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trans-Chloro[(*E*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl]bis(tricyclohexylphosphine)platinum(II)–*trans*-chloro[(*Z*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl]bis(tricyclohexylphosphine)platinum(II) (1/1) at 120 K

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.031
wR factor = 0.073
Data-to-parameter ratio = 16.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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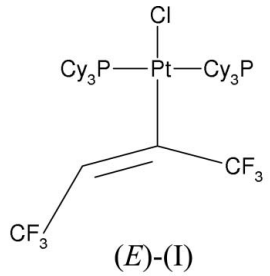
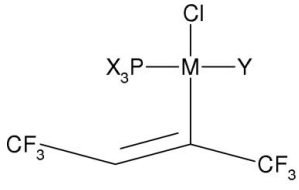
The title cocrystal, $[PtCl(C_4HF_6)(C_{18}H_{33}P)_2]$, contains molecules with a random distribution of *E* and *Z* alkenyl isomers in essentially equal numbers. This is indicative of the isomerization of the *E* form of the Pt complex in the course of attempting to carry out a reaction between it and tricyclohexyltin 4-chlorobenzenethiolate in acetone as solvent.

Comment

The cocrystal, (*E*/*Z*)-(I), a 1:1 mixture of *trans*-chloro[(*E*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl]bis(tricyclohexylphosphine)platinum(II), (*E*)-(I), and *trans*-chloro[(*Z*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl]bis(tricyclohexylphosphine)-platinum(II), (*Z*)-(I), was isolated from the attempted 1:1 reaction of a sample of (*E*)-(I) with tricyclohexyltin 4-chlorobenzenethiolate in Me_2CO. The starting compound, (*E*)-(I), had been prepared by the published procedure from *trans*-$[PtH\{P(C_6H_{11})_3\}_2(MeOH)]PF_6$ and $F_3CC{\equiv}CCF_3$, and had been shown by NMR to contain only an (*E*)-alkenyl group (Attig *et al.*, 1979).



(*E*)-(I)



(*Z*)-(I) X = Cy; Y = Cy_3P; M = Pt
(*Z*)-(II) X = Me; Y = Cp; M = Rh

Cy = Cyclohexyl
Cp = Cyclopentadienyl

The refinement of the structure was carried out on the basis of an asymmetric unit comprising a single 'average' molecule in which the alkenyl C atom not bonded to Pt and the CF_3 group attached to it are both distributed over pairs of sites of equal occupancy, with one set, C38*A* and C40*A* (Fig.1),

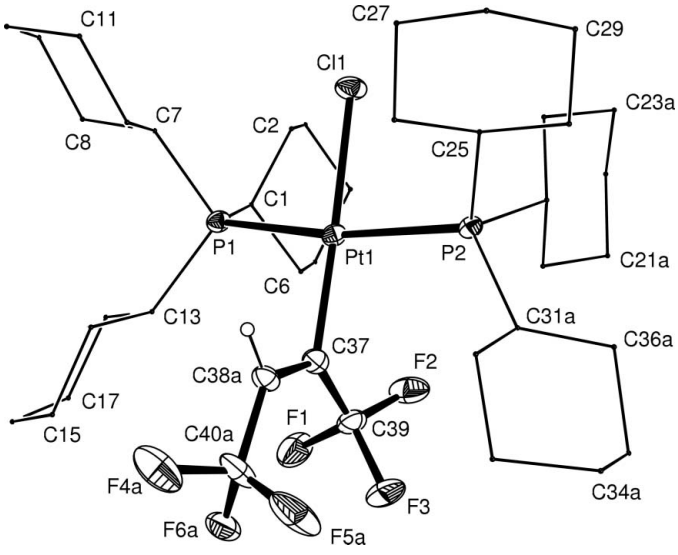


Figure 1
The *E* isomer of (I). Displacement ellipsoids are shown at the 20% probability level and the alkenyl H atom as a small sphere of arbitrary radius; other H atoms have been omitted. For clarity, the cyclohexyl groups are represented only by thin lines representing the bonds to their constituent C atoms, only some of which are labelled, because the strictly cyclic labelling of these groups allows the identity of the remainder to be worked out.

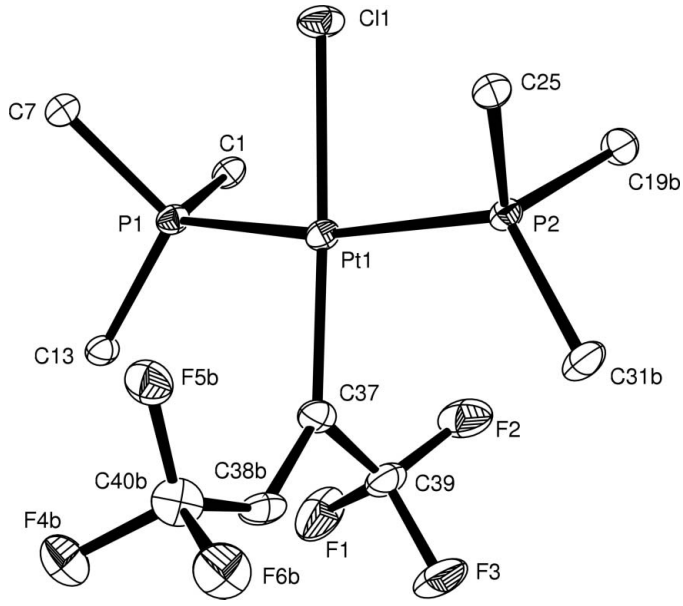


Figure 2
The *Z* isomer of (I). Displacement ellipsoids are shown at the 20% probability level. For clarity the cyclohexyl groups are represented by only the C atoms directly bonded to P, and all H atoms have been omitted.

corresponding to the *E* isomer with *cis* CF_3 groups and the other, C38*B* and C40*B* (Fig. 2), to the *Z* isomer with *trans* CF_3 groups. This is the justification for the presumption of a random distribution of essentially equal numbers of molecules with *E* and *Z* forms in the cocrystal. There is also disorder in two of the cyclohexyl groups attached to P2, which is not related in any obvious way to the disorder of the alkenyl group. In these groups defined, respectively, by C19–C24 and C30–C36, all of the atoms have been dealt with in pairs of equal occupancy, with suffix *A* for one orientation of the group and suffix *B* for the other. Selected geometric parameters for cocrystalline (*E*/*Z*)-(I) are given in Table 1. The coordination of Pt is square planar but with slight tetrahedral distortion, as shown by the displacements, all approximately 0.11 Å, of P1 and P2 to one side, and Cl1 and C37 to the other, of the plane defined by these four atoms. The displacement of the Pt atom from this plane is only 0.0283 (12) Å. The *E* and *Z* conformations of the butenyl groups are clearly seen from the torsion angles given in Table 1. The C—C distances in these groups are disappointingly disparate, with C═C distances of 1.327 (13) and 1.402 (13) Å and C—C (to the CF_3 groups) ranging over 1.398 (16)–1.496 (6) Å. This, along with the variation in bond angles in the butenyl groups, may be attributable to the superposition of the two conformations in the disordered 'average' molecule rather than to real differences in the bonding of the (*E*)- and (*Z*)-butenyl groups. The other bond lengths and bond angles in (*E*/*Z*)-(I), summarized in Table 2, are unremarkable. The only interaction between the molecules is in the form of van der Waals contacts. The content of the unit cell is shown in a highly schematic manner in Fig. 3.

