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1-Ferrocenylmethyl-2-phenyl-1*H*-1,3-benzimidazole

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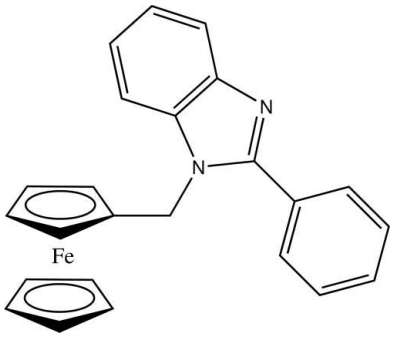
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.037; wR factor = 0.093; data-to-parameter ratio = 10.5.

In the title molecule, $[Fe(C_5H_5)(C_{19}H_{15}N_2)]$, the five-membered C_3N_2 imidazole ring forms dihedral angles of 84.71 (13) and 52.12 (11)°, respectively, with the substituted cyclopentadienyl and phenyl rings. In the crystal structure, in addition to a weak C—H···N interaction, there is a modest C—H···π(ring) interaction involving a C—H group of the unsubstituted cyclopentadienyl ring and the imidazole ring.

Related literature

For related ferrocene literature, see: Li *et al.*, (1998); Gallagher, Hanlon & Howarth, (2001); Gallagher, Hanlon, Howarth & Thomas, (2001); Howarth & Hanlon, (2001); Kazak *et al.*, (2006); Gallagher *et al.* (2007*a*,*b*). For the chemical synthesis and crystal structure of $[Fe(C_5H_5)_2CH_2N(CH_3)_3]^+[I]^-$, see: Pauson *et al.*, (1966); Ferguson *et al.* (1994).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{19}H_{15}N_2)]$
M_r = 392.27
Orthorhombic, $Pna2_1$
a = 11.6323 (12) Å
b = 13.7738 (10) Å
c = 11.5398 (7) Å
V = 1848.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 294 (1) K
0.50 × 0.50 × 0.35 mm

Data collection

Bruker $P4$ diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.683, T_{max} = 0.761
3270 measured reflections
2555 independent reflections
2435 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
3 standard reflections
every 197 reflections
intensity decay: 0.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.09
2555 reflections
244 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Absolute structure: Flack (1983), with 207 Friedel pairs
Flack parameter: 0.02 (2)

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

Cg is the centroid of the imidazole ring.

D—H···A	D—H	H···A	D···A	D—H···A
C23—H23···N1^{i}	0.93	2.69	3.346 (4)	128
C24—H24···*Cg*^{ii}	0.93	2.90	3.556 (3)	129

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

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: *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: LH2536).

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supplementary materials

Acta Cryst. (2007). E**63**, m2882 [**doi:10.1107/S1600536807053561**]

1-Ferrocenylmethyl-2-phenyl-1*H*-1,3-benzimidazole

J. F. Gallagher, K. Hanlon and J. Howarth

Comment

Benzimidazole systems continue to attract much attention in chemical synthesis, structural science and applied biological research (Li *et al.*, 1998; Gallagher, Hanlon & Howarth, 2001; Howarth & Hanlon, 2001; Gallagher, Hanlon, Howarth & Thomas, 2001; Kazak *et al.*, 2006). The title compound, 1-Ferrocenylmethyl-2-(phenyl)-1*H*-1,3-benzimidazole (Figures 1–3), is obtained from a series of reactions involving the chemical synthesis of 1-Ferrocenylmethyl-2-(phenyl)benzimidazole from 2-(phenyl)benzimidazole and (trimethylammonium)ferrocenylmethyl iodide (Pauson *et al.*, 1966; Ferguson *et al.*, 1994).

Bond lengths in the title compound 1-Ferrocenylmethyl-2-(phenyl)-1*H*-1,3-benzimidazole are normal and similar to our previously reported ferrocene derivatives (Gallagher, Hanlon & Howarth, 2001, 2007*a*,b; Gallagher, Hanlon, Howarth & Thomas, 2001).

The major conformation features are the orientation of the benzimidazole group to the ferrocenyl and phenyl rings. The five-membered imidazolyl ring forms dihedral angles of 84.71 (13)° and 52.12 (11)° with the substituted C_5H_4 and phenyl rings, respectively. These data ressemble the values 84.37 (9)°, 56.21 (8)° for a related 3-Cl substituted benzene ring system (Gallagher, Hanlon, Howarth & Thomas, 2001) and 88.61 (8)°, 42.15 (6)° for a 3,5-dimethyl substituted benzene ring system (Gallagher *et al.*, 2007*b*). Two related methoxy substituted derivatives differ somewhat from these values with [78.07 (8)°, 40.22 (9)°] and [73.86 (8)°, 70.02 (7)°] for a 4-OMe and a 3,4-$(OMe)_2$ pair (Gallagher, Hanlon & Howarth, 2001).

