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Crystal structures of two new six-coordinate iron(III) complexes with 1,2-bis(diphenylphosphane) ligands

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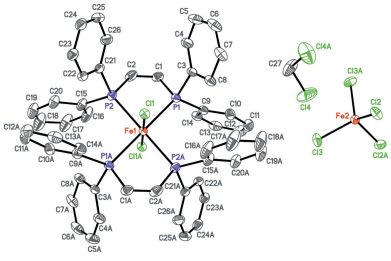
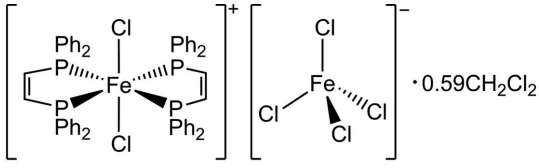
Structural characterization of the ionic complexes $[FeCl_2(C_{26}H_{22}P_2)_2][FeCl_4]\cdot 0.59CH_2Cl_2$ or $[(dppen)_2FeCl_2][FeCl_4]\cdot 0.59CH_2Cl_2$ (dppen = *cis*-1,2-bis(diphenylphosphane)ethylene, $P_2C_{26}H_{22}$) and $[FeCl_2(C_{30}H_{24}P_2)_2][FeCl_4]\cdot CH_2Cl_2$ or $[(dpbz)_2FeCl_2][FeCl_4]\cdot CH_2Cl_2$ (dpbz = 1,2-bis(diphenylphosphane)benzene, $P_2C_{30}H_{24}$) demonstrates *trans* coordination of two bidentate phosphane ligands (bisphosphanes) to a single iron(III) center, resulting in six-coordinate cationic complexes that are balanced in charge by tetrachloridoferrate(III) monoanions. The *trans* bisphosphane coordination is consistent will all previously reported molecular structures of six coordinate iron(III) complex cations with a $(PP)_2X_2$ (X = halido) donor set. The complex with dppen crystallizes in the centrosymmetric space group $C2/c$ as a partial-occupancy [0.592 (4)] dichloromethane solvate, while the dpbz-ligated complex crystallizes in the triclinic space group $P\overline{1}$ as a full dichloromethane monosolvate. Furthermore, the crystal studied of $[(dpbz)_2FeCl_2][FeCl_4]\cdot CH_2Cl_2$ was an inversion twin, whose component mass ratio refined to 0.76 (3):0.24 (3). Beyond a few very weak C—H···Cl and C—H···π interactions, there are no significant supramolecular features in either structure.

1. Chemical context

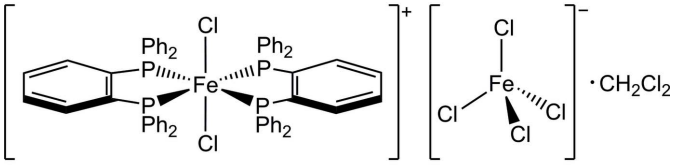
Bidentate phosphanes (bisphosphanes) are versatile supporting ligands in coordination chemistry because of the accessibility of various electronic and steric properties through manipulation of their backbone structures and phosphorus substituents. While these ligands are commonly used to stabilize low-valent metal complexes due to their function as both σ-donor and π-acceptor ligands, bisphosphane ligands have also been observed to support metal centers in higher oxidation states. For example, there exist a few structurally characterized examples of iron(III) complexes in which two bisphosphane ligands are coordinated to a single metal center, resulting in axial coordination of halido (X) ligands. These complex cations have been shown to be accessible through a variety of synthetic routes (Higgins *et al.*, 1985; Higgins & Levason, 1985; Field *et al.*, 1990, 2000; Evans *et al.*, 1992; Miller *et al.*, 2002; Hoffert *et al.*, 2011). A review of the literature finds that investigations into these complexes date back almost sixty years to the work of Chatt and Hayter, in which three distinct iron(III) bisphosphane complexes, formulated as complex salts with the molecular structures $[(PP)_2FeCl_2][FeCl_4]$ [PP = 1,2-bis(diethylphosphano)benzene (debz), 1,2-bis(diethylphosphano)ethane (depe), and 1,2-bis(dimethylphosphano)-ethane (dmpe)], were prepared through the reaction of



iron(III) chloride with one shoichiometric equivalent of bisphosphane (Chatt & Hayter, 1961; for later reports of various preparative methods of similar compounds, see: Levason *et al.*, 1975; Gargano *et al.*, 1975; Warren *et al.*, 1976; Higgins & Levason, 1985). Structural confirmation for this general molecular formula was achieved through the crystallographic characterization of $[(dmpe)_2FeCl_2][FeCl_4]$, although this synthesis employed photolytic oxidation of the iron(II) complex $(dmpe)_2FeCl_2$ and not direct reaction of an iron(III) precursor with bisphosphane (Field *et al.*, 1990). At the time of this report, the only other known molecular structure for a six-coordinate iron(III) complex cation bearing a $(PP)_2X_2$ ligand set was $[(o\text{-}C_6F_4(PMe_2)_2)_2FeCl_2][BF_4]$ (Higgins *et al.*, 1985; Higgins & Levason, 1985). This particular species was synthesized through metathesis of the original tetrachloridoferrate(III) anion with HBF_4. The initial salt, $[(o\text{-}C_6F_4(PMe_2)_2)_2FeCl_2][FeCl_4]$, prepared *via* a nearly 1:1 stoichiometric reaction of iron(III) chloride with $o\text{-}C_6F_4(PMe_2)_2$, was not structurally characterized.



1



2

Our group is interested in the application of bisphosphanes as supporting ligands within iron-catalyzed cross-coupling reactions. Numerous literature protocols for iron-catalyzed cross-coupling methods involve use of bisphosphanes as substoichiometric additives in conjunction with iron(II) or iron(III) salts, promoting the formation of the active catalyst *in situ*. Methods development in our laboratory using the dppen ligand in conjunction with iron(III) chloride resulted in the formation of $[(dppen)_2FeCl_2][FeCl_4]$ (**1**) from reaction mixtures and its subsequent structural characterization. As reported herein, **1** was then independently prepared *via* the method of Chatt & Hayter (1961). While we have not observed this compound to exhibit catalytic effectiveness in cross-coupling, a literature search indicated that this ionic complex was first synthesized in the 1970s using the same reaction stoichiometry (Levason *et al.*, 1975). This report lacked structural characterization of the complex, but its formulation as a complex salt was supported by magnetic susceptibility, Mössbauer, and IR absorption measurements. Upon confirming the structure of **1**, we sought to examine an analogous species, $[(dpbz)_2FeCl_2][FeCl_4]$ (**2**), by taking advantage of the same steric substitution at phosphorus, but with a slightly varied backbone character (*ortho*-phenylene in place of the C_2H_2 of dppen). Such studies are important as they expand the coordination chemistry library of iron(III) complexes bearing bisphosphane ligands. In addition, **1** and **2** join only two other structurally characterized examples of coordinatively saturated iron(III) monocations with a $(PP)_2X_2$ ligand set that have been synthesized without using oxidative methods (Miller *et al.*, 2002, Higgins & Levason, 1985).

2. Structural commentary

Both **1** and **2** are characterized as six-coordinate complex cations in which the iron(III) center is ligated by two bisphosphane ligands (dppen in **1**, dpbz in **2**) in a *trans* fashion (see Scheme). The two retained chlorido ligands are thus coordinated axially, and the displaced chlorido ligand results in generation of a single tetrachloridoferrate(III) anion in both cases. Compound **1** (Fig. 1) crystallizes in the centrosymmetric space group *C*2/*c*. The iron atom of the cation is located at a crystallographic inversion center, resulting in Cl—Fe—Cl and *trans* P—Fe—P angles of 180°. Deviation from ideal octahedral geometry is due to the 80.92 (2)° bite angles of the P—Fe—P chelate rings (Table 1). The Fe—P distances are considerably longer than those of the other structurally characterized iron(III) cations with a $(PP)_2X_2$ donor set (range 2.29–2.34 Å; Groom *et al.*, 2016, see *Database survey* below), but with shorter Fe—Cl distances than those of the other reported X = Cl compounds (range 2.23–2.25 Å). The ethylene backbones of each dppen ligand in the cation of **1** are bent out of the equatorial plane by 24.86 (8)°. The tetrachloridoferrate(III) anion lies along a crystallographic twofold axis that includes the metal center. Phenyl group C3—C8 (and thus its symmetry equivalent, Fig. 1) is modeled as disordered over two positions [0.561 (6):0.439 (6)].

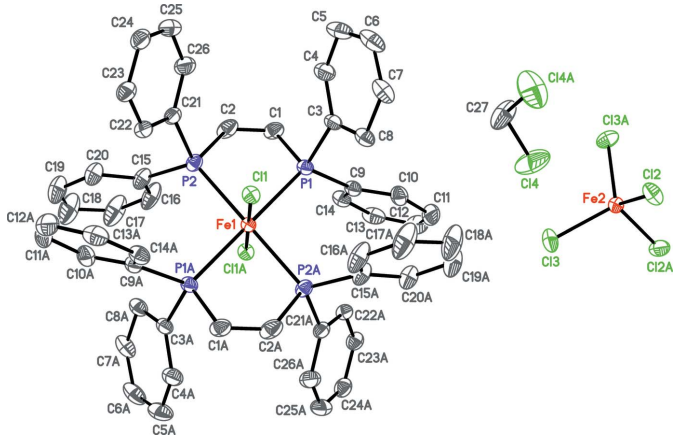


Figure 1
Displacement ellipsoid plot of **1** drawn at the 50% probability level with hydrogen atoms omitted. The full cation of the title formula is generated by a crystallographic inversion center $(1-x, 1-y, 1-z)$ at atom Fe1. The full anion is generated by a crystallographic twofold axis $(-x, y, \frac{3}{2}-z)$, which includes atom Fe2. The symmetry-equivalent atoms of the dichloromethane solvent molecule are generated by a crystallographic twofold axis $(1-x, y, \frac{3}{2}-z)$ that contains atom C27.

Table 1
Selected geometric parameters (Å, °) for **1**.

Fe1—Cl1	2.2135 (6)	Fe1—P2	2.3738 (6)
Fe1—P1	2.3662 (6)		
Cl1^{i}—Fe1—Cl1	180.0	Cl1—Fe1—P2^{i}	87.58 (2)
Cl1—Fe1—P1	92.38 (2)	Cl1—Fe1—P2	92.42 (2)
Cl1—Fe1—P1^{i}	87.62 (2)	P1—Fe1—P2	80.92 (2)
P1—Fe1—P1^{i}	180.0	P2^{i}—Fe1—P2	180.0

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2
Selected geometric parameters (Å, °) for **2**.

Fe1—Cl2	2.218 (2)	Fe1—P2	2.376 (2)
Fe1—Cl1	2.223 (2)	Fe1—P4	2.377 (2)
Fe1—P3	2.374 (2)	Fe1—P1	2.388 (2)
Cl2—Fe1—Cl1	179.87 (12)	P3—Fe1—P4	80.75 (8)
Cl2—Fe1—P3	87.69 (8)	P2—Fe1—P4	179.33 (10)
Cl1—Fe1—P3	92.26 (8)	Cl2—Fe1—P1	92.05 (8)
Cl2—Fe1—P2	92.82 (8)	Cl1—Fe1—P1	87.99 (7)
Cl1—Fe1—P2	87.30 (8)	P3—Fe1—P1	179.74 (10)
P3—Fe1—P2	98.58 (8)	P2—Fe1—P1	81.38 (8)
Cl2—Fe1—P4	87.23 (8)	P4—Fe1—P1	99.29 (8)
Cl1—Fe1—P4	92.65 (8)		

The asymmetric unit of **2** contains the cation, anion, and solvent molecule in general positions. The solvent molecule was modeled as disordered over three positions [0.740 (3):0.136 (3):0.124 (3)]. Despite the structural similarity of the backbone linkers and steric periphery of dppen and dpbz, the space group assignment and crystallographic symmetry of **2** contrasted from **1**. Metrically, however, **1** and **2** are quite similar. The axial chlorido ligands within the cation of **2** are located at Fe—Cl distances very close to that found in the cation of **1** and the Cl—Fe—Cl and *trans* P—Fe—P angles are very nearly linear (Fig. 2, Table 2). Additionally, the bite angles in the cation of **2** as well as Fe—Cl distances and Cl—Fe—Cl angles of its tetrachloridoferrate(III) anion are very similar to those of **1**. As observed for the ethylene backbones of the dppen ligands of **1**, the *ortho*-phenylene backbones of the dpbz ligands in **2** are also canted out the equatorial plane by 21.9 (1) and 22.9 (1)°. The crystal of **2** studied was an inversion twin, whose component mass ratio refined to 0.76 (3):0.24 (3).