Recourse to the Cambridge Structural Database (CSD; Version 5.26; Allen, 2002) by means of the Chemical Database Service of the EPSRC (CDS; Fletcher *et al.*, 1996) reveals the presence of data for only one analogue of (*E*/*Z*)-(I). This is the compound chloro-(*trans*-1,1,1,4,4,4-hexafluorobut-2-en-2-yl)-(η^5-pentamethylcyclopentadienyl)(trimethylphosphine)-rhodium (CSD code WIYZOT; Selmeczy & Jones, 2000), in which the CF_3 groups of the hexafluorobutenyl substituent are *trans* to one another and the compound is therefore here designated (*Z*)-(II). Although the *Z* conformation of the butenyl substituent is clearly established in the proposed structure of (*Z*)-(II), the internal geometry of the group is rather poorly defined; for example, the C═C bond length, calculated from the coordinates extracted from the CSD entry, is only 1.11 (3) Å, and the C—C bond lengths are very long. Nevertheless, the structure of (*Z*)-(II) clearly provides an authentic example of the butenyl substituent in the *Z* conformation. The paper of Selmeczy & Jones (2000) and the references within it also provide much information regarding the unpredictability of reactions such as those producing (*E*)-(I) and (*Z*)-(II), especially where hexafuorobut-2-yne is involved. Furthermore, Selmeczy & Jones (2000) also discuss, and summarize mechanisms for, the isomerization of such compounds. Thus, although no specific mechanism is invoked, the paper of Selmeczy & Jones (2000) clearly supports the interpretation of the structure of (*E*/*Z*)-(I) reported here as resulting from the partial isomerization of (*E*)-(I).

Experimental

A solution of (*E*)-(I) (Attig *et al.*, 1979) and $(C_6H_{11})_3SnSC_6H_4Cl$-*p* (each 1 mmol) in Me_2CO (15 ml) was refluxed for 30 min. Crystals of (*E*/*Z*)-(I) were formed on slow evaporation of the solvent at room temperature. IR (KBr): 1600 cm^{-1} (C═C).

Crystal data

$[PtCl(C_4HF_6)(C_{18}H_{33}P)_2]$	D_x = 1.524 Mg m^{-3}
M_r = 954.42	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 44847 reflections
a = 14.3933 (2) Å	θ = 2.9–27.5°
b = 17.5714 (3) Å	μ = 3.57 mm^{-1}
c = 17.5270 (3) Å	T = 120 (2) K
β = 110.2621 (10)°	Block, colourless
V = 4158.45 (12) Å^3	0.36 × 0.18 × 0.12 mm
Z = 4	

Data collection

Nonius KappaCD diffractometer	7588 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.042
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	θ_{max} = 27.5°
T_{min} = 0.457, T_{max} = 0.652	$h = -18 \rightarrow 18$
53705 measured reflections	$k = -22 \rightarrow 21$
9510 independent reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 5.1608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.031	$(\Delta/\sigma)_{max}$ = 0.003
$wR(F^2)$ = 0.074	$\Delta\rho_{max}$ = 0.88 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.98 e Å^{-3}
9510 reflections	
568 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Pt1—C37	2.033 (4)	C37—C38*A*	1.402 (13)
Pt1—P1	2.3426 (9)	C37—C39	1.496 (6)
Pt1—P2	2.3535 (9)	C38*A*—C40*A*	1.493 (13)
Pt1—Cl1	2.3688 (9)	C38*B*—C40*B*	1.398 (16)
C37—C38*B*	1.327 (13)		
C37—Pt1—P1	94.52 (10)	C38*A*—C37—C39	128.7 (5)
C37—Pt1—P2	95.55 (10)	C38*B*—C37—Pt1	138.9 (6)
P1—Pt1—P2	168.08 (3)	C38*A*—C37—Pt1	111.0 (5)
C37—Pt1—Cl1	175.69 (11)	C39—C37—Pt1	120.3 (3)
P1—Pt1—Cl1	86.29 (3)	C37—C38*A*—C40*A*	123.5 (10)
P2—Pt1—Cl1	84.14 (3)	C37—C38*B*—C40*B*	125.7 (10)
C38*B*—C37—C39	100.8 (6)		
Pt1—C37—C38*A*—C40*A*	178.6 (8)	C39—C37—C38*A*—C40*A*	−2.8 (14)
Pt1—C37—C38*B*—C40*B*	−2.2 (19)	C39—C37—C38*B*—C40*B*	178.5 (11)

Table 2
Geometric parameters (Å, °) for structural components of (*E*/*Z*)-(I) expressed as ranges; the ranges are somewhat extended by the inclusion of values associated with disordered atoms.

Group		Min.	Max.
CF_3	C—F	1.297 (10)	1.368 (9)
	F—C—F	102.0 (9)	106.5 (7)
	F—C—C	110.0 (10)	119.3 (9)
Phosphine	C—P	1.843 (3)	1.858 (4)
	C—P—Pt	108.61 (12)	118.53 (15)
	C—P—C	102.30 (17)	109.17 (19)
Cyclohexyl	C—C	1.402 (9)	1.628 (9)
	C—C—P	110.6 (2)	125.2 (4)
	C—C—C	103.5 (7)	116.7 (9)

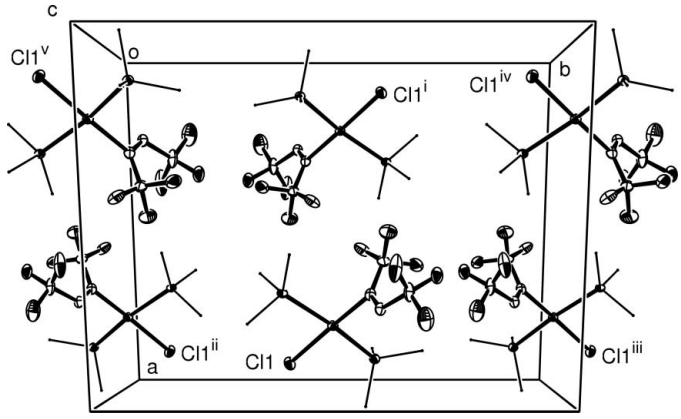


Figure 3
The packing of the molecules in the cell of (*E*/*Z*)-(I). Displacement ellipsoids are shown at the 20% probability level. For clarity, all H atoms have been omitted and the cyclohexyl groups are indicated simply by thin line P—C bonds. Selected atoms are labelled. The example shown employs molecules of the *E* form, as in Fig. 1. [Symmetry codes: (i) $1-x, 1-y, 1-z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$; (iii) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (iv) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$; (v) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$.]

The disorder in the hexafluorobutenyl substituent and in two of the four cyclohexyl groups noted in the *Comment* text was dealt with by standard techniques. Although subsidiary calculations, with isotropic displacement parameters constrained to be equal for atoms in pairs of the same type and connectivity, indicated occupancies of 0.441 (4) and 0.559 (4) for the disordered atoms of the *cis* (E form) and *trans* (*Z* form) hexafluorobutenyl groups, respectively, fixing these at 0.5 rather than at the refined values produced slightly better *R* values for the same mode of refinement. Some residual disorder is still apparent in this part of the molecule, as evidenced by rather extreme anisotropic displacement parameters as, for example, in the case of F4*A* and F5*A*. In order to permit interatomic distances within the disordered cyclohexyl groups to be restrained to be equal (within 0.02 Å) to those within a comparatively ordered cyclohexyl group (that defined by C1–C6 was used for this purpose), ordered atoms such as C19, C31, C32 and C35 were artificially split into pairs as, for example, C19*A*/C19*B*. For each such pair, the atomic coordinates were refined as free variables and the anisotropic displacement parameters of the two atoms were constrained to be equal. In this way, all six C atoms of the cyclohexyl group were made available for application of similarity restraints to the geometry of both orientations of the disordered groups. In the final stage of the calculations, H atoms were introduced in calculated positions, taking full account of the disorder noted above, with C—H set to 0.95, 0.99 and 1.00 Å for H atoms attached to alkene, methylene and tertiary C atoms, respectively, and refined with a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$ in all cases.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

We acknowledge the use of both the EPSRC's Chemical Database Service at Daresbury and X-ray crystallographic service at Southampton.

