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1′-Acetylferrocene-1-carbonitrile

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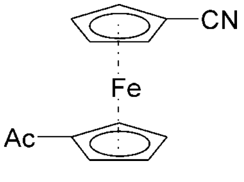
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.082; data-to-parameter ratio = 16.4.

In the title compound, $[Fe(C_6H_4N)(C_7H_7O)]$, the two cyclopentadienyl rings are nearly parallel, making a dihedral angle of 2.3 (1) Å, and are almost eclipsed as viewed down the normal to each ring. In the crystal structure, the molecules are stacked along the b axis, with a short distance of 3.749 (1) Å between the centroids of the cyclopentadienyl rings of neighbouring molecules. Weak intermolecular C—H···N and C—H···O hydrogen bonds link these stacks into two-dimensional sheets parallel to the bc plane.

Related literature

Transition metal complexes bearing a strongly electron-withdrawing cyano group at the cyclopentadienyl ring are relatively sparse and only three related structures have been published previously: (η^5-cyanocyclopentadienyl)-(η^4-tetraphenylcyclobutadiene)cobalt (Villa *et al.*, 1974), (η^5-cyanocyclopentadienyl)dicarbonylnitrosylchromium (Rogers *et al.*, 1988) and cyanoferrocene (Bell *et al.*, 1996). For related literature dealing with acetyl- and cyano-substituted ferrocenes, see: Nesmeyanov *et al.* (1962); Palenik (1970); Šťáva *et al.* (2007).



Experimental

Crystal data

$[Fe(C_6H_4N)(C_7H_7O)]$
M_r = 253.08
Triclinic, $P\overline{1}$
a = 5.7610 (5) Å
b = 6.8431 (5) Å
c = 14.1940 (14) Å
α = 99.264 (7)°
β = 99.666 (6)°
γ = 104.277 (7)°
V = 522.45 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 150 (1) K
0.16 × 0.10 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: integration (Gaussian; Coppens *et al.*, 1970)
$T_{\min}$ = 0.801, $T_{\max}$ = 0.931
6982 measured reflections
2383 independent reflections
2151 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.082
S = 1.08
2383 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.45 e Å^{-3}
$\Delta\rho_{\min}$ = −0.59 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N1$^{\rm i}$	0.93	2.72	3.411 (3)	132
C9—H9···N1$^{\rm i}$	0.93	2.73	3.463 (3)	137
C11—H11···O1$^{\rm ii}$	0.93	2.59	3.514 (3)	178

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+2, -y, -z$.

Table 2
Selected geometric parameters (Å, °).

Fe1···$Cg1$	1.6505 (10)
Fe1···$Cg2$	1.6479 (10)
$Cg2$···$Cg1^{\rm iii}$	3.749 (1)

$Cg1$ and $Cg2$ are the centroids defined by atoms C1–C5 and C8–C12, respectively. Symmetry code: (iii) $x, y+1, z$.

Data collection: *COLLECT* (Hooft, 1998) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *COLLECT* and *DENZO*; data reduction: *COLLECT* and *DENZO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2275).

References

Allen, F. H., Johnson, O., Shields, G. P., Smith, B. R. & Towler, M. (2004). *J. Appl. Cryst.* **37**, 335–338.
Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Bell, W., Ferguson, G. & Glidewell, C. (1996). *Acta Cryst.* C**52**, 1928–1930.
Coppens, P., Ahmed, F. R., Hall, S. R. & Huber, C. P. (1970). Editors. *Crystallographic Computing*. Copenhagen: Munksgaard.
Hooft, R. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Nesmeyanov, A. N., Perevalova, E. G., Yuryeva, L. P. & Grandberg, K. I. (1962). *Izv. Akad. Nauk. SSSR Ser. Khim.* pp. 1772–1777.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Palenik, G. J. (1970). *Inorg. Chem.* **9**, 2424–2430.

Rogers, R. D., Shakir, R., Atwood, J. L., Macomber, D. W., Wang, Y.-P. & Rausch, M. D. (1988). *J. Crystallogr. Spectrosc. Res.* **18**, 767–778.

Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Šťáva, V., Erben, M., Veselý, D. & Kalenda, P. (2007). *J. Phys. Chem. Solids*, **68**, 799–802.

Villa, A. C., Coghi, L., Manfredotti, A. G. & Guastini, C. (1974). *Acta Cryst.* B**30**, 2101–2112.

m2146 Erben *et al.* • [Fe(C_6H_4N)(C_7H_7O)] *Acta Cryst.* (2007). E**63**, m2145–m2146

supplementary materials

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1'-Acetylferrocene-1-carbonitrile

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Comment

Ferrocenes are well known class of organometallic compounds and the wealth of its derivatives is described in literature. Ferrocene compounds are widely used in homogenous catalysis, organic or organometallic synthesis and in material science. In last three years, utilization of ferrocene derivatives in drying of oxidizable paints has been investigated, and it was observed that ferrocenes bearing electron-withdrawing substituents showed the highest activity in drying processes Šťáva *et al.*, 2007). In the framework of investigation of ferrocene derivatives we prepared, spectroscopically characterized the title compound (I) and determined its molecular structure in the solid state.

Figure 1 shows typical sandwich structure of (I) with cyclopentadienyl ligands being very close to be eclipsed. The dihedral angle between a ring carbon, the two ring centroids and the carbon atom of opposite ring varies from 6.9 (2) to 8.2 (2)°. The exocyclic bond lengths C8—C13 and C1—C6 of 1.429 (3) Å and 1.466 (3) Å, respectively, are very close to those found in cyanoferrocene [1.432 (6) Å, (Bell *et al.*, 1996)] and diacetylferrocene [1.747 (8) Å, 1.768 (8) Å (Palenik, 1970)]. The interatomic distances and angles in the molecule of (I) are comparable to those observed for similar ferrocene derivatives, the principial interest lies in the intermolecular interactions.

The ring Cp2 of molecule at (x, y, z) is nearly coplanar with ring Cp1 of the molecule at $(x, 1 + y, z)$ with dihedral angle of 2.3 (1)°. The distance between the centriods of Cp rings was found to be 3.749 (1) Å indicating significant intermolecular $\pi\cdots\pi$ interaction between neighboring molecules of (I) along *b* axis.. Atom N1 in the molecule at (x, y, z) acts as hydrogen-bond acceptor from cyclopentadienyl carbon atoms C4 and C9 of the molecule at $(2 - x, 1 - y, 1 - z)$, *i.e.* (i), with C···N distances of 3.411 (3) and 3.464 (3) Å, respectively. Simultaneously, N1$^{\rm i}$ atom serves as hydrogen-bond acceptor from atoms C4 and C9 of molecule at (x, y, z) generating molecular pairs connected by four C—H···N hydrogen bonds. Thus each nitrogen atom exhibits trigonal coordination; an angle H4$^{\rm i}$···N1···H9$^{\rm i}$ was found to be 73°. Oxygen atom O1 of acetyl group also participates in intermolecular interactions, being hydrogen-bond acceptor from atom C11 of the molecule at $(2 - x, - y, - z)$. Reversely, atom C11 in the molecule at (x, y, z) acts as donor to the oxygen atom of the molecule at $(2 - x, - y, - z)$. Figure 2 depicts three molecules of (I) interconnected by weak hydrogen bonds.

The interplay of $\pi\cdots\pi$ stacking and weak hydrogen bonds is responsible for the observed structure giving two-dimensional sheets parallel to *bc*-plane

Experimental

The title compound (I) was synthesized by direct cyanation of acetylferrocene following published procedure (Nesmeyanov *et al.*, 1962). Melting point, IR, Raman and NMR spectra confirmed identity and purity of prepared compound. Crystals of (I) suitable for X-ray diffraction analysis were grown by sublimation in sealed ampoule at 0.1 Pa and 353 K.

