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Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for SDB04. 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}
Pt(1)	131(1)	113(1)	139(1)	5(1)	8(1)	23(1)
N(1)	142(16)	123(14)	175(16)	10(12)	9(12)	4(11)
N(2)	161(14)	167(16)	120(15)	-9(12)	32(12)	47(11)
C(1)	157(18)	147(19)	230(20)	55(16)	4(16)	5(14)
C(2)	201(19)	147(19)	240(20)	-11(16)	78(16)	36(16)
C(3)	206(18)	210(20)	170(20)	-9(17)	74(15)	-40(15)
C(4)	193(17)	123(18)	195(19)	-13(14)	72(15)	-80(13)
C(5)	215(18)	220(20)	126(18)	13(15)	-11(14)	-70(13)
C(6)	185(19)	171(19)	200(20)	55(16)	-53(15)	-41(14)
C(7)	134(15)	152(16)	222(19)	38(18)	21(17)	12(12)
C(8)	134(17)	125(17)	213(19)	10(15)	4(14)	-53(12)
C(9)	124(14)	145(16)	179(18)	-7(16)	37(12)	-34(14)
C(10)	163(17)	186(19)	114(15)	24(13)	-19(12)	81(14)
C(11)	127(19)	240(20)	150(18)	-6(15)	-14(14)	17(15)
C(12)	234(18)	150(17)	190(20)	-2(16)	-50(15)	22(13)
C(13)	242(18)	181(18)	160(20)	-18(15)	-26(15)	84(15)
C(14)	225(18)	220(20)	150(20)	86(15)	50(14)	74(15)
C(15)	193(15)	134(16)	225(17)	90(20)	14(16)	20(14)
C(16)	320(20)	128(17)	420(30)	-34(15)	-20(20)	-8(15)
C(17)	260(20)	260(20)	340(30)	110(20)	107(19)	133(17)
C(18)	157(19)	117(17)	175(18)	16(14)	3(14)	37(13)
C(19)	148(16)	260(20)	129(17)	-77(19)	-10(13)	24(18)
C(20)	224(19)	210(20)	180(20)	11(17)	-19(16)	-78(15)
C(21)	240(20)	143(18)	230(20)	30(15)	-41(17)	-25(17)
C(22)	204(18)	159(19)	140(19)	-35(16)	-21(15)	59(14)
C(23)	163(18)	199(19)	180(20)	23(15)	10(16)	80(15)
C(24)	177(17)	177(17)	290(20)	20(20)	-41(15)	22(17)
C(25)	201(19)	156(19)	230(20)	-14(17)	-19(16)	-30(15)

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Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for SDB04.

	x	y	z	U_{iso}
H(16A)	5025	9531	1044	43
H(16B)	3515	10012	764	43
H(16C)	4700	9540	231	43
H(17A)	-65	7289	1685	43
H(17B)	-14	5958	1427	43
H(17C)	-549	6968	913	43
H(1)	7560(40)	2260(30)	-100(20)	22(11)
H(2)	7860(40)	1830(30)	-1216(19)	17(10)
H(3)	6470(40)	2610(30)	-2070(20)	26(11)
H(5)	4460(40)	4230(30)	-2228(19)	23(11)
H(6)	3080(30)	5600(30)	-1856(18)	13(9)
H(7)	3100(30)	6060(30)	-714(18)	16(9)
H(11)	5120(40)	7300(30)	361(18)	15(11)
H(13)	1700(40)	8610(30)	1196(19)	27(11)
H(15)	2050(30)	5370(30)	810(20)	12(9)
H(18)	5200(40)	5490(30)	1741(18)	15(10)
H(19)	4270(40)	4470(30)	2608(19)	26(10)
H(20)	4520(50)	2720(40)	2780(20)	48(15)
H(21A)	6370(40)	1700(40)	2230(20)	40(13)
H(21B)	5130(40)	1610(30)	1830(20)	28(12)
H(22)	6620(30)	1940(30)	1031(17)	10(9)
H(23)	8350(40)	3270(40)	1100(20)	29(12)
H(24A)	9010(40)	4230(30)	2073(15)	9(8)
H(24B)	7850(40)	3560(30)	2410(20)	27(11)
H(25A)	7490(30)	5780(30)	1767(16)	9(8)
H(25B)	7120(30)	5490(30)	2529(19)	17(9)

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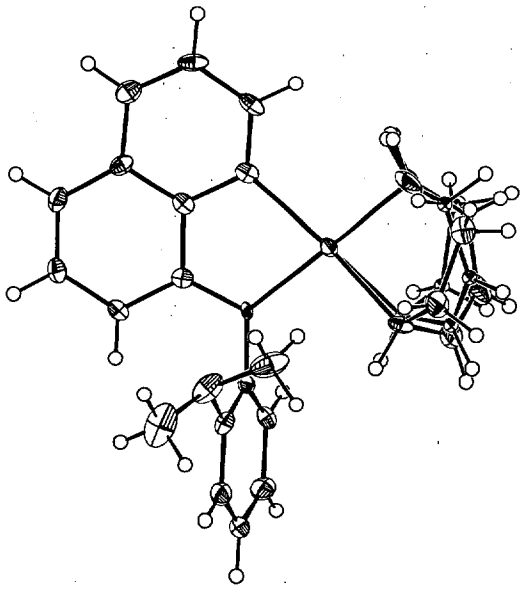
Crystal Structure Analysis of:

10b - jcp08

Contents



Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and have been placed on hold pending further instructions from us. The deposition number is 158906. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 158906."

Figures for jcp08.

Figure 1. Unlabeled Diamond view of the molecule, with 50% ellipsoids, showing both diastereomers. Hydrogen atoms are at arbitrary scale.

Figure 2. Unlabeled Diamond view of the molecule, with 50% ellipsoids. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms. Hydrogen atoms are at arbitrary scale.

Figure 3. Labeled Diamond view of the molecule, with 50% ellipsoids and hydrogen atoms omitted. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms.

Figure 4. Unlabeled Diamond view of the molecule, with 50% ellipsoids and hydrogen atoms omitted. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms.

Figure 5. Unlabeled Diamond view of the major diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale.

Figure 6. Unlabeled Diamond view of the minor diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale. The six non-overlapped atoms were refined with a common U_{iso}.

Figure 7. Unlabeled Diamond view of the major diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale.

Figure 8. Unlabeled Diamond view of the minor diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale. The six non-overlapped atoms were refined with a common U_{iso}.

Figure 9. Crystal packing viewed along the a-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

Figure 10. Crystal packing viewed along the b-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

Figure 11. Crystal packing viewed along the c-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

Figure 12. Overlap of jcp08 (solid lines) with jcp09 (dashed lines) based on best least-squares fit of all atoms.

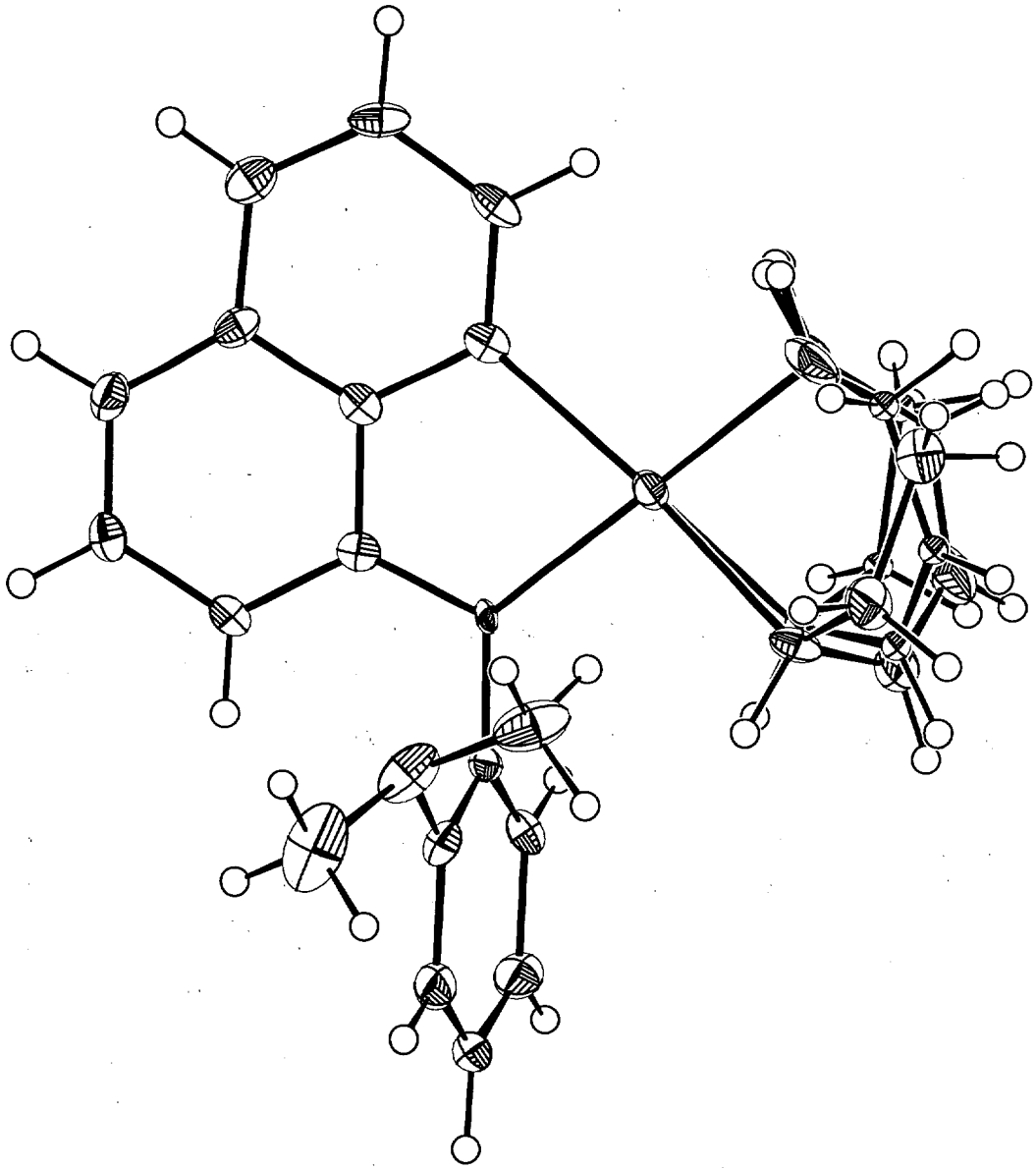


Figure 1. Unlabeled Diamond view of the molecule, with 50% ellipsoids, showing both diastereomers. Hydrogen atoms are at arbitrary scale.

