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(η^5-Cyclopentadienyl)(η^6-mesitylenyl)-iron(II) hexafluorophosphate chloroform solvate

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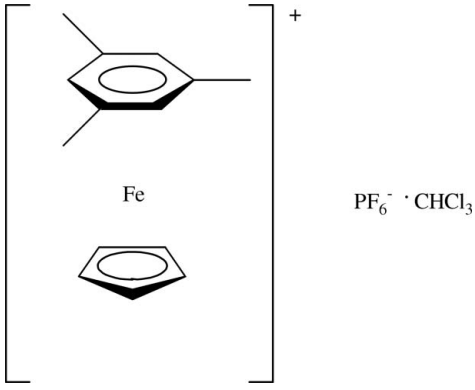
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.036; wR factor = 0.100; data-to-parameter ratio = 11.7.

The title compound, $[Fe(C_5H_5)(C_9H_{12})]PF_6{\cdot}CHCl_3$, crystallizes with $Z' = \frac{1}{3}$. The cation, anion and solvent molecule are all located on special positions with site symmetry 3m. The cyclopentadienyl ring is disordered, due to the symmetry of the special position.



Experimental

Crystal data

$[Fe(C_5H_5)(C_9H_{12})]PF_6{\cdot}CHCl_3$
M_r = 505.46
Hexagonal, $P6_3mc$
a = 9.3640 (11) Å
c = 13.3018 (19) Å
V = 1010.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.27 mm^{-1}
T = 173 (2) K
0.35 × 0.33 × 0.21 mm

Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.664, T_{max} = 0.776
4236 measured reflections
726 independent reflections
711 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.100
S = 1.13
726 reflections
62 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), with 332 Friedel pairs
Flack parameter: 0.02 (5)

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2319).

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supplementary materials

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(η^5-Cyclopentadienyl)(η^6-mesitylenyl)iron(II) hexafluorophosphate chloroform solvate

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Comment

The title compound, $[C_{14}H_{17}Fe]^+PF_6^-\cdot CHCl_3$, crystallizes with Z'=1/3. A l l there molecules are located on a special position with site symmetry 3 m. The cyclopentadienyl ring is disordered due to the symmetry of the special position.

Experimental

Ferrocene (2 g, 10.75 mmol) was dissolved in mesitylene and Al (0.29 g, 10.75 mmol), $AlCl_3$ (5.73 g, 43 mmol) and H_2O (0.22 ml, 10.75 mmol) were added. The crude mixture was heated at 373 K for 8 h followed by aqueous workup. The aqueous phase was treated with an ammonia solution and filtered. NH_4PF_6 was added to precipitate the title compound in 85% as a yellow solid. Single crystals were obtained from slow evaporation of a chloroform solution.

Refinement

H atoms were refined using a riding model with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(C_{methyl})] with C—H ranging from 0.95 Å to 1.00 Å. The cyclopentadienyl ring is disordered due to the symmetry of the special position. Since only nine sites were generated for the five atoms, the occupation factor of each site was set to 5/9 of is usual occupancy.

Figures

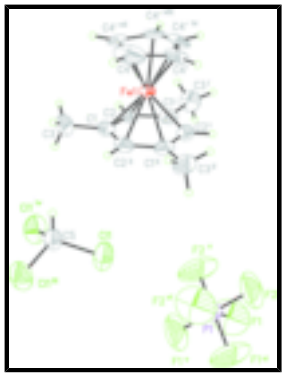


Fig. 1. Perspective view of the title compound with the atom numbering scheme; displacement ellipsoids are at the 50% probability level; H atoms are drawn as small spheres of arbitrary radii. Symmetry operators for generating equivalent atoms: (i) *x*, −*x*, *z*; (ii) −2x, *y*, *z*; (iii) −*y* + 1, *x*-*y* + 1, *z*; (iv) *y*-*x*, −*x* + 1, *z*; (v) −*x* + *y*+1, −*x* + 1, *z*; (vi) −*y* + 1, *x*-*y*, *z*; (vii) *y*-*x*, *y*, *z*; (viii) −*y*, −*x*, *z*; (ix) *y*-*x*, −*x*, *z*.