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supporting information

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trans-Chloro[(*E*)-1,1,1,4,4,4-hexafluorobut-2-en-2-yl]bis(tricyclohexylphosphine)platinum(II)–*trans*-chloro[(*Z*)-1,1,1,4,4,4-hexafluorobut-2-en-2yl]bis(tricyclohexylphosphine)platinum(II) (1/1) at 120 K

R. Alan Howie and James L. Wardell

***trans*-Chloro[(*E*)-1,1,1,4,4,4-hexafluorobut-2-en-2- yl]bis(tricyclohexylphosphine)platinum(II)–trans-chloro[(*Z*)-1,1,1,4,4,4-hexafluorobut-2-en-2- yl]bis(tricyclohexylphosphine)platinum(II) (1/1)**

Crystal data

$[PtCl(C_4HF_6)(C_{18}H_{33}P)_2]$
$M_r = 954.42$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.3933\ (2)$ Å
$b = 17.5714\ (3)$ Å
$c = 17.5270\ (3)$ Å
$\beta = 110.2621\ (10)°$
$V = 4158.45\ (12)$ Å^3
$Z = 4$
$F(000) = 1944$
$D_x = 1.524$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 44847 reflections
$\theta = 2.9–27.5°$
$\mu = 3.57$ mm^{-1}
$T = 120$ K
Block, colourless
0.36 × 0.18 × 0.12 mm

Data collection

Nonius KappaCD diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.457$, $T_{max} = 0.652$
53705 measured reflections
9510 independent reflections
7588 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -18\rightarrow18$
$k = -22\rightarrow21$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.074$
$S = 1.04$
9510 reflections
568 parameters
138 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 5.1608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.98$ e Å^{-3}

Special details

Experimental. Unit cell determined with *DIRAX* (Duisenberg, 1992; Duisenberg *et al.* 2000) but refined with the *DENZO*/*COLLECT HKL* package.
Refs as: Duisenberg, A. J. *M*. (1992). J. Appl. Cryst. 25, 92–96. Duisenberg, A. J. *M*., Hooft, *R*. W. W., Schreurs, A. *M. M*. & Kroon, J. (2000). J. Appl. Cryst. 33, 893–898.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.
Least-squares planes (*x*,*y*,*z* in crystal coordinates) and deviations from them (* indicates atom used to define plane)
3.7094 (105) *x* + 0.5402 (118) *y* + 14.3146 (73) *z* = 13.9386 (30)
* 0.1117 (0.0011) Cl1 * -0.1096 (0.0010) P1 * -0.1104 (0.0010) P2 * 0.1083 (0.0010) C37 0.0283 (0.0012) Pt1
Rms deviation of fitted atoms = 0.1100
9.3579 (238) *x* + 12.7506 (222) *y* - 7.6501 (290) *z* = 7.8235 (295)
Angle to previous plane (with approximate e.s.d.) = 88.41 (0.11)
* 0.0036 (0.0032) Pt1 * -0.0050 (0.0037) C39 * 0.0019 (0.0031) C37 * -0.0219 (0.0112) C38A_a * 0.0011 (0.0065) C40A_a * 0.0182 (0.0126) C38B_b * 0.0020 (0.0062) C40B_b
Rms deviation of fitted atoms = 0.0111

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* 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 $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.780491 (9)	0.493925 (7)	0.754821 (8)	0.03134 (5)	
Cl1	0.88937 (7)	0.40064 (5)	0.73595 (7)	0.0517 (3)	
P1	0.87733 (7)	0.58309 (5)	0.71673 (6)	0.0337 (2)	
C1	0.8549 (2)	0.5784 (2)	0.6061 (2)	0.0387 (8)	
H1	0.8934	0.6211	0.5938	0.046*	
C2	0.8881 (3)	0.5060 (2)	0.5748 (2)	0.0429 (9)	
H2A	0.8498	0.4621	0.5835	0.051*	
H2B	0.9590	0.4966	0.6056	0.051*	
C3	0.8722 (3)	0.5134 (2)	0.4840 (2)	0.0478 (10)	
H3A	0.9145	0.5549	0.4760	0.057*	
H3B	0.8923	0.4655	0.4643	0.057*	
C4	0.7647 (3)	0.5303 (3)	0.4349 (3)	0.0603 (12)	
H4A	0.7574	0.5379	0.3771	0.072*	
H4B	0.7232	0.4864	0.4380	0.072*	
C5	0.7293 (3)	0.6009 (3)	0.4663 (2)	0.0596 (12)	
H5A	0.6579	0.6086	0.4357	0.072*	
H5B	0.7656	0.6458	0.4571	0.072*	
C6	0.7457 (3)	0.5940 (2)	0.5570 (2)	0.0473 (10)	
H6A	0.7045	0.5520	0.5657	0.057*	
H6B	0.7248	0.6417	0.5764	0.057*	
C7	1.0111 (3)	0.5638 (2)	0.7655 (2)	0.0413 (9)	
H7	1.0222	0.5134	0.7434	0.050*	
C8	1.0804 (3)	0.6190 (2)	0.7443 (3)	0.0504 (10)	
H8A	1.0741	0.6702	0.7657	0.061*	

H8B	1.0610	0.6228	0.6845	0.061*	
C9	1.1882 (3)	0.5925 (3)	0.7805 (3)	0.0641 (13)	
H9A	1.1961	0.5437	0.7552	0.077*	
H9B	1.2319	0.6306	0.7685	0.077*	
C10	1.2183 (3)	0.5823 (3)	0.8716 (3)	0.0704 (15)	
H10A	1.2869	0.5626	0.8933	0.085*	
H10B	1.2169	0.6322	0.8972	0.085*	
C11	1.1503 (3)	0.5279 (3)	0.8932 (3)	0.0628 (13)	
H11A	1.1702	0.5248	0.9532	0.075*	
H11B	1.1574	0.4766	0.8727	0.075*	
C12	1.0422 (3)	0.5523 (2)	0.8578 (2)	0.0471 (9)	
H12A	1.0329	0.6004	0.8837	0.057*	
H12B	0.9998	0.5129	0.8695	0.057*	
C13	0.8532 (3)	0.68499 (19)	0.7312 (2)	0.0384 (8)	
H13	0.7797	0.6890	0.7166	0.046*	
C14	0.8966 (3)	0.7102 (2)	0.8199 (3)	0.0458 (10)	
H14A	0.9695	0.7143	0.8363	0.055*	
H14B	0.8814	0.6717	0.8551	0.055*	
C15	0.8535 (3)	0.7872 (2)	0.8314 (3)	0.0522 (11)	
H15A	0.7813	0.7821	0.8188	0.063*	
H15B	0.8837	0.8034	0.8888	0.063*	
C16	0.8730 (3)	0.8466 (2)	0.7768 (4)	0.0729 (16)	
H16A	0.8381	0.8941	0.7810	0.087*	
H16B	0.9448	0.8578	0.7957	0.087*	
C17	0.8395 (4)	0.8219 (2)	0.6896 (4)	0.0763 (16)	
H17A	0.8604	0.8605	0.6577	0.092*	
H17B	0.7662	0.8197	0.6681	0.092*	
C18	0.8804 (3)	0.7446 (2)	0.6775 (3)	0.0558 (11)	
H18A	0.9533	0.7475	0.6927	0.067*	
H18B	0.8520	0.7294	0.6196	0.067*	
P2	0.68959 (6)	0.38828 (5)	0.77267 (5)	0.02974 (19)	
C19A	0.6372 (3)	0.3377 (2)	0.6741 (2)	0.0401 (8)	0.50
H19A	0.5925	0.2980	0.6832	0.048*	0.50
C20A	0.5691 (10)	0.3909 (7)	0.6098 (7)	0.048 (3)	0.50
H20A	0.5223	0.4155	0.6324	0.057*	0.50
H20B	0.6096	0.4315	0.5977	0.057*	0.50
C21A	0.5101 (6)	0.3507 (5)	0.5308 (5)	0.0484 (19)	0.50
H21A	0.4612	0.3159	0.5405	0.058*	0.50
H21B	0.4735	0.3888	0.4898	0.058*	0.50
C22A	0.5778 (8)	0.3061 (6)	0.4990 (5)	0.057 (3)	0.50
H22A	0.6206	0.3417	0.4823	0.068*	0.50
H22B	0.5379	0.2769	0.4504	0.068*	0.50
C23A	0.6416 (6)	0.2522 (5)	0.5623 (4)	0.054 (2)	0.50
H23A	0.6866	0.2246	0.5402	0.065*	0.50
H23B	0.5991	0.2143	0.5761	0.065*	0.50
C24A	0.7039 (5)	0.2961 (4)	0.6408 (4)	0.0453 (19)	0.50
H24A	0.7449	0.2598	0.6818	0.054*	0.50
H24B	0.7488	0.3325	0.6277	0.054*	0.50