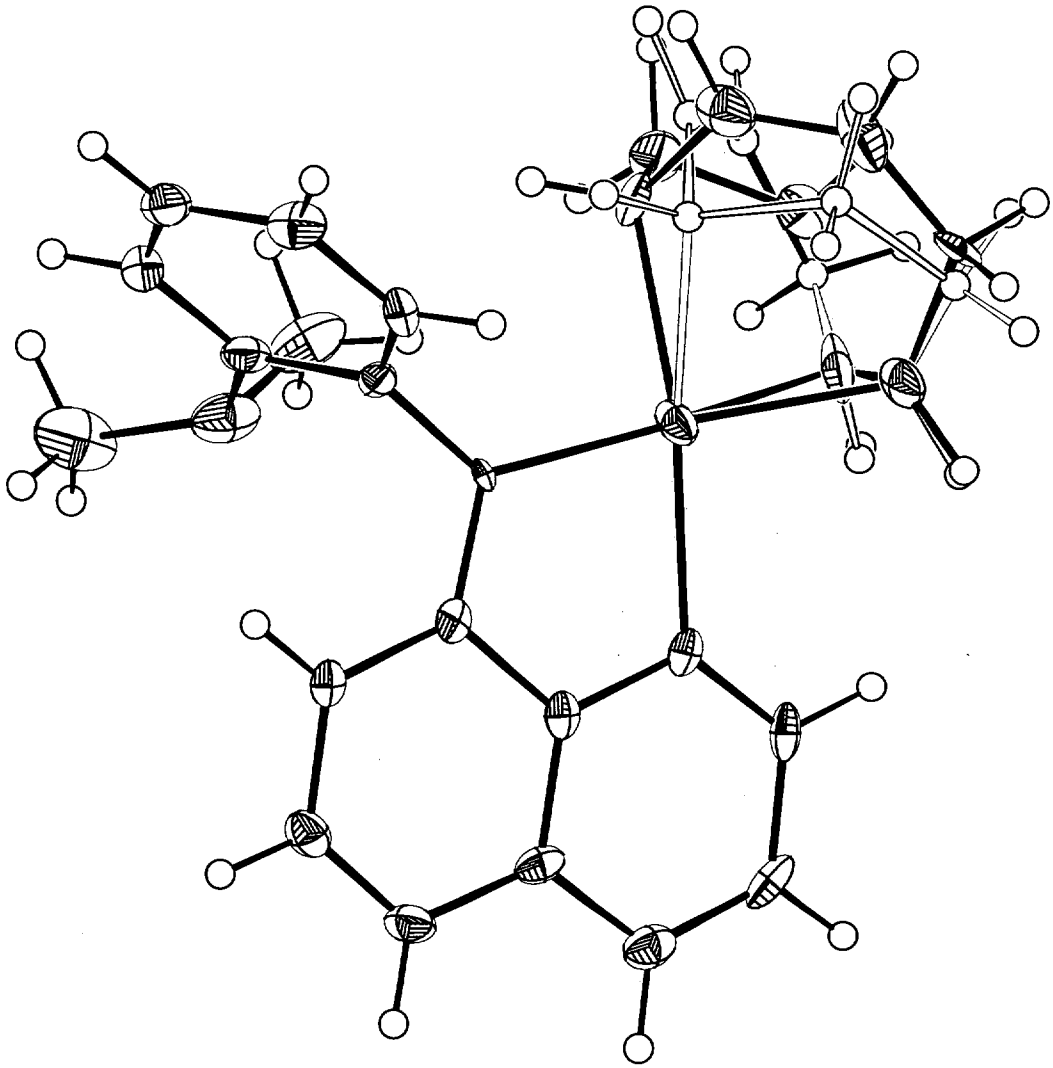


Figure 2. Unlabeled Diamond view of the molecule, with 50% ellipsoids. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms. Hydrogen atoms are at arbitrary scale.

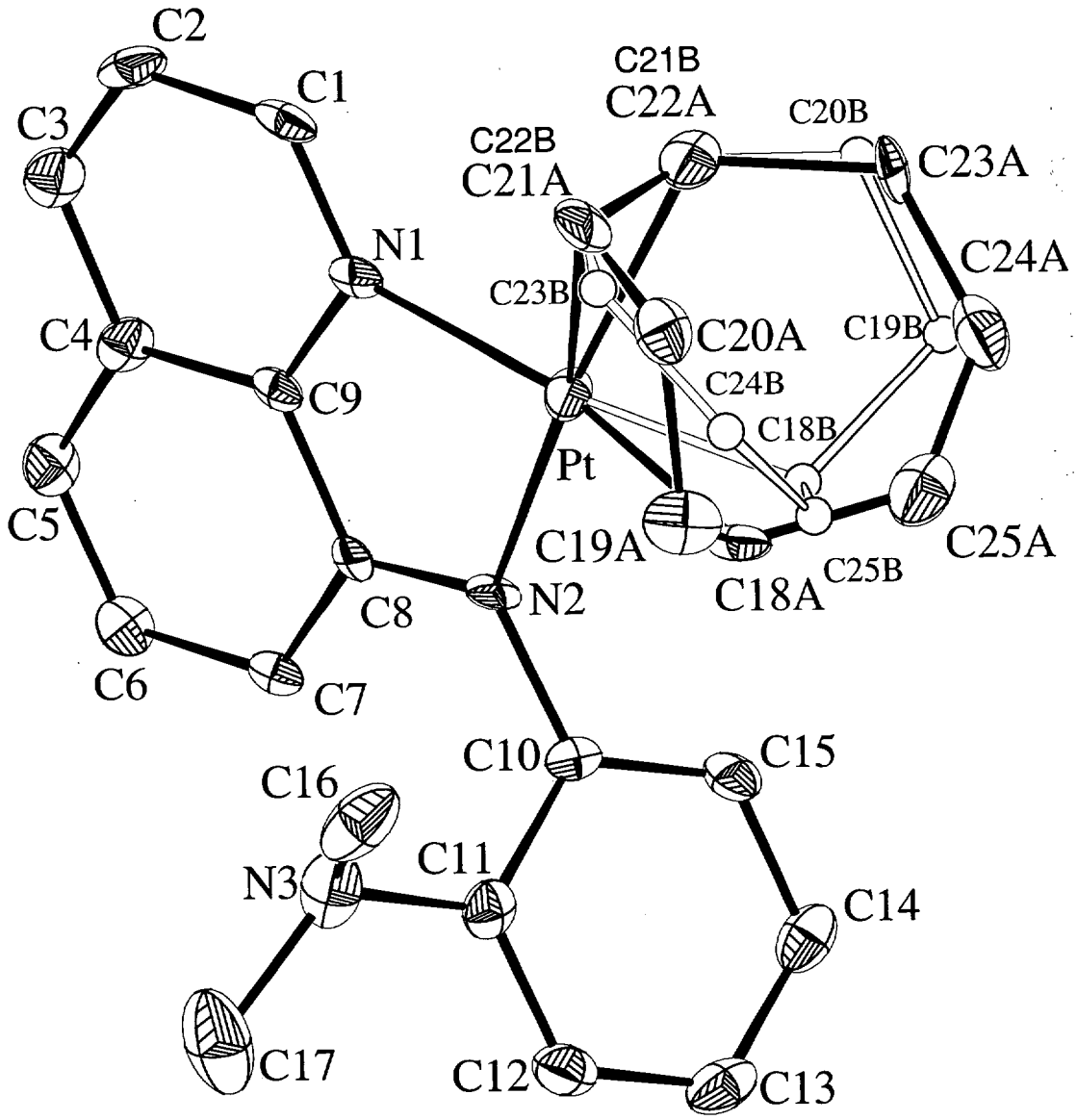


Figure 3. Labeled Diamond view of the molecule, with 50% ellipsoids and hydrogen atoms omitted. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms.

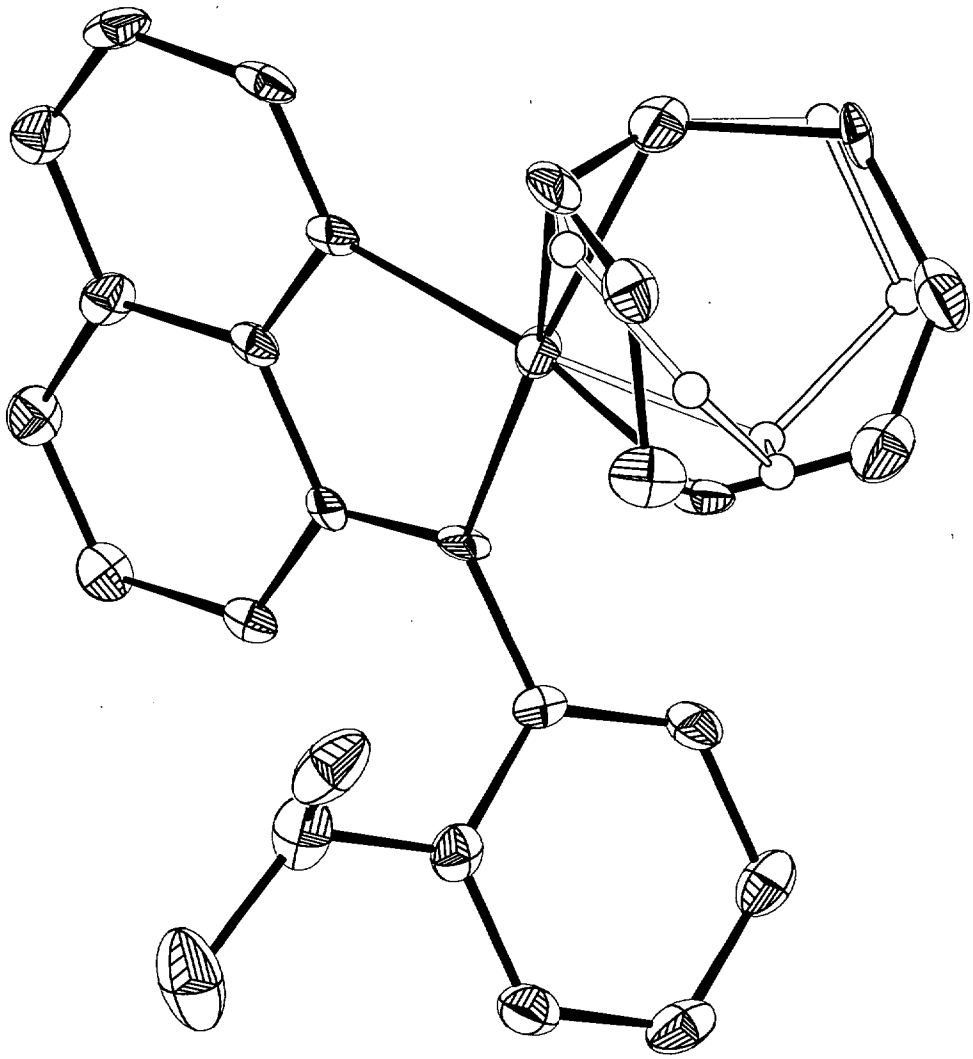


Figure 4. Unlabeled Diamond view of the molecule, with 50% ellipsoids and hydrogen atoms omitted. The six non-overlapping sites of the minor component are shown with hollow bonds and atoms.