η^5-Cyclopentadienyl-η^6-mesitylenyl-iron(III) hexafluoridophosphate chloroform solvate

Crystal data

$[Fe(C_5H_5)(C_9H_{12})]PF_6\cdot CHCl_3$ $Z = 2$

M_r = 505.46	F_{000} = 508
Hexagonal, $P6_3mc$	D_x = 1.662 Mg m^{-3}
Hall symbol: P 6c -2c	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.3640 (11) Å	Cell parameters from 4866 reflections
b = 9.3640 (11) Å	θ = 4.1–25.7º
c = 13.3018 (19) Å	μ = 1.27 mm^{-1}
α = 90º	T = 173 (2) K
β = 90º	Block, yellow
γ = 120º	0.35 × 0.33 × 0.21 mm
V = 1010.1 (2) Å^3	

Data collection

Stoe IPDS II two-circle diffractometer	726 independent reflections
Radiation source: fine-focus sealed tube	711 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.023
T = 173(2) K	θ_{max} = 25.6º
ω scans	θ_{min} = 4.0º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −11→11
T_{min} = 0.664, T_{max} = 0.776	k = −11→11
4236 measured reflections	l = −14→16

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2 + 0.3969P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.100	$(\Delta/\sigma)_{max} < 0.001$
S = 1.13	$\Delta\rho_{max}$ = 0.43 e Å^{-3}
726 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
62 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.021 (5)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 332 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (5)

Special details

Experimental.

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}	Occ. (<1)
Fe1	0.0000	0.0000	0.02847 (8)	0.0288 (3)	
C1	−0.0886 (3)	0.0886 (3)	0.1437 (3)	0.0403 (12)	
C2	−0.1726 (6)	−0.0863 (3)	0.1437 (3)	0.0402 (12)	
H2	−0.2897	−0.1449	0.1437	0.048*	
C3	−0.1813 (3)	0.1813 (3)	0.1387 (5)	0.0569 (13)	
H3A	−0.2044	0.2044	0.2052	0.085*	
H3B	−0.1156	0.2831	0.1033	0.085*	
C4	0.0681 (9)	0.1362 (19)	−0.1027 (15)	0.080 (10)	0.56
H4	0.1267	0.2533	−0.1048	0.096*	0.56
C4'	0.1380 (14)	0.0137 (13)	−0.0959 (6)	0.049 (3)	0.56
H4'	0.2481	0.0339	−0.0948	0.059*	0.56
P1	0.6667	0.3333	0.47038 (15)	0.0319 (4)	
F1	0.5906 (3)	0.1813 (7)	0.5415 (6)	0.140 (3)	
F2	0.7417 (3)	0.2583 (3)	0.3980 (5)	0.138 (2)	
C5	0.3333	0.6667	0.2813 (8)	0.0444 (17)	
H5	0.3333	0.6667	0.2061	0.053*	
Cl1	0.43613 (9)	0.56387 (9)	0.32191 (18)	0.0737 (5)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0348 (4)	0.0348 (4)	0.0170 (5)	0.01738 (19)	0.000	0.000
C1	0.052 (2)	0.052 (2)	0.025 (2)	0.031 (2)	0.0023 (9)	−0.0023 (9)
C2	0.039 (3)	0.050 (2)	0.027 (2)	0.0196 (13)	0.0036 (18)	0.0018 (9)
C3	0.062 (3)	0.062 (3)	0.060 (3)	0.042 (3)	0.0068 (12)	−0.0068 (12)
C4	0.14 (2)	0.042 (7)	0.029 (7)	0.021 (3)	0.006 (3)	0.011 (5)
C4'	0.051 (5)	0.071 (7)	0.018 (3)	0.024 (5)	0.012 (3)	−0.009 (4)
P1	0.0294 (5)	0.0294 (5)	0.0369 (9)	0.0147 (3)	0.000	0.000
F1	0.187 (6)	0.067 (3)	0.126 (5)	0.0334 (15)	0.0249 (18)	0.050 (4)
F2	0.187 (5)	0.187 (5)	0.119 (5)	0.154 (6)	0.0232 (14)	−0.0232 (14)
C5	0.039 (2)	0.039 (2)	0.055 (4)	0.0194 (12)	0.000	0.000
Cl1	0.0620 (7)	0.0620 (7)	0.1108 (13)	0.0411 (7)	−0.0044 (4)	0.0044 (4)