C19B	0.6372 (3)	0.3377 (2)	0.6741 (2)	0.0401 (8)	0.50
H19B	0.6989	0.3168	0.6680	0.048*	0.50
C20B	0.5776 (8)	0.2670 (5)	0.6658 (5)	0.071 (3)	0.50
H20C	0.5161	0.2796	0.6763	0.085*	0.50
H20D	0.6156	0.2306	0.7083	0.085*	0.50
C21B	0.5498 (9)	0.2282 (5)	0.5847 (5)	0.078 (3)	0.50
H21C	0.6075	0.1987	0.5827	0.094*	0.50
H21D	0.4957	0.1917	0.5799	0.094*	0.50
C22B	0.5173 (8)	0.2807 (5)	0.5139 (5)	0.070 (3)	0.50
H22C	0.4510	0.3011	0.5078	0.084*	0.50
H22D	0.5115	0.2519	0.4639	0.084*	0.50
C23B	0.5886 (8)	0.3467 (6)	0.5228 (5)	0.065 (3)	0.50
H23C	0.5618	0.3819	0.4762	0.078*	0.50
H23D	0.6531	0.3272	0.5226	0.078*	0.50
C24B	0.6040 (13)	0.3903 (7)	0.6040 (6)	0.086 (7)	0.50
H24C	0.6541	0.4308	0.6110	0.104*	0.50
H24D	0.5410	0.4147	0.6015	0.104*	0.50
C25	0.7717 (2)	0.31674 (19)	0.8418 (2)	0.0331 (7)	
H25	0.8092	0.2929	0.8094	0.040*	
C26	0.8509 (3)	0.3522 (2)	0.9158 (2)	0.0456 (9)	
H26A	0.8842	0.3944	0.8980	0.055*	
H26B	0.8194	0.3734	0.9532	0.055*	
C27	0.9271 (3)	0.2923 (3)	0.9601 (2)	0.0572 (12)	
H27A	0.9608	0.2730	0.9234	0.069*	
H27B	0.9778	0.3157	1.0079	0.069*	
C28	0.8783 (4)	0.2267 (3)	0.9877 (3)	0.0710 (15)	
H28A	0.8500	0.2451	1.0284	0.085*	
H28B	0.9286	0.1875	1.0139	0.085*	
C29	0.7965 (3)	0.1914 (2)	0.9163 (3)	0.0649 (13)	
H29A	0.7623	0.1518	0.9368	0.078*	
H29B	0.8263	0.1665	0.8796	0.078*	
C30	0.7210 (3)	0.2505 (2)	0.8683 (3)	0.0508 (10)	
H30A	0.6841	0.2701	0.9025	0.061*	
H30B	0.6728	0.2262	0.8197	0.061*	
C31A	0.5831 (3)	0.4050 (3)	0.8060 (2)	0.0489 (10)	0.50
H31A	0.5565	0.4542	0.7782	0.059*	0.50
C32A	0.6122 (3)	0.4270 (2)	0.8949 (2)	0.0443 (9)	0.50
H32A	0.6700	0.4617	0.9096	0.053*	0.50
H32B	0.6319	0.3808	0.9290	0.053*	0.50
C33A	0.5262 (6)	0.4666 (5)	0.9123 (6)	0.042 (2)	0.50
H33A	0.5458	0.4806	0.9705	0.051*	0.50
H33B	0.5055	0.5132	0.8790	0.051*	0.50
C34A	0.4422 (8)	0.4077 (7)	0.8894 (6)	0.053 (3)	0.50
H34A	0.3874	0.4249	0.9072	0.064*	0.50
H34B	0.4666	0.3580	0.9152	0.064*	0.50
C35A	0.4062 (3)	0.4009 (3)	0.7938 (3)	0.0759 (16)	0.50
H35A	0.3966	0.4518	0.7680	0.091*	0.50
H35B	0.3434	0.3720	0.7726	0.091*	0.50

