	3281(1)	6873(1)	21(1)
O	12069(1)	3073(1)	7791(1)	22(1)
C(1)	6130(1)	3237(1)	5950(1)	17(1)
C(2)	5392(1)	3141(1)	5939(1)	17(1)
C(3)	4739(1)	3321(1)	5731(1)	19(1)
C(4)	4094(1)	3169(1)	5791(1)	17(1)
C(5)	4124(1)	2822(1)	6127(1)	18(1)
C(6)	4778(1)	2635(1)	6284(1)	18(1)
C(7)	5404(1)	2785(1)	6186(1)	17(1)
C(8)	6142(1)	2656(1)	6315(1)	16(1)
C(9)	3410(1)	3366(1)	5440(1)	20(1)
C(10)	3408(1)	3454(1)	4785(1)	26(1)
C(11)	3207(1)	3729(1)	5733(1)	27(1)
C(12)	3521(1)	2660(1)	6383(1)	19(1)
C(13)	3137(1)	2308(1)	6064(1)	23(1)
C(14)	3757(1)	2576(1)	7060(1)	22(1)
C(15)	7001(1)	2202(1)	6623(1)	15(1)
C(16)	7225(1)	1833(1)	6873(1)	17(1)
C(17)	6858(1)	1528(1)	7025(1)	21(1)
C(18)	7200(1)	1200(1)	7275(1)	24(1)

C(19)	7973(1)	1196(1)	7408(1)	23(1)
C(20)	8320(1)	1498(1)	7212(1)	19(1)
C(21)	7959(1)	1814(1)	6946(1)	17(1)
C(22)	8177(1)	2171(1)	6730(1)	15(1)
C(23)	6698(1)	869(1)	7344(1)	37(1)
C(24)	6065(1)	794(1)	6784(2)	52(1)
C(25)	6395(1)	909(1)	7888(2)	56(1)
C(26)	8465(1)	898(1)	7788(1)	28(1)
C(27)	9097(1)	1074(1)	8271(1)	32(1)
C(28)	8752(1)	601(1)	7423(1)	36(1)
C(29)	9038(1)	2581(1)	6574(1)	16(1)
C(30)	9786(1)	2684(1)	6636(1)	16(1)
C(31)	10425(1)	2489(1)	6820(1)	17(1)
C(32)	11063(1)	2686(1)	6876(1)	18(1)
C(33)	11079(1)	3076(1)	6766(1)	19(1)
C(34)	10429(1)	3259(1)	6550(1)	19(1)
C(35)	9791(1)	3067(1)	6486(1)	17(1)
C(36)	9042(1)	3183(1)	6308(1)	16(1)
C(37)	8177(1)	3635(1)	5985(1)	16(1)
C(38)	7954(1)	4008(1)	5749(1)	18(1)
C(39)	8316(1)	4323(1)	5625(1)	20(1)
C(40)	7971(1)	4656(1)	5393(1)	22(1)
C(41)	7195(1)	4657(1)	5245(1)	23(1)
C(42)	6851(1)	4338(1)	5394(1)	21(1)
C(43)	7216(1)	4018(1)	5644(1)	18(1)
C(44)	6991(1)	3654(1)	5818(1)	17(1)
C(45)	6694(1)	4975(1)	4930(1)	32(1)
C(46)	6424(1)	5230(1)	5364(1)	45(1)
C(47)	6040(1)	4837(1)	4432(1)	48(1)
C(48)	8469(1)	4989(1)	5331(1)	26(1)
C(49)	8724(1)	4956(1)	4760(1)	36(1)
C(50)	9133(1)	5056(1)	5869(1)	33(1)
C(51)	12188(1)	3282(1)	7414(1)	19(1)
C(52)	12818(1)	3543(1)	7508(1)	27(1)
F(1)	4822(1)	2307(1)	6572(1)	24(1)
F(2)	4738(1)	3648(1)	5446(1)	26(1)
F(3)	2835(1)	3126(1)	5378(1)	26(1)
F(4)	3806(1)	3203(1)	4586(1)	37(1)
F(5)	3636(1)	3799(1)	4700(1)	31(1)
F(6)	2742(1)	3429(1)	4460(1)	37(1)
F(7)	3732(1)	3978(1)	5851(1)	36(1)
F(8)	2639(1)	3895(1)	5387(1)	44(1)
F(9)	3034(1)	3644(1)	6228(1)	47(1)
F(10)	2996(1)	2928(1)	6355(1)	24(1)

F(11)	2813(1)	2393(1)	5520(1)	37(1)
F(12)	2638(1)	2189(1)	6329(1)	37(1)
F(13)	3580(1)	2025(1)	6053(1)	32(1)
F(14)	3203(1)	2642(1)	7290(1)	29(1)
F(15)	3959(1)	2222(1)	7192(1)	32(1)
F(16)	4281(1)	2808(1)	7321(1)	34(1)
F(17)	6144(1)	1552(1)	6914(1)	29(1)
F(18)	9030(1)	1489(1)	7291(1)	24(1)
F(19)	7060(1)	534(1)	7407(1)	51(1)
F(20)	6244(1)	911(1)	6304(1)	56(1)
F(21)	5450(1)	955(1)	6805(1)	60(1)
F(22)	5943(1)	424(1)	6728(1)	81(1)
F(23)	6054(1)	1233(1)	7896(1)	62(1)
F(24)	5937(1)	626(1)	7898(1)	92(1)
F(25)	6915(1)	891(1)	8371(1)	77(1)
F(26)	8094(1)	700(1)	8115(1)	41(1)
F(27)	9235(1)	847(1)	8737(1)	49(1)
F(28)	9709(1)	1109(1)	8111(1)	38(1)
F(29)	8914(1)	1410(1)	8441(1)	39(1)
F(30)	9140(1)	757(1)	7093(1)	40(1)
F(31)	8218(1)	414(1)	7072(1)	52(1)
F(32)	9161(1)	349(1)	7774(1)	57(1)
F(33)	10447(1)	3629(1)	6423(1)	27(1)
F(34)	10451(1)	2120(1)	6937(1)	25(1)
F(35)	11679(1)	2493(1)	7026(1)	24(1)
F(36)	6139(1)	4332(1)	5286(1)	31(1)
F(37)	9030(1)	4303(1)	5739(1)	28(1)
F(38)	8116(1)	5326(1)	5303(1)	36(1)
F(39)	9114(1)	5256(1)	4698(1)	53(1)
F(40)	8166(1)	4939(1)	4303(1)	50(1)
F(41)	9112(1)	4647(1)	4753(1)	44(1)
F(42)	9265(1)	5426(1)	5918(1)	47(1)
F(43)	8981(1)	4940(1)	6358(1)	40(1)
F(44)	9732(1)	4892(1)	5819(1)	41(1)
F(45)	7045(1)	5209(1)	4632(1)	42(1)
F(46)	6962(1)	5423(1)	5690(1)	55(1)
F(47)	5941(1)	5476(1)	5082(1)	66(1)
F(48)	6126(1)	5025(1)	5714(1)	55(1)
F(49)	6200(1)	4518(1)	4196(1)	59(1)
F(50)	5902(1)	5098(1)	4015(1)	82(1)
F(51)	5439(1)	4787(1)	4599(1)	60(1)
C(1S)	7006(2)	3167(1)	4622(2)	39(1)
C(2S)	7699(2)	3292(1)	4652(2)	44(2)
C(3S)	7808(1)	3641(1)	4413(2)	42(1)

C(4S)	7224(2)	3863(1)	4144(1)	41(1)
C(5S)	6532(1)	3737(1)	4115(1)	36(1)
C(6S)	6423(1)	3389(1)	4354(2)	31(1)
C(7S)	5675(2)	3259(2)	4336(2)	43(1)
C(8S)	7138(3)	3506(1)	4413(2)	63(2)
C(9S)	7795(2)	3328(2)	4619(2)	71(4)
C(10S)	7825(2)	2969(2)	4864(2)	73(3)
C(11S)	7197(2)	2788(1)	4903(2)	51(2)
C(12S)	6539(2)	2966(1)	4697(2)	36(1)
C(13S)	6510(2)	3325(1)	4452(2)	42(2)
C(14S)	5802(3)	3517(2)	4225(3)	67(2)
C(1T)	1073(2)	3178(1)	5245(1)	56(1)
C(2T)	1016(2)	2801(1)	5385(1)	57(1)
C(3T)	358(2)	2626(1)	5259(1)	56(1)
C(4T)	-234(2)	2824(1)	4981(1)	57(1)
C(5T)	-176(2)	3194(1)	4838(2)	70(1)
C(6T)	473(2)	3381(1)	4968(2)	67(1)
C(7T)	540(3)	3788(1)	4811(4)	159(3)
C(1E)	7923(3)	5487(1)	2220(1)	113(2)
C(2E)	7254(2)	5415(1)	2321(1)	113(2)
C(3E)	7148(2)	5457(1)	2878(2)	94(2)
C(4E)	7712(2)	5571(1)	3334(1)	84(1)
C(5E)	8381(2)	5643(1)	3232(1)	84(1)
C(6E)	8487(2)	5601(1)	2675(2)	96(2)
C(7E)	9190(3)	5674(3)	2531(4)	176(4)
C(1K)	4951(3)	4457(1)	7521(2)	49(1)
C(2K)	5202(3)	4378(1)	7031(2)	48(1)
C(3K)	5310(3)	4004(1)	6887(2)	46(1)
C(4K)	5168(5)	3710(1)	7233(3)	50(2)
C(5K)	4916(4)	3790(1)	7723(3)	47(2)
C(6K)	4808(2)	4164(1)	7867(2)	40(1)
C(7K)	4548(3)	4247(2)	8402(2)	59(2)

Table S.3 Bond lengths [Å] and angles [deg] for **[NHAcF_{51}PcCo]$_2$·7(toluene)**.

Co-N(4)	1.9196(14)	Co-N(2)	1.9254(13)
Co-N(3)	1.9218(13)	Co-O#1	2.1586(13)
Co-N(1)	1.9231(13)		
N(1)-C(8)	1.373(2)	N(3)-C(29)	1.374(2)
N(1)-C(1)	1.375(2)	N(4)-C(37)	1.370(2)
N(2)-C(22)	1.369(2)	N(4)-C(44)	1.380(2)
N(2)-C(15)	1.375(2)	N(5)-C(44)	1.316(2)
N(3)-C(36)	1.373(2)	N(5)-C(1)	1.319(2)

N(6)-C(15)	1.315(2)	C(17)-C(18)	1.393(2)
N(6)-C(8)	1.320(2)	C(18)-C(19)	1.444(2)
N(7)-C(29)	1.317(2)	C(18)-C(23)	1.548(3)
N(7)-C(22)	1.321(2)	C(19)-C(20)	1.394(2)
N(8)-C(36)	1.317(2)	C(19)-C(26)	1.548(3)
N(8)-C(37)	1.323(2)	C(20)-F(18)	1.3337(19)
N(12)-C(51)	1.368(2)	C(20)-C(21)	1.383(2)
N(12)-C(33)	1.412(2)	C(21)-C(22)	1.458(2)
N(12)-H(12)	0.85(3)	C(23)-F(19)	1.362(2)
O-C(51)	1.220(2)	C(23)-C(25)	1.542(4)
C(1)-C(2)	1.453(2)	C(23)-C(24)	1.590(4)
C(2)-C(7)	1.386(2)	C(24)-F(21)	1.325(3)
C(2)-C(3)	1.386(2)	C(24)-F(22)	1.326(3)
C(3)-F(2)	1.3350(19)	C(24)-F(20)	1.333(4)
C(3)-C(4)	1.391(2)	C(25)-F(23)	1.320(3)
C(4)-C(5)	1.452(2)	C(25)-F(25)	1.325(4)
C(4)-C(9)	1.542(2)	C(25)-F(24)	1.336(3)
C(5)-C(6)	1.389(2)	C(26)-F(26)	1.365(2)
C(5)-C(12)	1.543(2)	C(26)-C(28)	1.544(3)
C(6)-F(1)	1.3353(18)	C(26)-C(27)	1.579(3)
C(6)-C(7)	1.386(2)	C(27)-F(29)	1.327(3)
C(7)-C(8)	1.450(2)	C(27)-F(28)	1.328(2)
C(9)-F(3)	1.3705(19)	C(27)-F(27)	1.337(2)
C(9)-C(11)	1.552(3)	C(28)-F(30)	1.324(3)
C(9)-C(10)	1.581(3)	C(28)-F(31)	1.328(3)
C(10)-F(5)	1.324(2)	C(28)-F(32)	1.335(3)
C(10)-F(6)	1.327(2)	C(29)-C(30)	1.458(2)
C(10)-F(4)	1.331(2)	C(30)-C(31)	1.384(2)
C(11)-F(7)	1.317(2)	C(30)-C(35)	1.396(2)
C(11)-F(9)	1.329(3)	C(31)-F(34)	1.3291(18)
C(11)-F(8)	1.331(2)	C(31)-C(32)	1.388(2)
C(12)-F(10)	1.3705(19)	C(32)-F(35)	1.3366(18)
C(12)-C(13)	1.547(2)	C(32)-C(33)	1.403(2)
C(12)-C(14)	1.582(3)	C(33)-C(34)	1.391(2)
C(13)-F(13)	1.320(2)	C(34)-F(33)	1.3426(19)
C(13)-F(11)	1.320(2)	C(34)-C(35)	1.378(2)
C(13)-F(12)	1.335(2)	C(35)-C(36)	1.458(2)
C(14)-F(15)	1.323(2)	C(37)-C(38)	1.453(2)
C(14)-F(16)	1.328(2)	C(38)-C(43)	1.381(2)
C(14)-F(14)	1.330(2)	C(38)-C(39)	1.382(2)
C(15)-C(16)	1.450(2)	C(39)-F(37)	1.3343(19)
C(16)-C(21)	1.381(2)	C(39)-C(40)	1.395(2)
C(16)-C(17)	1.382(2)	C(40)-C(41)	1.449(2)
C(17)-F(17)	1.3358(19)	C(40)-C(48)	1.546(2)

C(41)-C(42)	1.393(2)	C(8S)-H(8SA)	0.95
C(41)-C(45)	1.547(2)	C(9S)-C(10S)	1.39
C(42)-F(36)	1.3316(19)	C(9S)-H(9SA)	0.95
C(42)-C(43)	1.384(2)	C(10S)-C(11S)	1.39
C(43)-C(44)	1.449(2)	C(10S)-H(10A)	0.95
C(45)-F(45)	1.366(2)	C(11S)-C(12S)	1.39
C(45)-C(46)	1.548(4)	C(11S)-H(11A)	0.95
C(45)-C(47)	1.578(4)	C(12S)-C(13S)	1.39
C(46)-F(46)	1.319(3)	C(12S)-H(12A)	0.95
C(46)-F(47)	1.325(3)	C(13S)-C(14S)	1.499(3)
C(46)-F(48)	1.330(3)	C(14S)-H(14A)	0.98
C(47)-F(51)	1.322(3)	C(14S)-H(14B)	0.98
C(47)-F(49)	1.326(4)	C(14S)-H(14C)	0.98
C(47)-F(50)	1.329(3)	C(1T)-C(6T)	1.379(4)
C(48)-F(38)	1.364(2)	C(1T)-C(2T)	1.382(5)
C(48)-C(49)	1.550(3)	C(1T)-H(1TA)	0.95
C(48)-C(50)	1.587(3)	C(2T)-C(3T)	1.375(5)
C(49)-F(41)	1.324(3)	C(2T)-H(2TA)	0.95
C(49)-F(40)	1.327(3)	C(3T)-C(4T)	1.363(5)
C(49)-F(39)	1.328(3)	C(3T)-H(3TA)	0.95
C(50)-F(44)	1.320(3)	C(4T)-C(5T)	1.361(5)
C(50)-F(43)	1.326(3)	C(4T)-H(4TA)	0.95
C(50)-F(42)	1.330(2)	C(5T)-C(6T)	1.380(5)
C(51)-C(52)	1.494(2)	C(5T)-H(5TA)	0.95
C(52)-H(52A)	0.98	C(6T)-C(7T)	1.499(3)
C(52)-H(52B)	0.98	C(7T)-H(7TA)	0.98
C(52)-H(52C)	0.98	C(7T)-H(7TB)	0.98
C(1S)-C(2S)	1.39	C(7T)-H(7TC)	0.98
C(1S)-C(6S)	1.39	C(1E)-C(2E)	1.39
C(1S)-H(1SA)	0.95	C(1E)-C(6E)	1.39
C(2S)-C(3S)	1.39	C(1E)-H(1EA)	0.95
C(2S)-H(2SA)	0.95	C(2E)-C(3E)	1.39
C(3S)-C(4S)	1.39	C(2E)-H(2EA)	0.95
C(3S)-H(3SA)	0.95	C(3E)-C(4E)	1.39
C(4S)-C(5S)	1.39	C(3E)-H(3EA)	0.95
C(4S)-H(4SA)	0.95	C(4E)-C(5E)	1.39
C(5S)-C(6S)	1.39	C(4E)-H(4EA)	0.95
C(5S)-H(5SA)	0.95	C(5E)-C(6E)	1.39
C(6S)-C(7S)	1.500(3)	C(5E)-H(5EA)	0.95
C(7S)-H(7SA)	0.98	C(6E)-C(7E)	1.496(3)
C(7S)-H(7SB)	0.98	C(7E)-H(7EA)	0.98
C(7S)-H(7SC)	0.98	C(7E)-H(7EB)	0.98
C(8S)-C(9S)	1.39	C(7E)-H(7EC)	0.98
C(8S)-C(13S)	1.39	C(1K)-C(2K)	1.39

C(1K)-C(6K)	1.39
C(1K)-H(1KA)	0.95
C(2K)-C(3K)	1.39
C(2K)-H(2KA)	0.95
C(3K)-C(4K)	1.39
C(3K)-H(3KA)	0.95
C(4K)-C(5K)	1.39
C(4K)-H(4KA)	0.95
C(5K)-C(6K)	1.39
C(5K)-H(5KA)	0.95
C(6K)-C(7K)	1.499(3)
C(7K)-H(7KA)	0.98
C(7K)-H(7KB)	0.98
C(7K)-H(7KC)	0.98

N(4)-Co-N(3)	90.18(6)
N(4)-Co-N(1)	89.67(6)
N(3)-Co-N(1)	175.80(6)
N(4)-Co-N(2)	177.23(6)
N(3)-Co-N(2)	89.86(6)
N(1)-Co-N(2)	90.08(6)
N(4)-Co-O#1	94.60(6)
N(3)-Co-O#1	83.18(5)
N(1)-Co-O#1	101.02(5)
N(2)-Co-O#1	88.16(5)

C(8)-N(1)-C(1)	107.75(13)
C(8)-N(1)-Co	125.86(11)
C(1)-N(1)-Co	126.38(11)
C(22)-N(2)-C(15)	107.80(13)
C(22)-N(2)-Co	126.16(11)
C(15)-N(2)-Co	125.67(10)
C(36)-N(3)-C(29)	107.51(13)
C(36)-N(3)-Co	125.54(11)
C(29)-N(3)-Co	126.08(11)
C(37)-N(4)-C(44)	107.62(13)
C(37)-N(4)-Co	125.83(11)
C(44)-N(4)-Co	126.55(11)
C(44)-N(5)-C(1)	121.03(14)
C(15)-N(6)-C(8)	120.93(14)
C(29)-N(7)-C(22)	121.19(14)
C(36)-N(8)-C(37)	120.96(14)
C(51)-N(12)-C(33)	120.82(15)
C(51)-N(12)-H(12)	117.2(17)
C(33)-N(12)-H(12)	119.4(17)
C(51)-O-Co#1	144.62(12)
N(5)-C(1)-N(1)	128.27(14)
N(5)-C(1)-C(2)	122.40(14)
N(1)-C(1)-C(2)	109.27(14)
C(7)-C(2)-C(3)	119.07(15)
C(7)-C(2)-C(1)	106.71(14)
C(3)-C(2)-C(1)	134.19(15)
F(2)-C(3)-C(2)	117.68(14)
F(2)-C(3)-C(4)	119.60(14)
C(2)-C(3)-C(4)	122.67(15)
C(3)-C(4)-C(5)	117.72(14)
C(3)-C(4)-C(9)	115.88(14)
C(5)-C(4)-C(9)	126.12(14)
C(6)-C(5)-C(4)	117.33(15)
C(6)-C(5)-C(12)	115.93(14)
C(4)-C(5)-C(12)	126.43(14)
F(1)-C(6)-C(7)	117.81(14)
F(1)-C(6)-C(5)	119.33(14)
C(7)-C(6)-C(5)	122.75(15)
C(6)-C(7)-C(2)	119.47(14)
C(6)-C(7)-C(8)	133.81(15)
C(2)-C(7)-C(8)	106.64(14)
N(6)-C(8)-N(1)	128.45(14)
N(6)-C(8)-C(7)	122.01(14)
N(1)-C(8)-C(7)	109.52(13)
F(3)-C(9)-C(4)	109.86(13)
F(3)-C(9)-C(11)	105.86(14)
C(4)-C(9)-C(11)	114.09(15)
F(3)-C(9)-C(10)	101.99(14)
C(4)-C(9)-C(10)	114.53(15)
C(11)-C(9)-C(10)	109.48(14)
F(5)-C(10)-F(6)	106.51(14)
F(5)-C(10)-F(4)	108.50(17)
F(6)-C(10)-F(4)	107.84(17)
F(5)-C(10)-C(9)	114.11(16)
F(6)-C(10)-C(9)	109.11(16)
F(4)-C(10)-C(9)	110.53(14)
F(7)-C(11)-F(9)	107.93(18)
F(7)-C(11)-F(8)	108.09(16)
F(9)-C(11)-F(8)	107.37(17)
F(7)-C(11)-C(9)	112.46(16)
F(9)-C(11)-C(9)	110.49(16)
F(8)-C(11)-C(9)	110.32(17)

F(10)-C(12)-C(5)	109.96(13)	C(25)-C(23)-C(18)	113.0(2)
F(10)-C(12)-C(13)	105.68(13)	F(19)-C(23)-C(24)	102.2(2)
C(5)-C(12)-C(13)	114.88(15)	C(25)-C(23)-C(24)	110.0(2)
F(10)-C(12)-C(14)	101.82(14)	C(18)-C(23)-C(24)	114.15(19)
C(5)-C(12)-C(14)	114.16(13)	F(21)-C(24)-F(22)	106.8(2)
C(13)-C(12)-C(14)	109.20(14)	F(21)-C(24)-F(20)	108.5(2)
F(13)-C(13)-F(11)	107.83(16)	F(22)-C(24)-F(20)	107.3(3)
F(13)-C(13)-F(12)	108.17(16)	F(21)-C(24)-C(23)	114.0(3)
F(11)-C(13)-F(12)	107.96(15)	F(22)-C(24)-C(23)	109.2(2)
F(13)-C(13)-C(12)	112.59(14)	F(20)-C(24)-C(23)	110.78(19)
F(11)-C(13)-C(12)	110.51(15)	F(23)-C(25)-F(25)	107.6(3)
F(12)-C(13)-C(12)	109.63(16)	F(23)-C(25)-F(24)	108.4(2)
F(15)-C(14)-F(16)	108.96(15)	F(25)-C(25)-F(24)	108.0(2)
F(15)-C(14)-F(14)	106.58(15)	F(23)-C(25)-C(23)	112.5(2)
F(16)-C(14)-F(14)	107.19(16)	F(25)-C(25)-C(23)	110.8(2)
F(15)-C(14)-C(12)	114.33(15)	F(24)-C(25)-C(23)	109.4(3)
F(16)-C(14)-C(12)	110.70(15)	F(26)-C(26)-C(28)	106.12(16)
F(14)-C(14)-C(12)	108.76(14)	F(26)-C(26)-C(19)	110.29(15)
N(6)-C(15)-N(2)	128.64(14)	C(28)-C(26)-C(19)	112.88(18)
N(6)-C(15)-C(16)	121.85(14)	F(26)-C(26)-C(27)	101.93(17)
N(2)-C(15)-C(16)	109.47(13)	C(28)-C(26)-C(27)	110.78(16)
C(21)-C(16)-C(17)	120.07(15)	C(19)-C(26)-C(27)	114.00(16)
C(21)-C(16)-C(15)	106.74(14)	F(29)-C(27)-F(28)	108.85(19)
C(17)-C(16)-C(15)	133.18(15)	F(29)-C(27)-F(27)	107.35(19)
F(17)-C(17)-C(16)	117.76(15)	F(28)-C(27)-F(27)	106.20(17)
F(17)-C(17)-C(18)	119.47(15)	F(29)-C(27)-C(26)	110.90(16)
C(16)-C(17)-C(18)	122.75(15)	F(28)-C(27)-C(26)	114.20(18)
C(17)-C(18)-C(19)	117.04(15)	F(27)-C(27)-C(26)	109.02(18)
C(17)-C(18)-C(23)	115.51(16)	F(30)-C(28)-F(31)	107.4(2)
C(19)-C(18)-C(23)	127.34(16)	F(30)-C(28)-F(32)	108.21(19)
C(20)-C(19)-C(18)	118.16(15)	F(31)-C(28)-F(32)	107.98(18)
C(20)-C(19)-C(26)	116.00(15)	F(30)-C(28)-C(26)	112.13(16)
C(18)-C(19)-C(26)	125.71(16)	F(31)-C(28)-C(26)	111.03(18)
F(18)-C(20)-C(21)	117.83(14)	F(32)-C(28)-C(26)	110.0(2)
F(18)-C(20)-C(19)	119.43(15)	N(7)-C(29)-N(3)	128.24(14)
C(21)-C(20)-C(19)	122.73(15)	N(7)-C(29)-C(30)	121.79(14)
C(16)-C(21)-C(20)	118.71(15)	N(3)-C(29)-C(30)	109.79(13)
C(16)-C(21)-C(22)	106.64(14)	C(31)-C(30)-C(35)	120.10(14)
C(20)-C(21)-C(22)	134.55(15)	C(31)-C(30)-C(29)	133.41(15)
N(7)-C(22)-N(2)	128.14(14)	C(35)-C(30)-C(29)	106.45(13)
N(7)-C(22)-C(21)	122.51(14)	F(34)-C(31)-C(30)	122.63(14)
N(2)-C(22)-C(21)	109.32(13)	F(34)-C(31)-C(32)	118.89(14)
F(19)-C(23)-C(25)	106.05(19)	C(30)-C(31)-C(32)	118.48(15)
F(19)-C(23)-C(18)	110.54(16)	F(35)-C(32)-C(31)	118.39(15)

F(35)-C(32)-C(33)	119.41(14)	F(46)-C(46)-F(47)	108.12(19)
C(31)-C(32)-C(33)	122.18(15)	F(46)-C(46)-F(48)	108.3(3)
C(34)-C(33)-C(32)	117.82(15)	F(47)-C(46)-F(48)	108.3(2)
C(34)-C(33)-N(12)	120.29(15)	F(46)-C(46)-C(45)	110.21(19)
C(32)-C(33)-N(12)	121.89(15)	F(47)-C(46)-C(45)	110.7(3)
F(33)-C(34)-C(35)	121.79(14)	F(48)-C(46)-C(45)	111.17(18)
F(33)-C(34)-C(33)	117.68(14)	F(51)-C(47)-F(49)	108.7(2)
C(35)-C(34)-C(33)	120.51(15)	F(51)-C(47)-F(50)	106.5(2)
C(34)-C(35)-C(30)	120.66(14)	F(49)-C(47)-F(50)	107.6(3)
C(34)-C(35)-C(36)	133.09(15)	F(51)-C(47)-C(45)	114.5(3)
C(30)-C(35)-C(36)	106.16(13)	F(49)-C(47)-C(45)	110.61(19)
N(8)-C(36)-N(3)	128.31(14)	F(50)-C(47)-C(45)	108.7(2)
N(8)-C(36)-C(35)	121.67(14)	F(38)-C(48)-C(40)	110.78(15)
N(3)-C(36)-C(35)	110.02(13)	F(38)-C(48)-C(49)	106.44(16)
N(8)-C(37)-N(4)	128.37(14)	C(40)-C(48)-C(49)	111.17(17)
N(8)-C(37)-C(38)	122.13(14)	F(38)-C(48)-C(50)	101.77(16)
N(4)-C(37)-C(38)	109.49(13)	C(40)-C(48)-C(50)	115.64(16)
C(43)-C(38)-C(39)	119.25(15)	C(49)-C(48)-C(50)	110.30(17)
C(43)-C(38)-C(37)	106.76(14)	F(41)-C(49)-F(40)	107.4(2)
C(39)-C(38)-C(37)	134.00(15)	F(41)-C(49)-F(39)	108.71(19)
F(37)-C(39)-C(38)	117.54(14)	F(40)-C(49)-F(39)	108.30(19)
F(37)-C(39)-C(40)	119.35(15)	F(41)-C(49)-C(48)	111.79(17)
C(38)-C(39)-C(40)	123.11(15)	F(40)-C(49)-C(48)	110.39(18)
C(39)-C(40)-C(41)	117.43(15)	F(39)-C(49)-C(48)	110.1(2)
C(39)-C(40)-C(48)	115.60(15)	F(44)-C(50)-F(43)	109.03(19)
C(41)-C(40)-C(48)	126.97(15)	F(44)-C(50)-F(42)	106.61(17)
C(42)-C(41)-C(40)	117.49(15)	F(43)-C(50)-F(42)	107.71(19)
C(42)-C(41)-C(45)	115.50(15)	F(44)-C(50)-C(48)	114.40(19)
C(40)-C(41)-C(45)	127.00(16)	F(43)-C(50)-C(48)	110.43(16)
F(36)-C(42)-C(43)	117.36(15)	F(42)-C(50)-C(48)	108.39(17)
F(36)-C(42)-C(41)	119.65(15)	O-C(51)-N(12)	119.24(15)
C(43)-C(42)-C(41)	122.98(16)	O-C(51)-C(52)	123.54(16)
C(38)-C(43)-C(42)	119.49(15)	N(12)-C(51)-C(52)	117.22(15)
C(38)-C(43)-C(44)	106.82(14)	C(51)-C(52)-H(52A)	109.5
C(42)-C(43)-C(44)	133.63(15)	C(51)-C(52)-H(52B)	109.5
N(5)-C(44)-N(4)	128.05(15)	H(52A)-C(52)-H(52B)	109.5
N(5)-C(44)-C(43)	122.64(14)	C(51)-C(52)-H(52C)	109.5
N(4)-C(44)-C(43)	109.30(14)	H(52A)-C(52)-H(52C)	109.5
F(45)-C(45)-C(41)	111.14(16)	H(52B)-C(52)-H(52C)	109.5
F(45)-C(45)-C(46)	106.18(17)	C(2S)-C(1S)-C(6S)	120
C(41)-C(45)-C(46)	111.9(2)	C(2S)-C(1S)-H(1SA)	120
F(45)-C(45)-C(47)	101.76(19)	C(6S)-C(1S)-H(1SA)	120
C(41)-C(45)-C(47)	115.18(17)	C(1S)-C(2S)-C(3S)	120
C(46)-C(45)-C(47)	109.9(2)	C(1S)-C(2S)-H(2SA)	120

C(3S)-C(2S)-H(2SA)	120	C(6T)-C(1T)-H(1TA)	119.8
C(4S)-C(3S)-C(2S)	120	C(2T)-C(1T)-H(1TA)	119.8
C(4S)-C(3S)-H(3SA)	120	C(3T)-C(2T)-C(1T)	120.3(3)
C(2S)-C(3S)-H(3SA)	120	C(3T)-C(2T)-H(2TA)	119.8
C(3S)-C(4S)-C(5S)	120	C(1T)-C(2T)-H(2TA)	119.8
C(3S)-C(4S)-H(4SA)	120	C(4T)-C(3T)-C(2T)	119.4(3)
C(5S)-C(4S)-H(4SA)	120	C(4T)-C(3T)-H(3TA)	120.3
C(6S)-C(5S)-C(4S)	120	C(2T)-C(3T)-H(3TA)	120.3
C(6S)-C(5S)-H(5SA)	120	C(5T)-C(4T)-C(3T)	120.3(3)
C(4S)-C(5S)-H(5SA)	120	C(5T)-C(4T)-H(4TA)	119.9
C(5S)-C(6S)-C(1S)	120	C(3T)-C(4T)-H(4TA)	119.9
C(5S)-C(6S)-C(7S)	119.9(3)	C(4T)-C(5T)-C(6T)	121.8(3)
C(1S)-C(6S)-C(7S)	120.1(3)	C(4T)-C(5T)-H(5TA)	119.1
C(6S)-C(7S)-H(7SA)	109.5	C(6T)-C(5T)-H(5TA)	119.1
C(6S)-C(7S)-H(7SB)	109.5	C(1T)-C(6T)-C(5T)	117.8(3)
H(7SA)-C(7S)-H(7SB)	109.5	C(1T)-C(6T)-C(7T)	120.2(4)
C(6S)-C(7S)-H(7SC)	109.5	C(5T)-C(6T)-C(7T)	122.0(4)
H(7SA)-C(7S)-H(7SC)	109.5	C(6T)-C(7T)-H(7TA)	109.5
H(7SB)-C(7S)-H(7SC)	109.5	C(6T)-C(7T)-H(7TB)	109.5
C(9S)-C(8S)-C(13S)	120	H(7TA)-C(7T)-H(7TB)	109.5
C(9S)-C(8S)-H(8SA)	120	C(6T)-C(7T)-H(7TC)	109.5
C(13S)-C(8S)-H(8SA)	120	H(7TA)-C(7T)-H(7TC)	109.5
C(8S)-C(9S)-C(10S)	120	H(7TB)-C(7T)-H(7TC)	109.5
C(8S)-C(9S)-H(9SA)	120	C(2E)-C(1E)-C(6E)	120
C(10S)-C(9S)-H(9SA)	120	C(2E)-C(1E)-H(1EA)	120
C(9S)-C(10S)-C(11S)	120	C(6E)-C(1E)-H(1EA)	120
C(9S)-C(10S)-H(10A)	120	C(1E)-C(2E)-C(3E)	120
C(11S)-C(10S)-H(10A)	120	C(1E)-C(2E)-H(2EA)	120
C(12S)-C(11S)-C(10S)	120	C(3E)-C(2E)-H(2EA)	120
C(12S)-C(11S)-H(11A)	120	C(4E)-C(3E)-C(2E)	120
C(10S)-C(11S)-H(11A)	120	C(4E)-C(3E)-H(3EA)	120
C(11S)-C(12S)-C(13S)	120	C(2E)-C(3E)-H(3EA)	120
C(11S)-C(12S)-H(12A)	120	C(3E)-C(4E)-C(5E)	120
C(13S)-C(12S)-H(12A)	120	C(3E)-C(4E)-H(4EA)	120
C(12S)-C(13S)-C(8S)	120	C(5E)-C(4E)-H(4EA)	120
C(12S)-C(13S)-C(14S)	120.2(4)	C(6E)-C(5E)-C(4E)	120
C(8S)-C(13S)-C(14S)	119.8(4)	C(6E)-C(5E)-H(5EA)	120
C(13S)-C(14S)-H(14A)	109.5	C(4E)-C(5E)-H(5EA)	120
C(13S)-C(14S)-H(14B)	109.5	C(5E)-C(6E)-C(1E)	120
H(14A)-C(14S)-H(14B)	109.5	C(5E)-C(6E)-C(7E)	123.2(4)
C(13S)-C(14S)-H(14C)	109.5	C(1E)-C(6E)-C(7E)	116.8(4)
H(14A)-C(14S)-H(14C)	109.5	C(6E)-C(7E)-H(7EA)	109.5
H(14B)-C(14S)-H(14C)	109.5	C(6E)-C(7E)-H(7EB)	109.5
C(6T)-C(1T)-C(2T)	120.4(3)	H(7EA)-C(7E)-H(7EB)	109.5

C(6E)-C(7E)-H(7EC)	109.5	C(3K)-C(4K)-H(4KA)	120
H(7EA)-C(7E)-H(7EC)	109.5	C(4K)-C(5K)-C(6K)	120
H(7EB)-C(7E)-H(7EC)	109.5	C(4K)-C(5K)-H(5KA)	120
C(2K)-C(1K)-C(6K)	120	C(6K)-C(5K)-H(5KA)	120
C(2K)-C(1K)-H(1KA)	120	C(5K)-C(6K)-C(1K)	120
C(6K)-C(1K)-H(1KA)	120	C(5K)-C(6K)-C(7K)	119.7(4)
C(3K)-C(2K)-C(1K)	120	C(1K)-C(6K)-C(7K)	120.3(4)
C(3K)-C(2K)-H(2KA)	120	C(6K)-C(7K)-H(7KA)	109.5
C(1K)-C(2K)-H(2KA)	120	C(6K)-C(7K)-H(7KB)	109.5
C(2K)-C(3K)-C(4K)	120	H(7KA)-C(7K)-H(7KB)	109.5
C(2K)-C(3K)-H(3KA)	120	C(6K)-C(7K)-H(7KC)	109.5
C(4K)-C(3K)-H(3KA)	120	H(7KA)-C(7K)-H(7KC)	109.5
C(5K)-C(4K)-C(3K)	120	H(7KB)-C(7K)-H(7KC)	109.5
C(5K)-C(4K)-H(4KA)	120		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table S.4 Anisotropic displacement parameters ($Å^2$ x 10^3) **[NHAcF$_{51}$PcCo]$_2$·7(toluene)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [h2 a*^{2} U^{11} + ... + 2 h k a* b* U^{12}].

	U^{11}	**U^{22}**	**U^{33}**	**U^{23}**	**U^{13}**	**U^{12}**
Co	10(1)	12(1)	18(1)	1(1)	2(1)	1(1)
N(1)	12(1)	15(1)	18(1)	1(1)	2(1)	1(1)
N(2)	12(1)	14(1)	19(1)	0(1)	3(1)	1(1)
N(3)	13(1)	14(1)	17(1)	0(1)	3(1)	0(1)
N(4)	11(1)	15(1)	21(1)	1(1)	2(1)	1(1)
N(5)	13(1)	16(1)	24(1)	4(1)	4(1)	0(1)
N(6)	13(1)	15(1)	20(1)	2(1)	2(1)	1(1)
N(7)	13(1)	14(1)	20(1)	0(1)	3(1)	0(1)
N(8)	14(1)	16(1)	22(1)	3(1)	3(1)	2(1)
N(12)	15(1)	24(1)	24(1)	9(1)	1(1)	-3(1)
O	22(1)	21(1)	21(1)	3(1)	4(1)	-3(1)
C(1)	12(1)	18(1)	20(1)	2(1)	2(1)	1(1)
C(2)	12(1)	17(1)	22(1)	1(1)	2(1)	0(1)
C(3)	14(1)	16(1)	24(1)	4(1)	2(1)	0(1)
C(4)	11(1)	16(1)	23(1)	2(1)	1(1)	1(1)
C(5)	13(1)	17(1)	21(1)	1(1)	2(1)	0(1)
C(6)	14(1)	15(1)	24(1)	4(1)	3(1)	1(1)
C(7)	12(1)	17(1)	22(1)	1(1)	1(1)	1(1)
C(8)	12(1)	16(1)	19(1)	0(1)	2(1)	0(1)
C(9)	14(1)	18(1)	27(1)	3(1)	0(1)	1(1)
C(10)	24(1)	21(1)	29(1)	6(1)	-2(1)	0(1)
C(11)	20(1)	23(1)	38(1)	4(1)	5(1)	5(1)
C(12)	11(1)	20(1)	23(1)	2(1)	2(1)	1(1)
C(13)	17(1)	25(1)	26(1)	2(1)	1(1)	-4(1)

C(14)	15(1)	28(1)	24(1)	3(1)	4(1)	1(1)
C(15)	13(1)	13(1)	18(1)	0(1)	2(1)	1(1)
C(16)	15(1)	15(1)	22(1)	2(1)	3(1)	2(1)
C(17)	14(1)	19(1)	30(1)	4(1)	5(1)	0(1)
C(18)	18(1)	18(1)	36(1)	7(1)	7(1)	0(1)
C(19)	20(1)	17(1)	32(1)	5(1)	7(1)	2(1)
C(20)	14(1)	16(1)	27(1)	2(1)	5(1)	1(1)
C(21)	15(1)	14(1)	22(1)	1(1)	4(1)	0(1)
C(22)	14(1)	13(1)	19(1)	0(1)	3(1)	2(1)
C(23)	22(1)	23(1)	67(2)	20(1)	11(1)	0(1)
C(24)	29(1)	23(1)	98(2)	11(1)	2(1)	-8(1)
C(25)	33(1)	61(2)	82(2)	43(2)	28(1)	10(1)
C(26)	22(1)	21(1)	42(1)	13(1)	10(1)	4(1)
C(27)	29(1)	35(1)	32(1)	11(1)	8(1)	7(1)
C(28)	32(1)	18(1)	57(1)	4(1)	13(1)	4(1)
C(29)	12(1)	16(1)	19(1)	-1(1)	2(1)	1(1)
C(30)	12(1)	15(1)	18(1)	1(1)	2(1)	1(1)
C(31)	15(1)	15(1)	20(1)	3(1)	3(1)	2(1)
C(32)	12(1)	21(1)	21(1)	3(1)	2(1)	4(1)
C(33)	14(1)	22(1)	21(1)	6(1)	3(1)	0(1)
C(34)	14(1)	18(1)	24(1)	6(1)	3(1)	0(1)
C(35)	11(1)	18(1)	21(1)	4(1)	2(1)	1(1)
C(36)	12(1)	17(1)	18(1)	1(1)	2(1)	1(1)
C(37)	14(1)	14(1)	20(1)	3(1)	3(1)	1(1)
C(38)	15(1)	15(1)	24(1)	3(1)	4(1)	1(1)
C(39)	14(1)	17(1)	31(1)	4(1)	6(1)	1(1)
C(40)	18(1)	16(1)	32(1)	5(1)	7(1)	0(1)
C(41)	18(1)	16(1)	34(1)	6(1)	6(1)	3(1)
C(42)	14(1)	17(1)	33(1)	6(1)	5(1)	3(1)
C(43)	14(1)	15(1)	26(1)	4(1)	4(1)	1(1)
C(44)	14(1)	14(1)	23(1)	2(1)	3(1)	2(1)
C(45)	22(1)	18(1)	54(1)	15(1)	7(1)	4(1)
C(46)	30(1)	20(1)	88(2)	8(1)	21(1)	6(1)
C(47)	35(1)	36(1)	62(2)	22(1)	-7(1)	3(1)
C(48)	21(1)	18(1)	40(1)	8(1)	10(1)	0(1)
C(49)	33(1)	34(1)	43(1)	14(1)	15(1)	0(1)
C(50)	28(1)	23(1)	46(1)	2(1)	8(1)	-7(1)
C(51)	15(1)	18(1)	24(1)	2(1)	4(1)	1(1)
C(52)	21(1)	26(1)	32(1)	4(1)	2(1)	-8(1)
F(1)	16(1)	18(1)	36(1)	11(1)	6(1)	2(1)
F(2)	18(1)	19(1)	39(1)	13(1)	4(1)	1(1)
F(3)	14(1)	26(1)	35(1)	8(1)	-3(1)	-3(1)
F(4)	49(1)	32(1)	28(1)	4(1)	8(1)	10(1)
F(5)	30(1)	24(1)	35(1)	12(1)	0(1)	-4(1)

F(6)	30(1)	35(1)	35(1)	11(1)	-13(1)	-7(1)
F(7)	29(1)	25(1)	53(1)	-9(1)	7(1)	-2(1)
F(8)	27(1)	33(1)	66(1)	4(1)	-2(1)	16(1)
F(9)	68(1)	32(1)	54(1)	5(1)	37(1)	11(1)
F(10)	15(1)	26(1)	32(1)	6(1)	5(1)	7(1)
F(11)	39(1)	33(1)	29(1)	1(1)	-10(1)	-7(1)
F(12)	26(1)	41(1)	47(1)	-4(1)	14(1)	-16(1)
F(13)	26(1)	23(1)	42(1)	-4(1)	3(1)	-1(1)
F(14)	21(1)	40(1)	28(1)	5(1)	10(1)	5(1)
F(15)	31(1)	34(1)	30(1)	12(1)	9(1)	11(1)
F(16)	24(1)	48(1)	26(1)	-5(1)	0(1)	-10(1)
F(17)	13(1)	24(1)	50(1)	11(1)	7(1)	0(1)
F(18)	14(1)	19(1)	38(1)	6(1)	5(1)	2(1)
F(19)	30(1)	20(1)	101(1)	22(1)	12(1)	0(1)
F(20)	46(1)	42(1)	70(1)	-9(1)	-4(1)	-12(1)
F(21)	21(1)	38(1)	113(2)	22(1)	3(1)	-7(1)
F(22)	46(1)	26(1)	156(2)	6(1)	-4(1)	-16(1)
F(23)	49(1)	70(1)	77(1)	33(1)	38(1)	19(1)
F(24)	52(1)	80(1)	159(2)	73(2)	55(1)	3(1)
F(25)	52(1)	122(2)	67(1)	50(1)	31(1)	29(1)
F(26)	30(1)	38(1)	58(1)	28(1)	17(1)	6(1)
F(27)	44(1)	57(1)	43(1)	26(1)	6(1)	11(1)
F(28)	22(1)	46(1)	44(1)	11(1)	5(1)	6(1)
F(29)	39(1)	41(1)	36(1)	-1(1)	6(1)	7(1)
F(30)	40(1)	26(1)	61(1)	-4(1)	24(1)	0(1)
F(31)	46(1)	28(1)	84(1)	-13(1)	19(1)	-9(1)
F(32)	56(1)	30(1)	86(1)	20(1)	21(1)	25(1)
F(33)	18(1)	18(1)	41(1)	10(1)	2(1)	-2(1)
F(34)	19(1)	14(1)	38(1)	4(1)	2(1)	2(1)
F(35)	13(1)	24(1)	34(1)	3(1)	3(1)	4(1)
F(36)	13(1)	22(1)	56(1)	12(1)	5(1)	4(1)
F(37)	13(1)	22(1)	48(1)	9(1)	7(1)	1(1)
F(38)	29(1)	16(1)	65(1)	8(1)	14(1)	2(1)
F(39)	54(1)	45(1)	71(1)	19(1)	35(1)	-8(1)
F(40)	49(1)	64(1)	38(1)	16(1)	10(1)	5(1)
F(41)	46(1)	44(1)	49(1)	8(1)	25(1)	10(1)
F(42)	44(1)	24(1)	70(1)	0(1)	6(1)	-14(1)
F(43)	43(1)	37(1)	40(1)	0(1)	7(1)	-9(1)
F(44)	22(1)	35(1)	65(1)	8(1)	8(1)	-5(1)
F(45)	31(1)	29(1)	64(1)	24(1)	9(1)	2(1)
F(46)	44(1)	35(1)	90(1)	-16(1)	26(1)	-3(1)
F(47)	38(1)	22(1)	140(2)	15(1)	25(1)	15(1)
F(48)	49(1)	32(1)	100(1)	1(1)	46(1)	5(1)
F(49)	60(1)	60(1)	47(1)	3(1)	-8(1)	-11(1)

F(50)	55(1)	78(1)	92(2)	59(1)	-26(1)	-11(1)
F(51)	22(1)	41(1)	105(1)	31(1)	-6(1)	2(1)
C(1S)	40(2)	43(2)	29(2)	-6(2)	2(2)	14(2)
C(2S)	37(3)	57(4)	35(4)	-13(3)	4(2)	13(3)
C(3S)	38(2)	52(3)	38(2)	-14(2)	11(2)	1(2)
C(4S)	46(3)	39(2)	37(2)	-8(2)	8(2)	0(2)
C(5S)	37(2)	37(2)	30(2)	-8(2)	1(2)	8(2)
C(6S)	31(2)	37(2)	23(2)	-9(2)	3(2)	6(2)
C(7S)	38(2)	49(3)	39(3)	-12(2)	3(2)	1(2)
C(8S)	87(5)	70(4)	36(3)	-19(3)	23(3)	-37(4)
C(9S)	54(5)	122(10)	46(5)	-38(5)	29(4)	-41(6)
C(10S)	43(3)	134(8)	39(3)	-39(4)	7(3)	17(4)
C(11S)	57(3)	59(3)	35(3)	-13(2)	6(2)	20(3)
C(12S)	41(3)	34(2)	32(2)	-6(2)	6(2)	-2(2)
C(13S)	58(4)	42(3)	21(2)	-4(2)	2(2)	-7(3)
C(14S)	93(6)	45(3)	49(4)	1(3)	-14(3)	9(3)
C(1T)	30(1)	83(2)	56(2)	14(2)	14(1)	7(1)
C(2T)	54(2)	76(2)	45(2)	11(1)	16(1)	36(2)
C(3T)	86(2)	38(1)	50(2)	-4(1)	27(2)	13(1)
C(4T)	54(2)	59(2)	56(2)	-12(1)	8(1)	-8(1)
C(5T)	38(2)	75(2)	87(3)	24(2)	-6(2)	9(2)
C(6T)	45(2)	65(2)	87(2)	35(2)	9(2)	3(1)
C(7T)	102(4)	97(4)	261(9)	114(5)	11(5)	-5(3)
C(1E)	172(6)	60(3)	100(4)	-9(3)	21(4)	18(3)
C(2E)	195(7)	44(2)	100(4)	-2(2)	35(4)	-8(3)
C(3E)	138(4)	32(2)	108(4)	13(2)	24(3)	-7(2)
C(4E)	145(4)	33(2)	82(3)	20(2)	45(3)	20(2)
C(5E)	107(4)	49(2)	92(3)	12(2)	19(3)	17(2)
C(6E)	107(4)	75(3)	127(4)	22(3)	67(4)	21(3)
C(7E)	169(7)	211(9)	162(7)	-62(7)	67(6)	-40(7)
C(1K)	49(3)	31(2)	66(3)	7(6)	10(2)	6(4)
C(2K)	53(3)	37(3)	50(3)	6(2)	7(2)	-3(2)
C(3K)	41(3)	44(3)	49(3)	-3(2)	1(2)	-1(2)
C(4K)	54(4)	33(3)	56(4)	4(3)	-4(3)	2(3)
C(5K)	48(4)	27(2)	55(4)	2(2)	-7(3)	-3(3)
C(6K)	34(2)	34(2)	48(3)	6(2)	1(2)	2(2)
C(7K)	51(3)	65(4)	63(4)	6(3)	18(3)	11(3)

Table S.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **[NHAcF$_{51}$PcCo]$_2$·7(toluene)**.

	x	**y**	**z**	**U(eq)**
H(12)	11779(13)	3456(7)	6638(11)	26
H(52A)	12992	3596	7925	41

H(52B)	12675	3780	7297	41
H(52C)	13201	3423	7364	41
H(1SA)	6932	2929	4786	46
H(2SA)	8097	3140	4835	53
H(3SA)	8281	3727	4433	51
H(4SA)	7299	4101	3981	49
H(5SA)	6133	3889	3932	43
H(7SA)	5403	3235	3930	65
H(7SB)	5441	3443	4537	65
H(7SC)	5694	3012	4530	65
H(8SA)	7117	3752	4245	75
H(9SA)	8224	3452	4592	85
H(10A)	8274	2847	5004	87
H(11A)	7217	2542	5071	61
H(12A)	6110	2842	4724	44
H(14A)	5445	3329	4036	101
H(14B)	5850	3711	3941	101
H(14C)	5648	3636	4548	101
H(1TA)	1528	3299	5340	67
H(2TA)	1433	2663	5570	69
H(3TA)	317	2368	5365	68
H(4TA)	-689	2704	4887	69
H(5TA)	-595	3328	4642	84
H(7TA)	140	3933	4891	239
H(7TB)	530	3807	4396	239
H(7TC)	993	3891	5042	239
H(1EA)	7996	5458	1839	135
H(2EA)	6868	5337	2009	136
H(3EA)	6690	5408	2947	112
H(4EA)	7639	5600	3714	101
H(5EA)	8767	5721	3544	100
H(7EA)	9507	5812	2853	264
H(7EB)	9112	5827	2175	264
H(7EC)	9412	5433	2471	264
H(1KA)	4876	4713	7619	59
H(2KA)	5299	4578	6794	57
H(3KA)	5482	3949	6552	56
H(4KA)	5242	3455	7135	60
H(5KA)	4819	3589	7960	56
H(7KA)	4189	4059	8441	88
H(7KB)	4333	4501	8368	88
H(7KC)	4952	4238	8745	88

Table S.6 Torsion angles [deg] for **[NHAcF$_{51}$PcCo]$_2$·7(toluene)**.