Geometric parameters (Å, °)

Fe1—C4'	2.063 (9)	C3—H3A	0.9600
Fe1—C4'^{i}	2.063 (9)	C3—H3B	0.9608

Fe1—C4'^{ii}	2.063 (9)	C4—C4'^{i}	1.583 (9)
Fe1—C4'^{iii}	2.063 (9)	C4—C4'	1.583 (9)
Fe1—C4'^{iv}	2.063 (9)	C4—H4	0.9501
Fe1—C4'^{v}	2.063 (9)	C4'—C4'^{iv}	1.42 (2)
Fe1—C4^{iii}	2.065 (19)	C4'—H4'	0.9500
Fe1—C4	2.065 (19)	P1—F2^{vi}	1.552 (5)
Fe1—C4^{v}	2.065 (19)	P1—F2	1.552 (5)
Fe1—C2^{iii}	2.076 (5)	P1—F2^{vii}	1.552 (5)
Fe1—C2	2.076 (5)	P1—F1^{vii}	1.554 (5)
Fe1—C2^{v}	2.076 (5)	P1—F1^{vi}	1.554 (5)
C1—C2	1.419 (4)	P1—F1	1.554 (5)
C1—C2^{iii}	1.419 (4)	C5—Cl1^{viii}	1.753 (4)
C1—C3	1.505 (7)	C5—Cl1^{ix}	1.753 (4)
C2—C1^{v}	1.419 (4)	C5—Cl1	1.753 (4)
C2—H2	0.9500	C5—H5	1.0000
C4'—Fe1—C2^{iii}	123.8 (3)	Fe1—C2—H2	132.4
C4'^{i}—Fe1—C2^{iii}	123.8 (3)	C1—C3—H3A	110.5
C4'^{ii}—Fe1—C2^{iii}	105.2 (3)	C1—C3—H3B	109.0
C4'^{iii}—Fe1—C2^{iii}	163.3 (3)	H3A—C3—H3B	109.4
C4'^{iv}—Fe1—C2^{iii}	163.3 (3)	C4'^{ii}—C4—C4'^{i}	132 (2)
C4'^{v}—Fe1—C2^{iii}	105.2 (3)	C4'^{v}—C4—C4'	132 (2)
C4^{iii}—Fe1—C2^{iii}	143.54 (12)	C4'^{i}—C4—C4'	101.8 (13)
C4—Fe1—C2^{iii}	105.3 (5)	C4'^{v}—C4—C4^{iii}	112.1 (18)
C4^{v}—Fe1—C2^{iii}	143.54 (12)	C4'^{ii}—C4—C4^{v}	112.1 (18)
C4'—Fe1—C2	163.3 (3)	C4'^{ii}—C4—H4	97.8
C4'^{i}—Fe1—C2	105.2 (3)	C4'^{v}—C4—H4	97.8
C4'^{ii}—Fe1—C2	163.3 (3)	C4'^{i}—C4—H4	129.0
C4'^{iii}—Fe1—C2	105.2 (3)	C4'—C4—H4	129.0
C4'^{iv}—Fe1—C2	123.8 (3)	Fe1—C4—H4	124.0
C4'^{v}—Fe1—C2	123.8 (3)	C4^{iii}—C4'—C4'^{ii}	127.3 (18)
C4^{iii}—Fe1—C2	143.54 (12)	C4'^{ii}—C4'—C4'^{iv}	119.998 (3)
C4—Fe1—C2	143.54 (12)	C4^{iii}—C4'—C4	106 (2)
C4^{v}—Fe1—C2	105.3 (5)	C4^{iii}—C4'—H4'	122.1
C2^{iii}—Fe1—C2	71.5 (2)	C4'^{ii}—C4'—H4'	110.1
C4'—Fe1—C2^{v}	105.2 (3)	Fe1—C4'—H4'	125.7
C4'^{i}—Fe1—C2^{v}	163.3 (3)	F2^{vi}—P1—F2	85.5 (4)
C4'^{ii}—Fe1—C2^{v}	123.8 (3)	F2^{vi}—P1—F2^{vii}	85.5 (4)
C4'^{iii}—Fe1—C2^{v}	123.8 (3)	F2—P1—F2^{vii}	85.5 (4)
C4'^{iv}—Fe1—C2^{v}	105.2 (3)	F2^{vi}—P1—F1^{vii}	179.2 (4)
C4'^{v}—Fe1—C2^{v}	163.3 (3)	F2—P1—F1^{vii}	93.8 (3)
C4^{iii}—Fe1—C2^{v}	105.3 (5)	F2^{vii}—P1—F1^{vii}	93.8 (3)