The angles at N2 differ, with C2—N2—(C1/C3) 128.7 (2)°, 124.2 (2)° (a 4.5° difference) and C1—N2—C3 is 106.1 (2)°. The C2—N2—C1/C3 difference is 4°, 5° in the 3-Cl, 3,5-Me_2 derivatives, though extending to 7° in the 4-OMe and closing to 0° in the 3,4-$(OMe)_2$ system (Gallagher, Hanlon & Howarth, 2001), thus displaying a significant variation in the angles at the N2 atom by remote atom site variation on the benzene ring {C31,···,C36}. No clear trend has been established and it is most probably due to the different crystal packing forces at the ferrocenyl–benzimidazole C2 bridge atom that effects subtle differences in the C2—N2—C1/C3 angles. For the C11—C2—N2 angles a small variation of *ca* 1° is observed for our five previously reported structures and for Fe1—C11—C2 the range is similarly small (127.4 (2)° for the title compound), 127.81 (13)° (3-Cl) and 128.43 (13)° for the 3,5-$(Me)_2$ systems. A greater deviation in the bond angle data values is 126.56 (13)° [for 4-(OMe)] and 125.74 (15)° [for 3,4-$(OMe)_2$], these latter two systems also display the greatest differences at N2 (see above). A wide range of angles is observed between the imidazolyl and C_6 aromatic rings in these structures due to a lack of steric hindrance and differing crystal packing forces about the C1—C31 bond.

Of interest is the fact that there are no strong intermolecular interactions in the crystal structure of the title compound and the optimal acceptor N1 only has a closest H23 atom at a distance of 2.69 Å (Table 1). A weak $_{cp}$C24—H24···π(C═N) is also present with a C24···Cg^{i} distance of 3.556 (3) Å, where *Cg* is the ring centroid of the C_3N_2 ring and the symmetry operation i = 3/2 − *x*, *y* + 1/2, *z* − 1/2: the closest C24···(C1,N1) distances are 3.564 (4), 3.572 (4) Å. The corresponding H24···(C1,N1) distances and C24—H24···(C1,N1) angles are 2.72, 2.84 Å and 136°, 152°, respectively. We have noted that

in the absence of strong donors and acceptors that the primary interactions in the related derivatives arise from weaker interactions and contacts *e.g.* C—H···π(arene).

The obvious lack of formation (*via* C—H···N interactions) of a centrosymmetric $R^2_2(8)$ type hydrogen bonded ring involving molecules of the title compound (about inversion centres) can be explained by the presence of a myriad of weak C—H···π(arene) contacts (the shortest is a C—H···π(C═N) interaction, Table 1) which overall are more energetically favoured in the crystal structure than a series of localized 'hydrogen bonded dimers'. Weak interactions involving the N1 atom is a related 3,5-dimethylbenzene derivative have also been commented upon by us (Gallagher, Hanlon, Howarth, 2007) though the C···N contact distance is long at 3.658 (2) Å.

Examination of the structure with *PLATON* (Spek, 2003) showed that there were no solvent accessible voids in the crystal lattice.

Experimental

Synthesis and chemical characteristion of the title compound *N*-Ferrocenylmethyl-2-(phenyl)benzimidazole $[(C_5H_5)Fe(C_5H_4)CH_2(C_7H_4N_2)C_6H_5]$

To a mixture of 2-phenylbenzimidazole (2.5 g, 13 mmol) and K_2CO_3 (2.7 g, 19.5 mmol) in CH_3CN (150 ml) was added (trimethylammonium)ferrocenylmethyl iodide ($[FcCH_2N(CH_3)_3]^+[I]^-$) (10.0 g, 13 mmol) (Pauson *et al.*, 1966; Ferguson *et al.*, 1994) and the mixture was heated to reflux temperatures for 12 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 an orange gum. The crude product was purified by column chromatography on silica gel using CH_2Cl_2:CH_3OH (97:3) as eluent.

Yield 6.9 g (67%), m.p. 405–409 K (uncorrected). Compound (I) was obtained as a light orange solid. IR (KBr, ν cm^{-1}) (>1500 cm^{-1}): 3016, 1724, 1658.