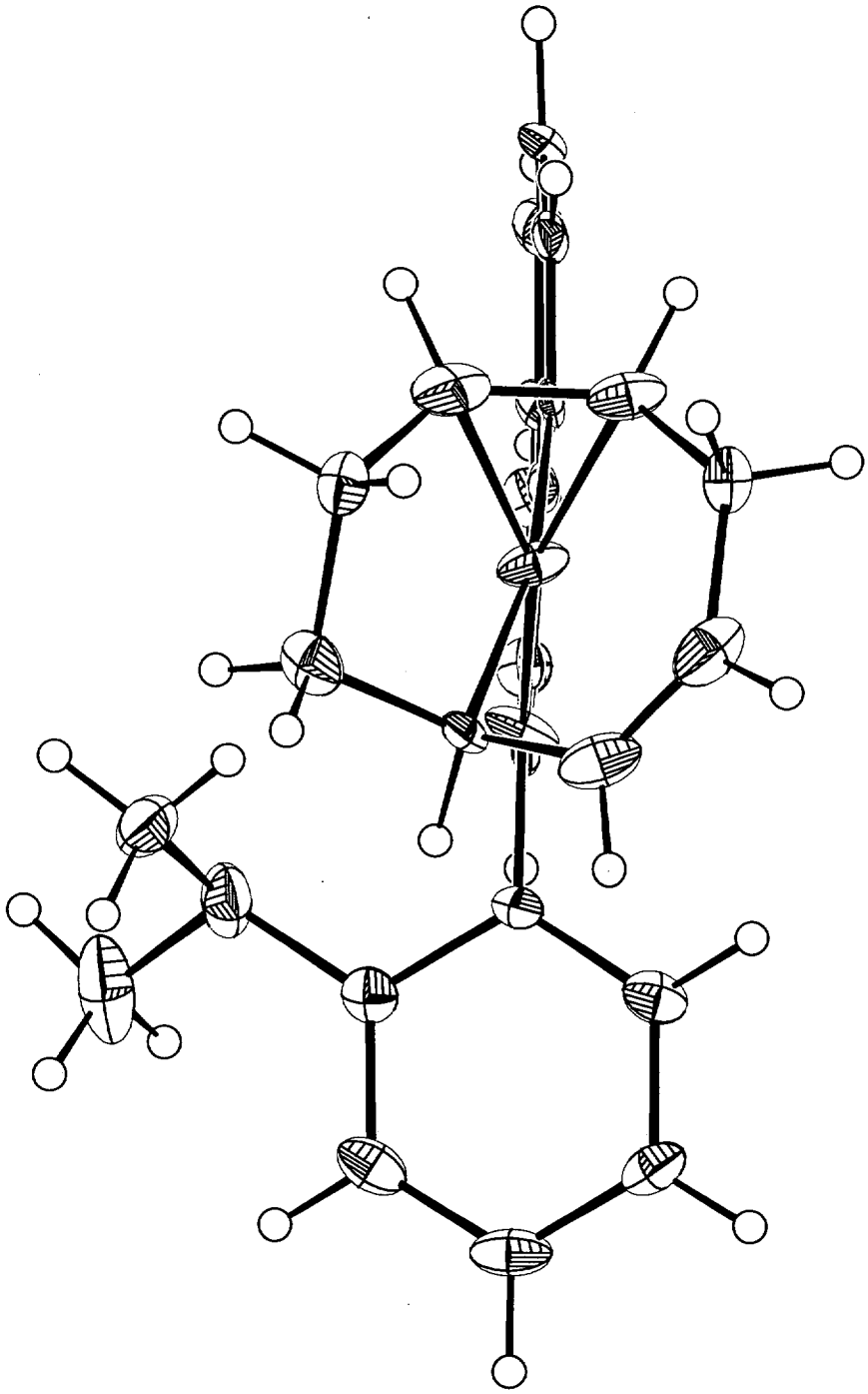


Figure 5. Unlabeled Diamond view of the major diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale.

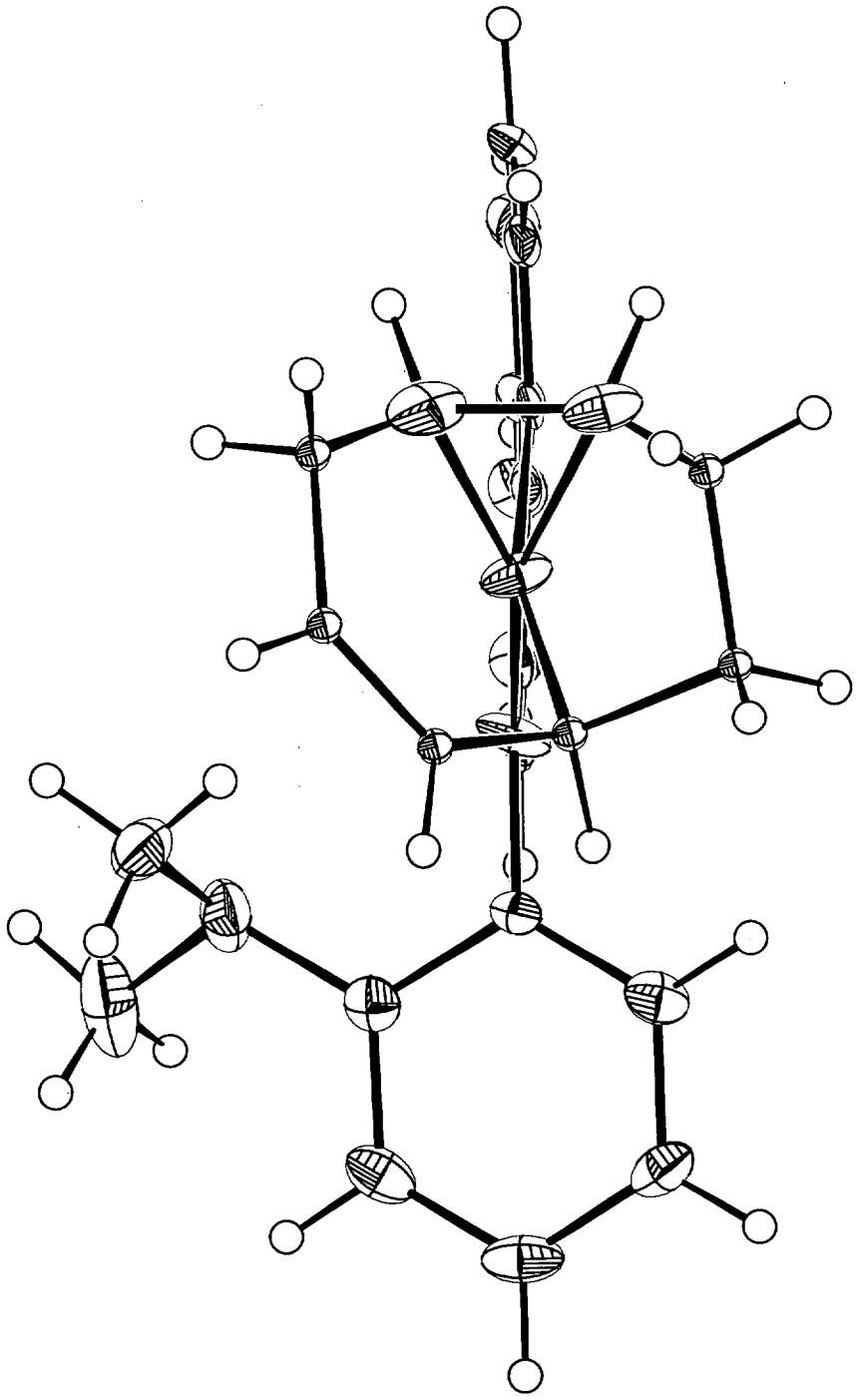


Figure 6. Unlabeled Diamond view of the minor diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale. The six non-overlapped atoms were refined with a common U_{iso}.

