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Bis(pentafluorobenzenethiolato-κS){(pentafluorophenyl)phenyl[3,4,5,6-tetrafluoro-2-(pentafluorophenylsulfanyl)phenyl]phosphane-$\kappa^2 P,S$}-platinum(II) dichloromethane hemisolvate

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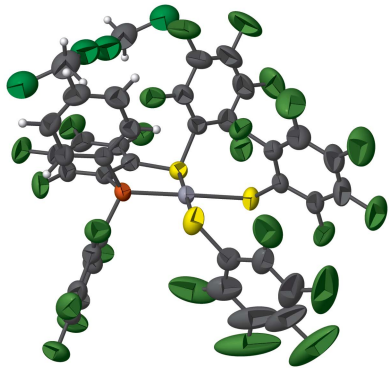
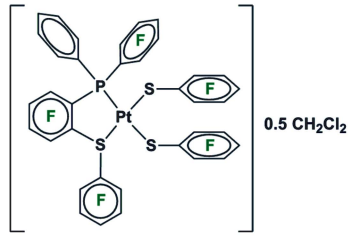
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[Pt(C_6F_5S)_2(C_{24}H_5F_{14}PS)]\cdot 0.5CH_2Cl_2$, the complex features a square-planar Pt^{II} atom coordinated by two thiolate ligands and one chelating bidentate P/S ligand, forming a five-membered metallacycle. The monodentate SC_6F_5 ligands give a weak parallel displaced π–π interaction. In the chelating ligand, the geometry for both S and P donor atoms is consistent with sp^3 hybridization. The complex conformation is identical to that previously described for the compound bearing 2,3,5,6-tetrafluorophenylthiolate in place of pentafluorophenylthiolate groups. The lattice solvent, CH_2Cl_2, is disordered over inversion centers in $P\overline{1}$, affording a hemisolvate.

3D view



Chemical scheme



Structure description

The title complex, $[Pt(SC_6F_5)_2(1,2\text{-}C_6F_4(SC_6F_5)(PPh(C_6F_5)))]$ (Fig. 1), is a product resulting from the C—F bond activation of $[Pt_2(\mu\text{-}SC_6F_5)_2(SC_6F_5)_2(PPh(C_6F_5)_2)_2]$. The chemistry has been described for this compound and for other related compounds with different fluorinated thiolate groups and phosphanes (Villanueva *et al.*, 2004; Bernès *et al.*, 2016).

The Pt^{II} center is coordinated by two *cis* thiolates and one chelating bidentate ligand, giving a square-planar coordination geometry. The thiolates have their C_6F_5 rings almost parallel, giving a parallel displaced π–π interaction; the angle between rings is 4.8 (4)°, and the distance between ring centroids is 4.322 (6) Å. One C_6F_5 ring is affected by libration, clearly visible on C3—F3, C4—F4 and C5—F5 groups (see Fig. 1). The chelate ring coordinates *via* P and S donors, at normal distances [Pt1—P1 = 2.2315 (11) Å; Pt1—

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Pt(C_6F_5S)_2(C_{24}H_5F_{14}PS)]\cdot 0.5CH_2Cl_2$
M_r	1258.10
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	11.2908 (10), 13.8516 (14), 14.6956 (17)
α, β, γ (°)	104.477 (8), 96.359 (8), 111.675 (7)
V (Å^3)	2014.6 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.89
Crystal size (mm)	0.65 × 0.40 × 0.24
Data collection	
Diffractometer	Bruker P4
Absorption correction	ψ scan (*XSCANS*; Bruker, 1997)
T_{min}, T_{max}	0.521, 0.897
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15487, 9078, 7392
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.089, 1.02
No. of reflections	9078
No. of parameters	614
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.99, −0.74

Computer programs: *XSCANS* (Bruker, 1997), *SHELXS2013* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

S3 = 2.2757 (12) Å, shorter than Pt—$S_{thiolate}$ bond lengths]. Both S and P atoms are tetrahedrally hybridized, assuming that one lone pair is present on S3. Angles around P1 are in the range 104.1 (2)–116.75 (15)°, while bond angles around S3 are in the range 102.4 (2)–109.13 (17)°. The complex conformation is identical to that previously described for the compound bearing 2,3,5,6-tetrafluorophenylthiolate in place of pentafluorophenylthiolate groups (Villanueva *et al.*, 2004).

The complex crystallized with dichloromethane as a lattice solvent. The molecule is located close to the inversion centers of the triclinic cell, and its occupancy was then fixed to 1/2. As the main complex is in a general position, the chemical composition thus corresponds to a hemisolvate.

Synthesis and crystallization

The synthesis and crystallization of this complex is similar to that described for $[Pt(SC_6F_4H)_2(1,2\text{-}C_6F_4(SC_6F_4H)(PPh(C_6F_5)))]$ in: Villanueva *et al.* (2004).

