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N-Ferrocenylmethyl-2-(3-methylstyryl)-*N*′-methylbenzimidazolium hexafluorophosphate

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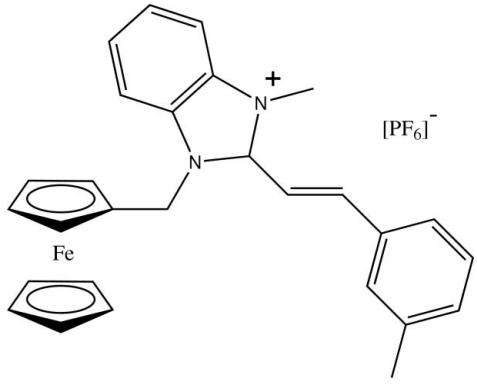
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.047; wR factor = 0.113; data-to-parameter ratio = 12.6.

In the title compound, $[Fe(C_5H_5)(C_{23}H_{22}N_2)]PF_6$, the F atoms of the $[PF_6]^-$ anion are disordered over four different orientations with equal occupancies. In the cation, the five-membered imidazolium ring forms dihedral angles of 71.48 (10) and 19.83 (10)° with the substituted C_5H_4 ring and the benzene ring of the styryl group, respectively. In the crystal structure, there is a significant C—H$\cdots\pi(\eta^5$-$C_5H_4)$ interaction.

Related literature

For related ferrocene literature, see: Benito *et al.* (1995); Li *et al.* (1998); Gallagher, Hanlon & Howarth (2001); Gallagher, Hanlon, Howarth & Thomas (2001); Howarth & Hanlon, (2001). For the chemical synthesis and crystal structure of $[FcCH_2N(CH_3)_3]^+[I]^-$, see: Pauson *et al.* (1966); Ferguson *et al.* (1994).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{23}H_{22}N_2)]PF_6$
M_r = 592.34
Monoclinic, $P2_1/a$
a = 13.5150 (10) Å
b = 12.8743 (10) Å
c = 15.2839 (9) Å
β = 94.037 (5)°
V = 2652.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.69 mm^{-1}
T = 294 (1) K
0.29 × 0.25 × 0.17 mm

Data collection

Bruker P4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.826, T_{max} = 0.889
8107 measured reflections
6387 independent reflections
3922 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
3 standard reflections
every 197 reflections
intensity decay: 0.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.113
S = 1.01
6387 reflections
507 parameters
228 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

*Cg*1 is the centroid of the C_5H_4 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C34—H34$\cdots Cg1^{i}$	0.93	2.65	3.472 (3)	149

Symmetry code: (i) $x-\frac{3}{2}, -y+\frac{3}{2}, z$.

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PREP8* (Ferguson, 1998).

JFG thanks Dublin City University for the purchase of a Bruker P4 diffractometer in 1998.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2519).

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supplementary materials

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N-Ferrocenylmethyl-2-(3-methylstyryl)-*N*'-methylbenzimidazolium hexafluorophosphate

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Comment

Benzimidazole systems have attracted considerable attention in synthetic and structural as well as in applied biological research (Gallagher, Hanlon & Howarth, 2001; Howarth & Hanlon, 2001; Gallagher, Hanlon, Howarth & Thomas, 2001). The title compound (Figures 1–3) was obtained from a series of reactions involving synthesis of the parent *N*-Ferrocenylmethyl-2-(3-methylstyryl)benzimidazole from 2-(3-methylstyryl)benzimidazole and (trimethylammonium)ferrocenylmethyl iodide: subsequent treatment of the product with methyl iodide and replacement of the iodo salt with the hexafluorophosphate anion yields the $[PF_6]^-$ salt.

Bond lengths and angles are normal and similar to those reported in the literature (Gallagher, Hanlon & Howarth, 2001; Gallagher, Hanlon, Howarth & Thomas, 2001). There is no disorder in the cation although the unsubstituted C_5H_5 ring displays large displacement parameters as could be expected given the geometry and the low energy barrier to rotation for Fe···η^5-C_5H_5 π-bonding. The $[PF_6]^-$ anion is disordered and a discussion of the treatment of this disorder is detailed below. The C_3N_2 5-membered imidazolium ring is almost orthogonal to the substituted C_5H_4 ring at 71.48 (10)° and deviates from co-planarity with the aromatic styryl C_6 ring by 19.83 (10)°: the latter C_6 ring is oriented at an angle of 85.52 (9)° to the C_5H_4 ring.

In the crystal structure there is only one intermolecular interaction of note (as detailed in Table 1) and involving C34—H34···*Cg*1^{i} (where *Cg*1 is the ring centroid of C_5H_4 and the symmetry operation i = $x-3/2,3/2-y,z$). Several C—H···F contacts involving the disordered $[PF_6]^-$ are present but are not important as they are relatively weak and involve the partial occupancy F atom sites.

Related structures include *N*-ferrocenylmethyl-2-ferrocenylbenzimidazole (Benito *et al.*, 1995) and the salt *N*-ferrocenylmethyl-2-ferrocenyl-benzimidazolium tetrafluoroborate (Li *et al.*, 1998) which differ from the title compound by having a ferrocenyl moiety at the 2-position of the benzimidazolium ring instead of the 3-methylstyryl group.

Experimental

Synthesis of the neutral starting material *N*-Ferrocenylmethyl-2-(3-methylstyryl)benzimidazole $[(C_5H_5)Fe(C_5H_4)CH_2(C_7H_4N_2)CH{=}CHC_6H_4CH_3]$

To a mixture of 2-(3-methylstyryl)benzimidazole (1.9 g, 8 mmol) and K_2CO_3 (1.66 g, 12 mmol) in CH_3CN (100 ml) was added (trimethylammonium)ferrocenylmethyl iodide ($[FcCH_2N(CH_3)_3]^+[I]^-$) (3.09 g, 8 mmol) (Pauson *et al.*, 1966; Ferguson *et al.*, 1994) and the mixture was heated to reflux temperatures for 10 h. The reaction was cooled to room temperature, water was added and the suspension extracted into $CHCl_3$. The organic layer was washed with water, dried $MgSO_4$

and evaporated under vacuum to leave a brown semi-solid. The crude product was purified by column chromatography on silica gel using CH_2Cl_2:CH_3OH (97:3) as eluent.

Yield 2.6 g (74%), m.p. 429–433 K (uncorrected). Compound (I) was obtained as a light orange solid. IR (KBr, ν cm^{-1}) (>1500 cm^{-1}): 3062, 2982, 2925, 2685, 2308, 1713, 1632 1604, 1581. ^{1}H NMR [400 MHz, δH (p.p.m.), $CDCl_3$], 7.90 (d, 1H, CH=CH, J=15.6 Hz), 7.69 (m, 1H, benz-H), 7.33 (m, 3H, benz-H + aryl-H), 7.19 (m, 3H, aryl-H + benz H), 7.10 (m, 2H, CH=CH + aryl-H), 5.06 (s, 2H, Fc—CH_2), 4.16 (m, 2H, cpd-H), 4.07 (m, 7H, cpd-H), 2.32 (s, 3H, CH_3). ^{13}C NMR [δC, $CDCl_3$], 150.93, 143.48, 138.94, 137.71, 136.47, 135.63, 130.35, 129.23, 128.43, 124.74, 123.0, 122.91, 119.78, 113.56, 109.96, 83.96, 69.24, 68.89, 68.84, 43.32, 21.92.

Synthesis of the *N*-Ferrocenylmethyl-2-(3-methylstyryl)-*N*'-methylbenzimidazolium iodide and hexafluorophosphate salts, $[(C_5H_5)Fe(C_5H_4)CH_2(C_7H_4N_2CH_3)CH{=}CHC_6H_4CH_3]^+$ $[I]^-$ and $[PF_6]^-$ salts.