C(44)-N(5)-C(1)-N(1)	0.2(3)	C(6)-C(7)-C(8)-N(1)	-173.16(19)
C(44)-N(5)-C(1)-C(2)	177.20(16)	C(2)-C(7)-C(8)-N(1)	3.30(19)
C(8)-N(1)-C(1)-N(5)	177.33(17)	C(3)-C(4)-C(9)-F(3)	160.08(15)
Co-N(1)-C(1)-N(5)	-1.7(3)	C(5)-C(4)-C(9)-F(3)	-13.6(2)
C(8)-N(1)-C(1)-C(2)	-0.01(18)	C(3)-C(4)-C(9)-C(11)	-81.2(2)
Co-N(1)-C(1)-C(2)	-179.07(11)	C(5)-C(4)-C(9)-C(11)	105.0(2)
N(5)-C(1)-C(2)-C(7)	-175.45(16)	C(3)-C(4)-C(9)-C(10)	46.0(2)
N(1)-C(1)-C(2)-C(7)	2.07(19)	C(5)-C(4)-C(9)-C(10)	-127.69(18)
N(5)-C(1)-C(2)-C(3)	6.5(3)	F(3)-C(9)-C(10)-F(5)	147.58(15)
N(1)-C(1)-C(2)-C(3)	-175.96(19)	C(4)-C(9)-C(10)-F(5)	-93.83(18)
C(7)-C(2)-C(3)-F(2)	-173.69(16)	C(11)-C(9)-C(10)-F(5)	35.8(2)
C(1)-C(2)-C(3)-F(2)	4.2(3)	F(3)-C(9)-C(10)-F(6)	28.60(18)
C(7)-C(2)-C(3)-C(4)	4.0(3)	C(4)-C(9)-C(10)-F(6)	147.20(15)
C(1)-C(2)-C(3)-C(4)	-178.19(18)	C(11)-C(9)-C(10)-F(6)	-83.21(18)
F(2)-C(3)-C(4)-C(5)	-177.30(15)	F(3)-C(9)-C(10)-F(4)	-89.82(17)
C(2)-C(3)-C(4)-C(5)	5.1(3)	C(4)-C(9)-C(10)-F(4)	28.8(2)
F(2)-C(3)-C(4)-C(9)	8.4(2)	C(11)-C(9)-C(10)-F(4)	158.37(15)
C(2)-C(3)-C(4)-C(9)	-169.17(16)	F(3)-C(9)-C(11)-F(7)	176.24(15)
C(3)-C(4)-C(5)-C(6)	-10.2(2)	C(4)-C(9)-C(11)-F(7)	55.3(2)
C(9)-C(4)-C(5)-C(6)	163.40(17)	C(10)-C(9)-C(11)-F(7)	-74.51(19)
C(3)-C(4)-C(5)-C(12)	163.04(16)	F(3)-C(9)-C(11)-F(9)	55.57(19)
C(9)-C(4)-C(5)-C(12)	-23.3(3)	C(4)-C(9)-C(11)-F(9)	-65.4(2)
C(4)-C(5)-C(6)-F(1)	-177.28(15)	C(10)-C(9)-C(11)-F(9)	164.82(16)
C(12)-C(5)-C(6)-F(1)	8.8(2)	F(3)-C(9)-C(11)-F(8)	-63.0(2)
C(4)-C(5)-C(6)-C(7)	6.8(3)	C(4)-C(9)-C(11)-F(8)	176.08(15)
C(12)-C(5)-C(6)-C(7)	-167.16(16)	C(10)-C(9)-C(11)-F(8)	46.2(2)
F(1)-C(6)-C(7)-C(2)	-173.76(15)	C(6)-C(5)-C(12)-F(10)	160.96(15)
C(5)-C(6)-C(7)-C(2)	2.2(3)	C(4)-C(5)-C(12)-F(10)	-12.4(2)
F(1)-C(6)-C(7)-C(8)	2.3(3)	C(6)-C(5)-C(12)-C(13)	-80.00(19)
C(5)-C(6)-C(7)-C(8)	178.32(18)	C(4)-C(5)-C(12)-C(13)	106.67(19)
C(3)-C(2)-C(7)-C(6)	-7.7(3)	C(6)-C(5)-C(12)-C(14)	47.3(2)
C(1)-C(2)-C(7)-C(6)	173.90(16)	C(4)-C(5)-C(12)-C(14)	-126.07(18)
C(3)-C(2)-C(7)-C(8)	175.23(16)	F(10)-C(12)-C(13)-F(13)	179.66(14)
C(1)-C(2)-C(7)-C(8)	-3.16(19)	C(5)-C(12)-C(13)-F(13)	58.2(2)
C(15)-N(6)-C(8)-N(1)	0.3(3)	C(14)-C(12)-C(13)-F(13)	-71.49(19)
C(15)-N(6)-C(8)-C(7)	178.73(16)	F(10)-C(12)-C(13)-F(11)	59.00(19)
C(1)-N(1)-C(8)-N(6)	176.57(17)	C(5)-C(12)-C(13)-F(11)	-62.40(19)
Co-N(1)-C(8)-N(6)	-4.4(3)	C(14)-C(12)-C(13)-F(11)	167.86(15)
C(1)-N(1)-C(8)-C(7)	-2.00(18)	F(10)-C(12)-C(13)-F(12)	-59.87(18)
Co-N(1)-C(8)-C(7)	177.07(11)	C(5)-C(12)-C(13)-F(12)	178.72(14)
C(6)-C(7)-C(8)-N(6)	8.2(3)	C(14)-C(12)-C(13)-F(12)	48.98(19)
C(2)-C(7)-C(8)-N(6)	-175.38(16)	F(10)-C(12)-C(14)-F(15)	146.90(14)

C(5)-C(12)-C(14)-F(15)	-94.66(18)	C(15)-N(2)-C(22)-N(7)	-178.81(16)
C(13)-C(12)-C(14)-F(15)	35.47(19)	Co-N(2)-C(22)-N(7)	-5.5(3)
F(10)-C(12)-C(14)-F(16)	-89.60(16)	C(15)-N(2)-C(22)-C(21)	-0.74(18)
C(5)-C(12)-C(14)-F(16)	28.8(2)	Co-N(2)-C(22)-C(21)	172.61(11)
C(13)-C(12)-C(14)-F(16)	158.97(15)	C(16)-C(21)-C(22)-N(7)	179.20(16)
F(10)-C(12)-C(14)-F(14)	27.92(18)	C(20)-C(21)-C(22)-N(7)	2.9(3)
C(5)-C(12)-C(14)-F(14)	146.37(15)	C(16)-C(21)-C(22)-N(2)	1.00(19)
C(13)-C(12)-C(14)-F(14)	-83.51(18)	C(20)-C(21)-C(22)-N(2)	-175.34(19)
C(8)-N(6)-C(15)-N(2)	-0.4(3)	C(17)-C(18)-C(23)-F(19)	160.0(2)
C(8)-N(6)-C(15)-C(16)	177.04(15)	C(19)-C(18)-C(23)-F(19)	-15.9(3)
C(22)-N(2)-C(15)-N(6)	177.95(16)	C(17)-C(18)-C(23)-C(25)	-81.3(2)
Co-N(2)-C(15)-N(6)	4.6(2)	C(19)-C(18)-C(23)-C(25)	102.8(2)
C(22)-N(2)-C(15)-C(16)	0.21(18)	C(17)-C(18)-C(23)-C(24)	45.5(3)
Co-N(2)-C(15)-C(16)	-173.18(11)	C(19)-C(18)-C(23)-C(24)	-130.5(2)
N(6)-C(15)-C(16)-C(21)	-177.50(15)	F(19)-C(23)-C(24)-F(21)	143.8(2)
N(2)-C(15)-C(16)-C(21)	0.42(19)	C(25)-C(23)-C(24)-F(21)	31.5(3)
N(6)-C(15)-C(16)-C(17)	3.6(3)	C(18)-C(23)-C(24)-F(21)	-96.8(3)
N(2)-C(15)-C(16)-C(17)	-178.52(19)	F(19)-C(23)-C(24)-F(22)	24.4(3)
C(21)-C(16)-C(17)-F(17)	-175.99(16)	C(25)-C(23)-C(24)-F(22)	-87.9(3)
C(15)-C(16)-C(17)-F(17)	2.8(3)	C(18)-C(23)-C(24)-F(22)	143.8(2)
C(21)-C(16)-C(17)-C(18)	2.5(3)	F(19)-C(23)-C(24)-F(20)	-93.5(2)
C(15)-C(16)-C(17)-C(18)	-178.64(19)	C(25)-C(23)-C(24)-F(20)	154.2(2)
F(17)-C(17)-C(18)-C(19)	-177.60(17)	C(18)-C(23)-C(24)-F(20)	25.9(3)
C(16)-C(17)-C(18)-C(19)	3.9(3)	F(19)-C(23)-C(25)-F(23)	177.3(2)
F(17)-C(17)-C(18)-C(23)	6.0(3)	C(18)-C(23)-C(25)-F(23)	56.0(3)
C(16)-C(17)-C(18)-C(23)	-172.50(19)	C(24)-C(23)-C(25)-F(23)	-72.9(3)
C(17)-C(18)-C(19)-C(20)	-8.0(3)	F(19)-C(23)-C(25)-F(25)	56.8(3)
C(23)-C(18)-C(19)-C(20)	167.9(2)	C(18)-C(23)-C(25)-F(25)	-64.5(3)
C(17)-C(18)-C(19)-C(26)	167.61(19)	C(24)-C(23)-C(25)-F(25)	166.6(2)
C(23)-C(18)-C(19)-C(26)	-16.5(3)	F(19)-C(23)-C(25)-F(24)	-62.2(3)
C(18)-C(19)-C(20)-F(18)	-175.18(17)	C(18)-C(23)-C(25)-F(24)	176.50(19)
C(26)-C(19)-C(20)-F(18)	8.8(3)	C(24)-C(23)-C(25)-F(24)	47.6(3)
C(18)-C(19)-C(20)-C(21)	6.2(3)	C(20)-C(19)-C(26)-F(26)	158.61(18)
C(26)-C(19)-C(20)-C(21)	-169.87(18)	C(18)-C(19)-C(26)-F(26)	-17.1(3)
C(17)-C(16)-C(21)-C(20)	-4.7(3)	C(20)-C(19)-C(26)-C(28)	-82.9(2)
C(15)-C(16)-C(21)-C(20)	176.20(16)	C(18)-C(19)-C(26)-C(28)	101.4(2)
C(17)-C(16)-C(21)-C(22)	178.27(16)	C(20)-C(19)-C(26)-C(27)	44.7(2)
C(15)-C(16)-C(21)-C(22)	-0.83(18)	C(18)-C(19)-C(26)-C(27)	-131.0(2)
F(18)-C(20)-C(21)-C(16)	-178.42(16)	F(26)-C(26)-C(27)-F(29)	-89.79(18)
C(19)-C(20)-C(21)-C(16)	0.3(3)	C(28)-C(26)-C(27)-F(29)	157.65(17)
F(18)-C(20)-C(21)-C(22)	-2.4(3)	C(19)-C(26)-C(27)-F(29)	29.0(2)
C(19)-C(20)-C(21)-C(22)	176.27(19)	F(26)-C(26)-C(27)-F(28)	146.79(17)
C(29)-N(7)-C(22)-N(2)	1.6(3)	C(28)-C(26)-C(27)-F(28)	34.2(2)
C(29)-N(7)-C(22)-C(21)	-176.26(15)	C(19)-C(26)-C(27)-F(28)	-94.4(2)

F(26)-C(26)-C(27)-F(27)	28.2(2)	C(31)-C(30)-C(35)-C(34)	-3.8(3)
C(28)-C(26)-C(27)-F(27)	-84.4(2)	C(29)-C(30)-C(35)-C(34)	174.16(16)
C(19)-C(26)-C(27)-F(27)	147.03(17)	C(31)-C(30)-C(35)-C(36)	179.40(15)
F(26)-C(26)-C(28)-F(30)	-178.46(18)	C(29)-C(30)-C(35)-C(36)	-2.69(18)
C(19)-C(26)-C(28)-F(30)	60.6(2)	C(37)-N(8)-C(36)-N(3)	1.0(3)
C(27)-C(26)-C(28)-F(30)	-68.6(2)	C(37)-N(8)-C(36)-C(35)	-178.13(16)
F(26)-C(26)-C(28)-F(31)	61.4(2)	C(29)-N(3)-C(36)-N(8)	-179.16(17)
C(19)-C(26)-C(28)-F(31)	-59.5(2)	Co-N(3)-C(36)-N(8)	-9.3(3)
C(27)-C(26)-C(28)-F(31)	171.27(18)	C(29)-N(3)-C(36)-C(35)	0.08(18)
F(26)-C(26)-C(28)-F(32)	-58.0(2)	Co-N(3)-C(36)-C(35)	169.91(11)
C(19)-C(26)-C(28)-F(32)	-178.94(17)	C(34)-C(35)-C(36)-N(8)	4.7(3)
C(27)-C(26)-C(28)-F(32)	51.8(2)	C(30)-C(35)-C(36)-N(8)	-178.98(16)
C(22)-N(7)-C(29)-N(3)	-0.6(3)	C(34)-C(35)-C(36)-N(3)	-174.57(18)
C(22)-N(7)-C(29)-C(30)	174.06(15)	C(30)-C(35)-C(36)-N(3)	1.72(19)
C(36)-N(3)-C(29)-N(7)	173.37(16)	C(36)-N(8)-C(37)-N(4)	3.9(3)
Co-N(3)-C(29)-N(7)	3.6(2)	C(36)-N(8)-C(37)-C(38)	-175.67(16)
C(36)-N(3)-C(29)-C(30)	-1.81(18)	C(44)-N(4)-C(37)-N(8)	-179.60(17)
Co-N(3)-C(29)-C(30)	-171.57(11)	Co-N(4)-C(37)-N(8)	0.2(3)
N(7)-C(29)-C(30)-C(31)	4.9(3)	C(44)-N(4)-C(37)-C(38)	-0.02(19)
N(3)-C(29)-C(30)-C(31)	-179.60(18)	Co-N(4)-C(37)-C(38)	179.73(11)
N(7)-C(29)-C(30)-C(35)	-172.66(15)	N(8)-C(37)-C(38)-C(43)	179.47(16)
N(3)-C(29)-C(30)-C(35)	2.89(19)	N(4)-C(37)-C(38)-C(43)	-0.1(2)
C(35)-C(30)-C(31)-F(34)	-176.12(16)	N(8)-C(37)-C(38)-C(39)	-0.8(3)
C(29)-C(30)-C(31)-F(34)	6.6(3)	N(4)-C(37)-C(38)-C(39)	179.6(2)
C(35)-C(30)-C(31)-C(32)	3.0(2)	C(43)-C(38)-C(39)-F(37)	179.31(16)
C(29)-C(30)-C(31)-C(32)	-174.29(17)	C(37)-C(38)-C(39)-F(37)	-0.5(3)
F(34)-C(31)-C(32)-F(35)	2.3(2)	C(43)-C(38)-C(39)-C(40)	-0.4(3)
C(30)-C(31)-C(32)-F(35)	-176.81(15)	C(37)-C(38)-C(39)-C(40)	179.87(19)
F(34)-C(31)-C(32)-C(33)	-179.43(16)	F(37)-C(39)-C(40)-C(41)	176.44(17)
C(30)-C(31)-C(32)-C(33)	1.5(3)	C(38)-C(39)-C(40)-C(41)	-3.9(3)
F(35)-C(32)-C(33)-C(34)	173.23(16)	F(37)-C(39)-C(40)-C(48)	-4.4(3)
C(31)-C(32)-C(33)-C(34)	-5.0(3)	C(38)-C(39)-C(40)-C(48)	175.25(18)
F(35)-C(32)-C(33)-N(12)	-7.5(3)	C(39)-C(40)-C(41)-C(42)	5.7(3)
C(31)-C(32)-C(33)-N(12)	174.26(17)	C(48)-C(40)-C(41)-C(42)	-173.29(19)
C(51)-N(12)-C(33)-C(34)	122.96(19)	C(39)-C(40)-C(41)-C(45)	-173.7(2)
C(51)-N(12)-C(33)-C(32)	-56.3(3)	C(48)-C(40)-C(41)-C(45)	7.3(3)
C(32)-C(33)-C(34)-F(33)	-177.41(16)	C(40)-C(41)-C(42)-F(36)	177.60(17)
N(12)-C(33)-C(34)-F(33)	3.3(3)	C(45)-C(41)-C(42)-F(36)	-2.9(3)
C(32)-C(33)-C(34)-C(35)	4.2(3)	C(40)-C(41)-C(42)-C(43)	-3.7(3)
N(12)-C(33)-C(34)-C(35)	-175.10(17)	C(45)-C(41)-C(42)-C(43)	175.79(19)
F(33)-C(34)-C(35)-C(30)	-178.27(16)	C(39)-C(38)-C(43)-C(42)	2.7(3)
C(33)-C(34)-C(35)-C(30)	0.1(3)	C(37)-C(38)-C(43)-C(42)	-177.49(17)
F(33)-C(34)-C(35)-C(36)	-2.4(3)	C(39)-C(38)-C(43)-C(44)	-179.58(16)
C(33)-C(34)-C(35)-C(36)	175.91(18)	C(37)-C(38)-C(43)-C(44)	0.24(19)

F(36)-C(42)-C(43)-C(38)	178.16(17)
C(41)-C(42)-C(43)-C(38)	-0.6(3)
F(36)-C(42)-C(43)-C(44)	1.2(3)
C(41)-C(42)-C(43)-C(44)	-177.6(2)
C(1)-N(5)-C(44)-N(4)	0.2(3)
C(1)-N(5)-C(44)-C(43)	-179.15(17)
C(37)-N(4)-C(44)-N(5)	-179.26(17)
Co-N(4)-C(44)-N(5)	1.0(3)
C(37)-N(4)-C(44)-C(43)	0.17(19)
Co-N(4)-C(44)-C(43)	-179.58(12)
C(38)-C(43)-C(44)-N(5)	179.21(17)
C(42)-C(43)-C(44)-N(5)	-3.5(3)
C(38)-C(43)-C(44)-N(4)	-0.3(2)
C(42)-C(43)-C(44)-N(4)	177.0(2)
C(42)-C(41)-C(45)-F(45)	-159.40(19)
C(40)-C(41)-C(45)-F(45)	20.0(3)
C(42)-C(41)-C(45)-C(46)	82.1(2)
C(40)-C(41)-C(45)-C(46)	-98.5(2)
C(42)-C(41)-C(45)-C(47)	-44.4(3)
C(40)-C(41)-C(45)-C(47)	135.1(2)
F(45)-C(45)-C(46)-F(46)	-54.6(2)
C(41)-C(45)-C(46)-F(46)	66.8(2)
C(47)-C(45)-C(46)-F(46)	-163.9(2)
F(45)-C(45)-C(46)-F(47)	64.9(2)
C(41)-C(45)-C(46)-F(47)	-173.63(17)
C(47)-C(45)-C(46)-F(47)	-44.4(2)
F(45)-C(45)-C(46)-F(48)	-174.7(2)
C(41)-C(45)-C(46)-F(48)	-53.2(3)
C(47)-C(45)-C(46)-F(48)	76.0(3)
F(45)-C(45)-C(47)-F(51)	-144.88(19)
C(41)-C(45)-C(47)-F(51)	94.8(2)
C(46)-C(45)-C(47)-F(51)	-32.7(3)
F(45)-C(45)-C(47)-F(49)	91.9(2)
C(41)-C(45)-C(47)-F(49)	-28.4(3)
C(46)-C(45)-C(47)-F(49)	-155.9(2)
F(45)-C(45)-C(47)-F(50)	-26.0(3)
C(41)-C(45)-C(47)-F(50)	-146.3(2)
C(46)-C(45)-C(47)-F(50)	86.2(3)
C(39)-C(40)-C(48)-F(38)	-158.51(18)
C(41)-C(40)-C(48)-F(38)	20.5(3)
C(39)-C(40)-C(48)-C(49)	83.4(2)
C(41)-C(40)-C(48)-C(49)	-97.6(2)
C(39)-C(40)-C(48)-C(50)	-43.4(2)
C(41)-C(40)-C(48)-C(50)	135.6(2)
F(38)-C(48)-C(49)-F(41)	176.43(18)
C(40)-C(48)-C(49)-F(41)	-62.8(2)
C(50)-C(48)-C(49)-F(41)	66.8(2)
F(38)-C(48)-C(49)-F(40)	-64.1(2)
C(40)-C(48)-C(49)-F(40)	56.7(2)
C(50)-C(48)-C(49)-F(40)	-173.69(17)
F(38)-C(48)-C(49)-F(39)	55.5(2)
C(40)-C(48)-C(49)-F(39)	176.20(17)
C(50)-C(48)-C(49)-F(39)	-54.2(2)
F(38)-C(48)-C(50)-F(44)	-144.88(17)
C(40)-C(48)-C(50)-F(44)	95.0(2)
C(49)-C(48)-C(50)-F(44)	-32.2(2)
F(38)-C(48)-C(50)-F(43)	91.68(18)
C(40)-C(48)-C(50)-F(43)	-28.5(2)
C(49)-C(48)-C(50)-F(43)	-155.66(17)
F(38)-C(48)-C(50)-F(42)	-26.1(2)
C(40)-C(48)-C(50)-F(42)	-146.23(18)
C(49)-C(48)-C(50)-F(42)	86.6(2)
Co#1-O-C(51)-N(12)	-174.28(14)
Co#1-O-C(51)-C(52)	5.8(3)
C(33)-N(12)-C(51)-O	7.2(3)
C(33)-N(12)-C(51)-C(52)	-172.85(17)
C(6S)-C(1S)-C(2S)-C(3S)	0
C(1S)-C(2S)-C(3S)-C(4S)	0
C(2S)-C(3S)-C(4S)-C(5S)	0
C(3S)-C(4S)-C(5S)-C(6S)	0
C(4S)-C(5S)-C(6S)-C(1S)	0
C(4S)-C(5S)-C(6S)-C(7S)	178.4(4)
C(2S)-C(1S)-C(6S)-C(5S)	0
C(2S)-C(1S)-C(6S)-C(7S)	-178.4(4)
C(13S)-C(8S)-C(9S)-C(10S)	0
C(8S)-C(9S)-C(10S)-C(11S)	0
C(9S)-C(10S)-C(11S)-C(12S)	0
C(10S)-C(11S)-C(12S)-C(13S)	0
C(11S)-C(12S)-C(13S)-C(8S)	0
C(11S)-C(12S)-C(13S)-C(14S)	179.4(5)
C(9S)-C(8S)-C(13S)-C(12S)	0
C(9S)-C(8S)-C(13S)-C(14S)	-179.4(5)

C(6T)-C(1T)-C(2T)-C(3T)	-1.1(5)	C(4E)-C(5E)-C(6E)-C(1E)	0
C(1T)-C(2T)-C(3T)-C(4T)	1.7(5)	C(4E)-C(5E)-C(6E)-C(7E)	179.7(5)
C(2T)-C(3T)-C(4T)-C(5T)	-1.0(5)	C(2E)-C(1E)-C(6E)-C(5E)	0
C(3T)-C(4T)-C(5T)-C(6T)	-0.3(6)	C(2E)-C(1E)-C(6E)-C(7E)	-179.8(5)
C(2T)-C(1T)-C(6T)-C(5T)	-0.2(6)	C(6K)-C(1K)-C(2K)-C(3K)	0
C(2T)-C(1T)-C(6T)-C(7T)	-179.2(5)	C(1K)-C(2K)-C(3K)-C(4K)	0
C(4T)-C(5T)-C(6T)-C(1T)	0.9(6)	C(2K)-C(3K)-C(4K)-C(5K)	0
C(4T)-C(5T)-C(6T)-C(7T)	179.9(5)	C(3K)-C(4K)-C(5K)-C(6K)	0
C(6E)-C(1E)-C(2E)-C(3E)	0	C(4K)-C(5K)-C(6K)-C(1K)	0
C(1E)-C(2E)-C(3E)-C(4E)	0	C(4K)-C(5K)-C(6K)-C(7K)	-179.0(4)
C(2E)-C(3E)-C(4E)-C(5E)	0	C(2K)-C(1K)-C(6K)-C(5K)	0
C(3E)-C(4E)-C(5E)-C(6E)	0	C(2K)-C(1K)-C(6K)-C(7K)	179.0(4)

Appendix T: Crystal structure of [NMeAcF$_{51}$PcCo]$_2$·7(toluene)

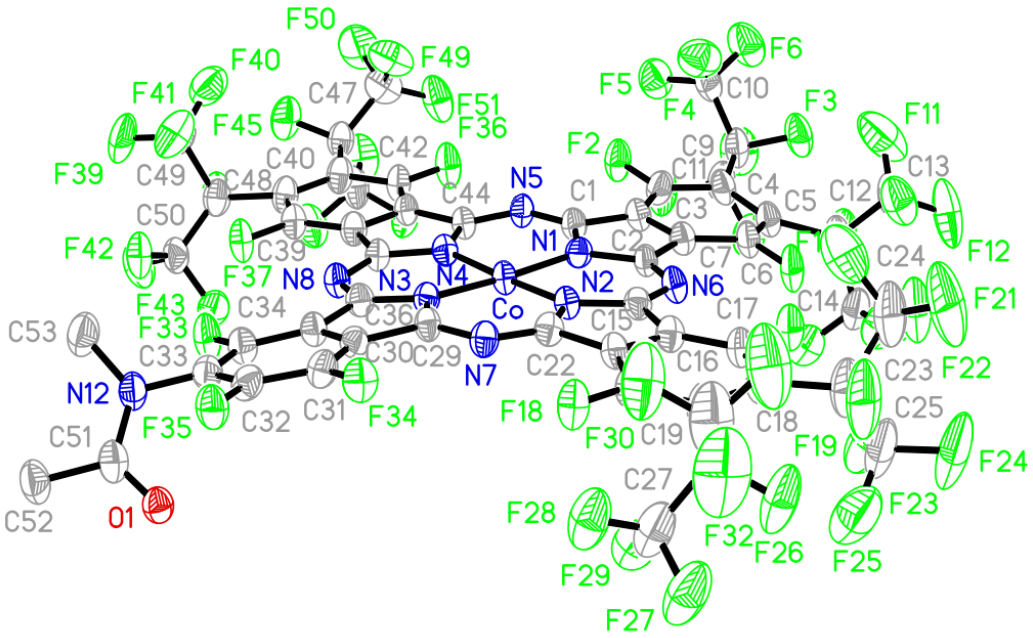


Figure T.1 ORTEP representation of **NMeAcF$_{51}$PcCo** X-ray crystal structure, at 50% probability.

Table T.1 Crystal data and structure refinement for **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**.

Empirical formula	C155 H68 Co2 F102 N18 O2	
Formula weight	4270.13	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, C2/c	
Unit cell dimensions	a = 19.627(5) Å	alpha = 90 deg.
	b = 35.191(9) Å	beta = 106.675(6) deg.
	c = 23.892(6) Å	gamma = 90 deg.
Volume	15808(7) Å^3	
Z, Calculated density	4, 1.794 g/cm^3	
Absorption coefficient	0.393 mm^{-1}	
F(000)	8448	
Crystal size	0.560 x 0.490 x 0.210 mm	
Theta range for data collection	1.322 to 25.026 deg.	
Limiting indices	-23<=h<=23, -41<=k<=41, -28<=l<=28	
Reflections collected / unique	142617 / 13966 [R(int) = 0.0387]	
Completeness to theta = 25.000	99.9 %	
Absorption correction	Empirical	
Max. and min. transmission	0.7461 and 0.6848	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13966 / 175 / 1312	

Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0918, wR2 = 0.2274
R indices (all data)	R1 = 0.1174, wR2 = 0.2591
Extinction coefficient	n/a
Largest diff. peak and hole	2.676 and -0.982 e.$Å^{-3}$

Table T.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7577(1)	2905(1)	6328(1)	23(1)
N(1)	6559(2)	2924(1)	6189(2)	22(1)
N(2)	7583(2)	2386(1)	6578(2)	24(1)
N(3)	8575(2)	2871(1)	6404(2)	22(1)
N(4)	7557(2)	3416(1)	6034(2)	26(1)
N(5)	6296(2)	3553(1)	5766(2)	27(1)
N(6)	6346(2)	2307(1)	6557(2)	27(1)
N(7)	8829(2)	2229(1)	6766(2)	24(1)
N(8)	8818(2)	3518(1)	6176(2)	27(1)
N(12)	11660(2)	3272(1)	6849(2)	31(1)
C(53)	11744(3)	3499(2)	6352(3)	44(2)
O	12030(2)	3073(1)	7766(2)	32(1)
C(1)	6127(3)	3222(1)	5943(2)	27(1)
C(2)	5397(3)	3128(2)	5930(2)	27(1)
C(3)	4752(3)	3311(2)	5707(2)	31(1)
C(4)	4120(3)	3171(2)	5778(3)	32(1)
C(5)	4162(3)	2832(2)	6130(3)	33(1)
C(6)	4797(3)	2637(2)	6286(3)	31(1)
C(7)	5414(3)	2780(2)	6187(2)	28(1)
C(8)	6147(3)	2646(1)	6331(2)	25(1)
C(9)	3438(3)	3386(2)	5434(3)	38(1)
C(10)	3383(3)	3464(2)	4770(3)	43(2)
C(11)	3320(3)	3754(2)	5734(3)	42(1)
C(12)	3566(3)	2684(2)	6389(3)	36(1)
C(13)	3151(3)	2340(2)	6071(3)	43(1)
C(14)	3811(3)	2602(2)	7063(3)	42(1)
C(15)	7008(3)	2193(1)	6664(2)	23(1)
C(16)	7242(3)	1826(1)	6920(2)	26(1)
C(17)	6894(3)	1526(2)	7088(2)	30(1)
C(18)	7234(3)	1197(2)	7339(3)	35(1)
C(19)	7999(3)	1186(2)	7457(3)	34(1)
C(20)	8328(3)	1482(1)	7247(2)	28(1)
C(21)	7961(3)	1801(1)	6983(2)	25(1)

C(22)	8169(3)	2156(1)	6763(2)	23(1)
C(23)	6751(3)	877(2)	7445(4)	51(2)
C(24)	6063(4)	799(2)	6901(5)	66(2)
C(25)	6518(4)	936(3)	8003(4)	70(2)
C(26)	8507(3)	882(2)	7826(3)	45(2)
C(27)	9170(3)	1061(2)	8303(3)	50(2)
C(28)	8745(4)	586(2)	7454(4)	61(2)
C(29)	9007(3)	2564(1)	6599(2)	24(1)
C(30)	9750(3)	2669(2)	6664(2)	26(1)
C(31)	10387(3)	2472(2)	6822(2)	29(1)
C(32)	11007(3)	2673(2)	6863(2)	30(1)
C(33)	11017(3)	3064(2)	6771(2)	29(1)
C(34)	10371(3)	3254(2)	6606(2)	31(1)
C(35)	9744(3)	3055(2)	6541(2)	27(1)
C(36)	9005(3)	3173(1)	6360(2)	25(1)
C(37)	8137(3)	3623(1)	6005(2)	25(1)
C(38)	7915(3)	3988(1)	5753(2)	27(1)
C(39)	8265(3)	4301(2)	5615(2)	31(1)
C(40)	7924(3)	4626(2)	5359(3)	34(1)
C(41)	7153(3)	4636(2)	5217(3)	34(1)
C(42)	6818(3)	4317(2)	5367(3)	32(1)
C(43)	7185(3)	4000(1)	5629(2)	27(1)
C(44)	6971(3)	3637(1)	5812(2)	26(1)
C(45)	6651(3)	4959(2)	4917(3)	38(1)
C(46)	6407(5)	5212(2)	5357(4)	70(2)
C(47)	6005(6)	4833(3)	4400(4)	92(4)
C(48)	8412(4)	4956(2)	5268(4)	58(2)
C(49)	8627(5)	4912(3)	4727(5)	82(3)
C(50)	9121(4)	5031(2)	5852(4)	53(2)
C(51)	12145(3)	3268(2)	7386(3)	32(1)
C(52)	12792(3)	3514(2)	7486(3)	41(1)
F(1)	4843(2)	2309(1)	6579(2)	40(1)
F(2)	4743(2)	3629(1)	5396(2)	39(1)
F(3)	2852(2)	3166(1)	5393(2)	46(1)
F(4)	3744(2)	3205(1)	4566(2)	55(1)
F(5)	3603(2)	3804(1)	4664(2)	49(1)
F(6)	2703(2)	3438(1)	4459(2)	60(1)
F(7)	3823(2)	4013(1)	5766(2)	49(1)
F(8)	2696(2)	3909(1)	5459(2)	63(1)
F(9)	3319(2)	3690(1)	6288(2)	51(1)
F(10)	3074(2)	2963(1)	6360(2)	45(1)
F(11)	2850(2)	2416(1)	5516(2)	65(1)
F(12)	2640(2)	2246(1)	6318(2)	68(1)
F(13)	3556(2)	2036(1)	6107(2)	54(1)

F(14)	3267(2)	2657(1)	7280(2)	59(1)
F(15)	4036(2)	2251(1)	7211(2)	59(1)
F(16)	4319(2)	2835(1)	7335(2)	65(1)
F(17)	6188(2)	1557(1)	6994(2)	39(1)
F(18)	9024(2)	1468(1)	7314(2)	34(1)
F(19)	7092(2)	536(1)	7499(2)	69(1)
F(20)	6190(2)	906(1)	6403(2)	70(1)
F(21)	5483(2)	966(1)	6938(2)	72(1)
F(22)	5936(3)	429(1)	6862(3)	102(2)
F(23)	6191(2)	1258(2)	8009(2)	74(1)
F(24)	6087(3)	653(2)	8056(3)	106(2)
F(25)	7084(3)	928(2)	8475(2)	88(2)
F(26)	8172(2)	692(1)	8171(2)	60(1)
F(27)	9336(2)	837(2)	8776(2)	72(1)
F(28)	9752(2)	1081(1)	8128(2)	55(1)
F(29)	9021(2)	1399(1)	8471(2)	53(1)
F(30)	9101(2)	737(1)	7114(2)	60(1)
F(31)	8185(3)	403(1)	7110(3)	79(2)
F(32)	9161(3)	328(1)	7797(3)	85(2)
F(33)	10365(2)	3629(1)	6526(2)	38(1)
F(34)	10420(2)	2100(1)	6917(2)	36(1)
F(35)	11620(2)	2477(1)	6983(2)	36(1)
F(36)	6113(2)	4313(1)	5247(2)	44(1)
F(37)	8971(2)	4278(1)	5739(2)	38(1)
F(38)	8102(3)	5312(1)	5307(3)	93(2)
F(39)	9021(3)	5198(2)	4640(3)	116(2)
F(40)	8027(3)	4931(2)	4297(3)	110(2)
F(41)	8953(3)	4591(2)	4713(2)	91(2)
F(42)	9255(3)	5404(1)	5830(3)	98(2)
F(43)	9023(3)	4933(1)	6316(2)	74(1)
F(44)	9685(2)	4852(1)	5751(3)	85(2)
F(45)	6990(2)	5212(1)	4670(3)	90(2)
F(46)	6977(3)	5405(2)	5691(3)	88(2)
F(47)	5939(2)	5458(1)	5106(3)	72(1)
F(48)	6167(2)	4997(1)	5717(2)	60(1)
F(49)	6079(3)	4525(2)	4168(2)	83(2)
F(50)	5832(3)	5116(2)	4010(2)	88(2)
F(51)	5398(2)	4792(1)	4627(3)	108(3)
C(1S)	7094(5)	3176(2)	4614(4)	50(3)
C(2S)	7780(4)	3294(2)	4646(4)	66(11)
C(3S)	7888(4)	3639(3)	4402(4)	61(4)
C(4S)	7311(5)	3866(2)	4125(4)	60(4)
C(5S)	6624(4)	3748(2)	4092(4)	55(3)
C(6S)	6516(4)	3403(3)	4337(4)	47(4)

C(7S)	5772(6)	3281(5)	4322(7)	64(4)
C(8S)	7182(11)	3496(4)	4418(7)	109(13)
C(9S)	7818(8)	3298(6)	4631(7)	90(20)
C(10S)	7818(7)	2939(6)	4874(7)	99(10)
C(11S)	7184(9)	2778(4)	4903(6)	76(7)
C(12S)	6548(7)	2975(4)	4690(6)	60(5)
C(13S)	6547(8)	3334(4)	4447(7)	62(9)
C(14S)	5837(11)	3529(7)	4207(11)	96(10)
C(1T)	985(5)	3051(3)	5022(4)	76(3)
C(2T)	933(5)	2709(3)	5295(4)	80(3)
C(3T)	291(5)	2566(3)	5309(4)	70(2)
C(4T)	-289(5)	2773(3)	5059(5)	89(3)
C(5T)	-218(6)	3111(4)	4798(7)	124(5)
C(6T)	406(5)	3257(3)	4774(5)	93(3)
C(7T)	492(9)	3638(4)	4507(9)	187(10)
C(1E)	7893(7)	5469(2)	2106(4)	125(4)
C(2E)	7217(6)	5435(2)	2178(4)	133(4)
C(3E)	7130(5)	5447(2)	2734(5)	135(4)
C(4E)	7717(7)	5494(2)	3219(3)	144(5)
C(5E)	8393(6)	5528(2)	3147(4)	139(5)
C(6E)	8480(5)	5516(2)	2590(5)	142(5)
C(7E)	9242(8)	5583(7)	2592(12)	234(10)
C(1K)	4916(12)	4437(3)	7525(7)	73(5)
C(2K)	5175(10)	4368(3)	7051(7)	79(6)
C(3K)	5313(9)	3998(4)	6912(6)	59(4)
C(4K)	5193(17)	3697(3)	7247(10)	73(9)
C(5K)	4933(16)	3766(3)	7721(10)	64(8)
C(6K)	4795(9)	4136(4)	7860(6)	69(6)
C(7K)	4510(9)	4195(6)	8379(7)	74(5)

Table T.3 Bond lengths [Å] and angles [deg] for **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**.

Co-N(3)	1.917(4)	N(4)-C(37)	1.371(6)
Co-N(2)	1.922(4)	N(5)-C(1)	1.314(7)
Co-N(4)	1.926(4)	N(5)-C(44)	1.330(7)
Co-N(1)	1.930(4)	N(6)-C(15)	1.314(6)
Co-O#1	2.161(4)	N(6)-C(8)	1.322(7)
N(1)-C(1)	1.370(6)	N(7)-C(22)	1.317(6)
N(1)-C(8)	1.374(6)	N(7)-C(29)	1.324(7)
N(2)-C(22)	1.371(6)	N(8)-C(36)	1.309(7)
N(2)-C(15)	1.381(6)	N(8)-C(37)	1.332(7)
N(3)-C(29)	1.371(6)	N(12)-C(51)	1.361(7)
N(3)-C(36)	1.378(6)	N(12)-C(33)	1.425(7)
N(4)-C(44)	1.363(7)	N(12)-C(53)	1.478(7)

C(53)-H(53A)	0.98	C(20)-C(21)	1.382(7)
C(53)-H(53B)	0.98	C(21)-C(22)	1.461(7)
C(53)-H(53C)	0.98	C(23)-F(19)	1.361(7)
O-C(51)	1.209(7)	C(23)-C(25)	1.543(12)
C(1)-C(2)	1.461(7)	C(23)-C(24)	1.607(12)
C(2)-C(7)	1.367(7)	C(24)-F(21)	1.305(9)
C(2)-C(3)	1.384(7)	C(24)-F(22)	1.323(8)
C(3)-F(2)	1.341(6)	C(24)-F(20)	1.339(10)
C(3)-C(4)	1.389(7)	C(25)-F(23)	1.305(10)
C(4)-C(5)	1.448(8)	C(25)-F(24)	1.337(9)
C(4)-C(9)	1.550(8)	C(25)-F(25)	1.337(10)
C(5)-C(6)	1.377(8)	C(26)-F(26)	1.367(7)
C(5)-C(12)	1.563(7)	C(26)-C(28)	1.527(11)
C(6)-F(1)	1.339(6)	C(26)-C(27)	1.593(10)
C(6)-C(7)	1.394(7)	C(27)-F(29)	1.315(8)
C(7)-C(8)	1.457(7)	C(27)-F(28)	1.325(7)
C(9)-F(3)	1.367(6)	C(27)-F(27)	1.338(7)
C(9)-C(11)	1.532(9)	C(28)-F(30)	1.324(9)
C(9)-C(10)	1.581(9)	C(28)-F(32)	1.334(8)
C(10)-F(5)	1.322(7)	C(28)-F(31)	1.334(10)
C(10)-F(4)	1.330(8)	C(29)-C(30)	1.470(7)
C(10)-F(6)	1.331(7)	C(30)-C(31)	1.384(7)
C(11)-F(8)	1.330(7)	C(30)-C(35)	1.389(7)
C(11)-F(7)	1.330(7)	C(31)-F(34)	1.328(6)
C(11)-F(9)	1.343(8)	C(31)-C(32)	1.387(8)
C(12)-F(10)	1.365(6)	C(32)-F(35)	1.346(6)
C(12)-C(13)	1.533(9)	C(32)-C(33)	1.395(8)
C(12)-C(14)	1.569(9)	C(33)-C(34)	1.387(8)
C(13)-F(11)	1.314(8)	C(34)-F(33)	1.331(6)
C(13)-F(13)	1.320(7)	C(34)-C(35)	1.384(7)
C(13)-F(12)	1.343(7)	C(35)-C(36)	1.451(7)
C(14)-F(16)	1.312(8)	C(37)-C(38)	1.432(7)
C(14)-F(15)	1.323(7)	C(38)-C(43)	1.378(7)
C(14)-F(14)	1.328(7)	C(38)-C(39)	1.387(7)
C(15)-C(16)	1.446(7)	C(39)-F(37)	1.333(6)
C(16)-C(21)	1.378(7)	C(39)-C(40)	1.379(8)
C(16)-C(17)	1.379(7)	C(40)-C(41)	1.455(8)
C(17)-F(17)	1.344(6)	C(40)-C(48)	1.559(8)
C(17)-C(18)	1.382(8)	C(41)-C(42)	1.398(8)
C(18)-C(19)	1.446(8)	C(41)-C(45)	1.539(8)
C(18)-C(23)	1.540(8)	C(42)-F(36)	1.330(6)
C(19)-C(20)	1.395(8)	C(42)-C(43)	1.376(7)
C(19)-C(26)	1.552(8)	C(43)-C(44)	1.452(7)
C(20)-F(18)	1.330(6)	C(45)-F(45)	1.344(7)

C(45)-C(46)	1.553(11)	C(11S)-H(11A)	0.95
C(45)-C(47)	1.559(11)	C(12S)-C(13S)	1.39
C(46)-F(47)	1.279(9)	C(12S)-H(12A)	0.95
C(46)-F(48)	1.330(10)	C(13S)-C(14S)	1.513(9)
C(46)-F(46)	1.356(10)	C(14S)-H(14A)	0.98
C(47)-F(49)	1.247(10)	C(14S)-H(14B)	0.98
C(47)-F(50)	1.339(10)	C(14S)-H(14C)	0.98
C(47)-F(51)	1.449(14)	C(1T)-C(6T)	1.336(14)
C(48)-F(38)	1.408(9)	C(1T)-C(2T)	1.387(14)
C(48)-C(49)	1.478(13)	C(1T)-H(1TA)	0.95
C(48)-C(50)	1.685(12)	C(2T)-C(3T)	1.366(13)
C(49)-F(41)	1.303(12)	C(2T)-H(2TA)	0.95
C(49)-F(39)	1.321(10)	C(3T)-C(4T)	1.339(14)
C(49)-F(40)	1.324(12)	C(3T)-H(3TA)	0.95
C(50)-F(43)	1.226(9)	C(4T)-C(5T)	1.368(16)
C(50)-F(42)	1.341(8)	C(4T)-H(4TA)	0.95
C(50)-F(44)	1.356(9)	C(5T)-C(6T)	1.346(15)
C(51)-C(52)	1.499(8)	C(5T)-H(5TA)	0.95
C(52)-H(52A)	0.98	C(6T)-C(7T)	1.513(9)
C(52)-H(52B)	0.98	C(7T)-H(7TA)	0.98
C(52)-H(52C)	0.98	C(7T)-H(7TB)	0.98
C(1S)-C(2S)	1.39	C(7T)-H(7TC)	0.98
C(1S)-C(6S)	1.39	C(1E)-C(2E)	1.39
C(1S)-H(1SA)	0.95	C(1E)-C(6E)	1.39
C(2S)-C(3S)	1.39	C(1E)-H(1EA)	0.95
C(2S)-H(2SA)	0.95	C(2E)-C(3E)	1.39
C(3S)-C(4S)	1.39	C(2E)-H(2EA)	0.95
C(3S)-H(3SA)	0.95	C(3E)-C(4E)	1.39
C(4S)-C(5S)	1.39	C(3E)-H(3EA)	0.95
C(4S)-H(4SA)	0.95	C(4E)-C(5E)	1.39
C(5S)-C(6S)	1.39	C(4E)-H(4EA)	0.95
C(5S)-H(5SA)	0.95	C(5E)-C(6E)	1.39
C(6S)-C(7S)	1.513(9)	C(5E)-H(5EA)	0.95
C(7S)-H(7SA)	0.98	C(6E)-C(7E)	1.512(9)
C(7S)-H(7SB)	0.98	C(7E)-H(7EA)	0.98
C(7S)-H(7SC)	0.98	C(7E)-H(7EB)	0.98
C(8S)-C(9S)	1.39	C(7E)-H(7EC)	0.98
C(8S)-C(13S)	1.39	C(1K)-C(2K)	1.39
C(8S)-H(8SA)	0.95	C(1K)-C(6K)	1.39
C(9S)-C(10S)	1.39	C(1K)-H(1KA)	0.95
C(9S)-H(9SA)	0.95	C(2K)-C(3K)	1.39
C(10S)-C(11S)	1.39	C(2K)-H(2KA)	0.95
C(10S)-H(10A)	0.95	C(3K)-C(4K)	1.39
C(11S)-C(12S)	1.39	C(3K)-H(3KA)	0.95

C(4K)-C(5K)	1.39	C(6K)-C(7K)	1.513(9)
C(4K)-H(4KA)	0.95	C(7K)-H(7KA)	0.98
C(5K)-C(6K)	1.39	C(7K)-H(7KB)	0.98
C(5K)-H(5KA)	0.95	C(7K)-H(7KC)	0.98

N(3)-Co-N(2)	89.79(17)	C(7)-C(2)-C(3)	119.4(5)
N(3)-Co-N(4)	90.37(17)	C(7)-C(2)-C(1)	107.2(4)
N(2)-Co-N(4)	176.82(18)	C(3)-C(2)-C(1)	133.4(5)
N(3)-Co-N(1)	175.35(17)	F(2)-C(3)-C(2)	117.8(5)
N(2)-Co-N(1)	89.99(17)	F(2)-C(3)-C(4)	119.6(5)
N(4)-Co-N(1)	89.58(17)	C(2)-C(3)-C(4)	122.6(5)
N(3)-Co-O#1	82.07(16)	C(3)-C(4)-C(5)	117.3(5)
N(2)-Co-O#1	88.86(16)	C(3)-C(4)-C(9)	115.3(5)
N(4)-Co-O#1	94.30(17)	C(5)-C(4)-C(9)	127.2(5)
N(1)-Co-O#1	102.57(16)	C(6)-C(5)-C(4)	117.6(5)
C(1)-N(1)-C(8)	108.4(4)	C(6)-C(5)-C(12)	116.7(5)
C(1)-N(1)-Co	125.6(3)	C(4)-C(5)-C(12)	125.5(5)
C(8)-N(1)-Co	126.0(3)	F(1)-C(6)-C(5)	119.4(5)
C(22)-N(2)-C(15)	107.9(4)	F(1)-C(6)-C(7)	117.9(5)
C(22)-N(2)-Co	126.2(3)	C(5)-C(6)-C(7)	122.6(5)
C(15)-N(2)-Co	125.5(3)	C(2)-C(7)-C(6)	119.3(5)
C(29)-N(3)-C(36)	107.5(4)	C(2)-C(7)-C(8)	107.0(4)
C(29)-N(3)-Co	126.6(3)	C(6)-C(7)-C(8)	133.7(5)
C(36)-N(3)-Co	125.2(3)	N(6)-C(8)-N(1)	128.2(4)
C(44)-N(4)-C(37)	107.3(4)	N(6)-C(8)-C(7)	123.0(4)
C(44)-N(4)-Co	126.9(3)	N(1)-C(8)-C(7)	108.8(4)
C(37)-N(4)-Co	125.7(3)	F(3)-C(9)-C(11)	106.0(5)
C(1)-N(5)-C(44)	120.4(4)	F(3)-C(9)-C(4)	110.1(4)
C(15)-N(6)-C(8)	120.9(4)	C(11)-C(9)-C(4)	112.8(5)
C(22)-N(7)-C(29)	121.0(4)	F(3)-C(9)-C(10)	102.3(5)
C(36)-N(8)-C(37)	121.3(4)	C(11)-C(9)-C(10)	110.3(5)
C(51)-N(12)-C(33)	118.0(4)	C(4)-C(9)-C(10)	114.6(5)
C(51)-N(12)-C(53)	123.7(5)	F(5)-C(10)-F(4)	108.2(5)
C(33)-N(12)-C(53)	118.2(4)	F(5)-C(10)-F(6)	106.5(5)
N(12)-C(53)-H(53A)	109.5	F(4)-C(10)-F(6)	107.6(5)
N(12)-C(53)-H(53B)	109.5	F(5)-C(10)-C(9)	114.7(5)
H(53A)-C(53)-H(53B)	109.5	F(4)-C(10)-C(9)	111.0(5)
N(12)-C(53)-H(53C)	109.5	F(6)-C(10)-C(9)	108.5(5)
H(53A)-C(53)-H(53C)	109.5	F(8)-C(11)-F(7)	108.0(5)
H(53B)-C(53)-H(53C)	109.5	F(8)-C(11)-F(9)	107.2(5)
C(51)-O-Co#1	144.8(4)	F(7)-C(11)-F(9)	105.7(5)
N(5)-C(1)-N(1)	129.4(4)	F(8)-C(11)-C(9)	110.9(5)
N(5)-C(1)-C(2)	122.0(5)	F(7)-C(11)-C(9)	113.4(5)
N(1)-C(1)-C(2)	108.6(4)	F(9)-C(11)-C(9)	111.3(5)