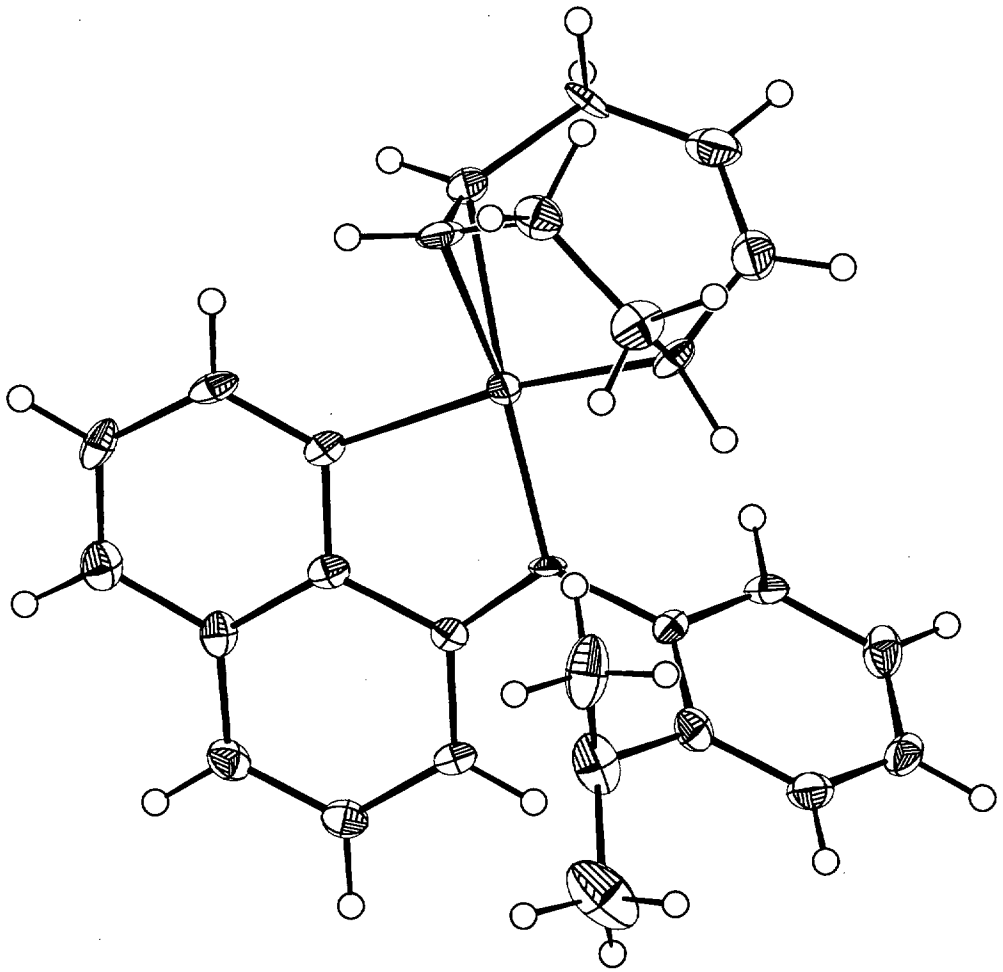


Figure 7. Unlabeled Diamond view of the major diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale.

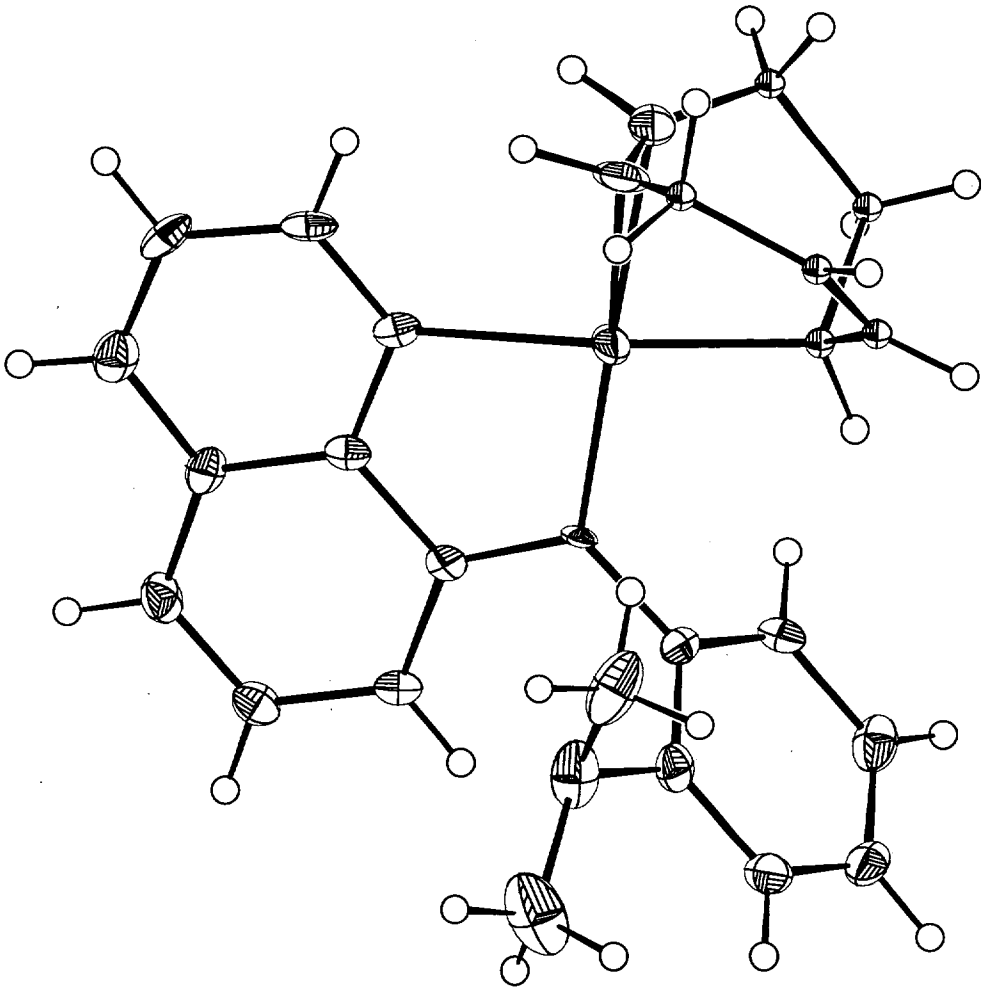


Figure 8. Unlabeled Diamond view of the minor diastereomer, with 50% ellipsoids and hydrogen atoms at arbitrary scale. The six non-overlapped atoms were refined with a common U_{iso}.

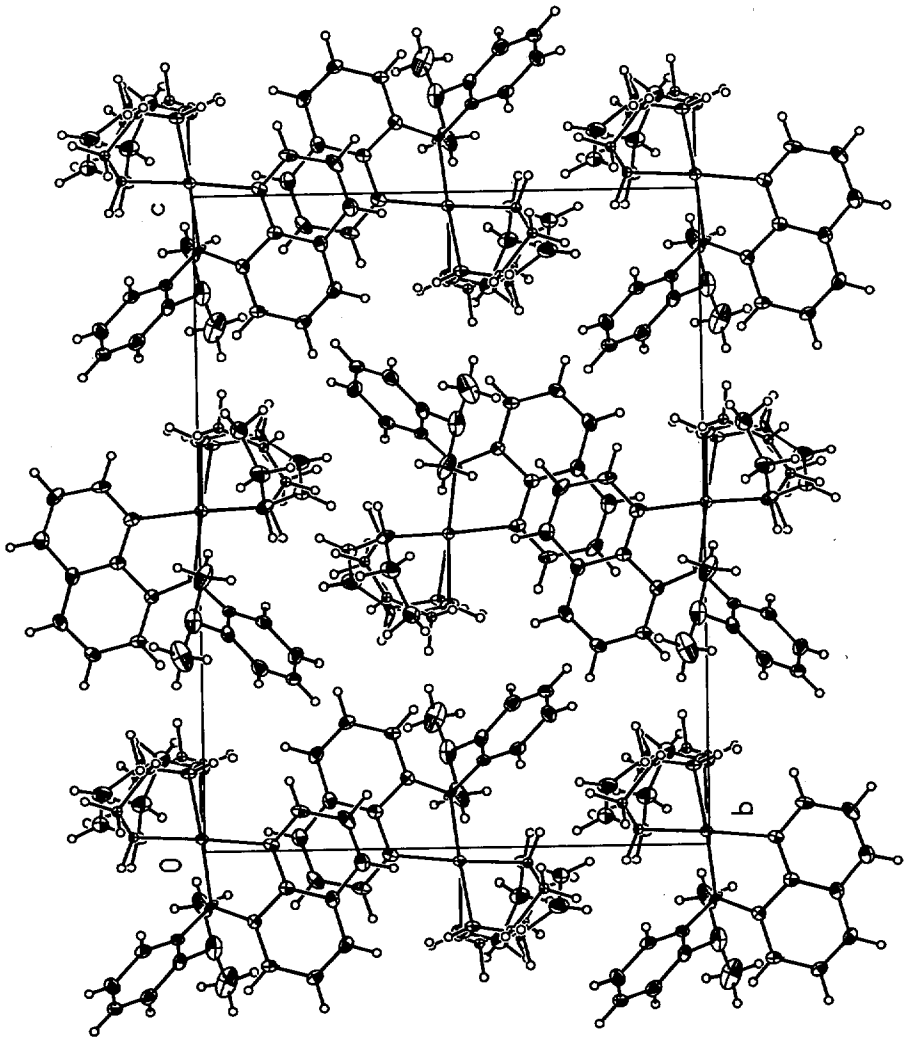


Figure 9. Crystal packing viewed along the a-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

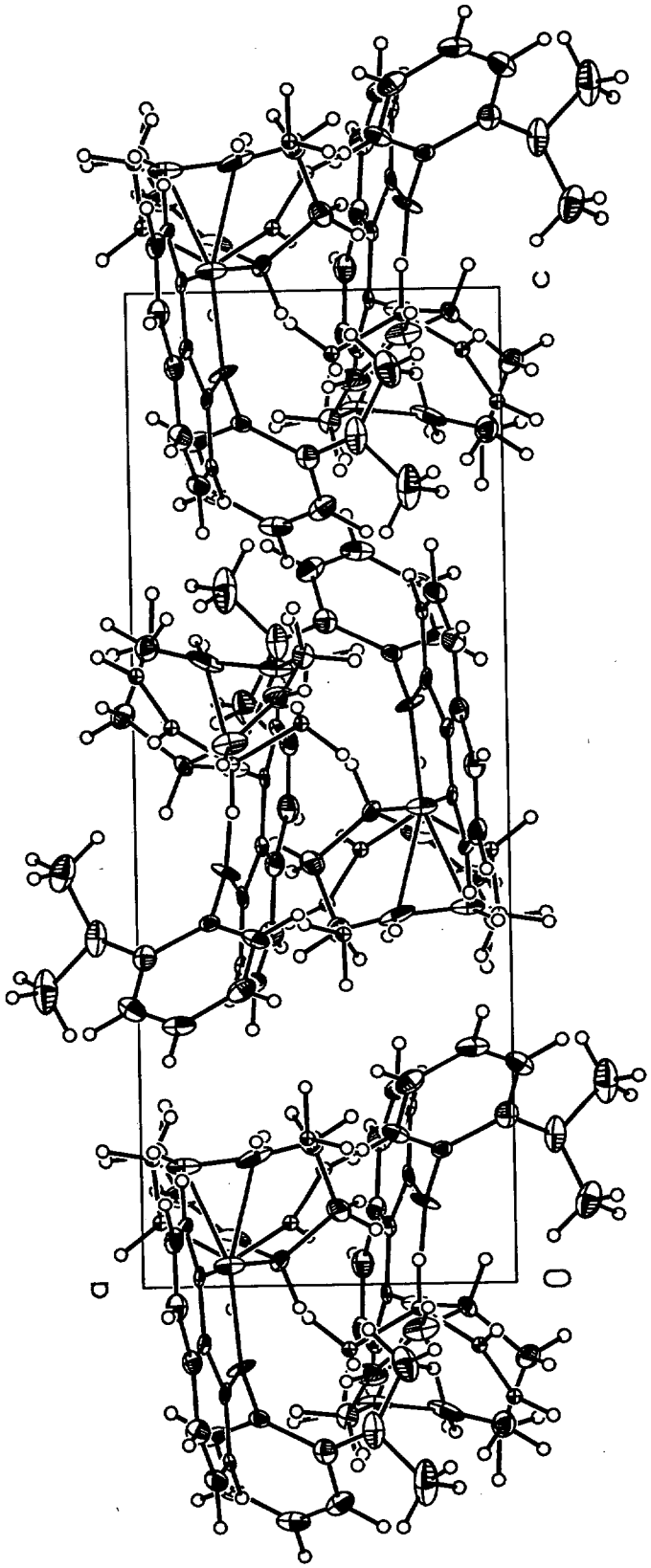


Figure 10. Crystal packing viewed along the b-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