N-Ferrocenylmethyl-2-(3-methylstyryl)benzimidazole (1.3 g, 3 mmol) was heated to reflux in excess methyl iodide (7 ml) for 2 h. The resultant orange precipitate was filtered and washed several times with ether to provide the iodo salt.

Yield 1.46 g (85 mmol) (74%), m.p. 492–495 K (uncorrected). IR (KBr, ν cm^{-1}) (>1500 cm^{-1}): 3062, 2994, 1649, 1637.

^{1}H NMR [400 MHz, δH (p.p.m.), $CDCl_3$], 8.24 (m, 1H, benz-H), 8.06 (m, 1H, benz-H), 7.82 (m, 2H, Aryl-H), 7.78 (m, 2H, CH=CH), 7.72 (m, 2H, Benz-H), 7.50 (t, 1H, aryl-H, J=7.6 Hz), 7.39 (d, 1H, Aryl-H, J=7.6 Hz), 5.74 (s, 2H, Fc—CH_2), 4.36 (m, 2H, cpd-H), 4.28 (s, 5H, cpd-H), 4.12 (s, 5H, cpd-H + N—CH_3), 2.32 (s, 3H, CH_3). ^{13}C NMR [δC, $CDCl_3$], 150.93, 143.48, 138.94, 137.71, 136.47, 135.63, 130.35, 129.23, 128.43, 124.74, 123.0, 122.91, 119.78, 113.56, 109.96, 83.96, 69.24, 68.89, 68.84, 43.32, 21.92.

The $[PF_6]^-$ salt was obtained by stirring the iodide derivative (from above) (0.4 g, 0.7 mmol) and ammonium hexafluorophosphate (0.12 g, 0.7 mmol) in methanol (50 ml) at room temperature for 24 h. The resultant orange-red precipitate was filtered and washed several times with methanol.

Yield 0.35 g (85%), m.p. 442–445 K (uncorrected). IR (KBr, ν cm^{-1}) (>1500 cm^{-1}): 3062, 2994, 1648, 1639.

^{1}H NMR [400 MHz, δH (p.p.m.), $CDCl_3$], 8.22 (m, 1H, benz-H), 8.06 (m, 1H, benz-H), 7.80 (m, 2H, Aryl-H), 7.76–7.73 (m, 2H, CH=CH), 7.71 (m, 2H, Benz-H), 7.49 (t, 1H, aryl-H, J=7.6 Hz), 7.39 (d, 1H, Aryl-H, J=7.6 Hz), 5.71 (s, 2H, Fc—CH_2), 4.35 (m, 2H, cpd-H), 4.28 (s, 5H, cpd-H), 4.14 (s, 5H, cpd-H + N—CH_3), 2.43 (s, 3H, CH_3). ^{13}C NMR [δC, $CDCl_3$], 148.09, 147.07, 138.89, 134.61, 132.62, 132.28, 130.78, 129.45, 126.96, 125.99, 113.65, 113.57, 108.39, 81.27, 69.32, 68.93, 44.95, 33.81, 21.30.

Analysis for $C_{28}H_{27}N_2FePF_6$: Calc. C: 56.78, H: 4.59, 4.73; Found C: 56.78, H 4.55, N 4.80.

Refinement

In the refinement all H atoms were allowed for as riding atoms with C—H distances of 0.93, 0.97 & 0.96 Å for the aromatic, methylene and methyl C—H [using the *SHELXL97* (Sheldrick, 1997) defaults at 294 K].

There is considerable disorder in the hexafluorophosphate anion The commonly observed disorder over two sites of the $[PF_6]^-$ moiety was further complicated by the presence of significant peaks of electron density between the modelled F atom site positions. The F atom sites were fixed using soft *DFIX* restraints [in *SHELXL97* (Sheldrick, 1997)] for distance (P—F 1.579 Å) and angle (*cis*-F at 2.233 and *trans*-F at 3.158 Å) with soft parameters used for the DELU/ISOR restraints [in *SHELXL97* (Sheldrick, 1997)]. The P atom is not disordered.

A satisfactory model was developed and the results are as follows: Two orientations of the $[PF_6]^-$ moiety were discernible and input with 25% site occupancy per F atom for site positions labelled as A/C where A and C are related by a 30° rotation about one of the F—P—F axes (two A/C F atom sites are almost coincident whilst the other four are separated by the 30° rotation). Two remaining $[PF_6]^-$ orientations (each with 25% F site occupancy) were subsequently included in a reasonable manner in the disorder model. The residual electron density in the final difference maps is +0.26/-0.28 e.Å^{-3} and therefore the disorder treatment can be said to have achieved a satisfactory conclusion. One *PLATON* (Spek, 2003) Alert B for a short intermolecular F4A···F4A contact can be disregarded as all F atom sites are modelled with 25% site occupancy.

Overall, the extensive disorder in the $[PF_6]^-$ counterion is not surprising given that the $[PF_6]^-$ anion occupies a void in the lattice of volume 215 Å^3 or *ca* 30.7 Å^3 per P/F atom: this is almost twice the average value expected for non-H atoms. Two voids of 64 Å^3 per unit cell remain after the final refinement and analysis but these voids are featureless and are devoid of electron density.

Figures

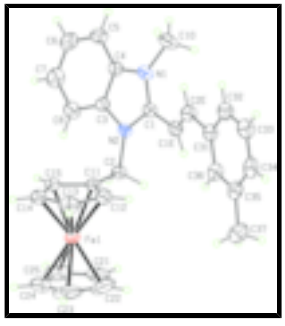

Fig. 1. A view of the cation with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

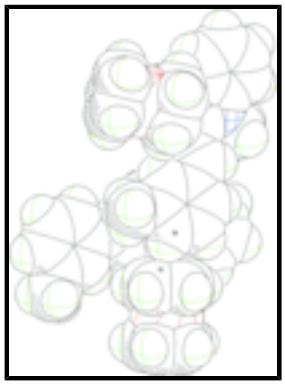

Fig. 2. A view of the C34—H34···π(C_5H_4) interaction in the crystal structure with atoms drawn as their van der Waals spheres. The C34 atom is labelled with a '*' and the η-$C_5H_4^i$ ring with a '#'.

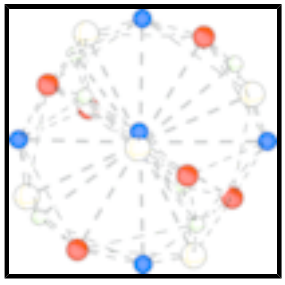

Fig. 3. A view of the disorder in the $[PF_6]^-$ anion with each of the four orientations depicted as coloured spheres of arbitrary radii.