C36A	0.4950 (4)	0.3559 (3)	0.7779 (4)	0.0249 (13)	0.50
H36A	0.5081	0.3072	0.8083	0.030*	0.50
H36B	0.4774	0.3445	0.7193	0.030*	0.50
C31B	0.5831 (3)	0.4050 (3)	0.8060 (2)	0.0489 (10)	0.50
H31B	0.5666	0.3505	0.8117	0.059*	0.50
C32B	0.6122 (3)	0.4270 (2)	0.8949 (2)	0.0443 (9)	0.50
H32C	0.6368	0.4801	0.9016	0.053*	0.50
H32D	0.6673	0.3939	0.9274	0.053*	0.50
C33B	0.5268 (7)	0.4206 (8)	0.9287 (6)	0.071 (3)	0.50
H33C	0.5225	0.3670	0.9445	0.085*	0.50
H33D	0.5442	0.4517	0.9789	0.085*	0.50
C34B	0.4285 (8)	0.4442 (9)	0.8746 (7)	0.072 (5)	0.50
H34C	0.4274	0.4998	0.8649	0.087*	0.50
H34D	0.3781	0.4320	0.8993	0.087*	0.50
C35B	0.4062 (3)	0.4009 (3)	0.7938 (3)	0.0759 (16)	0.50
H35C	0.3387	0.4130	0.7562	0.091*	0.50
H35D	0.4108	0.3453	0.8036	0.091*	0.50
C36B	0.4887 (6)	0.4284 (8)	0.7554 (5)	0.090 (4)	0.50
H36C	0.4736	0.4060	0.7006	0.108*	0.50
H36D	0.4871	0.4845	0.7500	0.108*	0.50
C37	0.6927 (3)	0.5734 (2)	0.7802 (2)	0.0408 (9)	
C39	0.6011 (3)	0.6009 (2)	0.7148 (3)	0.0541 (11)	
F1	0.6128 (2)	0.67065 (17)	0.6855 (2)	0.0983 (11)	
F2	0.57053 (19)	0.55666 (17)	0.64982 (17)	0.0774 (8)	
F3	0.5209 (2)	0.61073 (19)	0.7352 (2)	0.1052 (12)	
C38A	0.7296 (9)	0.5939 (6)	0.8625 (8)	0.040 (2)	0.50
H38A	0.7878	0.5693	0.8969	0.048*	0.50
C40A	0.6824 (8)	0.6523 (5)	0.8991 (6)	0.072 (3)	0.50
F4A	0.7516 (8)	0.6848 (6)	0.9645 (7)	0.117 (4)	0.50
F5A	0.6174 (7)	0.6236 (3)	0.9322 (5)	0.132 (4)	0.50
F6A	0.6384 (4)	0.7102 (3)	0.8556 (4)	0.0712 (15)	0.50
C38B	0.6898 (9)	0.6144 (8)	0.8429 (8)	0.050 (3)	0.50
H38B	0.6367	0.6495	0.8331	0.060*	0.50
C40B	0.7581 (7)	0.6105 (5)	0.9221 (6)	0.058 (2)	0.50
F4B	0.7977 (6)	0.6787 (4)	0.9529 (5)	0.067 (2)	0.50
F5B	0.8343 (4)	0.5635 (3)	0.9327 (3)	0.0573 (12)	0.50
F6B	0.7135 (4)	0.5881 (3)	0.9757 (3)	0.0708 (15)	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.03075 (8)	0.03668 (8)	0.03080 (8)	0.00114 (6)	0.01600 (6)	0.00202 (6)
Cl1	0.0546 (6)	0.0428 (5)	0.0764 (7)	0.0099 (4)	0.0466 (6)	0.0089 (5)
P1	0.0316 (5)	0.0368 (5)	0.0375 (5)	0.0015 (4)	0.0180 (4)	0.0028 (4)
C1	0.0328 (19)	0.048 (2)	0.040 (2)	0.0013 (16)	0.0187 (16)	0.0045 (16)
C2	0.042 (2)	0.050 (2)	0.043 (2)	0.0006 (17)	0.0212 (18)	0.0012 (17)
C3	0.048 (2)	0.060 (3)	0.043 (2)	0.0017 (19)	0.0250 (19)	−0.0012 (18)
C4	0.055 (3)	0.086 (3)	0.041 (2)	0.005 (2)	0.018 (2)	0.002 (2)

C5	0.049 (2)	0.087 (3)	0.044 (3)	0.015 (2)	0.017 (2)	0.013 (2)
C6	0.037 (2)	0.064 (3)	0.043 (2)	0.0087 (18)	0.0173 (18)	0.0082 (19)
C7	0.0309 (18)	0.045 (2)	0.049 (2)	0.0019 (16)	0.0148 (17)	−0.0035 (17)
C8	0.035 (2)	0.059 (3)	0.062 (3)	−0.0033 (18)	0.022 (2)	−0.006 (2)
C9	0.032 (2)	0.073 (3)	0.087 (4)	−0.002 (2)	0.020 (2)	−0.023 (3)
C10	0.034 (2)	0.074 (3)	0.090 (4)	0.010 (2)	0.005 (2)	−0.028 (3)
C11	0.060 (3)	0.054 (3)	0.059 (3)	0.022 (2)	0.001 (2)	−0.019 (2)
C12	0.049 (2)	0.042 (2)	0.045 (2)	0.0099 (18)	0.0091 (19)	−0.0051 (17)
C13	0.0355 (19)	0.0348 (19)	0.051 (2)	0.0001 (15)	0.0231 (17)	0.0019 (16)
C14	0.038 (2)	0.039 (2)	0.068 (3)	−0.0012 (16)	0.028 (2)	−0.0109 (19)
C15	0.041 (2)	0.039 (2)	0.085 (3)	−0.0044 (17)	0.034 (2)	−0.013 (2)
C16	0.063 (3)	0.036 (2)	0.148 (5)	−0.003 (2)	0.073 (3)	−0.003 (3)
C17	0.095 (4)	0.043 (3)	0.125 (5)	0.017 (2)	0.080 (4)	0.028 (3)
C18	0.062 (3)	0.040 (2)	0.085 (3)	0.0046 (19)	0.050 (3)	0.009 (2)
P2	0.0257 (4)	0.0365 (5)	0.0282 (5)	0.0011 (3)	0.0109 (4)	−0.0005 (4)
C19A	0.040 (2)	0.046 (2)	0.033 (2)	0.0000 (16)	0.0103 (16)	−0.0065 (16)
C20A	0.056 (6)	0.041 (6)	0.042 (7)	−0.005 (4)	0.013 (5)	−0.001 (4)
C21A	0.048 (5)	0.059 (5)	0.034 (4)	0.010 (4)	0.009 (4)	−0.009 (4)
C22A	0.045 (6)	0.088 (8)	0.037 (6)	0.004 (6)	0.013 (5)	−0.024 (5)
C23A	0.072 (6)	0.056 (5)	0.031 (4)	0.024 (4)	0.016 (4)	−0.011 (4)
C24A	0.047 (4)	0.046 (4)	0.041 (4)	0.016 (4)	0.013 (4)	0.000 (3)
C19B	0.040 (2)	0.046 (2)	0.033 (2)	0.0000 (16)	0.0103 (16)	−0.0065 (16)
C20B	0.092 (7)	0.046 (5)	0.048 (5)	−0.007 (5)	−0.010 (5)	−0.008 (4)
C21B	0.101 (8)	0.067 (7)	0.045 (6)	0.003 (6)	−0.001 (6)	−0.016 (5)
C22B	0.069 (7)	0.076 (7)	0.046 (6)	0.016 (6)	−0.004 (6)	−0.022 (5)
C23B	0.070 (7)	0.099 (9)	0.023 (5)	0.011 (7)	0.013 (5)	−0.011 (5)
C24B	0.140 (17)	0.072 (9)	0.027 (6)	−0.039 (10)	0.003 (8)	0.002 (6)
C25	0.0316 (18)	0.0366 (19)	0.0333 (19)	0.0028 (14)	0.0140 (15)	0.0018 (14)
C26	0.045 (2)	0.052 (2)	0.036 (2)	0.0085 (18)	0.0086 (18)	−0.0042 (17)
C27	0.055 (3)	0.076 (3)	0.033 (2)	0.022 (2)	0.007 (2)	0.002 (2)
C28	0.084 (4)	0.085 (4)	0.050 (3)	0.042 (3)	0.030 (3)	0.030 (3)
C29	0.072 (3)	0.053 (3)	0.086 (4)	0.019 (2)	0.048 (3)	0.027 (2)
C30	0.051 (2)	0.045 (2)	0.065 (3)	0.0076 (18)	0.031 (2)	0.014 (2)
C31A	0.0271 (19)	0.082 (3)	0.040 (2)	−0.0004 (18)	0.0134 (17)	−0.016 (2)
C32A	0.0311 (19)	0.063 (3)	0.040 (2)	0.0038 (17)	0.0136 (17)	−0.0090 (18)
C33A	0.042 (5)	0.055 (5)	0.037 (5)	0.016 (4)	0.022 (4)	−0.001 (4)
C34A	0.030 (6)	0.086 (9)	0.056 (7)	0.007 (5)	0.029 (5)	−0.003 (6)
C35A	0.027 (2)	0.141 (5)	0.065 (3)	−0.015 (3)	0.023 (2)	−0.031 (3)
C36A	0.020 (3)	0.031 (3)	0.027 (3)	−0.006 (2)	0.013 (3)	0.001 (3)
C31B	0.0271 (19)	0.082 (3)	0.040 (2)	−0.0004 (18)	0.0134 (17)	−0.016 (2)
C32B	0.0311 (19)	0.063 (3)	0.040 (2)	0.0038 (17)	0.0136 (17)	−0.0090 (18)
C33B	0.053 (7)	0.116 (10)	0.044 (6)	0.040 (7)	0.018 (5)	−0.002 (7)
C34B	0.043 (6)	0.114 (13)	0.070 (8)	0.010 (7)	0.032 (6)	−0.017 (8)
C35B	0.027 (2)	0.141 (5)	0.065 (3)	−0.015 (3)	0.023 (2)	−0.031 (3)
C36B	0.043 (5)	0.176 (13)	0.052 (6)	0.020 (7)	0.017 (5)	−0.016 (7)
C37	0.048 (2)	0.037 (2)	0.051 (2)	−0.0033 (16)	0.0351 (19)	−0.0001 (17)
C39	0.043 (2)	0.052 (3)	0.081 (3)	0.0038 (19)	0.039 (2)	0.006 (2)
F1	0.0573 (17)	0.0695 (19)	0.162 (3)	0.0108 (14)	0.0300 (19)	0.047 (2)