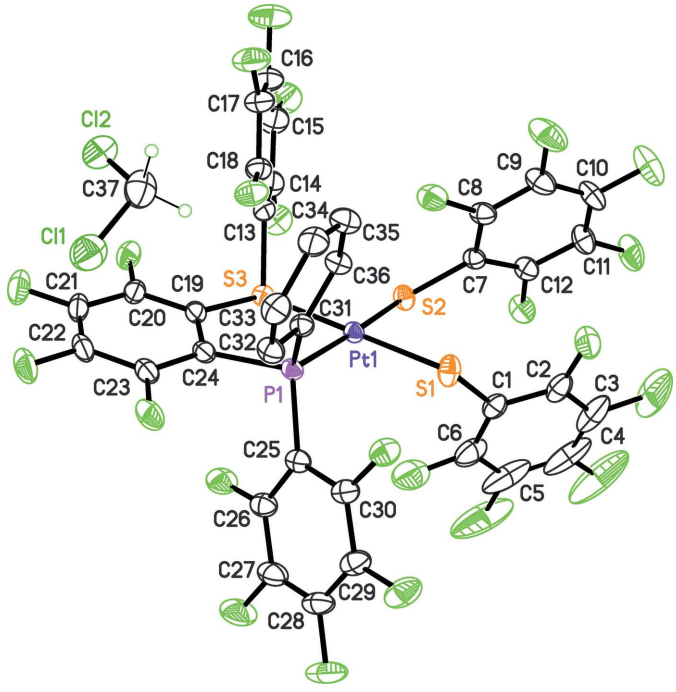


Figure 1
The structure of the title compound, with displacement ellipsoids for non-H atoms at the 20% probability level. Labels for F atoms (green ellipsoids) are identical to those of the C atom to which they are bonded.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. A free refinement of the occupancy for dichloromethane C37/Cl1/Cl2 converged to 0.47. In the final cycles, this parameter was fixed to 1/2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x160696 [doi:10.1107/S2414314616006969]

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Crystal data

$[Pt(C_6F_5S)_2(C_{24}H_5F_{14}PS)]\cdot 0.5CH_2Cl_2$
M_r = 1258.10
Triclinic, $P\overline{1}$
a = 11.2908 (10) Å
b = 13.8516 (14) Å
c = 14.6956 (17) Å
α = 104.477 (8)°
β = 96.359 (8)°
γ = 111.675 (7)°
V = 2014.6 (4) Å^3
Z = 2
$F(000)$ = 1198
D_x = 2.074 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 75 reflections
θ = 3.6–12.5°
μ = 3.89 mm^{-1}
T = 296 K
Plate, yellow
0.65 × 0.40 × 0.24 mm

Data collection

Bruker P4 diffractometer
Radiation source: fine-focus sealed tube, FN4
Graphite monochromator
$2\theta/\omega$ scans
Absorption correction: ψ scan (*XSCANS*; Bruker, 1997)
T_{min} = 0.521, T_{max} = 0.897
15487 measured reflections
9078 independent reflections
7392 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −14→8
k = −16→16
l = −19→19
3 standard reflections every 97 reflections
intensity decay: 1.5%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.089
S = 1.02
9078 reflections
614 parameters
0 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.2045P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Pt1	0.65934 (2)	0.65231 (2)	0.20934 (2)	0.04309 (7)	
P1	0.66292 (11)	0.81991 (9)	0.24844 (8)	0.0446 (2)	
S1	0.67412 (16)	0.65984 (11)	0.36926 (9)	0.0672 (4)	
S2	0.64217 (13)	0.47144 (9)	0.15065 (9)	0.0547 (3)	
S3	0.64754 (11)	0.64869 (9)	0.05284 (8)	0.0475 (2)	
C1	0.5663 (6)	0.5315 (4)	0.3703 (3)	0.0612 (13)	
C2	0.6101 (8)	0.4739 (5)	0.4213 (4)	0.0757 (17)	
F2	0.7365 (5)	0.5210 (4)	0.4704 (3)	0.1082 (13)	
C3	0.5288 (14)	0.3739 (7)	0.4240 (7)	0.127 (4)	
F3	0.5813 (10)	0.3252 (5)	0.4758 (6)	0.210 (4)	
C4	0.4052 (16)	0.3291 (8)	0.3786 (9)	0.157 (7)	
F4	0.3278 (10)	0.2290 (5)	0.3779 (6)	0.282 (6)	
C5	0.3544 (11)	0.3813 (12)	0.3270 (7)	0.165 (7)	
F5	0.2305 (6)	0.3384 (8)	0.2828 (4)	0.268 (6)	
C6	0.4387 (8)	0.4863 (7)	0.3266 (5)	0.101 (2)	
F6	0.3857 (4)	0.5362 (7)	0.2785 (4)	0.164 (3)	
C7	0.7545 (4)	0.4551 (4)	0.2305 (3)	0.0497 (10)	
C8	0.8822 (5)	0.5310 (4)	0.2722 (4)	0.0620 (13)	
F8	0.9267 (3)	0.6259 (3)	0.2523 (3)	0.0864 (10)	
C9	0.9678 (6)	0.5139 (5)	0.3327 (5)	0.0808 (17)	
F9	1.0905 (4)	0.5897 (4)	0.3704 (4)	0.1235 (16)	
C10	0.9278 (6)	0.4175 (5)	0.3555 (5)	0.0793 (17)	
F10	1.0090 (5)	0.3995 (4)	0.4144 (4)	0.1265 (17)	
C11	0.8028 (6)	0.3391 (4)	0.3152 (5)	0.0739 (15)	
F11	0.7620 (4)	0.2454 (3)	0.3374 (3)	0.1091 (13)	
C12	0.7197 (5)	0.3587 (4)	0.2537 (4)	0.0582 (12)	
F12	0.5975 (3)	0.2795 (2)	0.2166 (3)	0.0790 (9)	
C13	0.7970 (5)	0.6531 (4)	0.0211 (3)	0.0537 (11)	
C14	0.7924 (6)	0.5610 (5)	−0.0456 (4)	0.0671 (14)	
F14	0.6794 (4)	0.4732 (3)	−0.0847 (3)	0.0896 (11)	
C15	0.9053 (8)	0.5589 (6)	−0.0719 (5)	0.092 (2)	
F15	0.8988 (6)	0.4678 (4)	−0.1353 (4)	0.142 (2)	
C16	1.0213 (8)	0.6482 (7)	−0.0332 (6)	0.096 (2)	
F16	1.1287 (5)	0.6446 (5)	−0.0603 (4)	0.153 (2)	
C17	1.0287 (6)	0.7398 (6)	0.0309 (5)	0.0805 (17)	
F17	1.1407 (4)	0.8280 (4)	0.0671 (4)	0.1148 (14)	
C18	0.9160 (5)	0.7421 (4)	0.0597 (4)	0.0607 (12)	
F18	0.9254 (3)	0.8324 (3)	0.1254 (2)	0.0766 (9)	
C19	0.6525 (4)	0.7785 (4)	0.0507 (3)	0.0508 (11)	
C20	0.6550 (5)	0.8036 (4)	−0.0341 (4)	0.0579 (12)	
F20	0.6669 (3)	0.7372 (3)	−0.1115 (2)	0.0757 (9)	
C21	0.6500 (5)	0.8998 (5)	−0.0397 (4)	0.0694 (15)	
F21	0.6537 (4)	0.9256 (3)	−0.1213 (3)	0.0968 (12)	
C22	0.6388 (5)	0.9701 (4)	0.0404 (5)	0.0675 (15)	
F22	0.6332 (4)	1.0638 (3)	0.0362 (3)	0.0926 (11)	