_N_-Ferrocenylmethyl-2-(3-methylstyryl)-_N_'-methylbenzimidazolium hexafluorophosphate

Crystal data

$[Fe(C_5H_5)(C_{23}H_{22}N_2)]PF_6$	F_{000} = 1216
M_r = 592.34	D_x = 1.483 Mg m^{-3}
Monoclinic, $P2_1/a$	Melting point: 483 K
Hall symbol: -P 2yab	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.5150 (10) Å	Cell parameters from 85 reflections
b = 12.8743 (10) Å	θ = 8.9–30.4º
c = 15.2839 (9) Å	μ = 0.69 mm^{-1}
β = 94.037 (5)º	T = 294 (1) K
V = 2652.7 (3) Å^3	Block, red
Z = 4	0.29 × 0.25 × 0.17 mm

Data collection

Bruker P4 diffractometer	R_{int} = 0.025
Radiation source: X-ray tube	θ_{max} = 28.0º
Monochromator: graphite	θ_{min} = 2.1º
T = 294(1) K	h = −17→1
ω scans	k = −1→17
Absorption correction: ψ scan (North *et al.*, 1968)	l = −20→20
T_{min} = 0.826, T_{max} = 0.889	3 standard reflections
8107 measured reflections	every 197 reflections
6387 independent reflections	intensity decay: 0.5%
3922 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.113	$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.5898P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
6387 reflections	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
507 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
228 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Fe1	0.82902 (3)	0.82379 (3)	0.11263 (2)	0.04913 (13)	
P1	0.54550 (6)	0.93397 (6)	0.33825 (5)	0.0581 (2)	
F1A	0.6347 (14)	0.8544 (17)	0.360 (2)	0.106 (11)	0.25
F2A	0.559 (3)	0.919 (2)	0.2396 (11)	0.143 (11)	0.25
F3A	0.4607 (14)	1.0136 (15)	0.321 (2)	0.105 (10)	0.25
F4A	0.533 (2)	0.947 (2)	0.4403 (8)	0.119 (9)	0.25
F5A	0.4701 (12)	0.8394 (9)	0.3395 (19)	0.083 (10)	0.25
F6A	0.6243 (14)	1.0236 (17)	0.345 (2)	0.120 (13)	0.25
F1C	0.6291 (19)	0.8609 (17)	0.312 (2)	0.145 (12)	0.25
F2C	0.522 (3)	0.9619 (16)	0.2384 (9)	0.115 (9)	0.25
F3C	0.4564 (14)	1.0103 (15)	0.362 (2)	0.123 (9)	0.25
F4C	0.5611 (19)	0.9047 (17)	0.4371 (11)	0.106 (9)	0.25
F5C	0.4652 (18)	0.8425 (15)	0.3265 (18)	0.129 (15)	0.25
F6C	0.6175 (16)	1.0283 (12)	0.3520 (15)	0.085 (10)	0.25
F1B	0.4510 (13)	0.876 (2)	0.3717 (18)	0.105 (8)	0.25
F2B	0.556 (2)	0.8398 (15)	0.2719 (13)	0.100 (7)	0.25
F3B	0.6385 (12)	0.9846 (19)	0.303 (2)	0.110 (9)	0.25
F4B	0.531 (3)	1.0242 (15)	0.4024 (15)	0.164 (10)	0.25
F5B	0.6096 (15)	0.8745 (16)	0.4128 (13)	0.087 (8)	0.25
F6B	0.4771 (17)	0.989 (2)	0.2649 (17)	0.085 (8)	0.25
F1D	0.487 (2)	0.9106 (15)	0.4142 (14)	0.107 (6)	0.25
F2D	0.5115 (15)	0.8346 (10)	0.2877 (12)	0.071 (4)	0.25
F3D	0.6158 (18)	0.9605 (14)	0.2560 (13)	0.102 (7)	0.25
F4D	0.5959 (16)	1.0353 (11)	0.3844 (13)	0.077 (7)	0.25
F5D	0.6401 (15)	0.8699 (16)	0.3792 (19)	0.085 (10)	0.25
F6D	0.4659 (15)	1.008 (2)	0.2932 (19)	0.087 (10)	0.25
N1	1.00823 (15)	1.13875 (16)	0.40497 (12)	0.0454 (5)	
N2	0.94783 (14)	0.99330 (14)	0.35027 (12)	0.0387 (4)	
C1	0.92886 (17)	1.09458 (18)	0.36126 (14)	0.0409 (5)	
C2	0.88229 (18)	0.91633 (18)	0.30194 (15)	0.0425 (6)	
C3	1.04403 (17)	0.97278 (19)	0.38485 (14)	0.0405 (5)	
C4	1.08141 (18)	1.06479 (19)	0.41968 (15)	0.0433 (6)	
C5	1.1776 (2)	1.0705 (2)	0.45951 (17)	0.0583 (7)	
C6	1.2326 (2)	0.9824 (3)	0.46061 (19)	0.0695 (9)	
C7	1.1952 (2)	0.8897 (3)	0.42499 (19)	0.0686 (8)	
C8	1.0999 (2)	0.8825 (2)	0.38654 (17)	0.0552 (7)	
C10	1.0168 (2)	1.2464 (2)	0.4364 (2)	0.0673 (8)	
C11	0.89295 (17)	0.91959 (18)	0.20553 (15)	0.0394 (5)	