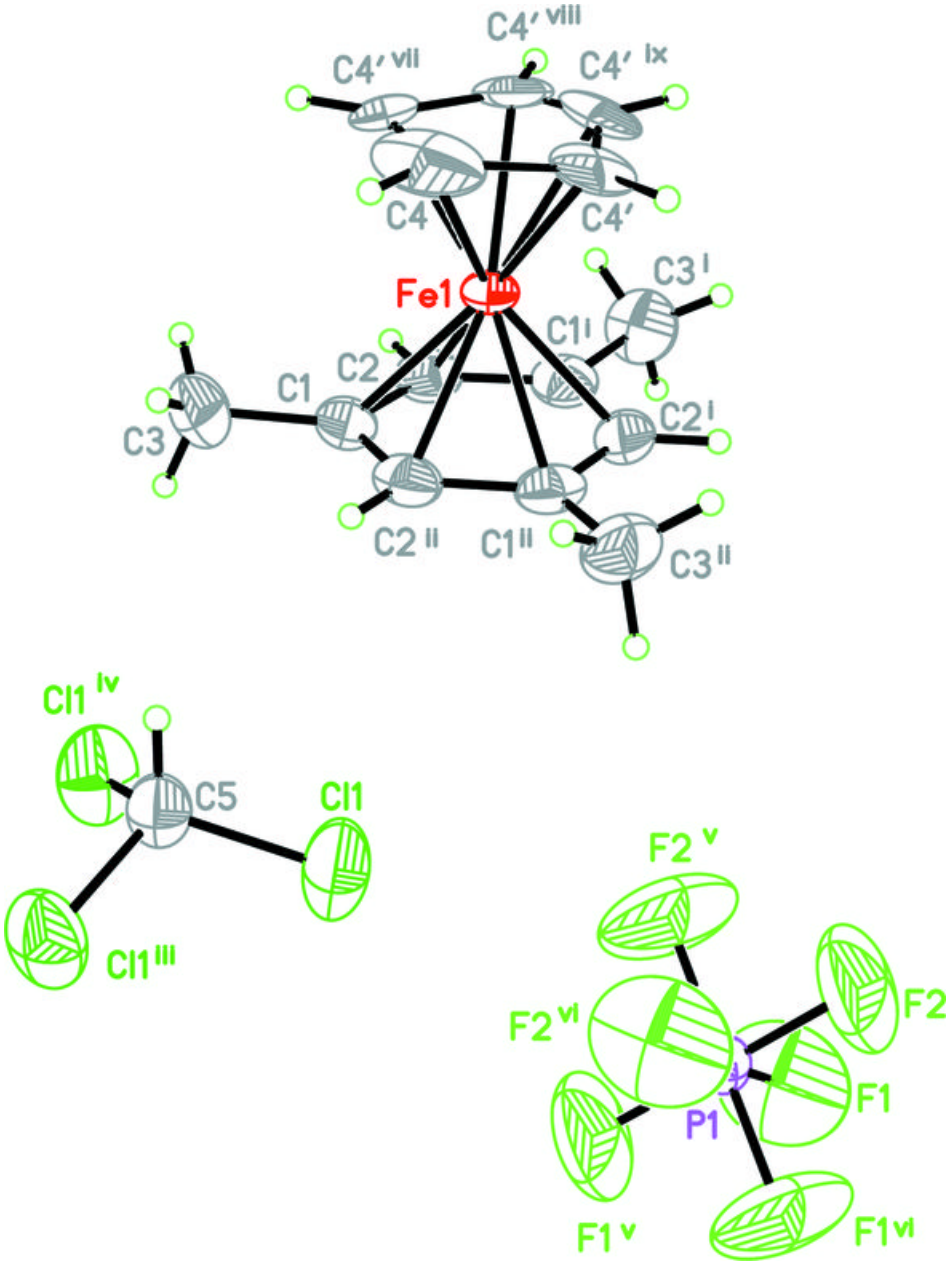
C4—Fe1—C2^{v}	143.54 (12)	F2^{vi}—P1—F1^{vi}	93.8 (3)
C4^{v}—Fe1—C2^{v}	143.54 (12)	F2—P1—F1^{vi}	179.2 (4)
C2^{iii}—Fe1—C2^{v}	71.5 (2)	F2^{vii}—P1—F1^{vi}	93.8 (3)
C2—Fe1—C2^{v}	71.5 (2)	F1^{vii}—P1—F1^{vi}	86.8 (4)
C2—C1—C2^{iii}	117.4 (4)	F2^{vi}—P1—F1	93.8 (3)
C2—C1—C3	121.3 (2)	F2—P1—F1	93.8 (3)
C2^{iii}—C1—C3	121.3 (2)	F2^{vii}—P1—F1	179.2 (5)
C2—C1—Fe1	69.2 (2)	F1^{vii}—P1—F1	86.8 (4)
C2^{iii}—C1—Fe1	69.2 (2)	F1^{vi}—P1—F1	86.8 (4)
C3—C1—Fe1	130.7 (4)	Cl1^{viii}—C5—Cl1^{ix}	110.9 (3)
C1^{v}—C2—C1	122.6 (4)	Cl1^{viii}—C5—Cl1	110.9 (3)
C1^{v}—C2—Fe1	71.1 (2)	Cl1^{ix}—C5—Cl1	110.9 (3)
C1—C2—Fe1	71.1 (2)	Cl1^{viii}—C5—H5	108.0
C1^{v}—C2—H2	118.7	Cl1^{ix}—C5—H5	108.0
C1—C2—H2	118.7	Cl1—C5—H5	108.0
C4'—Fe1—C1—C2	174.8 (8)	C4'^{i}—Fe1—C4—C4'	−114.4 (12)
C4'^{i}—Fe1—C1—C2	99.0 (3)	C4'^{ii}—Fe1—C4—C4'	30.1 (14)
C4'^{ii}—Fe1—C1—C2	163.4 (4)	C4'^{iii}—Fe1—C4—C4'	−73.0 (7)
C4'^{iii}—Fe1—C1—C2	64.5 (4)	C4'^{iv}—Fe1—C4—C4'	−41.4 (6)
C4'^{iv}—Fe1—C1—C2	53.0 (8)	C4'^{v}—Fe1—C4—C4'	−145 (2)
C4'^{v}—Fe1—C1—C2	128.8 (4)	C4^{iii}—Fe1—C4—C4'	−22.9 (7)
C4^{iii}—Fe1—C1—C2	113.9 (2)	C4^{v}—Fe1—C4—C4'	−91.6 (5)