F2	0.0616 (17)	0.089 (2)	0.0743 (19)	0.0347 (15)	0.0140 (15)	0.0071 (16)
F3	0.0667 (19)	0.104 (2)	0.177 (4)	0.0031 (17)	0.083 (2)	−0.015 (2)
C38A	0.051 (7)	0.036 (6)	0.041 (7)	0.000 (4)	0.027 (6)	−0.004 (5)
C40A	0.116 (9)	0.034 (5)	0.078 (7)	0.002 (6)	0.048 (7)	−0.017 (5)
F4A	0.181 (12)	0.083 (5)	0.092 (6)	0.008 (7)	0.053 (7)	−0.032 (4)
F5A	0.244 (10)	0.052 (4)	0.194 (8)	−0.022 (5)	0.196 (8)	−0.026 (4)
F6A	0.088 (4)	0.044 (3)	0.106 (4)	0.000 (3)	0.064 (4)	−0.012 (3)
C38B	0.050 (7)	0.056 (8)	0.059 (8)	0.010 (5)	0.038 (6)	0.004 (6)
C40B	0.074 (7)	0.054 (6)	0.052 (6)	0.005 (5)	0.029 (5)	0.015 (5)
F4B	0.088 (5)	0.048 (4)	0.067 (5)	−0.008 (3)	0.028 (4)	−0.007 (3)
F5B	0.066 (3)	0.061 (3)	0.047 (3)	0.000 (2)	0.022 (2)	−0.009 (2)
F6B	0.090 (4)	0.073 (4)	0.061 (3)	−0.006 (3)	0.042 (3)	0.006 (3)

Geometric parameters (Å, º)

Pt1—C37	2.033 (4)	C19B—H19B	1.0000
Pt1—P1	2.3426 (9)	C20B—C21B	1.499 (10)
Pt1—P2	2.3535 (9)	C20B—H20C	0.9900
Pt1—Cl1	2.3688 (9)	C20B—H20D	0.9900
P1—C7	1.848 (4)	C21B—C22B	1.486 (10)
P1—C1	1.854 (4)	C21B—H21C	0.9900
P1—C13	1.858 (4)	C21B—H21D	0.9900
C1—C2	1.525 (5)	C22B—C23B	1.520 (11)
C1—C6	1.533 (5)	C22B—H22C	0.9900
C1—H1	1.0000	C22B—H22D	0.9900
C2—C3	1.534 (5)	C23B—C24B	1.563 (12)
C2—H2A	0.9900	C23B—H23C	0.9900
C2—H2B	0.9900	C23B—H23D	0.9900
C3—C4	1.517 (6)	C24B—H24C	0.9900
C3—H3A	0.9900	C24B—H24D	0.9900
C3—H3B	0.9900	C25—C30	1.530 (5)
C4—C5	1.515 (6)	C25—C26	1.533 (5)
C4—H4A	0.9900	C25—H25	1.0000
C4—H4B	0.9900	C26—C27	1.524 (5)
C5—C6	1.530 (5)	C26—H26A	0.9900
C5—H5A	0.9900	C26—H26B	0.9900
C5—H5B	0.9900	C27—C28	1.514 (6)
C6—H6A	0.9900	C27—H27A	0.9900
C6—H6B	0.9900	C27—H27B	0.9900
C7—C8	1.526 (5)	C28—C29	1.521 (7)
C7—C12	1.536 (5)	C28—H28A	0.9900
C7—H7	1.0000	C28—H28B	0.9900
C8—C9	1.531 (5)	C29—C30	1.528 (5)
C8—H8A	0.9900	C29—H29A	0.9900
C8—H8B	0.9900	C29—H29B	0.9900
C9—C10	1.512 (7)	C30—H30A	0.9900
C9—H9A	0.9900	C30—H30B	0.9900
C9—H9B	0.9900	C31A—C36A	1.471 (6)

C10—C11	1.507 (7)	C31A—C32A	1.516 (5)
C10—H10A	0.9900	C31A—H31A	1.0000
C10—H10B	0.9900	C32A—C33A	1.540 (8)
C11—C12	1.523 (6)	C32A—H32A	0.9900
C11—H11A	0.9900	C32A—H32B	0.9900
C11—H11B	0.9900	C33A—C34A	1.536 (11)
C12—H12A	0.9900	C33A—H33A	0.9900
C12—H12B	0.9900	C33A—H33B	0.9900
C13—C14	1.527 (5)	C34A—C35A	1.578 (10)
C13—C18	1.546 (5)	C34A—H34A	0.9900
C13—H13	1.0000	C34A—H34B	0.9900
C14—C15	1.529 (5)	C35A—C36A	1.607 (7)
C14—H14A	0.9900	C35A—H35A	0.9900
C14—H14B	0.9900	C35A—H35B	0.9900
C15—C16	1.507 (6)	C36A—H36A	0.9900
C15—H15A	0.9900	C36A—H36B	0.9900
C15—H15B	0.9900	C31B—C36B	1.402 (9)
C16—C17	1.499 (7)	C31B—C32B	1.516 (5)
C16—H16A	0.9900	C31B—H31B	1.0000
C16—H16B	0.9900	C32B—C33B	1.543 (9)
C17—C18	1.525 (6)	C32B—H32C	0.9900
C17—H17A	0.9900	C32B—H32D	0.9900
C17—H17B	0.9900	C33B—C34B	1.464 (11)
C18—H18A	0.9900	C33B—H33C	0.9900
C18—H18B	0.9900	C33B—H33D	0.9900
P2—C31B	1.843 (3)	C34B—C35B	1.540 (11)
P2—C31A	1.843 (3)	C34B—H34C	0.9900
P2—C19A	1.855 (4)	C34B—H34D	0.9900
P2—C19B	1.855 (4)	C35B—C36B	1.628 (9)
P2—C25	1.858 (3)	C35B—H35C	0.9900
C19A—C24A	1.478 (7)	C35B—H35D	0.9900
C19A—C20A	1.529 (11)	C36B—H36C	0.9900
C19A—H19A	1.0000	C36B—H36D	0.9900
C20A—C21A	1.525 (12)	C37—C38B	1.327 (13)
C20A—H20A	0.9900	C37—C38A	1.402 (13)
C20A—H20B	0.9900	C37—C39	1.496 (6)
C21A—C22A	1.499 (9)	C39—F2	1.322 (5)
C21A—H21A	0.9900	C39—F3	1.332 (4)
C21A—H21B	0.9900	C39—F1	1.361 (5)
C22A—C23A	1.506 (10)	C38A—C40A	1.493 (13)
C22A—H22A	0.9900	C38A—H38A	0.9500
C22A—H22B	0.9900	C40A—F6A	1.297 (10)
C23A—C24A	1.561 (9)	C40A—F5A	1.357 (10)
C23A—H23A	0.9900	C40A—F4A	1.358 (11)
C23A—H23B	0.9900	C38B—C40B	1.398 (16)
C24A—H24A	0.9900	C38B—H38B	0.9500
C24A—H24B	0.9900	C40B—F5B	1.333 (9)
C19B—C24B	1.478 (12)	C40B—F4B	1.356 (10)