C12	0.83444 (19)	0.9779 (2)	0.14174 (17)	0.0519 (6)
C13	0.8722 (2)	0.9597 (2)	0.05876 (17)	0.0613 (8)
C14	0.9536 (2)	0.8921 (2)	0.07054 (17)	0.0562 (7)
C15	0.96684 (18)	0.8670 (2)	0.16044 (17)	0.0479 (6)
C21	0.7325 (4)	0.7294 (4)	0.1683 (3)	0.0947 (13)
C22	0.6852 (3)	0.7801 (4)	0.0999 (4)	0.1069 (14)
C23	0.7315 (4)	0.7541 (5)	0.0254 (3)	0.1191 (19)
C24	0.8057 (4)	0.6891 (4)	0.0457 (4)	0.1104 (17)
C25	0.8105 (4)	0.6704 (3)	0.1362 (4)	0.1108 (16)
C1E	0.83780 (19)	1.1431 (2)	0.32685 (16)	0.0471 (6)
C2E	0.8272 (2)	1.2409 (2)	0.30173 (17)	0.0511 (6)
C31	0.73912 (19)	1.28689 (19)	0.25643 (16)	0.0477 (6)
C32	0.7369 (2)	1.3941 (2)	0.24249 (18)	0.0571 (7)
C33	0.6559 (2)	1.4394 (2)	0.19980 (19)	0.0632 (8)
C34	0.5766 (2)	1.3800 (2)	0.16931 (17)	0.0599 (8)
C35	0.57701 (19)	1.2725 (2)	0.17876 (17)	0.0536 (7)
C36	0.65917 (19)	1.2276 (2)	0.22400 (16)	0.0503 (6)
C37	0.4940 (2)	1.2062 (3)	0.1393 (2)	0.0773 (9)
H2A	0.8138	0.9305	0.3131	0.051*
H2B	0.8985	0.8472	0.3237	0.051*
H5	1.2027	1.1320	0.4841	0.070*
H6	1.2973	0.9839	0.4859	0.083*
H7	1.2354	0.8310	0.4272	0.082*
H8	1.0746	0.8205	0.3631	0.066*
H10A	1.0431	1.2891	0.3920	0.101*
H10B	1.0605	1.2489	0.4887	0.101*
H10C	0.9525	1.2717	0.4490	0.101*
H12	0.7810	1.0204	0.1526	0.062*
H13	0.8473	0.9877	0.0056	0.074*
H14	0.9921	0.8680	0.0267	0.067*
H15	1.0156	0.8235	0.1860	0.057*
H21	0.7164	0.7327	0.2265	0.114*
H22	0.6312	0.8244	0.1027	0.128*
H23	0.7134	0.7785	−0.0308	0.143*
H24	0.8476	0.6605	0.0064	0.132*
H25	0.8555	0.6282	0.1683	0.133*
H1E	0.7814	1.1016	0.3219	0.057*
H2E	0.8811	1.2847	0.3141	0.061*
H32	0.7908	1.4347	0.2623	0.069*
H33	0.6545	1.5110	0.1914	0.076*
H34	0.5213	1.4122	0.1417	0.072*
H36	0.6605	1.1561	0.2327	0.060*
H37A	0.4331	1.2448	0.1373	0.116*
H37B	0.4878	1.1451	0.1744	0.116*
H37C	0.5081	1.1864	0.0809	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0420 (2)	0.0572 (2)	0.0479 (2)	−0.01612 (18)	0.00050 (15)	−0.01005 (18)
P1	0.0602 (5)	0.0412 (4)	0.0721 (5)	−0.0013 (4)	−0.0008 (4)	0.0038 (4)
F1A	0.106 (15)	0.056 (11)	0.16 (2)	0.005 (8)	0.015 (16)	0.015 (14)
F2A	0.20 (3)	0.15 (3)	0.073 (10)	0.05 (2)	0.011 (13)	−0.037 (14)
F3A	0.081 (13)	0.090 (13)	0.15 (2)	0.066 (10)	0.021 (13)	0.049 (15)
F4A	0.170 (18)	0.14 (2)	0.042 (7)	−0.016 (17)	−0.016 (8)	−0.014 (9)
F5A	0.065 (10)	0.035 (8)	0.15 (3)	−0.009 (7)	−0.007 (14)	0.021 (10)
F6A	0.055 (11)	0.11 (2)	0.20 (3)	−0.015 (11)	0.030 (14)	0.014 (17)
F1C	0.108 (17)	0.14 (2)	0.19 (2)	0.003 (14)	0.075 (17)	−0.020 (19)
F2C	0.20 (3)	0.085 (13)	0.063 (8)	0.021 (15)	0.014 (13)	−0.004 (7)
F3C	0.078 (10)	0.099 (12)	0.20 (2)	0.006 (8)	0.036 (12)	−0.033 (16)
F4C	0.119 (17)	0.086 (14)	0.111 (14)	−0.037 (12)	−0.016 (12)	0.059 (11)
F5C	0.14 (3)	0.125 (19)	0.12 (2)	−0.083 (16)	−0.011 (18)	−0.022 (14)
F6C	0.13 (2)	0.039 (9)	0.078 (13)	−0.046 (11)	−0.006 (12)	0.027 (9)
F1B	0.079 (11)	0.15 (2)	0.091 (15)	−0.010 (12)	0.031 (11)	0.018 (13)
F2B	0.130 (18)	0.072 (9)	0.106 (10)	−0.011 (12)	0.053 (12)	−0.029 (8)
F3B	0.060 (8)	0.105 (18)	0.17 (2)	−0.019 (11)	0.017 (14)	0.029 (17)
F4B	0.18 (2)	0.099 (13)	0.21 (2)	0.051 (18)	0.00 (2)	−0.065 (13)
F5B	0.082 (16)	0.084 (12)	0.090 (12)	−0.001 (10)	−0.032 (10)	0.002 (10)
F6B	0.087 (12)	0.078 (14)	0.090 (18)	0.019 (9)	0.002 (9)	0.019 (14)
F1D	0.15 (2)	0.113 (14)	0.059 (11)	−0.002 (13)	0.033 (10)	0.020 (10)
F2D	0.069 (10)	0.066 (7)	0.078 (11)	−0.029 (8)	−0.001 (7)	−0.002 (8)
F3D	0.128 (19)	0.089 (10)	0.093 (13)	−0.016 (11)	0.043 (11)	−0.019 (10)
F4D	0.078 (12)	0.050 (7)	0.095 (14)	0.016 (9)	−0.036 (10)	−0.021 (8)
F5D	0.058 (10)	0.039 (7)	0.15 (2)	0.027 (6)	−0.047 (13)	−0.021 (11)
F6D	0.069 (13)	0.096 (16)	0.094 (18)	0.016 (10)	−0.017 (12)	0.004 (13)
N1	0.0533 (12)	0.0407 (11)	0.0415 (11)	−0.0010 (10)	−0.0019 (9)	−0.0064 (9)
N2	0.0409 (10)	0.0370 (11)	0.0376 (10)	0.0020 (9)	−0.0025 (8)	−0.0021 (8)
C1	0.0445 (13)	0.0398 (13)	0.0381 (12)	0.0008 (11)	0.0018 (10)	−0.0018 (10)
C2	0.0423 (13)	0.0371 (13)	0.0472 (13)	−0.0030 (11)	−0.0023 (11)	−0.0001 (11)
C3	0.0391 (12)	0.0449 (14)	0.0369 (12)	0.0034 (11)	−0.0026 (10)	−0.0003 (11)
C4	0.0445 (13)	0.0479 (14)	0.0369 (12)	0.0011 (12)	−0.0017 (10)	−0.0016 (11)
C5	0.0535 (16)	0.0706 (19)	0.0491 (15)	−0.0076 (15)	−0.0088 (13)	−0.0081 (14)
C6	0.0470 (16)	0.098 (3)	0.0608 (18)	0.0082 (17)	−0.0147 (13)	−0.0026 (18)
C7	0.0584 (17)	0.077 (2)	0.0682 (19)	0.0236 (16)	−0.0116 (15)	0.0043 (17)
C8	0.0582 (16)	0.0515 (16)	0.0544 (15)	0.0113 (14)	−0.0064 (13)	0.0007 (13)
C10	0.085 (2)	0.0451 (16)	0.0694 (19)	−0.0046 (15)	−0.0150 (16)	−0.0169 (14)
C11	0.0372 (12)	0.0361 (12)	0.0442 (13)	−0.0058 (10)	−0.0018 (10)	−0.0029 (10)
C12	0.0503 (15)	0.0499 (15)	0.0545 (15)	0.0042 (13)	−0.0042 (12)	−0.0005 (13)
C13	0.0752 (19)	0.0642 (18)	0.0436 (14)	−0.0138 (16)	−0.0023 (14)	0.0049 (13)
C14	0.0522 (16)	0.0639 (18)	0.0539 (16)	−0.0187 (14)	0.0126 (13)	−0.0122 (14)
C15	0.0374 (13)	0.0475 (14)	0.0586 (15)	−0.0063 (11)	0.0018 (11)	−0.0084 (12)
C21	0.109 (3)	0.098 (3)	0.080 (3)	−0.068 (3)	0.025 (2)	−0.021 (2)
C22	0.050 (2)	0.119 (3)	0.149 (4)	−0.037 (2)	−0.006 (3)	−0.009 (3)

C23	0.106 (3)	0.168 (5)	0.079 (3)	−0.083 (4)	−0.022 (3)	−0.015 (3)
C24	0.094 (3)	0.103 (3)	0.137 (4)	−0.052 (3)	0.031 (3)	−0.065 (3)
C25	0.099 (3)	0.055 (2)	0.172 (5)	−0.039 (2)	−0.034 (3)	0.012 (3)
C1E	0.0447 (14)	0.0464 (14)	0.0500 (14)	0.0048 (11)	0.0009 (11)	−0.0019 (12)
C2E	0.0507 (15)	0.0495 (16)	0.0525 (15)	0.0016 (12)	−0.0004 (12)	0.0014 (12)
C31	0.0504 (15)	0.0443 (14)	0.0488 (14)	0.0087 (12)	0.0060 (12)	0.0060 (12)
C32	0.0613 (17)	0.0476 (15)	0.0625 (17)	0.0062 (14)	0.0058 (14)	0.0023 (13)
C33	0.074 (2)	0.0455 (16)	0.0698 (18)	0.0131 (15)	0.0060 (16)	0.0083 (14)
C34	0.0616 (18)	0.0650 (19)	0.0538 (16)	0.0264 (16)	0.0079 (14)	0.0135 (14)
C35	0.0481 (15)	0.0679 (18)	0.0454 (14)	0.0065 (14)	0.0074 (12)	0.0093 (13)
C36	0.0506 (15)	0.0484 (15)	0.0522 (15)	0.0078 (13)	0.0057 (12)	0.0113 (12)
C37	0.0588 (18)	0.100 (3)	0.071 (2)	0.0011 (18)	−0.0060 (16)	0.0133 (18)

Geometric parameters (Å, °)