^{1}H NMR [400 MHz, δH (p.p.m.), $CDCl_3$], 7.83 (m, 2H, Benz-H), 7.73 (m, 1H, aryl-H), 7.65 (m, 4H, aryl-H), 7.25 (m, 2H, Benz-H), 5.20 (s, 2H, Fc—CH_2), 4.17 (m, 2H, cpd-H), 4.07 (s, 5H, cpd-H), 4.04 (m, 2H, cpd-H). ^{13}C NMR [δC, $CDCl_3$], 153.21, 138.11, 135.50, 131.27, 130.62, 127.12, 122.41, 122.05, 119.13, 111.28, 82.95, 68.85, 68.79, 68.15, 43.61.

Refinement

The molecule crystallizes in the orthorhombic system; space group $Pc2_1n$ (No. 33) or Pcmn (No. 62) from the systematic absences. Space group $Pna2_1$ chosen from successful solution and refinement analysis (after transformation from the non-standard setting).

In the refinement, all H atoms were allowed for as riding atoms with C—H distances of 0.93 Å and 0.97 Å for the aromatic and methylene C—H (at 294 K).

The top five peaks in the final difference maps (+0.60 to +0.40 e.$Å^{-3}$) are within 0.90 Å of the Fe atom.

Figures

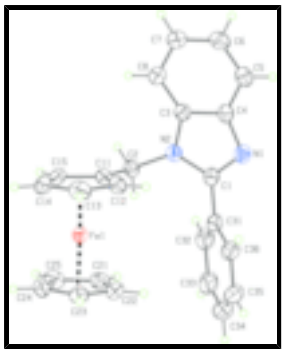

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

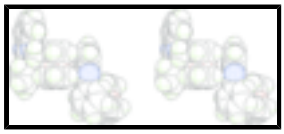

Fig. 2. A stereoview of the main $_{cp}$C—H···π-(C═N) interaction in the crystal structure with atoms depicted as their van der Waals spheres.

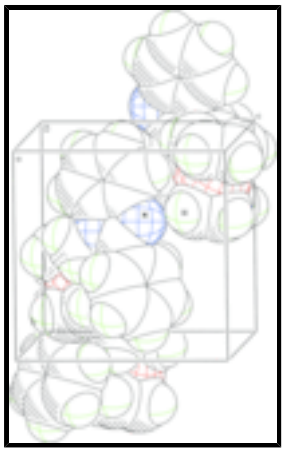

Fig. 3. A view of the C—H···N contact in the crystal structure with the N1 atom represented by a '*' and with H24 by a '#' located at symmetry position 1 − *x*,-*y*,-1/2 + *z*, (atoms depicted as for Fig. 2).

1-Ferrocenylmethyl-2-phenyl-1*H*-1,3-benzimidazole

Crystal data

$[Fe(C_5H_5)(C_{19}H_{15}N_2)]$	D_x = 1.409 Mg m^{-3}
M_r = 392.27	Melting point: 407 K
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 47 reflections
a = 11.6323 (12) Å	θ = 7.0–35.6º
b = 13.7738 (10) Å	μ = 0.83 mm^{-1}
c = 11.5398 (7) Å	*T* = 294 (1) K
V = 1848.9 (3) Å^3	Block, red
Z = 4	0.50 × 0.50 × 0.35 mm
F_{000} = 816	

Data collection

Bruker P4 diffractometer	R_{int} = 0.029
Radiation source: X-ray tube	θ_{max} = 28.0º
Monochromator: graphite	θ_{min} = 2.3º
T = 294(1) K	h = 0→15
ω scans	k = 0→18
Absorption correction: ψ scan (North *et al.*, 1968)	l = −15→1
T_{min} = 0.683, T_{max} = 0.761	3 standard reflections
3270 measured reflections	every 197 reflections
2555 independent reflections	intensity decay: 0.5%
2435 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.0565P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.093	$(\Delta/\sigma)_{max} < 0.001$
S = 1.09	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
2555 reflections	$\Delta\rho_{min}$ = −0.26 e Å^{-3}
244 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 207 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (2)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}
Fe1	0.81242 (3)	0.03598 (2)	0.24237 (5)	0.04083 (11)
N1	0.52595 (19)	−0.17950 (18)	0.5475 (2)	0.0498 (5)
N2	0.71032 (18)	−0.15801 (17)	0.4965 (2)	0.0440 (5)
C1	0.6004 (2)	−0.18169 (18)	0.4623 (3)	0.0440 (5)
C2	0.81119 (19)	−0.1389 (2)	0.4244 (3)	0.0455 (6)
C3	0.7034 (2)	−0.1362 (2)	0.6134 (3)	0.0464 (5)
C4	0.5876 (2)	−0.15079 (19)	0.6437 (3)	0.0467 (5)
C5	0.5527 (3)	−0.1356 (2)	0.7572 (3)	0.0566 (7)
C6	0.6312 (3)	−0.1046 (2)	0.8361 (3)	0.0638 (8)
C7	0.7468 (3)	−0.0896 (3)	0.8057 (3)	0.0680 (9)
C8	0.7846 (3)	−0.1045 (3)	0.6928 (3)	0.0606 (8)
C11	0.8254 (2)	−0.03259 (19)	0.4000 (3)	0.0437 (6)
C12	0.7383 (3)	0.0407 (2)	0.4034 (3)	0.0512 (6)