F(10)-C(12)-C(13)	106.0(4)	C(18)-C(23)-C(25)	113.1(6)
F(10)-C(12)-C(5)	109.8(4)	F(19)-C(23)-C(24)	101.7(6)
C(13)-C(12)-C(5)	114.7(5)	C(18)-C(23)-C(24)	114.0(6)
F(10)-C(12)-C(14)	101.0(5)	C(25)-C(23)-C(24)	109.5(6)
C(13)-C(12)-C(14)	109.1(5)	F(21)-C(24)-F(22)	107.3(6)
C(5)-C(12)-C(14)	115.1(5)	F(21)-C(24)-F(20)	108.7(7)
F(11)-C(13)-F(13)	108.6(6)	F(22)-C(24)-F(20)	107.0(8)
F(11)-C(13)-F(12)	108.5(5)	F(21)-C(24)-C(23)	114.6(8)
F(13)-C(13)-F(12)	106.4(5)	F(22)-C(24)-C(23)	108.8(6)
F(11)-C(13)-C(12)	111.1(5)	F(20)-C(24)-C(23)	110.1(6)
F(13)-C(13)-C(12)	112.5(5)	F(23)-C(25)-F(24)	108.6(6)
F(12)-C(13)-C(12)	109.5(5)	F(23)-C(25)-F(25)	107.5(9)
F(16)-C(14)-F(15)	107.7(5)	F(24)-C(25)-F(25)	107.5(7)
F(16)-C(14)-F(14)	107.3(6)	F(23)-C(25)-C(23)	113.4(6)
F(15)-C(14)-F(14)	106.1(5)	F(24)-C(25)-C(23)	109.5(8)
F(16)-C(14)-C(12)	111.0(5)	F(25)-C(25)-C(23)	110.2(6)
F(15)-C(14)-C(12)	115.2(6)	F(26)-C(26)-C(28)	107.4(5)
F(14)-C(14)-C(12)	109.1(5)	F(26)-C(26)-C(19)	109.7(5)
N(6)-C(15)-N(2)	128.8(4)	C(28)-C(26)-C(19)	113.1(6)
N(6)-C(15)-C(16)	122.0(4)	F(26)-C(26)-C(27)	101.4(5)
N(2)-C(15)-C(16)	109.1(4)	C(28)-C(26)-C(27)	111.2(5)
C(21)-C(16)-C(17)	119.7(5)	C(19)-C(26)-C(27)	113.2(5)
C(21)-C(16)-C(15)	107.2(4)	F(29)-C(27)-F(28)	109.5(6)
C(17)-C(16)-C(15)	133.2(5)	F(29)-C(27)-F(27)	107.2(6)
F(17)-C(17)-C(16)	117.5(5)	F(28)-C(27)-F(27)	106.0(5)
F(17)-C(17)-C(18)	119.2(5)	F(29)-C(27)-C(26)	111.6(5)
C(16)-C(17)-C(18)	123.3(5)	F(28)-C(27)-C(26)	113.4(6)
C(17)-C(18)-C(19)	117.0(5)	F(27)-C(27)-C(26)	108.8(6)
C(17)-C(18)-C(23)	116.1(5)	F(30)-C(28)-F(32)	108.2(6)
C(19)-C(18)-C(23)	126.9(5)	F(30)-C(28)-F(31)	107.6(8)
C(20)-C(19)-C(18)	118.1(5)	F(32)-C(28)-F(31)	107.5(6)
C(20)-C(19)-C(26)	115.6(5)	F(30)-C(28)-C(26)	112.7(5)
C(18)-C(19)-C(26)	126.3(5)	F(32)-C(28)-C(26)	110.0(7)
F(18)-C(20)-C(21)	118.0(4)	F(31)-C(28)-C(26)	110.6(6)
F(18)-C(20)-C(19)	119.6(5)	N(7)-C(29)-N(3)	127.9(4)
C(21)-C(20)-C(19)	122.4(5)	N(7)-C(29)-C(30)	122.2(4)
C(16)-C(21)-C(20)	119.1(5)	N(3)-C(29)-C(30)	109.6(4)
C(16)-C(21)-C(22)	106.7(4)	C(31)-C(30)-C(35)	120.0(5)
C(20)-C(21)-C(22)	134.1(5)	C(31)-C(30)-C(29)	134.0(5)
N(7)-C(22)-N(2)	128.3(4)	C(35)-C(30)-C(29)	106.0(4)
N(7)-C(22)-C(21)	122.7(4)	F(34)-C(31)-C(30)	122.4(5)
N(2)-C(22)-C(21)	109.0(4)	F(34)-C(31)-C(32)	119.6(5)
F(19)-C(23)-C(18)	110.6(5)	C(30)-C(31)-C(32)	117.9(5)
F(19)-C(23)-C(25)	107.2(6)	F(35)-C(32)-C(31)	117.7(5)

F(35)-C(32)-C(33)	119.3(5)	F(47)-C(46)-F(48)	110.3(7)
C(31)-C(32)-C(33)	123.0(5)	F(47)-C(46)-F(46)	107.2(7)
C(34)-C(33)-C(32)	117.9(5)	F(48)-C(46)-F(46)	107.0(8)
C(34)-C(33)-N(12)	119.5(5)	F(47)-C(46)-C(45)	112.9(8)
C(32)-C(33)-N(12)	122.6(5)	F(48)-C(46)-C(45)	110.3(6)
F(33)-C(34)-C(35)	121.0(5)	F(46)-C(46)-C(45)	108.9(7)
F(33)-C(34)-C(33)	119.1(5)	F(49)-C(47)-F(50)	112.0(9)
C(35)-C(34)-C(33)	119.8(5)	F(49)-C(47)-F(51)	107.1(9)
C(34)-C(35)-C(30)	121.2(5)	F(50)-C(47)-F(51)	105.3(7)
C(34)-C(35)-C(36)	132.0(5)	F(49)-C(47)-C(45)	115.3(7)
C(30)-C(35)-C(36)	106.8(4)	F(50)-C(47)-C(45)	109.1(8)
N(8)-C(36)-N(3)	128.4(5)	F(51)-C(47)-C(45)	107.5(8)
N(8)-C(36)-C(35)	121.7(4)	F(38)-C(48)-C(49)	112.9(7)
N(3)-C(36)-C(35)	109.9(4)	F(38)-C(48)-C(40)	111.0(5)
N(8)-C(37)-N(4)	127.7(5)	C(49)-C(48)-C(40)	112.6(7)
N(8)-C(37)-C(38)	122.4(4)	F(38)-C(48)-C(50)	94.4(6)
N(4)-C(37)-C(38)	109.9(4)	C(49)-C(48)-C(50)	111.5(6)
C(43)-C(38)-C(39)	118.7(5)	C(40)-C(48)-C(50)	113.2(5)
C(43)-C(38)-C(37)	106.9(4)	F(41)-C(49)-F(39)	110.0(8)
C(39)-C(38)-C(37)	134.4(5)	F(41)-C(49)-F(40)	110.9(10)
F(37)-C(39)-C(40)	119.2(5)	F(39)-C(49)-F(40)	105.6(8)
F(37)-C(39)-C(38)	117.1(5)	F(41)-C(49)-C(48)	112.3(7)
C(40)-C(39)-C(38)	123.7(5)	F(39)-C(49)-C(48)	112.6(9)
C(39)-C(40)-C(41)	117.6(5)	F(40)-C(49)-C(48)	105.1(8)
C(39)-C(40)-C(48)	116.2(5)	F(43)-C(50)-F(42)	113.1(7)
C(41)-C(40)-C(48)	126.2(5)	F(43)-C(50)-F(44)	112.3(7)
C(42)-C(41)-C(40)	117.1(5)	F(42)-C(50)-F(44)	105.6(5)
C(42)-C(41)-C(45)	115.3(5)	F(43)-C(50)-C(48)	113.5(5)
C(40)-C(41)-C(45)	127.6(5)	F(42)-C(50)-C(48)	104.2(6)
F(36)-C(42)-C(43)	117.7(5)	F(44)-C(50)-C(48)	107.5(6)
F(36)-C(42)-C(41)	119.3(5)	O-C(51)-N(12)	119.0(5)
C(43)-C(42)-C(41)	123.0(5)	O-C(51)-C(52)	122.7(5)
C(42)-C(43)-C(38)	119.9(5)	N(12)-C(51)-C(52)	118.4(5)
C(42)-C(43)-C(44)	133.8(5)	C(51)-C(52)-H(52A)	109.5
C(38)-C(43)-C(44)	106.3(4)	C(51)-C(52)-H(52B)	109.5
N(5)-C(44)-N(4)	127.9(5)	H(52A)-C(52)-H(52B)	109.5
N(5)-C(44)-C(43)	122.5(5)	C(51)-C(52)-H(52C)	109.5
N(4)-C(44)-C(43)	109.5(4)	H(52A)-C(52)-H(52C)	109.5
F(45)-C(45)-C(41)	111.2(5)	H(52B)-C(52)-H(52C)	109.5
F(45)-C(45)-C(46)	101.8(6)	C(2S)-C(1S)-C(6S)	120
C(41)-C(45)-C(46)	112.8(6)	C(2S)-C(1S)-H(1SA)	120
F(45)-C(45)-C(47)	103.5(7)	C(6S)-C(1S)-H(1SA)	120
C(41)-C(45)-C(47)	115.2(5)	C(3S)-C(2S)-C(1S)	120
C(46)-C(45)-C(47)	111.1(7)	C(3S)-C(2S)-H(2SA)	120

C(1S)-C(2S)-H(2SA)	120
C(4S)-C(3S)-C(2S)	120
C(4S)-C(3S)-H(3SA)	120
C(2S)-C(3S)-H(3SA)	120
C(3S)-C(4S)-C(5S)	120
C(3S)-C(4S)-H(4SA)	120
C(5S)-C(4S)-H(4SA)	120
C(4S)-C(5S)-C(6S)	120
C(4S)-C(5S)-H(5SA)	120
C(6S)-C(5S)-H(5SA)	120
C(5S)-C(6S)-C(1S)	120
C(5S)-C(6S)-C(7S)	120.1(10)
C(1S)-C(6S)-C(7S)	119.8(10)
C(6S)-C(7S)-H(7SA)	109.5
C(6S)-C(7S)-H(7SB)	109.5
H(7SA)-C(7S)-H(7SB)	109.5
C(6S)-C(7S)-H(7SC)	109.5
H(7SA)-C(7S)-H(7SC)	109.5
H(7SB)-C(7S)-H(7SC)	109.5
C(9S)-C(8S)-C(13S)	120
C(9S)-C(8S)-H(8SA)	120
C(13S)-C(8S)-H(8SA)	120
C(10S)-C(9S)-C(8S)	120
C(10S)-C(9S)-H(9SA)	120
C(8S)-C(9S)-H(9SA)	120
C(9S)-C(10S)-C(11S)	120
C(9S)-C(10S)-H(10A)	120
C(11S)-C(10S)-H(10A)	120
C(12S)-C(11S)-C(10S)	120
C(12S)-C(11S)-H(11A)	120
C(10S)-C(11S)-H(11A)	120
C(11S)-C(12S)-C(13S)	120
C(11S)-C(12S)-H(12A)	120
C(13S)-C(12S)-H(12A)	120
C(12S)-C(13S)-C(8S)	120
C(12S)-C(13S)-C(14S)	117.5(16)
C(8S)-C(13S)-C(14S)	122.5(16)
C(13S)-C(14S)-H(14A)	109.5
C(13S)-C(14S)-H(14B)	109.5
H(14A)-C(14S)-H(14B)	109.5
C(13S)-C(14S)-H(14C)	109.5
H(14A)-C(14S)-H(14C)	109.5
H(14B)-C(14S)-H(14C)	109.5
C(6T)-C(1T)-C(2T)	120.8(9)
C(6T)-C(1T)-H(1TA)	119.6
C(2T)-C(1T)-H(1TA)	119.6
C(3T)-C(2T)-C(1T)	121.6(9)
C(3T)-C(2T)-H(2TA)	119.2
C(1T)-C(2T)-H(2TA)	119.2
C(4T)-C(3T)-C(2T)	117.5(10)
C(4T)-C(3T)-H(3TA)	121.3
C(2T)-C(3T)-H(3TA)	121.3
C(3T)-C(4T)-C(5T)	119.4(10)
C(3T)-C(4T)-H(4TA)	120.3
C(5T)-C(4T)-H(4TA)	120.3
C(6T)-C(5T)-C(4T)	124.4(11)
C(6T)-C(5T)-H(5TA)	117.8
C(4T)-C(5T)-H(5TA)	117.8
C(1T)-C(6T)-C(5T)	116.2(10)
C(1T)-C(6T)-C(7T)	119.0(10)
C(5T)-C(6T)-C(7T)	124.7(11)
C(6T)-C(7T)-H(7TA)	109.5
C(6T)-C(7T)-H(7TB)	109.5
H(7TA)-C(7T)-H(7TB)	109.5
C(6T)-C(7T)-H(7TC)	109.5
H(7TA)-C(7T)-H(7TC)	109.5
H(7TB)-C(7T)-H(7TC)	109.5
C(2E)-C(1E)-C(6E)	120
C(2E)-C(1E)-H(1EA)	120
C(6E)-C(1E)-H(1EA)	120
C(1E)-C(2E)-C(3E)	120
C(1E)-C(2E)-H(2EA)	120
C(3E)-C(2E)-H(2EA)	120
C(4E)-C(3E)-C(2E)	120
C(4E)-C(3E)-H(3EA)	120
C(2E)-C(3E)-H(3EA)	120
C(3E)-C(4E)-C(5E)	120
C(3E)-C(4E)-H(4EA)	120
C(5E)-C(4E)-H(4EA)	120
C(4E)-C(5E)-C(6E)	120
C(4E)-C(5E)-H(5EA)	120
C(6E)-C(5E)-H(5EA)	120
C(5E)-C(6E)-C(1E)	120
C(5E)-C(6E)-C(7E)	112.7(13)
C(1E)-C(6E)-C(7E)	127.2(13)

C(6E)-C(7E)-H(7EA)	109.5	C(3K)-C(4K)-H(4KA)	120
C(6E)-C(7E)-H(7EB)	109.5	C(6K)-C(5K)-C(4K)	120
H(7EA)-C(7E)-H(7EB)	109.5	C(6K)-C(5K)-H(5KA)	120
C(6E)-C(7E)-H(7EC)	109.5	C(4K)-C(5K)-H(5KA)	120
H(7EA)-C(7E)-H(7EC)	109.5	C(5K)-C(6K)-C(1K)	120
H(7EB)-C(7E)-H(7EC)	109.5	C(5K)-C(6K)-C(7K)	117.9(12)
C(2K)-C(1K)-C(6K)	120	C(1K)-C(6K)-C(7K)	122.1(12)
C(2K)-C(1K)-H(1KA)	120	C(6K)-C(7K)-H(7KA)	109.5
C(6K)-C(1K)-H(1KA)	120	C(6K)-C(7K)-H(7KB)	109.5
C(3K)-C(2K)-C(1K)	120	H(7KA)-C(7K)-H(7KB)	109.5
C(3K)-C(2K)-H(2KA)	120	C(6K)-C(7K)-H(7KC)	109.5
C(1K)-C(2K)-H(2KA)	120	H(7KA)-C(7K)-H(7KC)	109.5
C(2K)-C(3K)-C(4K)	120	H(7KB)-C(7K)-H(7KC)	109.5
C(2K)-C(3K)-H(3KA)	120		
C(4K)-C(3K)-H(3KA)	120		
C(5K)-C(4K)-C(3K)	120		
C(5K)-C(4K)-H(4KA)	120		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table T.4 Anisotropic displacement parameters ($Å^2$ x 10^3) **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**. 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}
Co	16(1)	19(1)	33(1)	0(1)	8(1)	-1(1)
N(1)	21(2)	20(2)	26(2)	1(2)	8(2)	1(2)
N(2)	19(2)	22(2)	30(2)	-2(2)	7(2)	-2(2)
N(3)	23(2)	20(2)	25(2)	-1(2)	9(2)	-1(2)
N(4)	17(2)	25(2)	36(2)	0(2)	8(2)	-2(2)
N(5)	19(2)	25(2)	39(2)	7(2)	10(2)	-1(2)
N(6)	20(2)	22(2)	39(2)	0(2)	9(2)	0(2)
N(7)	20(2)	22(2)	31(2)	-3(2)	10(2)	0(2)
N(8)	20(2)	25(2)	33(2)	1(2)	5(2)	-2(2)
N(12)	22(2)	34(2)	36(2)	11(2)	9(2)	2(2)
C(53)	33(3)	48(4)	51(4)	19(3)	15(3)	2(3)
O	26(2)	29(2)	39(2)	5(2)	9(2)	-4(2)
C(1)	20(2)	27(3)	33(3)	2(2)	7(2)	-3(2)
C(2)	19(2)	28(3)	34(3)	0(2)	7(2)	-3(2)
C(3)	25(3)	27(3)	40(3)	8(2)	9(2)	0(2)
C(4)	19(2)	33(3)	42(3)	3(2)	8(2)	0(2)
C(5)	23(3)	30(3)	46(3)	6(2)	9(2)	-5(2)
C(6)	20(2)	26(3)	45(3)	8(2)	7(2)	-3(2)
C(7)	16(2)	30(3)	37(3)	2(2)	5(2)	-1(2)
C(8)	19(2)	23(2)	34(3)	0(2)	8(2)	-3(2)

C(9)	22(3)	35(3)	56(4)	8(3)	11(3)	-6(2)
C(10)	34(3)	30(3)	58(4)	8(3)	1(3)	-6(2)
C(11)	29(3)	39(3)	58(4)	17(3)	12(3)	4(2)
C(12)	17(2)	34(3)	57(4)	12(3)	12(2)	3(2)
C(13)	28(3)	47(4)	54(4)	6(3)	12(3)	-5(3)
C(14)	30(3)	45(3)	54(4)	13(3)	14(3)	2(3)
C(15)	23(2)	20(2)	25(2)	-3(2)	8(2)	-4(2)
C(16)	24(2)	22(2)	32(3)	-2(2)	10(2)	0(2)
C(17)	26(3)	26(3)	40(3)	3(2)	13(2)	0(2)
C(18)	32(3)	27(3)	49(3)	9(2)	17(3)	-1(2)
C(19)	35(3)	23(3)	48(3)	4(2)	19(3)	4(2)
C(20)	25(3)	22(2)	40(3)	1(2)	13(2)	3(2)
C(21)	23(2)	23(2)	31(3)	-1(2)	9(2)	-2(2)
C(22)	26(2)	18(2)	29(3)	-2(2)	12(2)	2(2)
C(23)	30(3)	34(3)	88(5)	26(3)	18(3)	2(3)
C(24)	53(5)	31(3)	116(7)	13(4)	25(5)	-11(3)
C(25)	49(4)	75(6)	96(6)	42(5)	39(5)	1(4)
C(26)	35(3)	35(3)	68(4)	25(3)	22(3)	5(3)
C(27)	38(3)	59(4)	57(4)	27(3)	20(3)	12(3)
C(28)	52(4)	29(3)	108(6)	17(4)	31(4)	13(3)
C(29)	19(2)	26(2)	30(3)	-2(2)	10(2)	0(2)
C(30)	23(3)	30(3)	27(3)	-2(2)	9(2)	-2(2)
C(31)	27(3)	27(3)	34(3)	4(2)	12(2)	4(2)
C(32)	21(3)	43(3)	28(3)	4(2)	9(2)	9(2)
C(33)	24(3)	35(3)	28(3)	5(2)	6(2)	0(2)
C(34)	26(3)	30(3)	36(3)	4(2)	9(2)	-3(2)
C(35)	22(2)	27(3)	33(3)	4(2)	7(2)	1(2)
C(36)	22(2)	23(2)	30(3)	-3(2)	9(2)	-1(2)
C(37)	20(2)	26(2)	30(3)	0(2)	9(2)	-2(2)
C(38)	26(3)	24(2)	33(3)	0(2)	12(2)	1(2)
C(39)	26(3)	30(3)	39(3)	1(2)	13(2)	-2(2)
C(40)	32(3)	27(3)	48(3)	7(2)	18(3)	-1(2)
C(41)	33(3)	28(3)	43(3)	5(2)	15(2)	2(2)
C(42)	25(3)	26(3)	47(3)	7(2)	14(2)	2(2)
C(43)	25(3)	24(2)	34(3)	1(2)	13(2)	-4(2)
C(44)	23(2)	22(2)	32(3)	2(2)	8(2)	0(2)
C(45)	35(3)	25(3)	55(4)	10(3)	15(3)	0(2)
C(46)	63(5)	53(5)	92(6)	-1(4)	19(5)	3(4)
C(47)	109(8)	52(5)	75(6)	-6(4)	-38(6)	35(5)
C(48)	37(4)	44(4)	100(6)	37(4)	31(4)	3(3)
C(49)	71(6)	97(7)	86(7)	23(6)	36(5)	-16(5)
C(50)	45(4)	35(3)	84(5)	-4(3)	29(4)	-16(3)
C(51)	25(3)	30(3)	45(3)	2(2)	14(2)	3(2)
C(52)	31(3)	39(3)	51(4)	8(3)	9(3)	-10(2)

F(1)	23(2)	28(2)	66(2)	16(2)	11(2)	-2(1)
F(2)	24(2)	33(2)	61(2)	21(2)	13(2)	2(1)
F(3)	21(2)	43(2)	66(2)	18(2)	1(2)	-4(1)
F(4)	62(3)	51(2)	48(2)	2(2)	10(2)	6(2)
F(5)	43(2)	42(2)	56(2)	16(2)	4(2)	-6(2)
F(6)	40(2)	58(2)	67(3)	21(2)	-11(2)	-9(2)
F(7)	44(2)	36(2)	73(3)	6(2)	28(2)	-4(2)
F(8)	35(2)	54(2)	96(3)	17(2)	12(2)	16(2)
F(9)	49(2)	48(2)	63(2)	7(2)	29(2)	3(2)
F(10)	26(2)	44(2)	70(2)	19(2)	19(2)	9(1)
F(11)	58(3)	54(2)	64(3)	8(2)	-11(2)	-12(2)
F(12)	41(2)	73(3)	95(3)	-2(2)	29(2)	-24(2)
F(13)	45(2)	35(2)	74(3)	3(2)	6(2)	-6(2)
F(14)	44(2)	75(3)	69(3)	30(2)	32(2)	19(2)
F(15)	55(2)	63(3)	63(3)	27(2)	23(2)	22(2)
F(16)	66(3)	83(3)	47(2)	-4(2)	20(2)	-23(2)
F(17)	24(2)	30(2)	64(2)	11(2)	14(2)	0(1)
F(18)	26(2)	26(2)	52(2)	8(1)	16(1)	5(1)
F(19)	48(2)	31(2)	130(4)	29(2)	31(2)	3(2)
F(20)	63(3)	49(2)	87(3)	-12(2)	5(2)	-10(2)
F(21)	35(2)	51(2)	128(4)	29(3)	17(2)	-8(2)
F(22)	68(3)	32(2)	190(6)	13(3)	8(4)	-22(2)
F(23)	61(3)	87(3)	91(3)	33(3)	49(3)	21(3)
F(24)	67(3)	104(4)	164(6)	77(4)	62(4)	3(3)
F(25)	64(3)	130(5)	78(3)	49(3)	34(3)	22(3)
F(26)	46(2)	56(2)	87(3)	42(2)	32(2)	11(2)
F(27)	50(2)	93(3)	73(3)	49(3)	20(2)	19(2)
F(28)	34(2)	66(3)	69(3)	27(2)	19(2)	12(2)
F(29)	47(2)	62(3)	53(2)	9(2)	18(2)	10(2)
F(30)	63(3)	31(2)	98(3)	-1(2)	44(2)	3(2)
F(31)	71(3)	36(2)	136(5)	-9(3)	39(3)	-9(2)
F(32)	79(3)	43(2)	141(5)	34(3)	45(3)	33(2)
F(33)	24(2)	27(2)	63(2)	10(2)	10(2)	-1(1)
F(34)	28(2)	30(2)	50(2)	5(1)	11(1)	5(1)
F(35)	22(2)	38(2)	48(2)	6(1)	10(1)	6(1)
F(36)	23(2)	32(2)	78(3)	16(2)	13(2)	3(1)
F(37)	22(2)	32(2)	63(2)	6(2)	15(2)	-3(1)
F(38)	59(3)	39(2)	194(6)	38(3)	56(3)	7(2)
F(39)	77(4)	152(6)	132(5)	71(5)	50(4)	-20(4)
F(40)	73(4)	136(6)	109(5)	64(4)	8(3)	-11(4)
F(41)	86(4)	129(5)	79(3)	42(3)	57(3)	48(4)
F(42)	70(3)	43(3)	190(6)	-9(3)	49(4)	-21(2)
F(43)	60(3)	62(3)	96(4)	-15(3)	18(3)	-12(2)
F(44)	49(3)	66(3)	146(5)	21(3)	38(3)	-5(2)

F(45)	48(2)	55(3)	163(5)	61(3)	24(3)	4(2)
F(46)	73(3)	70(3)	123(5)	-29(3)	31(3)	-13(3)
F(47)	55(3)	34(2)	130(4)	3(2)	30(3)	18(2)
F(48)	60(3)	52(2)	83(3)	-3(2)	42(2)	-3(2)
F(49)	109(4)	71(3)	61(3)	-17(2)	12(3)	-20(3)
F(50)	71(3)	93(4)	79(3)	40(3)	-10(3)	3(3)
F(51)	31(2)	61(3)	210(7)	57(4)	-1(3)	3(2)
C(1S)	61(8)	57(8)	31(6)	-9(5)	11(6)	1(7)
C(2S)	37(11)	80(20)	72(18)	-41(15)	0(10)	8(11)
C(3S)	72(9)	61(9)	58(8)	-29(7)	31(7)	-11(7)
C(4S)	88(10)	47(7)	47(7)	-9(6)	25(7)	-1(7)
C(5S)	61(8)	48(7)	53(7)	-20(6)	11(6)	8(6)
C(6S)	49(11)	56(9)	33(7)	-14(7)	7(6)	6(7)
C(7S)	61(9)	71(10)	62(9)	-16(8)	21(7)	-9(8)
C(8S)	170(30)	110(20)	60(15)	-49(15)	65(19)	-80(20)
C(9S)	120(40)	140(50)	40(20)	-10(20)	50(20)	-20(30)
C(10S)	84(19)	150(30)	69(16)	-38(17)	28(13)	22(18)
C(11S)	89(16)	84(15)	49(11)	-21(10)	11(10)	21(13)
C(12S)	73(13)	53(10)	51(10)	-12(8)	12(9)	-2(9)
C(13S)	90(30)	69(15)	18(9)	-9(10)	10(11)	-7(15)
C(14S)	140(30)	53(13)	67(15)	-11(12)	-21(15)	2(15)
C(1T)	57(5)	105(7)	68(5)	-10(5)	20(4)	-16(5)
C(2T)	69(6)	80(6)	85(6)	-3(5)	13(5)	7(5)
C(3T)	79(6)	65(5)	69(5)	-11(4)	29(5)	-6(5)
C(4T)	61(6)	100(8)	110(8)	4(6)	30(6)	-12(5)
C(5T)	67(7)	124(10)	180(14)	59(10)	32(8)	22(7)
C(6T)	57(6)	101(8)	106(8)	22(6)	0(5)	-7(5)
C(7T)	136(14)	151(15)	250(20)	129(16)	19(14)	-5(11)
C(1E)	214(12)	67(6)	95(7)	16(6)	45(7)	5(9)
C(2E)	207(12)	73(7)	114(8)	-3(7)	38(9)	-30(9)
C(3E)	219(13)	63(6)	122(8)	19(7)	47(8)	-27(8)
C(4E)	234(13)	59(6)	123(9)	30(7)	27(8)	-11(9)
C(5E)	214(12)	69(7)	109(7)	21(7)	8(9)	7(9)
C(6E)	207(11)	75(7)	136(8)	15(8)	35(8)	8(9)
C(7E)	237(15)	200(20)	270(30)	-90(20)	92(16)	-37(18)
C(1K)	84(14)	36(6)	89(11)	13(17)	11(10)	9(12)
C(2K)	95(15)	45(11)	92(15)	-7(11)	18(12)	-14(11)
C(3K)	61(10)	48(10)	63(12)	-1(8)	8(9)	-10(8)
C(4K)	83(18)	43(10)	83(19)	-3(11)	9(15)	7(12)
C(5K)	73(14)	26(7)	71(17)	-4(7)	-16(14)	-2(10)
C(6K)	46(10)	70(15)	79(15)	29(12)	-2(9)	9(10)
C(7K)	51(9)	83(13)	89(13)	9(11)	20(9)	0(9)

Table T.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**.

	x	y	z	U(eq)
H(53A)	11277	3587	6115	65
H(53B)	11962	3342	6112	65
H(53C)	12049	3719	6500	65
H(52A)	13110	3467	7879	62
H(52B)	12649	3782	7449	62
H(52C)	13041	3453	7195	62
H(1SA)	7019	2940	4781	60
H(2SA)	8175	3139	4836	80
H(3SA)	8357	3719	4424	73
H(4SA)	7385	4102	3957	72
H(5SA)	6230	3903	3903	66
H(7SA)	5465	3286	3918	96
H(7SB)	5583	3455	4561	96
H(7SC)	5786	3022	4478	96
H(8SA)	7182	3741	4252	131
H(9SA)	8251	3409	4610	111
H(10A)	8253	2805	5019	119
H(11A)	7184	2532	5069	91
H(12A)	6114	2864	4711	72
H(14A)	5496	3351	3962	144
H(14B)	5893	3749	3973	144
H(14C)	5661	3614	4531	144
H(1TA)	1439	3140	5011	91
H(2TA)	1355	2571	5477	96
H(3TA)	258	2329	5490	84
H(4TA)	-746	2686	5062	107
H(5TA)	-638	3251	4621	149
H(7TA)	294	3838	4699	281
H(7TB)	238	3634	4089	281
H(7TC)	998	3687	4560	281
H(1EA)	7953	5460	1725	150
H(2EA)	6816	5403	1846	160
H(3EA)	6668	5424	2784	162
H(4EA)	7657	5503	3599	172
H(5EA)	8794	5560	3478	166
H(7EA)	9324	5856	2567	351
H(7EB)	9331	5454	2257	351
H(7EC)	9564	5482	2954	351
H(1KA)	4821	4690	7620	87
H(2KA)	5258	4574	6822	95
H(3KA)	5491	3951	6588	71
H(4KA)	5287	3444	7152	87
H(5KA)	4850	3560	7950	77
H(7KA)	4185	3987	8398	112
H(7KB)	4253	4437	8336	112
H(7KC)	4906	4199	8738	112

Table T.6 Torsion angles [deg] for **[NMeAcF$_{51}$PcCo]$_2$·7(toluene)**.

C(44)-N(5)-C(1)-N(1)	0.4(9)	C(2)-C(7)-C(8)-N(1)	3.4(6)
C(44)-N(5)-C(1)-C(2)	176.5(5)	C(6)-C(7)-C(8)-N(1)	-172.8(6)
C(8)-N(1)-C(1)-N(5)	176.7(5)	C(3)-C(4)-C(9)-F(3)	162.1(5)
Co-N(1)-C(1)-N(5)	-1.9(8)	C(5)-C(4)-C(9)-F(3)	-13.7(9)
C(8)-N(1)-C(1)-C(2)	0.2(6)	C(3)-C(4)-C(9)-C(11)	-79.8(7)
Co-N(1)-C(1)-C(2)	-178.4(3)	C(5)-C(4)-C(9)-C(11)	104.4(7)
N(5)-C(1)-C(2)-C(7)	-174.9(5)	C(3)-C(4)-C(9)-C(10)	47.5(7)
N(1)-C(1)-C(2)-C(7)	1.9(6)	C(5)-C(4)-C(9)-C(10)	-128.4(6)
N(5)-C(1)-C(2)-C(3)	7.2(10)	F(3)-C(9)-C(10)-F(5)	144.8(5)
N(1)-C(1)-C(2)-C(3)	-176.0(6)	C(11)-C(9)-C(10)-F(5)	32.4(7)
C(7)-C(2)-C(3)-F(2)	-172.1(5)	C(4)-C(9)-C(10)-F(5)	-96.1(6)
C(1)-C(2)-C(3)-F(2)	5.6(9)	F(3)-C(9)-C(10)-F(4)	-92.3(5)
C(7)-C(2)-C(3)-C(4)	5.8(9)	C(11)-C(9)-C(10)-F(4)	155.4(5)
C(1)-C(2)-C(3)-C(4)	-176.4(6)	C(4)-C(9)-C(10)-F(4)	26.8(7)
F(2)-C(3)-C(4)-C(5)	-178.4(5)	F(3)-C(9)-C(10)-F(6)	25.8(6)
C(2)-C(3)-C(4)-C(5)	3.6(9)	C(11)-C(9)-C(10)-F(6)	-86.6(6)
F(2)-C(3)-C(4)-C(9)	5.3(8)	C(4)-C(9)-C(10)-F(6)	144.9(5)
C(2)-C(3)-C(4)-C(9)	-172.7(5)	F(3)-C(9)-C(11)-F(8)	-53.2(6)
C(3)-C(4)-C(5)-C(6)	-10.6(8)	C(4)-C(9)-C(11)-F(8)	-173.7(5)
C(9)-C(4)-C(5)-C(6)	165.2(6)	C(10)-C(9)-C(11)-F(8)	56.8(6)
C(3)-C(4)-C(5)-C(12)	164.3(6)	F(3)-C(9)-C(11)-F(7)	-175.0(5)
C(9)-C(4)-C(5)-C(12)	-19.9(10)	C(4)-C(9)-C(11)-F(7)	64.5(7)
C(4)-C(5)-C(6)-F(1)	-175.7(5)	C(10)-C(9)-C(11)-F(7)	-65.0(6)
C(12)-C(5)-C(6)-F(1)	8.9(8)	F(3)-C(9)-C(11)-F(9)	66.0(6)
C(4)-C(5)-C(6)-C(7)	8.8(9)	C(4)-C(9)-C(11)-F(9)	-54.4(6)
C(12)-C(5)-C(6)-C(7)	-166.6(5)	C(10)-C(9)-C(11)-F(9)	176.0(5)
C(3)-C(2)-C(7)-C(6)	-8.0(8)	C(6)-C(5)-C(12)-F(10)	160.5(5)
C(1)-C(2)-C(7)-C(6)	173.7(5)	C(4)-C(5)-C(12)-F(10)	-14.6(8)
C(3)-C(2)-C(7)-C(8)	175.2(5)	C(6)-C(5)-C(12)-C(13)	-80.4(7)
C(1)-C(2)-C(7)-C(8)	-3.1(6)	C(4)-C(5)-C(12)-C(13)	104.6(7)
F(1)-C(6)-C(7)-C(2)	-174.9(5)	C(6)-C(5)-C(12)-C(14)	47.3(7)
C(5)-C(6)-C(7)-C(2)	0.6(9)	C(4)-C(5)-C(12)-C(14)	-127.7(6)
F(1)-C(6)-C(7)-C(8)	0.8(10)	F(10)-C(12)-C(13)-F(11)	63.1(6)
C(5)-C(6)-C(7)-C(8)	176.4(6)	C(5)-C(12)-C(13)-F(11)	-58.1(7)
C(15)-N(6)-C(8)-N(1)	-1.5(8)	C(14)-C(12)-C(13)-F(11)	171.2(5)
C(15)-N(6)-C(8)-C(7)	177.9(5)	F(10)-C(12)-C(13)-F(13)	-174.8(5)
C(1)-N(1)-C(8)-N(6)	177.3(5)	C(5)-C(12)-C(13)-F(13)	64.0(7)
Co-N(1)-C(8)-N(6)	-4.1(8)	C(14)-C(12)-C(13)-F(13)	-66.8(6)
C(1)-N(1)-C(8)-C(7)	-2.2(6)	F(10)-C(12)-C(13)-F(12)	-56.7(6)
Co-N(1)-C(8)-C(7)	176.4(3)	C(5)-C(12)-C(13)-F(12)	-178.0(5)
C(2)-C(7)-C(8)-N(6)	-176.1(5)	C(14)-C(12)-C(13)-F(12)	51.3(6)
C(6)-C(7)-C(8)-N(6)	7.7(10)	F(10)-C(12)-C(14)-F(16)	-85.8(6)

C(13)-C(12)-C(14)-F(16)	162.9(5)	C(15)-N(2)-C(22)-N(7)	-179.3(5)
C(5)-C(12)-C(14)-F(16)	32.4(7)	Co-N(2)-C(22)-N(7)	-6.0(7)
F(10)-C(12)-C(14)-F(15)	151.5(5)	C(15)-N(2)-C(22)-C(21)	-0.4(5)
C(13)-C(12)-C(14)-F(15)	40.2(6)	Co-N(2)-C(22)-C(21)	172.9(3)
C(5)-C(12)-C(14)-F(15)	-90.3(6)	C(16)-C(21)-C(22)-N(7)	179.1(5)
F(10)-C(12)-C(14)-F(14)	32.2(6)	C(20)-C(21)-C(22)-N(7)	3.1(9)
C(13)-C(12)-C(14)-F(14)	-79.1(6)	C(16)-C(21)-C(22)-N(2)	0.2(6)
C(5)-C(12)-C(14)-F(14)	150.4(5)	C(20)-C(21)-C(22)-N(2)	-175.8(6)
C(8)-N(6)-C(15)-N(2)	0.7(8)	C(17)-C(18)-C(23)-F(19)	159.2(6)
C(8)-N(6)-C(15)-C(16)	178.9(5)	C(19)-C(18)-C(23)-F(19)	-18.5(10)
C(22)-N(2)-C(15)-N(6)	178.9(5)	C(17)-C(18)-C(23)-C(25)	-80.5(7)
Co-N(2)-C(15)-N(6)	5.6(7)	C(19)-C(18)-C(23)-C(25)	101.7(7)
C(22)-N(2)-C(15)-C(16)	0.5(5)	C(17)-C(18)-C(23)-C(24)	45.3(8)
Co-N(2)-C(15)-C(16)	-172.8(3)	C(19)-C(18)-C(23)-C(24)	-132.4(7)
N(6)-C(15)-C(16)-C(21)	-178.9(5)	F(19)-C(23)-C(24)-F(21)	144.0(6)
N(2)-C(15)-C(16)-C(21)	-0.4(6)	C(18)-C(23)-C(24)-F(21)	-97.0(7)
N(6)-C(15)-C(16)-C(17)	2.1(9)	C(25)-C(23)-C(24)-F(21)	30.7(8)
N(2)-C(15)-C(16)-C(17)	-179.4(6)	F(19)-C(23)-C(24)-F(22)	23.9(9)
C(21)-C(16)-C(17)-F(17)	-177.1(5)	C(18)-C(23)-C(24)-F(22)	142.9(7)
C(15)-C(16)-C(17)-F(17)	1.8(9)	C(25)-C(23)-C(24)-F(22)	-89.4(8)
C(21)-C(16)-C(17)-C(18)	2.4(9)	F(19)-C(23)-C(24)-F(20)	-93.1(6)
C(15)-C(16)-C(17)-C(18)	-178.7(6)	C(18)-C(23)-C(24)-F(20)	25.9(8)
F(17)-C(17)-C(18)-C(19)	-177.0(5)	C(25)-C(23)-C(24)-F(20)	153.6(6)
C(16)-C(17)-C(18)-C(19)	3.5(9)	F(19)-C(23)-C(25)-F(23)	179.1(6)
F(17)-C(17)-C(18)-C(23)	5.0(8)	C(18)-C(23)-C(25)-F(23)	56.9(9)
C(16)-C(17)-C(18)-C(23)	-174.5(6)	C(24)-C(23)-C(25)-F(23)	-71.3(8)
C(17)-C(18)-C(19)-C(20)	-7.6(8)	F(19)-C(23)-C(25)-F(24)	-59.5(8)
C(23)-C(18)-C(19)-C(20)	170.1(6)	C(18)-C(23)-C(25)-F(24)	178.3(6)
C(17)-C(18)-C(19)-C(26)	169.0(6)	C(24)-C(23)-C(25)-F(24)	50.1(8)
C(23)-C(18)-C(19)-C(26)	-13.3(10)	F(19)-C(23)-C(25)-F(25)	58.5(8)
C(18)-C(19)-C(20)-F(18)	-175.7(5)	C(18)-C(23)-C(25)-F(25)	-63.6(8)
C(26)-C(19)-C(20)-F(18)	7.4(8)	C(24)-C(23)-C(25)-F(25)	168.1(6)
C(18)-C(19)-C(20)-C(21)	6.3(9)	C(20)-C(19)-C(26)-F(26)	158.4(5)
C(26)-C(19)-C(20)-C(21)	-170.7(5)	C(18)-C(19)-C(26)-F(26)	-18.3(9)
C(17)-C(16)-C(21)-C(20)	-4.0(8)	C(20)-C(19)-C(26)-C(28)	-81.8(7)
C(15)-C(16)-C(21)-C(20)	176.8(5)	C(18)-C(19)-C(26)-C(28)	101.6(7)
C(17)-C(16)-C(21)-C(22)	179.3(5)	C(20)-C(19)-C(26)-C(27)	45.9(7)
C(15)-C(16)-C(21)-C(22)	0.1(6)	C(18)-C(19)-C(26)-C(27)	-130.8(6)
F(18)-C(20)-C(21)-C(16)	-178.5(5)	F(26)-C(26)-C(27)-F(29)	-89.7(6)
C(19)-C(20)-C(21)-C(16)	-0.4(8)	C(28)-C(26)-C(27)-F(29)	156.3(5)
F(18)-C(20)-C(21)-C(22)	-2.9(9)	C(19)-C(26)-C(27)-F(29)	27.7(7)
C(19)-C(20)-C(21)-C(22)	175.2(6)	F(26)-C(26)-C(27)-F(28)	145.9(5)
C(29)-N(7)-C(22)-N(2)	3.2(8)	C(28)-C(26)-C(27)-F(28)	32.0(7)
C(29)-N(7)-C(22)-C(21)	-175.5(5)	C(19)-C(26)-C(27)-F(28)	-96.6(6)

F(26)-C(26)-C(27)-F(27)	28.3(7)	F(33)-C(34)-C(35)-C(36)	3.5(9)
C(28)-C(26)-C(27)-F(27)	-85.6(7)	C(33)-C(34)-C(35)-C(36)	-178.0(5)
C(19)-C(26)-C(27)-F(27)	145.7(5)	C(31)-C(30)-C(35)-C(34)	-3.9(8)
F(26)-C(26)-C(28)-F(30)	-177.8(6)	C(29)-C(30)-C(35)-C(34)	174.9(5)
C(19)-C(26)-C(28)-F(30)	61.1(8)	C(31)-C(30)-C(35)-C(36)	176.9(5)
C(27)-C(26)-C(28)-F(30)	-67.6(8)	C(29)-C(30)-C(35)-C(36)	-4.3(6)
F(26)-C(26)-C(28)-F(32)	-56.9(7)	C(37)-N(8)-C(36)-N(3)	1.0(8)
C(19)-C(26)-C(28)-F(32)	-178.1(5)	C(37)-N(8)-C(36)-C(35)	179.3(5)
C(27)-C(26)-C(28)-F(32)	53.2(7)	C(29)-N(3)-C(36)-N(8)	177.8(5)
F(26)-C(26)-C(28)-F(31)	61.7(7)	Co-N(3)-C(36)-N(8)	-11.5(8)
C(19)-C(26)-C(28)-F(31)	-59.5(7)	C(29)-N(3)-C(36)-C(35)	-0.6(6)
C(27)-C(26)-C(28)-F(31)	171.8(5)	Co-N(3)-C(36)-C(35)	170.0(3)
C(22)-N(7)-C(29)-N(3)	-0.6(8)	C(34)-C(35)-C(36)-N(8)	5.6(9)
C(22)-N(7)-C(29)-C(30)	172.4(5)	C(30)-C(35)-C(36)-N(8)	-175.4(5)
C(36)-N(3)-C(29)-N(7)	171.6(5)	C(34)-C(35)-C(36)-N(3)	-175.8(6)
Co-N(3)-C(29)-N(7)	1.1(8)	C(30)-C(35)-C(36)-N(3)	3.3(6)
C(36)-N(3)-C(29)-C(30)	-2.1(5)	C(36)-N(8)-C(37)-N(4)	5.6(8)
Co-N(3)-C(29)-C(30)	-172.6(3)	C(36)-N(8)-C(37)-C(38)	-174.3(5)
N(7)-C(29)-C(30)-C(31)	8.6(9)	C(44)-N(4)-C(37)-N(8)	179.9(5)
N(3)-C(29)-C(30)-C(31)	-177.3(5)	Co-N(4)-C(37)-N(8)	-0.9(8)
N(7)-C(29)-C(30)-C(35)	-170.0(5)	C(44)-N(4)-C(37)-C(38)	-0.2(6)
N(3)-C(29)-C(30)-C(35)	4.1(6)	Co-N(4)-C(37)-C(38)	179.0(3)
C(35)-C(30)-C(31)-F(34)	-176.7(5)	N(8)-C(37)-C(38)-C(43)	180.0(5)
C(29)-C(30)-C(31)-F(34)	4.9(9)	N(4)-C(37)-C(38)-C(43)	0.0(6)
C(35)-C(30)-C(31)-C(32)	1.3(8)	N(8)-C(37)-C(38)-C(39)	1.1(10)
C(29)-C(30)-C(31)-C(32)	-177.1(5)	N(4)-C(37)-C(38)-C(39)	-178.8(6)
F(34)-C(31)-C(32)-F(35)	1.8(7)	C(43)-C(38)-C(39)-F(37)	-179.7(5)
C(30)-C(31)-C(32)-F(35)	-176.2(5)	C(37)-C(38)-C(39)-F(37)	-0.9(9)
F(34)-C(31)-C(32)-C(33)	-179.7(5)	C(43)-C(38)-C(39)-C(40)	0.0(8)
C(30)-C(31)-C(32)-C(33)	2.2(8)	C(37)-C(38)-C(39)-C(40)	178.8(6)
F(35)-C(32)-C(33)-C(34)	175.4(5)	F(37)-C(39)-C(40)-C(41)	178.5(5)
C(31)-C(32)-C(33)-C(34)	-3.1(8)	C(38)-C(39)-C(40)-C(41)	-1.3(9)
F(35)-C(32)-C(33)-N(12)	-5.4(8)	F(37)-C(39)-C(40)-C(48)	-3.5(8)
C(31)-C(32)-C(33)-N(12)	176.1(5)	C(38)-C(39)-C(40)-C(48)	176.8(6)
C(51)-N(12)-C(33)-C(34)	119.4(6)	C(39)-C(40)-C(41)-C(42)	1.7(8)
C(53)-N(12)-C(33)-C(34)	-56.9(7)	C(48)-C(40)-C(41)-C(42)	-176.1(6)
C(51)-N(12)-C(33)-C(32)	-59.7(7)	C(39)-C(40)-C(41)-C(45)	-178.3(6)
C(53)-N(12)-C(33)-C(32)	123.9(6)	C(48)-C(40)-C(41)-C(45)	3.9(10)
C(32)-C(33)-C(34)-F(33)	178.9(5)	C(40)-C(41)-C(42)-F(36)	179.8(5)
N(12)-C(33)-C(34)-F(33)	-0.3(8)	C(45)-C(41)-C(42)-F(36)	-0.2(8)
C(32)-C(33)-C(34)-C(35)	0.4(8)	C(40)-C(41)-C(42)-C(43)	-1.0(9)
N(12)-C(33)-C(34)-C(35)	-178.8(5)	C(45)-C(41)-C(42)-C(43)	178.9(5)
F(33)-C(34)-C(35)-C(30)	-175.5(5)	F(36)-C(42)-C(43)-C(38)	179.0(5)
C(33)-C(34)-C(35)-C(30)	3.1(8)	C(41)-C(42)-C(43)-C(38)	-0.2(9)

F(36)-C(42)-C(43)-C(44)	1.0(10)	C(39)-C(40)-C(48)-C(50)	-44.1(8)
C(41)-C(42)-C(43)-C(44)	-178.2(6)	C(41)-C(40)-C(48)-C(50)	133.8(6)
C(39)-C(38)-C(43)-C(42)	0.7(8)	F(38)-C(48)-C(49)-F(41)	176.0(7)
C(37)-C(38)-C(43)-C(42)	-178.3(5)	C(40)-C(48)-C(49)-F(41)	-57.3(10)
C(39)-C(38)-C(43)-C(44)	179.2(5)	C(50)-C(48)-C(49)-F(41)	71.3(9)
C(37)-C(38)-C(43)-C(44)	0.1(6)	F(38)-C(48)-C(49)-F(39)	51.2(11)
C(1)-N(5)-C(44)-N(4)	-0.6(9)	C(40)-C(48)-C(49)-F(39)	177.9(7)
C(1)-N(5)-C(44)-C(43)	-179.3(5)	C(50)-C(48)-C(49)-F(39)	-53.6(10)
C(37)-N(4)-C(44)-N(5)	-178.5(5)	F(38)-C(48)-C(49)-F(40)	-63.3(9)
Co-N(4)-C(44)-N(5)	2.2(8)	C(40)-C(48)-C(49)-F(40)	63.4(9)
C(37)-N(4)-C(44)-C(43)	0.3(6)	C(50)-C(48)-C(49)-F(40)	-168.1(7)
Co-N(4)-C(44)-C(43)	-178.9(3)	F(38)-C(48)-C(50)-F(43)	88.5(6)
C(42)-C(43)-C(44)-N(5)	-3.2(10)	C(49)-C(48)-C(50)-F(43)	-154.8(7)
C(38)-C(43)-C(44)-N(5)	178.6(5)	C(40)-C(48)-C(50)-F(43)	-26.5(9)
C(42)-C(43)-C(44)-N(4)	177.9(6)	F(38)-C(48)-C(50)-F(42)	-35.0(6)
C(38)-C(43)-C(44)-N(4)	-0.3(6)	C(49)-C(48)-C(50)-F(42)	81.7(8)
C(42)-C(41)-C(45)-F(45)	-165.8(6)	C(40)-C(48)-C(50)-F(42)	-150.0(6)
C(40)-C(41)-C(45)-F(45)	14.1(9)	F(38)-C(48)-C(50)-F(44)	-146.7(5)
C(42)-C(41)-C(45)-C(46)	80.5(7)	C(49)-C(48)-C(50)-F(44)	-30.0(8)
C(40)-C(41)-C(45)-C(46)	-99.5(7)	C(40)-C(48)-C(50)-F(44)	98.3(7)
C(42)-C(41)-C(45)-C(47)	-48.5(9)	Co#1-O-C(51)-N(12)	-177.7(4)
C(40)-C(41)-C(45)-C(47)	131.4(8)	Co#1-O-C(51)-C(52)	0.7(10)
F(45)-C(45)-C(46)-F(47)	66.9(8)	C(33)-N(12)-C(51)-O	3.9(8)
C(41)-C(45)-C(46)-F(47)	-173.8(6)	C(53)-N(12)-C(51)-O	-179.9(5)
C(47)-C(45)-C(46)-F(47)	-42.7(9)	C(33)-N(12)-C(51)-C(52)	-174.5(5)
F(45)-C(45)-C(46)-F(48)	-169.1(6)	C(53)-N(12)-C(51)-C(52)	1.7(8)
C(41)-C(45)-C(46)-F(48)	-49.9(8)	C(6S)-C(1S)-C(2S)-C(3S)	0
C(47)-C(45)-C(46)-F(48)	81.2(8)	C(1S)-C(2S)-C(3S)-C(4S)	0
F(45)-C(45)-C(46)-F(46)	-52.0(8)	C(2S)-C(3S)-C(4S)-C(5S)	0
C(41)-C(45)-C(46)-F(46)	67.2(8)	C(3S)-C(4S)-C(5S)-C(6S)	0
C(47)-C(45)-C(46)-F(46)	-161.7(7)	C(4S)-C(5S)-C(6S)-C(1S)	0
F(45)-C(45)-C(47)-F(49)	99.5(10)	C(4S)-C(5S)-C(6S)-C(7S)	177.7(10)
C(41)-C(45)-C(47)-F(49)	-22.1(13)	C(2S)-C(1S)-C(6S)-C(5S)	0
C(46)-C(45)-C(47)-F(49)	-152.0(9)	C(2S)-C(1S)-C(6S)-C(7S)	-177.7(10)
F(45)-C(45)-C(47)-F(50)	-27.5(10)	C(13S)-C(8S)-C(9S)-C(10S)	0
C(41)-C(45)-C(47)-F(50)	-149.1(7)	C(8S)-C(9S)-C(10S)-C(11S)	0
C(46)-C(45)-C(47)-F(50)	81.0(10)	C(9S)-C(10S)-C(11S)-C(12S)	0
F(45)-C(45)-C(47)-F(51)	-141.2(6)	C(10S)-C(11S)-C(12S)-C(13S)	0
C(41)-C(45)-C(47)-F(51)	97.2(6)	C(11S)-C(12S)-C(13S)-C(8S)	0
C(46)-C(45)-C(47)-F(51)	-32.7(8)	C(11S)-C(12S)-C(13S)-C(14S)	178.2(16)
C(39)-C(40)-C(48)-F(38)	-148.7(6)	C(9S)-C(8S)-C(13S)-C(12S)	0
C(41)-C(40)-C(48)-F(38)	29.1(10)	C(9S)-C(8S)-C(13S)-C(14S)	-178.1(17)
C(39)-C(40)-C(48)-C(49)	83.6(8)	C(6T)-C(1T)-C(2T)-C(3T)	1.6(16)
C(41)-C(40)-C(48)-C(49)	-98.6(8)	C(1T)-C(2T)-C(3T)-C(4T)	-1.3(15)

C(2T)-C(3T)-C(4T)-C(5T)	0.7(17)	C(4E)-C(5E)-C(6E)-C(7E)	176.3(13)
C(3T)-C(4T)-C(5T)-C(6T)	0(2)	C(2E)-C(1E)-C(6E)-C(5E)	0
C(2T)-C(1T)-C(6T)-C(5T)	-1.1(18)	C(2E)-C(1E)-C(6E)-C(7E)	-175.7(15)
C(2T)-C(1T)-C(6T)-C(7T)	176.9(14)	C(6K)-C(1K)-C(2K)-C(3K)	0
C(4T)-C(5T)-C(6T)-C(1T)	0(2)	C(1K)-C(2K)-C(3K)-C(4K)	0
C(4T)-C(5T)-C(6T)-C(7T)	-177.4(17)	C(2K)-C(3K)-C(4K)-C(5K)	0
C(6E)-C(1E)-C(2E)-C(3E)	0	C(3K)-C(4K)-C(5K)-C(6K)	0
C(1E)-C(2E)-C(3E)-C(4E)	0	C(4K)-C(5K)-C(6K)-C(1K)	0
C(2E)-C(3E)-C(4E)-C(5E)	0	C(4K)-C(5K)-C(6K)-C(7K)	179.7(13)
C(3E)-C(4E)-C(5E)-C(6E)	0	C(2K)-C(1K)-C(6K)-C(5K)	0
C(4E)-C(5E)-C(6E)-C(1E)	0	C(2K)-C(1K)-C(6K)-C(7K)	-179.7(14)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Appendix U: Crystal structure of [(NHAcF$_{51}$PcCo)$_2$OH]·7(toluene)

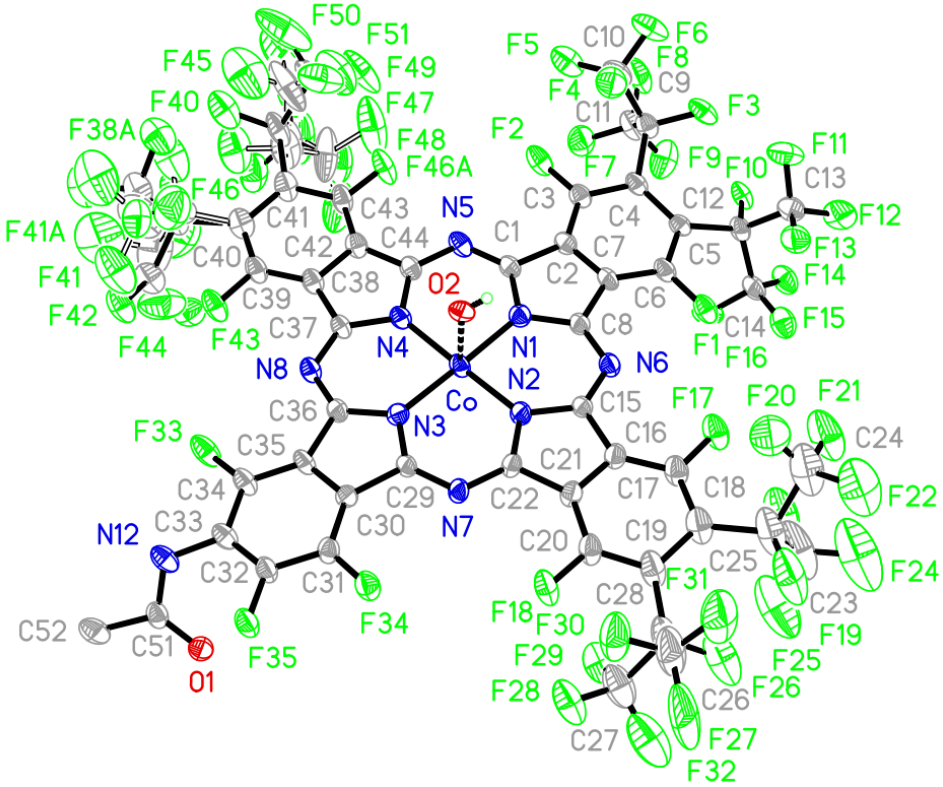


Figure U.1 ORTEP representation of **NHAcF$_{51}$PcCo-OH** X-ray crystal structure, at 50% probability.