C23	0.6337 (5)	0.9442 (4)	0.1259 (4)	0.0591 (12)	
F23	0.6178 (3)	1.0127 (3)	0.1998 (3)	0.0800 (9)	
C24	0.6438 (4)	0.8506 (4)	0.1336 (4)	0.0515 (11)	
C25	0.5295 (4)	0.8324 (3)	0.3027 (4)	0.0511 (11)	
C26	0.4054 (5)	0.7983 (4)	0.2474 (4)	0.0616 (13)	
F26	0.3832 (3)	0.7639 (3)	0.1508 (3)	0.0839 (10)	
C27	0.3012 (5)	0.7975 (5)	0.2881 (5)	0.0782 (17)	
F27	0.1825 (3)	0.7649 (4)	0.2310 (4)	0.1137 (15)	
C28	0.3180 (6)	0.8296 (5)	0.3867 (5)	0.0766 (18)	
F28	0.2158 (4)	0.8293 (3)	0.4255 (4)	0.1141 (15)	
C29	0.4365 (6)	0.8610 (4)	0.4428 (5)	0.0700 (16)	
F29	0.4538 (4)	0.8940 (3)	0.5394 (3)	0.0961 (12)	
C30	0.5405 (5)	0.8624 (4)	0.4017 (4)	0.0580 (12)	
F30	0.6563 (3)	0.8964 (3)	0.4627 (2)	0.0738 (8)	
C31	0.8149 (4)	0.9318 (4)	0.3230 (3)	0.0478 (10)	
C32	0.8251 (5)	1.0370 (4)	0.3632 (4)	0.0572 (12)	
H32A	0.7514	1.0521	0.3567	0.069*	
C33	0.9454 (5)	1.1192 (4)	0.4130 (4)	0.0663 (14)	
H33A	0.9529	1.1900	0.4403	0.080*	
C34	1.0556 (5)	1.0972 (5)	0.4227 (4)	0.0708 (15)	
H34A	1.1370	1.1533	0.4551	0.085*	
C35	1.0437 (5)	0.9921 (5)	0.3841 (4)	0.0688 (14)	
H35A	1.1169	0.9766	0.3920	0.083*	
C36	0.9245 (4)	0.9097 (4)	0.3341 (3)	0.0545 (11)	
H36A	0.9174	0.8388	0.3077	0.065*	
C37	1.0152 (16)	1.0944 (13)	0.1602 (11)	0.102 (5)	0.5
H37A	0.9769	1.0370	0.1884	0.123*	0.5
H37B	1.1064	1.1356	0.1937	0.123*	0.5
Cl1	0.9371 (4)	1.1786 (4)	0.1773 (3)	0.1127 (13)	0.5
Cl2	1.0064 (5)	1.0342 (4)	0.0376 (3)	0.1166 (14)	0.5

