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C—H···F, C—F···π and C—F···F—C interactions in a palladium(II) benzenethiolate complex

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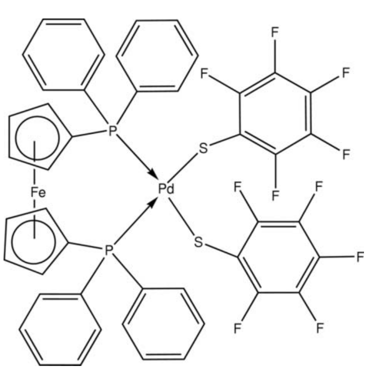
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.043; wR factor = 0.064; data-to-parameter ratio = 13.0.

The title compound, [1,1′-bis(diphenylphosphino)ferrocene-κ^2P,P']bis(2,3,4,5,6-pentafluorobenzenethiolato-κS)palladium(II), $[FePd(C_6F_5S)_2(C_{17}H_{14}P)_2]$, crystallizes with two independent molecules in the asymmetric unit. The complex has the palladium metal center in a slightly distorted square-planar environment with the 1,10-bis(diphenylphosphino)ferrocene (dppf) ligand coordinated in a bidentate fashion and, completing the coordination environment, the two $-SC_6F_5$ thiolates in a *cis* configuration. The molecules are linked by weak C—F···π, C—F···F—C and C—H···F stacking interactions.

Related literature

For general background, see: Bandoli & Dolmella, 2000); Cordero-Pensado *et al.*, 2006; Crespo *et al.*, 1999; Dilworth & Hu, 1993; Dilworth *et al.*, 2002; Estudiante-Negrete *et al.*, 2007; Maisela *et al.*, 2001. For related structures, see: Garcés-Rodríguez *et al.*, 2007; Herrera-Alvarez *et al.*, 2004; Thalladi *et al.*,1998); Althoff *et al.*, 2006). For structure analysis tools used, see: Janiak (2000).



Experimental

Crystal data

$[FePd(C_6F_5S)_2(C_{17}H_{14}P)_2]$
M_r = 1058.99
Monoclinic, $P2_1/n$
a = 19.7191 (12) Å
b = 22.0781 (11) Å
c = 19.7875 (13) Å
β = 106.665 (1)°
V = 8252.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 298 (2) K
0.36 × 0.20 × 0.14 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: integration (*SHELXTL*; Sheldrick, 2006)
T_{min} = 0.761, T_{max} = 0.914
66003 measured reflections
14535 independent reflections
9020 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.064
S = 0.82
14535 reflections
1117 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C22—H22···F6	0.93	2.44	3.306 (6)	156
C28—H28···F5	0.93	2.80	3.487 (5)	132
C59—H59···F1	0.93	2.76	3.681 (6)	170
C73—H73···F2	0.93	2.43	3.272 (6)	151
C74—H74···F16	0.93	2.70	3.629 (6)	177
C27—H27···F5^{i}	0.93	2.48	3.253 (6)	141
C62—H62···F19^{ii}	0.93	2.66	3.511 (6)	153
C67—H67···F13^{ii}	0.93	2.75	3.335 (6)	122
C19—H19···F3^{ii}	0.93	2.70	3.531 (7)	149
C32—H32···F14^{iii}	0.93	2.70	3.562 (6)	154
C50—H50···F8^{iv}	0.93	2.78	3.399 (6)	125
C77—H77···F10^{v}	0.93	2.72	3.231 (5)	116
C71—H71···F18^{v}	0.93	2.57	3.322 (6)	138

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Table 2
Intermolecular and intramolecular C-F–π, C-H–π and π–π interactions in (I) (Å).

H/F/centroid	centroid	distance	Symmetry code
H26	C35–C40	3.206	(i)
H60	C17–C22	3.425	(ii)
F11	C87–C92	3.237	
F20	C81–C86	3.295	
F10	C35–C40	3.072	
F1	C41–C46	3.691	
F19	C63–C68	2.996	(ii)
C41–C46	C81–C86	3.683	(iii)

Symmetry codes: (i) $-x+1, -y, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2006); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2163).

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supplementary materials

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C-H...F, C-F...π and C-F...F-C interactions in a palladium(II) benzenethiolate complex

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Comment

The, 1,1'-bis(diphenylphosphino)ferrocene (dppf) has been employed profusely for the synthesis of complexes otherwise difficult or in some cases almost impossible to isolate with other diphosphines (*e.g.* dppe)·(Bandoli & Dolmella, 2000)). In addition, platinum group metal complexes containing dppf and thiolate ligands on its structure are rare (Maisela *et al.*, 2001; Crespo *et al.*,1999) due in part to the well known tendency of these complexes to polymerize (Dilworth & Hu, 1993) affording in most of the cases intractable solids. Thus, given our continuous interest in the synthesis of transition metal complexes bearing thiolates (Garcés-Rodríguez *et al.*, 2007; Dilworth *et al.*, 2002; Estudiante-Negrete *et al.*, 2007; Cordero-Pensado *et al.*, 2006) we would like to report the crystal structure of the palladium(II) complex [Pd(dppf)(SC_6F_5)$_2$] (I) which represents a polymorph of a previously reported X-ray crystal structure determination for the same compound (Herrera-Alvarez, *et al.*, 2004).

Two independent molecules of (I) were found in the asymmetric unit. Both showing geometrical and conformational differences (Fig. 1). The structures can be defined as slightly distorted square planar with r.m.s. deviations from the plane constituted by the atoms bonded directly to the Pd atoms of 0.187 (1) %A, for molecule 1 and of 0.138 (2)%A for molecule 2. The dihedral angles between the phenyl rings in molecule 1 are 50.45 (1)° and 81.7 (1)° while in molecule 2 the dihedral angles are 66.4 (1)° and 71.9 (1)°, these dihedral angles differing from those reported for the polymorph [77.4 (1)° and 66.2 (2)°] (Herrera-Alvarez, *et al.*, 2004).

The fragments C_6F_5– are almost co-planar in both molecules and they are rotated by 64.2 (1)° and 74.3 (1)° in molecule 1 and 64.0 (1)° and 65.7 (1)° in molecule 2. The pentaflurophenylthiolate ligands in both molecules, are found in an anti conformation around the plane of the metal center. This conformation allow the C—F–π intermolecular interactions type offset π-stacked, the distances centroid-F being of 3.071 A° and 3.691 A° in molecule 1 and of 3.295 A° and 3.237 A° in molecule 2 (Table 1)(Janiak, 2000).

As a consequence of this conformation the molecules in the crystal are linked by weak C—H—F, C—F—F—C and C—H–π intramolecular and intermolecular interactions (Tables 1, 2.). Moreover, one benzenethiolate ring of molecule 1 is involved in face-to-face π–π stacking interactions with a crystallographically equivalent benzenethiolate ring of molecule 2 (Althoff *et al.*, 2006, Thalladi *et al.*, 1998). For this interactions, the centroid-to-centroid distances between the benzenethiolate rings are of 3.425 (2) A° (Janiak 2000). The anti conformation presented for compound (I), has been observed previously for the polymorph and the analogous Pt(II) derivative (Garcés-Rodríguez *et al.*, 2007, Herrera-Alvarez, *et al.*, 2004).

Experimental

Synthesis of [Pd(dppf)(SC_6F_5)$_2$] (1). The title compound was synthesized as previously described (Herrera-Alvarez, *et al.*, 2004) by metathetical reaction of [Pd(dppf)Cl_2] with [Pb(SC_6F_5)$_2$] in dichloromethane (Scheme 1). The compound was obtained as an orange microcrystalline powder after being recrystallized from a CH_2Cl_2/Hexane solvent system.

Refinement

H atoms were included in calculated positions (C—H = 0.93 Å), and refined using a riding model,with U_{iso}(H) = 1.2U_{eq} of the carrier atom.

Figures


Fig. 1. The two independent molecules in (I) with the atom-labeling scheme. Displacement ellipsoids are shown at the 40% probability level. H atoms have been omitted for clarity.

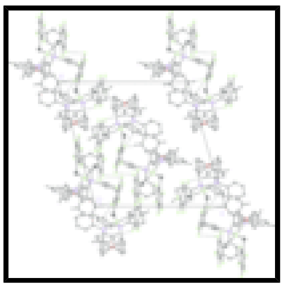


Fig. 2. Crystal packing of (I). Broken lines indicate C—H···F interactions.

[1,1'-bis(diphenylphosphino)ferrocene-κ^2*P*,*P*']bis(2,3,4,5,6- pentafluorobenzenethiolato-κ*S*)palladium(II)

Crystal data

[FePd(C_6F_5S)$_2$($C_{17}H_{14}P_1$)$_2$]	F_{000} = 4224
M_r = 1058.99	D_x = 1.705 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 9945 reflections
a = 19.7191 (12) Å	θ = 2.3–24.2º
b = 22.0781 (11) Å	μ = 1.05 mm^{-1}
c = 19.7875 (13) Å	*T* = 298 (2) K
β = 106.665 (1)º	Prism, orange
V = 8252.9 (8) Å^3	0.36 × 0.20 × 0.14 mm
Z = 8	

Data collection

Bruker SMART APEX AXS CCD area-detector diffractometer	14535 independent reflections
Radiation source: fine-focus sealed tube	9020 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.082
Detector resolution: 0.83 pixels mm^{-1}	θ_{max} = 25.0º
T = 298(2) K	θ_{min} = 1.6º
ω scans	*h* = −23→23
Absorption correction: integration	*k* = −26→26

(SHELXTL; Sheldrick, 2006)	
T_{min} = 0.761, T_{max} = 0.914	$l = -23 \rightarrow 23$
66003 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.064$	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.82$	$(\Delta/\sigma)_{max} = 0.001$
14535 reflections	$\Delta\rho_{max}$ = 0.90 e Å^{-3}
1117 parameters	$\Delta\rho_{min}$ = −0.76 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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.

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Pd1	0.373762 (17)	0.113792 (14)	0.627204 (17)	0.03282 (9)
Fe1	0.17220 (3)	0.04161 (3)	0.53565 (3)	0.03885 (17)
S1	0.43294 (7)	0.20565 (5)	0.61704 (6)	0.0485 (3)
S2	0.42193 (6)	0.11253 (5)	0.75128 (6)	0.0451 (3)
P1	0.30694 (6)	0.12752 (5)	0.50961 (6)	0.0358 (3)
P2	0.33331 (6)	0.01836 (5)	0.64001 (6)	0.0324 (3)
F1	0.54195 (16)	0.29322 (14)	0.69166 (16)	0.0922 (11)
F2	0.67792 (18)	0.27319 (16)	0.76062 (18)	0.1291 (15)
F3	0.73410 (17)	0.16069 (16)	0.77047 (16)	0.1080 (12)
F4	0.65054 (16)	0.06718 (16)	0.70589 (16)	0.0898 (11)
F5	0.51684 (14)	0.08494 (13)	0.63477 (14)	0.0668 (8)
F6	0.30252 (14)	0.20056 (13)	0.73164 (15)	0.0788 (9)
F7	0.30771 (18)	0.31647 (14)	0.77412 (17)	0.1074 (12)
F8	0.43199 (18)	0.36635 (13)	0.84519 (16)	0.1025 (11)
F9	0.55216 (17)	0.29898 (14)	0.87308 (17)	0.1041 (12)

F10	0.54768 (14)	0.18421 (12)	0.83278 (13)	0.0665 (8)
C1	0.2397 (2)	0.01744 (18)	0.6286 (2)	0.0328 (11)
C2	0.1874 (2)	−0.0283 (2)	0.6038 (2)	0.0448 (12)
H2	0.1961	−0.0682	0.5937	0.054*
C3	0.1205 (2)	−0.0029 (2)	0.5973 (2)	0.0512 (14)
H3	0.0774	−0.0231	0.5822	0.061*
C4	0.1296 (2)	0.0574 (2)	0.6172 (2)	0.0486 (13)
H4	0.0936	0.0845	0.6174	0.058*
C5	0.2024 (2)	0.07075 (19)	0.6369 (2)	0.0387 (12)
H5	0.2227	0.1081	0.6528	0.046*
C6	0.2245 (2)	0.0859 (2)	0.4761 (2)	0.0387 (11)
C7	0.2148 (2)	0.0240 (2)	0.4558 (2)	0.0441 (12)
H7	0.2507	−0.0037	0.4566	0.053*
C8	0.1415 (3)	0.0116 (2)	0.4343 (2)	0.0525 (14)
H8	0.1208	−0.0257	0.4192	0.063*
C9	0.1056 (2)	0.0647 (2)	0.4394 (2)	0.0532 (14)
H9	0.0567	0.0692	0.4279	0.064*
C10	0.1558 (2)	0.1103 (2)	0.4648 (2)	0.0453 (12)
H10	0.1456	0.1503	0.4730	0.054*
C11	0.3472 (2)	0.1214 (2)	0.4374 (2)	0.0411 (12)
C12	0.3097 (3)	0.1029 (3)	0.3716 (3)	0.091 (2)
H12	0.2633	0.0898	0.3641	0.109*
C13	0.3389 (3)	0.1031 (3)	0.3156 (3)	0.105 (2)
H13	0.3124	0.0898	0.2713	0.125*
C14	0.4060 (3)	0.1227 (3)	0.3257 (3)	0.085 (2)
H14	0.4258	0.1231	0.2883	0.103*
C15	0.4438 (3)	0.1415 (3)	0.3895 (3)	0.090 (2)
H15	0.4899	0.1552	0.3963	0.108*
C16	0.4148 (3)	0.1408 (2)	0.4460 (3)	0.0679 (16)
H16	0.4420	0.1537	0.4902	0.082*
C17	0.2727 (2)	0.2049 (2)	0.5032 (2)	0.0385 (12)
C18	0.2541 (2)	0.2368 (2)	0.4404 (3)	0.0545 (14)
H18	0.2639	0.2210	0.4007	0.065*
C19	0.2210 (3)	0.2924 (2)	0.4369 (3)	0.0698 (17)
H19	0.2092	0.3140	0.3948	0.084*
C20	0.2057 (3)	0.3158 (2)	0.4935 (3)	0.0672 (17)
H20	0.1818	0.3526	0.4896	0.081*
C21	0.2246 (3)	0.2863 (2)	0.5564 (3)	0.0663 (16)
H21	0.2155	0.3033	0.5959	0.080*
C22	0.2577 (2)	0.2306 (2)	0.5609 (3)	0.0511 (13)
H22	0.2700	0.2100	0.6037	0.061*
C23	0.3537 (2)	−0.03595 (19)	0.5802 (2)	0.0341 (11)
C24	0.3330 (2)	−0.0958 (2)	0.5781 (2)	0.0400 (12)
H24	0.3085	−0.1091	0.6091	0.048*
C25	0.3477 (2)	−0.1361 (2)	0.5314 (2)	0.0512 (13)
H25	0.3313	−0.1757	0.5293	0.061*
C26	0.3865 (3)	−0.1177 (2)	0.4882 (3)	0.0613 (15)
H26	0.3969	−0.1451	0.4569	0.074*
C27	0.4105 (3)	−0.0590 (2)	0.4906 (3)	0.0603 (15)