C4—Fe1—C1—C2	144.9 (4)	C2^{iii}—Fe1—C4—C4'	122.8 (6)
C4^{v}—Fe1—C1—C2	83.0 (4)	C2—Fe1—C4—C4'	−157.9 (5)
C2^{iii}—Fe1—C1—C2	−132.1 (4)	C2^{v}—Fe1—C4—C4'	43.5 (11)
C2^{v}—Fe1—C1—C2	−66.1 (2)	C4'—Fe1—C4—C4^{iii}	22.9 (7)
C4'—Fe1—C1—C2^{iii}	−53.0 (8)	C4'^{i}—Fe1—C4—C4^{iii}	−91.6 (5)
C4'^{i}—Fe1—C1—C2^{iii}	−128.8 (4)	C4'^{ii}—Fe1—C4—C4^{iii}	53 (2)
C4'^{ii}—Fe1—C1—C2^{iii}	−64.5 (4)	C4'^{iii}—Fe1—C4—C4^{iii}	−50.2 (3)
C4'^{iii}—Fe1—C1—C2^{iii}	−163.4 (4)	C4'^{iv}—Fe1—C4—C4^{iii}	−18.5 (4)
C4'^{iv}—Fe1—C1—C2^{iii}	−174.8 (8)	C4'^{v}—Fe1—C4—C4^{iii}	−121.7 (17)
C4'^{v}—Fe1—C1—C2^{iii}	−99.0 (3)	C4^{v}—Fe1—C4—C4^{iii}	−68.7 (3)
C4^{iii}—Fe1—C1—C2^{iii}	−113.9 (2)	C2^{iii}—Fe1—C4—C4^{iii}	145.65 (14)
C4—Fe1—C1—C2^{iii}	−83.0 (4)	C2—Fe1—C4—C4^{iii}	−135.0 (8)
C4^{v}—Fe1—C1—C2^{iii}	−144.9 (4)	C2^{v}—Fe1—C4—C4^{iii}	66.3 (5)
C2—Fe1—C1—C2^{iii}	132.1 (4)	C4'—Fe1—C4—C4^{v}	91.6 (5)
C2^{v}—Fe1—C1—C2^{iii}	66.1 (2)	C4'^{i}—Fe1—C4—C4^{v}	−22.9 (7)
C4'—Fe1—C1—C3	60.9 (8)	C4'^{ii}—Fe1—C4—C4^{v}	121.7 (17)
C4'^{i}—Fe1—C1—C3	−14.9 (3)	C4'^{iii}—Fe1—C4—C4^{v}	18.5 (4)
C4'^{ii}—Fe1—C1—C3	49.5 (4)	C4'^{iv}—Fe1—C4—C4^{v}	50.2 (3)
C4'^{iii}—Fe1—C1—C3	−49.5 (4)	C4'^{v}—Fe1—C4—C4^{v}	−53 (2)