Both **1** and **2** are dichloromethane solvates under the common crystallization procedure used (see below). In **1**, the solvent molecule is located along a crystallographic twofold axis that includes the carbon atom. Crystal desolvation is suspected, since its occupancy only refined to 0.592 (4). In contrast, **2** was found to possess full occupation of co-crystallized dichloromethane, modeled as disordered over three general positions [0.740 (3):0.136 (3):0.124 (3)].

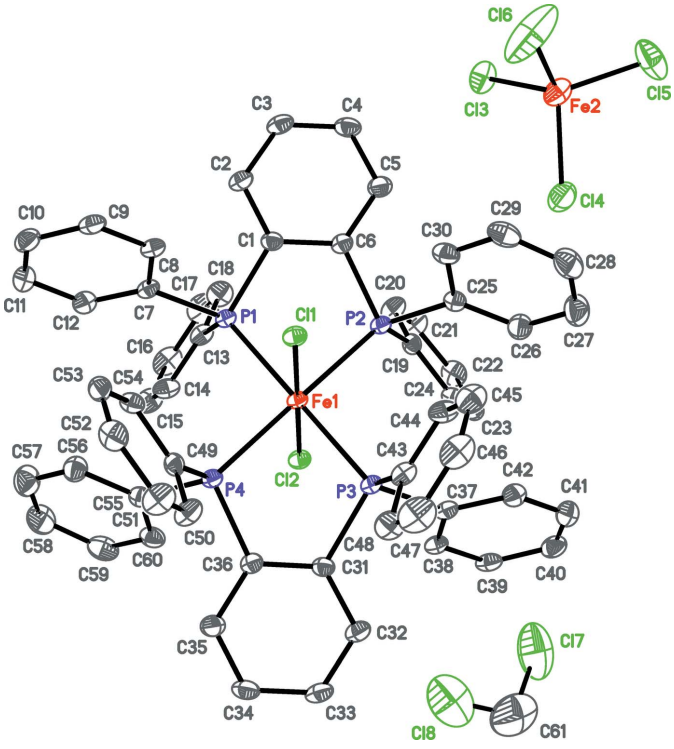


Figure 2
Displacement ellipsoid plot of **2** drawn at the 50% probability level with hydrogen atoms omitted. Only the major component of disorder of the dichloromethane solvent molecule is shown.

3. Supramolecular features

There are no significant supramolecular features beyond a few very weak C—H···Cl and C—H···π interactions.

4. Database survey

Outside of **1** and **2** reported herein, there are eight examples of ionic iron(III) compounds bearing *trans*-coordinating bisphosphane ligands in an overall $(PP)_2A_2$ (*A* = formally monoanionic ligand) environment reported in the Cambridge Structural Database (CSD, Version 5.39, update No. 2, February 2018; Groom *et al.*, 2016). The axial *A* ligands of the cations include two chlorido (CSD refcode DABCEO, Higgins *et al.*, 1985; recode VOBHUP, Field *et al.*, 1990; recode XAZZIH, Field *et al.*, 2000; refcode BAJLAA, Miller *et al.*, 2002), bromido and hydrido (refcode PABSUG; Evans *et al.*, 1992), and chlorido and alkynyl (refcodes NAWMIJ, NAWMOP, NAWMUV; Hoffert *et al.*, 2011). These structures include a variety of counter-anions: $[FeCl_4]^-$, $[BF_4]^-$, $[BPh_4]^-$, $[Cl]^-$, $[SO_3CF_3]^-$, and $[B(3,5\text{-}CF_3Ph)_4]^-$. Only one of these examples, *trans*-$[(o\text{-}C_6F_4(PMe_2)_2)_2FeCl_2][BF_4]$, contains a bisphosphane ligand with an unsaturated backbone linker (Higgins *et al.*, 1985). Just as in **1** and **2**, the fluoro-substituted *ortho*-phenylene backbone of *trans*-$[(o\text{-}C_6F_4(PMe_2)_2)_2\text{-}FeCl_2][BF_4]$ is also bent out of from the FeP_4 equatorial plane (17.6 °).

5. Synthesis and crystallization

Anhydrous $FeCl_3$ (98%, Alfa Aesar), *cis*-1,2-bis(diphenylphosphanel)ethylene (dppen, 98%, Strem), and 1,2-bis(di-

Table 3
Experimental details.

	1	2
Crystal data		
Chemical formula	$[FeCl_2(C_{26}H_{22}P_2)_2][FeCl_4]\cdot0.59CH_2Cl_2$	$[FeCl_2(C_{30}H_{24}P_2)_2][FeCl_4]\cdot CH_2Cl_2$
M_r	1167.47	1302.19
Crystal system, space group	Monoclinic, $C2/c$	Triclinic, $P\overline{1}$
Temperature (K)	100	100
a, b, c (Å)	9.7528 (7), 23.6871 (17), 23.6871 (17)	9.8771 (7), 12.6516 (8), 12.8258 (8)
α, β, γ (°)	90, 100.541 (2), 90	81.058 (1), 83.050 (1), 68.335 (1)
V (Å^3)	5379.7 (7)	1467.87 (17)
Z	4	1
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (mm^{-1})	1.05	1.01
Crystal size (mm)	0.22 × 0.22 × 0.10	0.24 × 0.20 × 0.08
Data collection		
Diffractometer	Bruker SMART APEX II CCD platform	Bruker SMART APEX II CCD platform
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.643, 0.746	0.644, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	71735, 8962, 6273	27211, 22268, 11890
R_{int}	0.091	0.050
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.736	0.807
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.119, 1.05	0.073, 0.182, 1.00
No. of reflections	8962	22268
No. of parameters	325	488
No. of restraints	33	34
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.74, −0.67	1.23, −1.39
Absolute structure	–	Refined as an inversion twin.
Absolute structure parameter	–	0.24 (3)

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2013), *SHELXT2014*/5 (Sheldrick, 2015*a*), *SHELXL2016*/6 (Sheldrick, 2015*b*), *SHELXL2018*/3 (Sheldrick, 2015*b*), *SHELXTL* (Sheldrick, 2008).

phenylphosphane)benzene (dpbz, 98%, Strem) were used in the synthesis of **1** and **2** without further purification. The syntheses of both compounds were performed under a dinitrogen atmosphere in a drybox. 80 mg $FeCl_3$ (0.49 mmol) was dissolved in 5 ml THF (Aldrich, anhydrous, 99.9%, inhibitor-free), resulting in a yellow–green solution. In a separate vial, 200 mg dppen (or 225 mg dpbz for **2**, 0.50 mmol in either case) was dissolved in 10 ml THF. At room temperature, the solution of bisphosphane was added to the stirring solution of $FeCl_3$, resulting in immediate formation of a dark green precipitate in both cases. Each reaction was stirred for 5 min following complete addition of the bisphosphane solution, filtered, and the resulting green solid was dried under vacuum. In both cases, analytically pure microcrystalline solid was isolated in nearly quantitative yield. $[FeCl_2(dppen)_2][FeCl_4]$: Yield: 94%. Elemental analysis: calculated: 55.903 C, 3.970 H; found: 56.327 C, 4.342 H. $[FeCl_2(dpbz)_2][FeCl_4]$: Yield: 89%. Elemental analysis: calculated: 59.199 C, 3.974 H; found: 59.526 C, 4.452.

Once isolated and dried, solid **1** and **2** were found to be indefinitely stable outside of an inert atmosphere (greater than one year). Both complexes were crystallized by layering toluene over a concentrated dichloromethane solution of the complex and allowing the layers to diffuse at room temperature (anhydrous solvents were not used during crystallizations). Red–green dichroic single crystals suitable for X-ray diffraction studies were generally observed to crystallize within 24 h. Out of a large number of polar and non-polar common organic solvents examined, only dichloromethane, chloroform, acetone, and nitromethane appreciably solubilized **1** and **2**. During preparation of crystallizations, dichloromethane solutions of **1** and **2** were observed under incandescent light to be green at low concentrations and red at high concentrations.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Phenyl ring C3–C8 of **1** was modeled as disordered over two general positions [0.561 (6):0.439 (6)]. Analogous bond lengths and angles between the two positions and in both directions around the rings were restrained to be similar. Additionally the P1—C3 and P1—C3′ bond lengths were restrained to be similar. Anisotropic displacement parameters for pairs of proximal atoms were constrained to be equivalent. The occupancy of the cocrystallized dichloromethane solvent molecule refined to 0.592 (4), which is consistent with crystal desolvation.

2 was refined as an inversion twin in $P\overline{1}$ whose twin component mass ratio refined to 0.76 (3):0.24 (3). Because of significant parameter correlation, anisotropic displacement parameters for pseudosymmetrically related atom pairs were constrained to be equivalent. The co-crystallized dichloro-

methane solvent molecule is modeled as disordered over three positions [0.740 (3):0.136 (3):0.124 (3)]. Analogous bond lengths and angles among the three positions of the disordered dichloromethane solvent molecule were restrained to be similar. Anisotropic displacement parameters for proximal and pseudosymmetrically related atoms were constrained to be equivalent.

A solution and refinement of **2** in centrosymmetric space group $P\overline{1}$ caused an increase in the $R1$ residual (strong data) from 0.071 to 0.118, which was not unexpected given the uneven twin component mass ratio when refined in $P1$. In the centrosymmetric model, the anion and solvent were modeled pairwise as disordered over a crystallographic inversion center.

H atoms were given riding models: aromatic/sp^2, C—H = 0.95 Å, and methylene, C—H = 0.99 Å, with U_{iso}(H) = 1.2U_{eq}(C).

For **1** the maximum residual peak of 0.74 e$^-$ Å^{-3} and the deepest hole of −0.67 e$^-$ Å^{-3} are found 0.72 and 0.82 Å, respectively, from atom CL4.

For **2** the maximum residual peak of 1.23 e$^-$ Å^{-3} and the deepest hole of −1.39 e$^-$ Å^{-3} are found 0.22 and 0.05 Å from atoms CL5 and C61 of the disordered solvent molcule, respectively.

Acknowledgements

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Crystal structures of two new six-coordinate iron(III) complexes with 1,2-bis(diphenylphosphane) ligands

Derek L. McNeil, Daihlia J. Beckford, Jared L. Kneebone, Stephanie H. Carpenter, William W. Brennessel and Michael L. Neidig

Computing details

For both structures, data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: SHELXT-2014/5 (Sheldrick, 2015a). Program(s) used to refine structure: *SHELXL2016*/6 (Sheldrick, 2015b) for (1); *SHELXL2018*/3 (Sheldrick, 2015b) for (2). For both structures, molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

trans-Bis[1,2-bis(diphenylphosphane)ethylene]dichloridoiron(III) tetrachloridoferrate(III) dichloromethane 0.59-solvate (1)

Crystal data

$[FeCl_2(C_{26}H_{22}P_2)_2][FeCl_4]\cdot 0.59CH_2Cl_2$
M_r = 1167.47
Monoclinic, *C*2/*c*
a = 9.7528 (7) Å
b = 23.6871 (17) Å
c = 23.6871 (17) Å
β = 100.541 (2)°
V = 5379.7 (7) Å^3
Z = 4
F(000) = 2380
D_x = 1.441 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4040 reflections
θ = 2.3–29.5°
μ = 1.05 mm^{-1}
T = 100 K
Plate, red-violet
0.22 × 0.22 × 0.10 mm

Data collection

Bruker SMART APEX II CCD platform diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.643, T_{max} = 0.746
71735 measured reflections
8962 independent reflections
6273 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
θ_{max} = 31.5°, θ_{min} = 1.7°
h = −14→14
k = −34→34
l = −34→34

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.119
S = 1.05
8962 reflections
325 parameters
33 restraints
Primary atom site location: dual

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 11.3134P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.74$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Phenyl ring C3-C8 is modeled as disordered over two positions (56:44). Analogous bond lengths and angles between the two positions were restrained to be similar. Anisotropic displacement parameters for pairs of proximal atoms were constrained to be equivalent.