C13	0.7909 (4)	0.1313 (2)	0.3750 (3)	0.0649 (8)
C14	0.9097 (3)	0.1143 (2)	0.3543 (3)	0.0635 (8)
C15	0.9307 (2)	0.0137 (3)	0.3697 (3)	0.0567 (7)
C21	0.7798 (3)	−0.0671 (2)	0.1200 (3)	0.0588 (7)
C22	0.6901 (3)	0.0032 (3)	0.1212 (3)	0.0591 (7)
C23	0.7390 (3)	0.0943 (2)	0.0966 (3)	0.0557 (7)
C24	0.8585 (3)	0.0820 (2)	0.0807 (3)	0.0542 (7)
C25	0.8831 (3)	−0.0172 (2)	0.0952 (3)	0.0564 (7)
C31	0.5694 (2)	−0.2044 (2)	0.3413 (2)	0.0484 (6)
C32	0.6256 (3)	−0.2752 (3)	0.2775 (3)	0.0641 (8)
C33	0.5939 (4)	−0.2929 (4)	0.1637 (4)	0.0829 (13)
C34	0.5049 (5)	−0.2420 (4)	0.1146 (4)	0.0933 (14)
C35	0.4467 (4)	−0.1738 (4)	0.1776 (4)	0.0842 (13)
C36	0.4770 (3)	−0.1544 (3)	0.2923 (3)	0.0632 (8)
H2A	0.8036	−0.1737	0.3518	0.055*
H2B	0.8793	−0.1629	0.4635	0.055*
H5	0.4768	−0.1464	0.7790	0.068*
H6	0.6079	−0.0930	0.9119	0.077*
H7	0.7989	−0.0695	0.8619	0.082*
H8	0.8606	−0.0936	0.6715	0.073*
H12	0.6611	0.0311	0.4211	0.061*
H13	0.7539	0.1910	0.3707	0.078*
H14	0.9641	0.1609	0.3342	0.076*
H15	1.0014	−0.0169	0.3614	0.068*
H21	0.7719	−0.1334	0.1331	0.071*
H22	0.6128	−0.0090	0.1357	0.071*
H23	0.6993	0.1527	0.0915	0.067*
H24	0.9113	0.1307	0.0639	0.065*
H25	0.9555	−0.0454	0.0893	0.068*
H32	0.6848	−0.3108	0.3112	0.077*
H33	0.6330	−0.3394	0.1205	0.100*
H34	0.4841	−0.2540	0.0381	0.112*
H35	0.3862	−0.1400	0.1436	0.101*
H36	0.4364	−0.1088	0.3354	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.03973 (17)	0.03969 (17)	0.04307 (18)	−0.00482 (11)	−0.00106 (18)	0.00165 (16)
N1	0.0424 (10)	0.0536 (11)	0.0533 (11)	−0.0006 (9)	0.0036 (9)	−0.0052 (10)
N2	0.0394 (9)	0.0446 (11)	0.0479 (11)	−0.0005 (8)	0.0016 (9)	0.0027 (9)
C1	0.0422 (11)	0.0374 (11)	0.0524 (12)	−0.0008 (10)	0.0007 (11)	0.0003 (10)
C2	0.0395 (12)	0.0473 (13)	0.0496 (13)	0.0019 (10)	0.0035 (10)	0.0042 (11)
C3	0.0469 (13)	0.0450 (12)	0.0472 (13)	−0.0029 (10)	−0.0008 (11)	0.0051 (11)
C4	0.0425 (12)	0.0437 (12)	0.0541 (14)	0.0001 (10)	0.0037 (11)	−0.0008 (11)
C5	0.0570 (14)	0.0573 (14)	0.0556 (18)	0.0027 (12)	0.0117 (13)	−0.0037 (13)
C6	0.079 (2)	0.0670 (18)	0.0453 (14)	0.0004 (17)	0.0054 (15)	−0.0046 (13)
C7	0.071 (2)	0.082 (2)	0.0516 (17)	−0.0148 (18)	−0.0088 (17)	−0.0010 (15)