H27	0.4378	−0.0469	0.4618	0.072*
C28	0.3936 (2)	−0.0180 (2)	0.5361 (2)	0.0428 (12)
H28	0.4092	0.0218	0.5373	0.051*
C29	0.3734 (2)	−0.01790 (17)	0.7242 (2)	0.0342 (11)
C30	0.4444 (2)	−0.03349 (19)	0.7423 (2)	0.0462 (13)
H30	0.4705	−0.0260	0.7107	0.055*
C31	0.4770 (3)	−0.0599 (2)	0.8066 (3)	0.0570 (15)
H31	0.5246	−0.0704	0.8181	0.068*
C32	0.4392 (3)	−0.0706 (2)	0.8529 (3)	0.0705 (18)
H32	0.4612	−0.0880	0.8964	0.085*
C33	0.3686 (3)	−0.0558 (2)	0.8358 (3)	0.0700 (17)
H33	0.3430	−0.0633	0.8678	0.084*
C34	0.3358 (3)	−0.0299 (2)	0.7716 (2)	0.0505 (13)
H34	0.2879	−0.0205	0.7600	0.061*
C35	0.5219 (2)	0.1902 (2)	0.6609 (2)	0.0470 (13)
C36	0.5672 (3)	0.2360 (3)	0.6933 (3)	0.0643 (16)
C37	0.6374 (4)	0.2265 (3)	0.7290 (3)	0.083 (2)
C38	0.6654 (3)	0.1702 (3)	0.7350 (3)	0.0726 (19)
C39	0.6240 (3)	0.1238 (3)	0.7028 (3)	0.0624 (15)
C40	0.5536 (3)	0.1336 (3)	0.6660 (3)	0.0526 (14)
C41	0.4247 (2)	0.18812 (19)	0.7783 (2)	0.0362 (11)
C42	0.3652 (3)	0.2242 (2)	0.7671 (2)	0.0471 (13)
C43	0.3673 (3)	0.2831 (3)	0.7879 (3)	0.0624 (16)
C44	0.4302 (4)	0.3082 (2)	0.8235 (3)	0.0659 (17)
C45	0.4903 (3)	0.2744 (2)	0.8377 (3)	0.0588 (15)
C46	0.4867 (3)	0.2153 (2)	0.8157 (2)	0.0456 (13)
Pd2	0.728272 (17)	0.365112 (15)	0.481499 (17)	0.03521 (10)
Fe2	0.60731 (3)	0.51461 (3)	0.36853 (3)	0.04017 (18)
S3	0.76545 (7)	0.28164 (6)	0.42804 (7)	0.0588 (4)
S4	0.82221 (6)	0.36135 (5)	0.58798 (6)	0.0483 (3)
P3	0.63013 (6)	0.36369 (5)	0.38330 (6)	0.0341 (3)
P4	0.70483 (6)	0.45721 (5)	0.52760 (6)	0.0369 (3)
F11	0.82982 (15)	0.16369 (12)	0.48196 (15)	0.0722 (9)
F12	0.96514 (16)	0.13341 (14)	0.52599 (16)	0.0971 (11)
F13	1.06712 (16)	0.21807 (16)	0.53507 (17)	0.1109 (13)
F14	1.02966 (17)	0.33339 (15)	0.49664 (17)	0.1032 (12)
F15	0.89390 (16)	0.36452 (13)	0.44768 (15)	0.0795 (9)
F16	0.71365 (14)	0.26038 (12)	0.59018 (14)	0.0685 (8)
F17	0.74354 (15)	0.14550 (13)	0.63006 (15)	0.0813 (9)
F18	0.87904 (15)	0.10782 (12)	0.67927 (14)	0.0792 (9)
F19	0.98578 (14)	0.18594 (12)	0.68588 (14)	0.0763 (9)
F20	0.95811 (13)	0.30139 (12)	0.64685 (14)	0.0645 (8)
C47	0.6163 (2)	0.43188 (18)	0.3316 (2)	0.0351 (11)
C48	0.6715 (2)	0.46942 (19)	0.3234 (2)	0.0437 (12)
H48	0.7196	0.4625	0.3434	0.052*
C49	0.6419 (3)	0.5190 (2)	0.2802 (2)	0.0545 (14)
H49	0.6668	0.5502	0.2667	0.065*
C50	0.5679 (3)	0.5128 (2)	0.2612 (2)	0.0544 (14)
H50	0.5354	0.5398	0.2335	0.065*

C51	0.5513 (2)	0.4594 (2)	0.2910 (2)	0.0448 (12)
H51	0.5060	0.4442	0.2855	0.054*
C52	0.6450 (2)	0.51255 (19)	0.4745 (2)	0.0375 (11)
C53	0.6624 (2)	0.5681 (2)	0.4484 (2)	0.0498 (13)
H53	0.7080	0.5828	0.4550	0.060*
C54	0.6000 (3)	0.5976 (2)	0.4111 (2)	0.0555 (14)
H54	0.5969	0.6347	0.3881	0.067*
C55	0.5426 (3)	0.5609 (2)	0.4145 (2)	0.0538 (14)
H55	0.4950	0.5699	0.3948	0.065*
C56	0.5694 (2)	0.5088 (2)	0.4527 (2)	0.0472 (13)
H56	0.5427	0.4770	0.4623	0.057*
C57	0.5511 (2)	0.34657 (18)	0.4095 (2)	0.0368 (11)
C58	0.5562 (2)	0.33439 (19)	0.4793 (2)	0.0471 (13)
H58	0.5997	0.3389	0.5131	0.057*
C59	0.4992 (3)	0.3160 (2)	0.4997 (3)	0.0619 (15)
H59	0.5043	0.3072	0.5469	0.074*
C60	0.4343 (3)	0.3105 (2)	0.4510 (3)	0.0671 (17)
H60	0.3951	0.2989	0.4652	0.081*
C61	0.4271 (3)	0.3221 (2)	0.3810 (3)	0.0598 (15)
H61	0.3832	0.3181	0.3476	0.072*
C62	0.4852 (2)	0.3396 (2)	0.3608 (2)	0.0525 (14)
H62	0.4802	0.3469	0.3134	0.063*
C63	0.6273 (2)	0.30619 (19)	0.3171 (2)	0.0327 (11)
C64	0.6048 (2)	0.2476 (2)	0.3255 (2)	0.0487 (13)
H64	0.5906	0.2377	0.3651	0.058*
C65	0.6034 (3)	0.2042 (2)	0.2747 (3)	0.0602 (15)
H65	0.5885	0.1650	0.2800	0.072*
C66	0.6244 (3)	0.2193 (2)	0.2166 (3)	0.0630 (16)
H66	0.6232	0.1901	0.1824	0.076*
C67	0.6465 (2)	0.2756 (2)	0.2082 (3)	0.0577 (15)
H67	0.6602	0.2852	0.1682	0.069*
C68	0.6489 (2)	0.3190 (2)	0.2582 (2)	0.0447 (13)
H68	0.6653	0.3576	0.2524	0.054*
C69	0.6762 (2)	0.4599 (2)	0.6076 (2)	0.0386 (12)
C70	0.6555 (2)	0.5146 (2)	0.6294 (2)	0.0514 (14)
H70	0.6535	0.5488	0.6015	0.062*
C71	0.6380 (3)	0.5192 (3)	0.6909 (3)	0.0653 (16)
H71	0.6265	0.5568	0.7058	0.078*
C72	0.6371 (3)	0.4692 (3)	0.7309 (3)	0.0627 (16)
H72	0.6245	0.4723	0.7726	0.075*
C73	0.6551 (3)	0.4144 (3)	0.7090 (3)	0.0623 (15)
H73	0.6542	0.3800	0.7358	0.075*
C74	0.6747 (2)	0.4093 (2)	0.6472 (2)	0.0482 (13)
H74	0.6867	0.3717	0.6328	0.058*
C75	0.7905 (2)	0.49639 (18)	0.5512 (2)	0.0375 (12)
C76	0.8191 (3)	0.52560 (19)	0.6151 (2)	0.0499 (13)
H76	0.7930	0.5283	0.6474	0.060*
C77	0.8854 (3)	0.5504 (2)	0.6308 (3)	0.0641 (16)
H77	0.9042	0.5697	0.6739	0.077*

C78	0.9242 (3)	0.5471 (2)	0.5840 (3)	0.0571 (15)
H78	0.9691	0.5644	0.5952	0.069*
C79	0.8977 (3)	0.5187 (2)	0.5210 (3)	0.0521 (14)
H79	0.9244	0.5164	0.4892	0.063*
C80	0.8307 (2)	0.4930 (2)	0.5045 (2)	0.0499 (13)
H80	0.8127	0.4733	0.4615	0.060*
C81	0.8552 (2)	0.2662 (2)	0.4641 (2)	0.0400 (12)
C82	0.8782 (3)	0.2073 (2)	0.4839 (2)	0.0460 (13)
C83	0.9475 (3)	0.1909 (3)	0.5073 (3)	0.0599 (15)
C84	0.9980 (3)	0.2330 (3)	0.5119 (3)	0.0684 (18)
C85	0.9794 (3)	0.2918 (3)	0.4924 (3)	0.0631 (16)
C86	0.9093 (3)	0.3076 (2)	0.4682 (2)	0.0500 (13)
C87	0.8346 (2)	0.2860 (2)	0.6156 (2)	0.0391 (12)
C88	0.7826 (3)	0.2438 (2)	0.6142 (2)	0.0488 (13)
C89	0.7965 (3)	0.1846 (2)	0.6347 (3)	0.0521 (14)
C90	0.8653 (3)	0.1656 (2)	0.6592 (2)	0.0504 (14)
C91	0.9184 (3)	0.2051 (2)	0.6637 (2)	0.0475 (13)
C92	0.9028 (2)	0.2640 (2)	0.6429 (2)	0.0429 (12)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pd1	0.0351 (2)	0.0307 (2)	0.0312 (2)	−0.00328 (16)	0.00703 (16)	0.00062 (17)
Fe1	0.0343 (4)	0.0381 (4)	0.0430 (4)	−0.0017 (3)	0.0091 (3)	0.0008 (3)
S1	0.0536 (9)	0.0432 (8)	0.0436 (8)	−0.0135 (6)	0.0059 (7)	0.0058 (6)
S2	0.0642 (9)	0.0322 (7)	0.0335 (7)	−0.0044 (6)	0.0054 (6)	−0.0016 (6)
P1	0.0340 (7)	0.0385 (8)	0.0341 (7)	−0.0012 (6)	0.0086 (6)	0.0046 (6)
P2	0.0337 (7)	0.0306 (7)	0.0324 (7)	0.0013 (6)	0.0087 (6)	0.0008 (6)
F1	0.100 (3)	0.058 (2)	0.092 (2)	−0.035 (2)	−0.014 (2)	0.011 (2)
F2	0.104 (3)	0.116 (3)	0.122 (3)	−0.060 (2)	−0.040 (2)	0.014 (2)
F3	0.053 (2)	0.174 (4)	0.078 (2)	−0.011 (2)	−0.0109 (19)	0.019 (2)
F4	0.071 (2)	0.112 (3)	0.089 (3)	0.019 (2)	0.0266 (19)	0.001 (2)
F5	0.055 (2)	0.074 (2)	0.076 (2)	−0.0027 (16)	0.0255 (17)	−0.0217 (18)
F6	0.050 (2)	0.097 (2)	0.086 (2)	0.0030 (18)	0.0132 (18)	−0.0260 (19)
F7	0.108 (3)	0.091 (3)	0.120 (3)	0.049 (2)	0.026 (2)	−0.013 (2)
F8	0.164 (3)	0.042 (2)	0.098 (3)	0.004 (2)	0.033 (2)	−0.0119 (19)
F9	0.105 (3)	0.077 (2)	0.106 (3)	−0.042 (2)	−0.008 (2)	−0.027 (2)
F10	0.053 (2)	0.071 (2)	0.061 (2)	−0.0008 (16)	−0.0070 (16)	−0.0070 (16)
C1	0.036 (3)	0.027 (3)	0.037 (3)	−0.002 (2)	0.014 (2)	0.003 (2)
C2	0.043 (3)	0.038 (3)	0.055 (3)	−0.005 (2)	0.016 (3)	0.003 (2)
C3	0.035 (3)	0.063 (4)	0.055 (3)	−0.015 (3)	0.012 (3)	0.007 (3)
C4	0.043 (3)	0.057 (4)	0.050 (3)	0.007 (3)	0.021 (3)	0.003 (3)
C5	0.040 (3)	0.038 (3)	0.042 (3)	0.003 (2)	0.018 (2)	0.001 (2)
C6	0.035 (3)	0.044 (3)	0.035 (3)	0.008 (2)	0.006 (2)	0.007 (2)
C7	0.044 (3)	0.045 (3)	0.039 (3)	0.001 (2)	0.006 (3)	−0.004 (2)
C8	0.059 (4)	0.053 (4)	0.043 (3)	−0.012 (3)	0.010 (3)	−0.003 (3)
C9	0.034 (3)	0.067 (4)	0.051 (3)	−0.004 (3)	−0.001 (3)	0.004 (3)
C10	0.042 (3)	0.040 (3)	0.046 (3)	0.001 (3)	0.002 (3)	0.007 (2)