The occupancy of the cocrystallized dichloromethane solvent molecule refined to 0.592 (4).

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.500000	0.500000	0.500000	0.01605 (10)	
Cl1	0.71798 (6)	0.53023 (2)	0.52215 (2)	0.02045 (12)	
P1	0.46240 (6)	0.51308 (3)	0.59502 (3)	0.01981 (13)	
P2	0.56127 (7)	0.40841 (3)	0.53686 (3)	0.02134 (13)	
C1	0.4343 (3)	0.44397 (12)	0.62312 (12)	0.0295 (6)	
H1	0.390120	0.440031	0.655474	0.035*	
C2	0.4761 (3)	0.39907 (12)	0.59802 (13)	0.0321 (6)	
H2	0.461628	0.362302	0.611842	0.038*	
C3	0.605 (2)	0.5342 (6)	0.6520 (8)	0.0227 (16)	0.439 (6)
C4	0.6555 (15)	0.4985 (4)	0.6979 (5)	0.0311 (15)	0.439 (6)
H4	0.618358	0.461673	0.699969	0.037*	0.439 (6)
C5	0.7618 (11)	0.5184 (4)	0.7406 (4)	0.0393 (15)	0.439 (6)
H5	0.798729	0.494642	0.772091	0.047*	0.439 (6)
C6	0.8136 (10)	0.5718 (4)	0.7377 (4)	0.0386 (16)	0.439 (6)
H6	0.885234	0.584895	0.767556	0.046*	0.439 (6)
C7	0.7637 (10)	0.6067 (4)	0.6925 (4)	0.0322 (13)	0.439 (6)
H7	0.801045	0.643578	0.690908	0.039*	0.439 (6)
C8	0.6576 (15)	0.5879 (5)	0.6487 (6)	0.0258 (14)	0.439 (6)
H8	0.622193	0.611721	0.617137	0.031*	0.439 (6)
C3′	0.5987 (16)	0.5479 (4)	0.6468 (6)	0.0227 (16)	0.561 (6)
C4′	0.6649 (11)	0.5188 (3)	0.6964 (4)	0.0311 (15)	0.561 (6)
H4′	0.640148	0.480827	0.702639	0.037*	0.561 (6)
C5′	0.7671 (8)	0.5460 (3)	0.7365 (3)	0.0393 (15)	0.561 (6)
H5′	0.810045	0.526376	0.770080	0.047*	0.561 (6)
C6′	0.8060 (7)	0.6004 (3)	0.7280 (3)	0.0386 (16)	0.561 (6)
H6′	0.875271	0.618286	0.755653	0.046*	0.561 (6)
C7′	0.7444 (7)	0.6293 (3)	0.6793 (3)	0.0322 (13)	0.561 (6)
H7′	0.771181	0.667151	0.673465	0.039*	0.561 (6)
C8′	0.6426 (11)	0.6029 (3)	0.6384 (4)	0.0258 (14)	0.561 (6)
H8′	0.602754	0.622673	0.604511	0.031*	0.561 (6)

C9	0.3051 (2)	0.54964 (11)	0.60637 (10)	0.0213 (5)	
C10	0.3035 (3)	0.60629 (12)	0.62219 (12)	0.0283 (5)	
H10	0.388476	0.626830	0.630628	0.034*	
C11	0.1786 (3)	0.63282 (14)	0.62566 (13)	0.0377 (7)	
H11	0.177872	0.671691	0.635490	0.045*	
C12	0.0553 (3)	0.60285 (15)	0.61486 (13)	0.0404 (8)	
H12	−0.030285	0.621444	0.616380	0.048*	
C13	0.0553 (3)	0.54595 (14)	0.60185 (12)	0.0338 (6)	
H13	−0.029162	0.524979	0.596454	0.041*	
C14	0.1798 (2)	0.51970 (12)	0.59672 (11)	0.0249 (5)	
H14	0.179670	0.480912	0.586525	0.030*	
C15	0.4992 (3)	0.34577 (11)	0.49472 (13)	0.0292 (6)	
C16	0.3571 (3)	0.33373 (12)	0.48605 (16)	0.0409 (8)	
H16	0.296816	0.356038	0.504190	0.049*	
C17	0.3039 (4)	0.28904 (13)	0.4508 (2)	0.0542 (10)	
H17	0.206782	0.281126	0.444628	0.065*	
C18	0.3916 (4)	0.25578 (13)	0.4246 (2)	0.0554 (10)	
H18	0.354057	0.226315	0.399149	0.066*	
C19	0.5340 (3)	0.26585 (13)	0.43563 (17)	0.0434 (8)	
H19	0.594411	0.241985	0.419199	0.052*	
C20	0.5891 (3)	0.31054 (11)	0.47053 (13)	0.0323 (6)	
H20	0.686832	0.317231	0.477997	0.039*	
C21	0.7448 (3)	0.39546 (10)	0.56642 (11)	0.0235 (5)	
C22	0.8443 (3)	0.40043 (10)	0.53138 (11)	0.0230 (5)	
H22	0.815723	0.409121	0.491821	0.028*	
C23	0.9851 (3)	0.39282 (11)	0.55371 (12)	0.0270 (5)	
H23	1.052194	0.395727	0.529381	0.032*	
C24	1.0276 (3)	0.38094 (11)	0.61176 (13)	0.0311 (6)	
H24	1.123860	0.376665	0.627434	0.037*	
C25	0.9290 (3)	0.37537 (14)	0.64658 (13)	0.0383 (7)	
H25	0.957818	0.366739	0.686137	0.046*	
C26	0.7883 (3)	0.38229 (13)	0.62420 (12)	0.0345 (6)	
H26	0.721343	0.378035	0.648409	0.041*	
Fe2	0.000000	0.80718 (2)	0.750000	0.02335 (12)	
Cl2	0.18469 (8)	0.86224 (3)	0.76337 (3)	0.03463 (16)	
Cl3	−0.00845 (8)	0.75564 (3)	0.67250 (3)	0.03743 (17)	
C27	0.500000	0.6989 (3)	0.750000	0.055 (3)	0.592 (4)
H27A	0.480195	0.674166	0.781219	0.066*	0.2960 (19)
H27B	0.519802	0.674164	0.718782	0.066*	0.2960 (19)
Cl4	0.35377 (18)	0.73688 (9)	0.72448 (9)	0.0700 (8)	0.592 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0147 (2)	0.0175 (2)	0.0161 (2)	−0.00051 (16)	0.00312 (16)	−0.00011 (17)
Cl1	0.0159 (2)	0.0237 (3)	0.0217 (3)	−0.0022 (2)	0.00337 (19)	−0.0017 (2)
P1	0.0166 (3)	0.0264 (3)	0.0167 (3)	0.0014 (2)	0.0037 (2)	0.0001 (2)
P2	0.0204 (3)	0.0198 (3)	0.0252 (3)	0.0025 (2)	0.0079 (2)	0.0039 (2)

C1	0.0302 (13)	0.0347 (14)	0.0263 (13)	0.0083 (11)	0.0126 (11)	0.0114 (11)
C2	0.0319 (14)	0.0316 (14)	0.0368 (15)	0.0083 (11)	0.0173 (12)	0.0163 (12)
C3	0.0173 (17)	0.034 (5)	0.016 (3)	0.006 (4)	0.0023 (13)	−0.002 (3)
C4	0.031 (2)	0.040 (5)	0.0219 (15)	0.002 (4)	0.0027 (14)	0.000 (3)
C5	0.034 (2)	0.058 (5)	0.0226 (19)	0.000 (4)	−0.0047 (16)	0.002 (4)
C6	0.0271 (19)	0.065 (5)	0.023 (3)	−0.007 (4)	0.0028 (18)	−0.012 (3)
C7	0.026 (2)	0.046 (4)	0.026 (3)	−0.011 (3)	0.009 (2)	−0.011 (3)
C8	0.021 (2)	0.036 (4)	0.020 (3)	−0.002 (3)	0.0026 (19)	−0.004 (3)
C3′	0.0173 (17)	0.034 (5)	0.016 (3)	0.006 (4)	0.0023 (13)	−0.002 (3)
C4′	0.031 (2)	0.040 (5)	0.0219 (15)	0.002 (4)	0.0027 (14)	0.000 (3)
C5′	0.034 (2)	0.058 (5)	0.0226 (19)	0.000 (4)	−0.0047 (16)	0.002 (4)
C6′	0.0271 (19)	0.065 (5)	0.023 (3)	−0.007 (4)	0.0028 (18)	−0.012 (3)
C7′	0.026 (2)	0.046 (4)	0.026 (3)	−0.011 (3)	0.009 (2)	−0.011 (3)
C8′	0.021 (2)	0.036 (4)	0.020 (3)	−0.002 (3)	0.0026 (19)	−0.004 (3)
C9	0.0175 (10)	0.0288 (12)	0.0181 (11)	0.0019 (9)	0.0044 (8)	−0.0001 (9)
C10	0.0304 (13)	0.0308 (13)	0.0259 (13)	0.0005 (11)	0.0108 (10)	−0.0028 (11)
C11	0.0471 (18)	0.0383 (16)	0.0328 (16)	0.0147 (14)	0.0204 (13)	0.0000 (12)
C12	0.0314 (15)	0.060 (2)	0.0336 (16)	0.0217 (14)	0.0166 (12)	0.0098 (15)
C13	0.0194 (12)	0.0573 (19)	0.0249 (13)	0.0028 (12)	0.0049 (10)	0.0055 (13)
C14	0.0197 (11)	0.0357 (14)	0.0200 (12)	−0.0018 (10)	0.0056 (9)	−0.0004 (10)
C15	0.0264 (12)	0.0180 (11)	0.0436 (16)	0.0006 (10)	0.0076 (11)	0.0021 (11)
C16	0.0257 (13)	0.0199 (13)	0.079 (2)	−0.0008 (11)	0.0139 (15)	0.0006 (14)
C17	0.0311 (16)	0.0241 (15)	0.106 (3)	−0.0062 (12)	0.0070 (18)	−0.0078 (18)
C18	0.0420 (18)	0.0233 (15)	0.097 (3)	−0.0058 (13)	0.0033 (19)	−0.0179 (17)
C19	0.0376 (16)	0.0255 (14)	0.067 (2)	0.0009 (12)	0.0100 (16)	−0.0107 (14)
C20	0.0289 (13)	0.0230 (13)	0.0455 (17)	0.0009 (10)	0.0083 (12)	−0.0008 (12)
C21	0.0243 (11)	0.0218 (11)	0.0245 (12)	0.0052 (9)	0.0049 (9)	0.0028 (9)
C22	0.0231 (11)	0.0226 (11)	0.0227 (12)	0.0022 (9)	0.0023 (9)	0.0021 (9)
C23	0.0221 (11)	0.0265 (13)	0.0319 (14)	0.0030 (10)	0.0034 (10)	0.0004 (10)
C24	0.0271 (13)	0.0269 (13)	0.0364 (15)	0.0047 (10)	−0.0022 (11)	−0.0031 (11)
C25	0.0423 (17)	0.0458 (18)	0.0245 (14)	0.0140 (14)	−0.0001 (12)	0.0050 (12)
C26	0.0362 (15)	0.0416 (16)	0.0270 (14)	0.0135 (13)	0.0091 (12)	0.0083 (12)
Fe2	0.0267 (3)	0.0208 (2)	0.0222 (3)	0.000	0.0037 (2)	0.000
Cl2	0.0376 (4)	0.0405 (4)	0.0270 (3)	−0.0135 (3)	0.0093 (3)	−0.0080 (3)
Cl3	0.0409 (4)	0.0326 (4)	0.0387 (4)	−0.0027 (3)	0.0071 (3)	−0.0155 (3)
C27	0.026 (4)	0.030 (4)	0.101 (8)	0.000	−0.010 (4)	0.000
Cl4	0.0446 (9)	0.0845 (14)	0.0813 (14)	0.0320 (9)	0.0126 (8)	0.0329 (10)