Table U.1 Crystal data and structure refinement for **[(NHAcF$_{51}$PcCo)$_2$OH]·7(toluene)**.

Empirical formula	C153 H65 Co2 F102 N18 O3	
Formula weight	4259.09	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.247(5) Å	α = 90°.
	b = 35.337(9) Å	β = 104.732(6)°.
	c = 23.857(6) Å	γ = 90°.
Volume	15692(6) Å^3	
Z	4	
Density (calculated)	1.803 g/cm^3	
Absorption coefficient	0.396 mm^{-1}	
F(000)	8420	
Crystal size	0.870 x 0.480 x 0.370 mm^3	
Theta range for data collection	1.348 to 30.536°.	

Index ranges	-27<=h<=27, -50<=k<=50, -34<=l<=33
Reflections collected	228254
Independent reflections	23951 [R(int) = 0.0526]
Completeness to theta = 25.000°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6740
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	23951 / 298 / 1497
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.1057, wR2 = 0.1889
R indices (all data)	R1 = 0.1611, wR2 = 0.2250
Extinction coefficient	n/a
Largest diff. peak and hole	1.200 and -1.490 e.$Å^{-3}$

Table U.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **[(NHAcF$_{51}$PcCo)$_2$OH]·7(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7589(1)	2906(1)	6302(1)	25(1)
N(1)	6564(2)	2928(1)	6188(2)	27(1)
N(2)	7586(2)	2388(1)	6548(2)	27(1)
N(3)	8604(2)	2876(1)	6379(1)	24(1)
N(4)	7587(2)	3417(1)	6029(2)	27(1)
N(5)	6310(2)	3559(1)	5786(2)	29(1)
N(6)	6327(2)	2309(1)	6526(2)	27(1)
N(7)	8853(2)	2237(1)	6744(2)	27(1)
N(8)	8859(2)	3520(1)	6142(2)	28(1)
N(12)	11736(2)	3272(1)	6895(2)	34(1)
O(1)	12088(2)	3060(1)	7810(1)	30(1)
C(1)	6130(2)	3228(1)	5957(2)	27(1)
C(2)	5389(2)	3131(1)	5947(2)	28(1)
C(3)	4742(2)	3318(1)	5748(2)	29(1)
C(4)	4090(2)	3166(1)	5802(2)	28(1)
C(5)	4121(2)	2818(1)	6133(2)	26(1)
C(6)	4776(2)	2630(1)	6287(2)	29(1)
C(7)	5401(2)	2781(1)	6189(2)	28(1)
C(8)	6138(2)	2649(1)	6322(2)	26(1)
C(9)	3404(2)	3368(1)	5459(2)	32(1)
C(10)	3401(3)	3466(1)	4812(2)	41(1)

C(11)	3213(3)	3725(1)	5765(2)	42(1)
C(12)	3518(2)	2654(1)	6383(2)	29(1)
C(13)	3130(2)	2304(1)	6058(2)	35(1)
C(14)	3752(2)	2567(1)	7049(2)	34(1)
C(15)	6997(2)	2193(1)	6633(2)	23(1)
C(16)	7223(2)	1826(1)	6879(2)	28(1)
C(17)	6861(2)	1528(1)	7042(2)	36(1)
C(18)	7202(3)	1201(1)	7305(3)	46(1)
C(19)	7981(3)	1195(1)	7423(3)	46(1)
C(20)	8322(2)	1491(1)	7209(2)	35(1)
C(21)	7958(2)	1805(1)	6945(2)	28(1)
C(22)	8175(2)	2161(1)	6729(2)	24(1)
C(23)	6707(3)	882(2)	7406(4)	73(2)
C(24)	6042(4)	797(2)	6852(6)	98(4)
C(25)	6421(4)	943(3)	7935(5)	99(3)
C(26)	8478(3)	902(2)	7807(3)	61(2)
C(27)	9119(3)	1082(2)	8273(3)	62(2)
C(28)	8747(4)	597(2)	7449(4)	79(2)
C(29)	9035(2)	2570(1)	6580(2)	26(1)
C(30)	9789(2)	2676(1)	6647(2)	25(1)
C(31)	10425(2)	2480(1)	6830(2)	27(1)
C(32)	11066(2)	2676(1)	6889(2)	30(1)
C(33)	11081(2)	3066(1)	6783(2)	31(1)
C(34)	10433(2)	3248(1)	6571(2)	33(1)
C(35)	9794(2)	3055(1)	6506(2)	28(1)
C(36)	9044(2)	3173(1)	6318(2)	26(1)
C(37)	8176(2)	3622(1)	5990(2)	26(1)
C(38)	7954(2)	3993(1)	5754(2)	30(1)
C(39)	8311(2)	4307(1)	5626(2)	33(1)
C(40)	7967(3)	4637(1)	5395(2)	38(1)
C(41)	7191(3)	4647(1)	5267(2)	39(1)
C(42)	6847(2)	4322(1)	5405(2)	35(1)
C(43)	7210(2)	4004(1)	5644(2)	29(1)
C(44)	6989(2)	3642(1)	5822(2)	27(1)
C(45)	6679(5)	4972(3)	4931(6)	43(3)
C(46)	6415(2)	5226(2)	5364(3)	68(3)
C(47)	6024(5)	4844(2)	4449(5)	67(4)
C(48)	8469(4)	4985(2)	5335(5)	32(2)
C(49)	8708(5)	4952(3)	4761(4)	46(2)
C(50)	9144(6)	5046(3)	5854(6)	46(3)
F(38)	8116(2)	5319(1)	5312(3)	49(1)
F(39)	9090(4)	5249(2)	4701(3)	71(2)
F(40)	8132(3)	4935(2)	4308(3)	66(2)
F(41)	9083(5)	4642(3)	4753(4)	60(2)

F(42)	9281(4)	5420(2)	5903(3)	64(2)
F(43)	9003(4)	4939(2)	6351(3)	52(2)
F(44)	9734(2)	4879(1)	5804(3)	51(1)
F(45)	7027(3)	5206(2)	4639(3)	59(2)
F(46)	6971(3)	5414(2)	5692(3)	76(2)
F(47)	5935(3)	5474(1)	5076(4)	93(3)
F(48)	6114(4)	5020(2)	5706(4)	73(3)
F(49)	6175(4)	4525(2)	4212(3)	82(2)
F(50)	5867(4)	5098(2)	4028(3)	117(4)
F(51)	5425(3)	4782(2)	4611(3)	81(3)
C(45A)	6718(9)	4971(5)	5170(8)	65(9)
C(46A)	6210(6)	5054(3)	5569(6)	88(14)
C(47A)	6278(6)	4979(3)	4532(6)	98(12)
C(48A)	8426(9)	4892(5)	5160(7)	52(7)
C(49A)	8983(11)	4737(5)	4841(9)	74(13)
C(50A)	8818(13)	5151(5)	5672(10)	106(13)
F(38A)	8013(6)	5133(4)	4763(7)	86(5)
F(39A)	8764(8)	4410(4)	4608(6)	89(4)
F(40A)	9633(6)	4684(4)	5201(7)	89(5)
F(41A)	9055(8)	4977(5)	4442(8)	111(6)
F(42A)	9236(11)	5401(5)	5488(11)	133(9)
F(43A)	9243(11)	4955(5)	6110(8)	96(8)
F(44A)	8358(10)	5352(4)	5875(9)	132(7)
F(45A)	7112(7)	5294(3)	5199(8)	91(5)
F(46A)	5559(6)	4902(3)	5383(7)	119(7)
F(47A)	6145(8)	5428(3)	5597(8)	119(7)
F(48A)	6513(8)	4922(4)	6098(5)	114(6)
F(49A)	6689(6)	4973(4)	4164(6)	118(7)
F(50A)	5888(7)	5292(3)	4421(8)	108(7)
F(51A)	5824(8)	4693(3)	4391(8)	92(6)
C(51)	12199(2)	3270(1)	7438(2)	30(1)
C(52)	12826(2)	3530(1)	7532(2)	41(1)
F(1)	4817(1)	2301(1)	6570(1)	34(1)
F(2)	4738(1)	3645(1)	5470(1)	39(1)
F(3)	2826(1)	3130(1)	5391(1)	40(1)
F(4)	3794(2)	3221(1)	4607(1)	52(1)
F(5)	3620(2)	3813(1)	4744(1)	50(1)
F(6)	2726(2)	3443(1)	4490(1)	54(1)
F(7)	3744(2)	3973(1)	5883(2)	54(1)
F(8)	2638(2)	3894(1)	5433(2)	64(1)
F(9)	3066(2)	3636(1)	6265(2)	65(1)
F(10)	2991(1)	2920(1)	6353(1)	36(1)
F(11)	2812(2)	2394(1)	5518(1)	54(1)
F(12)	2630(2)	2184(1)	6311(2)	51(1)

F(13)	3572(2)	2023(1)	6048(1)	48(1)
F(14)	3200(1)	2630(1)	7276(1)	43(1)
F(15)	3956(2)	2214(1)	7180(1)	44(1)
F(16)	4277(2)	2795(1)	7316(1)	46(1)
F(17)	6148(1)	1554(1)	6942(2)	45(1)
F(18)	9030(1)	1476(1)	7279(1)	43(1)
F(19)	7061(2)	544(1)	7472(3)	101(2)
F(20)	6201(2)	900(1)	6373(3)	93(2)
F(21)	5443(2)	965(1)	6891(3)	94(2)
F(22)	5913(3)	430(1)	6835(4)	139(3)
F(23)	6092(2)	1262(1)	7946(2)	93(2)
F(24)	5990(3)	660(2)	8001(3)	144(3)
F(25)	6973(3)	936(2)	8419(3)	121(2)
F(26)	8120(2)	714(1)	8146(2)	83(2)
F(27)	9275(2)	867(1)	8749(2)	94(2)
F(28)	9725(2)	1111(1)	8106(2)	68(1)
F(29)	8946(2)	1421(1)	8434(2)	67(1)
F(30)	9135(2)	741(1)	7116(2)	78(1)
F(31)	8205(2)	407(1)	7114(3)	106(2)
F(32)	9162(3)	349(1)	7815(3)	117(2)
F(33)	10450(1)	3617(1)	6449(1)	44(1)
F(34)	10454(1)	2112(1)	6948(1)	36(1)
F(35)	11685(1)	2482(1)	7045(1)	36(1)
F(36)	6134(1)	4318(1)	5304(2)	48(1)
F(37)	9027(1)	4286(1)	5737(1)	42(1)
C(1S)	6967(5)	3235(2)	4564(4)	112(4)
C(2S)	7671(4)	3336(2)	4585(4)	93(4)
C(3S)	7814(3)	3682(2)	4359(4)	89(3)
C(4S)	7254(5)	3926(2)	4112(3)	93(3)
C(5S)	6550(4)	3824(3)	4091(3)	122(4)
C(6S)	6407(3)	3479(3)	4317(4)	115(4)
C(7S)	5653(5)	3358(6)	4298(7)	152(8)
C(8S)	7184(12)	3501(5)	4427(8)	66(6)
C(9S)	7837(9)	3317(7)	4635(8)	71(7)
C(10S)	7856(8)	2959(6)	4881(7)	71(7)
C(11S)	7221(10)	2786(4)	4919(7)	61(6)
C(12S)	6568(8)	2970(4)	4711(8)	48(5)
C(13S)	6550(9)	3328(5)	4465(8)	50(5)
C(14S)	5854(12)	3535(7)	4238(17)	66(8)
C(1T)	1000(5)	3125(3)	5222(4)	106(3)
C(2T)	944(6)	2753(3)	5383(4)	98(3)
C(3T)	298(6)	2587(3)	5291(4)	92(3)
C(4T)	-307(6)	2787(3)	5023(4)	105(3)
C(5T)	-223(7)	3153(4)	4860(5)	123(4)

C(6T)	419(6)	3330(3)	4962(5)	114(4)
C(7T)	468(8)	3736(4)	4791(9)	238(11)
C(1E)	8083(10)	5506(3)	2267(5)	340(20)
C(2E)	7395(8)	5431(2)	2322(5)	209(11)
C(3E)	7242(5)	5465(2)	2859(6)	165(7)
C(4E)	7779(8)	5575(2)	3341(4)	142(5)
C(5E)	8467(6)	5649(3)	3285(6)	162(7)
C(6E)	8620(6)	5615(3)	2749(8)	221(11)
C(7E)	9204(11)	5705(8)	2457(10)	329(16)
C(1K)	4949(9)	4447(2)	7507(6)	72(4)
C(2K)	5217(8)	4363(2)	7032(5)	67(4)
C(3K)	5330(6)	3989(3)	6899(5)	64(4)
C(4K)	5174(11)	3698(2)	7241(7)	73(6)
C(5K)	4906(10)	3782(2)	7716(6)	56(4)
C(6K)	4794(6)	4157(3)	7848(4)	57(3)
C(7K)	4496(8)	4238(5)	8359(6)	79(4)
O(2)	7429(3)	2662(2)	5440(3)	26(1)

Table U.3 Bond lengths [Å] and angles [°] for **[(NHAcF_{51}PcCo)$_2$OH]·7(toluene)**.

Co-N(3)	1.919(3)	Co-N(1)	1.923(3)
Co-N(4)	1.919(4)	Co-O(1)#1	2.122(3)
Co-N(2)	1.922(4)	Co-O(2)	2.179(6)
N(1)-C(8)	1.373(5)	N(12)-C(33)	1.420(5)
N(1)-C(1)	1.374(5)	N(12)-H(12)	1.01(5)
N(2)-C(22)	1.366(5)	O(1)-C(51)	1.217(5)
N(2)-C(15)	1.384(5)	C(1)-C(2)	1.462(5)
N(3)-C(29)	1.374(5)	C(2)-C(7)	1.364(6)
N(3)-C(36)	1.377(5)	C(2)-C(3)	1.383(6)
N(4)-C(37)	1.368(5)	C(3)-F(2)	1.330(5)
N(4)-C(44)	1.381(5)	C(3)-C(4)	1.402(5)
N(5)-C(1)	1.315(5)	C(4)-C(5)	1.452(6)
N(5)-C(44)	1.321(5)	C(4)-C(9)	1.540(6)
N(6)-C(8)	1.313(5)	C(5)-C(6)	1.390(5)
N(6)-C(15)	1.314(5)	C(5)-C(12)	1.546(5)
N(7)-C(29)	1.315(5)	C(6)-F(1)	1.335(5)
N(7)-C(22)	1.324(5)	C(6)-C(7)	1.389(5)
N(8)-C(36)	1.316(5)	C(7)-C(8)	1.450(5)
N(8)-C(37)	1.322(5)	C(9)-F(3)	1.371(5)
N(12)-C(51)	1.373(6)	C(9)-C(11)	1.548(7)

C(9)-C(10)	1.583(7)	C(28)-F(31)	1.325(9)
C(10)-F(5)	1.319(5)	C(28)-F(32)	1.347(9)
C(10)-F(4)	1.322(6)	C(29)-C(30)	1.468(5)
C(10)-F(6)	1.332(5)	C(30)-C(31)	1.378(6)
C(11)-F(7)	1.321(6)	C(30)-C(35)	1.383(6)
C(11)-F(8)	1.329(5)	C(31)-F(34)	1.330(5)
C(11)-F(9)	1.330(6)	C(31)-C(32)	1.391(5)
C(12)-F(10)	1.371(5)	C(32)-F(35)	1.343(5)
C(12)-C(13)	1.548(6)	C(32)-C(33)	1.404(6)
C(12)-C(14)	1.568(6)	C(33)-C(34)	1.378(6)
C(13)-F(13)	1.313(6)	C(34)-F(33)	1.339(5)
C(13)-F(11)	1.317(5)	C(34)-C(35)	1.380(5)
C(13)-F(12)	1.329(5)	C(35)-C(36)	1.458(5)
C(14)-F(15)	1.320(5)	C(37)-C(38)	1.450(6)
C(14)-F(16)	1.322(5)	C(38)-C(39)	1.381(6)
C(14)-F(14)	1.328(5)	C(38)-C(43)	1.388(5)
C(15)-C(16)	1.445(5)	C(39)-F(37)	1.337(5)
C(16)-C(17)	1.371(6)	C(39)-C(40)	1.384(6)
C(16)-C(21)	1.385(5)	C(40)-C(41)	1.446(6)
C(17)-F(17)	1.336(5)	C(40)-C(48A)	1.47(2)
C(17)-C(18)	1.398(7)	C(40)-C(48)	1.592(9)
C(18)-C(19)	1.453(7)	C(41)-C(42)	1.407(6)
C(18)-C(23)	1.534(7)	C(41)-C(45A)	1.445(18)
C(19)-C(20)	1.397(6)	C(41)-C(45)	1.592(10)
C(19)-C(26)	1.543(7)	C(42)-F(36)	1.332(5)
C(20)-F(18)	1.332(5)	C(42)-C(43)	1.370(6)
C(20)-C(21)	1.378(6)	C(43)-C(44)	1.445(6)
C(21)-C(22)	1.460(5)	C(45)-F(45)	1.360(10)
C(23)-F(19)	1.365(7)	C(45)-C(47)	1.542(16)
C(23)-C(25)	1.516(13)	C(45)-C(46)	1.549(16)
C(23)-C(24)	1.618(13)	C(46)-F(46)	1.331(5)
C(24)-F(20)	1.307(12)	C(46)-F(48)	1.331(5)
C(24)-F(22)	1.320(7)	C(46)-F(47)	1.331(5)
C(24)-F(21)	1.321(8)	C(47)-F(51)	1.324(6)
C(25)-F(23)	1.296(9)	C(47)-F(49)	1.325(6)
C(25)-F(24)	1.333(8)	C(47)-F(50)	1.325(6)
C(25)-F(25)	1.357(11)	C(48)-F(38)	1.357(9)
C(26)-F(26)	1.362(7)	C(48)-C(49)	1.556(13)
C(26)-C(28)	1.544(10)	C(48)-C(50)	1.564(14)
C(26)-C(27)	1.571(10)	C(49)-F(39)	1.308(10)
C(27)-F(29)	1.327(8)	C(49)-F(41)	1.315(11)
C(27)-F(28)	1.328(7)	C(49)-F(40)	1.339(10)
C(27)-F(27)	1.336(7)	C(50)-F(44)	1.312(12)
C(28)-F(30)	1.324(9)	C(50)-F(43)	1.337(13)

C(50)-F(42)	1.348(11)	C(10S)-H(10A)	0.9500
C(45A)-F(45A)	1.362(16)	C(11S)-C(12S)	1.3900
C(45A)-C(47A)	1.543(19)	C(11S)-H(11A)	0.9500
C(45A)-C(46A)	1.554(19)	C(12S)-C(13S)	1.3900
C(46A)-F(48A)	1.331(5)	C(12S)-H(12A)	0.9500
C(46A)-F(47A)	1.331(5)	C(13S)-C(14S)	1.500(8)
C(46A)-F(46A)	1.331(5)	C(14S)-H(14A)	0.9800
C(47A)-F(51A)	1.324(6)	C(14S)-H(14B)	0.9800
C(47A)-F(50A)	1.325(6)	C(14S)-H(14C)	0.9800
C(47A)-F(49A)	1.325(6)	C(1T)-C(6T)	1.343(12)
C(48A)-F(38A)	1.368(16)	C(1T)-C(2T)	1.383(14)
C(48A)-C(50A)	1.56(2)	C(1T)-H(1TA)	0.9500
C(48A)-C(49A)	1.56(2)	C(2T)-C(3T)	1.340(14)
C(49A)-F(39A)	1.303(18)	C(2T)-H(2TA)	0.9500
C(49A)-F(41A)	1.309(17)	C(3T)-C(4T)	1.373(13)
C(49A)-F(40A)	1.339(19)	C(3T)-H(3TA)	0.9500
C(50A)-F(44A)	1.316(18)	C(4T)-C(5T)	1.371(15)
C(50A)-F(42A)	1.342(17)	C(4T)-H(4TA)	0.9500
C(50A)-F(43A)	1.343(19)	C(5T)-C(6T)	1.351(15)
C(51)-C(52)	1.487(6)	C(5T)-H(5TA)	0.9500
C(52)-H(52A)	0.9800	C(6T)-C(7T)	1.500(8)
C(52)-H(52B)	0.9800	C(7T)-H(7TA)	0.9800
C(52)-H(52C)	0.9800	C(7T)-H(7TB)	0.9800
C(1S)-C(2S)	1.3900	C(7T)-H(7TC)	0.9800
C(1S)-C(6S)	1.3900	C(1E)-C(2E)	1.3900
C(1S)-H(1SA)	0.9500	C(1E)-C(6E)	1.3900
C(2S)-C(3S)	1.3900	C(1E)-H(1EA)	0.9500
C(2S)-H(2SA)	0.9500	C(2E)-C(3E)	1.3900
C(3S)-C(4S)	1.3900	C(2E)-H(2EA)	0.9500
C(3S)-H(3SA)	0.9500	C(3E)-C(4E)	1.3900
C(4S)-C(5S)	1.3900	C(3E)-H(3EA)	0.9500
C(4S)-H(4SA)	0.9500	C(4E)-C(5E)	1.3900
C(5S)-C(6S)	1.3900	C(4E)-H(4EA)	0.9500
C(5S)-H(5SA)	0.9500	C(5E)-C(6E)	1.3900
C(6S)-C(7S)	1.501(8)	C(5E)-H(5EA)	0.9500
C(7S)-H(7SA)	0.9800	C(6E)-C(7E)	1.500(8)
C(7S)-H(7SB)	0.9800	C(7E)-H(7EA)	0.9800
C(7S)-H(7SC)	0.9800	C(7E)-H(7EB)	0.9800
C(8S)-C(9S)	1.3900	C(7E)-H(7EC)	0.9800
C(8S)-C(13S)	1.3900	C(1K)-C(2K)	1.3900
C(8S)-H(8SA)	0.9500	C(1K)-C(6K)	1.3900
C(9S)-C(10S)	1.3900	C(1K)-H(1KA)	0.9500
C(9S)-H(9SA)	0.9500	C(2K)-C(3K)	1.3900
C(10S)-C(11S)	1.3900	C(2K)-H(2KA)	0.9500

C(3K)-C(4K)	1.3900	C(6K)-C(7K)	1.500(8)
C(3K)-H(3KA)	0.9500	C(7K)-H(7KA)	0.9800
C(4K)-C(5K)	1.3900	C(7K)-H(7KB)	0.9800
C(4K)-H(4KA)	0.9500	C(7K)-H(7KC)	0.9800
C(5K)-C(6K)	1.3900	O(2)-H(2A)	0.62(11)
C(5K)-H(5KA)	0.9500		

N(3)-Co-N(4)	89.87(14)	N(2)-Co-O(1)#1	87.88(13)
N(3)-Co-N(2)	90.07(14)	N(1)-Co-O(1)#1	99.20(13)
N(4)-Co-N(2)	177.98(15)	N(3)-Co-O(2)	87.99(18)
N(3)-Co-N(1)	177.38(15)	N(4)-Co-O(2)	93.73(19)
N(4)-Co-N(1)	89.97(14)	N(2)-Co-O(2)	84.25(19)
N(2)-Co-N(1)	90.00(14)	N(1)-Co-O(2)	89.41(18)
N(3)-Co-O(1)#1	83.41(13)	O(1)#1-Co-O(2)	168.34(18)
N(4)-Co-O(1)#1	94.12(13)		

C(8)-N(1)-C(1)	108.0(3)	C(2)-C(3)-C(4)	122.2(4)
C(8)-N(1)-Co	126.1(3)	C(3)-C(4)-C(5)	117.5(3)
C(1)-N(1)-Co	125.9(3)	C(3)-C(4)-C(9)	116.0(4)
C(22)-N(2)-C(15)	107.8(3)	C(5)-C(4)-C(9)	126.3(3)
C(22)-N(2)-Co	126.1(3)	C(6)-C(5)-C(4)	117.2(3)
C(15)-N(2)-Co	125.8(3)	C(6)-C(5)-C(12)	116.0(4)
C(29)-N(3)-C(36)	107.7(3)	C(4)-C(5)-C(12)	126.5(3)
C(29)-N(3)-Co	125.8(3)	F(1)-C(6)-C(7)	118.5(3)
C(36)-N(3)-Co	126.0(3)	F(1)-C(6)-C(5)	118.9(3)
C(37)-N(4)-C(44)	107.5(3)	C(7)-C(6)-C(5)	122.5(4)
C(37)-N(4)-Co	126.2(3)	C(2)-C(7)-C(6)	119.9(4)
C(44)-N(4)-Co	126.3(3)	C(2)-C(7)-C(8)	107.2(3)
C(1)-N(5)-C(44)	120.7(4)	C(6)-C(7)-C(8)	132.9(4)
C(8)-N(6)-C(15)	121.6(4)	N(6)-C(8)-N(1)	128.2(4)
C(29)-N(7)-C(22)	120.5(3)	N(6)-C(8)-C(7)	122.7(4)
C(36)-N(8)-C(37)	120.7(4)	N(1)-C(8)-C(7)	109.1(3)
C(51)-N(12)-C(33)	120.5(4)	F(3)-C(9)-C(4)	109.9(3)
C(33)-N(12)-H(12)	120(3)	F(3)-C(9)-C(11)	105.7(4)
C(51)-N(12)-H(12)	112(3)	C(4)-C(9)-C(11)	113.7(4)
C(51)-O(1)-Co#1	145.5(3)	F(3)-C(9)-C(10)	102.6(3)
N(5)-C(1)-N(1)	129.0(3)	C(4)-C(9)-C(10)	114.3(4)
N(5)-C(1)-C(2)	122.4(4)	C(11)-C(9)-C(10)	109.8(4)
N(1)-C(1)-C(2)	108.5(3)	F(5)-C(10)-F(4)	109.4(4)
C(7)-C(2)-C(3)	119.8(4)	F(5)-C(10)-F(6)	106.4(4)
C(7)-C(2)-C(1)	107.1(4)	F(4)-C(10)-F(6)	108.2(4)
C(3)-C(2)-C(1)	133.1(4)	F(5)-C(10)-C(9)	113.7(4)
F(2)-C(3)-C(2)	118.5(3)	F(4)-C(10)-C(9)	110.8(4)
F(2)-C(3)-C(4)	119.3(4)	F(6)-C(10)-C(9)	108.1(4)

F(7)-C(11)-F(8)	108.0(4)	C(16)-C(21)-C(22)	106.9(4)
F(7)-C(11)-F(9)	107.1(5)	N(7)-C(22)-N(2)	128.5(4)
F(8)-C(11)-F(9)	107.8(4)	N(7)-C(22)-C(21)	122.3(4)
F(7)-C(11)-C(9)	112.2(4)	N(2)-C(22)-C(21)	109.1(3)
F(8)-C(11)-C(9)	110.4(4)	F(19)-C(23)-C(25)	107.8(6)
F(9)-C(11)-C(9)	111.1(4)	F(19)-C(23)-C(18)	110.5(4)
F(10)-C(12)-C(5)	109.9(3)	C(25)-C(23)-C(18)	113.5(7)
F(10)-C(12)-C(13)	105.4(3)	F(19)-C(23)-C(24)	101.4(6)
C(5)-C(12)-C(13)	114.8(4)	C(25)-C(23)-C(24)	109.1(6)
F(10)-C(12)-C(14)	101.9(3)	C(18)-C(23)-C(24)	113.7(6)
C(5)-C(12)-C(14)	114.4(3)	F(20)-C(24)-F(22)	109.4(9)
C(13)-C(12)-C(14)	109.2(4)	F(20)-C(24)-F(21)	109.8(8)
F(13)-C(13)-F(11)	107.9(4)	F(22)-C(24)-F(21)	106.5(5)
F(13)-C(13)-F(12)	108.3(4)	F(20)-C(24)-C(23)	110.5(5)
F(11)-C(13)-F(12)	108.2(4)	F(22)-C(24)-C(23)	108.2(7)
F(13)-C(13)-C(12)	112.4(4)	F(21)-C(24)-C(23)	112.4(8)
F(11)-C(13)-C(12)	110.0(4)	F(23)-C(25)-F(24)	109.2(6)
F(12)-C(13)-C(12)	109.8(4)	F(23)-C(25)-F(25)	106.2(10)
F(15)-C(14)-F(16)	108.5(4)	F(24)-C(25)-F(25)	105.3(7)
F(15)-C(14)-F(14)	106.3(4)	F(23)-C(25)-C(23)	115.0(6)
F(16)-C(14)-F(14)	107.1(4)	F(24)-C(25)-C(23)	111.1(9)
F(15)-C(14)-C(12)	114.7(4)	F(25)-C(25)-C(23)	109.5(6)
F(16)-C(14)-C(12)	110.9(4)	F(26)-C(26)-C(19)	110.4(4)
F(14)-C(14)-C(12)	109.0(3)	F(26)-C(26)-C(28)	106.2(5)
N(6)-C(15)-N(2)	128.0(4)	C(19)-C(26)-C(28)	112.7(6)
N(6)-C(15)-C(16)	122.4(4)	F(26)-C(26)-C(27)	101.7(6)
N(2)-C(15)-C(16)	109.6(3)	C(19)-C(26)-C(27)	113.9(5)
C(17)-C(16)-C(21)	120.3(4)	C(28)-C(26)-C(27)	111.2(5)
C(17)-C(16)-C(15)	133.1(4)	F(29)-C(27)-F(28)	108.9(5)
C(21)-C(16)-C(15)	106.6(3)	F(29)-C(27)-F(27)	106.7(6)
F(17)-C(17)-C(16)	118.1(4)	F(28)-C(27)-F(27)	105.9(5)
F(17)-C(17)-C(18)	118.7(4)	F(29)-C(27)-C(26)	111.2(5)
C(16)-C(17)-C(18)	123.2(4)	F(28)-C(27)-C(26)	114.2(6)
C(17)-C(18)-C(19)	116.3(4)	F(27)-C(27)-C(26)	109.6(5)
C(17)-C(18)-C(23)	116.0(4)	F(30)-C(28)-F(31)	108.2(8)
C(19)-C(18)-C(23)	127.7(5)	F(30)-C(28)-F(32)	108.0(6)
C(20)-C(19)-C(18)	118.4(4)	F(31)-C(28)-F(32)	107.9(6)
C(20)-C(19)-C(26)	116.2(4)	F(30)-C(28)-C(26)	112.5(5)
C(18)-C(19)-C(26)	125.3(4)	F(31)-C(28)-C(26)	111.3(5)
F(18)-C(20)-C(21)	118.3(4)	F(32)-C(28)-C(26)	108.8(8)
F(18)-C(20)-C(19)	119.1(4)	N(7)-C(29)-N(3)	128.8(3)
C(21)-C(20)-C(19)	122.6(4)	N(7)-C(29)-C(30)	121.7(4)
C(20)-C(21)-C(16)	118.7(4)	N(3)-C(29)-C(30)	109.2(3)
C(20)-C(21)-C(22)	134.3(4)	C(31)-C(30)-C(35)	120.3(3)

C(31)-C(30)-C(29)	132.9(4)	C(38)-C(43)-C(44)	106.7(4)
C(35)-C(30)-C(29)	106.7(3)	N(5)-C(44)-N(4)	128.1(4)
F(34)-C(31)-C(30)	123.0(4)	N(5)-C(44)-C(43)	122.4(4)
F(34)-C(31)-C(32)	118.6(4)	N(4)-C(44)-C(43)	109.5(3)
C(30)-C(31)-C(32)	118.4(4)	F(45)-C(45)-C(47)	102.4(9)
F(35)-C(32)-C(31)	118.4(4)	F(45)-C(45)-C(46)	106.1(8)
F(35)-C(32)-C(33)	119.6(4)	C(47)-C(45)-C(46)	108.9(6)
C(31)-C(32)-C(33)	122.0(4)	F(45)-C(45)-C(41)	111.9(6)
C(34)-C(33)-C(32)	117.7(4)	C(47)-C(45)-C(41)	116.5(7)
C(34)-C(33)-N(12)	120.6(4)	C(46)-C(45)-C(41)	110.4(8)
C(32)-C(33)-N(12)	121.7(4)	F(46)-C(46)-F(48)	108.8(5)
F(33)-C(34)-C(33)	117.6(4)	F(46)-C(46)-F(47)	108.9(5)
F(33)-C(34)-C(35)	121.7(4)	F(48)-C(46)-F(47)	108.9(5)
C(33)-C(34)-C(35)	120.7(4)	F(46)-C(46)-C(45)	109.3(6)
C(34)-C(35)-C(30)	120.7(4)	F(48)-C(46)-C(45)	111.1(8)
C(34)-C(35)-C(36)	132.8(4)	F(47)-C(46)-C(45)	109.8(7)
C(30)-C(35)-C(36)	106.5(3)	F(51)-C(47)-F(49)	106.6(6)
N(8)-C(36)-N(3)	128.2(4)	F(51)-C(47)-F(50)	106.5(6)
N(8)-C(36)-C(35)	122.0(4)	F(49)-C(47)-F(50)	106.5(6)
N(3)-C(36)-C(35)	109.8(3)	F(51)-C(47)-C(45)	116.1(8)
N(8)-C(37)-N(4)	128.5(4)	F(49)-C(47)-C(45)	110.1(7)
N(8)-C(37)-C(38)	121.8(4)	F(50)-C(47)-C(45)	110.5(8)
N(4)-C(37)-C(38)	109.7(3)	F(38)-C(48)-C(49)	106.7(7)
C(39)-C(38)-C(43)	119.0(4)	F(38)-C(48)-C(50)	102.7(8)
C(39)-C(38)-C(37)	134.4(4)	C(49)-C(48)-C(50)	109.6(7)
C(43)-C(38)-C(37)	106.6(4)	F(38)-C(48)-C(40)	111.4(5)
F(37)-C(39)-C(38)	117.2(4)	C(49)-C(48)-C(40)	110.1(7)
F(37)-C(39)-C(40)	119.4(4)	C(50)-C(48)-C(40)	115.8(7)
C(38)-C(39)-C(40)	123.4(4)	F(39)-C(49)-F(41)	109.9(8)
C(39)-C(40)-C(41)	117.9(4)	F(39)-C(49)-F(40)	108.7(7)
C(39)-C(40)-C(48A)	113.2(8)	F(41)-C(49)-F(40)	107.1(8)
C(41)-C(40)-C(48A)	126.4(7)	F(39)-C(49)-C(48)	109.7(8)
C(39)-C(40)-C(48)	116.5(5)	F(41)-C(49)-C(48)	111.1(7)
C(41)-C(40)-C(48)	125.5(5)	F(40)-C(49)-C(48)	110.2(7)
C(42)-C(41)-C(45A)	111.6(8)	F(44)-C(50)-F(43)	109.3(9)
C(42)-C(41)-C(40)	117.0(4)	F(44)-C(50)-F(42)	107.1(8)
C(45A)-C(41)-C(40)	128.9(8)	F(43)-C(50)-F(42)	106.2(10)
C(42)-C(41)-C(45)	116.1(5)	F(44)-C(50)-C(48)	115.4(10)
C(40)-C(41)-C(45)	126.7(5)	F(43)-C(50)-C(48)	110.4(7)
F(36)-C(42)-C(43)	117.4(4)	F(42)-C(50)-C(48)	107.9(9)
F(36)-C(42)-C(41)	119.4(4)	F(45A)-C(45A)-C(41)	109.6(12)
C(43)-C(42)-C(41)	123.2(4)	F(45A)-C(45A)-C(47A)	101.1(15)
C(42)-C(43)-C(38)	119.5(4)	C(41)-C(45A)-C(47A)	109.8(11)
C(42)-C(43)-C(44)	133.8(4)	F(45A)-C(45A)-C(46A)	103.9(12)

C(41)-C(45A)-C(46A)	121.4(14)	C(1S)-C(2S)-C(3S)	120.0
C(47A)-C(45A)-C(46A)	109.1(11)	C(1S)-C(2S)-H(2SA)	120.0
F(48A)-C(46A)-F(47A)	108.8(5)	C(3S)-C(2S)-H(2SA)	120.0
F(48A)-C(46A)-F(46A)	108.9(5)	C(4S)-C(3S)-C(2S)	120.0
F(47A)-C(46A)-F(46A)	108.9(5)	C(4S)-C(3S)-H(3SA)	120.0
F(48A)-C(46A)-C(45A)	108.8(11)	C(2S)-C(3S)-H(3SA)	120.0
F(47A)-C(46A)-C(45A)	107.5(10)	C(3S)-C(4S)-C(5S)	120.0
F(46A)-C(46A)-C(45A)	113.9(10)	C(3S)-C(4S)-H(4SA)	120.0
F(51A)-C(47A)-F(50A)	106.5(6)	C(5S)-C(4S)-H(4SA)	120.0
F(51A)-C(47A)-F(49A)	106.5(6)	C(6S)-C(5S)-C(4S)	120.0
F(50A)-C(47A)-F(49A)	106.5(6)	C(6S)-C(5S)-H(5SA)	120.0
F(51A)-C(47A)-C(45A)	113.4(13)	C(4S)-C(5S)-H(5SA)	120.0
F(50A)-C(47A)-C(45A)	110.8(12)	C(5S)-C(6S)-C(1S)	120.0
F(49A)-C(47A)-C(45A)	112.5(11)	C(5S)-C(6S)-C(7S)	121.5(11)
F(38A)-C(48A)-C(40)	110.2(12)	C(1S)-C(6S)-C(7S)	118.5(11)
F(38A)-C(48A)-C(50A)	104.8(16)	C(6S)-C(7S)-H(7SA)	109.5
C(40)-C(48A)-C(50A)	106.1(12)	C(6S)-C(7S)-H(7SB)	109.5
F(38A)-C(48A)-C(49A)	103.4(13)	H(7SA)-C(7S)-H(7SB)	109.5
C(40)-C(48A)-C(49A)	121.7(13)	C(6S)-C(7S)-H(7SC)	109.5
C(50A)-C(48A)-C(49A)	109.5(14)	H(7SA)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-F(41A)	110.4(18)	H(7SB)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-F(40A)	107.3(15)	C(9S)-C(8S)-C(13S)	120.0
F(41A)-C(49A)-F(40A)	107.6(16)	C(9S)-C(8S)-H(8SA)	120.0
F(39A)-C(49A)-C(48A)	109.3(14)	C(13S)-C(8S)-H(8SA)	120.0
F(41A)-C(49A)-C(48A)	109.8(15)	C(10S)-C(9S)-C(8S)	120.0
F(40A)-C(49A)-C(48A)	112.4(15)	C(10S)-C(9S)-H(9SA)	120.0
F(44A)-C(50A)-F(42A)	106.4(17)	C(8S)-C(9S)-H(9SA)	120.0
F(44A)-C(50A)-F(43A)	109(2)	C(9S)-C(10S)-C(11S)	120.0
F(42A)-C(50A)-F(43A)	107(2)	C(9S)-C(10S)-H(10A)	120.0
F(44A)-C(50A)-C(48A)	111.6(18)	C(11S)-C(10S)-H(10A)	120.0
F(42A)-C(50A)-C(48A)	109.8(17)	C(12S)-C(11S)-C(10S)	120.0
F(43A)-C(50A)-C(48A)	112.5(15)	C(12S)-C(11S)-H(11A)	120.0
O(1)-C(51)-N(12)	119.9(4)	C(10S)-C(11S)-H(11A)	120.0
O(1)-C(51)-C(52)	123.5(4)	C(11S)-C(12S)-C(13S)	120.0
N(12)-C(51)-C(52)	116.6(4)	C(11S)-C(12S)-H(12A)	120.0
C(51)-C(52)-H(52A)	109.5	C(13S)-C(12S)-H(12A)	120.0
C(51)-C(52)-H(52B)	109.5	C(12S)-C(13S)-C(8S)	120.0
H(52A)-C(52)-H(52B)	109.5	C(12S)-C(13S)-C(14S)	121.4(17)
C(51)-C(52)-H(52C)	109.5	C(8S)-C(13S)-C(14S)	118.6(17)
H(52A)-C(52)-H(52C)	109.5	C(13S)-C(14S)-H(14A)	109.5
H(52B)-C(52)-H(52C)	109.5	C(13S)-C(14S)-H(14B)	109.5
C(2S)-C(1S)-C(6S)	120.0	H(14A)-C(14S)-H(14B)	109.5
C(2S)-C(1S)-H(1SA)	120.0	C(13S)-C(14S)-H(14C)	109.5
C(6S)-C(1S)-H(1SA)	120.0	H(14A)-C(14S)-H(14C)	109.5

H(14B)-C(14S)-H(14C)	109.5	C(6E)-C(5E)-C(4E)	120.0
C(6T)-C(1T)-C(2T)	121.7(11)	C(6E)-C(5E)-H(5EA)	120.0
C(6T)-C(1T)-H(1TA)	119.1	C(4E)-C(5E)-H(5EA)	120.0
C(2T)-C(1T)-H(1TA)	119.1	C(5E)-C(6E)-C(1E)	120.0
C(3T)-C(2T)-C(1T)	120.3(9)	C(5E)-C(6E)-C(7E)	140.2(16)
C(3T)-C(2T)-H(2TA)	119.9	C(1E)-C(6E)-C(7E)	99.3(16)
C(1T)-C(2T)-H(2TA)	119.9	C(6E)-C(7E)-H(7EA)	109.5
C(2T)-C(3T)-C(4T)	119.6(10)	C(6E)-C(7E)-H(7EB)	109.5
C(2T)-C(3T)-H(3TA)	120.2	H(7EA)-C(7E)-H(7EB)	109.5
C(4T)-C(3T)-H(3TA)	120.2	C(6E)-C(7E)-H(7EC)	109.5
C(5T)-C(4T)-C(3T)	118.0(11)	H(7EA)-C(7E)-H(7EC)	109.5
C(5T)-C(4T)-H(4TA)	121.0	H(7EB)-C(7E)-H(7EC)	109.5
C(3T)-C(4T)-H(4TA)	121.0	C(2K)-C(1K)-C(6K)	120.0
C(6T)-C(5T)-C(4T)	123.6(10)	C(2K)-C(1K)-H(1KA)	120.0
C(6T)-C(5T)-H(5TA)	118.2	C(6K)-C(1K)-H(1KA)	120.0
C(4T)-C(5T)-H(5TA)	118.2	C(1K)-C(2K)-C(3K)	120.0
C(1T)-C(6T)-C(5T)	116.8(10)	C(1K)-C(2K)-H(2KA)	120.0
C(1T)-C(6T)-C(7T)	122.5(11)	C(3K)-C(2K)-H(2KA)	120.0
C(5T)-C(6T)-C(7T)	120.7(11)	C(4K)-C(3K)-C(2K)	120.0
C(6T)-C(7T)-H(7TA)	109.5	C(4K)-C(3K)-H(3KA)	120.0
C(6T)-C(7T)-H(7TB)	109.5	C(2K)-C(3K)-H(3KA)	120.0
H(7TA)-C(7T)-H(7TB)	109.5	C(3K)-C(4K)-C(5K)	120.0
C(6T)-C(7T)-H(7TC)	109.5	C(3K)-C(4K)-H(4KA)	120.0
H(7TA)-C(7T)-H(7TC)	109.5	C(5K)-C(4K)-H(4KA)	120.0
H(7TB)-C(7T)-H(7TC)	109.5	C(6K)-C(5K)-C(4K)	120.0
C(2E)-C(1E)-C(6E)	120.0	C(6K)-C(5K)-H(5KA)	120.0
C(2E)-C(1E)-H(1EA)	120.0	C(4K)-C(5K)-H(5KA)	120.0
C(6E)-C(1E)-H(1EA)	120.0	C(5K)-C(6K)-C(1K)	120.0
C(1E)-C(2E)-C(3E)	120.0	C(5K)-C(6K)-C(7K)	118.7(10)
C(1E)-C(2E)-H(2EA)	120.0	C(1K)-C(6K)-C(7K)	121.3(9)
C(3E)-C(2E)-H(2EA)	120.0	C(6K)-C(7K)-H(7KA)	109.5
C(4E)-C(3E)-C(2E)	120.0	C(6K)-C(7K)-H(7KB)	109.5
C(4E)-C(3E)-H(3EA)	120.0	H(7KA)-C(7K)-H(7KB)	109.5
C(2E)-C(3E)-H(3EA)	120.0	C(6K)-C(7K)-H(7KC)	109.5
C(3E)-C(4E)-C(5E)	120.0	H(7KA)-C(7K)-H(7KC)	109.5
C(3E)-C(4E)-H(4EA)	120.0	H(7KB)-C(7K)-H(7KC)	109.5
C(5E)-C(4E)-H(4EA)	120.0	Co-O(2)-H(2A)	113(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table U.4 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **[(NHAcF$_{51}$PcCo)$_2$OH]·7(toluene)**. 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}
Co	16(1)	27(1)	34(1)	1(1)	8(1)	-2(1)
N(1)	24(2)	26(2)	30(2)	-1(1)	7(1)	0(1)
N(2)	18(1)	30(2)	35(2)	-7(1)	11(1)	-3(1)
N(3)	24(2)	27(2)	25(2)	-2(1)	9(1)	-3(1)
N(4)	18(1)	33(2)	31(2)	-1(1)	7(1)	-2(1)
N(5)	18(1)	32(2)	39(2)	7(2)	9(1)	-4(1)
N(6)	21(2)	26(2)	35(2)	-1(1)	7(1)	1(1)
N(7)	21(2)	28(2)	36(2)	-7(1)	13(1)	-2(1)
N(8)	20(2)	28(2)	36(2)	3(1)	9(1)	1(1)
N(12)	22(2)	37(2)	41(2)	9(2)	6(1)	-5(1)
O(1)	28(1)	29(2)	34(2)	-2(1)	9(1)	-4(1)
C(1)	17(2)	32(2)	32(2)	-1(2)	7(1)	-2(1)
C(2)	17(2)	33(2)	36(2)	-3(2)	9(2)	-5(1)
C(3)	20(2)	29(2)	37(2)	3(2)	7(2)	-3(1)
C(4)	18(2)	30(2)	36(2)	3(2)	4(2)	-1(1)
C(5)	17(2)	30(2)	31(2)	2(2)	4(1)	-4(1)
C(6)	17(2)	29(2)	40(2)	2(2)	6(2)	-1(1)
C(7)	15(2)	34(2)	34(2)	0(2)	5(1)	1(1)
C(8)	19(2)	26(2)	31(2)	-3(2)	6(1)	-1(1)
C(9)	21(2)	28(2)	45(2)	2(2)	8(2)	-5(2)
C(10)	32(2)	37(2)	48(3)	11(2)	1(2)	-5(2)
C(11)	30(2)	38(2)	57(3)	12(2)	9(2)	4(2)
C(12)	16(2)	31(2)	43(2)	2(2)	11(2)	-1(1)
C(13)	27(2)	39(2)	39(2)	1(2)	7(2)	-8(2)
C(14)	19(2)	43(2)	39(2)	3(2)	7(2)	1(2)
C(15)	18(2)	24(2)	27(2)	-2(1)	7(1)	-2(1)
C(16)	26(2)	23(2)	38(2)	-3(2)	11(2)	0(1)
C(17)	26(2)	30(2)	57(3)	1(2)	17(2)	-2(2)
C(18)	32(2)	29(2)	82(4)	10(2)	24(2)	-2(2)
C(19)	31(2)	28(2)	84(4)	10(2)	22(2)	2(2)
C(20)	27(2)	24(2)	60(3)	1(2)	20(2)	-1(2)
C(21)	26(2)	22(2)	40(2)	-6(2)	15(2)	-5(1)
C(22)	25(2)	19(2)	31(2)	-2(1)	12(2)	0(1)
C(23)	37(3)	36(3)	153(7)	30(4)	37(4)	2(2)
C(24)	42(3)	32(3)	222(12)	3(5)	37(5)	-13(3)
C(25)	53(4)	88(6)	173(10)	73(6)	58(5)	10(4)
C(26)	40(3)	40(3)	110(5)	33(3)	32(3)	10(2)
C(27)	44(3)	65(4)	82(5)	32(3)	26(3)	11(3)
C(28)	54(4)	32(3)	155(8)	12(4)	36(5)	9(3)