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pt1	0.04474 (10)	0.03828 (10)	0.04831 (10)	0.01929 (7)	0.01035 (7)	0.01377 (7)
P1	0.0437 (6)	0.0404 (6)	0.0534 (6)	0.0214 (5)	0.0117 (5)	0.0142 (5)
S1	0.0982 (10)	0.0519 (7)	0.0473 (6)	0.0300 (7)	0.0092 (7)	0.0137 (5)
S2	0.0682 (7)	0.0411 (6)	0.0552 (7)	0.0264 (6)	0.0074 (6)	0.0123 (5)
S3	0.0457 (6)	0.0452 (6)	0.0483 (6)	0.0172 (5)	0.0088 (5)	0.0123 (5)
C1	0.073 (3)	0.064 (3)	0.045 (3)	0.027 (3)	0.021 (3)	0.014 (2)
C2	0.115 (5)	0.061 (3)	0.066 (3)	0.042 (4)	0.048 (4)	0.026 (3)
F2	0.131 (4)	0.145 (4)	0.097 (3)	0.089 (3)	0.035 (3)	0.065 (3)
C3	0.227 (12)	0.080 (5)	0.113 (7)	0.071 (7)	0.114 (8)	0.053 (5)
F3	0.390 (12)	0.148 (5)	0.229 (7)	0.166 (7)	0.191 (8)	0.150 (6)
C4	0.176 (13)	0.090 (7)	0.116 (9)	−0.032 (7)	0.101 (10)	−0.010 (6)
F4	0.396 (12)	0.098 (4)	0.229 (8)	−0.045 (6)	0.218 (9)	0.011 (4)
C5	0.107 (8)	0.191 (13)	0.078 (6)	−0.037 (8)	0.049 (6)	−0.017 (6)
F5	0.109 (4)	0.344 (11)	0.123 (4)	−0.084 (6)	0.048 (4)	−0.043 (6)

C6	0.089 (5)	0.132 (7)	0.058 (4)	0.023 (5)	0.027 (4)	0.020 (4)
F6	0.079 (3)	0.319 (9)	0.094 (3)	0.076 (4)	0.015 (2)	0.076 (5)
C7	0.052 (3)	0.044 (2)	0.059 (3)	0.027 (2)	0.016 (2)	0.015 (2)
C8	0.054 (3)	0.049 (3)	0.089 (4)	0.024 (2)	0.023 (3)	0.023 (3)
F8	0.0592 (18)	0.0622 (19)	0.140 (3)	0.0174 (15)	0.026 (2)	0.045 (2)
C9	0.052 (3)	0.068 (4)	0.110 (5)	0.021 (3)	−0.001 (3)	0.020 (3)
F9	0.061 (2)	0.094 (3)	0.184 (5)	0.018 (2)	−0.019 (3)	0.032 (3)
C10	0.072 (4)	0.071 (4)	0.100 (5)	0.043 (3)	−0.006 (3)	0.025 (3)
F10	0.119 (3)	0.110 (3)	0.143 (4)	0.059 (3)	−0.033 (3)	0.038 (3)
C11	0.090 (4)	0.053 (3)	0.088 (4)	0.040 (3)	0.008 (3)	0.025 (3)
F11	0.124 (3)	0.073 (2)	0.140 (4)	0.046 (2)	0.003 (3)	0.054 (2)
C12	0.062 (3)	0.044 (3)	0.067 (3)	0.026 (2)	0.012 (2)	0.012 (2)
F12	0.0678 (19)	0.0492 (16)	0.106 (3)	0.0121 (15)	0.0022 (18)	0.0277 (17)
C13	0.057 (3)	0.062 (3)	0.053 (3)	0.030 (2)	0.021 (2)	0.025 (2)
C14	0.086 (4)	0.064 (3)	0.059 (3)	0.039 (3)	0.023 (3)	0.016 (3)
F14	0.106 (3)	0.067 (2)	0.077 (2)	0.033 (2)	0.018 (2)	−0.0010 (17)
C15	0.120 (6)	0.099 (5)	0.092 (5)	0.073 (5)	0.054 (5)	0.029 (4)
F15	0.181 (5)	0.128 (4)	0.147 (4)	0.100 (4)	0.085 (4)	0.017 (3)
C16	0.092 (5)	0.132 (7)	0.107 (5)	0.076 (5)	0.058 (5)	0.049 (5)
F16	0.121 (4)	0.205 (6)	0.184 (5)	0.106 (4)	0.095 (4)	0.060 (4)
C17	0.056 (3)	0.101 (5)	0.092 (4)	0.033 (3)	0.031 (3)	0.038 (4)
F17	0.059 (2)	0.143 (4)	0.140 (4)	0.031 (2)	0.040 (2)	0.052 (3)
C18	0.060 (3)	0.066 (3)	0.060 (3)	0.030 (3)	0.020 (2)	0.017 (3)
F18	0.0597 (18)	0.071 (2)	0.077 (2)	0.0132 (15)	0.0176 (16)	0.0061 (17)
C19	0.042 (2)	0.055 (3)	0.059 (3)	0.020 (2)	0.009 (2)	0.026 (2)
C20	0.051 (3)	0.064 (3)	0.059 (3)	0.017 (2)	0.010 (2)	0.029 (2)
F20	0.087 (2)	0.086 (2)	0.0540 (17)	0.0305 (18)	0.0163 (16)	0.0286 (16)
C21	0.057 (3)	0.077 (4)	0.076 (4)	0.017 (3)	0.004 (3)	0.049 (3)
F21	0.099 (3)	0.102 (3)	0.092 (2)	0.026 (2)	0.011 (2)	0.065 (2)
C22	0.051 (3)	0.058 (3)	0.100 (4)	0.021 (2)	0.001 (3)	0.043 (3)
F22	0.087 (2)	0.068 (2)	0.134 (3)	0.0332 (18)	0.006 (2)	0.058 (2)
C23	0.051 (3)	0.052 (3)	0.078 (3)	0.026 (2)	0.008 (2)	0.024 (3)
F23	0.089 (2)	0.0583 (18)	0.105 (3)	0.0456 (17)	0.015 (2)	0.0261 (18)
C24	0.043 (2)	0.049 (2)	0.067 (3)	0.021 (2)	0.011 (2)	0.023 (2)
C25	0.048 (2)	0.037 (2)	0.065 (3)	0.0167 (19)	0.013 (2)	0.011 (2)
C26	0.056 (3)	0.054 (3)	0.073 (3)	0.024 (2)	0.017 (3)	0.016 (3)
F26	0.0481 (17)	0.100 (3)	0.089 (2)	0.0215 (17)	0.0051 (16)	0.024 (2)
C27	0.049 (3)	0.071 (4)	0.121 (6)	0.026 (3)	0.026 (3)	0.037 (4)
F27	0.051 (2)	0.137 (4)	0.156 (4)	0.039 (2)	0.022 (2)	0.050 (3)
C28	0.071 (4)	0.058 (3)	0.118 (5)	0.035 (3)	0.051 (4)	0.031 (3)
F28	0.089 (3)	0.104 (3)	0.178 (4)	0.052 (2)	0.086 (3)	0.047 (3)
C29	0.084 (4)	0.049 (3)	0.087 (4)	0.031 (3)	0.045 (3)	0.021 (3)
F29	0.126 (3)	0.068 (2)	0.099 (3)	0.039 (2)	0.066 (2)	0.0197 (19)
C30	0.057 (3)	0.042 (2)	0.074 (3)	0.019 (2)	0.024 (3)	0.015 (2)
F30	0.074 (2)	0.076 (2)	0.0663 (18)	0.0274 (17)	0.0228 (17)	0.0169 (16)
C31	0.047 (2)	0.046 (2)	0.049 (2)	0.019 (2)	0.012 (2)	0.0139 (19)
C32	0.054 (3)	0.047 (3)	0.068 (3)	0.022 (2)	0.011 (2)	0.014 (2)
C33	0.070 (3)	0.043 (3)	0.073 (3)	0.012 (2)	0.014 (3)	0.015 (2)