C8	0.0550 (15)	0.0713 (19)	0.0554 (15)	−0.0145 (15)	−0.0069 (15)	0.0059 (15)
C11	0.0456 (13)	0.0452 (15)	0.0405 (13)	−0.0041 (10)	−0.0001 (11)	0.0026 (10)
C12	0.0565 (16)	0.0510 (16)	0.0459 (14)	0.0001 (12)	0.0054 (13)	−0.0011 (11)
C13	0.096 (2)	0.0422 (14)	0.0565 (17)	−0.0031 (15)	0.0000 (17)	−0.0065 (13)
C14	0.0739 (19)	0.0588 (16)	0.0580 (16)	−0.0298 (15)	−0.0114 (15)	−0.0013 (14)
C15	0.0453 (13)	0.0701 (18)	0.0545 (15)	−0.0166 (13)	−0.0132 (12)	0.0096 (14)
C21	0.083 (2)	0.0484 (14)	0.0450 (14)	−0.0119 (16)	−0.0039 (15)	−0.0021 (12)
C22	0.0532 (16)	0.071 (2)	0.0530 (16)	−0.0131 (14)	−0.0077 (13)	−0.0035 (16)
C23	0.0563 (16)	0.0576 (16)	0.0533 (14)	0.0049 (14)	−0.0067 (13)	0.0069 (13)
C24	0.0517 (14)	0.0581 (16)	0.0527 (15)	−0.0075 (14)	0.0048 (12)	0.0105 (13)
C25	0.0615 (18)	0.0568 (15)	0.0509 (15)	0.0149 (15)	0.0064 (15)	0.0019 (13)
C31	0.0476 (13)	0.0488 (12)	0.0488 (13)	−0.0123 (11)	0.0005 (11)	−0.0016 (10)
C32	0.0659 (18)	0.0621 (17)	0.0642 (18)	−0.0134 (15)	0.0092 (14)	−0.0154 (15)
C33	0.084 (2)	0.093 (3)	0.072 (2)	−0.037 (2)	0.015 (2)	−0.031 (2)
C34	0.109 (3)	0.116 (3)	0.0549 (17)	−0.058 (3)	−0.006 (2)	−0.010 (2)
C35	0.082 (3)	0.094 (3)	0.076 (2)	−0.034 (2)	−0.031 (2)	0.022 (2)
C36	0.0640 (17)	0.0597 (18)	0.0658 (18)	−0.0129 (15)	−0.0125 (16)	0.0054 (15)

Geometric parameters (Å, °)

Fe1—C11	2.055 (3)	C22—C23	1.407 (5)
Fe1—C12	2.050 (3)	C23—C24	1.411 (4)
Fe1—C13	2.031 (3)	C24—C25	1.407 (5)
Fe1—C14	2.028 (3)	C31—C32	1.385 (4)
Fe1—C15	2.036 (3)	C31—C36	1.396 (4)
Fe1—C21	2.038 (3)	C32—C33	1.386 (6)
Fe1—C22	2.046 (3)	C33—C34	1.373 (8)
Fe1—C23	2.050 (3)	C34—C35	1.367 (7)
Fe1—C24	2.041 (3)	C35—C36	1.397 (5)
Fe1—C25	2.024 (3)	C2—H2A	0.9700
N1—C1	1.310 (4)	C2—H2B	0.9700
N1—C4	1.379 (4)	C5—H5	0.9300
N2—C1	1.378 (3)	C6—H6	0.9300
N2—C2	1.462 (3)	C7—H7	0.9300
N2—C3	1.384 (4)	C8—H8	0.9300
C1—C31	1.476 (4)	C12—H12	0.9300
C2—C11	1.501 (4)	C13—H13	0.9300
C3—C4	1.406 (4)	C14—H14	0.9300
C3—C8	1.386 (4)	C15—H15	0.9300
C4—C5	1.388 (4)	C21—H21	0.9300
C5—C6	1.358 (5)	C22—H22	0.9300
C6—C7	1.406 (6)	C23—H23	0.9300
C7—C8	1.390 (5)	C24—H24	0.9300
C11—C12	1.431 (4)	C25—H25	0.9300
C11—C15	1.424 (4)	C32—H32	0.9300
C12—C13	1.428 (4)	C33—H33	0.9300
C13—C14	1.422 (5)	C34—H34	0.9300
C14—C15	1.418 (5)	C35—H35	0.9300
C21—C22	1.423 (5)	C36—H36	0.9300