C11	0.036 (3)	0.050 (3)	0.037 (3)	0.004 (2)	0.011 (2)	0.006 (2)
C12	0.063 (4)	0.163 (6)	0.051 (4)	−0.042 (4)	0.023 (3)	−0.017 (4)
C13	0.078 (5)	0.193 (8)	0.046 (4)	−0.036 (5)	0.023 (4)	−0.022 (4)
C14	0.069 (5)	0.149 (6)	0.051 (4)	0.007 (4)	0.038 (4)	−0.007 (4)
C15	0.046 (4)	0.165 (7)	0.067 (4)	−0.013 (4)	0.030 (4)	0.001 (5)
C16	0.041 (3)	0.111 (5)	0.052 (4)	−0.016 (3)	0.014 (3)	−0.010 (3)
C17	0.027 (3)	0.043 (3)	0.043 (3)	−0.004 (2)	0.006 (2)	0.010 (3)
C18	0.051 (3)	0.055 (4)	0.051 (3)	−0.002 (3)	0.004 (3)	0.014 (3)
C19	0.062 (4)	0.060 (4)	0.076 (5)	0.008 (3)	0.002 (3)	0.027 (4)
C20	0.049 (4)	0.038 (4)	0.108 (5)	0.006 (3)	0.010 (4)	0.011 (4)
C21	0.070 (4)	0.051 (4)	0.081 (4)	0.004 (3)	0.026 (4)	−0.001 (3)
C22	0.052 (3)	0.044 (3)	0.060 (4)	0.007 (3)	0.020 (3)	0.013 (3)
C23	0.029 (3)	0.036 (3)	0.036 (3)	0.009 (2)	0.006 (2)	0.005 (2)
C24	0.042 (3)	0.042 (3)	0.033 (3)	0.001 (2)	0.006 (2)	−0.003 (2)
C25	0.057 (4)	0.038 (3)	0.054 (3)	0.001 (3)	0.008 (3)	−0.012 (3)
C26	0.068 (4)	0.062 (4)	0.055 (4)	0.008 (3)	0.019 (3)	−0.026 (3)
C27	0.062 (4)	0.067 (4)	0.061 (4)	0.005 (3)	0.033 (3)	−0.002 (3)
C28	0.041 (3)	0.040 (3)	0.049 (3)	0.002 (2)	0.015 (3)	−0.004 (3)
C29	0.040 (3)	0.021 (3)	0.038 (3)	−0.002 (2)	0.005 (2)	−0.005 (2)
C30	0.051 (4)	0.040 (3)	0.042 (3)	0.002 (3)	0.004 (3)	−0.001 (2)
C31	0.069 (4)	0.036 (3)	0.053 (4)	0.010 (3)	−0.005 (3)	−0.004 (3)
C32	0.110 (6)	0.043 (4)	0.041 (4)	0.009 (4)	−0.006 (4)	0.006 (3)
C33	0.110 (5)	0.062 (4)	0.042 (4)	0.001 (4)	0.027 (4)	0.009 (3)
C34	0.055 (4)	0.054 (3)	0.043 (3)	0.003 (3)	0.016 (3)	0.004 (3)
C35	0.053 (4)	0.055 (4)	0.032 (3)	−0.020 (3)	0.010 (3)	0.005 (3)
C36	0.074 (5)	0.058 (4)	0.052 (4)	−0.018 (4)	0.005 (3)	0.012 (3)
C37	0.076 (5)	0.088 (5)	0.066 (4)	−0.043 (4)	−0.009 (4)	0.009 (4)
C38	0.052 (4)	0.112 (6)	0.049 (4)	−0.021 (4)	0.006 (3)	0.012 (4)
C39	0.062 (4)	0.074 (5)	0.058 (4)	−0.001 (4)	0.026 (3)	0.008 (4)
C40	0.043 (4)	0.076 (4)	0.043 (3)	−0.011 (3)	0.020 (3)	−0.003 (3)
C41	0.048 (3)	0.035 (3)	0.025 (3)	−0.005 (2)	0.011 (2)	0.001 (2)
C42	0.049 (4)	0.050 (4)	0.039 (3)	−0.005 (3)	0.007 (3)	−0.006 (3)
C43	0.069 (5)	0.063 (4)	0.055 (4)	0.024 (4)	0.018 (3)	0.000 (3)
C44	0.112 (6)	0.026 (3)	0.054 (4)	0.000 (4)	0.015 (4)	−0.003 (3)
C45	0.075 (4)	0.044 (4)	0.046 (3)	−0.020 (3)	−0.002 (3)	−0.009 (3)
C46	0.052 (4)	0.040 (3)	0.040 (3)	0.001 (3)	0.006 (3)	0.002 (3)
Pd2	0.0320 (2)	0.0335 (2)	0.0370 (2)	0.00093 (17)	0.00480 (17)	−0.00317 (17)
Fe2	0.0421 (4)	0.0368 (4)	0.0417 (4)	0.0037 (3)	0.0122 (4)	0.0009 (3)
S3	0.0437 (9)	0.0577 (9)	0.0623 (9)	0.0144 (7)	−0.0050 (7)	−0.0234 (7)
S4	0.0441 (8)	0.0404 (8)	0.0491 (8)	0.0023 (6)	−0.0048 (6)	−0.0044 (6)
P3	0.0326 (7)	0.0342 (7)	0.0344 (7)	−0.0013 (6)	0.0081 (6)	−0.0017 (6)
P4	0.0362 (8)	0.0361 (7)	0.0367 (7)	0.0001 (6)	0.0076 (6)	−0.0042 (6)
F11	0.075 (2)	0.0464 (18)	0.097 (2)	−0.0037 (16)	0.0272 (19)	−0.0084 (17)
F12	0.103 (3)	0.074 (2)	0.100 (3)	0.049 (2)	0.007 (2)	0.006 (2)
F13	0.049 (2)	0.167 (4)	0.107 (3)	0.032 (2)	0.006 (2)	−0.033 (2)
F14	0.076 (2)	0.120 (3)	0.126 (3)	−0.039 (2)	0.049 (2)	−0.039 (2)
F15	0.108 (3)	0.0448 (19)	0.097 (2)	−0.0009 (18)	0.047 (2)	0.0055 (18)
F16	0.0424 (19)	0.071 (2)	0.088 (2)	−0.0014 (15)	0.0124 (17)	0.0050 (17)
F17	0.075 (2)	0.074 (2)	0.089 (2)	−0.0280 (18)	0.0133 (18)	0.0121 (18)

F18	0.106 (3)	0.049 (2)	0.071 (2)	0.0009 (17)	0.0069 (18)	0.0141 (17)
F19	0.052 (2)	0.077 (2)	0.086 (2)	0.0154 (16)	−0.0030 (17)	0.0252 (18)
F20	0.0390 (18)	0.067 (2)	0.076 (2)	−0.0043 (15)	−0.0020 (15)	0.0161 (16)
C47	0.038 (3)	0.037 (3)	0.031 (3)	0.001 (2)	0.011 (2)	−0.005 (2)
C48	0.042 (3)	0.045 (3)	0.044 (3)	−0.005 (3)	0.014 (3)	0.001 (3)
C49	0.071 (4)	0.047 (3)	0.052 (3)	−0.003 (3)	0.028 (3)	0.009 (3)
C50	0.067 (4)	0.051 (4)	0.043 (3)	0.012 (3)	0.012 (3)	0.011 (3)
C51	0.044 (3)	0.047 (3)	0.039 (3)	0.001 (3)	0.005 (3)	−0.001 (3)
C52	0.038 (3)	0.032 (3)	0.043 (3)	0.001 (2)	0.011 (2)	−0.007 (2)
C53	0.043 (3)	0.041 (3)	0.062 (4)	−0.002 (3)	0.010 (3)	−0.010 (3)
C54	0.077 (4)	0.029 (3)	0.056 (4)	0.015 (3)	0.012 (3)	−0.002 (3)
C55	0.048 (4)	0.056 (4)	0.055 (4)	0.015 (3)	0.011 (3)	−0.002 (3)
C56	0.049 (4)	0.051 (3)	0.043 (3)	0.004 (3)	0.016 (3)	−0.003 (3)
C57	0.034 (3)	0.034 (3)	0.040 (3)	0.001 (2)	0.007 (2)	0.003 (2)
C58	0.046 (3)	0.053 (3)	0.041 (3)	−0.005 (3)	0.011 (3)	−0.002 (3)
C59	0.072 (4)	0.065 (4)	0.056 (4)	−0.016 (3)	0.031 (3)	0.001 (3)
C60	0.055 (4)	0.067 (4)	0.093 (5)	−0.016 (3)	0.043 (4)	−0.006 (4)
C61	0.036 (3)	0.069 (4)	0.073 (4)	−0.005 (3)	0.012 (3)	0.007 (3)
C62	0.038 (3)	0.067 (4)	0.047 (3)	−0.005 (3)	0.005 (3)	0.009 (3)
C63	0.026 (3)	0.033 (3)	0.036 (3)	0.001 (2)	0.003 (2)	−0.001 (2)
C64	0.048 (3)	0.041 (3)	0.050 (3)	−0.001 (3)	0.003 (3)	0.001 (3)
C65	0.067 (4)	0.030 (3)	0.072 (4)	−0.007 (3)	0.001 (3)	−0.011 (3)
C66	0.053 (4)	0.058 (4)	0.070 (4)	0.002 (3)	0.004 (3)	−0.030 (3)
C67	0.057 (4)	0.060 (4)	0.059 (4)	−0.011 (3)	0.021 (3)	−0.025 (3)
C68	0.037 (3)	0.048 (3)	0.047 (3)	−0.007 (2)	0.009 (3)	−0.012 (3)
C69	0.036 (3)	0.041 (3)	0.035 (3)	0.003 (2)	0.005 (2)	−0.002 (2)
C70	0.059 (4)	0.047 (3)	0.050 (3)	0.006 (3)	0.018 (3)	−0.003 (3)
C71	0.076 (4)	0.070 (4)	0.057 (4)	0.018 (3)	0.029 (3)	−0.010 (3)
C72	0.061 (4)	0.090 (5)	0.039 (3)	0.006 (3)	0.016 (3)	−0.007 (3)
C73	0.068 (4)	0.069 (4)	0.051 (4)	−0.001 (3)	0.020 (3)	0.012 (3)
C74	0.052 (3)	0.048 (3)	0.042 (3)	−0.001 (3)	0.008 (3)	−0.008 (3)
C75	0.036 (3)	0.029 (3)	0.046 (3)	0.006 (2)	0.010 (3)	0.001 (2)
C76	0.054 (4)	0.047 (3)	0.049 (3)	−0.003 (3)	0.015 (3)	−0.011 (3)
C77	0.058 (4)	0.051 (4)	0.071 (4)	−0.018 (3)	−0.001 (3)	−0.015 (3)
C78	0.038 (3)	0.052 (4)	0.074 (4)	−0.006 (3)	0.003 (3)	0.014 (3)
C79	0.043 (3)	0.060 (4)	0.054 (4)	−0.009 (3)	0.015 (3)	0.004 (3)
C80	0.048 (3)	0.051 (3)	0.049 (3)	−0.004 (3)	0.012 (3)	−0.002 (3)
C81	0.042 (3)	0.044 (3)	0.031 (3)	0.002 (3)	0.006 (2)	−0.011 (2)
C82	0.044 (3)	0.047 (3)	0.046 (3)	0.001 (3)	0.011 (3)	−0.006 (3)
C83	0.061 (4)	0.057 (4)	0.057 (4)	0.025 (3)	0.008 (3)	−0.004 (3)
C84	0.037 (4)	0.103 (6)	0.058 (4)	0.024 (4)	0.002 (3)	−0.019 (4)
C85	0.042 (4)	0.080 (5)	0.072 (4)	−0.020 (4)	0.025 (3)	−0.029 (4)
C86	0.067 (4)	0.043 (4)	0.045 (3)	0.003 (3)	0.024 (3)	−0.006 (3)
C87	0.034 (3)	0.044 (3)	0.035 (3)	0.000 (2)	0.003 (2)	−0.001 (2)
C88	0.033 (3)	0.064 (4)	0.046 (3)	0.007 (3)	0.005 (3)	0.000 (3)
C89	0.052 (4)	0.050 (4)	0.054 (4)	−0.017 (3)	0.015 (3)	0.003 (3)
C90	0.070 (4)	0.036 (3)	0.038 (3)	0.008 (3)	0.005 (3)	0.013 (3)
C91	0.036 (3)	0.050 (4)	0.047 (3)	0.009 (3)	−0.003 (3)	0.008 (3)
C92	0.038 (3)	0.049 (3)	0.037 (3)	−0.005 (3)	0.002 (2)	0.003 (3)