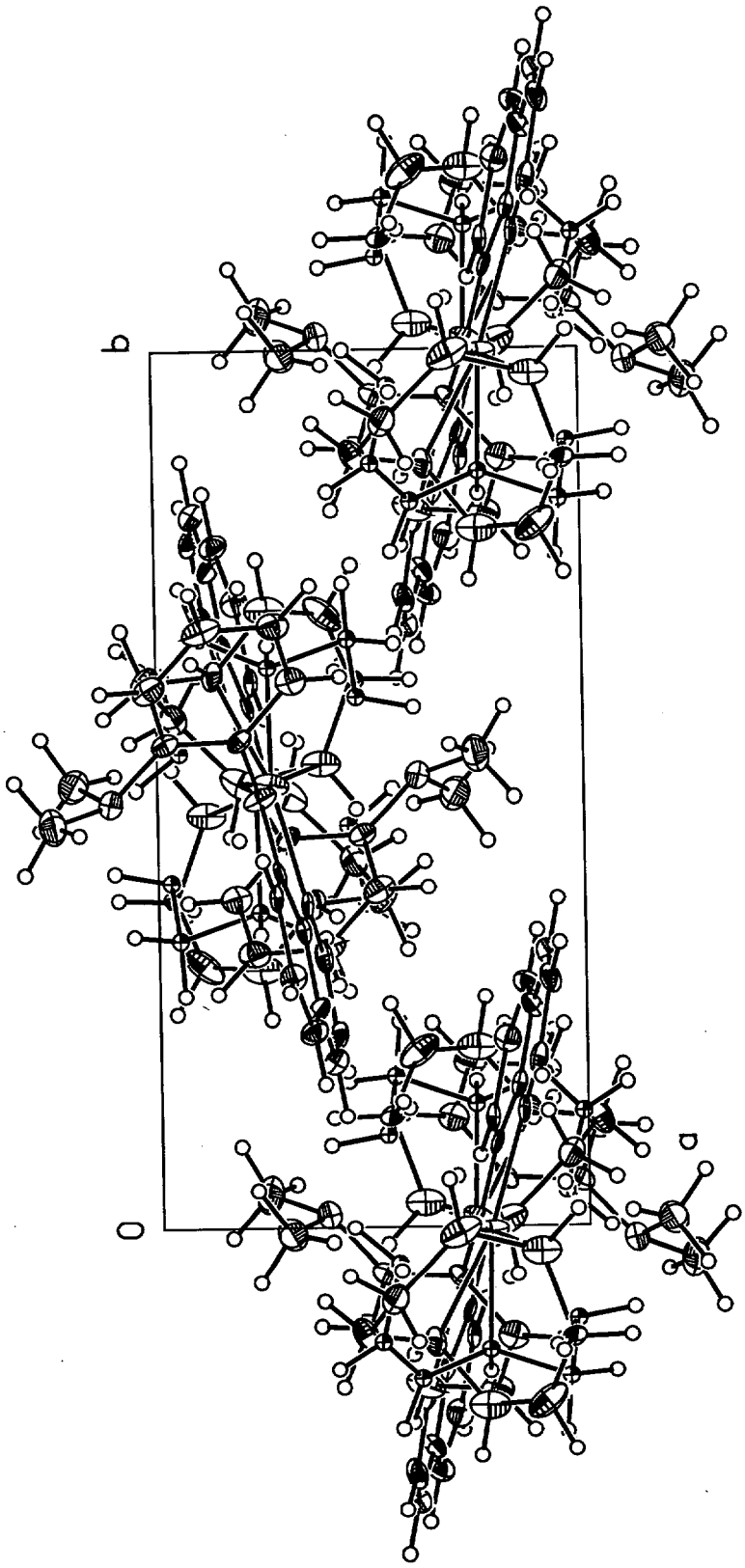


Figure 11. Crystal packing viewed along the c-axis, showing the unit cell boundaries, with 50% ellipsoids. Hydrogen atoms are at arbitrary scale.

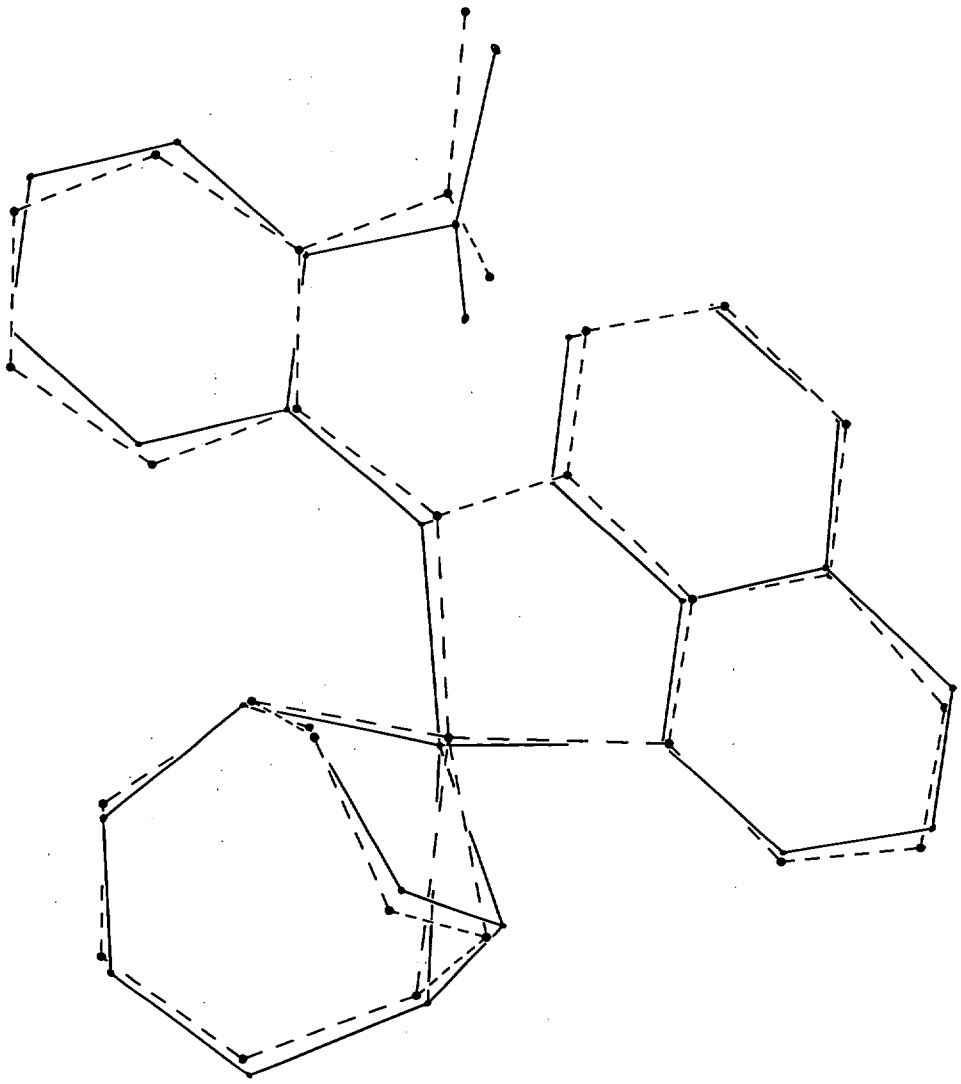


Figure 12. Overlap of jcp08 (solid lines) with jcp09 (dashed lines) based on best least-squares fit of all atoms.

Table 1. Crystal Data and Structure Analysis Details for jcp08.

Empirical formula	$C_{25}H_{27}N_3Pt$
Formula weight	564.59
Crystallization solvent	not specified
Crystal shape	column
Crystal color	red
Crystal size	0.22 x 0.26 x 0.31 mm

Data Collection

Preliminary photograph(s)	rotation
Type of diffractometer	Bruker SMART 1000 ccd
Wavelength	0.71073 Å MoKα
Data collection temperature	98 K
Theta range for 7778 reflections used in lattice determination	2.1 to 28.2°
Unit cell dimensions	a = 7.2129(6) Å α= 90° b = 14.8202(11) Å β= 90° c = 19.1861(15) Å γ = 90°
Volume	2050.9(3) $Å^3$
Z	4
Crystal system	monoclinic
Space group	$P2_12_12_1$ (# 19)
Density (calculated)	1.828 g/cm^3
F(000)	1104
Theta range for data collection	1.7 to 28.5°
Completeness to theta = 28.45°	96.3%
Index ranges	$-9 \le h \le 9, -19 \le k \le 18, -24 \le l \le 25$
Data collection scan type	ω scans at 5 fixed ϕ values
Reflections collected	30504
Independent reflections	4886 [R_{int}= 0.0393]
Reflections > 2σ(I)	4768
Average σ(I)/(net I)	0.0252
Absorption coefficient	6.86 mm^{-1}
Absorption correction	empirical
Max. and min. relative transmission	1.000 and 0.792
Reflections monitored for decay	first 75 scans recollected at end of runs
Decay of standards	within counting statistics

Table 1 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	4886 / 0 / 285
Treatment of hydrogen atoms	calculated, CH_3 groups allowed to rotate; U_{iso} fixed at 120% U_{eq} of attached atom
Goodness-of-fit on F^2	2.565
Final R indices [I>2σ(I), 4768 reflections]	R1 = 0.0364, wR2 = 0.0678
R indices (all data)	R1 = 0.0377, wR2 = 0.0679
Type of weighting scheme used	sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.038
Average shift/error	0.001
Absolute structure parameter	0.529(10)
Largest diff. peak and hole	4.27 and -4.22 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART v5.606
Data collection	Bruker SMART v5.606
Data reduction	Bruker SAINT v6.02
Structure solution	SHELXS-97 (Sheldrick, 1990)
Structure refinement	SHELXL-97 (Sheldrick, 1997)
Graphics	Diamond, Bruker SHELXTL v5.1

References

Bruker (1999) SMART (v5.606), SAINT (v6.02) and SHELXTL (v5.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Diamond 2.1. (2000) Crystal Impact GbR, Bonn, Germany.