Geometric parameters (Å, º)

Fe1—Cl1^{i}	2.2135 (6)	C10—C11	1.387 (4)
Fe1—Cl1	2.2135 (6)	C10—H10	0.9500
Fe1—P1	2.3662 (6)	C11—C12	1.379 (5)
Fe1—P1^{i}	2.3662 (6)	C11—H11	0.9500
Fe1—P2^{i}	2.3738 (6)	C12—C13	1.383 (5)
Fe1—P2	2.3738 (6)	C12—H12	0.9500
P1—C1	1.807 (3)	C13—C14	1.390 (4)
P1—C3	1.822 (6)	C13—H13	0.9500

P1—C9	1.824 (2)	C14—H14	0.9500
P1—C3′	1.832 (5)	C15—C16	1.393 (4)
P2—C2	1.811 (3)	C15—C20	1.406 (4)
P2—C21	1.825 (3)	C16—C17	1.388 (5)
P2—C15	1.829 (3)	C16—H16	0.9500
C1—C2	1.319 (4)	C17—C18	1.391 (5)
C1—H1	0.9500	C17—H17	0.9500
C2—H2	0.9500	C18—C19	1.386 (5)
C3—C8	1.379 (10)	C18—H18	0.9500
C3—C4	1.393 (10)	C19—C20	1.389 (4)
C4—C5	1.391 (10)	C19—H19	0.9500
C4—H4	0.9500	C20—H20	0.9500
C5—C6	1.369 (10)	C21—C26	1.392 (4)
C5—H5	0.9500	C21—C22	1.393 (4)
C6—C7	1.370 (10)	C22—C23	1.390 (3)
C6—H6	0.9500	C22—H22	0.9500
C7—C8	1.397 (10)	C23—C24	1.390 (4)
C7—H7	0.9500	C23—H23	0.9500
C8—H8	0.9500	C24—C25	1.383 (4)
C3′—C8′	1.396 (8)	C24—H24	0.9500
C3′—C4′	1.413 (8)	C25—C26	1.387 (4)
C4′—C5′	1.401 (8)	C25—H25	0.9500
C4′—H4′	0.9500	C26—H26	0.9500
C5′—C6′	1.368 (8)	Fe2—Cl3^{ii}	2.1936 (8)
C5′—H5′	0.9500	Fe2—Cl3	2.1937 (8)
C6′—C7′	1.382 (8)	Fe2—Cl2	2.1993 (8)
C6′—H6′	0.9500	Fe2—Cl2^{ii}	2.1993 (7)
C7′—C8′	1.401 (8)	C27—Cl4^{iii}	1.701 (4)
C7′—H7′	0.9500	C27—Cl4	1.701 (4)
C8′—H8′	0.9500	C27—H27A	0.9900
C9—C10	1.394 (4)	C27—H27B	0.9900
C9—C14	1.395 (3)		

Cl1^{i}—Fe1—Cl1	180.0	C3′—C8′—C7′	121.0 (6)
Cl1^{i}—Fe1—P1	87.63 (2)	C3′—C8′—H8′	119.5
Cl1—Fe1—P1	92.38 (2)	C7′—C8′—H8′	119.5
Cl1^{i}—Fe1—P1^{i}	92.38 (2)	C10—C9—C14	118.8 (2)
Cl1—Fe1—P1^{i}	87.62 (2)	C10—C9—P1	123.18 (19)
P1—Fe1—P1^{i}	180.0	C14—C9—P1	118.00 (19)
Cl1^{i}—Fe1—P2^{i}	92.42 (2)	C11—C10—C9	120.3 (3)
Cl1—Fe1—P2^{i}	87.58 (2)	C11—C10—H10	119.8
P1—Fe1—P2^{i}	99.08 (2)	C9—C10—H10	119.8
P1^{i}—Fe1—P2^{i}	80.92 (2)	C12—C11—C10	120.1 (3)
Cl1^{i}—Fe1—P2	87.58 (2)	C12—C11—H11	120.0
Cl1—Fe1—P2	92.42 (2)	C10—C11—H11	120.0
P1—Fe1—P2	80.92 (2)	C11—C12—C13	120.5 (3)
P1^{i}—Fe1—P2	99.08 (2)	C11—C12—H12	119.7
P2^{i}—Fe1—P2	180.0	C13—C12—H12	119.7

C1—P1—C3	97.0 (4)	C12—C13—C14	119.4 (3)
C1—P1—C9	100.81 (12)	C12—C13—H13	120.3
C3—P1—C9	108.1 (9)	C14—C13—H13	120.3
C1—P1—C3′	107.6 (3)	C13—C14—C9	120.8 (3)
C9—P1—C3′	102.4 (7)	C13—C14—H14	119.6
C1—P1—Fe1	106.98 (9)	C9—C14—H14	119.6
C3—P1—Fe1	120.7 (9)	C16—C15—C20	119.8 (3)
C9—P1—Fe1	118.90 (8)	C16—C15—P2	117.9 (2)
C3′—P1—Fe1	118.4 (7)	C20—C15—P2	122.4 (2)
C2—P2—C21	103.54 (13)	C17—C16—C15	119.8 (3)
C2—P2—C15	100.56 (14)	C17—C16—H16	120.1
C21—P2—C15	106.04 (12)	C15—C16—H16	120.1
C2—P2—Fe1	106.53 (9)	C16—C17—C18	120.5 (3)
C21—P2—Fe1	117.26 (9)	C16—C17—H17	119.7
C15—P2—Fe1	120.33 (9)	C18—C17—H17	119.7
C2—C1—P1	119.0 (2)	C19—C18—C17	119.6 (3)
C2—C1—H1	120.5	C19—C18—H18	120.2
P1—C1—H1	120.5	C17—C18—H18	120.2
C1—C2—P2	119.1 (2)	C18—C19—C20	120.6 (3)
C1—C2—H2	120.4	C18—C19—H19	119.7
P2—C2—H2	120.4	C20—C19—H19	119.7
C8—C3—C4	121.4 (7)	C19—C20—C15	119.5 (3)
C8—C3—P1	116.9 (8)	C19—C20—H20	120.3
C4—C3—P1	121.7 (8)	C15—C20—H20	120.3
C5—C4—C3	118.2 (8)	C26—C21—C22	119.0 (2)
C5—C4—H4	120.9	C26—C21—P2	121.0 (2)
C3—C4—H4	120.9	C22—C21—P2	119.92 (19)
C6—C5—C4	120.6 (8)	C23—C22—C21	120.6 (2)
C6—C5—H5	119.7	C23—C22—H22	119.7
C4—C5—H5	119.7	C21—C22—H22	119.7
C5—C6—C7	121.0 (8)	C22—C23—C24	119.8 (3)
C5—C6—H6	119.5	C22—C23—H23	120.1
C7—C6—H6	119.5	C24—C23—H23	120.1
C6—C7—C8	119.8 (8)	C25—C24—C23	119.7 (3)
C6—C7—H7	120.1	C25—C24—H24	120.1
C8—C7—H7	120.1	C23—C24—H24	120.1
C3—C8—C7	119.0 (8)	C24—C25—C26	120.5 (3)
C3—C8—H8	120.5	C24—C25—H25	119.7
C7—C8—H8	120.5	C26—C25—H25	119.7
C8′—C3′—C4′	117.9 (5)	C25—C26—C21	120.3 (3)
C8′—C3′—P1	121.9 (6)	C25—C26—H26	119.9
C4′—C3′—P1	120.2 (6)	C21—C26—H26	119.9
C5′—C4′—C3′	119.9 (6)	Cl3^{ii}—Fe2—Cl3	112.36 (5)
C5′—C4′—H4′	120.0	Cl3^{ii}—Fe2—Cl2	107.77 (3)
C3′—C4′—H4′	120.0	Cl3—Fe2—Cl2	110.79 (3)
C6′—C5′—C4′	121.0 (6)	Cl3^{ii}—Fe2—Cl2^{ii}	110.79 (3)
C6′—C5′—H5′	119.5	Cl3—Fe2—Cl2^{ii}	107.76 (3)
C4′—C5′—H5′	119.5	Cl2—Fe2—Cl2^{ii}	107.26 (5)

C5′—C6′—C7′	120.0 (6)	Cl4^{iii}—C27—Cl4	116.2 (5)
C5′—C6′—H6′	120.0	Cl4^{iii}—C27—H27A	108.2
C7′—C6′—H6′	120.0	Cl4—C27—H27A	108.2
C6′—C7′—C8′	120.0 (6)	Cl4^{iii}—C27—H27B	108.2
C6′—C7′—H7′	120.0	Cl4—C27—H27B	108.2
C8′—C7′—H7′	120.0	H27A—C27—H27B	107.4
C3—P1—C1—C2	−105.9 (10)	C1—P1—C9—C14	−38.8 (2)
C9—P1—C1—C2	144.1 (2)	C3—P1—C9—C14	−140.0 (5)
C3′—P1—C1—C2	−109.1 (8)	C3′—P1—C9—C14	−149.7 (4)
Fe1—P1—C1—C2	19.1 (3)	Fe1—P1—C9—C14	77.6 (2)
P1—C1—C2—P2	0.6 (4)	C14—C9—C10—C11	−2.9 (4)
C21—P2—C2—C1	104.4 (3)	P1—C9—C10—C11	174.8 (2)
C15—P2—C2—C1	−146.1 (3)	C9—C10—C11—C12	1.6 (4)
Fe1—P2—C2—C1	−19.9 (3)	C10—C11—C12—C13	1.5 (5)
C1—P1—C3—C8	−177 (2)	C11—C12—C13—C14	−3.4 (4)
C9—P1—C3—C8	−74 (2)	C12—C13—C14—C9	2.1 (4)
Fe1—P1—C3—C8	68 (2)	C10—C9—C14—C13	1.0 (4)
C1—P1—C3—C4	0 (2)	P1—C9—C14—C13	−176.8 (2)
C9—P1—C3—C4	104 (2)	C2—P2—C15—C16	47.9 (3)
Fe1—P1—C3—C4	−114 (2)	C21—P2—C15—C16	155.4 (2)
C8—C3—C4—C5	0 (4)	Fe1—P2—C15—C16	−68.5 (3)
P1—C3—C4—C5	−178.0 (16)	C2—P2—C15—C20	−133.1 (3)
C3—C4—C5—C6	1 (2)	C21—P2—C15—C20	−25.5 (3)
C4—C5—C6—C7	−0.9 (19)	Fe1—P2—C15—C20	110.6 (2)
C5—C6—C7—C8	0.5 (18)	C20—C15—C16—C17	−3.8 (5)
C4—C3—C8—C7	0 (4)	P2—C15—C16—C17	175.2 (3)
P1—C3—C8—C7	177.7 (14)	C15—C16—C17—C18	0.7 (6)
C6—C7—C8—C3	0 (3)	C16—C17—C18—C19	2.8 (6)
C1—P1—C3′—C8′	−178.4 (15)	C17—C18—C19—C20	−3.1 (6)
C9—P1—C3′—C8′	−72.6 (18)	C18—C19—C20—C15	0.0 (5)
Fe1—P1—C3′—C8′	60.3 (18)	C16—C15—C20—C19	3.5 (5)
C1—P1—C3′—C4′	2.9 (18)	P2—C15—C20—C19	−175.5 (3)
C9—P1—C3′—C4′	108.6 (15)	C2—P2—C21—C26	−0.4 (3)
Fe1—P1—C3′—C4′	−118.4 (14)	C15—P2—C21—C26	−105.7 (2)
C8′—C3′—C4′—C5′	3 (2)	Fe1—P2—C21—C26	116.6 (2)
P1—C3′—C4′—C5′	−178.7 (11)	C2—P2—C21—C22	−178.3 (2)
C3′—C4′—C5′—C6′	−1.0 (18)	C15—P2—C21—C22	76.3 (2)
C4′—C5′—C6′—C7′	−0.2 (13)	Fe1—P2—C21—C22	−61.4 (2)
C5′—C6′—C7′—C8′	−0.2 (13)	C26—C21—C22—C23	−0.5 (4)
C4′—C3′—C8′—C7′	−3 (3)	P2—C21—C22—C23	177.5 (2)
P1—C3′—C8′—C7′	178.3 (11)	C21—C22—C23—C24	−1.0 (4)
C6′—C7′—C8′—C3′	1.8 (19)	C22—C23—C24—C25	1.6 (4)
C1—P1—C9—C10	143.5 (2)	C23—C24—C25—C26	−0.9 (5)
C3—P1—C9—C10	42.3 (6)	C24—C25—C26—C21	−0.6 (5)