Geometric parameters (Å, °)

Pd1—P2	2.2926 (12)	Pd2—P3	2.3163 (11)
Pd1—P1	2.3418 (11)	Pd2—P4	2.3286 (12)
Pd1—S2	2.3651 (11)	Pd2—S3	2.3446 (12)
Pd1—S1	2.3769 (12)	Pd2—S4	2.3746 (12)
Fe1—C1	2.010 (4)	Fe2—C47	1.993 (4)
Fe1—C2	2.015 (4)	Fe2—C48	2.011 (4)
Fe1—C5	2.025 (4)	Fe2—C56	2.015 (4)
Fe1—C10	2.028 (4)	Fe2—C52	2.015 (4)
Fe1—C6	2.028 (4)	Fe2—C51	2.022 (4)
Fe1—C7	2.029 (4)	Fe2—C53	2.022 (4)
Fe1—C8	2.033 (4)	Fe2—C54	2.038 (4)
Fe1—C9	2.044 (4)	Fe2—C55	2.041 (4)
Fe1—C3	2.050 (4)	Fe2—C50	2.042 (4)
Fe1—C4	2.051 (4)	Fe2—C49	2.051 (4)
S1—C35	1.753 (5)	S3—C81	1.743 (4)
S2—C41	1.748 (4)	S4—C87	1.747 (4)
P1—C6	1.818 (4)	P3—C47	1.796 (4)
P1—C17	1.827 (4)	P3—C63	1.813 (4)
P1—C11	1.828 (4)	P3—C57	1.818 (4)
P2—C1	1.794 (4)	P4—C52	1.810 (4)
P2—C23	1.810 (4)	P4—C69	1.829 (4)
P2—C29	1.813 (4)	P4—C75	1.835 (4)
F1—C36	1.356 (6)	F11—C82	1.348 (5)
F2—C37	1.343 (6)	F12—C83	1.339 (5)
F3—C38	1.352 (6)	F13—C84	1.348 (5)
F3—F17	2.857 (4)	F14—C85	1.337 (5)
F4—C39	1.351 (6)	F15—C86	1.329 (5)
F5—C40	1.344 (5)	F16—C88	1.355 (5)
F6—C42	1.340 (5)	F17—C89	1.339 (5)
F7—C43	1.347 (5)	F18—C90	1.341 (5)
F8—C44	1.350 (5)	F19—C91	1.343 (5)
F9—C45	1.335 (5)	F20—C92	1.352 (5)
F10—C46	1.342 (5)	C47—C48	1.415 (5)
C1—C5	1.423 (5)	C47—C51	1.437 (5)
C1—C2	1.426 (5)	C48—C49	1.408 (5)
C2—C3	1.406 (5)	C48—H48	0.9300
C2—H2	0.9300	C49—C50	1.405 (6)
C3—C4	1.384 (6)	C49—H49	0.9300
C3—H3	0.9300	C50—C51	1.398 (5)
C4—C5	1.406 (5)	C50—H50	0.9300
C4—H4	0.9300	C51—H51	0.9300
C5—H5	0.9300	C52—C53	1.411 (5)
C6—C10	1.416 (5)	C52—C56	1.429 (5)
C6—C7	1.423 (5)	C53—C54	1.401 (5)
C7—C8	1.412 (5)	C53—H53	0.9300
C7—H7	0.9300	C54—C55	1.408 (6)

C8—C9	1.388 (6)	C54—H54	0.9300
C8—H8	0.9300	C55—C56	1.393 (5)
C9—C10	1.400 (5)	C55—H55	0.9300
C9—H9	0.9300	C56—H56	0.9300
C10—H10	0.9300	C57—C58	1.382 (5)
C11—C12	1.361 (6)	C57—C62	1.386 (5)
C11—C16	1.363 (5)	C58—C59	1.362 (6)
C12—C13	1.388 (6)	C58—H58	0.9300
C12—H12	0.9300	C59—C60	1.370 (6)
C13—C14	1.351 (7)	C59—H59	0.9300
C13—H13	0.9300	C60—C61	1.375 (6)
C14—C15	1.334 (6)	C60—H60	0.9300
C14—H14	0.9300	C61—C62	1.372 (6)
C15—C16	1.394 (6)	C61—H61	0.9300
C15—H15	0.9300	C62—H62	0.9300
C16—H16	0.9300	C63—C68	1.381 (5)
C17—C22	1.380 (6)	C63—C64	1.393 (5)
C17—C18	1.384 (5)	C64—C65	1.384 (6)
C18—C19	1.382 (6)	C64—H64	0.9300
C18—H18	0.9300	C65—C66	1.370 (6)
C19—C20	1.345 (6)	C65—H65	0.9300
C19—H19	0.9300	C66—C67	1.344 (6)
C20—C21	1.358 (6)	C66—H66	0.9300
C20—H20	0.9300	C67—C68	1.368 (5)
C21—C22	1.383 (6)	C67—H67	0.9300
C21—H21	0.9300	C68—H68	0.9300
C22—H22	0.9300	C69—C74	1.369 (5)
C23—C24	1.381 (5)	C69—C70	1.383 (5)
C23—C28	1.388 (5)	C70—C71	1.361 (6)
C24—C25	1.371 (5)	C70—H70	0.9300
C24—H24	0.9300	C71—C72	1.362 (6)
C25—C26	1.363 (6)	C71—H71	0.9300
C25—H25	0.9300	C72—C73	1.365 (6)
C26—C27	1.376 (6)	C72—H72	0.9300
C26—H26	0.9300	C73—C74	1.388 (6)
C27—C28	1.383 (5)	C73—H73	0.9300
C27—H27	0.9300	C74—H74	0.9300
C28—H28	0.9300	C75—C80	1.381 (5)
C29—C34	1.377 (5)	C75—C76	1.387 (5)
C29—C30	1.386 (5)	C76—C77	1.369 (6)
C30—C31	1.379 (5)	C76—H76	0.9300
C30—H30	0.9300	C77—C78	1.362 (6)
C31—C32	1.358 (6)	C77—H77	0.9300
C31—H31	0.9300	C78—C79	1.359 (6)
C32—C33	1.373 (7)	C78—H78	0.9300
C32—H32	0.9300	C79—C80	1.388 (5)
C33—C34	1.375 (6)	C79—H79	0.9300
C33—H33	0.9300	C80—H80	0.9300
C34—H34	0.9300	C81—C86	1.389 (6)

C35—C36	1.380 (6)	C81—C82	1.394 (6)
C35—C40	1.388 (6)	C82—C83	1.361 (6)
C36—C37	1.377 (7)	C83—C84	1.347 (7)
C37—C38	1.351 (7)	C84—C85	1.373 (7)
C38—C39	1.350 (7)	C85—C86	1.372 (6)
C39—C40	1.386 (6)	C87—C88	1.380 (6)
C41—C46	1.372 (5)	C87—C92	1.386 (5)
C41—C42	1.383 (6)	C88—C89	1.372 (6)
C42—C43	1.361 (6)	C89—C90	1.368 (6)
C43—C44	1.357 (7)	C90—C91	1.346 (6)
C44—C45	1.361 (7)	C91—C92	1.372 (6)
C45—C46	1.370 (6)		

P2—Pd1—P1	96.56 (4)	P3—Pd2—P4	97.38 (4)
P2—Pd1—S2	85.61 (4)	P3—Pd2—S3	84.55 (4)
P1—Pd1—S2	167.71 (4)	P4—Pd2—S3	170.39 (5)
P2—Pd1—S1	171.24 (4)	P3—Pd2—S4	174.47 (4)
P1—Pd1—S1	87.45 (4)	P4—Pd2—S4	82.82 (4)
S2—Pd1—S1	92.13 (4)	S3—Pd2—S4	96.18 (4)
C1—Fe1—C2	41.51 (15)	C47—Fe2—C48	41.38 (15)
C1—Fe1—C5	41.29 (14)	C47—Fe2—C56	109.71 (18)
C2—Fe1—C5	68.63 (17)	C48—Fe2—C56	139.91 (19)
C1—Fe1—C10	139.83 (17)	C47—Fe2—C52	108.39 (17)
C2—Fe1—C10	178.42 (18)	C48—Fe2—C52	111.08 (18)
C5—Fe1—C10	112.94 (18)	C56—Fe2—C52	41.55 (15)
C1—Fe1—C6	110.27 (16)	C47—Fe2—C51	41.93 (15)
C2—Fe1—C6	139.11 (18)	C48—Fe2—C51	68.92 (17)
C5—Fe1—C6	111.59 (17)	C56—Fe2—C51	109.73 (19)
C10—Fe1—C6	40.87 (15)	C52—Fe2—C51	137.25 (18)
C1—Fe1—C7	110.38 (17)	C47—Fe2—C53	137.51 (18)
C2—Fe1—C7	111.03 (18)	C48—Fe2—C53	111.82 (18)
C5—Fe1—C7	139.62 (18)	C56—Fe2—C53	68.53 (18)
C10—Fe1—C7	67.97 (17)	C52—Fe2—C53	40.91 (15)
C6—Fe1—C7	41.06 (15)	C51—Fe2—C53	178.09 (19)
C1—Fe1—C8	138.49 (19)	C47—Fe2—C54	177.22 (18)
C2—Fe1—C8	110.89 (19)	C48—Fe2—C54	139.3 (2)
C5—Fe1—C8	179.46 (19)	C56—Fe2—C54	68.19 (19)
C10—Fe1—C8	67.54 (18)	C52—Fe2—C54	68.83 (17)
C6—Fe1—C8	68.92 (17)	C51—Fe2—C54	140.12 (19)
C7—Fe1—C8	40.69 (15)	C53—Fe2—C54	40.35 (16)
C1—Fe1—C9	178.08 (19)	C47—Fe2—C55	138.96 (19)
C2—Fe1—C9	138.39 (19)	C48—Fe2—C55	179.6 (2)
C5—Fe1—C9	140.44 (19)	C56—Fe2—C55	40.17 (16)
C10—Fe1—C9	40.23 (15)	C52—Fe2—C55	68.77 (17)
C6—Fe1—C9	68.64 (17)	C51—Fe2—C55	111.42 (19)
C7—Fe1—C9	67.74 (18)	C53—Fe2—C55	67.85 (18)
C8—Fe1—C9	39.79 (16)	C54—Fe2—C55	40.40 (16)
C1—Fe1—C3	68.90 (16)	C47—Fe2—C50	69.43 (17)
C2—Fe1—C3	40.44 (15)	C48—Fe2—C50	68.24 (18)
C5—Fe1—C3	67.57 (17)	C56—Fe2—C50	137.5 (2)