Spek, A.L. (1990). *Acta Cryst.*, A**46**, C-34.

Sheldrick, G. M. (1990). *Acta Cryst.*, A**46**, 467-473.

Sheldrick, G. M. (1997). SHELXL-97. Program for Structures Refinement. Univ. of Gottingen, Federal Republic of Germany.

Special Refinement Details

The crystals were clumps of translucent red columns, many with steps, feathered and/or rounded. Samples were mounted on a glass fiber with Paratone-N oil. The first crystal was a section cut from a column. The rocking curves showed tails on the sides of some peaks. Five runs of data were collected with 10 second (nominal) long, –0.3° wide ω–scans at five different values of φ (0, 72, 144, 216, and 288°) with the detector 5 cm (nominal) distant at a θ of -28° using SMART v5.606. The initial cell for data reduction was calculated from 999 centered reflections (eleven discarded in least-squares). For data processing with SAINT v6.02, all defaults were used, except: a fixed box size of 1.8 x 1.8 x 1.0 was used (some tailing was still observed in the z direction), periodic orientation matrix updating was disabled, the instrument error was set to zero, no Laue class integration restraints were used, and for the post-integration global least squares refinement, no constraints were applied. No decay correction was needed. The faces were not well formed and a face-indexed absorption correction had minimal effect and was subsequently not used. SADABS 2.03beta was used with g=0.520. Although no change in absorption ripples was observed, the correction of the esd's should help the refinement (the GOF is ~0.5 larger with SADABS).

No outlier reflections were omitted from the final; 102 of 30606 reflections were rejected, with 7 space group-absence violations and 0 inconsistent equivalents. Refinement of F^2 was against all reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

The structure was not trivial to solve. [More crystals were examined until a smaller fragment gave a good, different cell leading to a very nice refinement (jcp09) in $P\bar{1}$ (#2) of a single compound.] Solution nmr showed the existence of two species so the data for this crystal were reexamined. XPREP could not find any suitable space groups; a number of potential systematic absences were weak but not absent. The structure was eventually solved in the nonpolar, noncentrosymmetric space group $P2_12_12_1$ by direct methods with fully normalized data and the help of Patterson maps. The platinum coordinates of (0.77, 0.99, 1.02) make phasing ambiguous. The coordination about the platinum atom is approximately square planar, with bonds to two nitrogens of the amine and to a carbon and a double bond of the COD. In this arrangement, there are two COD carbon atoms not bonded to Pt on the same side of the platinum coordination plane as the dimethylamino group, and three COD carbon atoms not bonded to Pt on the opposite side (see figure 5). This is the same geometry as for jcp09, in which all hydrogen atoms could be located in difference maps and all hydrogen parameters successfully refined. Peaks in a difference map revealed a second conformation of the COD. In this isomer, the COD is reflected across the platinum coordination plane and there are three COD carbon atoms not bonded to Pt on the same side of the platinum coordination plane as the dimethylamino group, and two COD carbon atoms not bonded to Pt on the opposite side (see figure 6). The ratio of these two diastereomers (assuming hindered rotation about the phenyl-N2 bond), refined to 0.71:0.29. The two σ-bonded carbon atoms C18A (0.71 population) and C18B (0.29 population) are 0.94 Å apart. The coordinated double bonds of both isomers overlap too closely to refine the carbon atoms involved independently and so the four sites were modeled with only two sites, one for each of the atom pairs (C21A, C22B) and (C22A, C21B). [The averaged site (C21A, C22B) leads to a long C21A-C20A bond of 1.614(11) Å and a short C22B-C23B bond of 1.23(4) Å as the two atoms are probably several tenths of an Angstrom separate.] The other six atoms were modeled with two sites each. The minor constituent was modeled isotropically; even so, the U_{iso} of C18B went negative and so all six of these atoms were given a common U_{iso} parameter. The crystal was also twinned by inversion, and the Flack parameter, included in the full matrix, refined to 0.529(10). So even though this is a noncentrosymmetric space group, both enantiomers are present in statistically equal amounts.

The Platon listing of intermolecular distances shows that two minor conformation COD hydrogens (H25C and H19D) on neighboring molecules are within 2.2Å, producing more rearrangement when these diastereomers are adjacent. The largest peaks in the final difference map greater were 4.27 $e\cdot Å^{-3}$ (0.76Å from Pt) and –4.22 $e\cdot Å^{-3}$ (0.67Å from Pt); the two other peaks greater than |2| $e\cdot Å^{-3}$ are 2.16 $e\cdot Å^{-3}$ (1.20Å from Pt) and –2.65 $e\cdot Å^{-3}$ (0.41Å from Pt). Additionally there are 6 more peaks greater than |1| $e\cdot Å^{-3}$, all near the platinum atom except for a peak of 1.25 $e\cdot Å^{-3}$ (0.90Å from C21A).

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jcp08. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Pt	7676(1)	9946(1)	10206(1)	20(1)
N1	8493(6)	11320(3)	10098(2)	13(1)
N2	7412(6)	10107(2)	9172(2)	18(1)
N3	3897(6)	10146(3)	8527(3)	30(1)
C1	8855(8)	11906(4)	10600(3)	17(1)
C2	9153(7)	12820(4)	10465(3)	21(1)
C3	9113(7)	13116(3)	9794(3)	22(1)
C4	8724(7)	12511(3)	9242(3)	18(1)
C5	8605(7)	12766(4)	8542(3)	21(1)
C6	8131(8)	12138(3)	8054(3)	19(1)
C7	7764(7)	11235(3)	8233(3)	13(1)
C8	7852(7)	10955(3)	8919(3)	13(1)
C9	8391(7)	11609(3)	9425(3)	14(1)
C10	6948(7)	9436(3)	8663(3)	14(1)
C11	5194(8)	9473(4)	8323(3)	19(1)
C12	4825(9)	8849(4)	7806(3)	24(1)
C13	6082(9)	8185(4)	7630(3)	25(2)
C14	7770(10)	8133(3)	7979(3)	24(1)
C15	8172(8)	8756(3)	8493(3)	21(1)
C16	3025(7)	9932(4)	9191(3)	36(1)
C17	2521(9)	10387(4)	8001(4)	47(2)
C18A[a]	6330(9)	8689(5)	10246(4)	18(2)
C19A[a]	4723(11)	8773(6)	10751(5)	26(2)
C20A[a]	5410(11)	9176(7)	11430(5)	23(2)
C21A[a,c]	6962(8)	9938(5)	11287(3)	32(2)
C22A[a,c]	8855(9)	9714(4)	11208(3)	24(2)
C23A[a]	9589(19)	8733(6)	11325(8)	17(3)
C24A[a]	8946(14)	7998(6)	10915(5)	32(2)
C25A[a]	7585(14)	7953(5)	10460(4)	30(2)
C18B[b]	7620(30)	8599(10)	10251(10)	8(2)*
C19B[b]	9500(30)	8286(14)	10646(13)	8(2)*
C20B[b]	9700(60)	8950(20)	11290(20)	8(2)*
C21B[b,c]	8855(9)	9714(4)	11208(3)	24(2)
C22B[b,c]	6962(8)	9938(5)	11287(3)	32(2)
C23B[b]	5530(30)	9581(15)	11472(14)	8(2)*
C24B[b]	5110(30)	8692(15)	11156(14)	8(2)*
C25B[b]	6020(30)	8267(14)	10624(12)	8(2)*

[a] Population 0.714(10)

[b] Population 0.286(10)

[c] Except for population, C21A≡C22B and C22A≡C21B

* U_{iso}

Table 3. Selected bond lengths [Å] and angles [°] for jcp08.

Pt-N1	2.130(4)	C18A-Pt-N2	95.6(3)
Pt-N2	2.006(4)	C18B-Pt-N2	99.2(6)
Pt-C18A	2.103(8)	C18A-Pt-N1	168.2(2)
Pt-C18B	1.999(15)	C18B-Pt-N1	164.7(6)
Pt-C21A	2.137(5)	N2-Pt-N1	79.44(16)
Pt-C22A	2.130(6)	N1-Pt-C21A	99.6(2)
C18A-C25A	1.476(11)	N2-Pt-C21A	159.57(19)
C18A-C19A	1.516(10)	N1-Pt-C21B	97.6(2)
C19A-C20A	1.518(12)	N2-Pt-C21B	161.6(2)
C20A-C21A	1.614(11)	N1-Pt-C22A	97.6(2)
C21A-C22A	1.413(8)	N2-Pt-C22A	161.6(2)
C22A-C23A	1.564(12)	N1-Pt-C22B	99.6(2)
C23A-C24A	1.421(16)	N2-Pt-C22B	159.57(19)
C24A-C25A	1.315(12)	C18A-Pt-C22A	90.5(3)
C18B-C25B	1.44(3)	C18B-Pt-C22B	87.0(6)
C18B-C19B	1.62(3)	C18B-Pt-C21B	78.8(6)
C19B-C20B	1.58(5)	C18A-Pt-C21A	81.3(3)
C20B-C21B	1.32(4)	C22A-Pt-C21A	38.7(2)
C21B-C22B	1.413(8)	C22B-Pt-C21B	38.7(2)
C22B-C23B	1.23(4)	C25A-C18A-C19A	110.6(7)
C23B-C24B	1.48(3)	C18A-C19A-C20A	109.4(6)
C24B-C25B	1.37(3)	C19A-C20A-C21A	110.8(7)
		C22A-C21A-C20A	121.7(6)
		C21A-C22A-C23A	122.0(7)
		C24A-C23A-C22A	121.5(11)
		C25A-C24A-C23A	130.6(9)
		C24A-C25A-C18A	127.2(7)
		C25B-C18B-C19B	109.9(15)
		C20B-C19B-C18B	105(2)
		C19B-C20B-C21B	111(2)
		C20B-C21B-C22B	128(2)
		C21B-C22B-C23B	138(2)
		C22B-C23B-C24B	116(2)
		C25B-C24B-C23B	128(2)
		C24B-C25B-C18B	126.7(19)

Table 4. Bond lengths [Å] and angles [°] for jcp08.