C34	0.048 (3)	0.069 (4)	0.074 (4)	0.005 (3)	0.002 (3)	0.021 (3)
C35	0.052 (3)	0.078 (4)	0.072 (3)	0.028 (3)	0.009 (3)	0.016 (3)
C36	0.047 (2)	0.057 (3)	0.058 (3)	0.023 (2)	0.009 (2)	0.013 (2)
C37	0.099 (10)	0.095 (10)	0.093 (10)	0.021 (8)	0.002 (8)	0.035 (8)
Cl1	0.103 (3)	0.120 (3)	0.107 (3)	0.035 (2)	0.025 (2)	0.039 (2)
Cl2	0.107 (3)	0.123 (4)	0.132 (4)	0.043 (3)	0.047 (3)	0.060 (3)

Geometric parameters (Å, º)

Pt1—P1	2.2315 (11)	C17—F17	1.327 (8)
Pt1—S3	2.2757 (12)	C17—C18	1.392 (7)
Pt1—S1	2.3107 (13)	C18—F18	1.336 (6)
Pt1—S2	2.3627 (12)	C19—C20	1.375 (7)
P1—C31	1.821 (5)	C19—C24	1.407 (7)
P1—C25	1.823 (5)	C20—F20	1.327 (6)
P1—C24	1.851 (5)	C20—C21	1.376 (8)
S1—C1	1.750 (6)	C21—F21	1.335 (6)
S2—C7	1.747 (5)	C21—C22	1.379 (8)
S3—C13	1.784 (5)	C22—F22	1.339 (6)
S3—C19	1.787 (5)	C22—C23	1.391 (8)
C1—C6	1.344 (9)	C23—F23	1.330 (6)
C1—C2	1.396 (8)	C23—C24	1.373 (7)
C2—F2	1.353 (8)	C25—C26	1.384 (7)
C2—C3	1.364 (10)	C25—C30	1.387 (7)
C3—C4	1.314 (18)	C26—F26	1.341 (6)
C3—F3	1.356 (13)	C26—C27	1.376 (7)
C4—F4	1.335 (11)	C27—F27	1.348 (7)
C4—C5	1.38 (2)	C27—C28	1.374 (10)
C5—F5	1.313 (13)	C28—F28	1.341 (6)
C5—C6	1.416 (15)	C28—C29	1.343 (9)
C6—F6	1.338 (11)	C29—F29	1.345 (7)
C7—C12	1.387 (7)	C29—C30	1.376 (7)
C7—C8	1.386 (7)	C30—F30	1.344 (6)
C8—F8	1.343 (6)	C31—C36	1.383 (6)
C8—C9	1.366 (8)	C31—C32	1.385 (6)
C9—F9	1.339 (7)	C32—C33	1.377 (7)
C9—C10	1.383 (9)	C32—H32A	0.9300
C10—F10	1.324 (7)	C33—C34	1.386 (8)
C10—C11	1.372 (8)	C33—H33A	0.9300
C11—F11	1.344 (6)	C34—C35	1.374 (8)
C11—C12	1.377 (8)	C34—H34A	0.9300
C12—F12	1.349 (6)	C35—C36	1.371 (7)
C13—C18	1.380 (7)	C35—H35A	0.9300
C13—C14	1.380 (7)	C36—H36A	0.9300
C14—F14	1.334 (7)	C37—Cl1	1.692 (17)
C14—C15	1.381 (9)	C37—Cl2	1.760 (15)
C15—F15	1.339 (8)	C37—H37A	0.9700
C15—C16	1.362 (11)	C37—H37B	0.9700