C3′—P1—C9—C10	32.6 (5)	C22—C21—C26—C25	1.2 (4)
Fe1—P1—C9—C10	−100.1 (2)	P2—C21—C26—C25	−176.7 (2)

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

trans-Bis[1,2-bis(diphenylphosphane)benzene]dichloridoiron(III) tetrachloridoferrate(III) dichloromethane monosolvate (2)

Crystal data

$[FeCl_2(C_{30}H_{24}P_2)_2][FeCl_4]\cdot CH_2Cl_2$
M_r = 1302.19
Triclinic, *P*1
a = 9.8771 (7) Å
b = 12.6516 (8) Å
c = 12.8258 (8) Å
α = 81.058 (1)°
β = 83.050 (1)°
γ = 68.335 (1)°
V = 1467.87 (17) Å^3
Z = 1
F(000) = 664
D_x = 1.473 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 4051 reflections
θ = 2.3–30.7°
μ = 1.01 mm^{-1}
T = 100 K
Plate, dichroic red-green
0.24 × 0.20 × 0.08 mm

Data collection

Bruker SMART APEX II CCD platform diffractometer
Radiation source: fine-focus sealed tube
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.644, T_{max} = 0.747
27211 measured reflections
22268 independent reflections
11890 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 35.0°, θ_{min} = 2.2°
h = −15→15
k = −20→20
l = −20→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.182
S = 1.00
22268 reflections
488 parameters
34 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.23 e Å^{-3}
$\Delta\rho_{min}$ = −1.39 e Å^{-3}
Absolute structure: Refined as an inversion twin.
Absolute structure parameter: 0.24 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The structure was modeled as an inversion twin whose component mass ratio refined to 0.76 (3):0.24 (3). A solution and refinement in centrosymmetric space group P-1 caused an increase in the R1 residual (strong data) from 0.071 to 0.118.

The cocrystallized dichloromethane solvent molecule is modeled as disordered over three positions (0.740 (3):0.136 (3):0.124 (3)). Analogous bond lengths and angles among the three positions of the disordered dichloromethane solvent molecule were restrained to be similar. Anisotropic displacement parameters for proximal and pseudosymmetrically related atoms were constrained to be equivalent.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.50286 (14)	0.39706 (10)	0.63842 (10)	0.01341 (15)	
Cl1	0.68914 (19)	0.42220 (14)	0.69888 (14)	0.01712 (17)	
Cl2	0.31700 (19)	0.37173 (15)	0.57842 (14)	0.01712 (17)	
P1	0.3591 (2)	0.59048 (15)	0.66544 (16)	0.01471 (18)	
P2	0.5609 (2)	0.48921 (15)	0.47244 (15)	0.01494 (19)	
P3	0.6449 (2)	0.20476 (15)	0.61113 (16)	0.01471 (18)	
P4	0.4468 (2)	0.30281 (15)	0.80391 (15)	0.01494 (19)	
C1	0.4350 (8)	0.6828 (6)	0.5755 (6)	0.0168 (7)	
C2	0.4012 (9)	0.7982 (6)	0.5880 (7)	0.0203 (8)	
H2	0.342059	0.829432	0.647917	0.024*	
C3	0.4557 (9)	0.8671 (7)	0.5111 (7)	0.0224 (8)	
H3	0.430915	0.945688	0.518605	0.027*	
C4	0.5440 (10)	0.8228 (7)	0.4253 (7)	0.0230 (8)	
H4	0.580837	0.870627	0.374680	0.028*	
C5	0.5801 (10)	0.7077 (7)	0.4120 (7)	0.0231 (8)	
H5	0.641033	0.677084	0.352542	0.028*	
C6	0.5258 (9)	0.6381 (6)	0.4871 (6)	0.0168 (7)	
C7	0.3577 (9)	0.6416 (6)	0.7913 (6)	0.0170 (7)	
C8	0.4891 (9)	0.6487 (6)	0.8184 (7)	0.0185 (7)	
H8	0.573481	0.629636	0.770516	0.022*	
C9	0.4942 (10)	0.6834 (7)	0.9141 (7)	0.0216 (8)	
H9	0.582948	0.686509	0.932254	0.026*	
C10	0.3734 (10)	0.7134 (7)	0.9833 (7)	0.0253 (9)	
H10	0.378826	0.736978	1.049025	0.030*	
C11	0.2439 (10)	0.7094 (7)	0.9579 (7)	0.0276 (10)	
H11	0.159982	0.730938	1.005926	0.033*	
C12	0.2351 (9)	0.6736 (7)	0.8613 (7)	0.0217 (8)	
H12	0.145437	0.671463	0.843936	0.026*	
C13	0.1675 (9)	0.6443 (7)	0.6345 (7)	0.0205 (8)	
C14	0.0746 (9)	0.5937 (7)	0.6896 (7)	0.0234 (8)	
H14	0.110682	0.531331	0.743055	0.028*	
C15	−0.0721 (10)	0.6326 (8)	0.6681 (8)	0.0292 (10)	
H15	−0.134976	0.597322	0.707755	0.035*	
C16	−0.1257 (10)	0.7200 (8)	0.5913 (8)	0.0308 (10)	
H16	−0.225523	0.745221	0.576744	0.037*	
C17	−0.0333 (11)	0.7737 (8)	0.5330 (8)	0.0358 (11)	
H17	−0.069872	0.834910	0.478609	0.043*	
C18	0.1131 (10)	0.7356 (7)	0.5564 (7)	0.0272 (9)	
H18	0.175868	0.772242	0.518776	0.033*	
C19	0.4506 (8)	0.5019 (6)	0.3642 (6)	0.0165 (7)	
C20	0.3450 (9)	0.6064 (7)	0.3297 (7)	0.0254 (9)	
H20	0.333632	0.672703	0.361033	0.030*	
C21	0.2576 (10)	0.6151 (8)	0.2516 (7)	0.0292 (10)	
H21	0.184693	0.686828	0.230899	0.035*	
C22	0.2737 (10)	0.5204 (8)	0.2020 (7)	0.0262 (10)	

H22	0.215100	0.527670	0.145873	0.031*
C23	0.3766 (9)	0.4155 (7)	0.2358 (6)	0.0206 (9)
H23	0.389282	0.349815	0.202910	0.025*
C24	0.4610 (9)	0.4065 (7)	0.3178 (6)	0.0187 (8)
H24	0.527743	0.333368	0.342963	0.022*
C25	0.7486 (9)	0.4461 (7)	0.4165 (6)	0.0177 (7)
C26	0.7991 (9)	0.3814 (7)	0.3313 (7)	0.0246 (9)
H26	0.732100	0.362996	0.296982	0.030*
C27	0.9467 (10)	0.3436 (9)	0.2961 (8)	0.0345 (11)
H27	0.981402	0.297850	0.239587	0.041*
C28	1.0437 (10)	0.3753 (9)	0.3469 (8)	0.0346 (12)
H28	1.144813	0.348675	0.324980	0.041*
C29	0.9948 (10)	0.4427 (8)	0.4259 (8)	0.0303 (11)
H29	1.060584	0.465935	0.456527	0.036*
C30	0.8479 (9)	0.4781 (7)	0.4623 (7)	0.0228 (8)
H30	0.814661	0.524277	0.518586	0.027*
C31	0.5655 (8)	0.1115 (6)	0.7002 (6)	0.0168 (7)
C32	0.6008 (9)	−0.0039 (7)	0.6850 (7)	0.0203 (8)
H32	0.661938	−0.033872	0.625422	0.024*
C33	0.5457 (9)	−0.0727 (7)	0.7576 (7)	0.0224 (8)
H33	0.568623	−0.150634	0.748200	0.027*
C34	0.4560 (10)	−0.0278 (7)	0.8449 (7)	0.0230 (8)
H34	0.417449	−0.075317	0.894485	0.028*
C35	0.4230 (10)	0.0844 (7)	0.8600 (7)	0.0231 (8)
H35	0.363418	0.113538	0.920434	0.028*
C36	0.4772 (9)	0.1564 (6)	0.7861 (6)	0.0168 (7)
C37	0.6454 (9)	0.1559 (6)	0.4842 (6)	0.0170 (7)
C38	0.5193 (9)	0.1451 (6)	0.4567 (7)	0.0185 (7)
H38	0.435397	0.161863	0.505053	0.022*
C39	0.5133 (10)	0.1107 (7)	0.3611 (7)	0.0216 (8)
H39	0.426161	0.104035	0.343895	0.026*
C40	0.6362 (10)	0.0858 (7)	0.2894 (7)	0.0253 (9)
H40	0.632232	0.063705	0.222680	0.030*
C41	0.7640 (10)	0.0934 (7)	0.3162 (7)	0.0276 (10)
H41	0.848092	0.075253	0.268098	0.033*
C42	0.7695 (9)	0.1273 (7)	0.4130 (7)	0.0217 (8)
H42	0.857814	0.131138	0.431233	0.026*
C43	0.8368 (9)	0.1487 (7)	0.6415 (7)	0.0205 (8)
C44	0.9319 (9)	0.2031 (7)	0.5899 (7)	0.0234 (8)
H44	0.894856	0.268358	0.539493	0.028*
C45	1.0755 (10)	0.1651 (8)	0.6101 (8)	0.0292 (10)
H45	1.138383	0.201914	0.572957	0.035*
C46	1.1292 (10)	0.0697 (8)	0.6873 (8)	0.0308 (10)
H46	1.228576	0.042808	0.703517	0.037*
C47	1.0388 (11)	0.0167 (8)	0.7381 (8)	0.0358 (11)
H47	1.076749	−0.048303	0.788638	0.043*
C48	0.8941 (10)	0.0544 (7)	0.7185 (7)	0.0272 (9)
H48	0.832507	0.016987	0.756782	0.033*