Pt-N1	2.130(4)	C20A-H20A	0.9900
Pt-N2	2.006(4)	C20A-H20B	0.9900
Pt-C18A	2.103(8)	C21A-C22A	1.413(8)
Pt-C18B	1.999(15)	C21A-H21A	1.0000
Pt-C21A	2.137(5)	C22A-C23A	1.564(12)
Pt-C22A	2.130(6)	C22A-H22A	1.0000
N1-C1	1.322(7)	C23A-C24A	1.421(16)
N1-C9	1.362(7)	C23A-H23A	0.9900
N2-C8	1.383(6)	C23A-H23B	0.9900
N2-C10	1.434(6)	C24A-C25A	1.315(12)
N3-C11	1.424(7)	C24A-H24A	0.9500
N3-C16	1.454(7)	C25A-H25A	0.9500
N3-C17	1.460(8)	C18B-C25B	1.44(3)
C1-C2	1.395(8)	C18B-C19B	1.62(3)
C1-H1	0.9500	C18B-H18C	1.0000
C2-C3	1.361(8)	C19B-C20B	1.58(5)
C2-H2	0.9500	C19B-H19C	0.9900
C3-C4	1.415(8)	C19B-H19D	0.9900
C3-H3	0.9500	C20B-C21B	1.32(4)
C4-C5	1.399(8)	C20B-H20C	0.9900
C4-C9	1.403(7)	C20B-H20D	0.9900
C5-C6	1.363(8)	C21B-C22B	1.413(8)
C5-H5	0.9500	C21B-H21B	1.0000
C6-C7	1.406(7)	C22B-C23B	1.23(4)
C6-H6	0.9500	C22A-H22A	1.0000
C7-C8	1.381(7)	C23B-C24B	1.48(3)
C7-H7	0.9500	C23B-H23C	0.9900
C8-C9	1.427(7)	C23B-H23D	0.9900
C10-C15	1.380(7)	C24B-C25B	1.37(3)
C10-C11	1.424(8)	C24B-H24C	0.9500
C11-C12	1.382(8)	C25B-H25C	0.9500
C12-C13	1.379(9)		
C12-H12	0.9500	C18A-Pt-N2	95.6(3)
C13-C14	1.391(9)	C18B-Pt-N2	99.2(6)
C13-H13	0.9500	C18A-Pt-N1	168.2(2)
C14-C15	1.383(8)	C18B-Pt-N1	164.7(6)
C14-H14	0.9500	N2-Pt-N1	79.44(16)
C15-H15	0.9500	N1-Pt-C21A	99.6(2)
C16-H16A	0.9800	N2-Pt-C21A	159.57(19)
C16-H16B	0.9800	N1-Pt-C21B	97.6(2)
C16-H16C	0.9800	N2-Pt-C21B	161.6(2)
C17-H17A	0.9800	N1-Pt-C22A	97.6(2)
C17-H17B	0.9800	N2-Pt-C22A	161.6(2)
C17-H17C	0.9800	N1-Pt-C22B	99.6(2)
C18A-C25A	1.476(11)	N2-Pt-C22B	159.57(19)
C18A-C19A	1.516(10)	C18A-Pt-C22A	90.5(3)
C18A-H18	1.0000	C18B-Pt-C22B	87.0(6)
C19A-C20A	1.518(12)	C18B-Pt-C21B	78.8(6)
C19A-H19A	0.9900	C18A-Pt-C21A	81.3(3)
C19A-H19B	0.9900	C22A-Pt-C21A	38.7(2)
C20A-C21A	1.614(11)	C22B-Pt-C21B	38.7(2)

C1-N1-C9	119.6(5)	N3-C16-H16A	109.5
C1-N1-Pt	127.7(4)	N3-C16-H16B	109.5
C9-N1-Pt	112.2(3)	H16A-C16-H16B	109.5
C8-N2-C10	116.3(4)	N3-C16-H16C	109.5
C8-N2-Pt	115.7(3)	H16A-C16-H16C	109.5
C10-N2-Pt	127.8(3)	H16B-C16-H16C	109.5
C11-N3-C16	111.9(5)	N3-C17-H17A	109.5
C11-N3-C17	115.3(5)	N3-C17-H17B	109.5
C16-N3-C17	111.4(5)	H17A-C17-H17B	109.5
N1-C1-C2	122.2(6)	N3-C17-H17C	109.5
N1-C1-H1	118.9	H17A-C17-H17C	109.5
C2-C1-H1	118.9	H17B-C17-H17C	109.5
C3-C2-C1	119.0(5)	C25A-C18A-C19A	110.6(7)
C3-C2-H2	120.5	C25A-C18A-Pt	112.5(5)
C1-C2-H2	120.5	C19A-C18A-Pt	107.6(5)
C2-C3-C4	120.5(5)	C25A-C18A-H18	108.7
C2-C3-H3	119.8	C19A-C18A-H18	108.7
C4-C3-H3	119.8	Pt-C18A-H18	108.7
C5-C4-C9	119.2(5)	C18A-C19A-C20A	109.4(6)
C5-C4-C3	124.0(5)	C18A-C19A-H19A	109.8
C9-C4-C3	116.8(5)	C20A-C19A-H19A	109.8
C6-C5-C4	119.3(5)	C18A-C19A-H19B	109.8
C6-C5-H5	120.3	C20A-C19A-H19B	109.8
C4-C5-H5	120.3	H19A-C19A-H19B	108.2
C5-C6-C7	122.0(5)	C19A-C20A-C21A	110.8(7)
C5-C6-H6	119.0	C19A-C20A-H20A	109.5
C7-C6-H6	119.0	C21A-C20A-H20A	109.5
C8-C7-C6	120.7(5)	C19A-C20A-H20B	109.5
C8-C7-H7	119.7	C21A-C20A-H20B	109.5
C6-C7-H7	119.7	H20A-C20A-H20B	108.1
C7-C8-N2	126.7(4)	C22A-C21A-C20A	121.7(6)
C7-C8-C9	117.1(4)	C22A-C21A-Pt	70.4(3)
N2-C8-C9	116.1(5)	C20A-C21A-Pt	109.7(4)
N1-C9-C4	121.8(5)	C22A-C21A-H21A	115.5
N1-C9-C8	116.5(5)	C20A-C21A-H21A	115.5
C4-C9-C8	121.6(5)	Pt-C21A-H21A	115.5
C15-C10-C11	119.2(5)	C21A-C22A-C23A	122.0(7)
C15-C10-N2	121.2(5)	C21A-C22A-Pt	70.9(3)
C11-C10-N2	119.6(5)	C23A-C22A-Pt	114.5(6)
C12-C11-N3	122.7(5)	C21A-C22A-H22A	114.1
C12-C11-C10	118.4(5)	C23A-C22A-H22A	114.1
N3-C11-C10	118.9(5)	Pt-C22A-H22A	114.1
C13-C12-C11	121.7(6)	C24A-C23A-C22A	121.5(11)
C13-C12-H12	119.1	C24A-C23A-H23A	107.0
C11-C12-H12	119.1	C22A-C23A-H23A	107.0
C12-C13-C14	119.9(5)	C24A-C23A-H23B	107.0
C12-C13-H13	120.1	C22A-C23A-H23B	107.0
C14-C13-H13	120.1	H23A-C23A-H23B	106.7
C15-C14-C13	119.3(6)	C25A-C24A-C23A	130.6(9)
C15-C14-H14	120.3	C25A-C24A-H24A	114.7
C13-C14-H14	120.3	C23A-C24A-H24A	114.7
C10-C15-C14	121.5(6)	C24A-C25A-C18A	127.2(7)
C10-C15-H15	119.2	C24A-C25A-H25A	116.4
C14-C15-H15	119.2	C18A-C25A-H25A	116.4

C25B-C18B-C19B	109.9(15)	H20C-C20B-H20D	107.6
C25B-C18B-Pt	112.1(13)	C19B-C20B-C21B	111(2)
C19B-C18B-Pt	106.9(12)	C20B-C21B-C22B	128(2)
C25B-C18B-H18C	109.3	C21B-C22B-C23B	138(2)
C19B-C18B-H18C	109.3	C22B-C23B-C24B	116(2)
Pt-C18B-H18C	109.3	C24B-C23B-H23C	108.2
C20B-C19B-C18B	105(2)	C24B-C23B-H23D	108.2
C20B-C19B-H19C	110.7	H23C-C23B-H23D	107.4
C18B-C19B-H19C	110.7	C25B-C24B-C23B	128(2)
C20B-C19B-H19D	110.7	C25B-C24B-H24C	116.0
C18B-C19B-H19D	110.7	C23B-C24B-H24C	116.0
H19C-C19B-H19D	108.8	C24B-C25B-C18B	126.7(19)
C19B-C20B-H20C	108.7	C24B-C25B-H25C	116.6
C19B-C20B-H20D	108.7	C18B-C25B-H25C	116.6