Refinement

All H atoms were positioned geometrically and refined as riding on their parent C atoms, with C—H = 0.93 Å, U_{iso}(H) = 1.2Ueq(C) and C—H = 0.96 Å, U_{iso}(H) = 1.5Ueq(C) for cyclopentadienyl and methyl H atoms, respectively.

Figures

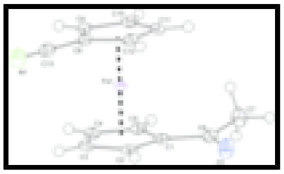


Fig. 1. *ORTEP* view of the title compound (I) with displacement ellipsoids drawn at the 50% probability.

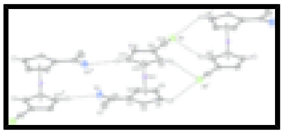


Fig. 2. A view of three molecules of (I) linked by weak C—H···N and C—H···O hydrogen bonds (dashed lines). H atoms not involved in contacts have been omitted. [Symmetry codes: (i) $2 - x$, $1 - y$, $1 - z$; (ii) $2 - x$, $- y$, $- z$]

1'-Acetylferrocene-1-carbonitrile

Crystal data

$[Fe(C_6H_4N)(C_7H_7O)]$	$Z = 2$
$M_r = 253.08$	$F_{000} = 260$
Triclinic, $P\overline{1}$	$D_x = 1.609$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 370 K
$a = 5.7610$ (5) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 6.8431$ (5) Å	Cell parameters from 7054 reflections
$c = 14.1940$ (14) Å	$\theta = 1–27.5°$
$\alpha = 99.264$ (7)°	$\mu = 1.42$ mm^{-1}
$\beta = 99.666$ (6)°	$T = 150$ (1) K
$\gamma = 104.277$ (7)°	Plate, red
$V = 522.45$ (8) Å^3	0.16 × 0.10 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	2383 independent reflections
Monochromator: graphite	2151 reflections with $I > 2\sigma(I)$
Detector resolution: 9.091 pixels mm^{-1}	$R_{int} = 0.052$
$T = 150(1)$ K	$\theta_{max} = 27.5°$
φ and ω scans to fill the Ewald sphere	$\theta_{min} = 3.7°$
Absorption correction: integration (Gaussian; Coppens *et al.*, 1970)	$h = -7\rightarrow7$
$T_{min} = 0.801$, $T_{max} = 0.931$	$k = -8\rightarrow8$
6982 measured reflections	$l = -18\rightarrow18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.032$	H-atom parameters constrained
$wR(F^2) = 0.082$	$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2 + 0.3168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
2383 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
145 parameters	$\Delta\rho_{min} = -0.59$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Melting point: 370–371 K. Spectroscopic analysis: ^{1}H NMR ($CDCl_3$, δ, p.p.m.): 2.40 (s, 3H), 4.40 (s, 2H), 4.62 (s, 4H), 4.87 (s, 2H). ^{13}C NMR ($CDCl_3$, δ, p.p.m.): 27.9, 53.9, 71.8, 72.4, 73.2, 74.5, 81.3, 118.9, 200.9. Uv-Vis (cyclohexane, maxima at nm): 447, 350s h, 314s h. IR (KBr disc, cm^{-1}): 3121 (*m*), 3104 (*m*), 3092 (*m*), 3078 (*s*), 2925 (*m*), 2856 (*m*), 2231 (*versus*), 1655 (*versus*), 1455 (*s*), 1400 (*m*), 1375 (*s*), 1356 (*m*), 1279 (*versus*), 1235 (*m*), 1117 (*m*), 1069 (w), 1039 (*m*), 966 (w), 917 (*m*), 896 (*m*), 854 (w), 833 (*s*), 667 (w), 623 (*m*), 556 (*s*), 527 (*s*), 512 (*m*), 483 (*s*). Raman (quartz capillary, cm^{-1}): 3122 (*m*), 3108 (*s*), 3092 (w), 3077 (*m*), 2925 (*m*), 2232 (*versus*), 1654 (*versus*), 1457 (w), 1446 (*m*), 1401 (w), 1378 (w), 1283 (*m*), 1234 (*s*), 1119 (*m*), 1077 (*m*), 1042 (*m*), 1034 (*m*), 917 (w), 673 (*m*), 641 (*m*), 625 (w), 555 (w), 527 (w), 483 (w), 358 (*m*), 314 (*versus*), 218 (*m*), 186 (*m*), 115 (*m*).