C(29)	15(2)	27(2)	36(2)	-6(2)	10(1)	-4(1)
C(30)	20(2)	29(2)	30(2)	-6(2)	11(1)	-7(1)
C(31)	25(2)	26(2)	35(2)	-1(2)	14(2)	-1(1)
C(32)	19(2)	34(2)	36(2)	0(2)	9(2)	2(2)
C(33)	21(2)	36(2)	37(2)	6(2)	7(2)	-3(2)
C(34)	18(2)	35(2)	44(2)	6(2)	8(2)	-1(2)
C(35)	16(2)	30(2)	37(2)	4(2)	6(1)	0(1)
C(36)	19(2)	30(2)	31(2)	-1(2)	9(1)	-1(1)
C(37)	18(2)	29(2)	32(2)	4(2)	7(1)	1(1)
C(38)	23(2)	30(2)	37(2)	3(2)	10(2)	0(2)
C(39)	21(2)	32(2)	49(3)	4(2)	12(2)	-1(2)
C(40)	34(2)	32(2)	52(3)	11(2)	16(2)	-1(2)
C(41)	32(2)	27(2)	61(3)	5(2)	16(2)	1(2)
C(42)	23(2)	30(2)	55(3)	2(2)	15(2)	1(2)
C(43)	22(2)	28(2)	39(2)	4(2)	12(2)	-3(1)
C(44)	22(2)	30(2)	31(2)	3(2)	9(2)	0(2)
C(45)	27(4)	25(4)	77(8)	23(4)	11(4)	8(3)
C(46)	37(4)	27(4)	146(11)	9(5)	36(6)	3(3)
C(47)	36(7)	58(8)	94(9)	28(8)	-7(6)	9(6)
C(48)	26(3)	17(4)	56(6)	7(4)	16(4)	-7(3)
C(49)	41(4)	46(5)	55(5)	21(4)	22(4)	-2(4)
C(50)	39(5)	26(5)	72(8)	8(5)	12(5)	-11(4)
F(38)	37(2)	21(2)	94(4)	9(2)	22(3)	-1(2)
F(39)	68(4)	58(4)	100(5)	24(4)	48(4)	-11(3)
F(40)	58(3)	87(4)	56(3)	27(3)	17(3)	9(3)
F(41)	59(5)	61(5)	66(5)	4(4)	29(4)	9(4)
F(42)	56(3)	32(3)	99(5)	-3(3)	10(4)	-19(2)
F(43)	51(3)	49(3)	58(4)	-4(3)	15(3)	-15(2)
F(44)	27(2)	45(3)	83(4)	13(3)	17(2)	-7(2)
F(45)	47(3)	39(3)	88(5)	32(3)	14(3)	5(2)
F(46)	62(4)	46(3)	127(6)	-24(3)	38(4)	-8(3)
F(47)	52(3)	24(3)	200(10)	10(4)	25(5)	16(2)
F(48)	60(5)	48(4)	129(8)	-13(4)	57(6)	-6(3)
F(49)	78(5)	85(5)	65(4)	5(4)	-17(4)	-10(4)
F(50)	74(5)	93(6)	146(9)	77(6)	-42(5)	-13(5)
F(51)	30(3)	50(3)	147(7)	41(4)	-5(3)	3(2)
C(45A)	62(14)	31(10)	110(20)	25(12)	33(14)	8(9)
C(46A)	120(30)	45(13)	130(20)	47(15)	90(20)	49(16)
C(47A)	43(14)	100(20)	140(30)	70(20)	18(17)	31(14)
C(48A)	56(11)	31(10)	58(13)	-1(9)	-4(9)	-4(8)
C(49A)	62(17)	70(20)	90(20)	57(18)	22(15)	-18(15)
C(50A)	130(30)	28(11)	190(40)	7(17)	110(30)	-13(16)
F(38A)	61(7)	72(8)	136(13)	56(9)	43(8)	6(6)
F(39A)	87(10)	99(11)	91(10)	-6(9)	42(8)	1(9)

F(40A)	51(7)	77(8)	141(13)	33(8)	31(8)	-14(6)
F(41A)	89(10)	124(14)	142(15)	46(13)	67(11)	-11(10)
F(42A)	115(14)	52(8)	230(30)	-7(14)	47(19)	-46(9)
F(43A)	116(18)	63(12)	85(16)	-9(11)	-16(12)	-14(12)
F(44A)	165(18)	68(10)	155(18)	-44(11)	27(14)	2(10)
F(45A)	83(9)	39(6)	159(16)	20(8)	46(10)	7(6)
F(46A)	72(9)	73(9)	240(20)	36(11)	84(13)	19(7)
F(47A)	127(15)	56(8)	190(20)	-3(11)	64(14)	42(9)
F(48A)	133(15)	113(13)	122(14)	-1(11)	78(12)	37(12)
F(49A)	101(12)	151(16)	107(12)	76(12)	33(10)	23(11)
F(50A)	78(10)	58(9)	170(19)	60(11)	2(11)	14(8)
F(51A)	69(12)	92(14)	112(14)	49(12)	18(11)	8(10)
C(51)	23(2)	26(2)	44(2)	1(2)	12(2)	-1(2)
C(52)	29(2)	39(2)	52(3)	3(2)	7(2)	-13(2)
F(1)	22(1)	31(1)	50(2)	11(1)	10(1)	0(1)
F(2)	24(1)	33(1)	59(2)	17(1)	7(1)	-1(1)
F(3)	22(1)	41(2)	50(2)	13(1)	-2(1)	-6(1)
F(4)	58(2)	56(2)	42(2)	7(1)	11(1)	10(2)
F(5)	40(2)	43(2)	61(2)	21(1)	2(1)	-6(1)
F(6)	40(2)	55(2)	53(2)	19(2)	-13(1)	-8(1)
F(7)	46(2)	37(2)	77(2)	-8(2)	13(2)	-3(1)
F(8)	40(2)	50(2)	95(3)	11(2)	6(2)	18(2)
F(9)	86(3)	50(2)	72(2)	5(2)	45(2)	10(2)
F(10)	20(1)	40(1)	47(2)	10(1)	8(1)	7(1)
F(11)	52(2)	53(2)	44(2)	1(1)	-12(1)	-13(2)
F(12)	33(1)	60(2)	63(2)	-6(2)	16(1)	-21(1)
F(13)	36(2)	43(2)	61(2)	-6(1)	6(1)	-6(1)
F(14)	30(1)	58(2)	44(2)	9(1)	14(1)	6(1)
F(15)	42(2)	48(2)	44(2)	13(1)	14(1)	10(1)
F(16)	34(1)	62(2)	38(2)	-4(1)	3(1)	-11(1)
F(17)	25(1)	36(1)	79(2)	10(1)	20(1)	-2(1)
F(18)	27(1)	30(1)	75(2)	10(1)	19(1)	5(1)
F(19)	46(2)	35(2)	225(6)	40(3)	40(3)	3(2)
F(20)	60(3)	61(3)	150(5)	-31(3)	12(3)	-18(2)
F(21)	37(2)	52(2)	192(5)	24(3)	25(3)	-10(2)
F(22)	66(3)	38(2)	300(9)	1(3)	23(4)	-21(2)
F(23)	71(3)	97(3)	132(4)	53(3)	61(3)	23(2)
F(24)	75(3)	116(4)	264(8)	116(5)	87(4)	13(3)
F(25)	75(3)	162(5)	142(5)	85(4)	57(3)	34(3)
F(26)	47(2)	70(2)	142(4)	61(3)	40(2)	12(2)
F(27)	64(3)	106(4)	115(4)	70(3)	27(2)	19(2)
F(28)	38(2)	71(2)	97(3)	28(2)	24(2)	12(2)
F(29)	54(2)	75(3)	74(2)	14(2)	21(2)	13(2)
F(30)	60(2)	38(2)	148(4)	-8(2)	49(3)	0(2)

F(31)	71(3)	38(2)	217(6)	-17(3)	50(3)	-9(2)
F(32)	83(3)	56(3)	223(7)	50(3)	60(4)	42(2)
F(33)	24(1)	35(1)	70(2)	16(1)	6(1)	-4(1)
F(34)	28(1)	28(1)	53(2)	2(1)	9(1)	1(1)
F(35)	22(1)	39(1)	48(2)	1(1)	10(1)	2(1)
F(36)	22(1)	37(2)	85(2)	15(2)	14(1)	6(1)
F(37)	21(1)	37(1)	69(2)	12(1)	13(1)	-2(1)
C(1S)	91(7)	160(11)	93(8)	-74(7)	37(6)	-49(6)
C(2S)	97(7)	89(7)	109(10)	-52(6)	57(7)	-24(6)
C(3S)	86(6)	87(6)	102(8)	-46(6)	38(6)	-9(5)
C(4S)	92(6)	106(8)	82(7)	-34(6)	24(6)	-7(5)
C(5S)	79(6)	187(12)	96(9)	-66(8)	17(6)	-20(7)
C(6S)	86(6)	196(12)	70(8)	-75(8)	31(6)	-37(7)
C(7S)	79(7)	280(20)	98(11)	-99(13)	26(7)	-65(10)
C(8S)	82(12)	84(15)	31(11)	-11(10)	14(10)	-20(10)
C(9S)	76(12)	114(17)	21(11)	-32(11)	7(10)	-15(11)
C(10S)	71(11)	109(16)	40(12)	-28(10)	29(10)	16(11)
C(11S)	74(11)	76(13)	45(11)	-13(9)	35(10)	32(9)
C(12S)	61(10)	47(10)	40(10)	-12(8)	19(9)	8(8)
C(13S)	69(11)	51(10)	23(10)	-11(8)	2(9)	1(8)
C(14S)	78(13)	42(13)	61(18)	7(12)	-16(15)	-6(11)
C(1T)	79(6)	143(9)	106(7)	32(7)	43(5)	46(6)
C(2T)	98(7)	133(9)	67(5)	14(5)	27(5)	65(7)
C(3T)	123(8)	84(6)	69(5)	-18(4)	24(5)	34(6)
C(4T)	114(8)	97(7)	89(7)	-31(6)	-2(6)	10(6)
C(5T)	105(8)	139(10)	107(8)	29(7)	-8(6)	42(8)
C(6T)	78(6)	144(10)	120(8)	49(7)	26(6)	23(7)
C(7T)	165(14)	178(15)	370(30)	188(18)	60(16)	36(12)
C(1E)	510(50)	149(18)	490(50)	130(20)	380(50)	190(30)
C(2E)	430(30)	68(7)	116(11)	-32(7)	49(15)	40(13)
C(3E)	215(16)	44(5)	199(16)	8(7)	-15(14)	-29(7)
C(4E)	246(18)	46(5)	134(11)	21(6)	48(12)	17(8)
C(5E)	160(14)	120(11)	201(18)	76(11)	36(12)	-12(10)
C(6E)	290(30)	158(17)	250(30)	65(18)	130(20)	11(17)
C(7E)	410(40)	360(40)	270(30)	-50(30)	200(30)	-20(30)
C(1K)	71(8)	45(5)	93(9)	19(17)	9(6)	4(13)
C(2K)	79(10)	55(9)	71(10)	0(7)	25(8)	-8(8)
C(3K)	47(7)	43(7)	93(11)	-14(7)	-2(7)	-5(6)
C(4K)	84(14)	42(7)	76(13)	6(7)	-10(10)	8(8)
C(5K)	45(8)	42(6)	76(12)	-1(7)	3(8)	2(6)
C(6K)	49(7)	41(7)	69(9)	-6(7)	-4(6)	3(6)
C(7K)	68(9)	76(10)	96(12)	8(9)	26(9)	17(8)
O(2)	19(2)	25(3)	34(3)	-3(2)	5(2)	-12(2)

Table U.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **[(NHAcF_{51}PcCo)$_2$OH]·7(toluene)**.

	x	y	z	U(eq)
H(52A)	12905	3649	7914	61
H(52B)	12731	3726	7232	61
H(52C)	13254	3387	7512	61
H(1SA)	6869	2999	4718	134
H(2SA)	8054	3169	4754	111
H(3SA)	8296	3751	4374	107
H(4SA)	7352	4162	3958	112
H(5SA)	6167	3991	3923	146
H(7SA)	5414	3272	3906	228
H(7SB)	5388	3573	4401	228
H(7SC)	5665	3151	4574	228
H(8SA)	7172	3746	4259	79
H(9SA)	8271	3436	4609	85
H(10A)	8302	2833	5022	85
H(11A)	7234	2541	5086	73
H(12A)	6134	2851	4737	58
H(14A)	5935	3754	4012	100
H(14B)	5670	3620	4563	100
H(14C)	5504	3365	3990	100
H(1TA)	1461	3240	5298	127
H(2TA)	1365	2614	5560	118
H(3TA)	259	2333	5410	110
H(4TA)	-770	2675	4952	126
H(5TA)	-639	3290	4666	148
H(7TA)	-3	3856	4736	357
H(7TB)	617	3747	4428	357
H(7TC)	821	3868	5096	357
H(1EA)	8187	5482	1900	404
H(2EA)	7028	5356	1993	250
H(3EA)	6772	5414	2896	198
H(4EA)	7675	5598	3707	170
H(5EA)	8834	5724	3615	194
H(7EA)	9663	5610	2692	494
H(7EB)	9235	5980	2413	494
H(7EC)	9095	5586	2074	494
H(1KA)	4872	4703	7597	86
H(2KA)	5323	4562	6799	81

H(3KA)	5513	3932	6575	77
H(4KA)	5251	3442	7150	87
H(5KA)	4800	3584	7949	67
H(7KA)	4063	4085	8331	118
H(7KB)	4372	4507	8361	118
H(7KC)	4856	4175	8717	118
H(2A)	7140(60)	2580(30)	5360(50)	31
H(12)	11770(30)	3512(15)	6680(20)	40

Appendix V: Crystal structure of $[(NHAcF_{51}PcCo)_2H_2O]\cdot 7(toluene)$

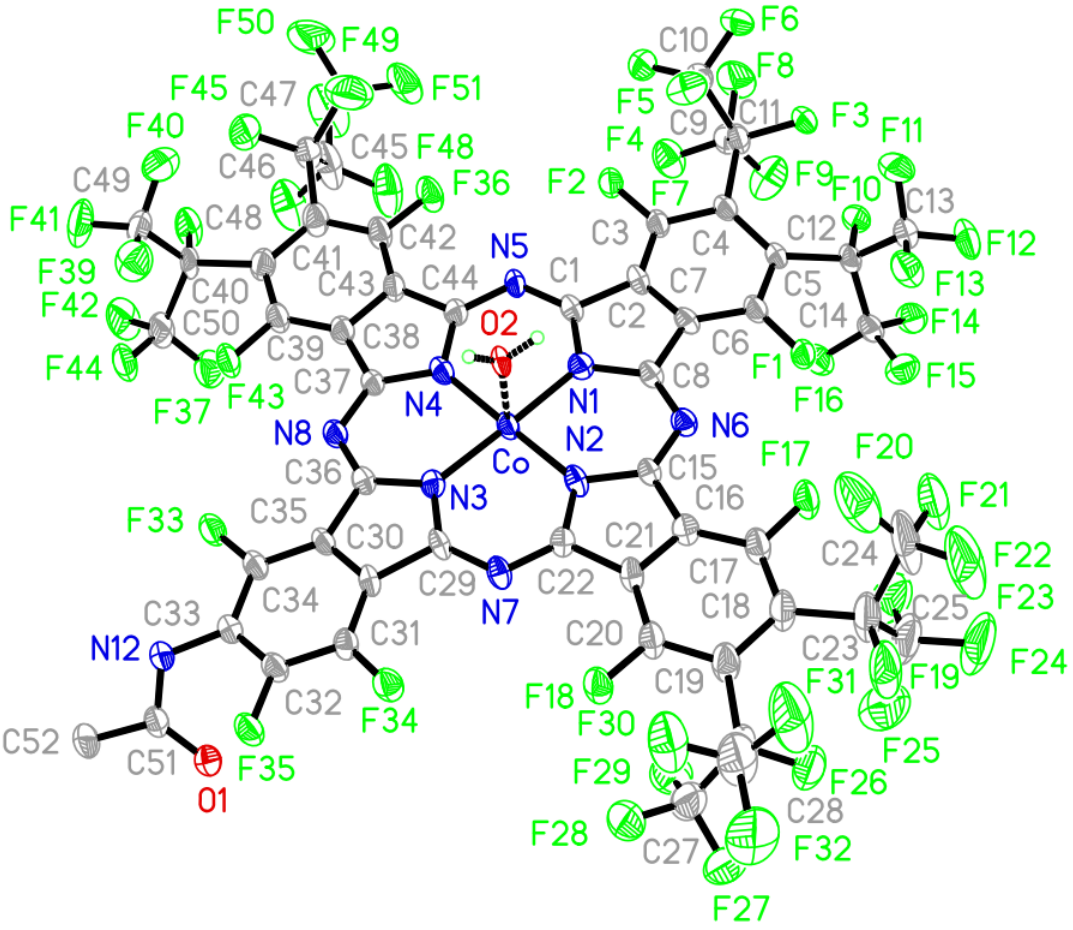


Figure V.1 ORTEP representation of **$NHAcF_{51}PcCo\text{-}OH_2$** X-ray crystal structure, at 50% probability.

Table V.1 Crystal data and structure refinement for **$[(NHAcF_{51}PcCo)_2H_2O]\cdot 7(toluene)$**.

Empirical formula	C153 H66 Co2 F102 N18 O3	
Formula weight	4260.09	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.247(5) Å	α = 90°.
	b = 35.337(9) Å	β = 104.732(6)°.
	c = 23.857(6) Å	γ = 90°.
Volume	15692(6) $Å^3$	
Z	4	
Density (calculated)	1.803 g/cm^3	

Absorption coefficient	0.396 mm^{-1}
F(000)	8424
Crystal size	0.870 x 0.480 x 0.370 mm^3
Theta range for data collection	1.348 to 30.536°.
Index ranges	-27<=h<=27, -50<=k<=50, -34<=l<=33
Reflections collected	228254
Independent reflections	23951 [R(int) = 0.0526]
Completeness to theta = 25.000°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6740
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	23951 / 301 / 1500
Goodness-of-fit on F^2	1.063
Final R indices [I>2sigma(I)]	R1 = 0.1057, wR2 = 0.1893
R indices (all data)	R1 = 0.1610, wR2 = 0.2254
Extinction coefficient	n/a
Largest diff. peak and hole	1.200 and -1.484 e.$Å^{-3}$

Table V.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[(NHAcF$_{51}$PcCo)$_2$H$_2$O]*7Toluene**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7589(1)	2906(1)	6302(1)	25(1)
N(1)	6564(2)	2928(1)	6188(2)	27(1)
N(2)	7586(2)	2388(1)	6548(2)	27(1)
N(3)	8604(2)	2876(1)	6379(1)	24(1)
N(4)	7587(2)	3417(1)	6029(2)	27(1)
N(5)	6310(2)	3559(1)	5786(2)	29(1)
N(6)	6328(2)	2309(1)	6526(2)	27(1)
N(7)	8853(2)	2237(1)	6744(2)	27(1)
N(8)	8859(2)	3520(1)	6142(2)	28(1)
N(12)	11736(2)	3272(1)	6895(2)	34(1)
O(1)	12088(2)	3060(1)	7810(1)	30(1)
C(1)	6130(2)	3228(1)	5957(2)	27(1)
C(2)	5389(2)	3131(1)	5947(2)	28(1)
C(3)	4742(2)	3318(1)	5748(2)	29(1)
C(4)	4090(2)	3166(1)	5802(2)	28(1)
C(5)	4121(2)	2818(1)	6133(2)	26(1)
C(6)	4776(2)	2630(1)	6287(2)	29(1)

C(7)	5401(2)	2781(1)	6189(2)	28(1)
C(8)	6138(2)	2649(1)	6322(2)	26(1)
C(9)	3404(2)	3368(1)	5459(2)	32(1)
C(10)	3401(3)	3466(1)	4812(2)	41(1)
C(11)	3213(3)	3725(1)	5765(2)	42(1)
C(12)	3518(2)	2654(1)	6383(2)	29(1)
C(13)	3130(2)	2304(1)	6058(2)	35(1)
C(14)	3752(2)	2567(1)	7049(2)	34(1)
C(15)	6997(2)	2193(1)	6633(2)	23(1)
C(16)	7223(2)	1826(1)	6879(2)	28(1)
C(17)	6861(2)	1528(1)	7042(2)	36(1)
C(18)	7202(3)	1201(1)	7305(3)	46(1)
C(19)	7981(3)	1195(1)	7423(3)	46(1)
C(20)	8322(2)	1491(1)	7209(2)	35(1)
C(21)	7958(2)	1805(1)	6945(2)	28(1)
C(22)	8175(2)	2161(1)	6729(2)	24(1)
C(23)	6707(3)	882(2)	7406(4)	73(2)
C(24)	6042(4)	797(2)	6851(6)	98(4)
C(25)	6421(4)	943(3)	7935(5)	99(3)
C(26)	8478(3)	902(2)	7807(3)	61(2)
C(27)	9119(3)	1082(2)	8273(3)	62(2)
C(28)	8747(4)	597(2)	7449(4)	79(2)
C(29)	9035(2)	2570(1)	6580(2)	26(1)
C(30)	9789(2)	2676(1)	6647(2)	25(1)
C(31)	10425(2)	2480(1)	6830(2)	27(1)
C(32)	11066(2)	2676(1)	6889(2)	30(1)
C(33)	11081(2)	3066(1)	6783(2)	31(1)
C(34)	10433(2)	3248(1)	6572(2)	33(1)
C(35)	9794(2)	3055(1)	6506(2)	28(1)
C(36)	9044(2)	3173(1)	6318(2)	26(1)
C(37)	8176(2)	3622(1)	5991(2)	26(1)
C(38)	7954(2)	3993(1)	5754(2)	30(1)
C(39)	8311(2)	4307(1)	5626(2)	33(1)
C(40)	7967(3)	4637(1)	5395(2)	38(1)
C(41)	7191(3)	4647(1)	5267(2)	39(1)
C(42)	6847(2)	4322(1)	5405(2)	35(1)
C(43)	7210(2)	4004(1)	5644(2)	29(1)
C(44)	6989(2)	3642(1)	5822(2)	27(1)
C(45)	6679(5)	4972(3)	4930(6)	43(3)
C(46)	6415(2)	5226(2)	5364(3)	68(3)
C(47)	6024(5)	4844(2)	4449(5)	67(4)
C(48)	8470(4)	4985(2)	5336(5)	32(2)
C(49)	8708(4)	4952(3)	4761(4)	46(2)
C(50)	9144(6)	5046(3)	5854(6)	46(3)

F(38)	8116(2)	5319(1)	5312(3)	49(1)
F(39)	9090(4)	5249(2)	4701(3)	71(2)
F(40)	8132(3)	4935(2)	4308(3)	66(2)
F(41)	9083(5)	4642(3)	4753(4)	60(2)
F(42)	9281(4)	5420(2)	5904(3)	64(2)
F(43)	9003(4)	4939(2)	6351(3)	52(2)
F(44)	9734(2)	4879(1)	5804(3)	51(1)
F(45)	7027(3)	5206(2)	4639(3)	59(2)
F(46)	6971(3)	5414(2)	5692(3)	76(2)
F(47)	5935(3)	5474(1)	5076(4)	93(3)
F(48)	6114(4)	5020(2)	5706(4)	73(3)
F(49)	6175(4)	4525(2)	4212(3)	82(2)
F(50)	5867(4)	5098(2)	4028(3)	117(4)
F(51)	5425(3)	4782(2)	4610(3)	81(3)
C(45A)	6717(9)	4971(5)	5170(8)	65(9)
C(46A)	6211(6)	5054(3)	5570(6)	88(14)
C(47A)	6278(6)	4979(3)	4532(6)	97(12)
C(48A)	8426(9)	4892(5)	5160(7)	51(7)
C(49A)	8983(11)	4737(5)	4841(9)	73(13)
C(50A)	8818(13)	5151(5)	5672(10)	105(13)
F(38A)	8013(6)	5133(4)	4763(7)	86(5)
F(39A)	8764(8)	4410(4)	4608(6)	89(4)
F(40A)	9633(6)	4684(4)	5201(7)	88(5)
F(41A)	9055(8)	4977(5)	4442(8)	111(6)
F(42A)	9236(11)	5401(5)	5488(11)	132(9)
F(43A)	9243(11)	4955(5)	6110(8)	95(8)
F(44A)	8358(10)	5351(4)	5875(9)	132(7)
F(45A)	7112(7)	5294(3)	5200(8)	91(5)
F(46A)	5560(6)	4902(3)	5384(7)	119(7)
F(47A)	6145(8)	5428(3)	5598(8)	119(7)
F(48A)	6514(8)	4922(4)	6098(5)	114(6)
F(49A)	6690(6)	4973(4)	4164(6)	118(7)
F(50A)	5888(7)	5292(3)	4420(8)	107(7)
F(51A)	5824(8)	4692(3)	4391(8)	91(6)
C(51)	12199(2)	3270(1)	7438(2)	30(1)
C(52)	12826(2)	3530(1)	7532(2)	41(1)
F(1)	4817(1)	2301(1)	6570(1)	34(1)
F(2)	4738(1)	3645(1)	5470(1)	39(1)
F(3)	2826(1)	3130(1)	5391(1)	40(1)
F(4)	3794(2)	3221(1)	4607(1)	52(1)
F(5)	3620(2)	3813(1)	4744(1)	50(1)
F(6)	2726(2)	3443(1)	4490(1)	54(1)
F(7)	3744(2)	3973(1)	5883(2)	54(1)
F(8)	2638(2)	3894(1)	5434(2)	64(1)

F(9)	3066(2)	3636(1)	6265(2)	65(1)
F(10)	2991(1)	2920(1)	6353(1)	36(1)
F(11)	2812(2)	2394(1)	5518(1)	54(1)
F(12)	2630(2)	2184(1)	6312(2)	51(1)
F(13)	3572(2)	2023(1)	6048(1)	48(1)
F(14)	3200(1)	2630(1)	7276(1)	43(1)
F(15)	3956(2)	2214(1)	7180(1)	44(1)
F(16)	4277(2)	2795(1)	7316(1)	46(1)
F(17)	6148(1)	1554(1)	6942(2)	45(1)
F(18)	9030(1)	1476(1)	7279(1)	43(1)
F(19)	7061(2)	544(1)	7472(3)	101(2)
F(20)	6201(2)	900(1)	6373(3)	93(2)
F(21)	5443(2)	965(1)	6891(3)	94(2)
F(22)	5913(3)	430(1)	6835(4)	139(3)
F(23)	6092(2)	1262(1)	7946(2)	93(2)
F(24)	5990(3)	660(2)	8001(3)	144(3)
F(25)	6974(3)	937(2)	8419(3)	121(2)
F(26)	8120(2)	714(1)	8146(2)	83(2)
F(27)	9275(2)	867(1)	8749(2)	94(2)
F(28)	9725(2)	1111(1)	8106(2)	68(1)
F(29)	8946(2)	1422(1)	8434(2)	67(1)
F(30)	9135(2)	741(1)	7116(2)	78(1)
F(31)	8205(2)	407(1)	7114(3)	106(2)
F(32)	9162(3)	349(1)	7815(3)	117(2)
F(33)	10450(1)	3617(1)	6449(1)	44(1)
F(34)	10454(1)	2112(1)	6948(1)	36(1)
F(35)	11685(1)	2482(1)	7045(1)	36(1)
F(36)	6134(1)	4318(1)	5304(2)	48(1)
F(37)	9027(1)	4286(1)	5737(1)	42(1)
C(1S)	6966(5)	3235(2)	4564(4)	113(4)
C(2S)	7670(4)	3336(2)	4585(4)	94(4)
C(3S)	7814(3)	3681(2)	4360(4)	90(3)
C(4S)	7254(5)	3925(2)	4113(3)	94(3)
C(5S)	6550(4)	3824(3)	4091(3)	123(4)
C(6S)	6406(3)	3479(3)	4317(4)	116(4)
C(7S)	5653(5)	3358(6)	4298(7)	153(8)
C(8S)	7180(12)	3504(5)	4425(8)	63(6)
C(9S)	7834(9)	3320(6)	4633(8)	67(7)
C(10S)	7854(8)	2962(6)	4879(8)	68(6)
C(11S)	7220(10)	2788(4)	4918(7)	58(6)
C(12S)	6566(8)	2972(4)	4710(8)	46(5)
C(13S)	6547(9)	3329(5)	4464(8)	47(5)
C(14S)	5850(12)	3535(8)	4238(17)	64(8)
C(1T)	1000(5)	3125(3)	5222(4)	106(3)

C(2T)	944(6)	2753(3)	5383(4)	98(3)
C(3T)	298(6)	2587(3)	5291(4)	92(3)
C(4T)	-307(6)	2787(3)	5023(4)	105(3)
C(5T)	-223(7)	3153(4)	4860(5)	123(4)
C(6T)	419(6)	3330(3)	4962(5)	114(4)
C(7T)	467(8)	3735(4)	4791(9)	239(11)
C(1E)	8082(10)	5506(3)	2266(5)	340(20)
C(2E)	7394(8)	5431(2)	2322(5)	209(11)
C(3E)	7242(5)	5466(2)	2859(6)	166(7)
C(4E)	7778(8)	5575(2)	3340(4)	142(5)
C(5E)	8467(6)	5649(3)	3285(6)	162(7)
C(6E)	8619(6)	5615(3)	2748(8)	221(11)
C(7E)	9203(11)	5705(8)	2456(10)	329(16)
C(1K)	4949(9)	4447(2)	7507(6)	72(4)
C(2K)	5217(8)	4363(2)	7032(5)	67(4)
C(3K)	5330(6)	3989(3)	6900(5)	64(4)
C(4K)	5174(11)	3698(2)	7241(7)	73(6)
C(5K)	4906(10)	3782(2)	7716(6)	56(4)
C(6K)	4794(6)	4157(3)	7849(4)	57(3)
C(7K)	4496(8)	4238(5)	8359(6)	79(4)
O(2)	7425(3)	2662(2)	5443(2)	26(1)

Table V.3 Bond lengths [Å] and angles [°] for **[(NHAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**.

Co-N(3)	1.919(3)	Co-N(1)	1.923(3)
Co-N(4)	1.919(4)	Co-O(1)#1	2.122(3)
Co-N(2)	1.923(4)	Co-O(2)	2.172(6)
N(1)-C(8)	1.373(5)	N(8)-C(36)	1.317(5)
N(1)-C(1)	1.374(5)	N(8)-C(37)	1.322(5)
N(2)-C(22)	1.366(5)	N(12)-C(51)	1.373(6)
N(2)-C(15)	1.384(5)	N(12)-C(33)	1.420(5)
N(3)-C(29)	1.374(5)	N(12)-H(12)	1.01(5)
N(3)-C(36)	1.377(5)	O(1)-C(51)	1.217(5)
N(4)-C(37)	1.368(5)	C(1)-C(2)	1.462(5)
N(4)-C(44)	1.381(5)	C(2)-C(7)	1.363(6)
N(5)-C(1)	1.315(5)	C(2)-C(3)	1.383(6)
N(5)-C(44)	1.321(5)	C(3)-F(2)	1.330(5)
N(6)-C(8)	1.313(5)	C(3)-C(4)	1.402(5)
N(6)-C(15)	1.314(5)	C(4)-C(5)	1.452(6)
N(7)-C(29)	1.315(5)	C(4)-C(9)	1.540(6)
N(7)-C(22)	1.324(5)	C(5)-C(6)	1.390(5)

C(5)-C(12)	1.546(5)	C(26)-C(28)	1.544(10)
C(6)-F(1)	1.335(5)	C(26)-C(27)	1.571(10)
C(6)-C(7)	1.389(5)	C(27)-F(29)	1.328(8)
C(7)-C(8)	1.450(5)	C(27)-F(28)	1.328(7)
C(9)-F(3)	1.371(5)	C(27)-F(27)	1.336(7)
C(9)-C(11)	1.548(7)	C(28)-F(30)	1.324(9)
C(9)-C(10)	1.583(7)	C(28)-F(31)	1.324(9)
C(10)-F(5)	1.319(5)	C(28)-F(32)	1.347(9)
C(10)-F(4)	1.322(6)	C(29)-C(30)	1.468(5)
C(10)-F(6)	1.332(5)	C(30)-C(31)	1.378(6)
C(11)-F(7)	1.320(6)	C(30)-C(35)	1.383(6)
C(11)-F(8)	1.329(5)	C(31)-F(34)	1.330(5)
C(11)-F(9)	1.330(6)	C(31)-C(32)	1.391(5)
C(12)-F(10)	1.371(5)	C(32)-F(35)	1.343(5)
C(12)-C(13)	1.548(6)	C(32)-C(33)	1.404(6)
C(12)-C(14)	1.569(6)	C(33)-C(34)	1.378(6)
C(13)-F(13)	1.314(6)	C(34)-F(33)	1.339(5)
C(13)-F(11)	1.317(5)	C(34)-C(35)	1.380(5)
C(13)-F(12)	1.329(5)	C(35)-C(36)	1.458(5)
C(14)-F(15)	1.320(5)	C(37)-C(38)	1.450(6)
C(14)-F(16)	1.322(5)	C(38)-C(39)	1.381(6)
C(14)-F(14)	1.328(5)	C(38)-C(43)	1.388(5)
C(15)-C(16)	1.445(5)	C(39)-F(37)	1.337(5)
C(16)-C(17)	1.370(6)	C(39)-C(40)	1.384(6)
C(16)-C(21)	1.385(5)	C(40)-C(41)	1.446(6)
C(17)-F(17)	1.336(5)	C(40)-C(48A)	1.47(2)
C(17)-C(18)	1.398(7)	C(40)-C(48)	1.592(9)
C(18)-C(19)	1.453(7)	C(41)-C(42)	1.407(6)
C(18)-C(23)	1.534(7)	C(41)-C(45A)	1.446(18)
C(19)-C(20)	1.397(6)	C(41)-C(45)	1.592(10)
C(19)-C(26)	1.543(7)	C(42)-F(36)	1.332(5)
C(20)-F(18)	1.331(5)	C(42)-C(43)	1.370(6)
C(20)-C(21)	1.378(6)	C(43)-C(44)	1.444(6)
C(21)-C(22)	1.460(5)	C(45)-F(45)	1.360(10)
C(23)-F(19)	1.366(7)	C(45)-C(47)	1.542(16)
C(23)-C(25)	1.516(13)	C(45)-C(46)	1.550(16)
C(23)-C(24)	1.619(13)	C(46)-F(46)	1.331(5)
C(24)-F(20)	1.307(12)	C(46)-F(48)	1.331(5)
C(24)-F(22)	1.320(7)	C(46)-F(47)	1.331(5)
C(24)-F(21)	1.321(8)	C(47)-F(51)	1.324(6)
C(25)-F(23)	1.296(9)	C(47)-F(49)	1.324(6)
C(25)-F(24)	1.333(8)	C(47)-F(50)	1.325(6)
C(25)-F(25)	1.357(11)	C(48)-F(38)	1.356(9)
C(26)-F(26)	1.362(7)	C(48)-C(49)	1.557(13)

C(48)-C(50)	1.563(14)	C(8S)-C(9S)	1.3900
C(49)-F(39)	1.307(10)	C(8S)-C(13S)	1.3900
C(49)-F(41)	1.315(11)	C(8S)-H(8SA)	0.9500
C(49)-F(40)	1.339(10)	C(9S)-C(10S)	1.3900
C(50)-F(44)	1.312(12)	C(9S)-H(9SA)	0.9500
C(50)-F(43)	1.337(13)	C(10S)-C(11S)	1.3900
C(50)-F(42)	1.348(11)	C(10S)-H(10A)	0.9500
C(45A)-F(45A)	1.362(16)	C(11S)-C(12S)	1.3900
C(45A)-C(47A)	1.543(19)	C(11S)-H(11A)	0.9500
C(45A)-C(46A)	1.555(19)	C(12S)-C(13S)	1.3900
C(46A)-F(48A)	1.331(5)	C(12S)-H(12A)	0.9500
C(46A)-F(46A)	1.331(5)	C(13S)-C(14S)	1.499(8)
C(46A)-F(47A)	1.331(5)	C(14S)-H(14A)	0.9800
C(47A)-F(51A)	1.324(6)	C(14S)-H(14B)	0.9800
C(47A)-F(50A)	1.324(6)	C(14S)-H(14C)	0.9800
C(47A)-F(49A)	1.324(6)	C(1T)-C(6T)	1.344(12)
C(48A)-F(38A)	1.368(16)	C(1T)-C(2T)	1.382(14)
C(48A)-C(50A)	1.56(2)	C(1T)-H(1TA)	0.9500
C(48A)-C(49A)	1.56(2)	C(2T)-C(3T)	1.341(14)
C(49A)-F(39A)	1.303(18)	C(2T)-H(2TA)	0.9500
C(49A)-F(41A)	1.309(17)	C(3T)-C(4T)	1.373(13)
C(49A)-F(40A)	1.339(19)	C(3T)-H(3TA)	0.9500
C(50A)-F(44A)	1.316(18)	C(4T)-C(5T)	1.371(15)
C(50A)-F(42A)	1.341(17)	C(4T)-H(4TA)	0.9500
C(50A)-F(43A)	1.343(19)	C(5T)-C(6T)	1.351(15)
C(51)-C(52)	1.487(6)	C(5T)-H(5TA)	0.9500
C(52)-H(52A)	0.9800	C(6T)-C(7T)	1.499(8)
C(52)-H(52B)	0.9800	C(7T)-H(7TA)	0.9800
C(52)-H(52C)	0.9800	C(7T)-H(7TB)	0.9800
C(1S)-C(2S)	1.3900	C(7T)-H(7TC)	0.9800
C(1S)-C(6S)	1.3900	C(1E)-C(2E)	1.3900
C(1S)-H(1SA)	0.9500	C(1E)-C(6E)	1.3900
C(2S)-C(3S)	1.3900	C(1E)-H(1EA)	0.9500
C(2S)-H(2SA)	0.9500	C(2E)-C(3E)	1.3900
C(3S)-C(4S)	1.3900	C(2E)-H(2EA)	0.9500
C(3S)-H(3SA)	0.9500	C(3E)-C(4E)	1.3900
C(4S)-C(5S)	1.3900	C(3E)-H(3EA)	0.9500
C(4S)-H(4SA)	0.9500	C(4E)-C(5E)	1.3900
C(5S)-C(6S)	1.3900	C(4E)-H(4EA)	0.9500
C(5S)-H(5SA)	0.9500	C(5E)-C(6E)	1.3900
C(6S)-C(7S)	1.499(8)	C(5E)-H(5EA)	0.9500
C(7S)-H(7SA)	0.9800	C(6E)-C(7E)	1.498(8)
C(7S)-H(7SB)	0.9800	C(7E)-H(7EA)	0.9800
C(7S)-H(7SC)	0.9800	C(7E)-H(7EB)	0.9800

C(7E)-H(7EC)	0.9800	C(4K)-H(4KA)	0.9500
C(1K)-C(2K)	1.3900	C(5K)-C(6K)	1.3900
C(1K)-C(6K)	1.3900	C(5K)-H(5KA)	0.9500
C(1K)-H(1KA)	0.9500	C(6K)-C(7K)	1.499(8)
C(2K)-C(3K)	1.3900	C(7K)-H(7KA)	0.9800
C(2K)-H(2KA)	0.9500	C(7K)-H(7KB)	0.9800
C(3K)-C(4K)	1.3900	C(7K)-H(7KC)	0.9800
C(3K)-H(3KA)	0.9500	O(2)-H(2A)	0.840(2)
C(4K)-C(5K)	1.3900	O(2)-H(2B)	0.840(2)

N(3)-Co-N(4)	89.87(14)	N(2)-Co-O(1)#1	87.88(13)
N(3)-Co-N(2)	90.07(14)	N(1)-Co-O(1)#1	99.20(13)
N(4)-Co-N(2)	177.98(15)	N(3)-Co-O(2)	88.24(17)
N(3)-Co-N(1)	177.39(15)	N(4)-Co-O(2)	93.79(18)
N(4)-Co-N(1)	89.97(14)	N(2)-Co-O(2)	84.19(18)
N(2)-Co-N(1)	89.99(14)	N(1)-Co-O(2)	89.16(17)
N(3)-Co-O(1)#1	83.41(13)	O(1)#1-Co-O(2)	168.48(17)
N(4)-Co-O(1)#1	94.12(13)		

C(8)-N(1)-C(1)	108.0(3)	C(7)-C(2)-C(1)	107.1(4)
C(8)-N(1)-Co	126.1(3)	C(3)-C(2)-C(1)	133.1(4)
C(1)-N(1)-Co	125.9(3)	F(2)-C(3)-C(2)	118.5(3)
C(22)-N(2)-C(15)	107.8(3)	F(2)-C(3)-C(4)	119.3(4)
C(22)-N(2)-Co	126.0(3)	C(2)-C(3)-C(4)	122.2(4)
C(15)-N(2)-Co	125.8(3)	C(3)-C(4)-C(5)	117.5(3)
C(29)-N(3)-C(36)	107.7(3)	C(3)-C(4)-C(9)	116.0(4)
C(29)-N(3)-Co	125.8(3)	C(5)-C(4)-C(9)	126.3(3)
C(36)-N(3)-Co	126.0(3)	C(6)-C(5)-C(4)	117.2(3)
C(37)-N(4)-C(44)	107.5(3)	C(6)-C(5)-C(12)	116.0(4)
C(37)-N(4)-Co	126.2(3)	C(4)-C(5)-C(12)	126.5(3)
C(44)-N(4)-Co	126.3(3)	F(1)-C(6)-C(7)	118.5(3)
C(1)-N(5)-C(44)	120.7(4)	F(1)-C(6)-C(5)	118.9(3)
C(8)-N(6)-C(15)	121.6(4)	C(7)-C(6)-C(5)	122.5(4)
C(29)-N(7)-C(22)	120.5(3)	C(2)-C(7)-C(6)	119.9(4)
C(36)-N(8)-C(37)	120.7(4)	C(2)-C(7)-C(8)	107.2(3)
C(51)-N(12)-C(33)	120.5(4)	C(6)-C(7)-C(8)	132.9(4)
		N(6)-C(8)-N(1)	128.2(4)
C(51)-N(12)-H(12)	112(3)	N(6)-C(8)-C(7)	122.7(4)
C(33)-N(12)-H(12)	120(3)	N(1)-C(8)-C(7)	109.1(3)
C(51)-O(1)-Co#1	145.5(3)	F(3)-C(9)-C(4)	109.9(3)
N(5)-C(1)-N(1)	129.0(3)	F(3)-C(9)-C(11)	105.7(4)
N(5)-C(1)-C(2)	122.4(4)	C(4)-C(9)-C(11)	113.7(4)
N(1)-C(1)-C(2)	108.5(4)	F(3)-C(9)-C(10)	102.6(3)
C(7)-C(2)-C(3)	119.8(4)	C(4)-C(9)-C(10)	114.3(4)

C(11)-C(9)-C(10)	109.8(4)	C(20)-C(19)-C(26)	116.2(4)
F(5)-C(10)-F(4)	109.4(4)	C(18)-C(19)-C(26)	125.3(4)
F(5)-C(10)-F(6)	106.4(4)	F(18)-C(20)-C(21)	118.3(4)
F(4)-C(10)-F(6)	108.2(4)	F(18)-C(20)-C(19)	119.1(4)
F(5)-C(10)-C(9)	113.7(4)	C(21)-C(20)-C(19)	122.6(4)
F(4)-C(10)-C(9)	110.8(4)	C(20)-C(21)-C(16)	118.7(4)
F(6)-C(10)-C(9)	108.1(4)	C(20)-C(21)-C(22)	134.3(4)
F(7)-C(11)-F(8)	108.0(4)	C(16)-C(21)-C(22)	106.9(4)
F(7)-C(11)-F(9)	107.1(5)	N(7)-C(22)-N(2)	128.5(4)
F(8)-C(11)-F(9)	107.7(4)	N(7)-C(22)-C(21)	122.3(4)
F(7)-C(11)-C(9)	112.2(4)	N(2)-C(22)-C(21)	109.1(3)
F(8)-C(11)-C(9)	110.4(4)	F(19)-C(23)-C(25)	107.8(6)
F(9)-C(11)-C(9)	111.1(4)	F(19)-C(23)-C(18)	110.4(4)
F(10)-C(12)-C(5)	109.9(3)	C(25)-C(23)-C(18)	113.5(7)
F(10)-C(12)-C(13)	105.5(3)	F(19)-C(23)-C(24)	101.4(6)
C(5)-C(12)-C(13)	114.8(4)	C(25)-C(23)-C(24)	109.1(6)
F(10)-C(12)-C(14)	101.9(3)	C(18)-C(23)-C(24)	113.7(6)
C(5)-C(12)-C(14)	114.4(3)	F(20)-C(24)-F(22)	109.4(9)
C(13)-C(12)-C(14)	109.2(4)	F(20)-C(24)-F(21)	109.8(8)
F(13)-C(13)-F(11)	107.9(4)	F(22)-C(24)-F(21)	106.4(5)
F(13)-C(13)-F(12)	108.3(4)	F(20)-C(24)-C(23)	110.5(5)
F(11)-C(13)-F(12)	108.2(4)	F(22)-C(24)-C(23)	108.1(7)
F(13)-C(13)-C(12)	112.4(4)	F(21)-C(24)-C(23)	112.3(8)
F(11)-C(13)-C(12)	110.0(4)	F(23)-C(25)-F(24)	109.2(6)
F(12)-C(13)-C(12)	109.8(4)	F(23)-C(25)-F(25)	106.2(10)
F(15)-C(14)-F(16)	108.5(4)	F(24)-C(25)-F(25)	105.3(7)
F(15)-C(14)-F(14)	106.3(4)	F(23)-C(25)-C(23)	115.0(6)
F(16)-C(14)-F(14)	107.1(4)	F(24)-C(25)-C(23)	111.0(9)
F(15)-C(14)-C(12)	114.7(4)	F(25)-C(25)-C(23)	109.5(6)
F(16)-C(14)-C(12)	110.9(4)	F(26)-C(26)-C(19)	110.4(4)
F(14)-C(14)-C(12)	109.0(3)	F(26)-C(26)-C(28)	106.2(5)
N(6)-C(15)-N(2)	128.0(4)	C(19)-C(26)-C(28)	112.7(6)
N(6)-C(15)-C(16)	122.4(4)	F(26)-C(26)-C(27)	101.7(6)
N(2)-C(15)-C(16)	109.5(3)	C(19)-C(26)-C(27)	113.8(5)
C(17)-C(16)-C(21)	120.3(4)	C(28)-C(26)-C(27)	111.2(5)
C(17)-C(16)-C(15)	133.1(4)	F(29)-C(27)-F(28)	108.9(5)
C(21)-C(16)-C(15)	106.6(3)	F(29)-C(27)-F(27)	106.7(6)
F(17)-C(17)-C(16)	118.1(4)	F(28)-C(27)-F(27)	105.9(5)
F(17)-C(17)-C(18)	118.7(4)	F(29)-C(27)-C(26)	111.2(5)
C(16)-C(17)-C(18)	123.2(4)	F(28)-C(27)-C(26)	114.2(6)
C(17)-C(18)-C(19)	116.3(4)	F(27)-C(27)-C(26)	109.6(5)
C(17)-C(18)-C(23)	116.0(4)	F(30)-C(28)-F(31)	108.2(8)
C(19)-C(18)-C(23)	127.7(5)	F(30)-C(28)-F(32)	108.0(6)
C(20)-C(19)-C(18)	118.4(4)	F(31)-C(28)-F(32)	107.9(6)

F(30)-C(28)-C(26)	112.4(5)	C(42)-C(41)-C(45)	116.1(5)
F(31)-C(28)-C(26)	111.3(5)	C(40)-C(41)-C(45)	126.7(5)
F(32)-C(28)-C(26)	108.8(8)	F(36)-C(42)-C(43)	117.4(4)
N(7)-C(29)-N(3)	128.8(3)	F(36)-C(42)-C(41)	119.4(4)
N(7)-C(29)-C(30)	121.7(4)	C(43)-C(42)-C(41)	123.2(4)
N(3)-C(29)-C(30)	109.2(3)	C(42)-C(43)-C(38)	119.5(4)
C(31)-C(30)-C(35)	120.3(3)	C(42)-C(43)-C(44)	133.8(4)
C(31)-C(30)-C(29)	132.9(4)	C(38)-C(43)-C(44)	106.7(4)
C(35)-C(30)-C(29)	106.7(3)	N(5)-C(44)-N(4)	128.1(4)
F(34)-C(31)-C(30)	123.0(4)	N(5)-C(44)-C(43)	122.4(4)
F(34)-C(31)-C(32)	118.6(4)	N(4)-C(44)-C(43)	109.5(3)
C(30)-C(31)-C(32)	118.4(4)	F(45)-C(45)-C(47)	102.4(9)
F(35)-C(32)-C(31)	118.4(4)	F(45)-C(45)-C(46)	106.1(8)
F(35)-C(32)-C(33)	119.6(4)	C(47)-C(45)-C(46)	108.9(6)
C(31)-C(32)-C(33)	122.0(4)	F(45)-C(45)-C(41)	111.9(6)
C(34)-C(33)-C(32)	117.7(4)	C(47)-C(45)-C(41)	116.5(7)
C(34)-C(33)-N(12)	120.6(4)	C(46)-C(45)-C(41)	110.3(8)
C(32)-C(33)-N(12)	121.7(4)	F(46)-C(46)-F(48)	108.8(5)
F(33)-C(34)-C(33)	117.6(4)	F(46)-C(46)-F(47)	108.9(5)
F(33)-C(34)-C(35)	121.7(4)	F(48)-C(46)-F(47)	108.9(5)
C(33)-C(34)-C(35)	120.7(4)	F(46)-C(46)-C(45)	109.3(6)
C(34)-C(35)-C(30)	120.7(4)	F(48)-C(46)-C(45)	111.1(8)
C(34)-C(35)-C(36)	132.8(4)	F(47)-C(46)-C(45)	109.8(7)
C(30)-C(35)-C(36)	106.4(3)	F(51)-C(47)-F(49)	106.6(6)
N(8)-C(36)-N(3)	128.2(4)	F(51)-C(47)-F(50)	106.5(6)
N(8)-C(36)-C(35)	122.0(4)	F(49)-C(47)-F(50)	106.6(6)
N(3)-C(36)-C(35)	109.8(3)	F(51)-C(47)-C(45)	116.1(8)
N(8)-C(37)-N(4)	128.5(4)	F(49)-C(47)-C(45)	110.0(7)
N(8)-C(37)-C(38)	121.8(4)	F(50)-C(47)-C(45)	110.5(8)
N(4)-C(37)-C(38)	109.7(3)	F(38)-C(48)-C(49)	106.6(7)
C(39)-C(38)-C(43)	119.0(4)	F(38)-C(48)-C(50)	102.7(8)
C(39)-C(38)-C(37)	134.4(4)	C(49)-C(48)-C(50)	109.6(7)
C(43)-C(38)-C(37)	106.5(4)	F(38)-C(48)-C(40)	111.4(5)
F(37)-C(39)-C(38)	117.2(4)	C(49)-C(48)-C(40)	110.1(7)
F(37)-C(39)-C(40)	119.4(4)	C(50)-C(48)-C(40)	115.9(7)
C(38)-C(39)-C(40)	123.4(4)	F(39)-C(49)-F(41)	109.9(8)
C(39)-C(40)-C(41)	117.9(4)	F(39)-C(49)-F(40)	108.7(7)
C(39)-C(40)-C(48A)	113.2(8)	F(41)-C(49)-F(40)	107.1(8)
C(41)-C(40)-C(48A)	126.4(7)	F(39)-C(49)-C(48)	109.7(8)
C(39)-C(40)-C(48)	116.5(5)	F(41)-C(49)-C(48)	111.1(7)
C(41)-C(40)-C(48)	125.5(5)	F(40)-C(49)-C(48)	110.2(7)
C(42)-C(41)-C(45A)	111.6(8)	F(44)-C(50)-F(43)	109.3(9)
C(42)-C(41)-C(40)	117.0(4)	F(44)-C(50)-F(42)	107.1(8)
C(45A)-C(41)-C(40)	128.9(8)	F(43)-C(50)-F(42)	106.2(10)