C4$'^{iv}$—Fe1—C1—C3	−60.9 (8)	C4^{iii}—Fe1—C4—C4^{v}	68.7 (3)
C4$'^{v}$—Fe1—C1—C3	14.9 (3)	C2^{iii}—Fe1—C4—C4^{v}	−145.65 (14)
C4^{iii}—Fe1—C1—C3	−0.002 (2)	C2—Fe1—C4—C4^{v}	−66.3 (5)
C4—Fe1—C1—C3	30.9 (3)	C2^{v}—Fe1—C4—C4^{v}	135.0 (8)
C4^{v}—Fe1—C1—C3	−30.9 (3)	C4$'^{ii}$—C4—C4'—C4^{iii}	180.003 (2)
C2^{iii}—Fe1—C1—C3	113.9 (2)	C4$'^{v}$—C4—C4'—C4^{iii}	21 (6)
C2—Fe1—C1—C3	−113.9 (2)	C4$'^{i}$—C4—C4'—C4^{iii}	13 (4)
C2^{v}—Fe1—C1—C3	180.0	C4^{v}—C4—C4'—C4^{iii}	8(2)
C2^{iii}—C1—C2—C1^{v}	−0.1 (7)	Fe1—C4—C4'—C4^{iii}	72 (3)
C3—C1—C2—C1^{v}	177.0 (4)	C4$'^{v}$—C4—C4'—C4$'^{ii}$	−159 (6)
Fe1—C1—C2—C1^{v}	51.3 (4)	C4$'^{i}$—C4—C4'—C4$'^{ii}$	−167 (4)
C2^{iii}—C1—C2—Fe1	−51.3 (4)	C4^{iii}—C4—C4'—C4$'^{ii}$	179.997 (2)
C3—C1—C2—Fe1	125.8 (4)	C4^{v}—C4—C4'—C4$'^{ii}$	−172 (2)
C4'—Fe1—C2—C1^{v}	51.1 (11)	Fe1—C4—C4'—C4$'^{ii}$	−108 (3)
C4$'^{i}$—Fe1—C2—C1^{v}	132.9 (3)	C4$'^{ii}$—C4—C4'—C4$'^{iv}$	172 (2)
C4$'^{ii}$—Fe1—C2—C1^{v}	172.9 (11)	C4$'^{v}$—C4—C4'—C4$'^{iv}$	13 (4)
C4$'^{iii}$—Fe1—C2—C1^{v}	91.1 (4)	C4$'^{i}$—C4—C4'—C4$'^{iv}$	4.6 (13)
C4$'^{iv}$—Fe1—C2—C1^{v}	66.2 (4)	C4^{iii}—C4—C4'—C4$'^{iv}$	−8(2)
C4$'^{v}$—Fe1—C2—C1^{v}	157.7 (4)	C4^{v}—C4—C4'—C4$'^{iv}$	0.0
C4^{iii}—Fe1—C2—C1^{v}	60.8 (8)	Fe1—C4—C4'—C4$'^{iv}$	63.7 (3)
C4—Fe1—C2—C1^{v}	163.2 (8)	C4$'^{ii}$—C4—C4'—Fe1	108 (3)