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 > 2sigma(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}
Fe1	0.92112 (5)	0.18493 (4)	0.26947 (2)	0.01257 (10)
C12	1.0895 (4)	0.4420 (3)	0.22364 (15)	0.0183 (4)
H12	1.2460	0.4734	0.2108	0.022*
O1	1.1803 (3)	−0.1467 (3)	0.09502 (12)	0.0281 (4)
C4	0.8082 (4)	−0.0211 (3)	0.35489 (16)	0.0192 (4)
H4	0.7015	−0.0130	0.3969	0.023*
C7	0.7473 (4)	−0.2488 (4)	0.03850 (17)	0.0277 (5)
H7A	0.7866	−0.2852	−0.0239	0.042*
H7B	0.6589	−0.1471	0.0362	0.042*

H7C	0.6478	−0.3693	0.0537	0.042*
C1	0.9600 (4)	−0.0971 (3)	0.21714 (15)	0.0151 (4)
C9	0.7666 (4)	0.4179 (3)	0.30431 (15)	0.0180 (4)
H9	0.6772	0.4308	0.3526	0.022*
C10	0.6706 (4)	0.3170 (3)	0.20418 (15)	0.0184 (4)
H10	0.5061	0.2521	0.1757	0.022*
C5	0.7397 (4)	−0.1180 (3)	0.25418 (15)	0.0163 (4)
H5	0.5806	−0.1833	0.2185	0.020*
C3	1.0686 (4)	0.0617 (3)	0.38067 (15)	0.0191 (4)
H3	1.1604	0.1340	0.4422	0.023*
C11	0.8676 (4)	0.3322 (3)	0.15519 (15)	0.0184 (4)
H11	0.8538	0.2791	0.0893	0.022*
C2	1.1633 (4)	0.0151 (3)	0.29684 (15)	0.0171 (4)
H2	1.3279	0.0508	0.2937	0.021*
C6	0.9806 (4)	−0.1621 (3)	0.11602 (15)	0.0184 (4)
N1	1.3441 (4)	0.6917 (3)	0.47474 (15)	0.0311 (5)
C8	1.0275 (4)	0.4956 (3)	0.31641 (15)	0.0173 (4)
C13	1.2006 (4)	0.6036 (3)	0.40509 (16)	0.0212 (4)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.01291 (15)	0.01076 (16)	0.01458 (16)	0.00420 (11)	0.00143 (10)	0.00445 (10)
C12	0.0214 (10)	0.0129 (9)	0.0237 (11)	0.0062 (8)	0.0075 (8)	0.0078 (8)
O1	0.0228 (8)	0.0363 (10)	0.0250 (8)	0.0086 (7)	0.0077 (7)	0.0026 (7)
C4	0.0236 (11)	0.0160 (10)	0.0217 (10)	0.0069 (8)	0.0075 (8)	0.0101 (8)
C7	0.0257 (12)	0.0293 (12)	0.0219 (11)	0.0039 (10)	−0.0006 (9)	0.0000 (9)
C1	0.0154 (9)	0.0094 (9)	0.0209 (10)	0.0044 (7)	0.0026 (8)	0.0044 (8)
C9	0.0213 (10)	0.0159 (10)	0.0208 (10)	0.0099 (8)	0.0059 (8)	0.0063 (8)
C10	0.0165 (10)	0.0178 (10)	0.0224 (11)	0.0082 (8)	0.0001 (8)	0.0073 (8)
C5	0.0155 (9)	0.0111 (9)	0.0219 (10)	0.0021 (7)	0.0027 (8)	0.0061 (8)
C3	0.0251 (11)	0.0162 (10)	0.0169 (10)	0.0087 (8)	−0.0003 (8)	0.0067 (8)
C11	0.0248 (11)	0.0165 (10)	0.0169 (10)	0.0086 (8)	0.0037 (8)	0.0083 (8)
C2	0.0145 (9)	0.0149 (10)	0.0237 (10)	0.0067 (8)	0.0014 (8)	0.0077 (8)
C6	0.0212 (10)	0.0130 (9)	0.0196 (10)	0.0037 (8)	0.0027 (8)	0.0034 (8)
N1	0.0316 (11)	0.0258 (11)	0.0293 (11)	0.0040 (9)	−0.0009 (9)	0.0010 (9)
C8	0.0202 (10)	0.0121 (9)	0.0199 (10)	0.0054 (8)	0.0032 (8)	0.0039 (8)
C13	0.0244 (11)	0.0134 (10)	0.0254 (11)	0.0052 (9)	0.0049 (9)	0.0039 (8)