C10—Fe1—C3	139.60 (19)	C52—Fe2—C50	177.48 (19)
C6—Fe1—C3	179.10 (19)	C51—Fe2—C50	40.26 (16)
C7—Fe1—C3	139.39 (19)	C53—Fe2—C50	141.6 (2)
C8—Fe1—C3	111.91 (19)	C54—Fe2—C50	113.34 (19)
C9—Fe1—C3	112.20 (18)	C55—Fe2—C50	111.9 (2)
C1—Fe1—C4	68.79 (17)	C47—Fe2—C49	69.21 (17)
C2—Fe1—C4	67.63 (18)	C48—Fe2—C49	40.55 (15)
C5—Fe1—C4	40.36 (15)	C56—Fe2—C49	177.5 (2)
C10—Fe1—C4	113.36 (18)	C52—Fe2—C49	140.7 (2)
C6—Fe1—C4	140.09 (19)	C51—Fe2—C49	67.94 (18)
C7—Fe1—C4	178.65 (18)	C53—Fe2—C49	113.8 (2)
C8—Fe1—C4	139.3 (2)	C54—Fe2—C49	113.0 (2)
C9—Fe1—C4	113.09 (19)	C55—Fe2—C49	139.4 (2)
C3—Fe1—C4	39.44 (16)	C50—Fe2—C49	40.14 (16)
C35—S1—Pd1	103.74 (17)	C81—S3—Pd2	112.43 (15)
C41—S2—Pd1	105.90 (14)	C87—S4—Pd2	108.33 (15)
C6—P1—C17	99.96 (19)	C47—P3—C63	101.98 (19)
C6—P1—C11	102.7 (2)	C47—P3—C57	109.48 (19)
C17—P1—C11	104.4 (2)	C63—P3—C57	102.06 (19)
C6—P1—Pd1	119.14 (14)	C47—P3—Pd2	114.84 (14)
C17—P1—Pd1	106.31 (15)	C63—P3—Pd2	117.44 (13)
C11—P1—Pd1	121.38 (15)	C57—P3—Pd2	110.02 (15)
C1—P2—C23	108.94 (19)	C52—P4—C69	99.7 (2)
C1—P2—C29	105.8 (2)	C52—P4—C75	103.2 (2)
C23—P2—C29	100.87 (18)	C69—P4—C75	104.8 (2)
C1—P2—Pd1	111.99 (14)	C52—P4—Pd2	122.13 (14)
C23—P2—Pd1	112.75 (15)	C69—P4—Pd2	120.84 (16)
C29—P2—Pd1	115.68 (13)	C75—P4—Pd2	103.85 (14)
C5—C1—C2	106.2 (4)	C48—C47—C51	106.3 (4)
C5—C1—P2	121.6 (3)	C48—C47—P3	124.0 (3)
C2—C1—P2	131.9 (3)	C51—C47—P3	129.7 (3)
C5—C1—Fe1	69.9 (2)	C48—C47—Fe2	70.0 (2)
C2—C1—Fe1	69.5 (2)	C51—C47—Fe2	70.1 (2)
P2—C1—Fe1	120.0 (2)	P3—C47—Fe2	125.1 (2)
C3—C2—C1	108.4 (4)	C49—C48—C47	109.0 (4)
C3—C2—Fe1	71.1 (3)	C49—C48—Fe2	71.3 (3)
C1—C2—Fe1	69.0 (2)	C47—C48—Fe2	68.7 (2)
C3—C2—H2	125.8	C49—C48—H48	125.5
C1—C2—H2	125.8	C47—C48—H48	125.5
Fe1—C2—H2	125.6	Fe2—C48—H48	126.1
C4—C3—C2	108.4 (4)	C50—C49—C48	107.8 (4)
C4—C3—Fe1	70.3 (3)	C50—C49—Fe2	69.6 (3)
C2—C3—Fe1	68.4 (2)	C48—C49—Fe2	68.2 (3)
C4—C3—H3	125.8	C50—C49—H49	126.1
C2—C3—H3	125.8	C48—C49—H49	126.1
Fe1—C3—H3	127.0	Fe2—C49—H49	127.7
C3—C4—C5	108.6 (4)	C51—C50—C49	108.6 (4)
C3—C4—Fe1	70.3 (3)	C51—C50—Fe2	69.1 (3)
C5—C4—Fe1	68.8 (2)	C49—C50—Fe2	70.3 (3)

C3—C4—H4	125.7	C51—C50—H50	125.7
C5—C4—H4	125.7	C49—C50—H50	125.7
Fe1—C4—H4	126.8	Fe2—C50—H50	126.5
C4—C5—C1	108.4 (4)	C50—C51—C47	108.3 (4)
C4—C5—Fe1	70.8 (3)	C50—C51—Fe2	70.6 (3)
C1—C5—Fe1	68.8 (2)	C47—C51—Fe2	68.0 (2)
C4—C5—H5	125.8	C50—C51—H51	125.9
C1—C5—H5	125.8	C47—C51—H51	125.9
Fe1—C5—H5	126.2	Fe2—C51—H51	127.1
C10—C6—C7	106.0 (4)	C53—C52—C56	106.3 (4)
C10—C6—P1	125.5 (3)	C53—C52—P4	127.8 (4)
C7—C6—P1	128.5 (3)	C56—C52—P4	125.9 (4)
C10—C6—Fe1	69.6 (2)	C53—C52—Fe2	69.8 (3)
C7—C6—Fe1	69.5 (2)	C56—C52—Fe2	69.2 (2)
P1—C6—Fe1	125.6 (2)	P4—C52—Fe2	127.1 (2)
C8—C7—C6	108.3 (4)	C54—C53—C52	109.1 (4)
C8—C7—Fe1	69.8 (3)	C54—C53—Fe2	70.4 (3)
C6—C7—Fe1	69.4 (2)	C52—C53—Fe2	69.3 (2)
C8—C7—H7	125.9	C54—C53—H53	125.4
C6—C7—H7	125.9	C52—C53—H53	125.4
Fe1—C7—H7	126.5	Fe2—C53—H53	126.4
C9—C8—C7	108.4 (4)	C53—C54—C55	107.7 (4)
C9—C8—Fe1	70.5 (3)	C53—C54—Fe2	69.2 (3)
C7—C8—Fe1	69.5 (3)	C55—C54—Fe2	69.9 (3)
C9—C8—H8	125.8	C53—C54—H54	126.2
C7—C8—H8	125.8	C55—C54—H54	126.2
Fe1—C8—H8	125.7	Fe2—C54—H54	126.3
C8—C9—C10	108.1 (4)	C56—C55—C54	108.4 (4)
C8—C9—Fe1	69.7 (3)	C56—C55—Fe2	68.9 (3)
C10—C9—Fe1	69.2 (3)	C54—C55—Fe2	69.7 (3)
C8—C9—H9	125.9	C56—C55—H55	125.8
C10—C9—H9	125.9	C54—C55—H55	125.8
Fe1—C9—H9	126.7	Fe2—C55—H55	127.2
C9—C10—C6	109.2 (4)	C55—C56—C52	108.5 (4)
C9—C10—Fe1	70.5 (3)	C55—C56—Fe2	70.9 (3)
C6—C10—Fe1	69.6 (2)	C52—C56—Fe2	69.2 (2)
C9—C10—H10	125.4	C55—C56—H56	125.7
C6—C10—H10	125.4	C52—C56—H56	125.7
Fe1—C10—H10	126.1	Fe2—C56—H56	125.7
C12—C11—C16	117.2 (4)	C58—C57—C62	117.3 (4)
C12—C11—P1	122.1 (4)	C58—C57—P3	120.1 (3)
C16—C11—P1	120.5 (4)	C62—C57—P3	122.3 (4)
C11—C12—C13	121.8 (5)	C59—C58—C57	121.7 (5)
C11—C12—H12	119.1	C59—C58—H58	119.2
C13—C12—H12	119.1	C57—C58—H58	119.2
C14—C13—C12	119.7 (5)	C58—C59—C60	120.1 (5)
C14—C13—H13	120.2	C58—C59—H59	119.9
C12—C13—H13	120.2	C60—C59—H59	119.9
C15—C14—C13	119.8 (5)	C59—C60—C61	119.9 (5)

C15—C14—H14	120.1	C59—C60—H60	120.1
C13—C14—H14	120.1	C61—C60—H60	120.1
C14—C15—C16	120.6 (5)	C62—C61—C60	119.4 (5)
C14—C15—H15	119.7	C62—C61—H61	120.3
C16—C15—H15	119.7	C60—C61—H61	120.3
C11—C16—C15	121.0 (5)	C61—C62—C57	121.6 (5)
C11—C16—H16	119.5	C61—C62—H62	119.2
C15—C16—H16	119.5	C57—C62—H62	119.2
C22—C17—C18	117.8 (4)	C68—C63—C64	118.5 (4)
C22—C17—P1	119.4 (3)	C68—C63—P3	120.9 (3)
C18—C17—P1	122.4 (4)	C64—C63—P3	120.6 (4)
C19—C18—C17	119.9 (5)	C65—C64—C63	119.9 (5)
C19—C18—H18	120.1	C65—C64—H64	120.1
C17—C18—H18	120.1	C63—C64—H64	120.1
C20—C19—C18	121.0 (5)	C66—C65—C64	119.5 (5)
C20—C19—H19	119.5	C66—C65—H65	120.2
C18—C19—H19	119.5	C64—C65—H65	120.2
C19—C20—C21	120.6 (5)	C67—C66—C65	121.0 (5)
C19—C20—H20	119.7	C67—C66—H66	119.5
C21—C20—H20	119.7	C65—C66—H66	119.5
C20—C21—C22	119.1 (5)	C66—C67—C68	120.3 (5)
C20—C21—H21	120.4	C66—C67—H67	119.9
C22—C21—H21	120.4	C68—C67—H67	119.9
C17—C22—C21	121.5 (5)	C67—C68—C63	120.8 (4)
C17—C22—H22	119.3	C67—C68—H68	119.6
C21—C22—H22	119.3	C63—C68—H68	119.6
C24—C23—C28	118.1 (4)	C74—C69—C70	118.5 (4)
C24—C23—P2	122.3 (3)	C74—C69—P4	122.1 (4)
C28—C23—P2	119.6 (3)	C70—C69—P4	119.3 (4)
C25—C24—C23	121.5 (4)	C71—C70—C69	121.1 (5)
C25—C24—H24	119.3	C71—C70—H70	119.4
C23—C24—H24	119.3	C69—C70—H70	119.4
C26—C25—C24	119.7 (5)	C70—C71—C72	120.6 (5)
C26—C25—H25	120.1	C70—C71—H71	119.7
C24—C25—H25	120.1	C72—C71—H71	119.7
C25—C26—C27	120.4 (5)	C71—C72—C73	119.0 (5)
C25—C26—H26	119.8	C71—C72—H72	120.5
C27—C26—H26	119.8	C73—C72—H72	120.5
C26—C27—C28	119.7 (5)	C72—C73—C74	121.1 (5)
C26—C27—H27	120.1	C72—C73—H73	119.5
C28—C27—H27	120.1	C74—C73—H73	119.5
C27—C28—C23	120.5 (4)	C69—C74—C73	119.6 (5)
C27—C28—H28	119.8	C69—C74—H74	120.2
C23—C28—H28	119.8	C73—C74—H74	120.2
C34—C29—C30	118.5 (4)	C80—C75—C76	118.3 (4)
C34—C29—P2	122.2 (4)	C80—C75—P4	117.9 (4)
C30—C29—P2	119.3 (4)	C76—C75—P4	123.7 (4)
C31—C30—C29	120.8 (5)	C77—C76—C75	120.4 (5)
C31—C30—H30	119.6	C77—C76—H76	119.8

C29—C30—H30	119.6	C75—C76—H76	119.8
C32—C31—C30	119.7 (5)	C78—C77—C76	120.7 (5)
C32—C31—H31	120.2	C78—C77—H77	119.7
C30—C31—H31	120.2	C76—C77—H77	119.7
C31—C32—C33	120.4 (5)	C79—C78—C77	120.3 (5)
C31—C32—H32	119.8	C79—C78—H78	119.8
C33—C32—H32	119.8	C77—C78—H78	119.8
C32—C33—C34	120.1 (5)	C78—C79—C80	119.6 (5)
C32—C33—H33	120.0	C78—C79—H79	120.2
C34—C33—H33	120.0	C80—C79—H79	120.2
C33—C34—C29	120.5 (5)	C75—C80—C79	120.7 (4)
C33—C34—H34	119.8	C75—C80—H80	119.6
C29—C34—H34	119.8	C79—C80—H80	119.6
C36—C35—C40	114.0 (5)	C86—C81—C82	114.6 (4)
C36—C35—S1	120.7 (4)	C86—C81—S3	124.5 (4)
C40—C35—S1	125.3 (4)	C82—C81—S3	120.5 (4)
F1—C36—C37	117.5 (5)	F11—C82—C83	116.9 (5)
F1—C36—C35	119.2 (5)	F11—C82—C81	119.2 (4)
C37—C36—C35	123.3 (6)	C83—C82—C81	123.9 (5)
F2—C37—C38	119.4 (6)	F12—C83—C84	120.5 (6)
F2—C37—C36	119.9 (7)	F12—C83—C82	120.2 (6)
C38—C37—C36	120.6 (6)	C84—C83—C82	119.3 (5)
C39—C38—C37	118.7 (6)	C83—C84—F13	120.6 (6)
C39—C38—F3	120.5 (7)	C83—C84—C85	120.0 (5)
C37—C38—F3	120.8 (6)	F13—C84—C85	119.3 (6)
C38—C39—F4	120.5 (6)	F14—C85—C86	120.1 (6)
C38—C39—C40	120.5 (6)	F14—C85—C84	119.9 (6)
F4—C39—C40	119.0 (6)	C86—C85—C84	120.0 (5)
F5—C40—C39	116.4 (5)	F15—C86—C85	117.8 (5)
F5—C40—C35	120.9 (5)	F15—C86—C81	120.1 (5)
C39—C40—C35	122.7 (5)	C85—C86—C81	122.1 (5)
C46—C41—C42	114.6 (4)	C88—C87—C92	113.9 (4)
C46—C41—S2	121.9 (4)	C88—C87—S4	126.9 (4)
C42—C41—S2	123.4 (4)	C92—C87—S4	119.2 (4)
F6—C42—C43	118.3 (5)	F16—C88—C89	117.2 (5)
F6—C42—C41	118.2 (4)	F16—C88—C87	119.3 (5)
C43—C42—C41	123.5 (5)	C89—C88—C87	123.5 (5)
F7—C43—C44	119.7 (6)	F17—C89—C90	120.1 (5)
F7—C43—C42	120.8 (6)	F17—C89—C88	120.5 (5)
C44—C43—C42	119.5 (5)	C90—C89—C88	119.4 (5)
F8—C44—C43	119.4 (6)	F18—C90—C91	120.6 (5)
F8—C44—C45	121.0 (6)	F18—C90—C89	119.5 (5)
C43—C44—C45	119.6 (5)	C91—C90—C89	119.8 (5)
F9—C45—C44	119.7 (5)	F19—C91—C90	119.7 (5)
F9—C45—C46	120.7 (5)	F19—C91—C92	120.8 (5)
C44—C45—C46	119.6 (5)	C90—C91—C92	119.5 (5)
F10—C46—C45	116.5 (5)	F20—C92—C91	117.0 (4)
F10—C46—C41	120.4 (4)	F20—C92—C87	119.1 (4)
C45—C46—C41	123.1 (5)	C91—C92—C87	123.9 (4)