C21—C25	1.414 (5)		
C25—Fe1—C14	120.02 (16)	C13—C14—Fe1	69.63 (18)
C25—Fe1—C13	156.34 (16)	C14—C15—C11	108.7 (3)
C14—Fe1—C13	41.00 (15)	C14—C15—Fe1	69.29 (17)
C25—Fe1—C15	106.06 (15)	C11—C15—Fe1	70.35 (17)
C14—Fe1—C15	40.84 (14)	C25—C21—C22	107.1 (3)
C13—Fe1—C15	68.71 (16)	C25—C21—Fe1	69.11 (19)
C25—Fe1—C21	40.72 (15)	C22—C21—Fe1	69.88 (19)
C14—Fe1—C21	156.31 (17)	C23—C22—C21	108.0 (3)
C13—Fe1—C21	161.63 (15)	C23—C22—Fe1	70.10 (18)
C15—Fe1—C21	121.40 (15)	C21—C22—Fe1	69.34 (18)
C25—Fe1—C24	40.48 (14)	C22—C23—C24	108.5 (3)
C14—Fe1—C24	105.66 (14)	C22—C23—Fe1	69.72 (19)
C13—Fe1—C24	121.30 (15)	C24—C23—Fe1	69.49 (17)
C15—Fe1—C24	121.92 (13)	C25—C24—C23	107.5 (3)
C21—Fe1—C24	68.44 (14)	C25—C24—Fe1	69.10 (17)
C25—Fe1—C22	68.20 (15)	C23—C24—Fe1	70.17 (17)
C14—Fe1—C22	160.24 (16)	C24—C25—C21	108.9 (3)
C13—Fe1—C22	124.90 (16)	C24—C25—Fe1	70.42 (17)
C15—Fe1—C22	158.44 (16)	C21—C25—Fe1	70.17 (18)
C21—Fe1—C22	40.78 (16)	C32—C31—C36	119.7 (3)
C24—Fe1—C22	68.07 (14)	C32—C31—C1	122.4 (3)
C25—Fe1—C12	160.58 (12)	C36—C31—C1	117.8 (3)
C14—Fe1—C12	68.94 (14)	C31—C32—C33	120.1 (4)
C13—Fe1—C12	40.96 (13)	C34—C33—C32	120.1 (4)
C15—Fe1—C12	68.59 (13)	C35—C34—C33	120.3 (4)
C21—Fe1—C12	124.88 (13)	C34—C35—C36	120.7 (5)
C24—Fe1—C12	158.24 (13)	C31—C36—C35	118.9 (4)
C22—Fe1—C12	109.52 (14)	N2—C2—H2A	109.3
C25—Fe1—C23	67.80 (14)	C11—C2—H2A	109.3
C14—Fe1—C23	123.13 (15)	N2—C2—H2B	109.3
C13—Fe1—C23	108.29 (15)	C11—C2—H2B	109.3
C15—Fe1—C23	158.81 (13)	H2A—C2—H2B	107.9
C21—Fe1—C23	68.08 (14)	C6—C5—H5	120.5
C24—Fe1—C23	40.35 (13)	C4—C5—H5	120.5
C22—Fe1—C23	40.18 (15)	C5—C6—H6	119.3
C12—Fe1—C23	123.80 (13)	C7—C6—H6	119.3
C25—Fe1—C11	123.12 (12)	C8—C7—H7	119.5
C14—Fe1—C11	68.90 (13)	C6—C7—H7	119.5
C13—Fe1—C11	68.87 (13)	C3—C8—H8	121.6
C15—Fe1—C11	40.76 (11)	C7—C8—H8	121.6
C21—Fe1—C11	107.86 (13)	C13—C12—H12	126.1
C24—Fe1—C11	158.77 (12)	C11—C12—H12	126.1
C22—Fe1—C11	123.68 (14)	Fe1—C12—H12	126.9
C12—Fe1—C11	40.81 (12)	C14—C13—H13	125.9
C23—Fe1—C11	159.53 (12)	C12—C13—H13	125.9
C1—N1—C4	105.5 (2)	Fe1—C13—H13	126.1
C1—N2—C2	128.7 (2)	C15—C14—H14	126.1
C1—N2—C3	106.1 (2)	C13—C14—H14	126.1