F(44)-C(50)-C(48)	115.5(10)	H(52A)-C(52)-H(52B)	109.5
F(43)-C(50)-C(48)	110.4(7)	C(51)-C(52)-H(52C)	109.5
F(42)-C(50)-C(48)	108.0(9)	H(52A)-C(52)-H(52C)	109.5
F(45A)-C(45A)-C(41)	109.5(12)	H(52B)-C(52)-H(52C)	109.5
F(45A)-C(45A)-C(47A)	101.2(15)	C(2S)-C(1S)-C(6S)	120.0
C(41)-C(45A)-C(47A)	109.8(11)	C(2S)-C(1S)-H(1SA)	120.0
F(45A)-C(45A)-C(46A)	103.8(12)	C(6S)-C(1S)-H(1SA)	120.0
C(41)-C(45A)-C(46A)	121.3(14)	C(1S)-C(2S)-C(3S)	120.0
C(47A)-C(45A)-C(46A)	109.2(11)	C(1S)-C(2S)-H(2SA)	120.0
F(48A)-C(46A)-F(46A)	108.9(5)	C(3S)-C(2S)-H(2SA)	120.0
F(48A)-C(46A)-F(47A)	108.9(5)	C(4S)-C(3S)-C(2S)	120.0
F(46A)-C(46A)-F(47A)	108.9(5)	C(4S)-C(3S)-H(3SA)	120.0
F(48A)-C(46A)-C(45A)	108.8(11)	C(2S)-C(3S)-H(3SA)	120.0
F(46A)-C(46A)-C(45A)	113.8(10)	C(3S)-C(4S)-C(5S)	120.0
F(47A)-C(46A)-C(45A)	107.5(10)	C(3S)-C(4S)-H(4SA)	120.0
F(51A)-C(47A)-F(50A)	106.5(6)	C(5S)-C(4S)-H(4SA)	120.0
F(51A)-C(47A)-F(49A)	106.6(6)	C(6S)-C(5S)-C(4S)	120.0
F(50A)-C(47A)-F(49A)	106.6(6)	C(6S)-C(5S)-H(5SA)	120.0
F(51A)-C(47A)-C(45A)	113.4(13)	C(4S)-C(5S)-H(5SA)	120.0
F(50A)-C(47A)-C(45A)	110.8(12)	C(5S)-C(6S)-C(1S)	120.0
F(49A)-C(47A)-C(45A)	112.6(11)	C(5S)-C(6S)-C(7S)	121.6(11)
F(38A)-C(48A)-C(40)	110.2(12)	C(1S)-C(6S)-C(7S)	118.4(11)
F(38A)-C(48A)-C(50A)	104.9(16)	C(6S)-C(7S)-H(7SA)	109.5
C(40)-C(48A)-C(50A)	106.1(12)	C(6S)-C(7S)-H(7SB)	109.5
F(38A)-C(48A)-C(49A)	103.4(13)	H(7SA)-C(7S)-H(7SB)	109.5
C(40)-C(48A)-C(49A)	121.6(13)	C(6S)-C(7S)-H(7SC)	109.5
C(50A)-C(48A)-C(49A)	109.5(14)	H(7SA)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-F(41A)	110.4(18)	H(7SB)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-F(40A)	107.3(15)	C(9S)-C(8S)-C(13S)	120.0
F(41A)-C(49A)-F(40A)	107.6(16)	C(9S)-C(8S)-H(8SA)	120.0
F(39A)-C(49A)-C(48A)	109.4(14)	C(13S)-C(8S)-H(8SA)	120.0
F(41A)-C(49A)-C(48A)	109.8(15)	C(8S)-C(9S)-C(10S)	120.0
F(40A)-C(49A)-C(48A)	112.4(15)	C(8S)-C(9S)-H(9SA)	120.0
F(44A)-C(50A)-F(42A)	106.3(17)	C(10S)-C(9S)-H(9SA)	120.0
F(44A)-C(50A)-F(43A)	109(2)	C(11S)-C(10S)-C(9S)	120.0
F(42A)-C(50A)-F(43A)	107(2)	C(11S)-C(10S)-H(10A)	120.0
F(44A)-C(50A)-C(48A)	111.6(18)	C(9S)-C(10S)-H(10A)	120.0
F(42A)-C(50A)-C(48A)	109.9(17)	C(10S)-C(11S)-C(12S)	120.0
F(43A)-C(50A)-C(48A)	112.5(15)	C(10S)-C(11S)-H(11A)	120.0
O(1)-C(51)-N(12)	119.9(4)	C(12S)-C(11S)-H(11A)	120.0
O(1)-C(51)-C(52)	123.5(4)	C(13S)-C(12S)-C(11S)	120.0
N(12)-C(51)-C(52)	116.6(4)	C(13S)-C(12S)-H(12A)	120.0
C(51)-C(52)-H(52A)	109.5	C(11S)-C(12S)-H(12A)	120.0
C(51)-C(52)-H(52B)	109.5	C(12S)-C(13S)-C(8S)	120.0

C(12S)-C(13S)-C(14S)	121.3(17)	C(3E)-C(4E)-H(4EA)	120.0
C(8S)-C(13S)-C(14S)	118.7(17)	C(5E)-C(4E)-H(4EA)	120.0
C(13S)-C(14S)-H(14A)	109.5	C(6E)-C(5E)-C(4E)	120.0
C(13S)-C(14S)-H(14B)	109.5	C(6E)-C(5E)-H(5EA)	120.0
H(14A)-C(14S)-H(14B)	109.5	C(4E)-C(5E)-H(5EA)	120.0
C(13S)-C(14S)-H(14C)	109.5	C(5E)-C(6E)-C(1E)	120.0
H(14A)-C(14S)-H(14C)	109.5	C(5E)-C(6E)-C(7E)	140.1(16)
H(14B)-C(14S)-H(14C)	109.5	C(1E)-C(6E)-C(7E)	99.4(16)
C(6T)-C(1T)-C(2T)	121.7(11)	C(6E)-C(7E)-H(7EA)	109.5
C(6T)-C(1T)-H(1TA)	119.1	C(6E)-C(7E)-H(7EB)	109.5
C(2T)-C(1T)-H(1TA)	119.1	H(7EA)-C(7E)-H(7EB)	109.5
C(3T)-C(2T)-C(1T)	120.3(9)	C(6E)-C(7E)-H(7EC)	109.5
C(3T)-C(2T)-H(2TA)	119.8	H(7EA)-C(7E)-H(7EC)	109.5
C(1T)-C(2T)-H(2TA)	119.8	H(7EB)-C(7E)-H(7EC)	109.5
C(2T)-C(3T)-C(4T)	119.6(10)	C(2K)-C(1K)-C(6K)	120.0
C(2T)-C(3T)-H(3TA)	120.2	C(2K)-C(1K)-H(1KA)	120.0
C(4T)-C(3T)-H(3TA)	120.2	C(6K)-C(1K)-H(1KA)	120.0
C(5T)-C(4T)-C(3T)	118.0(11)	C(3K)-C(2K)-C(1K)	120.0
C(5T)-C(4T)-H(4TA)	121.0	C(3K)-C(2K)-H(2KA)	120.0
C(3T)-C(4T)-H(4TA)	121.0	C(1K)-C(2K)-H(2KA)	120.0
C(6T)-C(5T)-C(4T)	123.7(10)	C(2K)-C(3K)-C(4K)	120.0
C(6T)-C(5T)-H(5TA)	118.2	C(2K)-C(3K)-H(3KA)	120.0
C(4T)-C(5T)-H(5TA)	118.2	C(4K)-C(3K)-H(3KA)	120.0
C(1T)-C(6T)-C(5T)	116.7(10)	C(5K)-C(4K)-C(3K)	120.0
C(1T)-C(6T)-C(7T)	122.6(11)	C(5K)-C(4K)-H(4KA)	120.0
C(5T)-C(6T)-C(7T)	120.7(11)	C(3K)-C(4K)-H(4KA)	120.0
C(6T)-C(7T)-H(7TA)	109.5	C(6K)-C(5K)-C(4K)	120.0
C(6T)-C(7T)-H(7TB)	109.5	C(6K)-C(5K)-H(5KA)	120.0
H(7TA)-C(7T)-H(7TB)	109.5	C(4K)-C(5K)-H(5KA)	120.0
C(6T)-C(7T)-H(7TC)	109.5	C(5K)-C(6K)-C(1K)	120.0
H(7TA)-C(7T)-H(7TC)	109.5	C(5K)-C(6K)-C(7K)	118.7(10)
H(7TB)-C(7T)-H(7TC)	109.5	C(1K)-C(6K)-C(7K)	121.3(10)
C(2E)-C(1E)-C(6E)	120.0	C(6K)-C(7K)-H(7KA)	109.5
C(2E)-C(1E)-H(1EA)	120.0	C(6K)-C(7K)-H(7KB)	109.5
C(6E)-C(1E)-H(1EA)	120.0	H(7KA)-C(7K)-H(7KB)	109.5
C(1E)-C(2E)-C(3E)	120.0	C(6K)-C(7K)-H(7KC)	109.5
C(1E)-C(2E)-H(2EA)	120.0	H(7KA)-C(7K)-H(7KC)	109.5
C(3E)-C(2E)-H(2EA)	120.0	H(7KB)-C(7K)-H(7KC)	109.5
C(4E)-C(3E)-C(2E)	120.0	Co-O(2)-H(2A)	120(4)
C(4E)-C(3E)-H(3EA)	120.0	Co-O(2)-H(2B)	133(4)
C(2E)-C(3E)-H(3EA)	120.0	H(2A)-O(2)-H(2B)	105.9(5
C(3E)-C(4E)-C(5E)	120.0		

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table V.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[(NHAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**. 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}
Co	16(1)	27(1)	34(1)	1(1)	8(1)	-2(1)
N(1)	24(2)	26(2)	30(2)	-1(1)	7(1)	0(1)
N(2)	18(1)	30(2)	35(2)	-7(1)	11(1)	-3(1)
N(3)	24(2)	26(2)	25(2)	-2(1)	9(1)	-3(1)
N(4)	18(1)	33(2)	31(2)	-1(1)	8(1)	-2(1)
N(5)	18(1)	32(2)	39(2)	7(2)	9(1)	-4(1)
N(6)	21(2)	26(2)	35(2)	-1(1)	7(1)	1(1)
N(7)	21(2)	27(2)	36(2)	-7(1)	13(1)	-2(1)
N(8)	20(2)	28(2)	36(2)	3(1)	9(1)	1(1)
N(12)	22(2)	37(2)	41(2)	9(2)	6(1)	-5(1)
O(1)	28(1)	29(2)	34(2)	-2(1)	9(1)	-4(1)
C(1)	17(2)	32(2)	32(2)	-1(2)	7(1)	-2(1)
C(2)	17(2)	33(2)	36(2)	-3(2)	9(2)	-5(1)
C(3)	20(2)	29(2)	37(2)	3(2)	7(2)	-3(1)
C(4)	17(2)	30(2)	36(2)	3(2)	4(2)	-1(1)
C(5)	17(2)	30(2)	31(2)	2(2)	4(1)	-4(1)
C(6)	17(2)	29(2)	40(2)	2(2)	6(2)	-1(1)
C(7)	15(2)	34(2)	34(2)	0(2)	5(1)	1(1)
C(8)	19(2)	26(2)	31(2)	-3(2)	6(1)	-1(1)
C(9)	21(2)	28(2)	45(2)	2(2)	8(2)	-5(2)
C(10)	32(2)	37(2)	48(3)	11(2)	1(2)	-5(2)
C(11)	30(2)	38(2)	57(3)	12(2)	9(2)	4(2)
C(12)	16(2)	31(2)	43(2)	2(2)	11(2)	-1(1)
C(13)	27(2)	39(2)	39(2)	1(2)	7(2)	-8(2)
C(14)	19(2)	43(2)	39(2)	3(2)	7(2)	1(2)
C(15)	18(2)	24(2)	27(2)	-2(1)	7(1)	-2(1)
C(16)	26(2)	23(2)	38(2)	-3(2)	11(2)	0(1)
C(17)	26(2)	30(2)	57(3)	1(2)	17(2)	-2(2)
C(18)	32(2)	29(2)	82(4)	10(2)	24(2)	-2(2)
C(19)	32(2)	28(2)	84(4)	10(2)	22(2)	2(2)
C(20)	27(2)	24(2)	60(3)	1(2)	20(2)	-1(2)
C(21)	26(2)	22(2)	40(2)	-6(2)	15(2)	-5(1)
C(22)	25(2)	19(2)	31(2)	-3(1)	12(2)	0(1)
C(23)	37(3)	36(3)	153(7)	30(4)	37(4)	2(2)
C(24)	42(3)	32(3)	222(12)	3(5)	37(5)	-13(3)
C(25)	53(4)	88(6)	173(10)	73(6)	58(5)	10(4)
C(26)	40(3)	40(3)	110(5)	33(3)	32(3)	10(2)
C(27)	44(3)	65(4)	83(5)	32(3)	26(3)	11(3)
C(28)	54(4)	32(3)	156(8)	12(4)	36(5)	9(3)

C(29)	15(2)	27(2)	36(2)	-6(2)	10(1)	-4(1)
C(30)	20(2)	29(2)	30(2)	-6(2)	11(1)	-7(1)
C(31)	25(2)	26(2)	35(2)	-1(2)	14(2)	-1(1)
C(32)	19(2)	34(2)	36(2)	0(2)	9(2)	2(2)
C(33)	21(2)	36(2)	37(2)	6(2)	7(2)	-3(2)
C(34)	18(2)	35(2)	44(2)	6(2)	8(2)	-1(2)
C(35)	16(2)	30(2)	37(2)	4(2)	6(1)	0(1)
C(36)	19(2)	30(2)	31(2)	-1(2)	9(1)	-1(1)
C(37)	18(2)	29(2)	32(2)	4(2)	7(1)	1(1)
C(38)	23(2)	30(2)	37(2)	3(2)	10(2)	0(2)
C(39)	21(2)	32(2)	49(3)	4(2)	12(2)	-1(2)
C(40)	34(2)	32(2)	52(3)	11(2)	16(2)	-1(2)
C(41)	32(2)	27(2)	61(3)	5(2)	16(2)	1(2)
C(42)	23(2)	30(2)	55(3)	2(2)	15(2)	1(2)
C(43)	22(2)	28(2)	39(2)	4(2)	12(2)	-3(1)
C(44)	22(2)	30(2)	31(2)	3(2)	9(2)	0(2)
C(45)	27(4)	25(4)	77(8)	23(4)	11(4)	8(3)
C(46)	37(4)	27(4)	146(11)	10(5)	36(6)	3(3)
C(47)	37(7)	58(8)	94(9)	28(8)	-7(6)	9(6)
C(48)	26(3)	17(4)	56(6)	7(4)	16(4)	-7(3)
C(49)	41(4)	46(5)	55(5)	21(4)	22(4)	-2(4)
C(50)	39(5)	26(5)	72(8)	8(5)	12(5)	-11(4)
F(38)	37(2)	21(2)	94(4)	9(2)	22(3)	-1(2)
F(39)	68(4)	58(4)	100(5)	24(4)	48(4)	-11(3)
F(40)	58(3)	87(4)	56(3)	27(3)	17(3)	9(3)
F(41)	59(5)	61(5)	66(5)	4(4)	29(4)	9(4)
F(42)	56(3)	33(3)	99(5)	-3(3)	11(4)	-19(2)
F(43)	51(3)	49(3)	58(4)	-4(3)	15(3)	-15(2)
F(44)	27(2)	45(3)	83(4)	13(3)	17(2)	-7(2)
F(45)	47(3)	39(3)	89(5)	32(3)	14(3)	5(2)
F(46)	62(4)	46(3)	127(6)	-24(3)	38(4)	-8(3)
F(47)	52(3)	24(3)	201(10)	10(4)	25(5)	16(2)
F(48)	60(5)	48(4)	129(8)	-13(4)	57(6)	-6(3)
F(49)	78(5)	85(5)	65(4)	5(4)	-17(4)	-10(4)
F(50)	74(5)	94(6)	146(9)	77(6)	-42(5)	-13(5)
F(51)	30(3)	50(3)	148(7)	41(4)	-6(3)	3(2)
C(45A)	62(14)	31(10)	110(20)	25(12)	33(14)	8(9)
C(46A)	120(30)	45(13)	130(20)	48(15)	90(20)	49(16)
C(47A)	44(14)	100(20)	140(30)	70(20)	17(17)	31(14)
C(48A)	56(11)	31(10)	58(13)	-1(9)	-4(9)	-4(8)
C(49A)	62(17)	70(20)	90(20)	57(18)	22(15)	-18(16)
C(50A)	130(30)	28(11)	190(40)	7(17)	110(30)	-13(16)
F(38A)	61(7)	71(8)	136(13)	55(9)	43(8)	6(6)
F(39A)	87(10)	99(11)	91(10)	-6(9)	42(8)	1(9)

F(40A)	51(7)	77(8)	141(13)	33(8)	31(8)	-14(6)
F(41A)	89(10)	124(14)	142(15)	46(13)	67(11)	-11(10)
F(42A)	115(14)	51(8)	230(30)	-7(14)	47(19)	-46(9)
F(43A)	115(18)	63(12)	85(16)	-9(11)	-15(12)	-14(11)
F(44A)	165(18)	69(10)	154(18)	-43(11)	27(14)	2(10)
F(45A)	83(9)	39(6)	158(16)	20(8)	46(10)	7(6)
F(46A)	72(9)	72(9)	240(20)	36(11)	84(13)	19(7)
F(47A)	128(15)	56(8)	190(20)	-3(11)	63(14)	42(9)
F(48A)	133(15)	113(13)	122(14)	-1(11)	78(12)	37(12)
F(49A)	101(12)	151(16)	106(12)	76(12)	33(10)	23(11)
F(50A)	78(10)	58(9)	169(19)	59(10)	2(11)	14(8)
F(51A)	69(12)	91(14)	112(14)	49(12)	18(11)	8(10)
C(51)	23(2)	26(2)	44(2)	1(2)	12(2)	-1(2)
C(52)	29(2)	39(2)	52(3)	3(2)	7(2)	-13(2)
F(1)	22(1)	31(1)	50(2)	11(1)	10(1)	0(1)
F(2)	24(1)	33(1)	59(2)	17(1)	7(1)	-1(1)
F(3)	22(1)	41(2)	50(2)	13(1)	-2(1)	-6(1)
F(4)	58(2)	56(2)	42(2)	7(1)	11(1)	10(2)
F(5)	40(2)	43(2)	61(2)	21(1)	2(1)	-6(1)
F(6)	40(2)	55(2)	53(2)	19(2)	-13(1)	-8(1)
F(7)	46(2)	37(2)	77(2)	-8(2)	13(2)	-3(1)
F(8)	40(2)	50(2)	95(3)	11(2)	6(2)	18(2)
F(9)	86(3)	50(2)	72(2)	5(2)	45(2)	10(2)
F(10)	20(1)	40(1)	47(2)	10(1)	8(1)	7(1)
F(11)	52(2)	54(2)	44(2)	1(1)	-12(1)	-13(2)
F(12)	33(1)	60(2)	63(2)	-6(2)	16(1)	-21(1)
F(13)	36(2)	43(2)	61(2)	-6(1)	6(1)	-6(1)
F(14)	30(1)	58(2)	44(2)	9(1)	14(1)	6(1)
F(15)	42(2)	48(2)	44(2)	13(1)	14(1)	10(1)
F(16)	34(1)	62(2)	38(2)	-4(1)	3(1)	-11(1)
F(17)	25(1)	36(1)	79(2)	10(1)	20(1)	-2(1)
F(18)	27(1)	30(1)	75(2)	10(1)	19(1)	5(1)
F(19)	46(2)	35(2)	225(6)	40(3)	40(3)	3(2)
F(20)	60(3)	61(3)	150(5)	-31(3)	12(3)	-18(2)
F(21)	37(2)	52(2)	192(5)	24(3)	25(3)	-10(2)
F(22)	66(3)	38(2)	300(9)	1(3)	23(4)	-21(2)
F(23)	71(3)	97(3)	132(4)	53(3)	61(3)	23(2)
F(24)	75(3)	116(4)	264(8)	116(5)	87(4)	13(3)
F(25)	75(3)	162(5)	142(5)	85(4)	57(3)	34(3)
F(26)	47(2)	70(2)	142(4)	61(3)	40(2)	12(2)
F(27)	64(3)	106(4)	115(4)	70(3)	27(2)	19(2)
F(28)	38(2)	71(2)	97(3)	28(2)	24(2)	12(2)
F(29)	54(2)	75(3)	74(2)	14(2)	21(2)	13(2)
F(30)	60(2)	38(2)	148(4)	-9(2)	49(3)	0(2)

F(31)	71(3)	38(2)	217(6)	-17(3)	50(3)	-9(2)
F(32)	82(3)	56(3)	223(7)	50(3)	60(4)	42(2)
F(33)	24(1)	35(1)	70(2)	16(1)	6(1)	-4(1)
F(34)	28(1)	28(1)	53(2)	2(1)	9(1)	1(1)
F(35)	22(1)	39(1)	48(2)	1(1)	10(1)	2(1)
F(36)	22(1)	37(2)	85(2)	15(2)	14(1)	6(1)
F(37)	21(1)	37(1)	69(2)	12(1)	13(1)	-2(1)
C(1S)	93(7)	160(11)	93(8)	-74(7)	38(6)	-49(6)
C(2S)	100(7)	90(7)	109(10)	-53(6)	58(7)	-26(6)
C(3S)	87(6)	88(6)	103(8)	-47(6)	39(6)	-9(5)
C(4S)	93(6)	107(8)	83(7)	-34(6)	24(6)	-7(5)
C(5S)	80(6)	188(12)	97(9)	-66(8)	17(6)	-20(7)
C(6S)	88(6)	197(12)	70(8)	-76(8)	31(6)	-37(7)
C(7S)	80(7)	280(20)	99(11)	-99(13)	26(7)	-66(10)
C(8S)	78(12)	81(15)	30(11)	-10(10)	14(10)	-18(10)
C(9S)	72(11)	107(17)	20(11)	-30(11)	8(10)	-14(11)
C(10S)	69(11)	103(16)	39(12)	-26(10)	29(10)	16(11)
C(11S)	70(11)	70(13)	44(11)	-12(9)	34(10)	32(9)
C(12S)	58(10)	44(9)	38(10)	-12(7)	17(9)	8(8)
C(13S)	66(11)	49(10)	22(10)	-10(8)	1(9)	2(8)
C(14S)	74(13)	41(13)	60(18)	8(13)	-16(15)	-5(11)
C(1T)	78(6)	144(9)	106(7)	32(7)	43(5)	46(6)
C(2T)	98(7)	132(9)	67(5)	15(5)	27(5)	65(7)
C(3T)	122(8)	84(6)	69(5)	-18(4)	24(5)	34(6)
C(4T)	114(8)	97(7)	89(7)	-31(6)	-2(6)	10(6)
C(5T)	105(8)	139(10)	107(8)	29(7)	-8(6)	42(8)
C(6T)	78(6)	144(10)	120(8)	49(7)	26(6)	23(7)
C(7T)	165(15)	179(15)	370(30)	189(18)	61(16)	37(12)
C(1E)	510(50)	150(18)	490(50)	130(20)	380(50)	190(30)
C(2E)	430(30)	68(7)	116(11)	-32(7)	49(15)	41(13)
C(3E)	215(16)	44(5)	200(16)	8(7)	-16(14)	-29(7)
C(4E)	246(18)	46(5)	134(11)	21(6)	47(12)	17(8)
C(5E)	160(14)	121(11)	200(18)	76(11)	36(12)	-12(10)
C(6E)	290(30)	158(17)	250(30)	66(18)	130(20)	11(17)
C(7E)	410(40)	360(40)	270(30)	-50(30)	200(30)	-30(30)
C(1K)	71(8)	45(5)	92(9)	19(17)	9(6)	4(13)
C(2K)	79(10)	55(9)	72(10)	0(7)	26(8)	-8(8)
C(3K)	47(7)	42(7)	93(11)	-14(7)	-2(7)	-5(6)
C(4K)	84(14)	41(7)	77(13)	7(7)	-10(10)	8(8)
C(5K)	45(8)	42(6)	75(12)	-1(7)	2(8)	2(6)
C(6K)	49(7)	41(7)	69(9)	-6(7)	-4(6)	3(6)
C(7K)	67(9)	76(10)	96(12)	8(9)	26(9)	17(8)
O(2)	19(2)	26(3)	32(3)	-4(2)	8(2)	-11(2)

Table V.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **[(NHAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**.

	x	y	z	U(eq)
H(12)	11770(30)	3512(15)	6680(20)	40
H(52A)	12919	3640	7921	61
H(52B)	12722	3733	7242	61
H(52C)	13249	3389	7494	61
H(1SA)	6867	2998	4718	135
H(2SA)	8053	3169	4754	113
H(3SA)	8296	3750	4374	108
H(4SA)	7353	4161	3959	113
H(5SA)	6167	3991	3923	147
H(7SA)	5414	3271	3907	229
H(7SB)	5388	3573	4401	229
H(7SC)	5666	3152	4575	229
H(8SA)	7167	3748	4257	76
H(9SA)	8267	3439	4606	81
H(10A)	8301	2837	5021	81
H(11A)	7234	2544	5086	69
H(12A)	6133	2853	4737	55
H(14A)	5929	3755	4012	96
H(14B)	5666	3620	4564	96
H(14C)	5501	3365	3990	96
H(1TA)	1461	3239	5298	127
H(2TA)	1365	2614	5560	117
H(3TA)	259	2333	5410	110
H(4TA)	-770	2675	4952	126
H(5TA)	-639	3290	4665	148
H(7TA)	-3	3856	4736	358
H(7TB)	617	3747	4428	358
H(7TC)	820	3868	5096	358
H(1EA)	8186	5482	1899	405
H(2EA)	7027	5356	1993	250
H(3EA)	6771	5414	2897	199
H(4EA)	7675	5598	3707	170
H(5EA)	8834	5724	3614	194
H(7EA)	9663	5611	2694	493
H(7EB)	9230	5980	2409	493
H(7EC)	9097	5583	2075	493
H(1KA)	4872	4703	7597	86

H(2KA)	5323	4562	6799	81
H(3KA)	5513	3932	6575	77
H(4KA)	5251	3442	7151	87
H(5KA)	4800	3584	7949	67
H(7KA)	4063	4085	8331	118
H(7KB)	4374	4507	8362	118
H(7KC)	4856	4174	8717	118
H(2A)	7046(19)	2542(19)	5290(30)	31
H(2B)	7690(20)	2640(20)	5210(20)	31

Appendix W: Crystal structure of [(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)

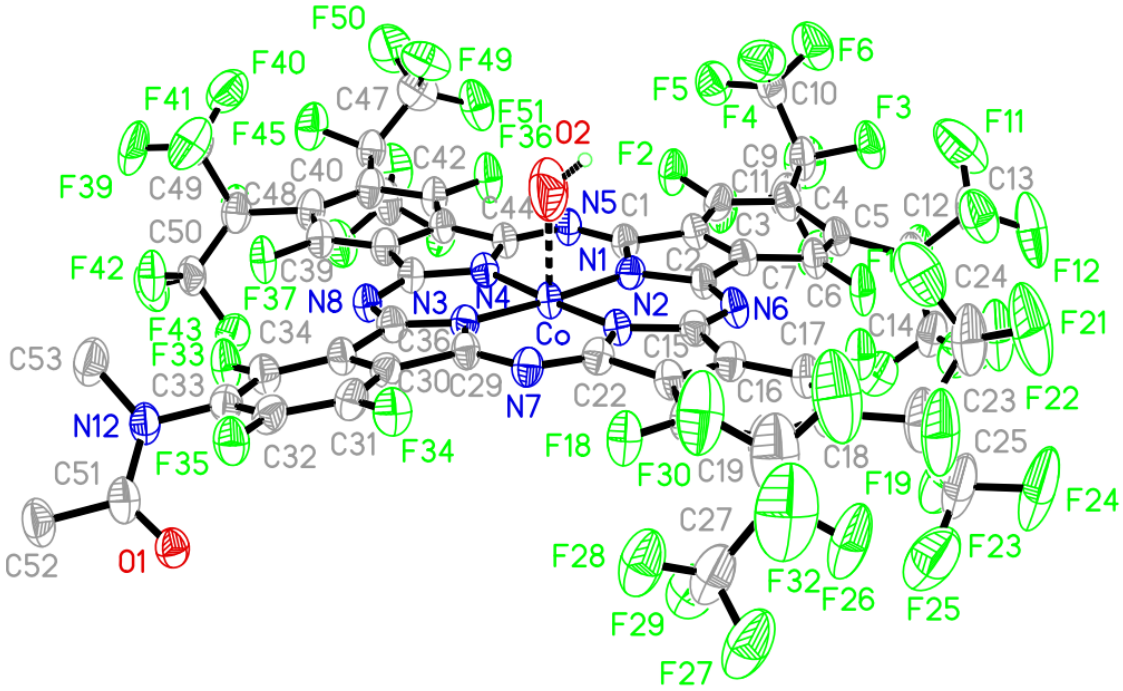


Figure W.1 ORTEP representation of **NMeAcF$_{51}$PcCo-OH** X-ray crystal structure, at 50% probability.

Table W.1 Crystal data and structure refinement for **[(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)**.

Empirical formula	C155 H69 Co2 F102 N18 O3	
Formula weight	4287.14	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.6464(18) Å	α = 90°.
	b = 35.227(3) Å	β = 107.096(3)°.
	c = 23.839(2) Å	γ = 90°.
Volume	15770(3) Å^3	
Z	4	
Density (calculated)	1.806 g/cm^3	
Absorption coefficient	0.394 mm^{-1}	
F(000)	8484	
Crystal size	0.600 x 0.280 x 0.050 mm^3	
Theta range for data collection	1.319 to 25.027°.	
Index ranges	-23<=h<=23, -41<=k<=41, -28<=l<=28	
Reflections collected	162989	

Independent reflections	13917 [R(int) = 0.0895]
Completeness to theta = 25.000°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6613
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13917 / 548 / 1473
Goodness-of-fit on F^2	1.064
Final R indices [I>2sigma(I)]	R1 = 0.0867, wR2 = 0.2042
R indices (all data)	R1 = 0.1344, wR2 = 0.2407
Extinction coefficient	n/a
Largest diff. peak and hole	0.731 and -0.744 e.$Å^{-3}$

Table W.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7583(1)	2897(1)	6331(1)	33(1)
N(1)	6572(3)	2919(1)	6202(2)	33(1)
N(2)	7587(2)	2376(1)	6582(2)	33(1)
N(3)	8581(2)	2864(1)	6409(2)	32(1)
N(4)	7570(3)	3408(1)	6045(2)	36(1)
N(5)	6308(3)	3550(1)	5782(2)	38(1)
N(6)	6355(3)	2302(1)	6558(2)	39(1)
N(7)	8830(3)	2219(1)	6765(2)	36(1)
N(8)	8825(3)	3508(1)	6185(2)	37(1)
N(12)	11666(3)	3250(2)	6845(3)	43(1)
O(1)	12041(2)	3062(1)	7770(2)	40(1)
C(1)	6136(3)	3218(2)	5958(3)	37(1)
C(2)	5415(3)	3123(2)	5945(3)	40(2)
C(3)	4769(3)	3315(2)	5728(3)	44(2)
C(4)	4131(3)	3172(2)	5791(3)	45(2)
C(5)	4169(3)	2829(2)	6132(3)	44(2)
C(6)	4798(3)	2635(2)	6278(3)	45(2)
C(7)	5427(3)	2776(2)	6197(3)	38(1)
C(8)	6152(3)	2641(2)	6338(3)	36(1)
C(9)	3452(4)	3387(2)	5440(4)	53(2)
C(10)	3394(4)	3473(2)	4782(4)	59(2)
C(11)	3332(4)	3750(2)	5742(4)	57(2)
C(12)	3573(3)	2674(2)	6376(4)	53(2)

C(13)	3169(4)	2333(2)	6044(5)	69(2)
C(14)	3815(4)	2582(2)	7047(4)	59(2)
C(15)	7011(3)	2188(2)	6663(3)	35(1)
C(16)	7243(3)	1818(2)	6918(3)	36(1)
C(17)	6896(3)	1518(2)	7085(3)	40(2)
C(18)	7238(4)	1191(2)	7340(3)	48(2)
C(19)	7993(4)	1176(2)	7447(4)	52(2)
C(20)	8324(3)	1471(2)	7237(3)	41(2)
C(21)	7963(3)	1793(2)	6978(3)	35(1)
C(22)	8166(3)	2148(2)	6758(3)	34(1)
C(23)	6748(4)	876(2)	7456(5)	68(3)
C(24)	6064(5)	793(2)	6923(6)	86(3)
C(25)	6519(5)	940(3)	7998(5)	89(3)
C(26)	8513(4)	877(2)	7825(5)	71(3)
C(27)	9167(5)	1046(3)	8293(5)	74(3)
C(28)	8733(5)	576(3)	7459(6)	94(4)
C(29)	9009(3)	2555(2)	6603(3)	33(1)
C(30)	9753(3)	2657(2)	6667(3)	35(1)
C(31)	10383(3)	2460(2)	6825(3)	39(2)
C(32)	11006(3)	2656(2)	6863(3)	41(2)
C(33)	11018(3)	3047(2)	6769(3)	40(2)
C(34)	10381(3)	3237(2)	6609(3)	42(2)
C(35)	9746(3)	3043(2)	6543(3)	36(1)
C(36)	9010(3)	3162(2)	6362(3)	36(1)
C(37)	8146(3)	3614(2)	6016(3)	35(1)
C(38)	7923(3)	3983(2)	5763(3)	39(2)
C(39)	8271(3)	4292(2)	5633(3)	41(2)
C(40)	7928(3)	4618(2)	5379(3)	45(2)
C(41)	7163(3)	4632(2)	5249(3)	44(2)
C(42)	6828(3)	4309(2)	5395(3)	43(2)
C(43)	7199(3)	3993(2)	5647(3)	36(1)
C(44)	6978(3)	3631(2)	5830(3)	34(1)
C(45)	6649(5)	4949(2)	4906(4)	46(2)
C(46)	6430(3)	5212(2)	5375(4)	59(3)
C(47)	5966(7)	4831(2)	4435(5)	58(5)
C(48)	8420(5)	4958(2)	5327(5)	46(2)
C(49)	8601(8)	4906(4)	4726(6)	61(3)
C(50)	9119(10)	5018(6)	5818(8)	50(5)
F(38)	8090(3)	5298(2)	5289(4)	58(2)
F(39)	9011(5)	5203(3)	4669(5)	86(3)
F(40)	8027(4)	4908(2)	4278(4)	77(2)
F(41)	8940(8)	4597(4)	4713(6)	75(4)
F(42)	9270(5)	5393(2)	5872(5)	72(3)
F(43)	9026(6)	4920(3)	6352(5)	58(3)

F(44)	9682(3)	4843(2)	5773(4)	60(2)
F(45)	6973(4)	5190(2)	4632(4)	62(2)
F(46)	6997(3)	5397(2)	5700(3)	73(2)
F(47)	5946(4)	5461(2)	5088(4)	74(3)
F(48)	6160(4)	5003(3)	5720(4)	61(3)
F(49)	6093(5)	4508(2)	4204(4)	79(3)
F(50)	5806(5)	5087(3)	4011(4)	97(4)
F(51)	5395(4)	4782(2)	4612(4)	71(2)
C(45A)	6667(8)	4983(3)	5038(7)	46(2)
C(46A)	6188(9)	5065(4)	5457(9)	120(20)
C(47A)	6249(8)	4946(4)	4397(8)	130(20)
C(48A)	8386(8)	4898(4)	5129(7)	46(2)
C(49A)	8986(12)	4734(7)	4873(11)	100(20)
C(50A)	8723(14)	5175(7)	5628(12)	100(13)
F(38A)	7959(7)	5111(4)	4692(8)	81(6)
F(39A)	8768(12)	4394(5)	4633(10)	86(7)
F(40A)	9603(6)	4687(5)	5257(8)	84(6)
F(41A)	9036(11)	4959(7)	4465(11)	115(9)
F(42A)	9157(14)	5414(6)	5448(14)	134(11)
F(43A)	9163(13)	4985(7)	6107(10)	75(10)
F(44A)	8270(12)	5373(5)	5805(11)	122(8)
F(45A)	7062(9)	5291(4)	5094(12)	103(8)
F(46A)	5553(8)	4904(5)	5251(12)	220(20)
F(47A)	6114(13)	5439(4)	5459(13)	164(17)
F(48A)	6492(14)	4945(7)	6001(9)	157(14)
F(49A)	6680(9)	4934(5)	4065(9)	130(9)
F(50A)	5839(11)	5248(4)	4239(13)	180(20)
F(51A)	5834(10)	4644(4)	4274(13)	155(18)
C(51)	12147(3)	3249(2)	7387(3)	44(2)
C(52)	12802(4)	3493(2)	7478(4)	57(2)
C(53)	11739(4)	3473(2)	6343(4)	61(2)
F(1)	4847(2)	2302(1)	6567(2)	56(1)
F(2)	4758(2)	3633(1)	5425(2)	56(1)
F(3)	2865(2)	3168(1)	5391(2)	66(1)
F(4)	3756(3)	3213(1)	4572(2)	77(1)
F(5)	3621(2)	3811(1)	4683(2)	70(1)
F(6)	2720(3)	3449(1)	4465(2)	85(2)
F(7)	3839(2)	4008(1)	5789(2)	68(1)
F(8)	2711(2)	3906(1)	5467(3)	84(2)
F(9)	3326(2)	3679(1)	6299(2)	71(1)
F(10)	3080(2)	2952(1)	6349(2)	64(1)
F(11)	2880(4)	2414(2)	5500(3)	125(3)
F(12)	2641(3)	2241(2)	6273(4)	124(3)
F(13)	3556(2)	2032(1)	6090(2)	77(2)

F(14)	3258(3)	2626(2)	7248(3)	99(2)
F(15)	4048(3)	2236(2)	7190(2)	82(2)
F(16)	4308(3)	2818(2)	7334(2)	85(2)
F(17)	6188(2)	1551(1)	6992(2)	52(1)
F(18)	9023(2)	1455(1)	7302(2)	50(1)
F(19)	7095(3)	533(1)	7507(3)	101(2)
F(20)	6179(3)	899(2)	6404(3)	93(2)
F(21)	5485(3)	966(1)	6944(3)	89(2)
F(22)	5926(3)	430(1)	6874(4)	130(3)
F(23)	6198(3)	1263(2)	8011(3)	92(2)
F(24)	6099(3)	659(2)	8071(4)	132(3)
F(25)	7099(3)	930(2)	8480(3)	116(2)
F(26)	8181(3)	689(2)	8174(3)	94(2)
F(27)	9345(3)	828(2)	8766(3)	107(2)
F(28)	9754(2)	1071(2)	8119(3)	83(2)
F(29)	9029(2)	1392(2)	8467(2)	74(1)
F(30)	9093(3)	722(1)	7110(3)	94(2)
F(31)	8176(3)	393(1)	7110(4)	117(2)
F(32)	9151(3)	321(2)	7807(4)	129(3)
F(33)	10377(2)	3614(1)	6521(2)	55(1)
F(34)	10415(2)	2085(1)	6921(2)	48(1)
F(35)	11617(2)	2459(1)	6987(2)	48(1)
F(36)	6126(2)	4311(1)	5281(2)	58(1)
F(37)	8980(2)	4269(1)	5748(2)	50(1)
C(1S)	7091(7)	3207(3)	4597(5)	114(5)
C(2S)	7776(5)	3320(3)	4620(5)	108(6)
C(3S)	7884(5)	3667(3)	4381(5)	109(5)
C(4S)	7307(7)	3900(3)	4118(4)	106(5)
C(5S)	6622(5)	3786(4)	4095(5)	118(5)
C(6S)	6514(5)	3439(4)	4334(5)	112(5)
C(7S)	5744(7)	3341(8)	4288(10)	152(9)
C(8S)	7191(13)	3489(5)	4437(11)	72(8)
C(9S)	7818(10)	3283(7)	4645(11)	86(12)
C(10S)	7804(10)	2922(7)	4877(10)	83(9)
C(11S)	7163(13)	2767(5)	4901(9)	66(7)
C(12S)	6535(10)	2973(6)	4693(10)	66(7)
C(13S)	6549(10)	3334(6)	4461(10)	60(8)
C(14S)	5852(13)	3552(8)	4230(20)	92(14)
C(1T)	970(5)	3037(3)	5046(5)	139(5)
C(2T)	916(5)	2689(3)	5304(4)	134(4)
C(3T)	254(6)	2554(2)	5313(4)	114(4)
C(4T)	-354(5)	2768(3)	5064(4)	137(4)
C(5T)	-300(5)	3117(3)	4807(5)	190(7)
C(6T)	362(7)	3251(2)	4798(5)	176(7)

C(7T)	429(13)	3652(5)	4578(12)	301(16)
C(1E)	7903(12)	5486(3)	2133(6)	153(7)
C(2E)	7223(9)	5452(3)	2195(7)	220(14)
C(3E)	7128(9)	5466(3)	2750(10)	290(20)
C(4E)	7712(13)	5512(3)	3243(6)	187(10)
C(5E)	8392(10)	5545(3)	3181(6)	192(11)
C(6E)	8487(8)	5532(3)	2626(9)	169(8)
C(7E)	9224(10)	5617(7)	2568(13)	272(14)
C(1K)	4908(15)	4436(3)	7526(9)	83(7)
C(2K)	5173(12)	4362(4)	7057(8)	105(10)
C(3K)	5314(12)	3991(5)	6928(9)	83(7)
C(4K)	5190(20)	3693(3)	7269(14)	100(16)
C(5K)	4920(20)	3767(4)	7737(13)	74(10)
C(6K)	4783(11)	4139(5)	7866(8)	82(7)
C(7K)	4472(12)	4210(7)	8372(9)	98(7)
O(2)	7420(8)	2659(4)	5450(8)	95(4)

Table W.3 Bond lengths [Å] and angles [°] for **[(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)**.

Co-N(3)	1.918(5)	Co-N(2)	1.929(5)
Co-N(1)	1.921(5)	Co-O(1)#1	2.133(5)
Co-N(4)	1.924(5)	Co-O(2)	2.195(17)
N(1)-C(1)	1.375(8)	O(1)-C(51)	1.194(8)
N(1)-C(8)	1.380(7)	C(1)-C(2)	1.447(8)
N(2)-C(22)	1.354(7)	C(2)-C(7)	1.357(9)
N(2)-C(15)	1.371(7)	C(2)-C(3)	1.395(9)
N(3)-C(36)	1.369(7)	C(3)-F(2)	1.332(7)
N(3)-C(29)	1.372(7)	C(3)-C(4)	1.400(9)
N(4)-C(37)	1.362(7)	C(4)-C(5)	1.443(9)
N(4)-C(44)	1.373(8)	C(4)-C(9)	1.549(9)
N(5)-C(44)	1.318(7)	C(5)-C(6)	1.364(9)
N(5)-C(1)	1.320(8)	C(5)-C(12)	1.552(9)
N(6)-C(15)	1.303(8)	C(6)-F(1)	1.350(7)
N(6)-C(8)	1.318(8)	C(6)-C(7)	1.399(8)
N(7)-C(29)	1.322(7)	C(7)-C(8)	1.444(8)
N(7)-C(22)	1.323(7)	C(9)-F(3)	1.365(7)
N(8)-C(36)	1.307(8)	C(9)-C(11)	1.518(11)
N(8)-C(37)	1.328(8)	C(9)-C(10)	1.567(12)
N(12)-C(51)	1.359(9)	C(10)-F(5)	1.315(8)
N(12)-C(33)	1.424(8)	C(10)-F(6)	1.321(8)
N(12)-C(53)	1.473(9)	C(10)-F(4)	1.345(10)

C(11)-F(8)	1.324(8)	C(30)-C(35)	1.391(9)
C(11)-F(7)	1.329(8)	C(31)-F(34)	1.337(7)
C(11)-F(9)	1.352(9)	C(31)-C(32)	1.385(9)
C(12)-F(10)	1.366(8)	C(32)-F(35)	1.343(7)
C(12)-C(13)	1.527(11)	C(32)-C(33)	1.398(9)
C(12)-C(14)	1.563(12)	C(33)-C(34)	1.369(9)
C(13)-F(11)	1.286(11)	C(34)-F(33)	1.344(7)
C(13)-F(13)	1.289(10)	C(34)-C(35)	1.388(8)
C(13)-F(12)	1.344(10)	C(35)-C(36)	1.444(8)
C(14)-F(16)	1.306(9)	C(37)-C(38)	1.446(8)
C(14)-F(15)	1.313(9)	C(38)-C(43)	1.369(8)
C(14)-F(14)	1.328(9)	C(38)-C(39)	1.371(9)
C(15)-C(16)	1.454(8)	C(39)-F(37)	1.339(7)
C(16)-C(17)	1.378(8)	C(39)-C(40)	1.379(9)
C(16)-C(21)	1.383(8)	C(40)-C(41)	1.444(9)
C(17)-F(17)	1.348(7)	C(40)-C(48A)	1.566(7)
C(17)-C(18)	1.381(9)	C(40)-C(48)	1.566(7)
C(18)-C(19)	1.430(10)	C(41)-C(42)	1.407(8)
C(18)-C(23)	1.547(9)	C(41)-C(45A)	1.565(7)
C(19)-C(20)	1.393(9)	C(41)-C(45)	1.566(7)
C(19)-C(26)	1.558(10)	C(42)-F(36)	1.325(7)
C(20)-F(18)	1.337(7)	C(42)-C(43)	1.367(9)
C(20)-C(21)	1.382(9)	C(43)-C(44)	1.454(8)
C(21)-C(22)	1.458(8)	C(45)-F(45)	1.341(10)
C(23)-F(19)	1.374(8)	C(45)-C(47)	1.533(17)
C(23)-C(25)	1.507(14)	C(45)-C(46)	1.607(15)
C(23)-C(24)	1.580(14)	C(46)-F(46)	1.325(6)
C(24)-F(21)	1.304(11)	C(46)-F(47)	1.326(6)
C(24)-F(22)	1.306(10)	C(46)-F(48)	1.326(6)
C(24)-F(20)	1.373(12)	C(47)-F(49)	1.321(7)
C(25)-F(23)	1.307(12)	C(47)-F(51)	1.321(7)
C(25)-F(24)	1.330(10)	C(47)-F(50)	1.321(7)
C(25)-F(25)	1.360(12)	C(48)-F(38)	1.355(11)
C(26)-F(26)	1.369(9)	C(48)-C(50)	1.53(2)
C(26)-C(28)	1.515(14)	C(48)-C(49)	1.585(16)
C(26)-C(27)	1.552(14)	C(49)-F(41)	1.282(17)
C(27)-F(27)	1.323(9)	C(49)-F(40)	1.305(15)
C(27)-F(29)	1.339(11)	C(49)-F(39)	1.351(15)
C(27)-F(28)	1.339(9)	C(50)-F(44)	1.30(2)
C(28)-F(31)	1.328(13)	C(50)-F(42)	1.35(2)
C(28)-F(32)	1.330(11)	C(50)-F(43)	1.38(2)
C(28)-F(30)	1.343(12)	C(45A)-F(45A)	1.317(16)
C(29)-C(30)	1.468(8)	C(45A)-C(47A)	1.512(19)
C(30)-C(31)	1.374(9)	C(45A)-C(46A)	1.587(19)

C(46A)-F(46A)	1.325(6)	C(11S)-C(12S)	1.3900
C(46A)-F(48A)	1.325(6)	C(11S)-H(11A)	0.9500
C(46A)-F(47A)	1.325(6)	C(12S)-C(13S)	1.3900
C(47A)-F(51A)	1.321(7)	C(12S)-H(12A)	0.9500
C(47A)-F(49A)	1.321(7)	C(13S)-C(14S)	1.525(10)
C(47A)-F(50A)	1.321(7)	C(14S)-H(14A)	0.9800
C(48A)-F(38A)	1.356(16)	C(14S)-H(14B)	0.9800
C(48A)-C(50A)	1.53(2)	C(14S)-H(14C)	0.9800
C(48A)-C(49A)	1.58(2)	C(1T)-C(2T)	1.3900
C(49A)-F(41A)	1.28(2)	C(1T)-C(6T)	1.3900
C(49A)-F(40A)	1.30(2)	C(1T)-H(1TA)	0.9500
C(49A)-F(39A)	1.34(2)	C(2T)-C(3T)	1.3900
C(50A)-F(44A)	1.30(2)	C(2T)-H(2TA)	0.9500
C(50A)-F(42A)	1.36(2)	C(3T)-C(4T)	1.3900
C(50A)-F(43A)	1.39(2)	C(3T)-H(3TA)	0.9500
C(51)-C(52)	1.508(9)	C(4T)-C(5T)	1.3900
C(52)-H(52A)	0.9800	C(4T)-H(4TA)	0.9500
C(52)-H(52B)	0.9800	C(5T)-C(6T)	1.3900
C(52)-H(52C)	0.9800	C(5T)-H(5TA)	0.9500
C(53)-H(53A)	0.9800	C(6T)-C(7T)	1.525(10)
C(53)-H(53B)	0.9800	C(7T)-H(7TA)	0.9800
C(53)-H(53C)	0.9800	C(7T)-H(7TB)	0.9800
C(1S)-C(2S)	1.3900	C(7T)-H(7TC)	0.9800
C(1S)-C(6S)	1.3900	C(1E)-C(2E)	1.3900
C(1S)-H(1SA)	0.9500	C(1E)-C(6E)	1.3900
C(2S)-C(3S)	1.3900	C(1E)-H(1EA)	0.9500
C(2S)-H(2SA)	0.9500	C(2E)-C(3E)	1.3900
C(3S)-C(4S)	1.3900	C(2E)-H(2EA)	0.9500
C(3S)-H(3SA)	0.9500	C(3E)-C(4E)	1.3900
C(4S)-C(5S)	1.3900	C(3E)-H(3EA)	0.9500
C(4S)-H(4SA)	0.9500	C(4E)-C(5E)	1.3900
C(5S)-C(6S)	1.3900	C(4E)-H(4EA)	0.9500
C(5S)-H(5SA)	0.9500	C(5E)-C(6E)	1.3900
C(6S)-C(7S)	1.525(10)	C(5E)-H(5EA)	0.9500
C(7S)-H(7SA)	0.9800	C(6E)-C(7E)	1.524(10)
C(7S)-H(7SB)	0.9800	C(7E)-H(7EA)	0.9800
C(7S)-H(7SC)	0.9800	C(7E)-H(7EB)	0.9800
C(8S)-C(9S)	1.3900	C(7E)-H(7EC)	0.9800
C(8S)-C(13S)	1.3900	C(1K)-C(2K)	1.3900
C(8S)-H(8SA)	0.9500	C(1K)-C(6K)	1.3900
C(9S)-C(10S)	1.3900	C(1K)-H(1KA)	0.9500
C(9S)-H(9SA)	0.9500	C(2K)-C(3K)	1.3900
C(10S)-C(11S)	1.3900	C(2K)-H(2KA)	0.9500
C(10S)-H(10A)	0.9500	C(3K)-C(4K)	1.3900

C(3K)-H(3KA)	0.9500	C(6K)-C(7K)	1.524(10)
C(4K)-C(5K)	1.3900	C(7K)-H(7KA)	0.9800
C(4K)-H(4KA)	0.9500	C(7K)-H(7KB)	0.9800
C(5K)-C(6K)	1.3900	C(7K)-H(7KC)	0.9800
C(5K)-H(5KA)	0.9500	O(2)-H(2A)	0.840(2)