Fe1—C11	2.028 (2)	C2E—C31	1.460 (4)
Fe1—C12	2.034 (3)	C31—C36	1.386 (4)
Fe1—C13	2.036 (3)	C31—C32	1.396 (4)
Fe1—C14	2.043 (3)	C32—C33	1.366 (4)
Fe1—C15	2.030 (2)	C33—C34	1.372 (4)
Fe1—C21	2.016 (3)	C34—C35	1.391 (4)
Fe1—C22	2.020 (3)	C35—C36	1.392 (3)
Fe1—C23	2.018 (3)	C35—C37	1.502 (4)
Fe1—C25	2.025 (4)	C2—H2A	0.9700
Fe1—C24	2.027 (4)	C2—H2B	0.9700
N1—C1	1.349 (3)	C5—H5	0.9300
N1—C4	1.380 (3)	C6—H6	0.9300
N1—C10	1.469 (3)	C7—H7	0.9300
N2—C1	1.342 (3)	C8—H8	0.9300
N2—C2	1.490 (3)	C1E—H1E	0.9300
N2—C3	1.394 (3)	C2E—H2E	0.9300
C1—C1E	1.446 (3)	C12—H12	0.9300
C2—C11	1.491 (3)	C13—H13	0.9300
C3—C4	1.380 (3)	C14—H14	0.9300
C3—C8	1.385 (3)	C15—H15	0.9300
C4—C5	1.398 (3)	C21—H21	0.9300
C5—C6	1.356 (4)	C22—H22	0.9300
C6—C7	1.392 (4)	C23—H23	0.9300
C7—C8	1.380 (4)	C24—H24	0.9300
C11—C15	1.424 (3)	C25—H25	0.9300
C11—C12	1.425 (3)	C32—H32	0.9300
C12—C13	1.420 (4)	C33—H33	0.9300
C13—C14	1.404 (4)	C34—H34	0.9300
C14—C15	1.410 (4)	C36—H36	0.9300
C21—C22	1.355 (6)	C10—H10A	0.9600
C21—C25	1.415 (6)	C10—H10B	0.9600
C22—C23	1.379 (6)	C10—H10C	0.9600
C23—C24	1.326 (6)	C37—H37A	0.9600
C24—C25	1.400 (6)	C37—H37B	0.9600

C1E—C2E	1.321 (3)	C37—H37C	0.9600
C21—Fe1—C23	66.35 (17)	C15—C11—Fe1	69.55 (13)
C21—Fe1—C22	39.22 (17)	C12—C11—Fe1	69.70 (14)
C23—Fe1—C22	39.94 (18)	C2—C11—Fe1	127.50 (16)
C21—Fe1—C25	41.00 (17)	C13—C12—C11	107.9 (2)
C23—Fe1—C25	66.5 (2)	C13—C12—Fe1	69.67 (16)
C22—Fe1—C25	67.38 (19)	C11—C12—Fe1	69.21 (14)
C21—Fe1—C24	67.33 (17)	C13—C12—H12	126.1
C23—Fe1—C24	38.27 (19)	C11—C12—H12	126.1
C22—Fe1—C24	66.32 (18)	Fe1—C12—H12	126.6
C25—Fe1—C24	40.43 (19)	C14—C13—C12	108.4 (2)
C21—Fe1—C11	109.13 (12)	C14—C13—Fe1	70.12 (16)
C23—Fe1—C11	163.6 (2)	C12—C13—Fe1	69.50 (16)
C22—Fe1—C11	126.64 (17)	C14—C13—H13	125.8
C25—Fe1—C11	121.36 (17)	C12—C13—H13	125.8
C24—Fe1—C11	156.6 (2)	Fe1—C13—H13	126.2
C21—Fe1—C15	128.19 (16)	C13—C14—C15	108.1 (2)
C23—Fe1—C15	154.1 (2)	C13—C14—Fe1	69.62 (16)
C22—Fe1—C15	164.46 (19)	C15—C14—Fe1	69.25 (14)
C25—Fe1—C15	108.97 (15)	C13—C14—H14	125.9
C24—Fe1—C15	121.50 (18)	C15—C14—H14	125.9
C11—Fe1—C15	41.08 (9)	Fe1—C14—H14	126.8
C21—Fe1—C12	120.70 (16)	C14—C15—C11	108.5 (2)
C23—Fe1—C12	126.2 (2)	C14—C15—Fe1	70.22 (14)
C22—Fe1—C12	108.21 (16)	C11—C15—Fe1	69.36 (13)
C25—Fe1—C12	156.2 (2)	C14—C15—H15	125.7
C24—Fe1—C12	161.3 (2)	C11—C15—H15	125.7
C11—Fe1—C12	41.09 (9)	Fe1—C15—H15	126.2
C15—Fe1—C12	68.64 (10)	C22—C21—C25	108.2 (4)
C21—Fe1—C13	154.4 (2)	C22—C21—Fe1	70.6 (2)
C23—Fe1—C13	107.88 (16)	C25—C21—Fe1	69.9 (2)
C22—Fe1—C13	120.11 (18)	C22—C21—H21	125.9
C25—Fe1—C13	162.1 (2)	C25—C21—H21	125.9
C24—Fe1—C13	124.74 (19)	Fe1—C21—H21	125.2
C11—Fe1—C13	68.93 (10)	C21—C22—C23	107.7 (4)
C15—Fe1—C13	68.17 (11)	C21—C22—Fe1	70.2 (2)
C12—Fe1—C13	40.83 (11)	C23—C22—Fe1	70.0 (2)
C21—Fe1—C14	164.81 (19)	C21—C22—H22	126.1
C23—Fe1—C14	119.83 (17)	C23—C22—H22	126.1
C22—Fe1—C14	153.94 (19)	Fe1—C22—H22	125.3
C25—Fe1—C14	126.19 (19)	C24—C23—C22	109.8 (5)
C24—Fe1—C14	108.17 (15)	C24—C23—Fe1	71.2 (2)
C11—Fe1—C14	68.82 (10)	C22—C23—Fe1	70.1 (2)
C15—Fe1—C14	40.52 (10)	C24—C23—H23	125.1
C12—Fe1—C14	68.35 (11)	C22—C23—H23	125.1
C13—Fe1—C14	40.26 (11)	Fe1—C23—H23	125.2
C1—N1—C4	109.00 (19)	C23—C24—C25	108.8 (4)
C1—N1—C10	127.0 (2)	C23—C24—Fe1	70.5 (2)
C4—N1—C10	124.0 (2)	C25—C24—Fe1	69.7 (2)