C2—N2—C3	124.2 (2)	Fe1—C14—H14	126.0
N1—C1—N2	113.1 (2)	C14—C15—H15	125.6
N1—C1—C31	123.6 (2)	C11—C15—H15	125.6
N2—C1—C31	123.2 (2)	Fe1—C15—H15	126.3
N2—C2—C11	111.8 (2)	C25—C21—H21	126.4
N2—C3—C4	105.5 (3)	C22—C21—H21	126.4
N2—C3—C8	132.3 (3)	Fe1—C21—H21	126.1
C4—C3—C8	122.2 (3)	C23—C22—H22	126.0
N1—C4—C3	109.8 (3)	C21—C22—H22	126.0
N1—C4—C5	130.6 (3)	Fe1—C22—H22	126.1
C3—C4—C5	119.6 (3)	C22—C23—H23	125.7
C6—C5—C4	118.9 (3)	C24—C23—H23	125.7
C5—C6—C7	121.5 (3)	Fe1—C23—H23	126.6
C6—C7—C8	121.0 (3)	C25—C24—H24	126.2
C3—C8—C7	116.8 (3)	C23—C24—H24	126.2
C12—C11—C15	107.4 (3)	Fe1—C24—H24	126.1
C15—C11—C2	125.3 (3)	C24—C25—H25	125.6
C12—C11—C2	127.3 (2)	C21—C25—H25	125.6
C15—C11—Fe1	68.90 (18)	Fe1—C25—H25	125.4
C12—C11—Fe1	69.41 (17)	C31—C32—H32	119.9
C2—C11—Fe1	127.4 (2)	C33—C32—H32	119.9
C13—C12—C11	107.8 (3)	C34—C33—H33	120.0
C13—C12—Fe1	68.8 (2)	C32—C33—H33	120.0
C11—C12—Fe1	69.77 (18)	C35—C34—H34	119.8
C14—C13—C12	108.2 (3)	C33—C34—H34	119.8
C14—C13—Fe1	69.37 (19)	C34—C35—H35	119.6
C12—C13—Fe1	70.22 (18)	C36—C35—H35	119.6
C15—C14—C13	107.9 (3)	C31—C36—H36	120.5
C15—C14—Fe1	69.87 (17)	C35—C36—H36	120.5
C4—N1—C1—N2	1.4 (3)	C4—C5—C6—C7	−1.3 (5)
C4—N1—C1—C31	−176.9 (3)	C5—C6—C7—C8	1.2 (6)
C3—N2—C1—N1	−1.8 (3)	N2—C3—C8—C7	180.0 (3)
C2—N2—C1—N1	−170.1 (3)	C4—C3—C8—C7	1.5 (5)
C3—N2—C1—C31	176.5 (2)	C6—C7—C8—C3	−1.2 (6)
C2—N2—C1—C31	8.2 (4)	N2—C2—C11—C15	156.6 (3)
C1—N2—C2—C11	93.8 (3)	N2—C2—C11—C12	−22.7 (4)
C3—N2—C2—C11	−72.6 (3)	N2—C2—C11—Fe1	−114.2 (3)
C1—N2—C3—C8	−177.3 (3)	N1—C1—C31—C32	−127.7 (3)
C2—N2—C3—C8	−8.3 (5)	N2—C1—C31—C32	54.1 (4)
C1—N2—C3—C4	1.4 (3)	N1—C1—C31—C36	49.9 (4)
C2—N2—C3—C4	170.4 (2)	N2—C1—C31—C36	−128.2 (3)
C1—N1—C4—C5	179.5 (3)	C36—C31—C32—C33	3.1 (5)
C1—N1—C4—C3	−0.4 (3)	C1—C31—C32—C33	−179.3 (3)
N2—C3—C4—N1	−0.6 (3)	C31—C32—C33—C34	−1.5 (6)
C8—C3—C4—N1	178.2 (3)	C32—C33—C34—C35	−0.3 (6)
N2—C3—C4—C5	179.4 (3)	C33—C34—C35—C36	0.4 (6)
C8—C3—C4—C5	−1.7 (4)	C32—C31—C36—C35	−2.9 (4)
N1—C4—C5—C6	−178.3 (3)	C1—C31—C36—C35	179.4 (3)
C3—C4—C5—C6	1.6 (4)	C34—C35—C36—C31	1.2 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C23—H23···N1^{i}	0.93	2.69	3.346 (4)	128
C24—H24···Cg^{ii}	0.93	2.90	3.556 (3)	129