P1—Pd1—S1—C35	−138.42 (17)	C42—C41—C46—C45	−2.9 (7)
S2—Pd1—S1—C35	53.88 (17)	S2—C41—C46—C45	−179.8 (4)
P2—Pd1—S2—C41	−151.92 (17)	P3—Pd2—S3—C81	163.84 (18)
P1—Pd1—S2—C41	−51.2 (3)	S4—Pd2—S3—C81	−21.67 (18)
S1—Pd1—S2—C41	36.55 (17)	P4—Pd2—S4—C87	145.26 (16)
P2—Pd1—P1—C6	25.66 (17)	S3—Pd2—S4—C87	−44.36 (17)
S2—Pd1—P1—C6	−73.9 (3)	P4—Pd2—P3—C47	50.04 (15)
S1—Pd1—P1—C6	−162.16 (17)	S3—Pd2—P3—C47	−120.48 (15)
P2—Pd1—P1—C17	137.34 (14)	P4—Pd2—P3—C63	169.92 (17)
S2—Pd1—P1—C17	37.8 (3)	S3—Pd2—P3—C63	−0.60 (17)
S1—Pd1—P1—C17	−50.47 (15)	P4—Pd2—P3—C57	−73.99 (15)
P2—Pd1—P1—C11	−103.78 (18)	S3—Pd2—P3—C57	115.48 (15)
S2—Pd1—P1—C11	156.7 (2)	P3—Pd2—P4—C52	−18.90 (18)
S1—Pd1—P1—C11	68.41 (18)	S4—Pd2—P4—C52	166.68 (18)
P1—Pd1—P2—C1	−62.08 (15)	P3—Pd2—P4—C69	108.49 (16)
S2—Pd1—P2—C1	105.77 (15)	S4—Pd2—P4—C69	−65.94 (16)
P1—Pd1—P2—C23	61.22 (14)	P3—Pd2—P4—C75	−134.56 (15)
S2—Pd1—P2—C23	−130.94 (14)	S4—Pd2—P4—C75	51.01 (15)
P1—Pd1—P2—C29	176.58 (17)	C63—P3—C47—C48	−95.4 (4)
S2—Pd1—P2—C29	−15.58 (17)	C57—P3—C47—C48	157.0 (3)
C23—P2—C1—C5	−146.7 (3)	Pd2—P3—C47—C48	32.7 (4)
C29—P2—C1—C5	105.6 (3)	C63—P3—C47—C51	84.0 (4)
Pd1—P2—C1—C5	−21.3 (4)	C57—P3—C47—C51	−23.6 (4)
C23—P2—C1—C2	25.4 (5)	Pd2—P3—C47—C51	−147.9 (3)
C29—P2—C1—C2	−82.3 (4)	C63—P3—C47—Fe2	176.4 (3)
Pd1—P2—C1—C2	150.9 (4)	C57—P3—C47—Fe2	68.8 (3)
C23—P2—C1—Fe1	−63.0 (3)	Pd2—P3—C47—Fe2	−55.5 (3)
C29—P2—C1—Fe1	−170.7 (2)	C56—Fe2—C47—C48	−145.4 (3)
Pd1—P2—C1—Fe1	62.4 (2)	C52—Fe2—C47—C48	−101.3 (3)
C2—Fe1—C1—C5	−117.0 (4)	C51—Fe2—C47—C48	116.7 (4)
C10—Fe1—C1—C5	64.3 (4)	C53—Fe2—C47—C48	−66.0 (4)
C6—Fe1—C1—C5	100.0 (3)	C55—Fe2—C47—C48	−179.8 (3)
C7—Fe1—C1—C5	143.9 (3)	C50—Fe2—C47—C48	80.0 (3)
C8—Fe1—C1—C5	−179.3 (3)	C49—Fe2—C47—C48	37.0 (3)
C3—Fe1—C1—C5	−79.6 (3)	C48—Fe2—C47—C51	−116.7 (4)
C4—Fe1—C1—C5	−37.2 (2)	C56—Fe2—C47—C51	97.9 (3)
C5—Fe1—C1—C2	117.0 (4)	C52—Fe2—C47—C51	142.0 (3)
C10—Fe1—C1—C2	−178.7 (3)	C53—Fe2—C47—C51	177.3 (3)
C6—Fe1—C1—C2	−143.0 (3)	C55—Fe2—C47—C51	63.5 (4)
C7—Fe1—C1—C2	−99.1 (3)	C50—Fe2—C47—C51	−36.7 (3)
C8—Fe1—C1—C2	−62.3 (4)	C49—Fe2—C47—C51	−79.7 (3)
C3—Fe1—C1—C2	37.4 (3)	C48—Fe2—C47—P3	118.2 (4)
C4—Fe1—C1—C2	79.8 (3)	C56—Fe2—C47—P3	−27.2 (3)
C2—Fe1—C1—P2	127.3 (4)	C52—Fe2—C47—P3	16.9 (3)
C5—Fe1—C1—P2	−115.7 (4)	C51—Fe2—C47—P3	−125.1 (4)
C10—Fe1—C1—P2	−51.4 (4)	C53—Fe2—C47—P3	52.2 (4)
C6—Fe1—C1—P2	−15.7 (3)	C55—Fe2—C47—P3	−61.6 (4)
C7—Fe1—C1—P2	28.3 (3)	C50—Fe2—C47—P3	−161.8 (3)
C8—Fe1—C1—P2	65.1 (4)	C49—Fe2—C47—P3	155.2 (3)

C3—Fe1—C1—P2	164.7 (3)	C51—C47—C48—C49	1.0 (5)
C4—Fe1—C1—P2	−152.9 (3)	P3—C47—C48—C49	−179.5 (3)
C5—C1—C2—C3	0.2 (5)	Fe2—C47—C48—C49	−60.1 (3)
P2—C1—C2—C3	−172.8 (3)	C51—C47—C48—Fe2	61.0 (3)
Fe1—C1—C2—C3	−60.5 (3)	P3—C47—C48—Fe2	−119.5 (3)
C5—C1—C2—Fe1	60.7 (3)	C47—Fe2—C48—C49	120.1 (4)
P2—C1—C2—Fe1	−112.4 (4)	C56—Fe2—C48—C49	176.3 (3)
C1—Fe1—C2—C3	119.2 (4)	C52—Fe2—C48—C49	−145.7 (3)
C5—Fe1—C2—C3	80.1 (3)	C51—Fe2—C48—C49	80.3 (3)
C6—Fe1—C2—C3	178.8 (3)	C53—Fe2—C48—C49	−101.6 (3)
C7—Fe1—C2—C3	−143.4 (3)	C54—Fe2—C48—C49	−64.1 (4)
C8—Fe1—C2—C3	−99.7 (3)	C50—Fe2—C48—C49	36.9 (3)
C9—Fe1—C2—C3	−63.7 (4)	C56—Fe2—C48—C47	56.2 (4)
C4—Fe1—C2—C3	36.4 (3)	C52—Fe2—C48—C47	94.2 (3)
C5—Fe1—C2—C1	−39.2 (2)	C51—Fe2—C48—C47	−39.8 (2)
C6—Fe1—C2—C1	59.6 (4)	C53—Fe2—C48—C47	138.3 (3)
C7—Fe1—C2—C1	97.4 (3)	C54—Fe2—C48—C47	175.9 (3)
C8—Fe1—C2—C1	141.1 (3)	C50—Fe2—C48—C47	−83.2 (3)
C9—Fe1—C2—C1	177.1 (3)	C49—Fe2—C48—C47	−120.1 (4)
C3—Fe1—C2—C1	−119.2 (4)	C47—C48—C49—C50	0.1 (5)
C4—Fe1—C2—C1	−82.8 (3)	Fe2—C48—C49—C50	−58.4 (3)
C1—C2—C3—C4	0.1 (5)	C47—C48—C49—Fe2	58.5 (3)
Fe1—C2—C3—C4	−59.1 (3)	C47—Fe2—C49—C50	82.4 (3)
C1—C2—C3—Fe1	59.2 (3)	C48—Fe2—C49—C50	120.1 (4)
C1—Fe1—C3—C4	81.9 (3)	C52—Fe2—C49—C50	176.3 (3)
C2—Fe1—C3—C4	120.2 (4)	C51—Fe2—C49—C50	37.2 (3)
C5—Fe1—C3—C4	37.3 (3)	C53—Fe2—C49—C50	−143.6 (3)
C10—Fe1—C3—C4	−62.3 (4)	C54—Fe2—C49—C50	−99.5 (3)
C7—Fe1—C3—C4	179.0 (3)	C55—Fe2—C49—C50	−60.5 (4)
C8—Fe1—C3—C4	−142.9 (3)	C47—Fe2—C49—C48	−37.7 (3)
C9—Fe1—C3—C4	−99.8 (3)	C52—Fe2—C49—C48	56.2 (4)
C1—Fe1—C3—C2	−38.3 (3)	C51—Fe2—C49—C48	−82.9 (3)
C5—Fe1—C3—C2	−82.9 (3)	C53—Fe2—C49—C48	96.3 (3)
C10—Fe1—C3—C2	177.6 (3)	C54—Fe2—C49—C48	140.4 (3)
C7—Fe1—C3—C2	58.8 (4)	C55—Fe2—C49—C48	179.5 (3)
C8—Fe1—C3—C2	96.9 (3)	C50—Fe2—C49—C48	−120.1 (4)
C9—Fe1—C3—C2	140.0 (3)	C48—C49—C50—C51	−1.1 (5)
C4—Fe1—C3—C2	−120.2 (4)	Fe2—C49—C50—C51	−58.7 (3)
C2—C3—C4—C5	−0.3 (5)	C48—C49—C50—Fe2	57.5 (3)
Fe1—C3—C4—C5	−58.3 (3)	C47—Fe2—C50—C51	38.1 (3)
C2—C3—C4—Fe1	57.9 (3)	C48—Fe2—C50—C51	82.7 (3)
C1—Fe1—C4—C3	−82.2 (3)	C56—Fe2—C50—C51	−59.0 (4)
C2—Fe1—C4—C3	−37.3 (3)	C53—Fe2—C50—C51	−179.3 (3)
C5—Fe1—C4—C3	−120.2 (4)	C54—Fe2—C50—C51	−141.6 (3)
C10—Fe1—C4—C3	141.3 (3)	C55—Fe2—C50—C51	−97.7 (3)
C6—Fe1—C4—C3	−178.8 (3)	C49—Fe2—C50—C51	119.9 (4)
C8—Fe1—C4—C3	59.1 (4)	C47—Fe2—C50—C49	−81.8 (3)
C9—Fe1—C4—C3	97.4 (3)	C48—Fe2—C50—C49	−37.3 (3)
C1—Fe1—C4—C5	38.0 (2)	C56—Fe2—C50—C49	−178.9 (3)