C19B—C20B	1.489 (8)	C40B—F6B	1.368 (9)
C37—Pt1—P1	94.52 (10)	C20B—C19B—P2	121.7 (4)
C37—Pt1—P2	95.55 (10)	C24B—C19B—H19B	100.7
P1—Pt1—P2	168.08 (3)	C20B—C19B—H19B	100.7
C37—Pt1—Cl1	175.69 (11)	P2—C19B—H19B	100.7
P1—Pt1—Cl1	86.29 (3)	C19B—C20B—C21B	115.3 (8)
P2—Pt1—Cl1	84.14 (3)	C19B—C20B—H20C	108.4
C7—P1—C1	104.57 (16)	C21B—C20B—H20C	108.4
C7—P1—C13	109.17 (17)	C19B—C20B—H20D	108.4
C1—P1—C13	102.30 (17)	C21B—C20B—H20D	108.4
C7—P1—Pt1	111.89 (13)	H20C—C20B—H20D	107.5
C1—P1—Pt1	111.27 (12)	C22B—C21B—C20B	114.4 (7)
C13—P1—Pt1	116.59 (11)	C22B—C21B—H21C	108.7
C2—C1—C6	109.6 (3)	C20B—C21B—H21C	108.7
C2—C1—P1	116.8 (3)	C22B—C21B—H21D	108.7
C6—C1—P1	110.6 (2)	C20B—C21B—H21D	108.7
C2—C1—H1	106.4	H21C—C21B—H21D	107.6
C6—C1—H1	106.4	C21B—C22B—C23B	112.4 (8)
P1—C1—H1	106.4	C21B—C22B—H22C	109.1
C1—C2—C3	110.4 (3)	C23B—C22B—H22C	109.1
C1—C2—H2A	109.6	C21B—C22B—H22D	109.1
C3—C2—H2A	109.6	C23B—C22B—H22D	109.1
C1—C2—H2B	109.6	H22C—C22B—H22D	107.8
C3—C2—H2B	109.6	C22B—C23B—C24B	110.2 (9)
H2A—C2—H2B	108.1	C22B—C23B—H23C	109.6
C4—C3—C2	111.2 (3)	C24B—C23B—H23C	109.6
C4—C3—H3A	109.4	C22B—C23B—H23D	109.6
C2—C3—H3A	109.4	C24B—C23B—H23D	109.6
C4—C3—H3B	109.4	H23C—C23B—H23D	108.1
C2—C3—H3B	109.4	C19B—C24B—C23B	110.6 (9)
H3A—C3—H3B	108.0	C19B—C24B—H24C	109.5
C5—C4—C3	111.0 (4)	C23B—C24B—H24C	109.5
C5—C4—H4A	109.4	C19B—C24B—H24D	109.5
C3—C4—H4A	109.4	C23B—C24B—H24D	109.5
C5—C4—H4B	109.4	H24C—C24B—H24D	108.1
C3—C4—H4B	109.4	C30—C25—C26	110.2 (3)
H4A—C4—H4B	108.0	C30—C25—P2	116.7 (2)
C4—C5—C6	111.3 (4)	C26—C25—P2	113.3 (2)
C4—C5—H5A	109.4	C30—C25—H25	105.1
C6—C5—H5A	109.4	C26—C25—H25	105.1
C4—C5—H5B	109.4	P2—C25—H25	105.1
C6—C5—H5B	109.4	C27—C26—C25	110.1 (3)
H5A—C5—H5B	108.0	C27—C26—H26A	109.6
C5—C6—C1	110.8 (3)	C25—C26—H26A	109.6
C5—C6—H6A	109.5	C27—C26—H26B	109.6
C1—C6—H6A	109.5	C25—C26—H26B	109.6
C5—C6—H6B	109.5	H26A—C26—H26B	108.2

C1—C6—H6B	109.5	C28—C27—C26	110.9 (4)
H6A—C6—H6B	108.1	C28—C27—H27A	109.5
C8—C7—C12	111.3 (3)	C26—C27—H27A	109.5
C8—C7—P1	115.8 (3)	C28—C27—H27B	109.5
C12—C7—P1	112.8 (3)	C26—C27—H27B	109.5
C8—C7—H7	105.3	H27A—C27—H27B	108.0
C12—C7—H7	105.3	C27—C28—C29	111.1 (4)
P1—C7—H7	105.3	C27—C28—H28A	109.4
C7—C8—C9	111.1 (4)	C29—C28—H28A	109.4
C7—C8—H8A	109.4	C27—C28—H28B	109.4
C9—C8—H8A	109.4	C29—C28—H28B	109.4
C7—C8—H8B	109.4	H28A—C28—H28B	108.0
C9—C8—H8B	109.4	C28—C29—C30	112.1 (4)
H8A—C8—H8B	108.0	C28—C29—H29A	109.2
C10—C9—C8	110.6 (4)	C30—C29—H29A	109.2
C10—C9—H9A	109.5	C28—C29—H29B	109.2
C8—C9—H9A	109.5	C30—C29—H29B	109.2
C10—C9—H9B	109.5	H29A—C29—H29B	107.9
C8—C9—H9B	109.5	C29—C30—C25	111.1 (3)
H9A—C9—H9B	108.1	C29—C30—H30A	109.4
C11—C10—C9	111.6 (4)	C25—C30—H30A	109.4
C11—C10—H10A	109.3	C29—C30—H30B	109.4
C9—C10—H10A	109.3	C25—C30—H30B	109.4
C11—C10—H10B	109.3	H30A—C30—H30B	108.0
C9—C10—H10B	109.3	C36A—C31A—C32A	113.1 (4)
H10A—C10—H10B	108.0	C36A—C31A—P2	121.0 (3)
C10—C11—C12	112.3 (4)	C32A—C31A—P2	113.7 (2)
C10—C11—H11A	109.1	C36A—C31A—H31A	101.8
C12—C11—H11A	109.1	C32A—C31A—H31A	101.8
C10—C11—H11B	109.1	P2—C31A—H31A	101.8
C12—C11—H11B	109.1	C31A—C32A—C33A	111.3 (4)
H11A—C11—H11B	107.9	C31A—C32A—H32A	109.4
C11—C12—C7	110.5 (3)	C33A—C32A—H32A	109.4
C11—C12—H12A	109.6	C31A—C32A—H32B	109.4
C7—C12—H12A	109.6	C33A—C32A—H32B	109.4
C11—C12—H12B	109.6	H32A—C32A—H32B	108.0
C7—C12—H12B	109.6	C34A—C33A—C32A	105.0 (7)
H12A—C12—H12B	108.1	C34A—C33A—H33A	110.8
C14—C13—C18	108.8 (3)	C32A—C33A—H33A	110.8
C14—C13—P1	112.9 (3)	C34A—C33A—H33B	110.8
C18—C13—P1	118.0 (2)	C32A—C33A—H33B	110.8
C14—C13—H13	105.3	H33A—C33A—H33B	108.8
C18—C13—H13	105.3	C33A—C34A—C35A	105.5 (7)
P1—C13—H13	105.3	C33A—C34A—H34A	110.6
C13—C14—C15	110.4 (3)	C35A—C34A—H34A	110.6
C13—C14—H14A	109.6	C33A—C34A—H34B	110.6
C15—C14—H14A	109.6	C35A—C34A—H34B	110.6
C13—C14—H14B	109.6	H34A—C34A—H34B	108.8