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

Fig. 1

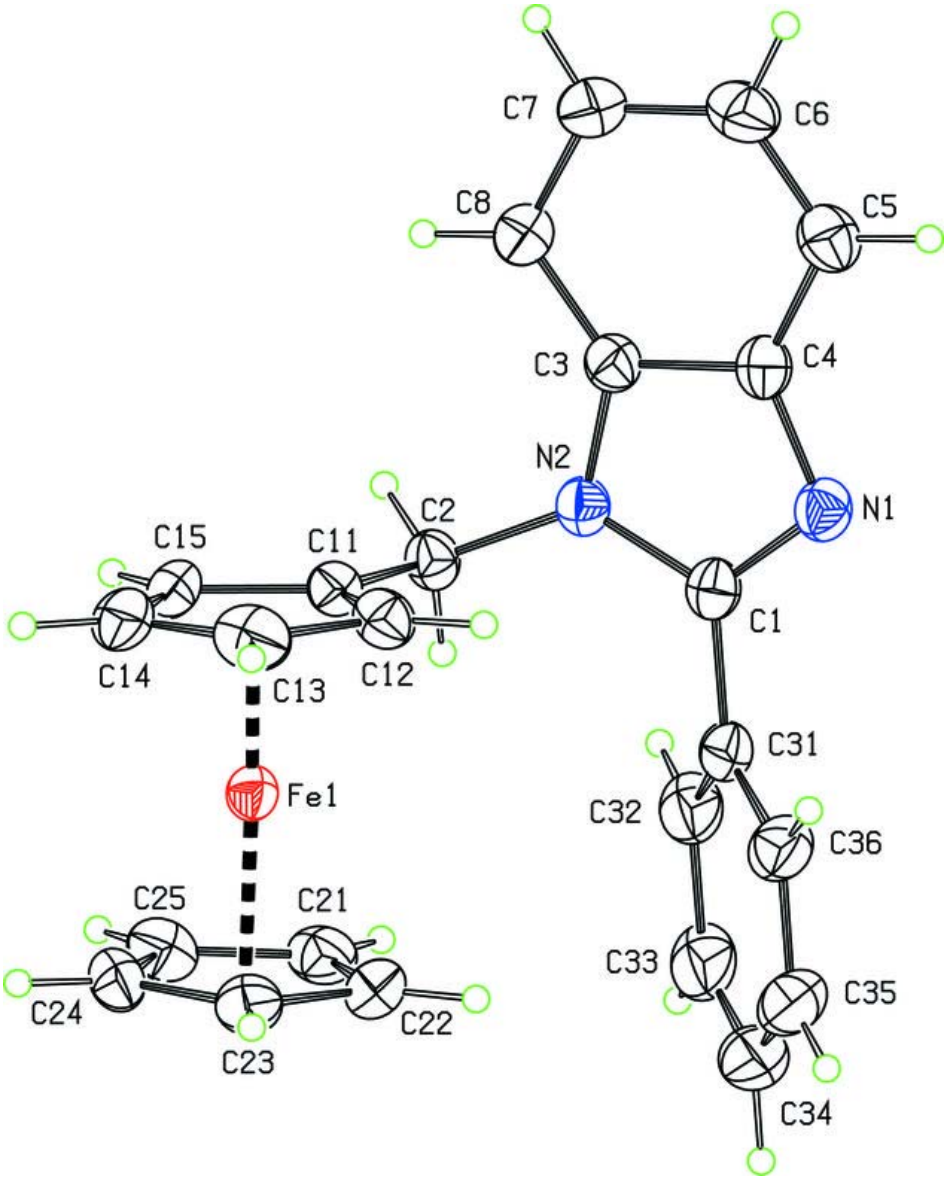

Fig. 2

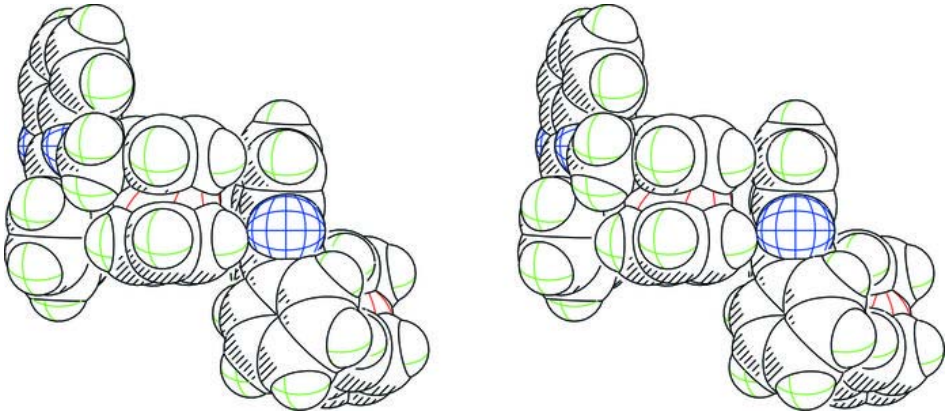

Fig. 3