C4^{v}—Fe1—C2—C1^{v}	112.0 (2)	C4$'^{v}$—C4—C4'—Fe1	−50 (4)
C2^{iii}—Fe1—C2—C1^{v}	−106.02 (18)	C4$'^{i}$—C4—C4'—Fe1	−59.2 (10)
C2^{v}—Fe1—C2—C1^{v}	−30.0 (2)	C4^{iii}—C4—C4'—Fe1	−72 (3)
C4'—Fe1—C2—C1	−172.9 (11)	C4^{v}—C4—C4'—Fe1	−63.7 (3)
C4$'^{i}$—Fe1—C2—C1	−91.1 (4)	C4$'^{i}$—Fe1—C4'—C4^{iii}	−70 (2)
C4$'^{ii}$—Fe1—C2—C1	−51.1 (11)	C4$'^{ii}$—Fe1—C4'—C4^{iii}	−133.0 (19)
C4$'^{iii}$—Fe1—C2—C1	−132.9 (3)	C4$'^{iii}$—Fe1—C4'—C4^{iii}	−27.6 (18)
C4$'^{iv}$—Fe1—C2—C1	−157.7 (4)	C4$'^{iv}$—Fe1—C4'—C4^{iii}	−3(2)
C4$'^{v}$—Fe1—C2—C1	−66.2 (4)	C4$'^{v}$—Fe1—C4'—C4^{iii}	−99.1 (17)
C4^{iii}—Fe1—C2—C1	−163.2 (8)	C4—Fe1—C4'—C4^{iii}	−112 (2)
C4—Fe1—C2—C1	−60.8 (8)	C4^{v}—Fe1—C4'—C4^{iii}	−49.2 (17)
C4^{v}—Fe1—C2—C1	−112.0 (2)	C2^{iii}—Fe1—C4'—C4^{iii}	170.5 (17)
C2^{iii}—Fe1—C2—C1	30.0 (2)	C2—Fe1—C4'—C4^{iii}	17 (3)
C2^{v}—Fe1—C2—C1	106.02 (18)	C2^{v}—Fe1—C4'—C4^{iii}	92.9 (19)
C4'—Fe1—C4—C4$'^{ii}$	−30.1 (14)	C4$'^{i}$—Fe1—C4'—C4$'^{ii}$	63.21 (18)
C4$'^{i}$—Fe1—C4—C4$'^{ii}$	−145 (2)	C4$'^{iii}$—Fe1—C4'—C4$'^{ii}$	105.4 (4)
C4$'^{iii}$—Fe1—C4—C4$'^{ii}$	−103 (2)	C4$'^{iv}$—Fe1—C4'—C4$'^{ii}$	130.19 (16)
C4$'^{iv}$—Fe1—C4—C4$'^{ii}$	−71.6 (16)	C4$'^{v}$—Fe1—C4'—C4$'^{ii}$	33.9 (4)
C4$'^{v}$—Fe1—C4—C4$'^{ii}$	−175 (4)	C4^{iii}—Fe1—C4'—C4$'^{ii}$	133.0 (19)
C4^{iii}—Fe1—C4—C4$'^{ii}$	−53 (2)	C4—Fe1—C4'—C4$'^{ii}$	20.8 (7)