C16—F16	1.332 (7)	Cl2—Cl2^{i}	1.217 (9)
C16—C17	1.346 (10)		
P1—Pt1—S3	89.63 (4)	F17—C17—C18	119.3 (6)
P1—Pt1—S1	89.40 (5)	C16—C17—C18	119.2 (6)
S3—Pt1—S1	178.81 (4)	F18—C18—C13	120.6 (4)
P1—Pt1—S2	173.59 (4)	F18—C18—C17	118.6 (5)
S3—Pt1—S2	84.72 (4)	C13—C18—C17	120.8 (5)
S1—Pt1—S2	96.28 (5)	C20—C19—C24	120.5 (5)
C31—P1—C25	107.8 (2)	C20—C19—S3	119.5 (4)
C31—P1—C24	104.1 (2)	C24—C19—S3	119.8 (4)
C25—P1—C24	106.7 (2)	F20—C20—C19	120.6 (5)
C31—P1—Pt1	116.75 (15)	F20—C20—C21	118.5 (5)
C25—P1—Pt1	114.57 (15)	C19—C20—C21	120.9 (5)
C24—P1—Pt1	105.86 (15)	F21—C21—C20	121.5 (6)
C1—S1—Pt1	106.76 (17)	F21—C21—C22	119.4 (5)
C7—S2—Pt1	108.35 (15)	C20—C21—C22	119.1 (5)
C13—S3—C19	102.4 (2)	F22—C22—C21	120.0 (5)
C13—S3—Pt1	109.13 (17)	F22—C22—C23	119.8 (6)
C19—S3—Pt1	105.85 (16)	C21—C22—C23	120.2 (5)
C6—C1—C2	117.3 (7)	F23—C23—C24	121.0 (5)
C6—C1—S1	122.4 (6)	F23—C23—C22	117.8 (5)
C2—C1—S1	120.2 (5)	C24—C23—C22	121.2 (5)
F2—C2—C3	120.0 (8)	C23—C24—C19	117.9 (5)
F2—C2—C1	118.2 (5)	C23—C24—P1	124.1 (4)
C3—C2—C1	121.8 (9)	C19—C24—P1	117.7 (3)
C4—C3—F3	122.7 (11)	C26—C25—C30	115.4 (4)
C4—C3—C2	120.3 (11)	C26—C25—P1	121.6 (4)
F3—C3—C2	117.0 (12)	C30—C25—P1	122.4 (4)
C3—C4—F4	119.8 (17)	F26—C26—C27	117.7 (5)
C3—C4—C5	121.3 (10)	F26—C26—C25	120.2 (4)
F4—C4—C5	118.8 (16)	C27—C26—C25	122.1 (5)
F5—C5—C4	121.9 (14)	F27—C27—C26	119.8 (6)
F5—C5—C6	120.0 (16)	F27—C27—C28	120.1 (5)
C4—C5—C6	118.1 (11)	C26—C27—C28	120.1 (6)
F6—C6—C1	122.2 (8)	F28—C28—C29	121.0 (7)
F6—C6—C5	116.7 (10)	F28—C28—C27	119.5 (6)
C1—C6—C5	121.1 (10)	C29—C28—C27	119.5 (5)
C12—C7—C8	114.9 (5)	C28—C29—F29	119.7 (5)
C12—C7—S2	120.0 (4)	C28—C29—C30	120.1 (6)
C8—C7—S2	125.0 (4)	F29—C29—C30	120.1 (6)
F8—C8—C9	117.2 (5)	F30—C30—C29	116.6 (5)
F8—C8—C7	119.6 (5)	F30—C30—C25	120.7 (4)
C9—C8—C7	123.2 (5)	C29—C30—C25	122.7 (5)
F9—C9—C8	120.7 (6)	C36—C31—C32	120.0 (4)
F9—C9—C10	119.4 (6)	C36—C31—P1	117.3 (3)
C8—C9—C10	119.9 (5)	C32—C31—P1	122.6 (4)
F10—C10—C11	119.8 (6)	C33—C32—C31	119.3 (5)