C2—Fe1—C4—C5	82.9 (3)	C51—Fe2—C50—C49	−119.9 (4)
C10—Fe1—C4—C5	−98.5 (3)	C53—Fe2—C50—C49	60.8 (4)
C6—Fe1—C4—C5	−58.6 (4)	C54—Fe2—C50—C49	98.5 (3)
C8—Fe1—C4—C5	179.3 (3)	C55—Fe2—C50—C49	142.4 (3)
C9—Fe1—C4—C5	−142.4 (3)	C49—C50—C51—C47	1.7 (5)
C3—Fe1—C4—C5	120.2 (4)	Fe2—C50—C51—C47	−57.7 (3)
C3—C4—C5—C1	0.5 (5)	C49—C50—C51—Fe2	59.4 (3)
Fe1—C4—C5—C1	−58.7 (3)	C48—C47—C51—C50	−1.7 (5)
C3—C4—C5—Fe1	59.1 (3)	P3—C47—C51—C50	178.9 (3)
C2—C1—C5—C4	−0.4 (5)	Fe2—C47—C51—C50	59.3 (3)
P2—C1—C5—C4	173.5 (3)	C48—C47—C51—Fe2	−61.0 (3)
Fe1—C1—C5—C4	60.0 (3)	P3—C47—C51—Fe2	119.6 (4)
C2—C1—C5—Fe1	−60.3 (3)	C47—Fe2—C51—C50	−120.1 (4)
P2—C1—C5—Fe1	113.6 (3)	C48—Fe2—C51—C50	−80.8 (3)
C1—Fe1—C5—C4	−119.5 (4)	C56—Fe2—C51—C50	142.1 (3)
C2—Fe1—C5—C4	−80.2 (3)	C52—Fe2—C51—C50	−179.5 (3)
C10—Fe1—C5—C4	99.6 (3)	C54—Fe2—C51—C50	62.8 (4)
C6—Fe1—C5—C4	143.9 (3)	C55—Fe2—C51—C50	99.1 (3)
C7—Fe1—C5—C4	−177.9 (3)	C49—Fe2—C51—C50	−37.1 (3)
C9—Fe1—C5—C4	61.7 (4)	C48—Fe2—C51—C47	39.3 (2)
C3—Fe1—C5—C4	−36.4 (3)	C56—Fe2—C51—C47	−97.9 (3)
C2—Fe1—C5—C1	39.4 (2)	C52—Fe2—C51—C47	−59.4 (4)
C10—Fe1—C5—C1	−140.9 (2)	C54—Fe2—C51—C47	−177.1 (3)
C6—Fe1—C5—C1	−96.5 (3)	C55—Fe2—C51—C47	−140.9 (3)
C7—Fe1—C5—C1	−58.4 (4)	C50—Fe2—C51—C47	120.1 (4)
C9—Fe1—C5—C1	−178.7 (3)	C49—Fe2—C51—C47	83.0 (3)
C3—Fe1—C5—C1	83.1 (3)	C69—P4—C52—C53	117.0 (4)
C4—Fe1—C5—C1	119.5 (4)	C75—P4—C52—C53	9.2 (4)
C17—P1—C6—C10	−11.9 (4)	Pd2—P4—C52—C53	−106.8 (4)
C11—P1—C6—C10	−119.3 (4)	C69—P4—C52—C56	−60.9 (4)
Pd1—P1—C6—C10	103.3 (4)	C75—P4—C52—C56	−168.7 (4)
C17—P1—C6—C7	168.0 (4)	Pd2—P4—C52—C56	75.3 (4)
C11—P1—C6—C7	60.6 (4)	C69—P4—C52—Fe2	−150.8 (3)
Pd1—P1—C6—C7	−76.9 (4)	C75—P4—C52—Fe2	101.4 (3)
C17—P1—C6—Fe1	−100.9 (3)	Pd2—P4—C52—Fe2	−14.6 (4)
C11—P1—C6—Fe1	151.7 (3)	C47—Fe2—C52—C53	143.4 (3)
Pd1—P1—C6—Fe1	14.2 (3)	C48—Fe2—C52—C53	99.4 (3)
C1—Fe1—C6—C10	−144.9 (3)	C56—Fe2—C52—C53	−117.4 (4)
C2—Fe1—C6—C10	177.6 (3)	C51—Fe2—C52—C53	−179.3 (3)
C5—Fe1—C6—C10	−100.6 (3)	C54—Fe2—C52—C53	−36.8 (3)
C7—Fe1—C6—C10	117.0 (4)	C55—Fe2—C52—C53	−80.3 (3)
C8—Fe1—C6—C10	79.6 (3)	C49—Fe2—C52—C53	64.0 (4)
C9—Fe1—C6—C10	36.8 (3)	C47—Fe2—C52—C56	−99.2 (3)
C4—Fe1—C6—C10	−64.1 (4)	C48—Fe2—C52—C56	−143.2 (3)
C1—Fe1—C6—C7	98.1 (3)	C51—Fe2—C52—C56	−61.9 (4)
C2—Fe1—C6—C7	60.6 (4)	C53—Fe2—C52—C56	117.4 (4)
C5—Fe1—C6—C7	142.5 (3)	C54—Fe2—C52—C56	80.6 (3)
C10—Fe1—C6—C7	−117.0 (4)	C55—Fe2—C52—C56	37.1 (3)
C8—Fe1—C6—C7	−37.4 (2)	C49—Fe2—C52—C56	−178.6 (3)

C9—Fe1—C6—C7	−80.2 (3)	C47—Fe2—C52—P4	20.7 (3)
C4—Fe1—C6—C7	178.9 (3)	C48—Fe2—C52—P4	−23.3 (3)
C1—Fe1—C6—P1	−25.2 (3)	C56—Fe2—C52—P4	119.9 (4)
C2—Fe1—C6—P1	−62.7 (4)	C51—Fe2—C52—P4	58.0 (4)
C5—Fe1—C6—P1	19.1 (3)	C53—Fe2—C52—P4	−122.7 (4)
C10—Fe1—C6—P1	119.7 (4)	C54—Fe2—C52—P4	−159.5 (4)
C7—Fe1—C6—P1	−123.3 (4)	C55—Fe2—C52—P4	157.0 (4)
C8—Fe1—C6—P1	−160.7 (3)	C49—Fe2—C52—P4	−58.7 (4)
C9—Fe1—C6—P1	156.5 (4)	C56—C52—C53—C54	−0.6 (5)
C4—Fe1—C6—P1	55.6 (4)	P4—C52—C53—C54	−178.8 (3)
C10—C6—C7—C8	−1.1 (5)	Fe2—C52—C53—C54	59.3 (3)
P1—C6—C7—C8	178.9 (3)	C56—C52—C53—Fe2	−59.9 (3)
Fe1—C6—C7—C8	59.2 (3)	P4—C52—C53—Fe2	121.9 (4)
C10—C6—C7—Fe1	−60.3 (3)	C47—Fe2—C53—C54	−177.3 (3)
P1—C6—C7—Fe1	119.8 (4)	C48—Fe2—C53—C54	142.1 (3)
C1—Fe1—C7—C8	142.5 (3)	C56—Fe2—C53—C54	−81.2 (3)
C2—Fe1—C7—C8	98.0 (3)	C52—Fe2—C53—C54	−120.4 (4)
C5—Fe1—C7—C8	179.3 (3)	C55—Fe2—C53—C54	−37.7 (3)
C10—Fe1—C7—C8	−80.7 (3)	C50—Fe2—C53—C54	60.0 (4)
C6—Fe1—C7—C8	−119.7 (4)	C49—Fe2—C53—C54	98.0 (3)
C9—Fe1—C7—C8	−37.1 (3)	C47—Fe2—C53—C52	−56.9 (4)
C3—Fe1—C7—C8	61.5 (4)	C48—Fe2—C53—C52	−97.4 (3)
C1—Fe1—C7—C6	−97.8 (3)	C56—Fe2—C53—C52	39.3 (2)
C2—Fe1—C7—C6	−142.3 (3)	C54—Fe2—C53—C52	120.4 (4)
C5—Fe1—C7—C6	−61.0 (4)	C55—Fe2—C53—C52	82.7 (3)
C10—Fe1—C7—C6	39.0 (2)	C50—Fe2—C53—C52	−179.5 (3)
C8—Fe1—C7—C6	119.7 (4)	C49—Fe2—C53—C52	−141.6 (3)
C9—Fe1—C7—C6	82.6 (3)	C52—C53—C54—C55	1.0 (5)
C3—Fe1—C7—C6	−178.8 (3)	Fe2—C53—C54—C55	59.6 (3)
C6—C7—C8—C9	1.2 (5)	C52—C53—C54—Fe2	−58.6 (3)
Fe1—C7—C8—C9	60.1 (3)	C48—Fe2—C54—C53	−60.9 (4)
C6—C7—C8—Fe1	−58.9 (3)	C56—Fe2—C54—C53	82.1 (3)
C1—Fe1—C8—C9	−178.7 (3)	C52—Fe2—C54—C53	37.3 (3)
C2—Fe1—C8—C9	142.4 (3)	C51—Fe2—C54—C53	177.1 (3)
C10—Fe1—C8—C9	−37.4 (3)	C55—Fe2—C54—C53	119.0 (4)
C6—Fe1—C8—C9	−81.5 (3)	C50—Fe2—C54—C53	−144.1 (3)
C7—Fe1—C8—C9	−119.2 (4)	C49—Fe2—C54—C53	−100.3 (3)
C3—Fe1—C8—C9	98.8 (3)	C48—Fe2—C54—C55	−179.8 (3)
C4—Fe1—C8—C9	62.8 (4)	C56—Fe2—C54—C55	−36.9 (3)
C1—Fe1—C8—C7	−59.5 (4)	C52—Fe2—C54—C55	−81.7 (3)
C2—Fe1—C8—C7	−98.4 (3)	C51—Fe2—C54—C55	58.2 (4)
C10—Fe1—C8—C7	81.9 (3)	C53—Fe2—C54—C55	−119.0 (4)
C6—Fe1—C8—C7	37.7 (3)	C50—Fe2—C54—C55	96.9 (3)
C9—Fe1—C8—C7	119.2 (4)	C49—Fe2—C54—C55	140.7 (3)
C3—Fe1—C8—C7	−141.9 (3)	C53—C54—C55—C56	−1.0 (5)
C4—Fe1—C8—C7	−177.9 (3)	Fe2—C54—C55—C56	58.2 (3)
C7—C8—C9—C10	−0.7 (5)	C53—C54—C55—Fe2	−59.1 (3)
Fe1—C8—C9—C10	58.7 (3)	C47—Fe2—C55—C56	55.6 (4)
C7—C8—C9—Fe1	−59.5 (3)	C52—Fe2—C55—C56	−38.3 (3)

C2—Fe1—C9—C8	−59.1 (4)	C51—Fe2—C55—C56	95.6 (3)
C5—Fe1—C9—C8	−179.2 (3)	C53—Fe2—C55—C56	−82.5 (3)
C10—Fe1—C9—C8	119.7 (4)	C54—Fe2—C55—C56	−120.2 (4)
C6—Fe1—C9—C8	82.3 (3)	C50—Fe2—C55—C56	139.1 (3)
C7—Fe1—C9—C8	37.9 (3)	C49—Fe2—C55—C56	176.3 (3)
C3—Fe1—C9—C8	−98.0 (3)	C47—Fe2—C55—C54	175.9 (3)
C4—Fe1—C9—C8	−140.9 (3)	C56—Fe2—C55—C54	120.2 (4)
C2—Fe1—C9—C10	−178.8 (3)	C52—Fe2—C55—C54	81.9 (3)
C5—Fe1—C9—C10	61.1 (4)	C51—Fe2—C55—C54	−144.2 (3)
C6—Fe1—C9—C10	−37.4 (3)	C53—Fe2—C55—C54	37.7 (3)
C7—Fe1—C9—C10	−81.7 (3)	C50—Fe2—C55—C54	−100.7 (3)
C8—Fe1—C9—C10	−119.7 (4)	C49—Fe2—C55—C54	−63.5 (4)
C3—Fe1—C9—C10	142.3 (3)	C54—C55—C56—C52	0.6 (5)
C4—Fe1—C9—C10	99.4 (3)	Fe2—C55—C56—C52	59.3 (3)
C8—C9—C10—C6	0.0 (5)	C54—C55—C56—Fe2	−58.6 (3)
Fe1—C9—C10—C6	59.0 (3)	C53—C52—C56—C55	0.0 (5)
C8—C9—C10—Fe1	−59.0 (3)	P4—C52—C56—C55	178.2 (3)
C7—C6—C10—C9	0.7 (5)	Fe2—C52—C56—C55	−60.3 (3)
P1—C6—C10—C9	−179.4 (3)	C53—C52—C56—Fe2	60.3 (3)
Fe1—C6—C10—C9	−59.6 (3)	P4—C52—C56—Fe2	−121.5 (3)
C7—C6—C10—Fe1	60.3 (3)	C47—Fe2—C56—C55	−144.8 (3)
P1—C6—C10—Fe1	−119.8 (3)	C48—Fe2—C56—C55	179.5 (3)
C1—Fe1—C10—C9	177.0 (3)	C52—Fe2—C56—C55	119.3 (4)
C5—Fe1—C10—C9	−142.7 (3)	C51—Fe2—C56—C55	−100.2 (3)
C6—Fe1—C10—C9	120.3 (4)	C53—Fe2—C56—C55	80.7 (3)
C7—Fe1—C10—C9	81.1 (3)	C54—Fe2—C56—C55	37.1 (3)
C8—Fe1—C10—C9	37.0 (3)	C50—Fe2—C56—C55	−64.1 (4)
C3—Fe1—C10—C9	−60.9 (4)	C47—Fe2—C56—C52	95.8 (3)
C4—Fe1—C10—C9	−98.7 (3)	C48—Fe2—C56—C52	60.1 (4)
C1—Fe1—C10—C6	56.8 (4)	C51—Fe2—C56—C52	140.5 (3)
C5—Fe1—C10—C6	97.0 (3)	C53—Fe2—C56—C52	−38.7 (2)
C7—Fe1—C10—C6	−39.2 (2)	C54—Fe2—C56—C52	−82.2 (3)
C8—Fe1—C10—C6	−83.3 (3)	C55—Fe2—C56—C52	−119.3 (4)
C9—Fe1—C10—C6	−120.3 (4)	C50—Fe2—C56—C52	176.5 (3)
C3—Fe1—C10—C6	178.8 (3)	C47—P3—C57—C58	−129.6 (4)
C4—Fe1—C10—C6	141.1 (3)	C63—P3—C57—C58	122.9 (4)
C6—P1—C11—C12	14.4 (5)	Pd2—P3—C57—C58	−2.5 (4)
C17—P1—C11—C12	−89.6 (5)	C47—P3—C57—C62	56.5 (4)
Pd1—P1—C11—C12	150.6 (4)	C63—P3—C57—C62	−51.0 (4)
C6—P1—C11—C16	−171.7 (4)	Pd2—P3—C57—C62	−176.4 (3)
C17—P1—C11—C16	84.3 (4)	C62—C57—C58—C59	0.3 (7)
Pd1—P1—C11—C16	−35.5 (5)	P3—C57—C58—C59	−173.9 (4)
C16—C11—C12—C13	0.5 (9)	C57—C58—C59—C60	−1.5 (8)
P1—C11—C12—C13	174.6 (5)	C58—C59—C60—C61	1.6 (8)
C11—C12—C13—C14	−0.8 (11)	C59—C60—C61—C62	−0.4 (8)
C12—C13—C14—C15	0.3 (11)	C60—C61—C62—C57	−0.8 (8)
C13—C14—C15—C16	0.3 (11)	C58—C57—C62—C61	0.9 (7)
C12—C11—C16—C15	0.1 (8)	P3—C57—C62—C61	174.9 (4)
P1—C11—C16—C15	−174.1 (4)	C47—P3—C63—C68	30.2 (4)