C1—N2—C3	108.54 (19)	C23—C24—H24	125.6
C1—N2—C2	126.60 (19)	C25—C24—H24	125.6
C3—N2—C2	124.62 (19)	Fe1—C24—H24	125.7
N2—C1—N1	108.6 (2)	C24—C25—C21	105.5 (4)
N2—C1—C1E	122.7 (2)	C24—C25—Fe1	69.8 (2)
N1—C1—C1E	128.7 (2)	C21—C25—Fe1	69.1 (2)
N2—C2—C11	112.06 (18)	C24—C25—H25	127.3
N2—C2—H2A	109.2	C21—C25—H25	127.3
C11—C2—H2A	109.2	Fe1—C25—H25	125.4
N2—C2—H2B	109.2	C2E—C1E—C1	126.1 (3)
C11—C2—H2B	109.2	C2E—C1E—H1E	116.9
H2A—C2—H2B	107.9	C1—C1E—H1E	116.9
C4—C3—C8	121.9 (2)	C1E—C2E—C31	126.3 (3)
C4—C3—N2	106.9 (2)	C1E—C2E—H2E	116.8
C8—C3—N2	131.2 (2)	C31—C2E—H2E	116.8
C3—C4—N1	106.9 (2)	C36—C31—C32	118.8 (2)
C3—C4—C5	121.1 (2)	C36—C31—C2E	122.4 (2)
N1—C4—C5	131.9 (2)	C32—C31—C2E	118.8 (3)
C6—C5—C4	117.0 (3)	C33—C32—C31	120.2 (3)
C6—C5—H5	121.5	C33—C32—H32	119.9
C4—C5—H5	121.5	C31—C32—H32	119.9
C5—C6—C7	121.9 (3)	C32—C33—C34	120.3 (3)
C5—C6—H6	119.1	C32—C33—H33	119.8
C7—C6—H6	119.1	C34—C33—H33	119.8
C8—C7—C6	121.8 (3)	C33—C34—C35	121.5 (3)
C8—C7—H7	119.1	C33—C34—H34	119.3
C6—C7—H7	119.1	C35—C34—H34	119.3
C7—C8—C3	116.3 (3)	C34—C35—C36	117.5 (3)
C7—C8—H8	121.9	C34—C35—C37	121.7 (3)
C3—C8—H8	121.9	C36—C35—C37	120.7 (3)
N1—C10—H10A	109.5	C31—C36—C35	121.6 (3)
N1—C10—H10B	109.5	C31—C36—H36	119.2
H10A—C10—H10B	109.5	C35—C36—H36	119.2
N1—C10—H10C	109.5	C35—C37—H37A	109.5
H10A—C10—H10C	109.5	C35—C37—H37B	109.5
H10B—C10—H10C	109.5	H37A—C37—H37B	109.5
C15—C11—C12	107.1 (2)	C35—C37—H37C	109.5
C15—C11—C2	125.8 (2)	H37A—C37—H37C	109.5
C12—C11—C2	127.1 (2)	H37B—C37—H37C	109.5
C3—N2—C1—N1	−2.5 (3)	C23—Fe1—C15—C14	48.9 (5)
C2—N2—C1—N1	−177.06 (19)	C22—Fe1—C15—C14	−162.4 (6)
C3—N2—C1—C1E	175.4 (2)	C25—Fe1—C15—C14	124.0 (3)
C2—N2—C1—C1E	0.8 (4)	C24—Fe1—C15—C14	81.1 (3)
C4—N1—C1—N2	2.2 (3)	C11—Fe1—C15—C14	−119.7 (2)
C10—N1—C1—N2	−175.3 (2)	C12—Fe1—C15—C14	−81.25 (17)
C4—N1—C1—C1E	−175.6 (2)	C13—Fe1—C15—C14	−37.19 (16)
C10—N1—C1—C1E	7.0 (4)	C21—Fe1—C15—C11	−74.5 (2)
C1—N2—C2—C11	82.7 (3)	C23—Fe1—C15—C11	168.7 (4)
C3—N2—C2—C11	−91.1 (3)	C22—Fe1—C15—C11	−42.7 (6)

C1—N2—C3—C4	1.9 (3)	C25—Fe1—C15—C11	−116.3 (3)
C2—N2—C3—C4	176.57 (19)	C24—Fe1—C15—C11	−159.1 (2)
C1—N2—C3—C8	−176.9 (3)	C12—Fe1—C15—C11	38.47 (14)
C2—N2—C3—C8	−2.2 (4)	C13—Fe1—C15—C11	82.53 (16)
C8—C3—C4—N1	178.4 (2)	C14—Fe1—C15—C11	119.7 (2)
N2—C3—C4—N1	−0.5 (3)	C23—Fe1—C21—C22	−38.1 (3)
C8—C3—C4—C5	−0.9 (4)	C25—Fe1—C21—C22	−118.8 (4)
N2—C3—C4—C5	−179.8 (2)	C24—Fe1—C21—C22	−79.8 (3)
C1—N1—C4—C3	−1.0 (3)	C11—Fe1—C21—C22	125.0 (3)
C10—N1—C4—C3	176.6 (2)	C15—Fe1—C21—C22	167.1 (3)
C1—N1—C4—C5	178.1 (3)	C12—Fe1—C21—C22	81.2 (3)
C10—N1—C4—C5	−4.3 (4)	C13—Fe1—C21—C22	44.0 (4)
C3—C4—C5—C6	1.3 (4)	C14—Fe1—C21—C22	−155.4 (5)
N1—C4—C5—C6	−177.7 (3)	C23—Fe1—C21—C25	80.8 (3)
C4—C5—C6—C7	−0.9 (4)	C22—Fe1—C21—C25	118.8 (4)
C5—C6—C7—C8	0.1 (5)	C24—Fe1—C21—C25	39.0 (3)
C6—C7—C8—C3	0.4 (4)	C11—Fe1—C21—C25	−116.1 (3)
C4—C3—C8—C7	0.0 (4)	C15—Fe1—C21—C25	−74.1 (3)
N2—C3—C8—C7	178.6 (3)	C12—Fe1—C21—C25	−159.9 (3)
N2—C2—C11—C15	84.2 (3)	C13—Fe1—C21—C25	162.9 (3)
N2—C2—C11—C12	−93.4 (3)	C14—Fe1—C21—C25	−36.6 (6)
N2—C2—C11—Fe1	174.77 (15)	C25—C21—C22—C23	0.2 (4)
C21—Fe1—C11—C15	126.7 (2)	Fe1—C21—C22—C23	60.2 (3)
C23—Fe1—C11—C15	−162.3 (5)	C25—C21—C22—Fe1	−60.0 (2)
C22—Fe1—C11—C15	166.9 (2)	C23—Fe1—C22—C21	118.4 (4)
C25—Fe1—C11—C15	83.1 (3)	C25—Fe1—C22—C21	38.5 (3)
C24—Fe1—C11—C15	49.7 (4)	C24—Fe1—C22—C21	82.6 (3)
C12—Fe1—C11—C15	−118.2 (2)	C11—Fe1—C22—C21	−74.6 (3)
C13—Fe1—C11—C15	−80.54 (17)	C15—Fe1—C22—C21	−40.9 (7)
C14—Fe1—C11—C15	−37.24 (15)	C12—Fe1—C22—C21	−116.5 (3)
C21—Fe1—C11—C12	−115.1 (2)	C13—Fe1—C22—C21	−159.7 (3)
C23—Fe1—C11—C12	−44.1 (6)	C14—Fe1—C22—C21	165.6 (3)
C22—Fe1—C11—C12	−74.9 (3)	C21—Fe1—C22—C23	−118.4 (4)
C25—Fe1—C11—C12	−158.7 (2)	C25—Fe1—C22—C23	−79.9 (4)
C24—Fe1—C11—C12	167.9 (4)	C24—Fe1—C22—C23	−35.7 (3)
C15—Fe1—C11—C12	118.2 (2)	C11—Fe1—C22—C23	167.0 (3)
C13—Fe1—C11—C12	37.63 (16)	C15—Fe1—C22—C23	−159.3 (5)
C14—Fe1—C11—C12	80.93 (16)	C12—Fe1—C22—C23	125.1 (3)
C21—Fe1—C11—C2	6.7 (3)	C13—Fe1—C22—C23	82.0 (4)
C23—Fe1—C11—C2	77.7 (6)	C14—Fe1—C22—C23	47.3 (5)
C22—Fe1—C11—C2	46.9 (3)	C21—C22—C23—C24	0.0 (5)
C25—Fe1—C11—C2	−36.9 (3)	Fe1—C22—C23—C24	60.4 (3)
C24—Fe1—C11—C2	−70.3 (4)	C21—C22—C23—Fe1	−60.3 (3)
C15—Fe1—C11—C2	−120.0 (3)	C21—Fe1—C23—C24	−82.9 (3)
C12—Fe1—C11—C2	121.8 (3)	C22—Fe1—C23—C24	−120.3 (5)
C13—Fe1—C11—C2	159.4 (2)	C25—Fe1—C23—C24	−37.9 (3)
C14—Fe1—C11—C2	−157.3 (2)	C11—Fe1—C23—C24	−160.1 (5)
C15—C11—C12—C13	0.6 (3)	C15—Fe1—C23—C24	47.2 (5)
C2—C11—C12—C13	178.6 (2)	C12—Fe1—C23—C24	165.4 (3)