C49	0.5653 (8)	0.2851 (6)	0.9099 (6)	0.0165 (7)	
C50	0.6609 (10)	0.1782 (7)	0.9469 (7)	0.0254 (9)	
H50	0.664284	0.112121	0.918717	0.030*	
C51	0.7527 (10)	0.1675 (8)	1.0259 (7)	0.0292 (10)	
H51	0.819167	0.094181	1.050727	0.035*	
C52	0.7467 (10)	0.2646 (8)	1.0683 (7)	0.0262 (10)	
H52	0.809821	0.257491	1.121332	0.031*	
C53	0.6490 (9)	0.3706 (7)	1.0329 (6)	0.0206 (9)	
H53	0.642575	0.436063	1.063628	0.025*	
C54	0.5595 (9)	0.3826 (7)	0.9523 (6)	0.0187 (8)	
H54	0.495090	0.456324	0.926328	0.022*	
C55	0.2583 (9)	0.3503 (7)	0.8622 (6)	0.0177 (7)	
C56	0.2117 (9)	0.4183 (7)	0.9441 (7)	0.0246 (9)	
H56	0.280279	0.438387	0.974875	0.030*	
C57	0.0671 (10)	0.4570 (9)	0.9813 (8)	0.0345 (11)	
H57	0.037337	0.503542	1.037323	0.041*	
C58	−0.0343 (10)	0.4296 (8)	0.9388 (8)	0.0346 (12)	
H58	−0.134230	0.458287	0.963586	0.041*	
C59	0.0112 (10)	0.3588 (8)	0.8584 (8)	0.0303 (11)	
H59	−0.057673	0.337013	0.829994	0.036*	
C60	0.1560 (9)	0.3200 (7)	0.8196 (7)	0.0228 (8)	
H60	0.185630	0.272858	0.764084	0.027*	
Fe2	0.74909 (13)	0.79207 (11)	0.09572 (11)	0.0302 (3)	
Cl3	0.5310 (2)	0.92270 (18)	0.11580 (17)	0.0339 (4)	
Cl4	0.7333 (3)	0.62264 (18)	0.13622 (18)	0.0437 (6)	
Cl5	0.8376 (3)	0.8101 (3)	−0.0681 (3)	0.0645 (6)	
Cl6	0.8890 (4)	0.8166 (3)	0.2034 (4)	0.0963 (15)	
Cl7	0.1337 (4)	0.0699 (5)	0.1131 (4)	0.0819 (15)	0.740 (3)
C61	0.1765 (12)	−0.0475 (9)	0.2177 (8)	0.0302 (3)	0.740 (3)
H61A	0.108903	−0.089082	0.218036	0.036*	0.740 (3)
H61B	0.276777	−0.101351	0.202280	0.036*	0.740 (3)
Cl8	0.1656 (4)	−0.0086 (4)	0.3389 (4)	0.0645 (6)	0.740 (3)
Cl7′	0.129 (3)	−0.012 (3)	0.087 (3)	0.0963 (15)	0.124 (3)
C61′	0.249 (5)	0.007 (7)	0.168 (3)	0.0302 (3)	0.124 (3)
H61C	0.332305	−0.066406	0.178368	0.036*	0.124 (3)
H61D	0.287840	0.064322	0.128480	0.036*	0.124 (3)
Cl8′	0.178 (2)	0.050 (2)	0.2923 (19)	0.0645 (6)	0.124 (3)
Cl7"	0.127 (2)	−0.0679 (19)	0.166 (2)	0.0645 (6)	0.136 (3)
C61"	0.276 (4)	−0.026 (3)	0.178 (6)	0.0302 (3)	0.136 (3)
H61E	0.327391	−0.066354	0.242501	0.036*	0.136 (3)
H61F	0.345977	−0.040293	0.115397	0.036*	0.136 (3)
Cl8"	0.191 (2)	0.119 (2)	0.187 (2)	0.0819 (15)	0.136 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0152 (4)	0.0115 (3)	0.0147 (4)	−0.0053 (3)	−0.0038 (3)	−0.0015 (3)
Cl1	0.0180 (4)	0.0166 (4)	0.0190 (4)	−0.0078 (3)	−0.0047 (3)	−0.0020 (3)

Cl2	0.0180 (4)	0.0166 (4)	0.0190 (4)	−0.0078 (3)	−0.0047 (3)	−0.0020 (3)
P1	0.0166 (4)	0.0123 (4)	0.0160 (5)	−0.0052 (3)	−0.0034 (4)	−0.0018 (3)
P2	0.0181 (5)	0.0128 (4)	0.0151 (5)	−0.0064 (4)	−0.0035 (4)	−0.0012 (3)
P3	0.0166 (4)	0.0123 (4)	0.0160 (5)	−0.0052 (3)	−0.0034 (4)	−0.0018 (3)
P4	0.0181 (5)	0.0128 (4)	0.0151 (5)	−0.0064 (4)	−0.0035 (4)	−0.0012 (3)
C1	0.0207 (18)	0.0144 (15)	0.0161 (18)	−0.0071 (14)	−0.0032 (14)	−0.0003 (13)
C2	0.027 (2)	0.0151 (16)	0.021 (2)	−0.0076 (15)	−0.0045 (16)	−0.0037 (14)
C3	0.030 (2)	0.0132 (16)	0.024 (2)	−0.0072 (15)	−0.0075 (17)	−0.0012 (15)
C4	0.032 (2)	0.0181 (17)	0.022 (2)	−0.0130 (17)	−0.0054 (17)	0.0039 (15)
C5	0.032 (2)	0.0185 (18)	0.020 (2)	−0.0115 (17)	−0.0020 (17)	−0.0025 (15)
C6	0.0188 (18)	0.0146 (15)	0.0169 (18)	−0.0053 (14)	−0.0030 (14)	−0.0020 (13)
C7	0.0207 (18)	0.0116 (15)	0.0191 (19)	−0.0052 (13)	−0.0045 (14)	−0.0017 (13)
C8	0.0198 (18)	0.0149 (16)	0.023 (2)	−0.0078 (14)	−0.0034 (15)	−0.0035 (14)
C9	0.031 (2)	0.0160 (16)	0.021 (2)	−0.0115 (16)	−0.0094 (16)	0.0006 (14)
C10	0.040 (3)	0.0204 (19)	0.019 (2)	−0.0132 (18)	−0.0048 (18)	−0.0042 (15)
C11	0.033 (2)	0.029 (2)	0.023 (2)	−0.0135 (19)	0.0038 (18)	−0.0086 (18)
C12	0.022 (2)	0.0203 (19)	0.023 (2)	−0.0073 (16)	−0.0021 (16)	−0.0038 (15)
C13	0.0206 (19)	0.0171 (17)	0.024 (2)	−0.0051 (15)	−0.0047 (15)	−0.0046 (14)
C14	0.022 (2)	0.0182 (18)	0.033 (2)	−0.0090 (15)	−0.0062 (17)	−0.0031 (16)
C15	0.020 (2)	0.029 (2)	0.042 (3)	−0.0091 (18)	−0.0049 (19)	−0.012 (2)
C16	0.019 (2)	0.029 (2)	0.042 (3)	−0.0007 (17)	−0.0151 (19)	−0.008 (2)
C17	0.030 (3)	0.029 (2)	0.040 (3)	0.0013 (19)	−0.019 (2)	0.003 (2)
C18	0.026 (2)	0.023 (2)	0.028 (2)	−0.0032 (17)	−0.0068 (18)	0.0002 (17)
C19	0.0190 (19)	0.0193 (17)	0.0110 (17)	−0.0068 (15)	−0.0015 (14)	−0.0008 (13)
C20	0.029 (2)	0.020 (2)	0.025 (2)	−0.0047 (17)	−0.0074 (17)	−0.0054 (17)
C21	0.027 (2)	0.026 (2)	0.031 (3)	−0.0029 (19)	−0.0128 (19)	−0.0014 (19)
C22	0.029 (2)	0.035 (2)	0.017 (2)	−0.014 (2)	−0.0094 (18)	0.0011 (17)
C23	0.024 (2)	0.026 (2)	0.017 (2)	−0.0141 (19)	0.0009 (17)	−0.0056 (16)
C24	0.019 (2)	0.0191 (17)	0.020 (2)	−0.0105 (16)	−0.0017 (16)	0.0001 (14)
C25	0.0182 (18)	0.0185 (17)	0.0173 (19)	−0.0081 (14)	−0.0023 (14)	−0.0002 (13)
C26	0.022 (2)	0.027 (2)	0.027 (2)	−0.0099 (17)	−0.0006 (17)	−0.0070 (17)
C27	0.026 (2)	0.040 (3)	0.038 (3)	−0.012 (2)	0.006 (2)	−0.013 (2)
C28	0.023 (2)	0.043 (3)	0.041 (3)	−0.017 (2)	0.005 (2)	−0.007 (2)
C29	0.024 (2)	0.034 (2)	0.038 (3)	−0.019 (2)	−0.007 (2)	0.002 (2)
C30	0.028 (2)	0.026 (2)	0.021 (2)	−0.0169 (17)	−0.0042 (16)	0.0003 (16)
C31	0.0207 (18)	0.0144 (15)	0.0161 (18)	−0.0071 (14)	−0.0032 (14)	−0.0003 (13)
C32	0.027 (2)	0.0151 (16)	0.021 (2)	−0.0076 (15)	−0.0045 (16)	−0.0037 (14)
C33	0.030 (2)	0.0132 (16)	0.024 (2)	−0.0072 (15)	−0.0075 (17)	−0.0012 (15)
C34	0.032 (2)	0.0181 (17)	0.022 (2)	−0.0130 (17)	−0.0054 (17)	0.0039 (15)
C35	0.032 (2)	0.0185 (18)	0.020 (2)	−0.0115 (17)	−0.0020 (17)	−0.0025 (15)
C36	0.0188 (18)	0.0146 (15)	0.0169 (18)	−0.0053 (14)	−0.0030 (14)	−0.0020 (13)
C37	0.0207 (18)	0.0116 (15)	0.0191 (19)	−0.0052 (13)	−0.0045 (14)	−0.0017 (13)
C38	0.0198 (18)	0.0149 (16)	0.023 (2)	−0.0078 (14)	−0.0034 (15)	−0.0035 (14)
C39	0.031 (2)	0.0160 (16)	0.021 (2)	−0.0115 (16)	−0.0094 (16)	0.0006 (14)
C40	0.040 (3)	0.0204 (19)	0.019 (2)	−0.0132 (18)	−0.0048 (18)	−0.0042 (15)
C41	0.033 (2)	0.029 (2)	0.023 (2)	−0.0135 (19)	0.0038 (18)	−0.0086 (18)
C42	0.022 (2)	0.0203 (19)	0.023 (2)	−0.0073 (16)	−0.0021 (16)	−0.0038 (15)
C43	0.0206 (19)	0.0171 (17)	0.024 (2)	−0.0051 (15)	−0.0047 (15)	−0.0046 (14)

C44	0.022 (2)	0.0182 (18)	0.033 (2)	−0.0090 (15)	−0.0062 (17)	−0.0031 (16)
C45	0.020 (2)	0.029 (2)	0.042 (3)	−0.0091 (18)	−0.0049 (19)	−0.012 (2)
C46	0.019 (2)	0.029 (2)	0.042 (3)	−0.0007 (17)	−0.0151 (19)	−0.008 (2)
C47	0.030 (3)	0.029 (2)	0.040 (3)	0.0013 (19)	−0.019 (2)	0.003 (2)
C48	0.026 (2)	0.023 (2)	0.028 (2)	−0.0032 (17)	−0.0068 (18)	0.0002 (17)
C49	0.0190 (19)	0.0193 (17)	0.0110 (17)	−0.0068 (15)	−0.0015 (14)	−0.0008 (13)
C50	0.029 (2)	0.020 (2)	0.025 (2)	−0.0047 (17)	−0.0074 (17)	−0.0054 (17)
C51	0.027 (2)	0.026 (2)	0.031 (3)	−0.0029 (19)	−0.0128 (19)	−0.0014 (19)
C52	0.029 (2)	0.035 (2)	0.017 (2)	−0.014 (2)	−0.0094 (18)	0.0011 (17)
C53	0.024 (2)	0.026 (2)	0.017 (2)	−0.0141 (19)	0.0009 (17)	−0.0056 (16)
C54	0.019 (2)	0.0191 (17)	0.020 (2)	−0.0105 (16)	−0.0017 (16)	0.0001 (14)
C55	0.0182 (18)	0.0185 (17)	0.0173 (19)	−0.0081 (14)	−0.0023 (14)	−0.0002 (13)
C56	0.022 (2)	0.027 (2)	0.027 (2)	−0.0099 (17)	−0.0006 (17)	−0.0070 (17)
C57	0.026 (2)	0.040 (3)	0.038 (3)	−0.012 (2)	0.006 (2)	−0.013 (2)
C58	0.023 (2)	0.043 (3)	0.041 (3)	−0.017 (2)	0.005 (2)	−0.007 (2)
C59	0.024 (2)	0.034 (2)	0.038 (3)	−0.019 (2)	−0.007 (2)	0.002 (2)
C60	0.028 (2)	0.026 (2)	0.021 (2)	−0.0169 (17)	−0.0042 (16)	0.0003 (16)
Fe2	0.0234 (6)	0.0251 (6)	0.0393 (7)	−0.0018 (4)	−0.0095 (5)	−0.0077 (5)
Cl3	0.0226 (9)	0.0378 (11)	0.0356 (12)	−0.0001 (8)	−0.0087 (8)	−0.0093 (9)
Cl4	0.0709 (17)	0.0271 (10)	0.0283 (11)	−0.0138 (11)	0.0042 (11)	−0.0046 (8)
Cl5	0.0335 (9)	0.0725 (13)	0.0668 (13)	−0.0075 (9)	0.0006 (8)	0.0200 (10)
Cl6	0.0488 (16)	0.090 (2)	0.146 (3)	0.0219 (15)	−0.0621 (19)	−0.077 (2)
Cl7	0.0330 (19)	0.128 (4)	0.070 (3)	−0.006 (2)	−0.0002 (18)	−0.027 (3)
C61	0.0234 (6)	0.0251 (6)	0.0393 (7)	−0.0018 (4)	−0.0095 (5)	−0.0077 (5)
Cl8	0.0335 (9)	0.0725 (13)	0.0668 (13)	−0.0075 (9)	0.0006 (8)	0.0200 (10)
Cl7′	0.0488 (16)	0.090 (2)	0.146 (3)	0.0219 (15)	−0.0621 (19)	−0.077 (2)
C61′	0.0234 (6)	0.0251 (6)	0.0393 (7)	−0.0018 (4)	−0.0095 (5)	−0.0077 (5)
Cl8′	0.0335 (9)	0.0725 (13)	0.0668 (13)	−0.0075 (9)	0.0006 (8)	0.0200 (10)
Cl7"	0.0335 (9)	0.0725 (13)	0.0668 (13)	−0.0075 (9)	0.0006 (8)	0.0200 (10)
C61"	0.0234 (6)	0.0251 (6)	0.0393 (7)	−0.0018 (4)	−0.0095 (5)	−0.0077 (5)
Cl8"	0.0330 (19)	0.128 (4)	0.070 (3)	−0.006 (2)	−0.0002 (18)	−0.027 (3)