Table 5. Anisotropic displacement parameters ($Å^2 x 10^3$) for jcp08. 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}
Pt	37.0(1)	13.6(1)	10.6(1)	0.1(1)	-1.7(1)	4.0(1)
N1	4(2)	21(2)	15(3)	-2(2)	-1(2)	1(2)
N2	31(2)	14(2)	10(2)	7(2)	-12(2)	-9(3)
N3	16(2)	23(3)	51(3)	0(3)	2(2)	-1(2)
C1	9(3)	31(3)	12(3)	-3(3)	-3(3)	4(2)
C2	13(3)	25(3)	25(3)	-12(3)	-2(2)	-5(2)
C3	17(3)	20(3)	29(3)	-1(3)	0(3)	-4(2)
C4	14(3)	16(3)	23(3)	-1(2)	1(2)	-6(2)
C5	22(3)	18(3)	24(3)	5(2)	1(2)	-4(2)
C6	20(3)	22(3)	16(3)	5(2)	3(2)	-1(2)
C7	5(2)	22(2)	12(3)	0(2)	2(2)	0(2)
C8	5(2)	16(2)	17(3)	-1(2)	-2(2)	5(2)
C9	6(2)	20(3)	15(3)	0(2)	-1(2)	3(2)
C10	16(3)	15(2)	10(3)	1(2)	2(2)	-6(2)
C11	20(3)	14(3)	22(3)	3(2)	2(2)	-4(2)
C12	29(3)	23(3)	22(3)	5(3)	-9(3)	-7(3)
C13	43(4)	20(3)	13(3)	0(2)	1(3)	-10(3)
C14	30(4)	19(2)	22(3)	-4(2)	9(3)	0(3)
C15	27(4)	22(3)	14(3)	4(2)	-7(3)	0(2)
C16	26(3)	30(3)	52(4)	-18(3)	11(2)	-4(3)
C17	21(3)	42(3)	78(5)	20(4)	0(4)	4(3)
C18A	13(4)	26(4)	16(4)	-6(4)	-4(3)	-2(3)
C19A	22(4)	33(5)	22(5)	4(4)	4(4)	-11(3)
C20A	20(4)	25(5)	25(5)	2(5)	2(4)	4(4)
C21A,C22B	49(3)	30(3)	15(3)	-4(3)	-17(2)	16(4)
C22A,C21B	44(4)	20(4)	9(3)	0(2)	-1(2)	1(2)
C23A	18(4)	12(6)	23(5)	12(5)	1(3)	4(5)
C24A	44(6)	35(5)	18(5)	2(4)	-2(5)	21(4)
C25A	49(6)	22(4)	18(4)	0(3)	6(4)	0(4)

Table 6. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for jcp08.

	x	y	z	U_{iso}
H1	891	1170	1107	21
H2	938	1323	1084	25
H3	935	1373	969	26
H5	885	1337	841	25
H6	805	1232	758	23
H7	745	1081	788	15
H12	368	888	756	29
H13	579	776	727	30
H14	864	767	786	29
H15	932	871	873	25
H16A	227	939	914	43
H16B	223	1044	933	43
H16C	398	983	954	43
H17A	314	1050	756	56
H17B	186	1093	815	56
H17C	163	989	795	56
H18	583	855	977	22
H19A	418	817	1084	31
H19B	375	916	1055	31
H20A	594	869	1173	28
H20B	435	945	1168	28
H21A	671	1054	1150	38
H22A	973	1020	1136	29
H23A	1095	875	1127	21
H23B	934	858	1182	21
H24A	961	745	1098	39
H25A	739	738	1025	36
H18C	762	835	977	10
H19C	940	765	1080	10
H19D	1059	834	1033	10
H20C	919	864	1171	10
H20D	1103	906	1137	10
H21C	967	1023	1135	29
H22C	691	1058	1144	38
H23C	449	999	1137	10
H23D	557	950	1198	10
H24C	407	838	1135	10
H25C	556	770	1049	10

Principal mean square atomic displacements U for jcp08 [Å^2]

0.0378	0.0130	0.0104	Pt
0.0217	0.0144	0.0037	N1
0.0412	0.0108	0.0035	N2
0.0512	0.0230	0.0160	N3
0.0321	0.0128	0.0067	C1
0.0371	0.0185	0.0077	C2
0.0289	0.0227	0.0143	C3
0.0239	0.0202	0.0092	C4
0.0274	0.0233	0.0124	C5
0.0247	0.0214	0.0122	C6
0.0218	0.0121	0.0047	C7
0.0193	0.0156	0.0028	C8
0.0209	0.0148	0.0057	C9
0.0214	0.0114	0.0082	C10
0.0234	0.0223	0.0113	C11
0.0394	0.0181	0.0159	C12
0.0467	0.0160	0.0131	C13
0.0362	0.0212	0.0141	C14
0.0305	0.0225	0.0101	C15
0.0653	0.0237	0.0189	C16
0.0874	0.0334	0.0200	C17
0.0288	0.0175	0.0076	C18A
0.0402	0.0248	0.0117	C19A
0.0293	0.0234	0.0177	C20A
0.0644	0.0227	0.0076	C21A
0.0445	0.0202	0.0089	C22A
0.0305	0.0178	0.0042	C23A
0.0612	0.0205	0.0155	C24A
0.0499	0.0221	0.0172	C25A
(0.0445	0.0202	0.0089	C21B)
(0.0644	0.0227	0.0076	C22B)

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MODEL FITTING FOR jcp08 in P2(1)2(1)2(1) with sadabs

ORTHOGONAL COORDINATES FROM jcp09

** MODEL INVERTED **

ATOM MODEL DEVIATION

PT	PT	0.148
N1	N1	0.109
N2	N2	0.196
N3	N3	0.270
C1	C1	0.084
C2	C2	0.263
C3	C3	0.239
C4	C4	0.066
C5	C5	0.073
C6	C6	0.121
C7	C7	0.193
C8	C8	0.207
C9	C9	0.133
C10	C10	0.130
C11	C15	0.068
C12	C14	0.201
C13	C13	0.305
C14	C12	0.315
C15	C11	0.236
C16	C17	0.399
C17	C16	0.425
C18A	C18	0.078
C19A	C25	0.093
C20A	C24	0.195
C21A	C23	0.163
C22A	C22	0.126
C23A	C21	0.317
C24A	C20	0.181
C25A	C19	0.115

WEIGHTED R.M.S. DEVIATION = 0.2111 ANGSTROMS

Summary of Shortest Inter Contacts with d(I-J) < R(I) + R(J) + 0.2 of Residue # 1 to Neighbouring ARU'S

Nr	ARU	Nr.Cont.	d(min)	Del	XHn	X	- At(I)		At(J)	- Y	YHn	Note	Partaking ARU's in Close Contact Resd.
1	[3455.01]	20	2.5025	0.10	0	C(23B)	-*H(23C)	...	H(5)	-C(5)	1		3455.01
2	[3555.01]	20	2.5025	0.10	1	C(5)	- H(5)	...	*H(23C)	-C(23B)	0		3555.01
3	[2565.01]	11	2.2806	-0.12	1	C(7)	- H(7)	...	*H(23D)	-C(23B)	0	<	2565.01
4	[4545.01]	1	3.0458	0.15	1	C(5)	- C(6)	...	H(13)	-C(13)	1		4545.01
5	[4645.01]	2	2.5938	0.19	1	C(6)	- H(6)	...	H(14)	-C(14)	1		4645.01
6	[1655.01]	6	2.4195	0.02	0	C(20B)	-*H(20D)	...	*H(24C)	-C(24B)	0		1655.01
7	[3465.01]	15	2.1954	-0.20	0	C(25B)	-*H(25C)	...	*H(19D)	-C(19B)	0	<<	3465.01
8	[3565.01]	15	2.1954	-0.20	0	C(19B)	-*H(19D)	...	*H(25C)	-C(25B)	0	<<	3565.01
9	[2465.01]	4	2.4581	0.06	3	C(17)	- H(17A)	...	*H(20B)	-C(20A)	1		2465.01
10	[1455.01]	6	2.4195	0.02	0	C(24B)	-*H(24C)	...	*H(20D)	-C(20B)	0		1455.01
11	[2564.01]	11	2.2806	-0.12	0	C(23B)	-*H(23D)	...	H(7)	-C(7)	1	<	2564.01
12	[4555.01]	1	3.0458	0.15	1	C(13)	- H(13)	...	C(6)	-C(5)	1		4555.01
13	[4655.01]	2	2.5938	0.19	1	C(14)	- H(14)	...	H(6)	-C(6)	1		4655.01
14	[2464.01]	4	2.4581	0.06	1	C(20A)	-*H(20B)	...	H(17A)	-C(17)	3		2464.01

Symbols :: < denotes contacts less than the sum of the van der Waals Radii and << contacts less than this sum minus 0.2 Angstrom.
NR.CONT. = Number of short contacts from current ARU to surrounding ARU's (from list above).

Asymmetric Residue Unit (= ARU) Code List

ARU-CODE	Symmetry-Code	sym	TX	TY	TZ	Ires	x(cen)	y(cen)	z(cen)
[3455.01]	= -1/2+x,1/2-y,-z	= [3	-1	0	0	1]	-0.270	-0.009	-0.007
[3555.01]	= 1/2+x,1/2-y,-z	= [3	0	0	0	1]	0.730	-0.009	-0.007
[2565.01]	= 1/2-x,1-y,1/2+z	= [2	0	1	0	1]	0.270	0.491	0.507
[4545.01]	= -x,-1/2+y,1/2-z	= [4	0	-1	0	1]	-0.230	0.009	0.493
[4645.01]	= 1-x,-1/2+y,1/2-z	= [4	1	-1	0	1]	0.770	0.009	0.493
[1655.01]	= 1+x,y,z	= [1	1	0	0	1]	1.230	0.509	0.007
[3465.01]	= -1/2+x,3/2-y,-z	= [3	-1	1	0	1]	-0.270	0.991	-0.007
[3565.01]	= 1/2+x,3/2-y,-z	= [3	0	1	0	1]	0.730	0.991	-0.007
[2465.01]	= -1/2-x,1-y,1/2+z	= [2	-1	1	0	1]	-0.730	0.491	0.507
[1455.01]	= -1+x,y,z	= [1	-1	0	0	1]	-0.770	0.509	0.007
[2564.01]	= 1/2-x,1-y,-1/2+z	= [2	0	1	-1	1]	0.270	0.491	-0.493
[4555.01]	= -x,1/2+y,1/2-z	= [4	0	0	0	1]	-0.230	1.009	0.493
[4655.01]	= 1-x,1/2+y,1/2-z	= [4	1	0	0	1]	0.770	1.009	0.493
[2464.01]	= -1/2-x,1-y,-1/2+z	= [2	-1	1	-1	1]	-0.730	0.491	-0.493

Note: Symmetry Operations Refer to the Coordinates listed in the Fractional Coordinate Table given above

X(J) = X(sym) + TX , Y(J) = Y(sym) + TY , Z(J) = Z(sym) + TZ,

SYM - Number of the Symmetry Operator.
Ires - Residue Number.
TX, TY, TZ - Unit Cell Translation