F10—C10—C9	120.9 (6)	C33—C32—H32A	120.3
C11—C10—C9	119.3 (5)	C31—C32—H32A	120.3
F11—C11—C10	120.0 (5)	C32—C33—C34	120.6 (5)
F11—C11—C12	120.7 (6)	C32—C33—H33A	119.7
C10—C11—C12	119.2 (5)	C34—C33—H33A	119.7
F12—C12—C11	117.0 (5)	C35—C34—C33	119.5 (5)
F12—C12—C7	119.5 (5)	C35—C34—H34A	120.2
C11—C12—C7	123.5 (5)	C33—C34—H34A	120.2
C18—C13—C14	118.5 (5)	C36—C35—C34	120.4 (5)
C18—C13—S3	124.0 (4)	C36—C35—H35A	119.8
C14—C13—S3	117.4 (4)	C34—C35—H35A	119.8
F14—C14—C13	120.5 (5)	C35—C36—C31	120.1 (5)
F14—C14—C15	119.4 (5)	C35—C36—H36A	119.9
C13—C14—C15	120.1 (6)	C31—C36—H36A	119.9
F15—C15—C16	120.9 (6)	Cl1—C37—Cl2	112.9 (9)
F15—C15—C14	119.0 (7)	Cl1—C37—H37A	109.0
C16—C15—C14	120.1 (6)	Cl2—C37—H37A	109.0
F16—C16—C17	119.7 (8)	Cl1—C37—H37B	109.0
F16—C16—C15	119.1 (7)	Cl2—C37—H37B	109.0
C17—C16—C15	121.2 (6)	H37A—C37—H37B	107.8
F17—C17—C16	121.5 (6)	Cl2^{i}—Cl2—C37	160.4 (8)

Pt1—S1—C1—C6	−55.3 (5)	C13—S3—C19—C20	61.7 (4)
Pt1—S1—C1—C2	127.6 (4)	Pt1—S3—C19—C20	176.0 (4)
C6—C1—C2—F2	−176.2 (5)	C13—S3—C19—C24	−123.0 (4)
S1—C1—C2—F2	1.1 (7)	Pt1—S3—C19—C24	−8.7 (4)
C6—C1—C2—C3	2.5 (8)	C24—C19—C20—F20	178.1 (4)
S1—C1—C2—C3	179.8 (5)	S3—C19—C20—F20	−6.7 (7)
F2—C2—C3—C4	178.2 (7)	C24—C19—C20—C21	0.4 (8)
C1—C2—C3—C4	−0.5 (11)	S3—C19—C20—C21	175.6 (4)
F2—C2—C3—F3	−1.2 (9)	F20—C20—C21—F21	1.6 (8)
C1—C2—C3—F3	−179.9 (5)	C19—C20—C21—F21	179.4 (5)
F3—C3—C4—F4	−3.8 (14)	F20—C20—C21—C22	−179.5 (5)
C2—C3—C4—F4	176.9 (7)	C19—C20—C21—C22	−1.8 (8)
F3—C3—C4—C5	179.5 (8)	F21—C21—C22—F22	−0.8 (8)
C2—C3—C4—C5	0.1 (15)	C20—C21—C22—F22	−179.7 (5)
C3—C4—C5—F5	−178.6 (8)	F21—C21—C22—C23	179.5 (5)
F4—C4—C5—F5	4.6 (16)	C20—C21—C22—C23	0.6 (8)
C3—C4—C5—C6	−1.8 (16)	F22—C22—C23—F23	2.8 (7)
F4—C4—C5—C6	−178.5 (7)	C21—C22—C23—F23	−177.5 (5)
C2—C1—C6—F6	177.9 (6)	F22—C22—C23—C24	−177.7 (4)
S1—C1—C6—F6	0.6 (9)	C21—C22—C23—C24	2.0 (8)
C2—C1—C6—C5	−4.1 (9)	F23—C23—C24—C19	176.2 (4)
S1—C1—C6—C5	178.6 (6)	C22—C23—C24—C19	−3.3 (7)
F5—C5—C6—F6	−1.1 (12)	F23—C23—C24—P1	−10.0 (7)
C4—C5—C6—F6	−178.0 (8)	C22—C23—C24—P1	170.5 (4)
F5—C5—C6—C1	−179.2 (7)	C20—C19—C24—C23	2.1 (7)
C4—C5—C6—C1	3.9 (13)	S3—C19—C24—C23	−173.1 (4)