Geometric parameters (Å, º)

Fe1—Cl2	2.218 (2)	C30—H30	0.9500
Fe1—Cl1	2.223 (2)	C31—C36	1.376 (11)
Fe1—P3	2.374 (2)	C31—C32	1.410 (10)
Fe1—P2	2.376 (2)	C32—C33	1.377 (11)
Fe1—P4	2.377 (2)	C32—H32	0.9500
Fe1—P1	2.388 (2)	C33—C34	1.396 (12)
P1—C1	1.810 (8)	C33—H33	0.9500
P1—C7	1.827 (8)	C34—C35	1.374 (11)
P1—C13	1.830 (8)	C34—H34	0.9500
P2—C25	1.817 (8)	C35—C36	1.408 (11)
P2—C19	1.819 (8)	C35—H35	0.9500
P2—C6	1.822 (7)	C37—C38	1.393 (11)
P3—C37	1.828 (8)	C37—C42	1.404 (11)
P3—C43	1.830 (8)	C38—C39	1.379 (11)

P3—C31	1.833 (8)	C38—H38	0.9500
P4—C36	1.811 (7)	C39—C40	1.398 (13)
P4—C49	1.834 (8)	C39—H39	0.9500
P4—C55	1.835 (8)	C40—C41	1.387 (12)
C1—C2	1.403 (10)	C40—H40	0.9500
C1—C6	1.410 (11)	C41—C42	1.389 (11)
C2—C3	1.404 (11)	C41—H41	0.9500
C2—H2	0.9500	C42—H42	0.9500
C3—C4	1.373 (12)	C43—C44	1.406 (11)
C3—H3	0.9500	C43—C48	1.411 (12)
C4—C5	1.399 (11)	C44—C45	1.362 (11)
C4—H4	0.9500	C44—H44	0.9500
C5—C6	1.396 (11)	C45—C46	1.415 (13)
C5—H5	0.9500	C45—H45	0.9500
C7—C12	1.387 (11)	C46—C47	1.355 (13)
C7—C8	1.421 (11)	C46—H46	0.9500
C8—C9	1.379 (10)	C47—C48	1.371 (12)
C8—H8	0.9500	C47—H47	0.9500
C9—C10	1.367 (12)	C48—H48	0.9500
C9—H9	0.9500	C49—C50	1.382 (11)
C10—C11	1.379 (12)	C49—C54	1.404 (10)
C10—H10	0.9500	C50—C51	1.398 (12)
C11—C12	1.406 (11)	C50—H50	0.9500
C11—H11	0.9500	C51—C52	1.398 (11)
C12—H12	0.9500	C51—H51	0.9500
C13—C14	1.374 (11)	C52—C53	1.377 (12)
C13—C18	1.392 (12)	C52—H52	0.9500
C14—C15	1.394 (11)	C53—C54	1.395 (11)
C14—H14	0.9500	C53—H53	0.9500
C15—C16	1.352 (13)	C54—H54	0.9500
C15—H15	0.9500	C55—C56	1.388 (11)
C16—C17	1.411 (14)	C55—C60	1.396 (11)
C16—H16	0.9500	C56—C57	1.378 (12)
C17—C18	1.400 (12)	C56—H56	0.9500
C17—H17	0.9500	C57—C58	1.367 (12)
C18—H18	0.9500	C57—H57	0.9500
C19—C24	1.392 (10)	C58—C59	1.394 (13)
C19—C20	1.394 (11)	C58—H58	0.9500
C20—C21	1.365 (12)	C59—C60	1.385 (12)
C20—H20	0.9500	C59—H59	0.9500
C21—C22	1.392 (12)	C60—H60	0.9500
C21—H21	0.9500	Fe2—Cl4	2.184 (2)
C22—C23	1.384 (12)	Fe2—Cl5	2.188 (3)
C22—H22	0.9500	Fe2—Cl3	2.193 (2)
C23—C24	1.385 (11)	Fe2—Cl6	2.197 (3)
C23—H23	0.9500	Cl7—C61	1.799 (11)
C24—H24	0.9500	C61—Cl8	1.682 (10)
C25—C26	1.399 (11)	C61—H61A	0.9900

C25—C30	1.406 (11)	C61—H61B	0.9900
C26—C27	1.397 (12)	Cl7′—C61′	1.77 (2)
C26—H26	0.9500	C61′—Cl8′	1.75 (2)
C27—C28	1.420 (13)	C61′—H61C	0.9900
C27—H27	0.9500	C61′—H61D	0.9900
C28—C29	1.354 (13)	Cl7"—C61"	1.76 (2)
C28—H28	0.9500	C61"—Cl8"	1.73 (2)
C29—C30	1.394 (12)	C61"—H61E	0.9900
C29—H29	0.9500	C61"—H61F	0.9900

Cl2—Fe1—Cl1	179.87 (12)	C27—C28—H28	119.4
Cl2—Fe1—P3	87.69 (8)	C28—C29—C30	120.1 (8)
Cl1—Fe1—P3	92.26 (8)	C28—C29—H29	119.9
Cl2—Fe1—P2	92.82 (8)	C30—C29—H29	119.9
Cl1—Fe1—P2	87.30 (8)	C29—C30—C25	120.7 (8)
P3—Fe1—P2	98.58 (8)	C29—C30—H30	119.7
Cl2—Fe1—P4	87.23 (8)	C25—C30—H30	119.7
Cl1—Fe1—P4	92.65 (8)	C36—C31—C32	121.2 (7)
P3—Fe1—P4	80.75 (8)	C36—C31—P3	117.5 (6)
P2—Fe1—P4	179.33 (10)	C32—C31—P3	121.2 (6)
Cl2—Fe1—P1	92.05 (8)	C33—C32—C31	119.3 (7)
Cl1—Fe1—P1	87.99 (7)	C33—C32—H32	120.4
P3—Fe1—P1	179.74 (10)	C31—C32—H32	120.4
P2—Fe1—P1	81.38 (8)	C32—C33—C34	119.9 (7)
P4—Fe1—P1	99.29 (8)	C32—C33—H33	120.1
C1—P1—C7	100.8 (3)	C34—C33—H33	120.1
C1—P1—C13	103.2 (4)	C35—C34—C33	120.7 (8)
C7—P1—C13	105.0 (4)	C35—C34—H34	119.7
C1—P1—Fe1	107.7 (3)	C33—C34—H34	119.7
C7—P1—Fe1	120.0 (3)	C34—C35—C36	120.3 (8)
C13—P1—Fe1	117.6 (2)	C34—C35—H35	119.9
C25—P2—C19	105.8 (4)	C36—C35—H35	119.9
C25—P2—C6	100.4 (4)	C31—C36—C35	118.7 (7)
C19—P2—C6	102.7 (4)	C31—C36—P4	118.2 (6)
C25—P2—Fe1	120.0 (3)	C35—C36—P4	122.9 (6)
C19—P2—Fe1	117.0 (3)	C38—C37—C42	118.3 (7)
C6—P2—Fe1	108.3 (3)	C38—C37—P3	119.4 (6)
C37—P3—C43	104.8 (4)	C42—C37—P3	122.3 (6)
C37—P3—C31	100.6 (3)	C39—C38—C37	121.6 (8)
C43—P3—C31	103.8 (4)	C39—C38—H38	119.2
C37—P3—Fe1	119.4 (3)	C37—C38—H38	119.2
C43—P3—Fe1	118.2 (2)	C38—C39—C40	119.7 (8)
C31—P3—Fe1	107.7 (3)	C38—C39—H39	120.2
C36—P4—C49	102.8 (4)	C40—C39—H39	120.2
C36—P4—C55	101.4 (4)	C41—C40—C39	119.7 (8)
C49—P4—C55	107.0 (4)	C41—C40—H40	120.1
C36—P4—Fe1	108.0 (3)	C39—C40—H40	120.1
C49—P4—Fe1	116.1 (3)	C40—C41—C42	120.3 (8)

C55—P4—Fe1	119.2 (3)	C40—C41—H41	119.9
C2—C1—C6	119.1 (7)	C42—C41—H41	119.9
C2—C1—P1	122.3 (6)	C41—C42—C37	120.5 (8)
C6—C1—P1	118.5 (6)	C41—C42—H42	119.8
C1—C2—C3	119.3 (7)	C37—C42—H42	119.8
C1—C2—H2	120.3	C44—C43—C48	117.6 (8)
C3—C2—H2	120.3	C44—C43—P3	119.8 (6)
C4—C3—C2	121.2 (7)	C48—C43—P3	122.6 (7)
C4—C3—H3	119.4	C45—C44—C43	122.0 (9)
C2—C3—H3	119.4	C45—C44—H44	119.0
C3—C4—C5	120.3 (8)	C43—C44—H44	119.0
C3—C4—H4	119.8	C44—C45—C46	118.7 (9)
C5—C4—H4	119.8	C44—C45—H45	120.6
C6—C5—C4	119.3 (8)	C46—C45—H45	120.6
C6—C5—H5	120.3	C47—C46—C45	119.9 (8)
C4—C5—H5	120.3	C47—C46—H46	120.0
C5—C6—C1	120.7 (7)	C45—C46—H46	120.0
C5—C6—P2	122.0 (6)	C46—C47—C48	121.8 (9)
C1—C6—P2	117.2 (6)	C46—C47—H47	119.1
C12—C7—C8	118.7 (7)	C48—C47—H47	119.1
C12—C7—P1	123.3 (6)	C47—C48—C43	119.9 (9)
C8—C7—P1	118.1 (6)	C47—C48—H48	120.1
C9—C8—C7	119.9 (8)	C43—C48—H48	120.1
C9—C8—H8	120.0	C50—C49—C54	119.9 (7)
C7—C8—H8	120.0	C50—C49—P4	121.2 (6)
C10—C9—C8	121.1 (8)	C54—C49—P4	118.9 (6)
C10—C9—H9	119.5	C49—C50—C51	120.0 (7)
C8—C9—H9	119.5	C49—C50—H50	120.0
C9—C10—C11	120.0 (8)	C51—C50—H50	120.0
C9—C10—H10	120.0	C50—C51—C52	120.0 (8)
C11—C10—H10	120.0	C50—C51—H51	120.0
C10—C11—C12	120.4 (8)	C52—C51—H51	120.0
C10—C11—H11	119.8	C53—C52—C51	119.8 (8)
C12—C11—H11	119.8	C53—C52—H52	120.1
C7—C12—C11	119.9 (8)	C51—C52—H52	120.1
C7—C12—H12	120.1	C52—C53—C54	120.6 (7)
C11—C12—H12	120.1	C52—C53—H53	119.7
C14—C13—C18	119.0 (8)	C54—C53—H53	119.7
C14—C13—P1	119.4 (7)	C53—C54—C49	119.6 (8)
C18—C13—P1	121.6 (7)	C53—C54—H54	120.2
C13—C14—C15	120.8 (9)	C49—C54—H54	120.2
C13—C14—H14	119.6	C56—C55—C60	118.6 (8)
C15—C14—H14	119.6	C56—C55—P4	122.9 (6)
C16—C15—C14	120.8 (9)	C60—C55—P4	118.4 (6)
C16—C15—H15	119.6	C57—C56—C55	120.7 (8)
C14—C15—H15	119.6	C57—C56—H56	119.6
C15—C16—C17	119.9 (8)	C55—C56—H56	119.6
C15—C16—H16	120.0	C58—C57—C56	121.1 (9)