Fe1—C11—C12—C13	−59.15 (19)	C13—Fe1—C23—C24	123.9 (3)
C15—C11—C12—Fe1	59.78 (16)	C14—Fe1—C23—C24	81.6 (3)
C2—C11—C12—Fe1	−122.3 (2)	C21—Fe1—C23—C22	37.4 (3)
C21—Fe1—C12—C13	−156.4 (2)	C25—Fe1—C23—C22	82.3 (3)
C23—Fe1—C12—C13	−74.7 (3)	C24—Fe1—C23—C22	120.3 (5)
C22—Fe1—C12—C13	−115.3 (2)	C11—Fe1—C23—C22	−39.8 (7)
C25—Fe1—C12—C13	169.7 (4)	C15—Fe1—C23—C22	167.5 (3)
C24—Fe1—C12—C13	−45.6 (5)	C12—Fe1—C23—C22	−74.3 (4)
C11—Fe1—C12—C13	119.4 (2)	C13—Fe1—C23—C22	−115.8 (3)
C15—Fe1—C12—C13	80.91 (18)	C14—Fe1—C23—C22	−158.2 (3)
C14—Fe1—C12—C13	37.20 (16)	C22—C23—C24—C25	−0.3 (5)
C21—Fe1—C12—C11	84.2 (2)	Fe1—C23—C24—C25	59.4 (3)
C23—Fe1—C12—C11	165.9 (2)	C22—C23—C24—Fe1	−59.7 (3)
C22—Fe1—C12—C11	125.3 (2)	C21—Fe1—C24—C23	80.1 (3)
C25—Fe1—C12—C11	50.3 (4)	C22—Fe1—C24—C23	37.3 (3)
C24—Fe1—C12—C11	−164.9 (4)	C25—Fe1—C24—C23	119.6 (4)
C15—Fe1—C12—C11	−38.47 (14)	C11—Fe1—C24—C23	166.0 (3)
C13—Fe1—C12—C11	−119.4 (2)	C15—Fe1—C24—C23	−157.9 (3)
C14—Fe1—C12—C11	−82.17 (16)	C12—Fe1—C24—C23	−39.4 (6)
C11—C12—C13—C14	−0.7 (3)	C13—Fe1—C24—C23	−74.0 (3)
Fe1—C12—C13—C14	−59.54 (19)	C14—Fe1—C24—C23	−115.4 (3)
C11—C12—C13—Fe1	58.87 (17)	C21—Fe1—C24—C25	−39.6 (3)
C21—Fe1—C13—C14	172.2 (3)	C23—Fe1—C24—C25	−119.6 (4)
C23—Fe1—C13—C14	−115.3 (3)	C22—Fe1—C24—C25	−82.4 (3)
C22—Fe1—C13—C14	−157.2 (2)	C11—Fe1—C24—C25	46.4 (5)
C25—Fe1—C13—C14	−46.8 (5)	C15—Fe1—C24—C25	82.4 (3)
C24—Fe1—C13—C14	−76.6 (3)	C12—Fe1—C24—C25	−159.0 (4)
C11—Fe1—C13—C14	81.72 (16)	C13—Fe1—C24—C25	166.4 (3)
C15—Fe1—C13—C14	37.43 (15)	C14—Fe1—C24—C25	125.0 (3)
C12—Fe1—C13—C14	119.6 (2)	C23—C24—C25—C21	0.4 (4)
C21—Fe1—C13—C12	52.6 (4)	Fe1—C24—C25—C21	60.3 (2)
C23—Fe1—C13—C12	125.1 (3)	C23—C24—C25—Fe1	−59.9 (3)
C22—Fe1—C13—C12	83.2 (2)	C22—C21—C25—C24	−0.3 (4)
C25—Fe1—C13—C12	−166.4 (5)	Fe1—C21—C25—C24	−60.8 (2)
C24—Fe1—C13—C12	163.8 (2)	C22—C21—C25—Fe1	60.4 (3)
C11—Fe1—C13—C12	−37.87 (15)	C21—Fe1—C25—C24	116.4 (4)
C15—Fe1—C13—C12	−82.16 (17)	C23—Fe1—C25—C24	36.0 (3)
C14—Fe1—C13—C12	−119.6 (2)	C22—Fe1—C25—C24	79.5 (3)
C12—C13—C14—C15	0.4 (3)	C11—Fe1—C25—C24	−160.3 (3)
Fe1—C13—C14—C15	−58.71 (18)	C15—Fe1—C25—C24	−116.7 (3)
C12—C13—C14—Fe1	59.15 (19)	C12—Fe1—C25—C24	163.4 (3)
C21—Fe1—C14—C13	−167.1 (5)	C13—Fe1—C25—C24	−39.1 (6)
C23—Fe1—C14—C13	82.6 (3)	C14—Fe1—C25—C24	−74.8 (3)
C22—Fe1—C14—C13	49.6 (4)	C23—Fe1—C25—C21	−80.4 (3)
C25—Fe1—C14—C13	163.9 (2)	C22—Fe1—C25—C21	−36.9 (2)
C24—Fe1—C14—C13	122.7 (3)	C24—Fe1—C25—C21	−116.4 (4)
C11—Fe1—C14—C13	−82.00 (16)	C11—Fe1—C25—C21	83.3 (3)
C15—Fe1—C14—C13	−119.7 (2)	C15—Fe1—C25—C21	127.0 (3)
C12—Fe1—C14—C13	−37.71 (16)	C12—Fe1—C25—C21	47.0 (5)

C21—Fe1—C14—C15	−47.4 (5)	C13—Fe1—C25—C21	−155.5 (4)
C23—Fe1—C14—C15	−157.7 (3)	C14—Fe1—C25—C21	168.8 (2)
C22—Fe1—C14—C15	169.4 (3)	N2—C1—C1E—C2E	−150.1 (3)
C25—Fe1—C14—C15	−76.4 (3)	N1—C1—C1E—C2E	27.4 (4)
C24—Fe1—C14—C15	−117.5 (3)	C1—C1E—C2E—C31	171.4 (2)
C11—Fe1—C14—C15	37.74 (15)	C1E—C2E—C31—C36	−8.8 (4)
C12—Fe1—C14—C15	82.03 (16)	C1E—C2E—C31—C32	173.6 (3)
C13—Fe1—C14—C15	119.7 (2)	C36—C31—C32—C33	1.9 (4)
C13—C14—C15—C11	−0.1 (3)	C2E—C31—C32—C33	179.6 (3)
Fe1—C14—C15—C11	−58.98 (16)	C31—C32—C33—C34	−0.8 (4)
C13—C14—C15—Fe1	58.93 (19)	C32—C33—C34—C35	−1.6 (4)
C12—C11—C15—C14	−0.4 (3)	C33—C34—C35—C36	2.9 (4)
C2—C11—C15—C14	−178.3 (2)	C33—C34—C35—C37	−175.0 (3)
Fe1—C11—C15—C14	59.52 (17)	C32—C31—C36—C35	−0.5 (4)
C12—C11—C15—Fe1	−59.87 (16)	C2E—C31—C36—C35	−178.1 (2)
C2—C11—C15—Fe1	122.2 (2)	C34—C35—C36—C31	−1.8 (4)
C21—Fe1—C15—C14	165.8 (2)	C37—C35—C36—C31	176.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C34—H34···Cg1^{i}	0.93	2.65	3.472 (3)	149