Geometric parameters (Å, °)

Fe1—C8	2.026 (2)	C7—H7A	0.9600
Fe1—C1	2.0332 (19)	C7—H7B	0.9600
Fe1—C5	2.036 (2)	C7—H7C	0.9600
Fe1—C9	2.042 (2)	C1—C5	1.438 (3)
Fe1—C12	2.049 (2)	C1—C2	1.440 (3)
Fe1—C2	2.052 (2)	C1—C6	1.466 (3)
Fe1—C10	2.055 (2)	C9—C10	1.426 (3)
Fe1—C4	2.060 (2)	C9—C8	1.436 (3)

Fe1—C11	2.062 (2)	C9—H9	0.9300
Fe1—C3	2.063 (2)	C10—C11	1.419 (3)
C12—C11	1.420 (3)	C10—H10	0.9300
C12—C8	1.436 (3)	C5—H5	0.9300
C12—H12	0.9300	C3—C2	1.413 (3)
O1—C6	1.221 (3)	C3—H3	0.9300
C4—C5	1.419 (3)	C11—H11	0.9300
C4—C3	1.426 (3)	C2—H2	0.9300
C4—H4	0.9300	N1—C13	1.145 (3)
C7—C6	1.506 (3)	C8—C13	1.429 (3)

C8—Fe1—C1	156.37 (9)	C6—C7—H7B	109.5
C8—Fe1—C5	160.78 (8)	H7A—C7—H7B	109.5
C1—Fe1—C5	41.38 (8)	C6—C7—H7C	109.5
C8—Fe1—C9	41.34 (8)	H7A—C7—H7C	109.5
C1—Fe1—C9	161.58 (8)	H7B—C7—H7C	109.5
C5—Fe1—C9	122.75 (8)	C5—C1—C2	107.46 (18)
C8—Fe1—C12	41.27 (8)	C5—C1—C6	127.67 (18)
C1—Fe1—C12	121.50 (8)	C2—C1—C6	124.73 (18)
C5—Fe1—C12	155.76 (9)	C5—C1—Fe1	69.43 (11)
C9—Fe1—C12	69.39 (8)	C2—C1—Fe1	70.06 (11)
C8—Fe1—C2	120.61 (8)	C6—C1—Fe1	122.50 (14)
C1—Fe1—C2	41.27 (8)	C10—C9—C8	107.00 (18)
C5—Fe1—C2	69.15 (8)	C10—C9—Fe1	70.11 (12)
C9—Fe1—C2	154.11 (9)	C8—C9—Fe1	68.71 (11)
C12—Fe1—C2	109.65 (8)	C10—C9—H9	126.5
C8—Fe1—C10	68.63 (8)	C8—C9—H9	126.5
C1—Fe1—C10	125.75 (8)	Fe1—C9—H9	126.2
C5—Fe1—C10	106.12 (8)	C11—C10—C9	108.71 (18)
C9—Fe1—C10	40.74 (8)	C11—C10—Fe1	70.12 (11)
C12—Fe1—C10	68.34 (8)	C9—C10—Fe1	69.15 (11)
C2—Fe1—C10	164.69 (9)	C11—C10—H10	125.6
C8—Fe1—C4	124.28 (9)	C9—C10—H10	125.6
C1—Fe1—C4	68.66 (8)	Fe1—C10—H10	126.7
C5—Fe1—C4	40.54 (8)	C4—C5—C1	107.80 (18)
C9—Fe1—C4	104.96 (8)	C4—C5—Fe1	70.63 (12)
C12—Fe1—C4	163.19 (9)	C1—C5—Fe1	69.19 (11)
C2—Fe1—C4	68.14 (8)	C4—C5—H5	126.1