C17—C16—H16	120.0	C58—C57—H57	119.5
C18—C17—C16	119.0 (9)	C56—C57—H57	119.5
C18—C17—H17	120.5	C57—C58—C59	118.9 (9)
C16—C17—H17	120.5	C57—C58—H58	120.5
C13—C18—C17	120.5 (9)	C59—C58—H58	120.5
C13—C18—H18	119.8	C60—C59—C58	120.6 (8)
C17—C18—H18	119.8	C60—C59—H59	119.7
C24—C19—C20	117.5 (7)	C58—C59—H59	119.7
C24—C19—P2	121.4 (6)	C59—C60—C55	120.0 (8)
C20—C19—P2	121.0 (6)	C59—C60—H60	120.0
C21—C20—C19	121.1 (8)	C55—C60—H60	120.0
C21—C20—H20	119.4	Cl4—Fe2—Cl5	109.67 (12)
C19—C20—H20	119.4	Cl4—Fe2—Cl3	108.95 (10)
C20—C21—C22	121.0 (8)	Cl5—Fe2—Cl3	110.14 (11)
C20—C21—H21	119.5	Cl4—Fe2—Cl6	110.12 (15)
C22—C21—H21	119.5	Cl5—Fe2—Cl6	110.26 (17)
C23—C22—C21	118.8 (8)	Cl3—Fe2—Cl6	107.67 (10)
C23—C22—H22	120.6	Cl8—C61—Cl7	114.4 (6)
C21—C22—H22	120.6	Cl8—C61—H61A	108.7
C22—C23—C24	119.8 (7)	Cl7—C61—H61A	108.7
C22—C23—H23	120.1	Cl8—C61—H61B	108.7
C24—C23—H23	120.1	Cl7—C61—H61B	108.7
C23—C24—C19	121.7 (8)	H61A—C61—H61B	107.6
C23—C24—H24	119.2	Cl8′—C61′—Cl7′	117 (3)
C19—C24—H24	119.2	Cl8′—C61′—H61C	107.9
C26—C25—C30	118.6 (8)	Cl7′—C61′—H61C	107.9
C26—C25—P2	123.1 (6)	Cl8′—C61′—H61D	107.9
C30—C25—P2	118.2 (6)	Cl7′—C61′—H61D	107.9
C27—C26—C25	120.8 (8)	H61C—C61′—H61D	107.2
C27—C26—H26	119.6	Cl8"—C61"—Cl7"	102 (2)
C25—C26—H26	119.6	Cl8"—C61"—H61E	111.3
C26—C27—C28	118.4 (8)	Cl7"—C61"—H61E	111.3
C26—C27—H27	120.8	Cl8"—C61"—H61F	111.3
C28—C27—H27	120.8	Cl7"—C61"—H61F	111.3
C29—C28—C27	121.2 (9)	H61E—C61"—H61F	109.2
C29—C28—H28	119.4		

C7—P1—C1—C2	−37.2 (7)	C37—P3—C31—C36	−145.7 (6)
C13—P1—C1—C2	71.2 (7)	C43—P3—C31—C36	106.0 (7)
Fe1—P1—C1—C2	−163.7 (6)	Fe1—P3—C31—C36	−20.1 (7)
C7—P1—C1—C6	145.8 (6)	C37—P3—C31—C32	38.2 (7)
C13—P1—C1—C6	−105.7 (7)	C43—P3—C31—C32	−70.1 (7)
Fe1—P1—C1—C6	19.3 (7)	Fe1—P3—C31—C32	163.8 (6)
C6—C1—C2—C3	1.5 (12)	C36—C31—C32—C33	0.1 (12)
P1—C1—C2—C3	−175.5 (6)	P3—C31—C32—C33	176.0 (6)
C1—C2—C3—C4	−1.5 (13)	C31—C32—C33—C34	0.0 (13)
C2—C3—C4—C5	0.9 (13)	C32—C33—C34—C35	−0.6 (13)
C3—C4—C5—C6	−0.2 (13)	C33—C34—C35—C36	1.2 (13)

C4—C5—C6—C1	0.2 (12)	C32—C31—C36—C35	0.5 (12)
C4—C5—C6—P2	177.1 (7)	P3—C31—C36—C35	−175.6 (6)
C2—C1—C6—C5	−0.9 (12)	C32—C31—C36—P4	176.2 (6)
P1—C1—C6—C5	176.2 (6)	P3—C31—C36—P4	0.1 (9)
C2—C1—C6—P2	−177.9 (6)	C34—C35—C36—C31	−1.2 (12)
P1—C1—C6—P2	−0.9 (9)	C34—C35—C36—P4	−176.6 (7)
C25—P2—C6—C5	38.1 (8)	C49—P4—C36—C31	−103.3 (7)
C19—P2—C6—C5	−70.8 (7)	C55—P4—C36—C31	146.1 (7)
Fe1—P2—C6—C5	164.8 (6)	Fe1—P4—C36—C31	20.0 (7)
C25—P2—C6—C1	−144.8 (6)	C49—P4—C36—C35	72.2 (7)
C19—P2—C6—C1	106.2 (7)	C55—P4—C36—C35	−38.4 (8)
Fe1—P2—C6—C1	−18.2 (7)	Fe1—P4—C36—C35	−164.6 (6)
C1—P1—C7—C12	128.4 (7)	C43—P3—C37—C38	155.9 (6)
C13—P1—C7—C12	21.4 (8)	C31—P3—C37—C38	48.5 (7)
Fe1—P1—C7—C12	−113.8 (6)	Fe1—P3—C37—C38	−68.9 (7)
C1—P1—C7—C8	−51.5 (7)	C43—P3—C37—C42	−23.3 (8)
C13—P1—C7—C8	−158.6 (6)	C31—P3—C37—C42	−130.7 (7)
Fe1—P1—C7—C8	66.3 (7)	Fe1—P3—C37—C42	111.9 (6)
C12—C7—C8—C9	2.1 (11)	C42—C37—C38—C39	−2.0 (11)
P1—C7—C8—C9	−177.9 (6)	P3—C37—C38—C39	178.8 (6)
C7—C8—C9—C10	−1.2 (12)	C37—C38—C39—C40	0.1 (12)
C8—C9—C10—C11	−0.1 (13)	C38—C39—C40—C41	1.4 (13)
C9—C10—C11—C12	0.6 (13)	C39—C40—C41—C42	−1.0 (13)
C8—C7—C12—C11	−1.6 (12)	C40—C41—C42—C37	−1.0 (13)
P1—C7—C12—C11	178.4 (6)	C38—C37—C42—C41	2.4 (12)
C10—C11—C12—C7	0.3 (13)	P3—C37—C42—C41	−178.3 (6)
C1—P1—C13—C14	−179.5 (6)	C37—P3—C43—C44	77.3 (7)
C7—P1—C13—C14	−74.3 (7)	C31—P3—C43—C44	−177.6 (6)
Fe1—P1—C13—C14	62.2 (7)	Fe1—P3—C43—C44	−58.5 (7)
C1—P1—C13—C18	0.4 (8)	C37—P3—C43—C48	−105.1 (7)
C7—P1—C13—C18	105.7 (7)	C31—P3—C43—C48	−0.1 (8)
Fe1—P1—C13—C18	−117.9 (6)	Fe1—P3—C43—C48	119.0 (6)
C18—C13—C14—C15	0.0 (12)	C48—C43—C44—C45	2.1 (12)
P1—C13—C14—C15	180.0 (6)	P3—C43—C44—C45	179.7 (6)
C13—C14—C15—C16	1.0 (13)	C43—C44—C45—C46	−1.7 (13)
C14—C15—C16—C17	−0.8 (13)	C44—C45—C46—C47	1.3 (13)
C15—C16—C17—C18	−0.4 (13)	C45—C46—C47—C48	−1.4 (14)
C14—C13—C18—C17	−1.2 (13)	C46—C47—C48—C43	1.8 (14)
P1—C13—C18—C17	178.8 (7)	C44—C43—C48—C47	−2.1 (12)
C16—C17—C18—C13	1.4 (13)	P3—C43—C48—C47	−179.7 (7)
C25—P2—C19—C24	66.4 (7)	C36—P4—C49—C50	7.1 (8)
C6—P2—C19—C24	171.3 (6)	C55—P4—C49—C50	113.5 (7)
Fe1—P2—C19—C24	−70.3 (7)	Fe1—P4—C49—C50	−110.5 (7)
C25—P2—C19—C20	−118.1 (7)	C36—P4—C49—C54	−174.0 (6)
C6—P2—C19—C20	−13.3 (8)	C55—P4—C49—C54	−67.6 (7)
Fe1—P2—C19—C20	105.2 (7)	Fe1—P4—C49—C54	68.4 (7)
C24—C19—C20—C21	−1.5 (13)	C54—C49—C50—C51	−0.6 (13)
P2—C19—C20—C21	−177.1 (7)	P4—C49—C50—C51	178.3 (7)

C19—C20—C21—C22	−1.7 (14)	C49—C50—C51—C52	0.7 (14)
C20—C21—C22—C23	2.4 (14)	C50—C51—C52—C53	0.7 (14)
C21—C22—C23—C24	0.0 (12)	C51—C52—C53—C54	−2.3 (13)
C22—C23—C24—C19	−3.3 (12)	C52—C53—C54—C49	2.5 (12)
C20—C19—C24—C23	4.0 (12)	C50—C49—C54—C53	−1.0 (12)
P2—C19—C24—C23	179.6 (6)	P4—C49—C54—C53	−179.9 (6)
C19—P2—C25—C26	−29.2 (8)	C36—P4—C55—C56	139.5 (7)
C6—P2—C25—C26	−135.8 (7)	C49—P4—C55—C56	32.2 (8)
Fe1—P2—C25—C26	105.9 (7)	Fe1—P4—C55—C56	−102.1 (7)
C19—P2—C25—C30	151.7 (7)	C36—P4—C55—C60	−42.9 (7)
C6—P2—C25—C30	45.2 (7)	C49—P4—C55—C60	−150.2 (7)
Fe1—P2—C25—C30	−73.2 (7)	Fe1—P4—C55—C60	75.4 (7)
C30—C25—C26—C27	3.6 (13)	C60—C55—C56—C57	−1.2 (13)
P2—C25—C26—C27	−175.4 (7)	P4—C55—C56—C57	176.3 (7)
C25—C26—C27—C28	−1.8 (14)	C55—C56—C57—C58	0.0 (15)
C26—C27—C28—C29	−1.5 (15)	C56—C57—C58—C59	1.7 (16)
C27—C28—C29—C30	3.0 (16)	C57—C58—C59—C60	−2.2 (15)
C28—C29—C30—C25	−1.1 (14)	C58—C59—C60—C55	1.0 (14)
C26—C25—C30—C29	−2.2 (13)	C56—C55—C60—C59	0.7 (13)
P2—C25—C30—C29	176.9 (7)	P4—C55—C60—C59	−177.0 (7)