C15—C14—H14B	109.6	C34A—C35A—C36A	103.5 (5)
H14A—C14—H14B	108.1	C34A—C35A—H35A	111.1
C16—C15—C14	110.9 (3)	C36A—C35A—H35A	111.1
C16—C15—H15A	109.5	C34A—C35A—H35B	111.1
C14—C15—H15A	109.5	C36A—C35A—H35B	111.1
C16—C15—H15B	109.5	H35A—C35A—H35B	109.0
C14—C15—H15B	109.5	C31A—C36A—C35A	107.3 (4)
H15A—C15—H15B	108.1	C31A—C36A—H36A	110.2
C17—C16—C15	112.4 (4)	C35A—C36A—H36A	110.2
C17—C16—H16A	109.1	C31A—C36A—H36B	110.2
C15—C16—H16A	109.1	C35A—C36A—H36B	110.2
C17—C16—H16B	109.1	H36A—C36A—H36B	108.5
C15—C16—H16B	109.1	C36B—C31B—C32B	116.0 (5)
H16A—C16—H16B	107.8	C36B—C31B—P2	125.2 (4)
C16—C17—C18	113.4 (4)	C32B—C31B—P2	113.7 (2)
C16—C17—H17A	108.9	C36B—C31B—H31B	97.6
C18—C17—H17A	108.9	C32B—C31B—H31B	97.6
C16—C17—H17B	108.9	P2—C31B—H31B	97.6
C18—C17—H17B	108.9	C31B—C32B—C33B	113.8 (5)
H17A—C17—H17B	107.7	C31B—C32B—H32C	108.8
C17—C18—C13	109.1 (3)	C33B—C32B—H32C	108.8
C17—C18—H18A	109.9	C31B—C32B—H32D	108.8
C13—C18—H18A	109.9	C33B—C32B—H32D	108.8
C17—C18—H18B	109.9	H32C—C32B—H32D	107.7
C13—C18—H18B	109.9	C34B—C33B—C32B	116.7 (9)
H18A—C18—H18B	108.3	C34B—C33B—H33C	108.1
C31B—P2—C19A	104.93 (16)	C32B—C33B—H33C	108.1
C31A—P2—C19A	104.93 (16)	C34B—C33B—H33D	108.1
C31B—P2—C19B	104.93 (16)	C32B—C33B—H33D	108.1
C31A—P2—C19B	104.93 (16)	H33C—C33B—H33D	107.3
C31B—P2—C25	108.22 (18)	C33B—C34B—C35B	107.7 (8)
C31A—P2—C25	108.22 (18)	C33B—C34B—H34C	110.2
C19A—P2—C25	104.16 (16)	C35B—C34B—H34C	110.2
C19B—P2—C25	104.16 (16)	C33B—C34B—H34D	110.2
C31B—P2—Pt1	118.53 (15)	C35B—C34B—H34D	110.2
C31A—P2—Pt1	118.53 (15)	H34C—C34B—H34D	108.5
C19A—P2—Pt1	108.61 (12)	C34B—C35B—C36B	106.5 (7)
C19B—P2—Pt1	108.61 (12)	C34B—C35B—H35C	110.4
C25—P2—Pt1	111.27 (11)	C36B—C35B—H35C	110.4
C24A—C19A—C20A	110.5 (6)	C34B—C35B—H35D	110.4
C24A—C19A—P2	119.6 (4)	C36B—C35B—H35D	110.4
C20A—C19A—P2	110.1 (5)	H35C—C35B—H35D	108.6
C24A—C19A—H19A	105.1	C31B—C36B—C35B	109.7 (7)
C20A—C19A—H19A	105.1	C31B—C36B—H36C	109.7
P2—C19A—H19A	105.1	C35B—C36B—H36C	109.7
C21A—C20A—C19A	113.5 (8)	C31B—C36B—H36D	109.7
C21A—C20A—H20A	108.9	C35B—C36B—H36D	109.7
C19A—C20A—H20A	108.9	H36C—C36B—H36D	108.2

C21A—C20A—H20B	108.9	C38B—C37—C39	100.8 (6)
C19A—C20A—H20B	108.9	C38A—C37—C39	128.7 (5)
H20A—C20A—H20B	107.7	C38B—C37—Pt1	138.9 (6)
C22A—C21A—C20A	110.5 (8)	C38A—C37—Pt1	111.0 (5)
C22A—C21A—H21A	109.5	C39—C37—Pt1	120.3 (3)
C20A—C21A—H21A	109.5	F2—C39—F3	104.3 (4)
C22A—C21A—H21B	109.5	F2—C39—F1	104.6 (4)
C20A—C21A—H21B	109.5	F3—C39—F1	102.5 (3)
H21A—C21A—H21B	108.1	F2—C39—C37	114.3 (3)
C21A—C22A—C23A	111.3 (7)	F3—C39—C37	116.9 (4)
C21A—C22A—H22A	109.4	F1—C39—C37	112.8 (3)
C23A—C22A—H22A	109.4	C37—C38A—C40A	123.5 (10)
C21A—C22A—H22B	109.4	C37—C38A—H38A	118.3
C23A—C22A—H22B	109.4	C40A—C38A—H38A	118.3
H22A—C22A—H22B	108.0	F6A—C40A—F5A	105.9 (9)
C22A—C23A—C24A	110.8 (7)	F6A—C40A—F4A	103.5 (8)
C22A—C23A—H23A	109.5	F5A—C40A—F4A	102.0 (9)
C24A—C23A—H23A	109.5	F6A—C40A—C38A	119.3 (9)
C22A—C23A—H23B	109.5	F5A—C40A—C38A	114.3 (8)
C24A—C23A—H23B	109.5	F4A—C40A—C38A	110.0 (10)
H23A—C23A—H23B	108.1	C37—C38B—C40B	125.7 (10)
C19A—C24A—C23A	109.8 (5)	C37—C38B—H38B	117.2
C19A—C24A—H24A	109.7	C40B—C38B—H38B	117.2
C23A—C24A—H24A	109.7	F5B—C40B—F4B	106.3 (8)
C19A—C24A—H24B	109.7	F5B—C40B—F6B	106.5 (7)
C23A—C24A—H24B	109.7	F4B—C40B—F6B	102.3 (8)
H24A—C24A—H24B	108.2	F5B—C40B—C38B	115.5 (9)
C24B—C19B—C20B	115.6 (7)	F4B—C40B—C38B	114.0 (9)
C24B—C19B—P2	112.6 (5)	F6B—C40B—C38B	111.1 (9)
Pt1—C37—C38A—C40A	178.6 (8)	C39—C37—C38A—C40A	−2.8 (14)
Pt1—C37—C38B—C40B	−2.2 (19)	C39—C37—C38B—C40B	178.5 (11)