N(3)-Co-N(1)	176.4(2)	N(4)-Co-O(1)#1	93.7(2)
N(3)-Co-N(4)	89.8(2)	N(2)-Co-O(1)#1	88.81(19)
N(1)-Co-N(4)	90.0(2)	N(3)-Co-O(2)	85.8(4)
N(3)-Co-N(2)	90.1(2)	N(1)-Co-O(2)	90.5(4)
N(1)-Co-N(2)	89.9(2)	N(4)-Co-O(2)	92.0(4)
N(4)-Co-N(2)	177.4(2)	N(2)-Co-O(2)	85.4(4)
N(3)-Co-O(1)#1	82.91(19)	O(1)#1-Co-O(2)	167.3(4)
N(1)-Co-O(1)#1	100.73(19)		

C(1)-N(1)-C(8)	107.6(5)	C(3)-C(4)-C(5)	117.4(6)
C(1)-N(1)-Co	125.9(4)	C(3)-C(4)-C(9)	114.8(6)
C(8)-N(1)-Co	126.5(4)	C(5)-C(4)-C(9)	127.5(5)
C(22)-N(2)-C(15)	108.9(5)	C(6)-C(5)-C(4)	117.2(6)
C(22)-N(2)-Co	125.9(4)	C(6)-C(5)-C(12)	116.9(6)
C(15)-N(2)-Co	125.0(4)	C(4)-C(5)-C(12)	125.8(6)
C(36)-N(3)-C(29)	107.7(5)	F(1)-C(6)-C(5)	119.3(5)
C(36)-N(3)-Co	125.6(4)	F(1)-C(6)-C(7)	116.6(6)
C(29)-N(3)-Co	126.0(4)	C(5)-C(6)-C(7)	123.8(6)
C(37)-N(4)-C(44)	107.7(5)	C(2)-C(7)-C(6)	118.7(6)
C(37)-N(4)-Co	126.2(4)	C(2)-C(7)-C(8)	106.8(5)
C(44)-N(4)-Co	126.1(4)	C(6)-C(7)-C(8)	134.5(6)
C(44)-N(5)-C(1)	120.5(5)	N(6)-C(8)-N(1)	127.2(5)
C(15)-N(6)-C(8)	121.4(5)	N(6)-C(8)-C(7)	123.7(5)
C(29)-N(7)-C(22)	120.8(5)	N(1)-C(8)-C(7)	109.1(5)
C(36)-N(8)-C(37)	121.2(5)	F(3)-C(9)-C(11)	105.7(6)
C(51)-N(12)-C(33)	117.8(5)	F(3)-C(9)-C(4)	109.9(5)
C(51)-N(12)-C(53)	124.5(6)	C(11)-C(9)-C(4)	112.6(6)
C(33)-N(12)-C(53)	117.5(6)	F(3)-C(9)-C(10)	102.2(6)
C(51)-O(1)-Co#1	146.4(5)	C(11)-C(9)-C(10)	109.7(6)
N(5)-C(1)-N(1)	128.9(5)	C(4)-C(9)-C(10)	115.8(6)
N(5)-C(1)-C(2)	122.7(6)	F(5)-C(10)-F(6)	106.9(6)
N(1)-C(1)-C(2)	108.4(5)	F(5)-C(10)-F(4)	107.8(7)
C(7)-C(2)-C(3)	119.7(6)	F(6)-C(10)-F(4)	107.1(7)
C(7)-C(2)-C(1)	108.0(6)	F(5)-C(10)-C(9)	115.1(7)
C(3)-C(2)-C(1)	132.3(6)	F(6)-C(10)-C(9)	109.1(7)
F(2)-C(3)-C(2)	118.5(6)	F(4)-C(10)-C(9)	110.4(6)
F(2)-C(3)-C(4)	119.3(6)	F(8)-C(11)-F(7)	108.4(6)
C(2)-C(3)-C(4)	122.1(6)	F(8)-C(11)-F(9)	106.9(6)

F(7)-C(11)-F(9)	105.4(7)	N(7)-C(22)-C(21)	122.1(5)
F(8)-C(11)-C(9)	111.3(7)	N(2)-C(22)-C(21)	109.1(5)
F(7)-C(11)-C(9)	113.5(6)	F(19)-C(23)-C(25)	108.6(8)
F(9)-C(11)-C(9)	111.1(6)	F(19)-C(23)-C(18)	109.2(6)
F(10)-C(12)-C(13)	106.6(6)	C(25)-C(23)-C(18)	113.8(8)
F(10)-C(12)-C(5)	109.5(5)	F(19)-C(23)-C(24)	101.1(7)
C(13)-C(12)-C(5)	114.8(7)	C(25)-C(23)-C(24)	108.6(8)
F(10)-C(12)-C(14)	101.2(6)	C(18)-C(23)-C(24)	114.5(7)
C(13)-C(12)-C(14)	108.8(6)	F(21)-C(24)-F(22)	107.5(7)
C(5)-C(12)-C(14)	114.9(6)	F(21)-C(24)-F(20)	106.5(9)
F(11)-C(13)-F(13)	110.0(9)	F(22)-C(24)-F(20)	105.6(10)
F(11)-C(13)-F(12)	107.3(7)	F(21)-C(24)-C(23)	115.5(9)
F(13)-C(13)-F(12)	105.9(7)	F(22)-C(24)-C(23)	110.9(9)
F(11)-C(13)-C(12)	110.7(7)	F(20)-C(24)-C(23)	110.3(7)
F(13)-C(13)-C(12)	113.5(6)	F(23)-C(25)-F(24)	108.8(8)
F(12)-C(13)-C(12)	109.1(8)	F(23)-C(25)-F(25)	107.1(10)
F(16)-C(14)-F(15)	107.9(7)	F(24)-C(25)-F(25)	105.6(8)
F(16)-C(14)-F(14)	107.5(8)	F(23)-C(25)-C(23)	114.7(8)
F(15)-C(14)-F(14)	106.0(6)	F(24)-C(25)-C(23)	110.7(10)
F(16)-C(14)-C(12)	111.1(6)	F(25)-C(25)-C(23)	109.5(8)
F(15)-C(14)-C(12)	115.8(7)	F(26)-C(26)-C(28)	106.2(7)
F(14)-C(14)-C(12)	108.2(6)	F(26)-C(26)-C(27)	100.9(8)
N(6)-C(15)-N(2)	129.5(6)	C(28)-C(26)-C(27)	111.7(8)
N(6)-C(15)-C(16)	121.7(5)	F(26)-C(26)-C(19)	109.3(6)
N(2)-C(15)-C(16)	108.8(5)	C(28)-C(26)-C(19)	113.0(8)
C(17)-C(16)-C(21)	119.8(6)	C(27)-C(26)-C(19)	114.8(7)
C(17)-C(16)-C(15)	133.5(6)	F(27)-C(27)-F(29)	107.0(9)
C(21)-C(16)-C(15)	106.6(5)	F(27)-C(27)-F(28)	105.4(6)
F(17)-C(17)-C(16)	117.4(5)	F(29)-C(27)-F(28)	107.9(7)
F(17)-C(17)-C(18)	119.3(5)	F(27)-C(27)-C(26)	110.2(7)
C(16)-C(17)-C(18)	123.3(6)	F(29)-C(27)-C(26)	111.9(7)
C(17)-C(18)-C(19)	117.0(6)	F(28)-C(27)-C(26)	114.0(8)
C(17)-C(18)-C(23)	115.5(6)	F(31)-C(28)-F(32)	108.0(8)
C(19)-C(18)-C(23)	127.5(6)	F(31)-C(28)-F(30)	106.6(11)
C(20)-C(19)-C(18)	118.5(6)	F(32)-C(28)-F(30)	107.7(8)
C(20)-C(19)-C(26)	114.6(6)	F(31)-C(28)-C(26)	112.2(8)
C(18)-C(19)-C(26)	126.7(6)	F(32)-C(28)-C(26)	109.9(10)
F(18)-C(20)-C(21)	117.4(5)	F(30)-C(28)-C(26)	112.2(7)
F(18)-C(20)-C(19)	119.9(6)	N(7)-C(29)-N(3)	128.2(5)
C(21)-C(20)-C(19)	122.6(6)	N(7)-C(29)-C(30)	122.2(5)
C(20)-C(21)-C(16)	118.3(6)	N(3)-C(29)-C(30)	109.4(5)
C(20)-C(21)-C(22)	134.9(6)	C(31)-C(30)-C(35)	120.3(6)
C(16)-C(21)-C(22)	106.7(5)	C(31)-C(30)-C(29)	133.9(6)
N(7)-C(22)-N(2)	128.8(5)	C(35)-C(30)-C(29)	105.8(5)

F(34)-C(31)-C(30)	122.6(5)	N(5)-C(44)-C(43)	122.8(5)
F(34)-C(31)-C(32)	119.1(5)	N(4)-C(44)-C(43)	108.6(5)
C(30)-C(31)-C(32)	118.2(6)	F(45)-C(45)-C(47)	104.7(7)
F(35)-C(32)-C(31)	118.1(6)	F(45)-C(45)-C(41)	112.5(7)
F(35)-C(32)-C(33)	119.4(6)	C(47)-C(45)-C(41)	118.8(7)
C(31)-C(32)-C(33)	122.5(6)	F(45)-C(45)-C(46)	103.7(7)
C(34)-C(33)-C(32)	117.9(6)	C(47)-C(45)-C(46)	108.0(6)
C(34)-C(33)-N(12)	120.1(6)	C(41)-C(45)-C(46)	108.2(7)
C(32)-C(33)-N(12)	122.0(6)	F(46)-C(46)-F(47)	109.4(6)
F(33)-C(34)-C(33)	119.2(5)	F(46)-C(46)-F(48)	109.3(6)
F(33)-C(34)-C(35)	120.2(6)	F(47)-C(46)-F(48)	109.3(6)
C(33)-C(34)-C(35)	120.6(6)	F(46)-C(46)-C(45)	109.8(8)
C(34)-C(35)-C(30)	120.3(6)	F(47)-C(46)-C(45)	108.7(8)
C(34)-C(35)-C(36)	132.8(6)	F(48)-C(46)-C(45)	110.3(8)
C(30)-C(35)-C(36)	106.9(5)	F(49)-C(47)-F(51)	107.6(7)
N(8)-C(36)-N(3)	128.4(5)	F(49)-C(47)-F(50)	107.5(7)
N(8)-C(36)-C(35)	121.6(5)	F(51)-C(47)-F(50)	107.5(7)
N(3)-C(36)-C(35)	109.9(5)	F(49)-C(47)-C(45)	107.8(8)
N(8)-C(37)-N(4)	127.6(6)	F(51)-C(47)-C(45)	116.4(9)
N(8)-C(37)-C(38)	122.2(5)	F(50)-C(47)-C(45)	109.6(9)
N(4)-C(37)-C(38)	110.1(5)	F(38)-C(48)-C(50)	103.4(10)
C(43)-C(38)-C(39)	119.4(6)	F(38)-C(48)-C(40)	112.7(7)
C(43)-C(38)-C(37)	106.2(5)	C(50)-C(48)-C(40)	118.7(10)
C(39)-C(38)-C(37)	134.4(6)	F(38)-C(48)-C(49)	105.9(9)
F(37)-C(39)-C(38)	117.5(6)	C(50)-C(48)-C(49)	108.6(9)
F(37)-C(39)-C(40)	119.1(5)	C(40)-C(48)-C(49)	106.9(8)
C(38)-C(39)-C(40)	123.4(6)	F(41)-C(49)-F(40)	108.4(12)
C(39)-C(40)-C(41)	117.7(5)	F(41)-C(49)-F(39)	109.1(13)
C(39)-C(40)-C(48A)	115.4(8)	F(40)-C(49)-F(39)	108.0(11)
C(41)-C(40)-C(48A)	125.3(8)	F(41)-C(49)-C(48)	112.1(10)
C(39)-C(40)-C(48)	115.9(6)	F(40)-C(49)-C(48)	111.6(11)
C(41)-C(40)-C(48)	126.0(6)	F(39)-C(49)-C(48)	107.5(11)
C(42)-C(41)-C(40)	117.0(5)	F(44)-C(50)-F(42)	107.7(13)
C(42)-C(41)-C(45A)	115.3(8)	F(44)-C(50)-F(43)	107.7(16)
C(40)-C(41)-C(45A)	127.2(8)	F(42)-C(50)-F(43)	104.0(15)
C(42)-C(41)-C(45)	115.5(6)	F(44)-C(50)-C(48)	117.5(14)
C(40)-C(41)-C(45)	127.2(6)	F(42)-C(50)-C(48)	109.3(15)
F(36)-C(42)-C(43)	118.8(5)	F(43)-C(50)-C(48)	109.8(14)
F(36)-C(42)-C(41)	118.6(5)	F(45A)-C(45A)-C(47A)	107.6(15)
C(43)-C(42)-C(41)	122.6(6)	F(45A)-C(45A)-C(41)	109.1(12)
C(42)-C(43)-C(38)	119.9(5)	C(47A)-C(45A)-C(41)	111.0(10)
C(42)-C(43)-C(44)	132.6(6)	F(45A)-C(45A)-C(46A)	103.2(13)
C(38)-C(43)-C(44)	107.5(5)	C(47A)-C(45A)-C(46A)	113.9(12)
N(5)-C(44)-N(4)	128.6(5)	C(41)-C(45A)-C(46A)	111.6(10)

F(46A)-C(46A)-F(48A)	109.4(6)	H(53B)-C(53)-H(53C)	109.5
F(46A)-C(46A)-F(47A)	109.4(6)	C(2S)-C(1S)-C(6S)	120.0
F(48A)-C(46A)-F(47A)	109.4(6)	C(2S)-C(1S)-H(1SA)	120.0
F(46A)-C(46A)-C(45A)	110.9(13)	C(6S)-C(1S)-H(1SA)	120.0
F(48A)-C(46A)-C(45A)	112.2(14)	C(1S)-C(2S)-C(3S)	120.0
F(47A)-C(46A)-C(45A)	105.5(13)	C(1S)-C(2S)-H(2SA)	120.0
F(51A)-C(47A)-F(49A)	107.5(7)	C(3S)-C(2S)-H(2SA)	120.0
F(51A)-C(47A)-F(50A)	107.5(7)	C(4S)-C(3S)-C(2S)	120.0
F(49A)-C(47A)-F(50A)	107.5(7)	C(4S)-C(3S)-H(3SA)	120.0
F(51A)-C(47A)-C(45A)	114.3(16)	C(2S)-C(3S)-H(3SA)	120.0
F(49A)-C(47A)-C(45A)	110.8(14)	C(5S)-C(4S)-C(3S)	120.0
F(50A)-C(47A)-C(45A)	108.9(15)	C(5S)-C(4S)-H(4SA)	120.0
F(38A)-C(48A)-C(50A)	105.8(16)	C(3S)-C(4S)-H(4SA)	120.0
F(38A)-C(48A)-C(40)	110.2(11)	C(4S)-C(5S)-C(6S)	120.0
C(50A)-C(48A)-C(40)	105.7(13)	C(4S)-C(5S)-H(5SA)	120.0
F(38A)-C(48A)-C(49A)	105.7(13)	C(6S)-C(5S)-H(5SA)	120.0
C(50A)-C(48A)-C(49A)	109.3(14)	C(5S)-C(6S)-C(1S)	120.0
C(40)-C(48A)-C(49A)	119.6(14)	C(5S)-C(6S)-C(7S)	116.0(14)
F(41A)-C(49A)-F(40A)	110(2)	C(1S)-C(6S)-C(7S)	124.0(14)
F(41A)-C(49A)-F(39A)	108(2)	C(6S)-C(7S)-H(7SA)	109.5
F(40A)-C(49A)-F(39A)	108(2)	C(6S)-C(7S)-H(7SB)	109.5
F(41A)-C(49A)-C(48A)	107.4(16)	H(7SA)-C(7S)-H(7SB)	109.5
F(40A)-C(49A)-C(48A)	115.0(19)	C(6S)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-C(48A)	108.0(19)	H(7SA)-C(7S)-H(7SC)	109.5
F(44A)-C(50A)-F(42A)	109(2)	H(7SB)-C(7S)-H(7SC)	109.5
F(44A)-C(50A)-F(43A)	108(2)	C(9S)-C(8S)-C(13S)	120.0
F(42A)-C(50A)-F(43A)	105(2)	C(9S)-C(8S)-H(8SA)	120.0
F(44A)-C(50A)-C(48A)	115(2)	C(13S)-C(8S)-H(8SA)	120.0
F(42A)-C(50A)-C(48A)	109(2)	C(8S)-C(9S)-C(10S)	120.0
F(43A)-C(50A)-C(48A)	111(2)	C(8S)-C(9S)-H(9SA)	120.0
O(1)-C(51)-N(12)	119.9(6)	C(10S)-C(9S)-H(9SA)	120.0
O(1)-C(51)-C(52)	122.5(7)	C(11S)-C(10S)-C(9S)	120.0
N(12)-C(51)-C(52)	117.5(6)	C(11S)-C(10S)-H(10A)	120.0
C(51)-C(52)-H(52A)	109.5	C(9S)-C(10S)-H(10A)	120.0
C(51)-C(52)-H(52B)	109.5	C(12S)-C(11S)-C(10S)	120.0
H(52A)-C(52)-H(52B)	109.5	C(12S)-C(11S)-H(11A)	120.0
C(51)-C(52)-H(52C)	109.5	C(10S)-C(11S)-H(11A)	120.0
H(52A)-C(52)-H(52C)	109.5	C(13S)-C(12S)-C(11S)	120.0
H(52B)-C(52)-H(52C)	109.5	C(13S)-C(12S)-H(12A)	120.0
N(12)-C(53)-H(53A)	109.5	C(11S)-C(12S)-H(12A)	120.0
N(12)-C(53)-H(53B)	109.5	C(12S)-C(13S)-C(8S)	120.0
H(53A)-C(53)-H(53B)	109.5	C(12S)-C(13S)-C(14S)	119(2)
N(12)-C(53)-H(53C)	109.5	C(8S)-C(13S)-C(14S)	121(2)
H(53A)-C(53)-H(53C)	109.5	C(13S)-C(14S)-H(14A)	109.5

C(13S)-C(14S)-H(14B)	109.5	C(5E)-C(4E)-H(4EA)	120.0
H(14A)-C(14S)-H(14B)	109.5	C(3E)-C(4E)-H(4EA)	120.0
C(13S)-C(14S)-H(14C)	109.5	C(4E)-C(5E)-C(6E)	120.0
H(14A)-C(14S)-H(14C)	109.5	C(4E)-C(5E)-H(5EA)	120.0
H(14B)-C(14S)-H(14C)	109.5	C(6E)-C(5E)-H(5EA)	120.0
C(2T)-C(1T)-C(6T)	120.0	C(5E)-C(6E)-C(1E)	120.0
C(2T)-C(1T)-H(1TA)	120.0	C(5E)-C(6E)-C(7E)	118.4(18)
C(6T)-C(1T)-H(1TA)	120.0	C(1E)-C(6E)-C(7E)	121.2(18)
C(3T)-C(2T)-C(1T)	120.0	C(6E)-C(7E)-H(7EA)	109.5
C(3T)-C(2T)-H(2TA)	120.0	C(6E)-C(7E)-H(7EB)	109.5
C(1T)-C(2T)-H(2TA)	120.0	H(7EA)-C(7E)-H(7EB)	109.5
C(2T)-C(3T)-C(4T)	120.0	C(6E)-C(7E)-H(7EC)	109.5
C(2T)-C(3T)-H(3TA)	120.0	H(7EA)-C(7E)-H(7EC)	109.5
C(4T)-C(3T)-H(3TA)	120.0	H(7EB)-C(7E)-H(7EC)	109.5
C(5T)-C(4T)-C(3T)	120.0	C(2K)-C(1K)-C(6K)	120.0
C(5T)-C(4T)-H(4TA)	120.0	C(2K)-C(1K)-H(1KA)	120.0
C(3T)-C(4T)-H(4TA)	120.0	C(6K)-C(1K)-H(1KA)	120.0
C(4T)-C(5T)-C(6T)	120.0	C(3K)-C(2K)-C(1K)	120.0
C(4T)-C(5T)-H(5TA)	120.0	C(3K)-C(2K)-H(2KA)	120.0
C(6T)-C(5T)-H(5TA)	120.0	C(1K)-C(2K)-H(2KA)	120.0
C(5T)-C(6T)-C(1T)	120.0	C(2K)-C(3K)-C(4K)	120.0
C(5T)-C(6T)-C(7T)	119.7(12)	C(2K)-C(3K)-H(3KA)	120.0
C(1T)-C(6T)-C(7T)	119.9(12)	C(4K)-C(3K)-H(3KA)	120.0
C(6T)-C(7T)-H(7TA)	109.5	C(3K)-C(4K)-C(5K)	120.0
C(6T)-C(7T)-H(7TB)	109.5	C(3K)-C(4K)-H(4KA)	120.0
H(7TA)-C(7T)-H(7TB)	109.5	C(5K)-C(4K)-H(4KA)	120.0
C(6T)-C(7T)-H(7TC)	109.5	C(6K)-C(5K)-C(4K)	120.0
H(7TA)-C(7T)-H(7TC)	109.5	C(6K)-C(5K)-H(5KA)	120.0
H(7TB)-C(7T)-H(7TC)	109.5	C(4K)-C(5K)-H(5KA)	120.0
C(2E)-C(1E)-C(6E)	120.0	C(5K)-C(6K)-C(1K)	120.0
C(2E)-C(1E)-H(1EA)	120.0	C(5K)-C(6K)-C(7K)	118.7(15)
C(6E)-C(1E)-H(1EA)	120.0	C(1K)-C(6K)-C(7K)	121.2(15)
C(3E)-C(2E)-C(1E)	120.0	C(6K)-C(7K)-H(7KA)	109.5
C(3E)-C(2E)-H(2EA)	120.0	C(6K)-C(7K)-H(7KB)	109.5
C(1E)-C(2E)-H(2EA)	120.0	H(7KA)-C(7K)-H(7KB)	109.5
C(2E)-C(3E)-C(4E)	120.0	C(6K)-C(7K)-H(7KC)	109.5
C(2E)-C(3E)-H(3EA)	120.0	H(7KA)-C(7K)-H(7KC)	109.5
C(4E)-C(3E)-H(3EA)	120.0	H(7KB)-C(7K)-H(7KC)	109.5
C(5E)-C(4E)-C(3E)	120.0	Co-O(2)-H(2A)	104(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table W.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)**. 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}
Co	27(1)	28(1)	46(1)	1(1)	13(1)	-3(1)
N(1)	37(3)	25(2)	39(3)	3(2)	12(2)	-1(2)
N(2)	28(3)	30(3)	42(3)	-1(2)	11(2)	-4(2)
N(3)	33(3)	26(2)	39(3)	0(2)	14(2)	-3(2)
N(4)	30(3)	38(3)	43(3)	-1(2)	13(2)	-5(2)
N(5)	28(3)	36(3)	51(3)	12(2)	12(2)	-2(2)
N(6)	31(3)	29(3)	57(4)	1(2)	11(2)	-6(2)
N(7)	33(3)	32(3)	47(3)	-1(2)	19(2)	1(2)
N(8)	32(3)	31(3)	50(3)	3(2)	13(2)	-4(2)
N(12)	29(3)	46(3)	55(4)	16(3)	11(3)	-2(2)
O(1)	38(2)	34(2)	48(3)	3(2)	13(2)	-3(2)
C(1)	35(3)	30(3)	48(4)	2(3)	12(3)	-4(3)
C(2)	32(3)	37(3)	50(4)	0(3)	11(3)	-7(3)
C(3)	40(4)	42(4)	53(4)	15(3)	16(3)	0(3)
C(4)	27(3)	42(4)	62(5)	5(3)	9(3)	-5(3)
C(5)	34(3)	34(3)	59(4)	8(3)	8(3)	-6(3)
C(6)	32(3)	37(4)	63(5)	9(3)	11(3)	-9(3)
C(7)	29(3)	35(3)	49(4)	2(3)	11(3)	-1(3)
C(8)	32(3)	31(3)	44(4)	3(3)	12(3)	-8(3)
C(9)	34(4)	46(4)	79(6)	12(4)	17(4)	-9(3)
C(10)	48(4)	39(4)	79(6)	11(4)	3(4)	-12(3)
C(11)	45(4)	47(4)	82(6)	22(4)	23(4)	3(3)
C(12)	26(3)	42(4)	90(6)	15(4)	16(4)	1(3)
C(13)	38(4)	62(5)	100(7)	19(5)	10(4)	-14(4)
C(14)	44(4)	59(5)	80(6)	23(4)	24(4)	-2(4)
C(15)	36(3)	28(3)	42(4)	-5(3)	15(3)	-5(3)
C(16)	38(3)	24(3)	49(4)	-5(3)	20(3)	-1(2)
C(17)	37(3)	29(3)	59(4)	1(3)	19(3)	-3(3)
C(18)	48(4)	31(3)	70(5)	5(3)	25(4)	-3(3)
C(19)	51(4)	31(3)	83(6)	10(3)	33(4)	4(3)
C(20)	41(4)	29(3)	61(5)	3(3)	26(3)	3(3)
C(21)	32(3)	29(3)	48(4)	-4(3)	16(3)	-2(2)
C(22)	38(3)	24(3)	42(4)	-4(3)	17(3)	0(2)
C(23)	48(4)	37(4)	123(8)	26(4)	32(5)	5(3)
C(24)	74(7)	44(5)	150(11)	11(6)	47(7)	-15(4)
C(25)	67(6)	85(7)	126(9)	48(7)	46(7)	-10(5)
C(26)	59(5)	44(4)	123(8)	38(5)	46(5)	8(4)
C(27)	55(5)	78(6)	99(7)	44(6)	38(5)	18(5)
C(28)	73(6)	41(5)	178(12)	20(6)	54(7)	13(5)

C(29)	27(3)	31(3)	44(4)	-4(3)	17(3)	-2(2)
C(30)	35(3)	38(3)	36(4)	-5(3)	15(3)	-5(3)
C(31)	39(4)	33(3)	51(4)	6(3)	20(3)	3(3)
C(32)	33(3)	50(4)	44(4)	5(3)	19(3)	8(3)
C(33)	36(3)	41(4)	43(4)	5(3)	13(3)	-4(3)
C(34)	34(3)	37(3)	54(4)	6(3)	11(3)	-2(3)
C(35)	28(3)	36(3)	46(4)	3(3)	13(3)	-2(3)
C(36)	32(3)	32(3)	45(4)	1(3)	12(3)	1(3)
C(37)	30(3)	34(3)	45(4)	2(3)	15(3)	-4(3)
C(38)	36(3)	31(3)	52(4)	0(3)	18(3)	0(3)
C(39)	33(3)	38(4)	56(4)	-1(3)	19(3)	-4(3)
C(40)	45(4)	29(3)	65(5)	4(3)	26(3)	-2(3)
C(41)	45(4)	26(3)	67(5)	3(3)	26(3)	-2(3)
C(42)	33(3)	34(3)	65(5)	8(3)	20(3)	-1(3)
C(43)	35(3)	29(3)	46(4)	1(3)	14(3)	-8(3)
C(44)	29(3)	29(3)	47(4)	0(3)	13(3)	-3(2)
C(45)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(46)	48(8)	36(7)	99(11)	-4(7)	30(7)	-4(6)
C(47)	66(12)	36(9)	65(9)	7(8)	8(8)	9(8)
C(48)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(49)	56(9)	74(9)	60(9)	19(7)	28(8)	-2(7)
C(50)	48(10)	42(8)	62(15)	5(10)	17(10)	-17(7)
F(38)	51(4)	29(3)	101(6)	10(4)	31(4)	3(3)
F(39)	79(6)	86(7)	109(8)	31(6)	54(5)	-18(6)
F(40)	79(6)	91(6)	68(5)	23(5)	31(5)	3(4)
F(41)	97(10)	58(7)	93(8)	13(7)	62(7)	12(7)
F(42)	59(5)	46(5)	107(7)	-7(5)	20(5)	-19(3)
F(43)	56(5)	63(5)	60(7)	-1(5)	25(4)	-7(4)
F(44)	40(4)	51(4)	98(6)	7(4)	33(4)	-5(3)
F(45)	55(4)	43(4)	92(6)	33(4)	27(4)	8(3)
F(46)	62(5)	57(4)	103(6)	-24(4)	32(4)	-9(4)
F(47)	57(5)	40(4)	127(9)	12(4)	30(5)	18(3)
F(48)	59(6)	50(5)	87(7)	5(5)	45(5)	0(4)
F(49)	82(7)	71(6)	67(5)	-10(5)	-2(5)	0(5)
F(50)	78(7)	92(9)	97(7)	49(7)	-11(5)	-6(6)
F(51)	36(4)	48(4)	116(7)	21(4)	4(4)	4(3)
C(45A)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(46A)	80(30)	50(20)	270(70)	50(30)	130(40)	19(17)
C(47A)	60(30)	90(30)	200(60)	70(30)	-20(30)	0(20)
C(48A)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(49A)	28(18)	120(40)	120(40)	60(40)	0(20)	-20(20)
C(50A)	80(30)	60(20)	160(40)	40(20)	30(30)	-11(19)
F(38A)	62(9)	64(10)	132(17)	41(11)	54(10)	6(7)
F(39A)	108(16)	54(12)	124(17)	15(13)	77(13)	19(11)

F(40A)	41(8)	84(11)	133(17)	35(11)	32(10)	-15(7)
F(41A)	95(14)	122(19)	170(20)	57(18)	99(15)	-1(15)
F(42A)	130(20)	60(12)	210(30)	1(18)	50(20)	-57(12)
F(43A)	70(16)	80(20)	70(30)	-20(20)	9(17)	-12(12)
F(44A)	141(19)	62(11)	160(20)	-17(13)	36(17)	35(11)
F(45A)	108(14)	35(9)	190(30)	30(12)	84(17)	2(8)
F(46A)	120(20)	82(16)	520(70)	110(30)	200(40)	53(16)
F(47A)	220(30)	33(11)	300(50)	-2(17)	180(30)	32(15)
F(48A)	220(40)	120(20)	180(30)	-10(20)	140(30)	30(20)
F(49A)	130(20)	104(16)	140(20)	45(15)	25(16)	-23(14)
F(50A)	78(16)	65(16)	350(60)	100(30)	-10(20)	12(12)
F(51A)	72(18)	90(20)	280(50)	110(20)	10(20)	-8(17)
C(51)	35(4)	34(3)	66(5)	1(3)	21(4)	0(3)
C(52)	41(4)	53(4)	75(6)	10(4)	14(4)	-15(3)
C(53)	45(4)	68(5)	71(6)	29(4)	21(4)	-2(4)
F(1)	32(2)	35(2)	99(3)	23(2)	16(2)	-5(2)
F(2)	37(2)	44(2)	85(3)	27(2)	17(2)	1(2)
F(3)	30(2)	57(3)	97(4)	25(2)	-3(2)	-7(2)
F(4)	87(4)	69(3)	69(3)	4(3)	12(3)	5(3)
F(5)	63(3)	58(3)	81(3)	22(2)	6(2)	-6(2)
F(6)	57(3)	75(3)	98(4)	27(3)	-15(3)	-6(2)
F(7)	64(3)	46(2)	105(4)	8(2)	43(3)	-5(2)
F(8)	53(3)	66(3)	128(5)	27(3)	19(3)	22(2)
F(9)	67(3)	63(3)	92(4)	9(3)	39(3)	2(2)
F(10)	34(2)	59(3)	103(4)	30(2)	25(2)	10(2)
F(11)	120(5)	72(4)	126(5)	19(4)	-51(4)	-25(3)
F(12)	57(3)	99(4)	226(8)	-10(5)	58(4)	-36(3)
F(13)	61(3)	50(3)	109(4)	6(3)	6(3)	-11(2)
F(14)	60(3)	126(5)	127(5)	75(4)	55(3)	33(3)
F(15)	73(3)	76(3)	99(4)	39(3)	29(3)	26(3)
F(16)	90(4)	98(4)	74(3)	4(3)	34(3)	-21(3)
F(17)	37(2)	37(2)	84(3)	12(2)	21(2)	-4(2)
F(18)	40(2)	34(2)	85(3)	11(2)	29(2)	5(2)
F(19)	65(3)	36(2)	213(7)	41(3)	57(4)	8(2)
F(20)	83(4)	64(3)	126(5)	-25(3)	21(4)	-14(3)
F(21)	53(3)	57(3)	160(5)	23(3)	35(3)	-13(2)
F(22)	94(4)	37(3)	252(9)	0(4)	40(5)	-25(3)
F(23)	82(4)	95(4)	121(5)	40(4)	64(3)	26(3)
F(24)	83(4)	125(5)	208(8)	96(5)	75(5)	2(4)
F(25)	82(4)	157(6)	121(5)	67(5)	47(4)	19(4)
F(26)	68(3)	76(3)	154(5)	66(4)	61(3)	22(3)
F(27)	69(3)	124(5)	137(5)	84(4)	46(3)	28(3)
F(28)	54(3)	85(3)	122(4)	45(3)	44(3)	21(2)
F(29)	62(3)	79(3)	86(4)	19(3)	29(3)	15(3)

F(30)	96(4)	40(3)	174(6)	-6(3)	83(4)	-1(2)
F(31)	98(4)	39(3)	227(8)	-11(4)	67(5)	-12(3)
F(32)	107(5)	53(3)	242(9)	50(4)	74(5)	41(3)
F(33)	35(2)	37(2)	93(3)	14(2)	20(2)	-4(2)
F(34)	44(2)	36(2)	66(3)	3(2)	20(2)	3(2)
F(35)	32(2)	45(2)	67(3)	5(2)	18(2)	4(2)
F(36)	33(2)	37(2)	103(3)	19(2)	21(2)	1(2)
F(37)	31(2)	39(2)	84(3)	7(2)	24(2)	-5(2)
C(1S)	117(10)	147(13)	84(11)	-54(9)	40(9)	-35(8)
C(2S)	120(10)	119(11)	99(15)	-45(10)	56(10)	-33(9)
C(3S)	126(10)	107(10)	109(12)	-53(8)	58(9)	-29(7)
C(4S)	127(10)	118(11)	85(10)	-51(8)	49(9)	-23(7)
C(5S)	119(9)	143(12)	102(11)	-56(9)	47(9)	-21(9)
C(6S)	109(9)	157(13)	80(12)	-55(10)	42(9)	-33(9)
C(7S)	109(10)	250(20)	112(15)	-85(18)	56(11)	-66(13)
C(8S)	102(16)	81(17)	32(15)	-19(13)	19(13)	-16(11)
C(9S)	99(17)	100(20)	50(30)	-21(18)	20(18)	-10(15)
C(10S)	102(16)	100(18)	52(17)	-21(14)	31(14)	8(14)
C(11S)	103(16)	73(15)	25(14)	-12(11)	26(13)	18(11)
C(12S)	96(15)	57(13)	48(15)	-7(11)	25(13)	4(11)
C(13S)	90(15)	60(13)	20(14)	-12(12)	1(13)	-4(11)
C(14S)	93(17)	39(15)	100(30)	-28(16)	-41(19)	-17(13)
C(1T)	152(10)	134(10)	124(11)	7(8)	31(9)	10(8)
C(2T)	143(9)	127(10)	128(11)	4(8)	33(9)	14(8)
C(3T)	147(9)	110(9)	87(8)	-31(6)	37(7)	0(6)
C(4T)	164(10)	133(10)	114(10)	-16(8)	40(9)	24(8)
C(5T)	157(11)	191(14)	200(16)	47(12)	16(13)	15(11)
C(6T)	138(10)	151(12)	187(14)	30(10)	-31(11)	-9(9)
C(7T)	260(20)	230(20)	350(30)	200(20)	-10(20)	12(17)
C(1E)	220(20)	106(12)	137(17)	16(10)	66(16)	-8(14)
C(2E)	410(50)	115(15)	130(17)	12(12)	70(20)	-20(20)
C(3E)	330(40)	52(9)	380(50)	45(18)	-80(30)	-43(14)
C(4E)	250(30)	81(11)	240(30)	55(13)	90(20)	4(15)
C(5E)	370(40)	84(10)	105(14)	18(9)	48(17)	36(16)
C(6E)	250(30)	81(10)	156(18)	1(11)	30(20)	18(13)
C(7E)	270(30)	200(30)	350(40)	-60(20)	100(30)	10(20)
C(1K)	92(18)	55(9)	108(15)	20(20)	39(12)	-2(15)
C(2K)	120(20)	45(13)	150(30)	-24(16)	43(19)	-24(15)
C(3K)	85(15)	51(14)	100(20)	-17(14)	9(14)	-8(11)
C(4K)	120(30)	43(12)	130(40)	5(14)	30(30)	5(16)
C(5K)	78(15)	49(11)	70(20)	-8(10)	-15(16)	8(13)
C(6K)	71(14)	59(18)	100(20)	22(15)	1(12)	24(14)
C(7K)	100(17)	91(16)	102(18)	-15(14)	29(14)	9(13)
O(2)	96(10)	65(8)	131(13)	-7(8)	43(10)	-37(7)

Table W.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$OH]·7(toluene)**.

	x	y	z	U(eq)
H(52A)	13110	3463	7881	85
H(52B)	12660	3760	7409	85
H(52C)	13061	3415	7203	85
H(53A)	12158	3385	6236	91
H(53B)	11796	3742	6450	91
H(53C)	11313	3439	6008	91
H(1SA)	7017	2970	4761	136
H(2SA)	8171	3161	4800	129
H(3SA)	8353	3745	4397	131
H(4SA)	7381	4136	3955	127
H(5SA)	6228	3945	3915	142
H(7SA)	5458	3344	3875	229
H(7SB)	5554	3528	4508	229
H(7SC)	5724	3088	4452	229
H(8SA)	7200	3735	4278	86
H(9SA)	8257	3389	4628	103
H(10A)	8233	2782	5019	100
H(11A)	7153	2521	5060	79
H(12A)	6097	2867	4710	80
H(14A)	5634	3492	3816	138
H(14B)	5946	3825	4276	138
H(14C)	5527	3478	4456	138
H(1TA)	1423	3129	5040	167
H(2TA)	1332	2542	5474	161
H(3TA)	218	2316	5489	137
H(4TA)	-806	2677	5070	164
H(5TA)	-716	3263	4637	229
H(7TA)	927	3702	4600	452
H(7TB)	131	3675	4170	452
H(7TC)	272	3836	4822	452
H(1EA)	7968	5477	1754	184
H(2EA)	6824	5421	1858	264
H(3EA)	6664	5443	2792	351
H(4EA)	7647	5521	3622	224
H(5EA)	8791	5577	3518	231
H(7EA)	9276	5891	2526	408
H(7EB)	9282	5487	2222	408

H(7EC)	9588	5527	2920	408
H(1KA)	4812	4690	7614	100
H(2KA)	5259	4565	6824	125
H(3KA)	5496	3940	6608	100
H(4KA)	5286	3439	7181	120
H(5KA)	4838	3564	7970	89
H(7KA)	4016	4076	8297	147
H(7KB)	4396	4483	8406	147
H(7KC)	4803	4116	8738	147
H(2A)	7010(30)	2560(30)	5370(100)	114

Appendix X: Crystal structure of [(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)

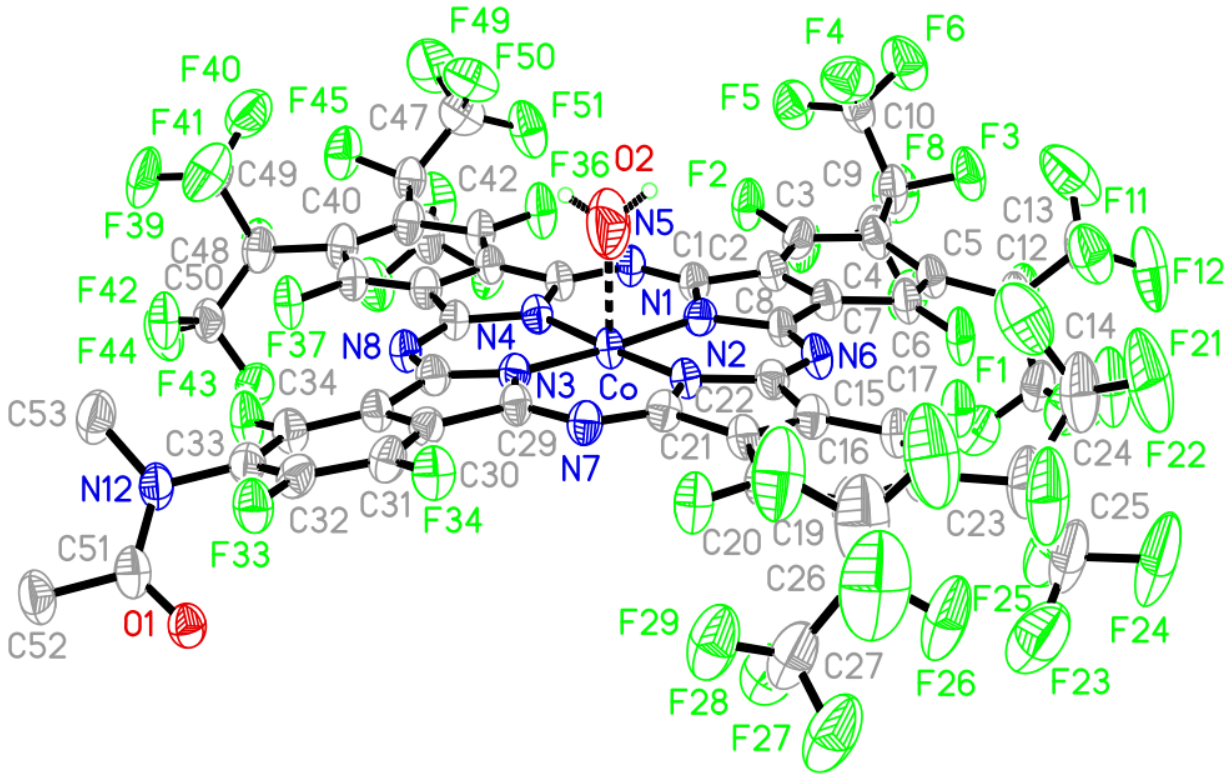


Figure X.1 ORTEP representation of **NMeAcF$_{51}$PcCo-OH$_2$** X-ray crystal structure, at 50% probability.

Table X.1 Crystal data and structure refinement for **[(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**.

Empirical formula	C155 H70 Co2 F102 N18 O3	
Formula weight	4288.15	
Temperature	130(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.6464(18) Å	α = 90°.
	b = 35.227(3) Å	β = 107.096(3)°.
	c = 23.839(2) Å	γ = 90°.
Volume	15770(3) Å^3	
Z	4	
Density (calculated)	1.806 g/cm^3	
Absorption coefficient	0.394 mm^{-1}	
F(000)	8488	
Crystal size	0.600 x 0.280 x 0.050 mm^3	
Theta range for data collection	1.319 to 25.027°.	

Index ranges	-23<=h<=23, -41<=k<=41, -28<=l<=28
Reflections collected	162989
Independent reflections	13917 [R(int) = 0.0895]
Completeness to theta = 25.000°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	0.7461 and 0.6613
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13917 / 550 / 1476
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0868, wR2 = 0.2052
R indices (all data)	R1 = 0.1344, wR2 = 0.2419
Extinction coefficient	n/a
Largest diff. peak and hole	0.733 and -0.743 e.$Å^{-3}$

Table X.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co	7583(1)	2897(1)	6331(1)	33(1)
N(1)	6572(3)	2919(1)	6202(2)	33(1)
N(2)	7587(2)	2376(1)	6582(2)	33(1)
N(3)	8581(2)	2864(1)	6409(2)	32(1)
N(4)	7570(3)	3408(1)	6045(2)	36(1)
N(5)	6308(3)	3550(1)	5782(2)	38(1)
N(6)	6355(3)	2302(1)	6558(2)	39(1)
N(7)	8830(3)	2219(1)	6765(2)	36(1)
N(8)	8825(3)	3508(1)	6185(2)	37(1)
N(12)	11666(3)	3250(2)	6845(3)	43(1)
O(1)	12041(2)	3062(1)	7770(2)	40(1)
C(1)	6136(3)	3218(2)	5958(3)	37(1)
C(2)	5415(3)	3123(2)	5945(3)	40(2)
C(3)	4769(3)	3315(2)	5728(3)	44(2)
C(4)	4131(3)	3172(2)	5792(3)	45(2)
C(5)	4170(3)	2829(2)	6132(3)	44(2)
C(6)	4798(3)	2635(2)	6278(3)	45(2)
C(7)	5427(3)	2776(2)	6197(3)	38(1)
C(8)	6152(3)	2641(2)	6338(3)	36(1)
C(9)	3452(4)	3387(2)	5440(4)	53(2)
C(10)	3394(4)	3473(2)	4782(4)	59(2)
C(11)	3332(4)	3750(2)	5742(4)	57(2)

C(12)	3573(3)	2674(2)	6376(4)	53(2)
C(13)	3169(4)	2333(2)	6045(5)	69(2)
C(14)	3815(4)	2582(2)	7047(4)	59(2)
C(15)	7011(3)	2188(2)	6663(3)	35(1)
C(16)	7243(3)	1818(2)	6919(3)	36(1)
C(17)	6896(3)	1518(2)	7085(3)	40(2)
C(18)	7238(4)	1191(2)	7340(3)	48(2)
C(19)	7993(4)	1176(2)	7447(4)	52(2)
C(20)	8324(3)	1471(2)	7237(3)	41(2)
C(21)	7963(3)	1793(2)	6978(3)	35(1)
C(22)	8166(3)	2148(2)	6758(3)	34(1)
C(23)	6748(4)	876(2)	7456(5)	68(3)
C(24)	6064(5)	793(2)	6923(6)	86(3)
C(25)	6520(6)	940(3)	7999(5)	89(3)
C(26)	8513(4)	877(2)	7825(5)	71(3)
C(27)	9167(5)	1046(3)	8294(5)	74(3)
C(28)	8732(5)	576(3)	7458(6)	94(4)
C(29)	9009(3)	2555(2)	6603(3)	33(1)
C(30)	9753(3)	2657(2)	6667(3)	35(1)
C(31)	10383(3)	2460(2)	6825(3)	39(2)
C(32)	11006(3)	2656(2)	6863(3)	41(2)
C(33)	11017(3)	3047(2)	6769(3)	40(2)
C(34)	10381(3)	3237(2)	6609(3)	42(2)
C(35)	9746(3)	3043(2)	6543(3)	36(1)
C(36)	9010(3)	3162(2)	6362(3)	36(1)
C(37)	8146(3)	3614(2)	6015(3)	35(1)
C(38)	7923(3)	3983(2)	5763(3)	39(2)
C(39)	8271(3)	4292(2)	5633(3)	41(2)
C(40)	7928(3)	4618(2)	5379(3)	45(2)
C(41)	7163(3)	4632(2)	5249(3)	44(2)
C(42)	6828(3)	4309(2)	5395(3)	43(2)
C(43)	7198(3)	3993(2)	5647(3)	36(1)
C(44)	6978(3)	3631(2)	5830(3)	34(1)
C(45)	6649(5)	4949(2)	4906(4)	46(2)
C(46)	6430(3)	5212(2)	5375(4)	59(3)
C(47)	5966(7)	4831(2)	4435(5)	58(5)
C(48)	8420(5)	4958(2)	5327(5)	46(2)
C(49)	8601(8)	4906(4)	4726(6)	61(4)
C(50)	9119(10)	5018(6)	5819(8)	50(5)
F(38)	8090(3)	5299(2)	5290(4)	58(2)
F(39)	9011(5)	5203(3)	4669(5)	86(3)
F(40)	8027(4)	4908(2)	4278(4)	77(2)
F(41)	8940(8)	4596(4)	4713(6)	75(4)
F(42)	9270(5)	5393(2)	5872(5)	72(3)

F(43)	9026(6)	4920(3)	6352(5)	58(3)
F(44)	9682(3)	4843(2)	5773(4)	60(2)
F(45)	6973(4)	5190(2)	4632(4)	62(2)
F(46)	6998(3)	5396(2)	5701(3)	73(2)
F(47)	5946(4)	5461(2)	5088(4)	74(3)
F(48)	6160(4)	5003(3)	5720(4)	61(3)
F(49)	6093(5)	4508(2)	4203(4)	79(3)
F(50)	5806(5)	5087(3)	4011(4)	97(4)
F(51)	5395(4)	4782(2)	4612(4)	71(2)
C(45A)	6667(8)	4983(3)	5038(7)	46(2)
C(46A)	6189(9)	5065(4)	5458(9)	120(20)
C(47A)	6249(8)	4946(4)	4397(8)	130(20)
C(48A)	8386(8)	4898(4)	5129(7)	46(2)
C(49A)	8986(12)	4734(7)	4873(11)	100(20)
C(50A)	8723(14)	5175(7)	5628(12)	100(13)
F(38A)	7959(7)	5111(4)	4692(9)	81(6)
F(39A)	8768(12)	4394(5)	4632(10)	86(7)
F(40A)	9603(6)	4687(5)	5257(8)	84(6)
F(41A)	9036(11)	4959(7)	4465(11)	115(9)
F(42A)	9157(14)	5414(6)	5448(14)	134(11)
F(43A)	9163(13)	4985(7)	6108(10)	75(10)
F(44A)	8270(12)	5373(5)	5805(11)	122(8)
F(45A)	7062(10)	5291(4)	5094(12)	104(8)
F(46A)	5554(8)	4904(5)	5252(12)	220(20)
F(47A)	6115(13)	5439(4)	5460(13)	164(17)
F(48A)	6494(14)	4945(7)	6001(9)	157(14)
F(49A)	6680(9)	4934(5)	4065(9)	130(9)
F(50A)	5839(11)	5249(4)	4239(13)	180(20)
F(51A)	5834(10)	4644(5)	4273(13)	154(18)
C(51)	12147(3)	3249(2)	7387(3)	44(2)
C(52)	12802(4)	3493(2)	7478(4)	57(2)
C(53)	11740(4)	3473(2)	6343(4)	61(2)
F(1)	4847(2)	2302(1)	6567(2)	56(1)
F(2)	4758(2)	3633(1)	5425(2)	56(1)
F(3)	2865(2)	3168(1)	5391(2)	66(1)
F(4)	3756(3)	3213(1)	4572(2)	77(1)
F(5)	3621(2)	3811(1)	4683(2)	70(1)
F(6)	2720(3)	3449(1)	4465(2)	85(2)
F(7)	3839(2)	4008(1)	5789(2)	68(1)
F(8)	2711(2)	3906(1)	5467(3)	84(2)
F(9)	3326(2)	3679(1)	6299(2)	71(1)
F(10)	3080(2)	2952(1)	6349(2)	64(1)
F(11)	2880(4)	2414(2)	5500(3)	125(3)
F(12)	2641(3)	2241(2)	6273(4)	124(3)

F(13)	3556(2)	2032(1)	6090(2)	77(2)
F(14)	3258(3)	2626(2)	7248(3)	99(2)
F(15)	4048(3)	2236(2)	7190(2)	82(2)
F(16)	4308(3)	2818(2)	7334(2)	85(2)
F(17)	6188(2)	1551(1)	6992(2)	52(1)
F(18)	9023(2)	1455(1)	7302(2)	50(1)
F(19)	7095(3)	533(1)	7507(3)	101(2)
F(20)	6179(3)	899(2)	6404(3)	93(2)
F(21)	5485(3)	966(1)	6944(3)	89(2)
F(22)	5926(3)	430(1)	6874(4)	130(3)
F(23)	6198(3)	1263(2)	8011(3)	92(2)
F(24)	6099(3)	659(2)	8071(4)	132(3)
F(25)	7100(3)	930(2)	8480(3)	116(2)
F(26)	8181(3)	689(2)	8174(3)	94(2)
F(27)	9345(3)	828(2)	8766(3)	107(2)
F(28)	9754(2)	1071(2)	8119(3)	83(2)
F(29)	9029(2)	1392(2)	8467(2)	74(1)
F(30)	9093(3)	722(1)	7110(3)	94(2)
F(31)	8177(3)	393(1)	7110(4)	117(2)
F(32)	9151(3)	321(2)	7807(4)	129(3)
F(33)	10377(2)	3614(1)	6521(2)	55(1)
F(34)	10415(2)	2085(1)	6921(2)	48(1)
F(35)	11617(2)	2459(1)	6987(2)	48(1)
F(36)	6126(2)	4311(1)	5281(2)	58(1)
F(37)	8980(2)	4269(1)	5748(2)	50(1)
C(1S)	7090(7)	3207(3)	4597(5)	115(5)
C(2S)	7776(5)	3320(3)	4620(5)	110(6)
C(3S)	7884(5)	3667(3)	4381(5)	111(5)
C(4S)	7308(7)	3900(3)	4118(4)	108(5)
C(5S)	6622(5)	3786(4)	4095(5)	120(5)
C(6S)	6513(5)	3440(4)	4334(5)	114(5)
C(7S)	5743(7)	3342(8)	4288(10)	155(9)
C(8S)	7186(13)	3491(5)	4435(11)	69(8)
C(9S)	7815(10)	3286(7)	4641(11)	82(12)
C(10S)	7803(10)	2925(7)	4873(10)	79(9)
C(11S)	7162(13)	2769(5)	4898(9)	62(7)
C(12S)	6534(10)	2974(6)	4692(10)	63(7)
C(13S)	6546(10)	3336(6)	4461(11)	57(8)
C(14S)	5848(13)	3552(8)	4230(20)	89(13)
C(1T)	971(5)	3037(3)	5047(5)	139(5)
C(2T)	917(5)	2688(3)	5304(4)	134(4)
C(3T)	255(6)	2554(2)	5313(4)	114(4)
C(4T)	-353(5)	2768(3)	5065(4)	137(4)
C(5T)	-300(5)	3117(3)	4807(5)	190(7)

C(6T)	362(7)	3251(2)	4798(5)	175(7)
C(7T)	429(13)	3651(5)	4578(12)	301(16)
C(1E)	7903(12)	5486(3)	2133(6)	153(7)
C(2E)	7223(9)	5452(3)	2194(7)	220(14)
C(3E)	7128(9)	5466(3)	2749(10)	290(20)
C(4E)	7711(13)	5512(3)	3242(6)	187(10)
C(5E)	8391(10)	5545(3)	3181(6)	192(11)
C(6E)	8487(8)	5532(3)	2626(9)	169(8)
C(7E)	9223(10)	5617(7)	2567(13)	272(14)
C(1K)	4908(15)	4436(3)	7526(9)	83(7)
C(2K)	5174(12)	4362(4)	7058(8)	104(10)
C(3K)	5314(12)	3990(5)	6929(9)	84(8)
C(4K)	5190(20)	3693(3)	7268(14)	100(16)
C(5K)	4923(19)	3767(4)	7737(12)	74(10)
C(6K)	4783(11)	4139(5)	7866(8)	82(7)
C(7K)	4472(12)	4210(7)	8372(9)	98(7)
O(2)	7416(8)	2659(4)	5459(7)	97(5)

Table X.3 Bond lengths [Å] and angles [°] for **[(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**.