C4^{v}—Fe1—C4—C4'^{ii}	−121.7 (17)	C4^{v}—Fe1—C4'—C4'^{ii}	83.7 (2)
C2^{iii}—Fe1—C4—C4'^{ii}	92.6 (19)	C2^{iii}—Fe1—C4'—C4'^{ii}	−56.5 (2)
C2—Fe1—C4—C4'^{ii}	171.9 (13)	C2—Fe1—C4'—C4'^{ii}	149.8 (11)
C2^{v}—Fe1—C4—C4'^{ii}	13 (2)	C2^{v}—Fe1—C4'—C4'^{ii}	−134.09 (14)
C4'—Fe1—C4—C4'^{v}	145 (2)	C4'^{i}—Fe1—C4'—C4'^{iv}	−66.98 (19)
C4'^{i}—Fe1—C4—C4'^{v}	30.1 (14)	C4'^{ii}—Fe1—C4'—C4'^{iv}	−130.19 (16)
C4'^{ii}—Fe1—C4—C4'^{v}	175 (4)	C4'^{iii}—Fe1—C4'—C4'^{iv}	−24.8 (4)
C4'^{iii}—Fe1—C4—C4'^{v}	71.6 (16)	C4'^{v}—Fe1—C4'—C4'^{iv}	−96.3 (5)
C4'^{iv}—Fe1—C4—C4'^{v}	103 (2)	C4^{iii}—Fe1—C4'—C4'^{iv}	3(2)
C4^{iii}—Fe1—C4—C4'^{v}	121.7 (17)	C4—Fe1—C4'—C4'^{iv}	−109.3 (6)
C4^{v}—Fe1—C4—C4'^{v}	53 (2)	C4^{v}—Fe1—C4'—C4'^{iv}	−46.4 (3)
C2^{iii}—Fe1—C4—C4'^{v}	−92.6 (19)	C2^{iii}—Fe1—C4'—C4'^{iv}	173.3 (3)
C2—Fe1—C4—C4'^{v}	−13 (2)	C2—Fe1—C4'—C4'^{iv}	19.7 (10)
C2^{v}—Fe1—C4—C4'^{v}	−171.9 (13)	C2^{v}—Fe1—C4'—C4'^{iv}	95.72 (14)
C4'—Fe1—C4—C4'^{i}	114.4 (12)	C4'^{i}—Fe1—C4'—C4	42.4 (7)
C4'^{ii}—Fe1—C4—C4'^{i}	145 (2)	C4'^{ii}—Fe1—C4'—C4	−20.8 (7)
C4'^{iii}—Fe1—C4—C4'^{i}	41.4 (6)	C4'^{iii}—Fe1—C4'—C4	84.6 (7)
C4'^{iv}—Fe1—C4—C4'^{i}	73.0 (7)	C4'^{iv}—Fe1—C4'—C4	109.3 (6)
C4'^{v}—Fe1—C4—C4'^{i}	−30.1 (14)	C4'^{v}—Fe1—C4'—C4	13.0 (8)
C4^{iii}—Fe1—C4—C4'^{i}	91.6 (5)	C4^{iii}—Fe1—C4'—C4	112 (2)
C4^{v}—Fe1—C4—C4'^{i}	22.9 (7)	C4^{v}—Fe1—C4'—C4	62.9 (8)
C2^{iii}—Fe1—C4—C4'^{i}	−122.8 (6)	C2^{iii}—Fe1—C4'—C4	−77.3 (8)
C2—Fe1—C4—C4'^{i}	−43.5 (11)	C2—Fe1—C4'—C4	129.0 (8)
C2^{v}—Fe1—C4—C4'^{i}	157.9 (5)	C2^{v}—Fe1—C4'—C4	−154.9 (6)

Symmetry codes: (i) −*x*+*y*, *y*, *z*; (ii) *x*, *x*−*y*, *z*; (iii) −*x*+*y*, −*x*, *z*; (iv) −*y*, −*x*, *z*; (v) −*y*, *x*−*y*, *z*; (vi) −*x*+*y*+1, −*x*+1, *z*; (vii) −*y*+1, *x*−*y*, *z*; (viii) −*x*+*y*, −*x*+1, *z*; (ix) −*y*+1, *x*−*y*+1, *z*.

Fig. 1


C4′viii
C4′vii
C4′ix
C4
C4′
Fe1
C3i
C1i
C2
C1
C2i
C3
C2ii
C1ii
C3ii
Cl1iv
C5
Cl1
Cl1iii
F2v
F2vi
F2
F1
P1
F1v
F1vi