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

Fig. 1

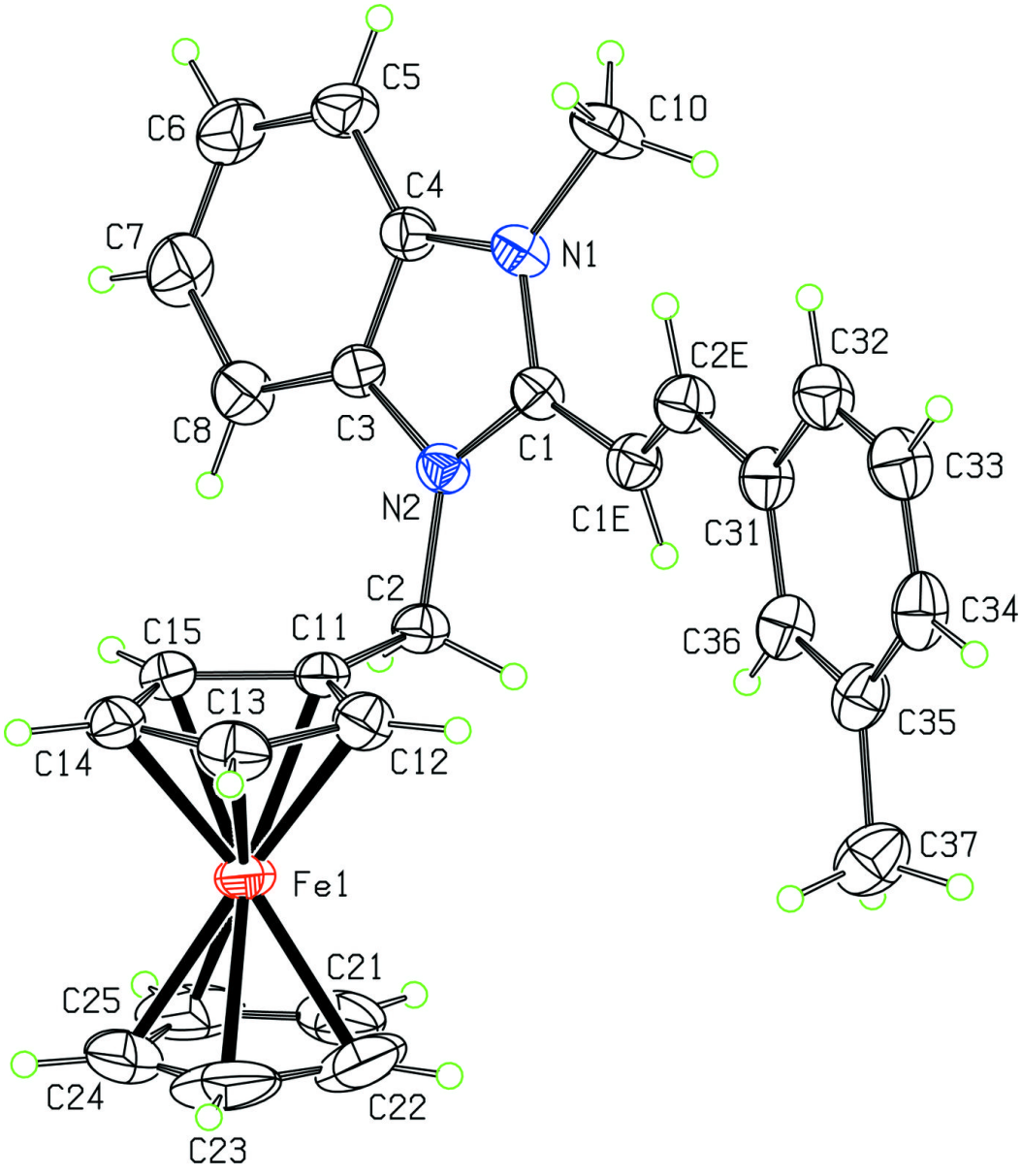
C5
C6
C10
C4
C7
N1
C2E
C32
C8
C3
C1
C33
N2
C1E
C31
C2
C34
C15
C11
C36
C13
C35
C14
C12
C37
Fe1
C21
C25
C24
C22
C23

Fig. 2

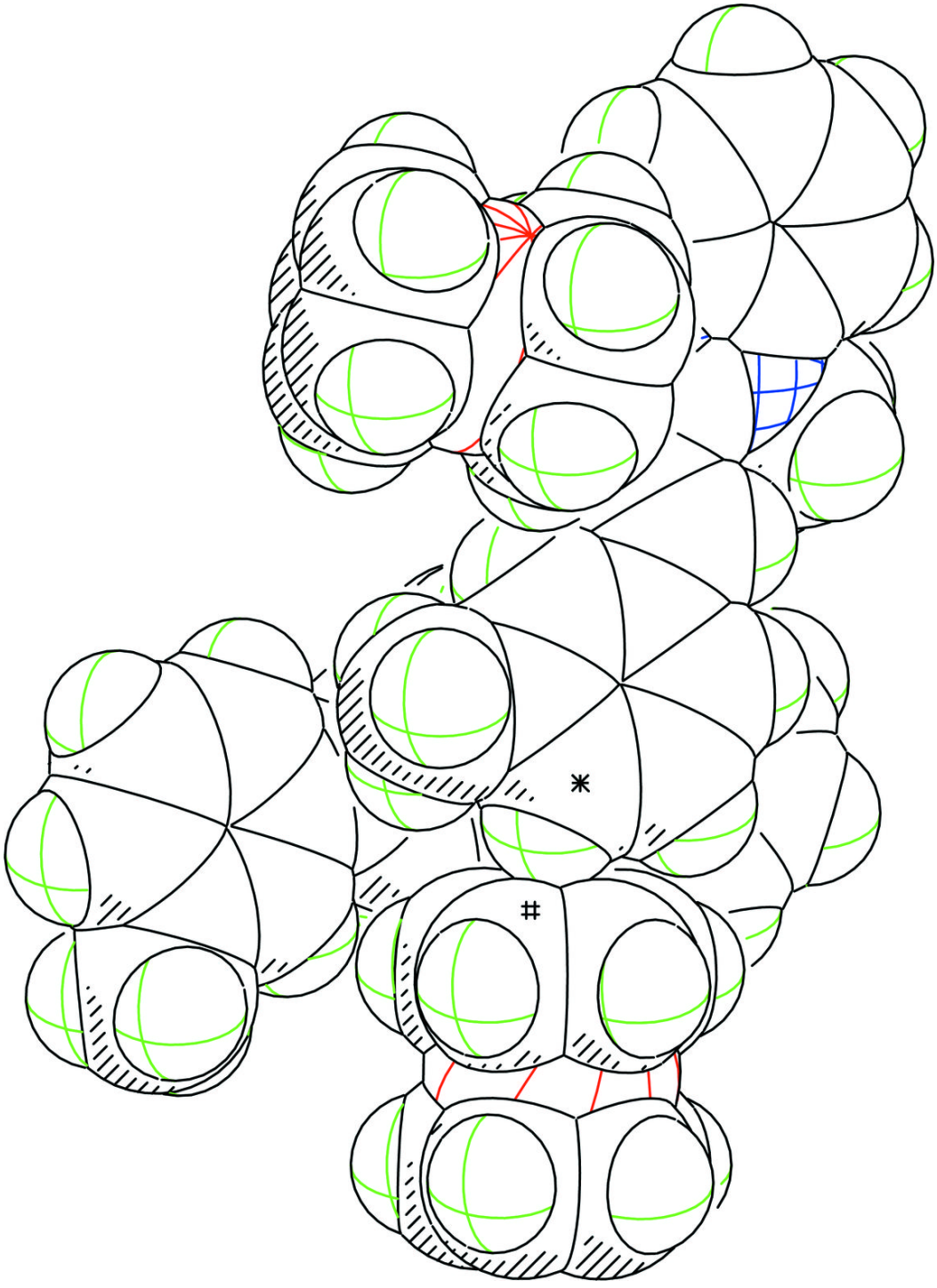

Fig. 3