C14—C15—C16—C11	−0.5 (10)	C57—P3—C63—C68	143.4 (3)
C6—P1—C17—C22	92.9 (4)	Pd2—P3—C63—C68	−96.3 (3)
C11—P1—C17—C22	−161.1 (4)	C47—P3—C63—C64	−151.3 (3)
Pd1—P1—C17—C22	−31.6 (4)	C57—P3—C63—C64	−38.1 (4)
C6—P1—C17—C18	−80.2 (4)	Pd2—P3—C63—C64	82.2 (3)
C11—P1—C17—C18	25.9 (4)	C68—C63—C64—C65	−1.0 (6)
Pd1—P1—C17—C18	155.3 (3)	P3—C63—C64—C65	−179.5 (3)
C22—C17—C18—C19	−0.6 (7)	C63—C64—C65—C66	0.0 (7)
P1—C17—C18—C19	172.6 (4)	C64—C65—C66—C67	0.3 (8)
C17—C18—C19—C20	−0.9 (8)	C65—C66—C67—C68	0.4 (8)
C18—C19—C20—C21	2.4 (9)	C66—C67—C68—C63	−1.5 (7)
C19—C20—C21—C22	−2.4 (8)	C64—C63—C68—C67	1.7 (6)
C18—C17—C22—C21	0.5 (7)	P3—C63—C68—C67	−179.8 (3)
P1—C17—C22—C21	−172.9 (4)	C52—P4—C69—C74	144.0 (4)
C20—C21—C22—C17	1.0 (8)	C75—P4—C69—C74	−109.5 (4)
C1—P2—C23—C24	−53.7 (4)	Pd2—P4—C69—C74	7.0 (4)
C29—P2—C23—C24	57.3 (4)	C52—P4—C69—C70	−36.2 (4)
Pd1—P2—C23—C24	−178.7 (3)	C75—P4—C69—C70	70.3 (4)
C1—P2—C23—C28	128.5 (3)	Pd2—P4—C69—C70	−173.2 (3)
C29—P2—C23—C28	−120.5 (3)	C74—C69—C70—C71	3.9 (7)
Pd1—P2—C23—C28	3.5 (4)	P4—C69—C70—C71	−175.9 (4)
C28—C23—C24—C25	−3.5 (6)	C69—C70—C71—C72	−3.2 (8)
P2—C23—C24—C25	178.7 (3)	C70—C71—C72—C73	0.9 (8)
C23—C24—C25—C26	3.2 (7)	C71—C72—C73—C74	0.6 (8)
C24—C25—C26—C27	−0.6 (7)	C70—C69—C74—C73	−2.3 (7)
C25—C26—C27—C28	−1.4 (8)	P4—C69—C74—C73	177.5 (3)
C26—C27—C28—C23	1.0 (7)	C72—C73—C74—C69	0.1 (7)
C24—C23—C28—C27	1.4 (6)	C52—P4—C75—C80	−86.4 (4)
P2—C23—C28—C27	179.3 (3)	C69—P4—C75—C80	169.7 (3)
C1—P2—C29—C34	−11.9 (4)	Pd2—P4—C75—C80	42.0 (4)
C23—P2—C29—C34	−125.4 (4)	C52—P4—C75—C76	98.1 (4)
Pd1—P2—C29—C34	112.7 (3)	C69—P4—C75—C76	−5.8 (4)
C1—P2—C29—C30	168.9 (3)	Pd2—P4—C75—C76	−133.5 (4)
C23—P2—C29—C30	55.4 (4)	C80—C75—C76—C77	0.2 (7)
Pd1—P2—C29—C30	−66.5 (4)	P4—C75—C76—C77	175.6 (4)
C34—C29—C30—C31	−0.6 (6)	C75—C76—C77—C78	0.3 (8)
P2—C29—C30—C31	178.6 (3)	C76—C77—C78—C79	−0.5 (8)
C29—C30—C31—C32	−0.3 (7)	C77—C78—C79—C80	0.1 (7)
C30—C31—C32—C33	0.7 (8)	C76—C75—C80—C79	−0.5 (7)
C31—C32—C33—C34	−0.1 (8)	P4—C75—C80—C79	−176.3 (3)
C32—C33—C34—C29	−0.8 (8)	C78—C79—C80—C75	0.4 (7)
C30—C29—C34—C33	1.2 (7)	Pd2—S3—C81—C86	−56.0 (4)
P2—C29—C34—C33	−178.0 (4)	Pd2—S3—C81—C82	131.7 (3)
Pd1—S1—C35—C36	−151.4 (4)	C86—C81—C82—F11	179.9 (4)
Pd1—S1—C35—C40	29.7 (4)	S3—C81—C82—F11	−7.1 (6)
C40—C35—C36—F1	179.9 (4)	C86—C81—C82—C83	1.6 (7)
S1—C35—C36—F1	0.9 (7)	S3—C81—C82—C83	174.6 (4)
C40—C35—C36—C37	−1.4 (8)	F11—C82—C83—F12	1.0 (7)
S1—C35—C36—C37	179.5 (4)	C81—C82—C83—F12	179.3 (4)

F1—C36—C37—F2	0.3 (8)	F11—C82—C83—C84	−178.4 (5)
C35—C36—C37—F2	−178.4 (5)	C81—C82—C83—C84	−0.1 (8)
F1—C36—C37—C38	177.5 (5)	F12—C83—C84—F13	0.4 (8)
C35—C36—C37—C38	−1.2 (10)	C82—C83—C84—F13	179.8 (4)
F2—C37—C38—C39	−179.9 (5)	F12—C83—C84—C85	179.8 (5)
C36—C37—C38—C39	2.8 (10)	C82—C83—C84—C85	−0.8 (8)
F2—C37—C38—F3	−2.2 (9)	C83—C84—C85—F14	−179.5 (5)
C36—C37—C38—F3	−179.4 (5)	F13—C84—C85—F14	−0.1 (8)
C37—C38—C39—F4	178.1 (5)	C83—C84—C85—C86	0.0 (9)
F3—C38—C39—F4	0.4 (8)	F13—C84—C85—C86	179.5 (4)
C37—C38—C39—C40	−1.8 (9)	F14—C85—C86—F15	1.8 (7)
F3—C38—C39—C40	−179.6 (4)	C84—C85—C86—F15	−177.7 (5)
C38—C39—C40—F5	179.0 (5)	F14—C85—C86—C81	−178.8 (4)
F4—C39—C40—F5	−0.9 (7)	C84—C85—C86—C81	1.7 (8)
C38—C39—C40—C35	−1.0 (8)	C82—C81—C86—F15	177.0 (4)
F4—C39—C40—C35	179.1 (4)	S3—C81—C86—F15	4.3 (6)
C36—C35—C40—F5	−177.5 (4)	C82—C81—C86—C85	−2.4 (7)
S1—C35—C40—F5	1.5 (7)	S3—C81—C86—C85	−175.1 (4)
C36—C35—C40—C39	2.5 (7)	Pd2—S4—C87—C88	−41.4 (4)
S1—C35—C40—C39	−178.5 (4)	Pd2—S4—C87—C92	139.2 (3)
Pd1—S2—C41—C46	−122.7 (3)	C92—C87—C88—F16	178.5 (4)
Pd1—S2—C41—C42	60.7 (4)	S4—C87—C88—F16	−1.0 (7)
C46—C41—C42—F6	−179.2 (4)	C92—C87—C88—C89	−2.9 (7)
S2—C41—C42—F6	−2.4 (6)	S4—C87—C88—C89	177.7 (4)
C46—C41—C42—C43	3.3 (7)	F16—C88—C89—F17	0.6 (7)
S2—C41—C42—C43	−179.8 (4)	C87—C88—C89—F17	−178.1 (4)
F6—C42—C43—F7	1.0 (7)	F16—C88—C89—C90	179.9 (4)
C41—C42—C43—F7	178.5 (4)	C87—C88—C89—C90	1.2 (8)
F6—C42—C43—C44	−179.6 (5)	F17—C89—C90—F18	−0.8 (7)
C41—C42—C43—C44	−2.2 (8)	C88—C89—C90—F18	179.9 (4)
F7—C43—C44—F8	0.5 (8)	F17—C89—C90—C91	180.0 (4)
C42—C43—C44—F8	−178.8 (4)	C88—C89—C90—C91	0.8 (8)
F7—C43—C44—C45	179.7 (5)	F18—C90—C91—F19	2.7 (7)
C42—C43—C44—C45	0.4 (8)	C89—C90—C91—F19	−178.1 (4)
F8—C44—C45—F9	−0.4 (8)	F18—C90—C91—C92	−179.9 (4)
C43—C44—C45—F9	−179.6 (5)	C89—C90—C91—C92	−0.7 (8)
F8—C44—C45—C46	179.3 (4)	F19—C91—C92—F20	−1.0 (7)
C43—C44—C45—C46	0.0 (8)	C90—C91—C92—F20	−178.4 (4)
F9—C45—C46—F10	1.2 (7)	F19—C91—C92—C87	176.2 (4)
C44—C45—C46—F10	−178.5 (5)	C90—C91—C92—C87	−1.2 (8)
F9—C45—C46—C41	−179.0 (4)	C88—C87—C92—F20	180.0 (4)
C44—C45—C46—C41	1.3 (8)	S4—C87—C92—F20	−0.5 (6)
C42—C41—C46—F10	177.0 (4)	C88—C87—C92—C91	2.9 (7)
S2—C41—C46—F10	0.0 (6)	S4—C87—C92—C91	−177.6 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C22—H22···F6	0.93	2.44	3.306 (6)	156

C28—H28···F5	0.93	2.80	3.487 (5)	132
C59—H59···F1	0.93	2.76	3.681 (6)	170
C73—H73···F2	0.93	2.43	3.272 (6)	151
C74—H74···F16	0.93	2.70	3.629 (6)	177
C27—H27···F5^{i}	0.93	2.48	3.253 (6)	141
C62—H62···F19^{ii}	0.93	2.66	3.511 (6)	153
C67—H67···F13^{ii}	0.93	2.75	3.335 (6)	122
C19—H19···F3^{ii}	0.93	2.70	3.531 (7)	149
C32—H32···F14^{iii}	0.93	2.70	3.562 (6)	154
C50—H50···F8^{iv}	0.93	2.78	3.399 (6)	125
C77—H77···F10^{v}	0.93	2.72	3.231 (5)	116
C71—H71···F18^{v}	0.93	2.57	3.322 (6)	138

Symmetry codes: (i) −*x*+1, −*y*, −*z*+1; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) −*x*+3/2, *y*−1/2, −*z*+3/2; (iv) −*x*+1, −*y*+1, −*z*+1; (v) −*x*+3/2, *y*+1/2, −*z*+3/2.

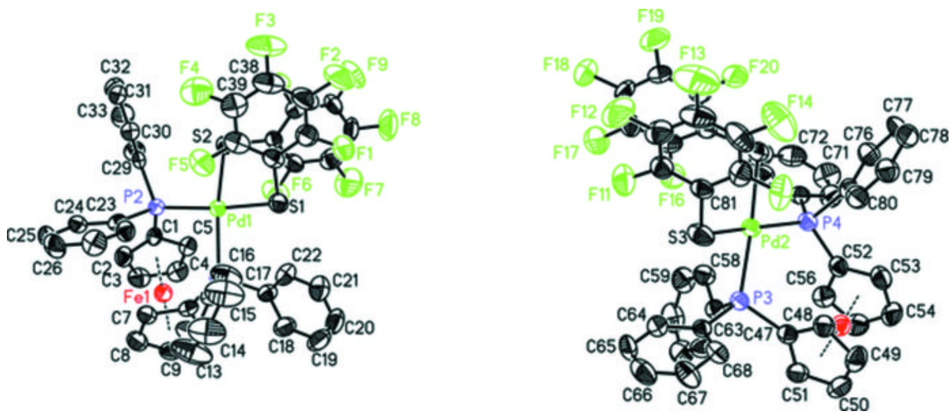
Table 2

Intermolecular and intramolecular C-F–π, C-H–π and π–π interactions in (I) (Å)

H/F/centroid	centroid	distance	Symmetry-code
H26	C35-C40	3.206	(i)
H60	C17-C22	3.425	(ii)
F11	C87-C92	3.237	
F20	C81-C86	3.295	
F10	C35-C40	3.072	
F1	C41-C46	3.691	
F19	C63-C68	2.996	(ii)
C41-C46	C81-C86	3.683	(iii)

(i) −*x* + 1, −*y*, −*z* + 1; (ii) *x* − 1/2, −*y* + 1/2', *z* − 1/2; (iii) *x* + 1/2, −*y* + 1/2, *z* − 1/2

Fig. 1


F3
F4
C38
F2
F9
C32
C31
C39
C33
C30
F8
S2
F1
F5
F6
C29
F7
P2
C24
C23
Pd1
S1
C1
C5
C25
C4
C16
C22
C26
C2
C3
C17
C21
Fe1
C15
C7
C20
C14
C18
C8
C19
C9
C13
F19
F18
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F14
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C77
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C76
C78
F17
C71
C79
F11
F16
C81
C80
P4
S3
Pd2
C52
C58
C53
C59
C56
P3
C48
C54
C64
C63
C47
C65
C49
C68
C66
C67
C51
C50

Fig. 2