Co-N(3)	1.918(5)	Co-N(2)	1.929(5)
Co-N(1)	1.921(5)	Co-O(1)#1	2.133(5)
Co-N(4)	1.924(5)	Co-O(2)	2.175(15)
N(1)-C(1)	1.374(8)	N(12)-C(53)	1.473(9)
N(1)-C(8)	1.380(7)	O(1)-C(51)	1.194(8)
N(2)-C(22)	1.354(7)	C(1)-C(2)	1.447(8)
N(2)-C(15)	1.372(7)	C(2)-C(7)	1.357(9)
N(3)-C(36)	1.369(7)	C(2)-C(3)	1.396(9)
N(3)-C(29)	1.372(7)	C(3)-F(2)	1.331(7)
N(4)-C(37)	1.362(7)	C(3)-C(4)	1.400(9)
N(4)-C(44)	1.373(8)	C(4)-C(5)	1.442(9)
N(5)-C(44)	1.318(7)	C(4)-C(9)	1.549(9)
N(5)-C(1)	1.320(8)	C(5)-C(6)	1.364(9)
N(6)-C(15)	1.303(8)	C(5)-C(12)	1.553(9)
N(6)-C(8)	1.318(8)	C(6)-F(1)	1.351(7)
N(7)-C(29)	1.322(7)	C(6)-C(7)	1.398(8)
N(7)-C(22)	1.323(7)	C(7)-C(8)	1.444(8)
N(8)-C(36)	1.307(8)	C(9)-F(3)	1.365(7)
N(8)-C(37)	1.328(8)	C(9)-C(11)	1.518(11)
N(12)-C(51)	1.359(9)	C(9)-C(10)	1.567(12)
N(12)-C(33)	1.424(8)	C(10)-F(5)	1.316(8)

C(10)-F(6)	1.321(8)	C(29)-C(30)	1.468(8)
C(10)-F(4)	1.345(10)	C(30)-C(31)	1.374(9)
C(11)-F(8)	1.324(8)	C(30)-C(35)	1.391(9)
C(11)-F(7)	1.329(8)	C(31)-F(34)	1.336(7)
C(11)-F(9)	1.352(9)	C(31)-C(32)	1.385(9)
C(12)-F(10)	1.366(8)	C(32)-F(35)	1.344(7)
C(12)-C(13)	1.527(11)	C(32)-C(33)	1.398(9)
C(12)-C(14)	1.564(12)	C(33)-C(34)	1.369(9)
C(13)-F(11)	1.287(11)	C(34)-F(33)	1.344(7)
C(13)-F(13)	1.289(10)	C(34)-C(35)	1.389(8)
C(13)-F(12)	1.344(10)	C(35)-C(36)	1.444(8)
C(14)-F(16)	1.306(9)	C(37)-C(38)	1.446(9)
C(14)-F(15)	1.313(9)	C(38)-C(43)	1.369(8)
C(14)-F(14)	1.327(9)	C(38)-C(39)	1.371(9)
C(15)-C(16)	1.454(8)	C(39)-F(37)	1.339(7)
C(16)-C(17)	1.378(8)	C(39)-C(40)	1.378(9)
C(16)-C(21)	1.383(8)	C(40)-C(41)	1.445(9)
C(17)-F(17)	1.348(7)	C(40)-C(48A)	1.565(7)
C(17)-C(18)	1.381(9)	C(40)-C(48)	1.566(7)
C(18)-C(19)	1.430(10)	C(41)-C(42)	1.407(8)
C(18)-C(23)	1.548(9)	C(41)-C(45A)	1.565(7)
C(19)-C(20)	1.393(9)	C(41)-C(45)	1.566(7)
C(19)-C(26)	1.558(10)	C(42)-F(36)	1.324(7)
C(20)-F(18)	1.337(7)	C(42)-C(43)	1.367(9)
C(20)-C(21)	1.382(9)	C(43)-C(44)	1.454(8)
C(21)-C(22)	1.458(8)	C(45)-F(45)	1.341(10)
C(23)-F(19)	1.373(8)	C(45)-C(47)	1.533(17)
C(23)-C(25)	1.507(15)	C(45)-C(46)	1.607(15)
C(23)-C(24)	1.581(14)	C(46)-F(46)	1.326(6)
C(24)-F(21)	1.303(11)	C(46)-F(47)	1.326(6)
C(24)-F(22)	1.306(10)	C(46)-F(48)	1.326(6)
C(24)-F(20)	1.373(12)	C(47)-F(49)	1.321(7)
C(25)-F(23)	1.307(12)	C(47)-F(51)	1.321(7)
C(25)-F(24)	1.330(10)	C(47)-F(50)	1.321(7)
C(25)-F(25)	1.360(12)	C(48)-F(38)	1.355(11)
C(26)-F(26)	1.369(9)	C(48)-C(50)	1.54(2)
C(26)-C(28)	1.515(14)	C(48)-C(49)	1.585(16)
C(26)-C(27)	1.553(14)	C(49)-F(41)	1.283(17)
C(27)-F(27)	1.323(9)	C(49)-F(40)	1.305(15)
C(27)-F(29)	1.339(11)	C(49)-F(39)	1.351(15)
C(27)-F(28)	1.340(9)	C(50)-F(44)	1.30(2)
C(28)-F(31)	1.327(13)	C(50)-F(42)	1.35(2)
C(28)-F(32)	1.330(11)	C(50)-F(43)	1.38(2)
C(28)-F(30)	1.343(12)	C(45A)-F(45A)	1.318(16)

C(45A)-C(47A)	1.513(19)	C(10S)-C(11S)	1.3900
C(45A)-C(46A)	1.587(19)	C(10S)-H(10A)	0.9500
C(46A)-F(46A)	1.326(6)	C(11S)-C(12S)	1.3900
C(46A)-F(48A)	1.326(6)	C(11S)-H(11A)	0.9500
C(46A)-F(47A)	1.326(6)	C(12S)-C(13S)	1.3900
C(47A)-F(51A)	1.321(7)	C(12S)-H(12A)	0.9500
C(47A)-F(49A)	1.321(7)	C(13S)-C(14S)	1.524(10)
C(47A)-F(50A)	1.321(7)	C(14S)-H(14A)	0.9800
C(48A)-F(38A)	1.356(16)	C(14S)-H(14B)	0.9800
C(48A)-C(50A)	1.53(2)	C(14S)-H(14C)	0.9800
C(48A)-C(49A)	1.59(2)	C(1T)-C(2T)	1.3900
C(49A)-F(41A)	1.28(2)	C(1T)-C(6T)	1.3900
C(49A)-F(40A)	1.30(2)	C(1T)-H(1TA)	0.9500
C(49A)-F(39A)	1.34(2)	C(2T)-C(3T)	1.3900
C(50A)-F(44A)	1.30(2)	C(2T)-H(2TA)	0.9500
C(50A)-F(42A)	1.35(2)	C(3T)-C(4T)	1.3900
C(50A)-F(43A)	1.39(2)	C(3T)-H(3TA)	0.9500
C(51)-C(52)	1.507(9)	C(4T)-C(5T)	1.3900
C(52)-H(52A)	0.9800	C(4T)-H(4TA)	0.9500
C(52)-H(52B)	0.9800	C(5T)-C(6T)	1.3900
C(52)-H(52C)	0.9800	C(5T)-H(5TA)	0.9500
C(53)-H(53A)	0.9800	C(6T)-C(7T)	1.524(10)
C(53)-H(53B)	0.9800	C(7T)-H(7TA)	0.9800
C(53)-H(53C)	0.9800	C(7T)-H(7TB)	0.9800
C(1S)-C(2S)	1.3900	C(7T)-H(7TC)	0.9800
C(1S)-C(6S)	1.3900	C(1E)-C(2E)	1.3900
C(1S)-H(1SA)	0.9500	C(1E)-C(6E)	1.3900
C(2S)-C(3S)	1.3900	C(1E)-H(1EA)	0.9500
C(2S)-H(2SA)	0.9500	C(2E)-C(3E)	1.3900
C(3S)-C(4S)	1.3900	C(2E)-H(2EA)	0.9500
C(3S)-H(3SA)	0.9500	C(3E)-C(4E)	1.3900
C(4S)-C(5S)	1.3900	C(3E)-H(3EA)	0.9500
C(4S)-H(4SA)	0.9500	C(4E)-C(5E)	1.3900
C(5S)-C(6S)	1.3900	C(4E)-H(4EA)	0.9500
C(5S)-H(5SA)	0.9500	C(5E)-C(6E)	1.3900
C(6S)-C(7S)	1.524(10)	C(5E)-H(5EA)	0.9500
C(7S)-H(7SA)	0.9800	C(6E)-C(7E)	1.523(10)
C(7S)-H(7SB)	0.9800	C(7E)-H(7EA)	0.9800
C(7S)-H(7SC)	0.9800	C(7E)-H(7EB)	0.9800
C(8S)-C(9S)	1.3900	C(7E)-H(7EC)	0.9800
C(8S)-C(13S)	1.3900	C(1K)-C(2K)	1.3900
C(8S)-H(8SA)	0.9500	C(1K)-C(6K)	1.3900
C(9S)-C(10S)	1.3900	C(1K)-H(1KA)	0.9500
C(9S)-H(9SA)	0.9500	C(2K)-C(3K)	1.3900

C(2K)-H(2KA)	0.9500	C(6K)-C(7K)	1.524(10)
C(3K)-C(4K)	1.3900	C(7K)-H(7KA)	0.9800
C(3K)-H(3KA)	0.9500	C(7K)-H(7KB)	0.9800
C(4K)-C(5K)	1.3900	C(7K)-H(7KC)	0.9800
C(4K)-H(4KA)	0.9500	O(2)-H(2A)	0.840(2)
C(5K)-C(6K)	1.3900	O(2)-H(2B)	0.840(2)
C(5K)-H(5KA)	0.9500		

N(3)-Co-N(1)	176.4(2)	N(4)-Co-O(1)#1	93.7(2)
N(3)-Co-N(4)	89.8(2)	N(2)-Co-O(1)#1	88.81(19)
N(1)-Co-N(4)	90.0(2)	N(3)-Co-O(2)	86.1(4)
N(3)-Co-N(2)	90.1(2)	N(1)-Co-O(2)	90.3(4)
N(1)-Co-N(2)	89.9(2)	N(4)-Co-O(2)	92.2(4)
N(4)-Co-N(2)	177.4(2)	N(2)-Co-O(2)	85.2(4)
N(3)-Co-O(1)#1	82.91(19)	O(1)#1-Co-O(2)	167.5(4)
N(1)-Co-O(1)#1	100.73(19)		

C(1)-N(1)-C(8)	107.6(5)	F(2)-C(3)-C(4)	119.4(6)
C(1)-N(1)-Co	125.9(4)	C(2)-C(3)-C(4)	122.1(6)
C(8)-N(1)-Co	126.5(4)	C(3)-C(4)-C(5)	117.4(6)
C(22)-N(2)-C(15)	108.9(5)	C(3)-C(4)-C(9)	114.8(6)
C(22)-N(2)-Co	125.9(4)	C(5)-C(4)-C(9)	127.5(5)
C(15)-N(2)-Co	125.0(4)	C(6)-C(5)-C(4)	117.2(6)
C(36)-N(3)-C(29)	107.7(5)	C(6)-C(5)-C(12)	116.9(6)
C(36)-N(3)-Co	125.6(4)	C(4)-C(5)-C(12)	125.7(6)
C(29)-N(3)-Co	126.0(4)	F(1)-C(6)-C(5)	119.3(5)
C(37)-N(4)-C(44)	107.6(5)	F(1)-C(6)-C(7)	116.6(6)
C(37)-N(4)-Co	126.2(4)	C(5)-C(6)-C(7)	123.8(6)
C(44)-N(4)-Co	126.1(4)	C(2)-C(7)-C(6)	118.7(6)
C(44)-N(5)-C(1)	120.5(5)	C(2)-C(7)-C(8)	106.8(5)
C(15)-N(6)-C(8)	121.4(5)	C(6)-C(7)-C(8)	134.5(6)
C(29)-N(7)-C(22)	120.8(5)	N(6)-C(8)-N(1)	127.3(5)
C(36)-N(8)-C(37)	121.2(5)	N(6)-C(8)-C(7)	123.7(5)
C(51)-N(12)-C(33)	117.9(5)	N(1)-C(8)-C(7)	109.1(5)
C(51)-N(12)-C(53)	124.5(6)	F(3)-C(9)-C(11)	105.7(6)
C(33)-N(12)-C(53)	117.5(6)	F(3)-C(9)-C(4)	109.8(5)
C(51)-O(1)-Co#1	146.4(5)	C(11)-C(9)-C(4)	112.6(6)
N(5)-C(1)-N(1)	128.9(5)	F(3)-C(9)-C(10)	102.2(6)
N(5)-C(1)-C(2)	122.7(6)	C(11)-C(9)-C(10)	109.7(6)
N(1)-C(1)-C(2)	108.4(5)	C(4)-C(9)-C(10)	115.8(6)
C(7)-C(2)-C(3)	119.7(6)	F(5)-C(10)-F(6)	106.9(6)
C(7)-C(2)-C(1)	108.0(6)	F(5)-C(10)-F(4)	107.8(7)
C(3)-C(2)-C(1)	132.3(6)	F(6)-C(10)-F(4)	107.1(7)
F(2)-C(3)-C(2)	118.5(6)	F(5)-C(10)-C(9)	115.1(7)

F(6)-C(10)-C(9)	109.1(7)	C(20)-C(21)-C(16)	118.3(6)
F(4)-C(10)-C(9)	110.4(6)	C(20)-C(21)-C(22)	134.9(6)
F(8)-C(11)-F(7)	108.4(6)	C(16)-C(21)-C(22)	106.7(5)
F(8)-C(11)-F(9)	106.9(6)	N(7)-C(22)-N(2)	128.8(5)
F(7)-C(11)-F(9)	105.4(7)	N(7)-C(22)-C(21)	122.1(5)
F(8)-C(11)-C(9)	111.3(7)	N(2)-C(22)-C(21)	109.1(5)
F(7)-C(11)-C(9)	113.5(6)	F(19)-C(23)-C(25)	108.7(8)
F(9)-C(11)-C(9)	111.1(6)	F(19)-C(23)-C(18)	109.3(6)
F(10)-C(12)-C(13)	106.6(6)	C(25)-C(23)-C(18)	113.8(8)
F(10)-C(12)-C(5)	109.5(5)	F(19)-C(23)-C(24)	101.1(7)
C(13)-C(12)-C(5)	114.8(7)	C(25)-C(23)-C(24)	108.6(8)
F(10)-C(12)-C(14)	101.2(6)	C(18)-C(23)-C(24)	114.5(7)
C(13)-C(12)-C(14)	108.8(6)	F(21)-C(24)-F(22)	107.5(7)
C(5)-C(12)-C(14)	114.9(6)	F(21)-C(24)-F(20)	106.5(9)
F(11)-C(13)-F(13)	110.0(9)	F(22)-C(24)-F(20)	105.6(10)
F(11)-C(13)-F(12)	107.3(8)	F(21)-C(24)-C(23)	115.5(9)
F(13)-C(13)-F(12)	106.0(7)	F(22)-C(24)-C(23)	110.9(9)
F(11)-C(13)-C(12)	110.7(7)	F(20)-C(24)-C(23)	110.3(7)
F(13)-C(13)-C(12)	113.5(6)	F(23)-C(25)-F(24)	108.8(8)
F(12)-C(13)-C(12)	109.1(8)	F(23)-C(25)-F(25)	107.1(10)
F(16)-C(14)-F(15)	107.9(7)	F(24)-C(25)-F(25)	105.7(8)
F(16)-C(14)-F(14)	107.5(8)	F(23)-C(25)-C(23)	114.7(8)
F(15)-C(14)-F(14)	106.0(6)	F(24)-C(25)-C(23)	110.7(10)
F(16)-C(14)-C(12)	111.1(6)	F(25)-C(25)-C(23)	109.5(8)
F(15)-C(14)-C(12)	115.8(7)	F(26)-C(26)-C(28)	106.2(7)
F(14)-C(14)-C(12)	108.2(6)	F(26)-C(26)-C(27)	100.9(8)
N(6)-C(15)-N(2)	129.5(6)	C(28)-C(26)-C(27)	111.7(8)
N(6)-C(15)-C(16)	121.7(5)	F(26)-C(26)-C(19)	109.3(6)
N(2)-C(15)-C(16)	108.8(5)	C(28)-C(26)-C(19)	113.0(9)
C(17)-C(16)-C(21)	119.8(6)	C(27)-C(26)-C(19)	114.7(7)
C(17)-C(16)-C(15)	133.5(6)	F(27)-C(27)-F(29)	107.0(9)
C(21)-C(16)-C(15)	106.6(5)	F(27)-C(27)-F(28)	105.4(6)
F(17)-C(17)-C(16)	117.4(5)	F(29)-C(27)-F(28)	107.9(7)
F(17)-C(17)-C(18)	119.3(5)	F(27)-C(27)-C(26)	110.2(7)
C(16)-C(17)-C(18)	123.3(6)	F(29)-C(27)-C(26)	111.9(7)
C(17)-C(18)-C(19)	117.0(6)	F(28)-C(27)-C(26)	114.0(8)
C(17)-C(18)-C(23)	115.5(6)	F(31)-C(28)-F(32)	108.0(8)
C(19)-C(18)-C(23)	127.5(6)	F(31)-C(28)-F(30)	106.6(11)
C(20)-C(19)-C(18)	118.5(6)	F(32)-C(28)-F(30)	107.7(8)
C(20)-C(19)-C(26)	114.6(6)	F(31)-C(28)-C(26)	112.2(8)
C(18)-C(19)-C(26)	126.7(6)	F(32)-C(28)-C(26)	109.9(10)
F(18)-C(20)-C(21)	117.4(5)	F(30)-C(28)-C(26)	112.1(7)
F(18)-C(20)-C(19)	119.9(6)	N(7)-C(29)-N(3)	128.2(5)
C(21)-C(20)-C(19)	122.6(6)	N(7)-C(29)-C(30)	122.2(5)

N(3)-C(29)-C(30)	109.4(5)	C(42)-C(43)-C(38)	119.9(5)
C(31)-C(30)-C(35)	120.3(6)	C(42)-C(43)-C(44)	132.7(6)
C(31)-C(30)-C(29)	133.9(6)	C(38)-C(43)-C(44)	107.4(5)
C(35)-C(30)-C(29)	105.8(5)	N(5)-C(44)-N(4)	128.6(5)
F(34)-C(31)-C(30)	122.6(5)	N(5)-C(44)-C(43)	122.8(5)
F(34)-C(31)-C(32)	119.1(5)	N(4)-C(44)-C(43)	108.6(5)
C(30)-C(31)-C(32)	118.2(6)	F(45)-C(45)-C(47)	104.7(7)
F(35)-C(32)-C(31)	118.1(6)	F(45)-C(45)-C(41)	112.5(7)
F(35)-C(32)-C(33)	119.3(6)	C(47)-C(45)-C(41)	118.7(7)
C(31)-C(32)-C(33)	122.6(6)	F(45)-C(45)-C(46)	103.7(7)
C(34)-C(33)-C(32)	117.9(6)	C(47)-C(45)-C(46)	108.1(6)
C(34)-C(33)-N(12)	120.1(6)	C(41)-C(45)-C(46)	108.2(7)
C(32)-C(33)-N(12)	122.0(6)	F(46)-C(46)-F(47)	109.4(6)
F(33)-C(34)-C(33)	119.2(5)	F(46)-C(46)-F(48)	109.3(6)
F(33)-C(34)-C(35)	120.2(6)	F(47)-C(46)-F(48)	109.3(6)
C(33)-C(34)-C(35)	120.6(6)	F(46)-C(46)-C(45)	109.8(8)
C(34)-C(35)-C(30)	120.3(6)	F(47)-C(46)-C(45)	108.7(8)
C(34)-C(35)-C(36)	132.8(6)	F(48)-C(46)-C(45)	110.3(8)
C(30)-C(35)-C(36)	106.9(5)	F(49)-C(47)-F(51)	107.6(7)
N(8)-C(36)-N(3)	128.4(5)	F(49)-C(47)-F(50)	107.5(7)
N(8)-C(36)-C(35)	121.6(5)	F(51)-C(47)-F(50)	107.5(7)
N(3)-C(36)-C(35)	109.9(5)	F(49)-C(47)-C(45)	107.8(8)
N(8)-C(37)-N(4)	127.6(6)	F(51)-C(47)-C(45)	116.4(9)
N(8)-C(37)-C(38)	122.2(5)	F(50)-C(47)-C(45)	109.6(9)
N(4)-C(37)-C(38)	110.1(5)	F(38)-C(48)-C(50)	103.4(10)
C(43)-C(38)-C(39)	119.4(6)	F(38)-C(48)-C(40)	112.7(7)
C(43)-C(38)-C(37)	106.2(5)	C(50)-C(48)-C(40)	118.6(10)
C(39)-C(38)-C(37)	134.4(6)	F(38)-C(48)-C(49)	105.9(9)
F(37)-C(39)-C(38)	117.5(6)	C(50)-C(48)-C(49)	108.6(9)
F(37)-C(39)-C(40)	119.1(5)	C(40)-C(48)-C(49)	106.9(8)
C(38)-C(39)-C(40)	123.4(6)	F(41)-C(49)-F(40)	108.4(12)
C(39)-C(40)-C(41)	117.7(5)	F(41)-C(49)-F(39)	109.1(13)
C(39)-C(40)-C(48A)	115.4(8)	F(40)-C(49)-F(39)	108.0(11)
C(41)-C(40)-C(48A)	125.3(8)	F(41)-C(49)-C(48)	112.1(10)
C(39)-C(40)-C(48)	115.9(6)	F(40)-C(49)-C(48)	111.6(11)
C(41)-C(40)-C(48)	125.9(6)	F(39)-C(49)-C(48)	107.5(11)
C(42)-C(41)-C(40)	117.0(5)	F(44)-C(50)-F(42)	107.7(13)
C(42)-C(41)-C(45A)	115.4(8)	F(44)-C(50)-F(43)	107.8(16)
C(40)-C(41)-C(45A)	127.2(8)	F(42)-C(50)-F(43)	104.1(15)
C(42)-C(41)-C(45)	115.5(6)	F(44)-C(50)-C(48)	117.5(14)
C(40)-C(41)-C(45)	127.2(6)	F(42)-C(50)-C(48)	109.2(15)
F(36)-C(42)-C(43)	118.8(5)	F(43)-C(50)-C(48)	109.8(14)
F(36)-C(42)-C(41)	118.6(5)	F(45A)-C(45A)-C(47A)	107.6(15)
C(43)-C(42)-C(41)	122.6(6)	F(45A)-C(45A)-C(41)	109.1(12)

C(47A)-C(45A)-C(41)	111.0(10)	N(12)-C(53)-H(53B)	109.5
F(45A)-C(45A)-C(46A)	103.2(13)	H(53A)-C(53)-H(53B)	109.5
C(47A)-C(45A)-C(46A)	114.0(12)	N(12)-C(53)-H(53C)	109.5
C(41)-C(45A)-C(46A)	111.5(10)	H(53A)-C(53)-H(53C)	109.5
F(46A)-C(46A)-F(48A)	109.4(6)	H(53B)-C(53)-H(53C)	109.5
F(46A)-C(46A)-F(47A)	109.4(6)	C(2S)-C(1S)-C(6S)	120.0
F(48A)-C(46A)-F(47A)	109.4(6)	C(2S)-C(1S)-H(1SA)	120.0
F(46A)-C(46A)-C(45A)	110.9(13)	C(6S)-C(1S)-H(1SA)	120.0
F(48A)-C(46A)-C(45A)	112.2(14)	C(3S)-C(2S)-C(1S)	120.0
F(47A)-C(46A)-C(45A)	105.5(13)	C(3S)-C(2S)-H(2SA)	120.0
F(51A)-C(47A)-F(49A)	107.5(7)	C(1S)-C(2S)-H(2SA)	120.0
F(51A)-C(47A)-F(50A)	107.5(7)	C(2S)-C(3S)-C(4S)	120.0
F(49A)-C(47A)-F(50A)	107.5(7)	C(2S)-C(3S)-H(3SA)	120.0
F(51A)-C(47A)-C(45A)	114.3(16)	C(4S)-C(3S)-H(3SA)	120.0
F(49A)-C(47A)-C(45A)	110.8(14)	C(3S)-C(4S)-C(5S)	120.0
F(50A)-C(47A)-C(45A)	108.9(15)	C(3S)-C(4S)-H(4SA)	120.0
F(38A)-C(48A)-C(50A)	105.8(16)	C(5S)-C(4S)-H(4SA)	120.0
F(38A)-C(48A)-C(40)	110.2(11)	C(6S)-C(5S)-C(4S)	120.0
C(50A)-C(48A)-C(40)	105.7(13)	C(6S)-C(5S)-H(5SA)	120.0
F(38A)-C(48A)-C(49A)	105.7(13)	C(4S)-C(5S)-H(5SA)	120.0
C(50A)-C(48A)-C(49A)	109.3(14)	C(5S)-C(6S)-C(1S)	120.0
C(40)-C(48A)-C(49A)	119.5(14)	C(5S)-C(6S)-C(7S)	116.0(14)
F(41A)-C(49A)-F(40A)	110(2)	C(1S)-C(6S)-C(7S)	124.0(14)
F(41A)-C(49A)-F(39A)	108(2)	C(6S)-C(7S)-H(7SA)	109.5
F(40A)-C(49A)-F(39A)	108(2)	C(6S)-C(7S)-H(7SB)	109.5
F(41A)-C(49A)-C(48A)	107.3(16)	H(7SA)-C(7S)-H(7SB)	109.5
F(40A)-C(49A)-C(48A)	115.0(19)	C(6S)-C(7S)-H(7SC)	109.5
F(39A)-C(49A)-C(48A)	108.0(19)	H(7SA)-C(7S)-H(7SC)	109.5
F(44A)-C(50A)-F(42A)	109(2)	H(7SB)-C(7S)-H(7SC)	109.5
F(44A)-C(50A)-F(43A)	108(2)	C(9S)-C(8S)-C(13S)	120.0
F(42A)-C(50A)-F(43A)	105(2)	C(9S)-C(8S)-H(8SA)	120.0
F(44A)-C(50A)-C(48A)	115(2)	C(13S)-C(8S)-H(8SA)	120.0
F(42A)-C(50A)-C(48A)	109(2)	C(8S)-C(9S)-C(10S)	120.0
F(43A)-C(50A)-C(48A)	111(2)	C(8S)-C(9S)-H(9SA)	120.0
O(1)-C(51)-N(12)	119.9(6)	C(10S)-C(9S)-H(9SA)	120.0
O(1)-C(51)-C(52)	122.5(7)	C(11S)-C(10S)-C(9S)	120.0
N(12)-C(51)-C(52)	117.6(6)	C(11S)-C(10S)-H(10A)	120.0
C(51)-C(52)-H(52A)	109.5	C(9S)-C(10S)-H(10A)	120.0
C(51)-C(52)-H(52B)	109.5	C(12S)-C(11S)-C(10S)	120.0
H(52A)-C(52)-H(52B)	109.5	C(12S)-C(11S)-H(11A)	120.0
C(51)-C(52)-H(52C)	109.5	C(10S)-C(11S)-H(11A)	120.0
H(52A)-C(52)-H(52C)	109.5	C(11S)-C(12S)-C(13S)	120.0
H(52B)-C(52)-H(52C)	109.5	C(11S)-C(12S)-H(12A)	120.0
N(12)-C(53)-H(53A)	109.5	C(13S)-C(12S)-H(12A)	120.0

C(12S)-C(13S)-C(8S)	120.0	C(3E)-C(4E)-C(5E)	120.0
C(12S)-C(13S)-C(14S)	119(2)	C(3E)-C(4E)-H(4EA)	120.0
C(8S)-C(13S)-C(14S)	121(2)	C(5E)-C(4E)-H(4EA)	120.0
C(13S)-C(14S)-H(14A)	109.5	C(6E)-C(5E)-C(4E)	120.0
C(13S)-C(14S)-H(14B)	109.5	C(6E)-C(5E)-H(5EA)	120.0
H(14A)-C(14S)-H(14B)	109.5	C(4E)-C(5E)-H(5EA)	120.0
C(13S)-C(14S)-H(14C)	109.5	C(5E)-C(6E)-C(1E)	120.0
H(14A)-C(14S)-H(14C)	109.5	C(5E)-C(6E)-C(7E)	118.7(18)
H(14B)-C(14S)-H(14C)	109.5	C(1E)-C(6E)-C(7E)	120.9(18)
C(2T)-C(1T)-C(6T)	120.0	C(6E)-C(7E)-H(7EA)	109.5
C(2T)-C(1T)-H(1TA)	120.0	C(6E)-C(7E)-H(7EB)	109.5
C(6T)-C(1T)-H(1TA)	120.0	H(7EA)-C(7E)-H(7EB)	109.5
C(1T)-C(2T)-C(3T)	120.0	C(6E)-C(7E)-H(7EC)	109.5
C(1T)-C(2T)-H(2TA)	120.0	H(7EA)-C(7E)-H(7EC)	109.5
C(3T)-C(2T)-H(2TA)	120.0	H(7EB)-C(7E)-H(7EC)	109.5
C(4T)-C(3T)-C(2T)	120.0	C(2K)-C(1K)-C(6K)	120.0
C(4T)-C(3T)-H(3TA)	120.0	C(2K)-C(1K)-H(1KA)	120.0
C(2T)-C(3T)-H(3TA)	120.0	C(6K)-C(1K)-H(1KA)	120.0
C(5T)-C(4T)-C(3T)	120.0	C(1K)-C(2K)-C(3K)	120.0
C(5T)-C(4T)-H(4TA)	120.0	C(1K)-C(2K)-H(2KA)	120.0
C(3T)-C(4T)-H(4TA)	120.0	C(3K)-C(2K)-H(2KA)	120.0
C(4T)-C(5T)-C(6T)	120.0	C(4K)-C(3K)-C(2K)	120.0
C(4T)-C(5T)-H(5TA)	120.0	C(4K)-C(3K)-H(3KA)	120.0
C(6T)-C(5T)-H(5TA)	120.0	C(2K)-C(3K)-H(3KA)	120.0
C(5T)-C(6T)-C(1T)	120.0	C(5K)-C(4K)-C(3K)	120.0
C(5T)-C(6T)-C(7T)	119.7(12)	C(5K)-C(4K)-H(4KA)	120.0
C(1T)-C(6T)-C(7T)	119.9(12)	C(3K)-C(4K)-H(4KA)	120.0
C(6T)-C(7T)-H(7TA)	109.5	C(4K)-C(5K)-C(6K)	120.0
C(6T)-C(7T)-H(7TB)	109.5	C(4K)-C(5K)-H(5KA)	120.0
H(7TA)-C(7T)-H(7TB)	109.5	C(6K)-C(5K)-H(5KA)	120.0
C(6T)-C(7T)-H(7TC)	109.5	C(5K)-C(6K)-C(1K)	120.0
H(7TA)-C(7T)-H(7TC)	109.5	C(5K)-C(6K)-C(7K)	118.8(15)
H(7TB)-C(7T)-H(7TC)	109.5	C(1K)-C(6K)-C(7K)	121.2(15)
C(2E)-C(1E)-C(6E)	120.0	C(6K)-C(7K)-H(7KA)	109.5
C(2E)-C(1E)-H(1EA)	120.0	C(6K)-C(7K)-H(7KB)	109.5
C(6E)-C(1E)-H(1EA)	120.0	H(7KA)-C(7K)-H(7KB)	109.5
C(3E)-C(2E)-C(1E)	120.0	C(6K)-C(7K)-H(7KC)	109.5
C(3E)-C(2E)-H(2EA)	120.0	H(7KA)-C(7K)-H(7KC)	109.5
C(1E)-C(2E)-H(2EA)	120.0	H(7KB)-C(7K)-H(7KC)	109.5
C(2E)-C(3E)-C(4E)	120.0	Co-O(2)-H(2A)	126(6)
C(2E)-C(3E)-H(3EA)	120.0	Co-O(2)-H(2B)	127(8)
C(4E)-C(3E)-H(3EA)	120.0	H(2A)-O(2)-H(2B)	105.8(6)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,y,-z+3/2

Table X.4 Anisotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**. 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}
Co	27(1)	28(1)	46(1)	1(1)	13(1)	-3(1)
N(1)	37(3)	25(2)	39(3)	3(2)	12(2)	-1(2)
N(2)	28(3)	30(3)	42(3)	-1(2)	11(2)	-4(2)
N(3)	33(3)	26(2)	39(3)	-1(2)	14(2)	-3(2)
N(4)	30(3)	38(3)	43(3)	-2(2)	13(2)	-5(2)
N(5)	28(3)	36(3)	51(3)	12(2)	12(2)	-2(2)
N(6)	31(3)	29(3)	57(4)	1(2)	11(2)	-6(2)
N(7)	33(3)	32(3)	47(3)	-1(2)	19(2)	1(2)
N(8)	32(3)	31(3)	50(3)	3(2)	13(2)	-4(2)
N(12)	29(3)	46(3)	55(4)	16(3)	11(3)	-2(2)
O(1)	38(2)	34(2)	48(3)	3(2)	13(2)	-3(2)
C(1)	35(3)	30(3)	48(4)	2(3)	12(3)	-4(3)
C(2)	32(3)	37(3)	50(4)	0(3)	11(3)	-7(3)
C(3)	40(4)	42(4)	53(4)	15(3)	16(3)	0(3)
C(4)	27(3)	42(4)	62(5)	5(3)	9(3)	-5(3)
C(5)	35(3)	34(3)	59(5)	8(3)	8(3)	-6(3)
C(6)	32(3)	37(4)	62(5)	9(3)	11(3)	-9(3)
C(7)	29(3)	35(3)	49(4)	2(3)	11(3)	-1(3)
C(8)	32(3)	31(3)	44(4)	3(3)	12(3)	-8(3)
C(9)	34(4)	46(4)	79(6)	12(4)	17(4)	-9(3)
C(10)	48(4)	39(4)	79(6)	11(4)	3(4)	-12(3)
C(11)	45(4)	47(4)	82(6)	22(4)	23(4)	3(3)
C(12)	26(3)	42(4)	90(6)	15(4)	16(4)	1(3)
C(13)	38(4)	62(5)	100(7)	19(5)	10(4)	-14(4)
C(14)	44(4)	59(5)	80(6)	23(4)	24(4)	-2(4)
C(15)	37(3)	29(3)	42(4)	-5(3)	15(3)	-5(3)
C(16)	38(3)	24(3)	49(4)	-5(3)	20(3)	-1(2)
C(17)	37(3)	29(3)	59(4)	1(3)	19(3)	-3(3)
C(18)	48(4)	31(3)	70(5)	5(3)	24(4)	-3(3)
C(19)	51(4)	31(3)	83(6)	10(3)	33(4)	4(3)
C(20)	41(4)	29(3)	61(5)	3(3)	26(3)	3(3)
C(21)	32(3)	29(3)	48(4)	-4(3)	16(3)	-2(2)
C(22)	38(3)	24(3)	42(4)	-4(3)	17(3)	0(2)
C(23)	48(4)	37(4)	123(8)	26(4)	32(5)	5(3)
C(24)	74(7)	44(5)	150(11)	11(6)	47(7)	-15(4)
C(25)	68(6)	85(7)	126(10)	48(7)	46(7)	-10(5)
C(26)	59(5)	44(4)	123(8)	38(5)	46(5)	8(4)
C(27)	55(5)	78(6)	99(7)	44(6)	38(5)	19(5)
C(28)	73(6)	41(5)	178(12)	20(6)	54(7)	13(5)
C(29)	27(3)	31(3)	44(4)	-4(3)	17(3)	-2(2)

C(30)	35(3)	38(3)	36(4)	-5(3)	15(3)	-5(3)
C(31)	39(4)	33(3)	51(4)	6(3)	20(3)	3(3)
C(32)	33(3)	50(4)	43(4)	5(3)	19(3)	8(3)
C(33)	36(3)	41(4)	43(4)	5(3)	13(3)	-4(3)
C(34)	34(3)	37(3)	54(4)	6(3)	11(3)	-2(3)
C(35)	28(3)	36(3)	46(4)	3(3)	13(3)	-2(3)
C(36)	32(3)	32(3)	45(4)	1(3)	12(3)	1(3)
C(37)	30(3)	34(3)	45(4)	2(3)	15(3)	-4(3)
C(38)	36(3)	31(3)	52(4)	0(3)	18(3)	0(3)
C(39)	33(3)	38(4)	56(4)	-1(3)	19(3)	-4(3)
C(40)	45(4)	29(3)	65(5)	4(3)	26(3)	-2(3)
C(41)	45(4)	26(3)	67(5)	3(3)	26(3)	-2(3)
C(42)	33(3)	34(3)	65(5)	8(3)	20(3)	-1(3)
C(43)	35(3)	29(3)	46(4)	1(3)	14(3)	-8(3)
C(44)	29(3)	29(3)	47(4)	0(3)	13(3)	-3(2)
C(45)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(46)	48(8)	36(7)	98(11)	-4(7)	30(7)	-4(6)
C(47)	66(12)	37(9)	65(9)	7(8)	8(8)	9(9)
C(48)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(49)	56(9)	75(9)	60(9)	19(7)	28(8)	-2(7)
C(50)	47(10)	42(8)	62(15)	5(10)	17(10)	-17(7)
F(38)	51(4)	29(3)	100(6)	10(4)	31(4)	3(3)
F(39)	79(6)	86(7)	109(8)	31(6)	54(5)	-18(6)
F(40)	79(6)	91(6)	68(5)	23(5)	31(5)	3(4)
F(41)	97(10)	58(7)	93(8)	13(7)	62(7)	12(7)
F(42)	59(5)	46(5)	107(7)	-7(5)	20(5)	-19(3)
F(43)	56(5)	63(5)	60(7)	0(5)	25(4)	-7(4)
F(44)	40(4)	51(4)	98(6)	7(4)	33(4)	-5(3)
F(45)	55(4)	43(4)	92(6)	33(4)	27(4)	8(3)
F(46)	62(5)	57(4)	103(6)	-24(4)	32(4)	-9(4)
F(47)	57(5)	40(4)	127(9)	12(4)	29(5)	18(3)
F(48)	59(6)	50(5)	88(7)	5(5)	45(5)	0(4)
F(49)	82(7)	71(6)	67(5)	-10(5)	-2(5)	0(5)
F(50)	78(7)	93(9)	97(7)	50(7)	-11(5)	-6(6)
F(51)	36(4)	48(4)	116(7)	21(4)	4(4)	4(3)
C(45A)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(46A)	80(30)	50(20)	270(70)	50(30)	130(40)	18(17)
C(47A)	60(30)	90(30)	200(60)	70(30)	-20(30)	0(20)
C(48A)	46(3)	33(3)	65(5)	4(3)	24(3)	-1(2)
C(49A)	28(18)	120(40)	120(40)	60(40)	0(20)	-20(20)
C(50A)	80(30)	60(20)	160(40)	40(20)	30(30)	-11(19)
F(38A)	62(9)	64(10)	133(17)	41(11)	54(10)	6(7)
F(39A)	108(16)	54(12)	124(17)	15(13)	77(13)	19(11)
F(40A)	40(8)	84(11)	133(17)	35(11)	33(10)	-15(7)

F(41A)	94(14)	123(19)	170(20)	57(18)	98(15)	-1(15)
F(42A)	130(20)	60(12)	210(30)	1(18)	50(20)	-57(12)
F(43A)	71(16)	80(20)	70(30)	-10(20)	9(17)	-12(12)
F(44A)	142(19)	62(11)	160(20)	-17(13)	36(17)	35(12)
F(45A)	109(15)	35(9)	190(30)	30(12)	84(17)	3(8)
F(46A)	120(20)	81(16)	520(70)	110(30)	200(40)	53(16)
F(47A)	220(30)	33(11)	300(50)	-2(17)	180(30)	32(15)
F(48A)	220(40)	120(20)	180(30)	-10(20)	140(30)	30(20)
F(49A)	130(20)	103(16)	140(20)	45(15)	25(16)	-23(14)
F(50A)	78(16)	65(16)	350(60)	100(30)	-10(20)	12(12)
F(51A)	72(18)	90(20)	280(50)	110(20)	10(20)	-7(17)
C(51)	35(4)	34(3)	66(5)	1(3)	21(4)	0(3)
C(52)	41(4)	53(4)	75(6)	10(4)	14(4)	-15(3)
C(53)	45(4)	68(5)	71(6)	29(4)	21(4)	-2(4)
F(1)	32(2)	35(2)	99(3)	23(2)	16(2)	-5(2)
F(2)	37(2)	44(2)	85(3)	27(2)	17(2)	1(2)
F(3)	30(2)	57(3)	97(4)	26(2)	-3(2)	-7(2)
F(4)	87(4)	69(3)	69(3)	4(3)	12(3)	5(3)
F(5)	63(3)	58(3)	81(3)	22(2)	6(2)	-6(2)
F(6)	57(3)	75(3)	98(4)	27(3)	-15(3)	-6(2)
F(7)	64(3)	46(2)	105(4)	8(2)	43(3)	-5(2)
F(8)	53(3)	66(3)	128(5)	27(3)	19(3)	22(2)
F(9)	67(3)	63(3)	92(4)	9(3)	39(3)	2(2)
F(10)	34(2)	59(3)	103(4)	30(2)	25(2)	10(2)
F(11)	120(5)	72(4)	126(5)	19(4)	-51(4)	-25(3)
F(12)	58(3)	99(4)	226(8)	-10(5)	58(4)	-36(3)
F(13)	61(3)	50(3)	109(4)	6(3)	6(3)	-10(2)
F(14)	60(3)	126(5)	127(5)	75(4)	55(3)	33(3)
F(15)	73(3)	76(3)	99(4)	39(3)	28(3)	26(3)
F(16)	89(4)	98(4)	74(3)	4(3)	34(3)	-21(3)
F(17)	37(2)	37(2)	83(3)	12(2)	21(2)	-4(2)
F(18)	40(2)	34(2)	85(3)	11(2)	29(2)	5(2)
F(19)	64(3)	36(2)	213(7)	42(3)	57(4)	8(2)
F(20)	83(4)	64(3)	126(5)	-25(3)	21(4)	-14(3)
F(21)	53(3)	57(3)	160(5)	23(3)	35(3)	-13(2)
F(22)	94(4)	37(3)	252(9)	-1(4)	40(5)	-25(3)
F(23)	82(4)	95(4)	121(5)	40(4)	64(3)	26(3)
F(24)	83(4)	125(5)	208(8)	96(5)	75(5)	2(4)
F(25)	82(4)	157(6)	121(5)	67(5)	47(4)	20(4)
F(26)	68(3)	76(3)	154(5)	66(4)	61(3)	22(3)
F(27)	69(3)	124(5)	137(5)	83(4)	46(3)	28(3)
F(28)	54(3)	85(3)	122(4)	45(3)	44(3)	21(2)
F(29)	62(3)	79(3)	86(4)	19(3)	29(3)	15(3)
F(30)	96(4)	40(3)	174(6)	-6(3)	83(4)	-1(3)

F(31)	99(4)	39(3)	227(8)	-11(4)	67(5)	-12(3)
F(32)	107(5)	53(3)	241(9)	50(4)	73(5)	41(3)
F(33)	35(2)	37(2)	93(3)	14(2)	20(2)	-4(2)
F(34)	44(2)	36(2)	66(3)	3(2)	20(2)	3(2)
F(35)	32(2)	45(2)	67(3)	5(2)	18(2)	4(2)
F(36)	34(2)	37(2)	103(3)	19(2)	21(2)	1(2)
F(37)	31(2)	39(2)	84(3)	7(2)	24(2)	-5(2)
C(1S)	120(10)	148(13)	84(11)	-55(9)	41(9)	-36(8)
C(2S)	124(10)	120(11)	100(15)	-46(10)	57(11)	-35(9)
C(3S)	128(10)	108(10)	111(12)	-54(8)	58(9)	-29(7)
C(4S)	129(10)	120(11)	86(10)	-52(8)	50(9)	-24(7)
C(5S)	121(9)	145(12)	103(12)	-56(9)	47(9)	-21(9)
C(6S)	112(10)	159(13)	81(12)	-56(10)	44(9)	-34(9)
C(7S)	112(11)	250(20)	113(15)	-86(18)	57(11)	-67(13)
C(8S)	97(16)	78(17)	30(15)	-18(13)	18(13)	-15(11)
C(9S)	94(17)	100(20)	50(30)	-19(18)	20(18)	-10(15)
C(10S)	99(15)	97(18)	48(17)	-19(14)	30(14)	8(14)
C(11S)	98(15)	70(15)	22(13)	-11(11)	24(12)	17(11)
C(12S)	92(15)	55(13)	45(15)	-7(11)	23(13)	4(10)
C(13S)	85(15)	58(13)	18(14)	-11(11)	0(12)	-3(10)
C(14S)	88(17)	38(15)	100(30)	-28(16)	-41(19)	-16(13)
C(1T)	152(10)	134(10)	124(11)	7(8)	32(9)	10(8)
C(2T)	143(9)	127(10)	127(11)	4(8)	33(9)	14(8)
C(3T)	146(9)	110(9)	87(8)	-31(6)	36(7)	0(6)
C(4T)	164(10)	133(10)	114(10)	-16(8)	40(9)	23(8)
C(5T)	157(11)	191(14)	200(16)	46(12)	16(13)	14(11)
C(6T)	138(10)	151(12)	187(14)	30(10)	-31(11)	-9(9)
C(7T)	260(20)	230(20)	350(30)	190(20)	-10(20)	12(17)
C(1E)	220(20)	105(12)	137(17)	15(10)	65(16)	-9(14)
C(2E)	410(50)	116(15)	131(17)	12(12)	80(20)	-20(20)
C(3E)	320(40)	52(9)	390(50)	45(18)	-80(30)	-43(14)
C(4E)	250(30)	81(11)	240(30)	55(14)	90(20)	4(15)
C(5E)	370(40)	84(10)	105(14)	19(9)	48(17)	36(16)
C(6E)	250(30)	81(10)	157(18)	1(11)	30(20)	18(13)
C(7E)	270(30)	200(30)	340(40)	-60(20)	100(30)	10(20)
C(1K)	93(18)	55(9)	108(15)	20(20)	39(12)	-2(15)
C(2K)	120(20)	45(13)	150(30)	-24(16)	43(19)	-23(15)
C(3K)	86(15)	51(14)	100(20)	-18(14)	8(14)	-8(11)
C(4K)	120(30)	43(12)	130(40)	5(14)	30(30)	5(16)
C(5K)	78(16)	49(11)	70(20)	-8(10)	-15(17)	9(13)
C(6K)	71(14)	59(18)	100(20)	22(15)	1(12)	24(14)
C(7K)	100(17)	91(16)	102(18)	-15(14)	29(14)	8(13)
O(2)	102(11)	67(8)	132(13)	-9(8)	50(10)	-40(8)

Table X.5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **[(NMeAcF$_{51}$PcCo)$_2$H$_2$O]·7(toluene)**.

	x	y	z	U(eq)
H(52A)	13109	3463	7882	85
H(52B)	12660	3760	7408	85
H(52C)	13061	3415	7204	85
H(53A)	12159	3385	6237	91
H(53B)	11795	3742	6450	91
H(53C)	11314	3439	6007	91
H(1SA)	7016	2970	4760	138
H(2SA)	8170	3161	4800	132
H(3SA)	8353	3744	4397	133
H(4SA)	7382	4136	3955	129
H(5SA)	6228	3945	3915	144
H(7SA)	5457	3345	3874	232
H(7SB)	5554	3529	4507	232
H(7SC)	5722	3088	4451	232
H(8SA)	7194	3738	4277	82
H(9SA)	8252	3392	4624	98
H(10A)	8232	2784	5013	95
H(11A)	7154	2522	5056	74
H(12A)	6096	2868	4710	76
H(14A)	5630	3493	3816	133
H(14B)	5941	3825	4277	133
H(14C)	5523	3478	4456	133
H(1TA)	1423	3129	5040	166
H(2TA)	1333	2542	5474	161
H(3TA)	219	2316	5489	137
H(4TA)	-806	2676	5071	164
H(5TA)	-716	3263	4637	229
H(7TA)	927	3701	4600	451
H(7TB)	131	3675	4170	451
H(7TC)	271	3835	4822	451
H(1EA)	7968	5476	1754	184
H(2EA)	6824	5421	1857	264
H(3EA)	6663	5443	2791	352
H(4EA)	7646	5522	3621	225
H(5EA)	8790	5577	3518	231
H(7EA)	9274	5891	2524	408
H(7EB)	9280	5486	2221	408

H(7EC)	9587	5528	2918	408
H(1KA)	4813	4690	7614	100
H(2KA)	5260	4565	6825	125
H(3KA)	5496	3940	6608	100
H(4KA)	5284	3439	7180	120
H(5KA)	4837	3564	7969	89
H(7KA)	4014	4078	8295	147
H(7KB)	4399	4483	8408	147
H(7KC)	4801	4115	8737	147
H(2A)	7060(30)	2540(30)	5260(40)	116
H(2B)	7650(30)	2710(40)	5230(20)	116