Pt1—S2—C7—C12	139.5 (4)	C20—C19—C24—P1	−172.1 (4)
Pt1—S2—C7—C8	−42.9 (4)	S3—C19—C24—P1	12.7 (5)
C12—C7—C8—F8	178.2 (4)	C31—P1—C24—C23	−60.2 (4)
S2—C7—C8—F8	0.5 (7)	C25—P1—C24—C23	53.7 (5)
C12—C7—C8—C9	−0.8 (8)	Pt1—P1—C24—C23	176.2 (4)
S2—C7—C8—C9	−178.5 (5)	C31—P1—C24—C19	113.6 (4)
F8—C8—C9—F9	0.4 (9)	C25—P1—C24—C19	−132.5 (4)
C7—C8—C9—F9	179.4 (6)	Pt1—P1—C24—C19	−10.0 (4)
F8—C8—C9—C10	−179.7 (6)	C31—P1—C25—C26	149.1 (4)
C7—C8—C9—C10	−0.7 (10)	C24—P1—C25—C26	37.7 (5)
F9—C9—C10—F10	0.3 (11)	Pt1—P1—C25—C26	−79.1 (4)
C8—C9—C10—F10	−179.6 (6)	C31—P1—C25—C30	−39.8 (5)
F9—C9—C10—C11	−178.7 (6)	C24—P1—C25—C30	−151.1 (4)
C8—C9—C10—C11	1.4 (10)	Pt1—P1—C25—C30	92.0 (4)
F10—C10—C11—F11	1.7 (10)	C30—C25—C26—F26	−177.6 (5)
C9—C10—C11—F11	−179.4 (6)	P1—C25—C26—F26	−6.0 (7)
F10—C10—C11—C12	−179.6 (6)	C30—C25—C26—C27	1.9 (8)
C9—C10—C11—C12	−0.7 (10)	P1—C25—C26—C27	173.6 (4)
F11—C11—C12—F12	−0.7 (8)	F26—C26—C27—F27	−1.3 (8)
C10—C11—C12—F12	−179.4 (5)	C25—C26—C27—F27	179.1 (5)
F11—C11—C12—C7	177.8 (5)	F26—C26—C27—C28	178.5 (5)
C10—C11—C12—C7	−0.9 (9)	C25—C26—C27—C28	−1.0 (9)
C8—C7—C12—F12	−179.9 (4)	F27—C27—C28—F28	−0.7 (9)
S2—C7—C12—F12	−2.1 (6)	C26—C27—C28—F28	179.4 (5)
C8—C7—C12—C11	1.5 (8)	F27—C27—C28—C29	179.4 (6)
S2—C7—C12—C11	179.4 (4)	C26—C27—C28—C29	−0.4 (9)
C19—S3—C13—C18	45.1 (5)	F28—C28—C29—F29	−0.8 (8)
Pt1—S3—C13—C18	−66.8 (5)	C27—C28—C29—F29	179.0 (5)
C19—S3—C13—C14	−135.4 (4)	F28—C28—C29—C30	−179.0 (5)
Pt1—S3—C13—C14	112.7 (4)	C27—C28—C29—C30	0.8 (9)
C18—C13—C14—F14	180.0 (5)	C28—C29—C30—F30	179.0 (5)
S3—C13—C14—F14	0.5 (7)	F29—C29—C30—F30	0.8 (7)
C18—C13—C14—C15	0.6 (8)	C28—C29—C30—C25	0.2 (8)
S3—C13—C14—C15	−178.9 (5)	F29—C29—C30—C25	−178.1 (4)
F14—C14—C15—F15	−0.8 (10)	C26—C25—C30—F30	179.7 (4)
C13—C14—C15—F15	178.6 (6)	P1—C25—C30—F30	8.1 (7)
F14—C14—C15—C16	179.5 (6)	C26—C25—C30—C29	−1.5 (7)
C13—C14—C15—C16	−1.1 (11)	P1—C25—C30—C29	−173.1 (4)
F15—C15—C16—F16	0.9 (12)	C25—P1—C31—C36	143.3 (4)
C14—C15—C16—F16	−179.4 (7)	C24—P1—C31—C36	−103.6 (4)
F15—C15—C16—C17	−179.7 (7)	Pt1—P1—C31—C36	12.6 (4)
C14—C15—C16—C17	0.0 (12)	C25—P1—C31—C32	−40.3 (5)
F16—C16—C17—F17	1.1 (12)	C24—P1—C31—C32	72.8 (4)
C15—C16—C17—F17	−178.3 (7)	Pt1—P1—C31—C32	−171.0 (3)
F16—C16—C17—C18	−179.1 (6)	C36—C31—C32—C33	1.0 (7)
C15—C16—C17—C18	1.5 (12)	P1—C31—C32—C33	−175.3 (4)
C14—C13—C18—F18	−179.2 (5)	C31—C32—C33—C34	0.1 (8)
S3—C13—C18—F18	0.3 (8)	C32—C33—C34—C35	−1.4 (9)

C14—C13—C18—C17	1.0 (8)	C33—C34—C35—C36	1.7 (9)
S3—C13—C18—C17	−179.5 (5)	C34—C35—C36—C31	−0.6 (8)
F17—C17—C18—F18	−2.0 (9)	C32—C31—C36—C35	−0.7 (7)
C16—C17—C18—F18	178.1 (6)	P1—C31—C36—C35	175.8 (4)
F17—C17—C18—C13	177.8 (5)	Cl1—C37—Cl2—Cl2^{i}	−137 (2)
C16—C17—C18—C13	−2.0 (10)		

Symmetry code: (i) −*x*+2, −*y*+2, −*z*.