C10—Fe1—C4	118.35 (9)	C1—C5—H5	126.1
C8—Fe1—C11	68.51 (8)	Fe1—C5—H5	125.7
C1—Fe1—C11	109.10 (8)	C2—C3—C4	108.44 (18)
C5—Fe1—C11	120.23 (8)	C2—C3—Fe1	69.49 (11)
C9—Fe1—C11	68.56 (8)	C4—C3—Fe1	69.65 (11)
C12—Fe1—C11	40.41 (8)	C2—C3—H3	125.8
C2—Fe1—C11	128.46 (9)	C4—C3—H3	125.8
C10—Fe1—C11	40.31 (8)	Fe1—C3—H3	126.7
C4—Fe1—C11	153.79 (9)	C10—C11—C12	108.58 (18)
C8—Fe1—C3	107.35 (8)	C10—C11—Fe1	69.56 (11)
C1—Fe1—C3	68.57 (8)	C12—C11—Fe1	69.28 (11)
C5—Fe1—C3	68.50 (8)	C10—C11—H11	125.7

C9—Fe1—C3	118.52 (9)	C12—C11—H11	125.7
C12—Fe1—C3	127.16 (9)	Fe1—C11—H11	127.0
C2—Fe1—C3	40.17 (8)	C3—C2—C1	107.97 (18)
C10—Fe1—C3	153.12 (9)	C3—C2—Fe1	70.34 (12)
C4—Fe1—C3	40.48 (8)	C1—C2—Fe1	68.68 (11)
C11—Fe1—C3	165.04 (9)	C3—C2—H2	126.0
C11—C12—C8	107.36 (18)	C1—C2—H2	126.0
C11—C12—Fe1	70.31 (11)	Fe1—C2—H2	126.5
C8—C12—Fe1	68.50 (11)	O1—C6—C1	121.19 (19)
C11—C12—H12	126.3	O1—C6—C7	120.82 (19)
C8—C12—H12	126.3	C1—C6—C7	117.99 (18)
Fe1—C12—H12	126.4	C13—C8—C9	126.81 (19)
C5—C4—C3	108.33 (19)	C13—C8—C12	124.83 (19)
C5—C4—Fe1	68.83 (11)	C9—C8—C12	108.35 (18)
C3—C4—Fe1	69.87 (12)	C13—C8—Fe1	124.42 (15)
C5—C4—H4	125.8	C9—C8—Fe1	69.95 (11)
C3—C4—H4	125.8	C12—C8—Fe1	70.23 (11)
Fe1—C4—H4	127.0	N1—C13—C8	178.1 (2)
C6—C7—H7A	109.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N1^{i}	0.93	2.72	3.411 (3)	132
C9—H9···N1^{i}	0.93	2.73	3.463 (3)	137
C11—H11···O1^{ii}	0.93	2.59	3.514 (3)	178

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+2, -y, -z$.

Selected geometric parameters (Å, °).

Fe1···*Cg*1	1.6505 (10)
Fe1···*Cg*2	1.6479 (10)
*Cg*2···*Cg*1^{iii}	3.749 (1)

*Cg*1 and *Cg*2 are the centroids defined by atoms C1–C5 and C8–C12, respectively. Symmetry code: (iii) $x, 1 + y, z$.

Fig. 1

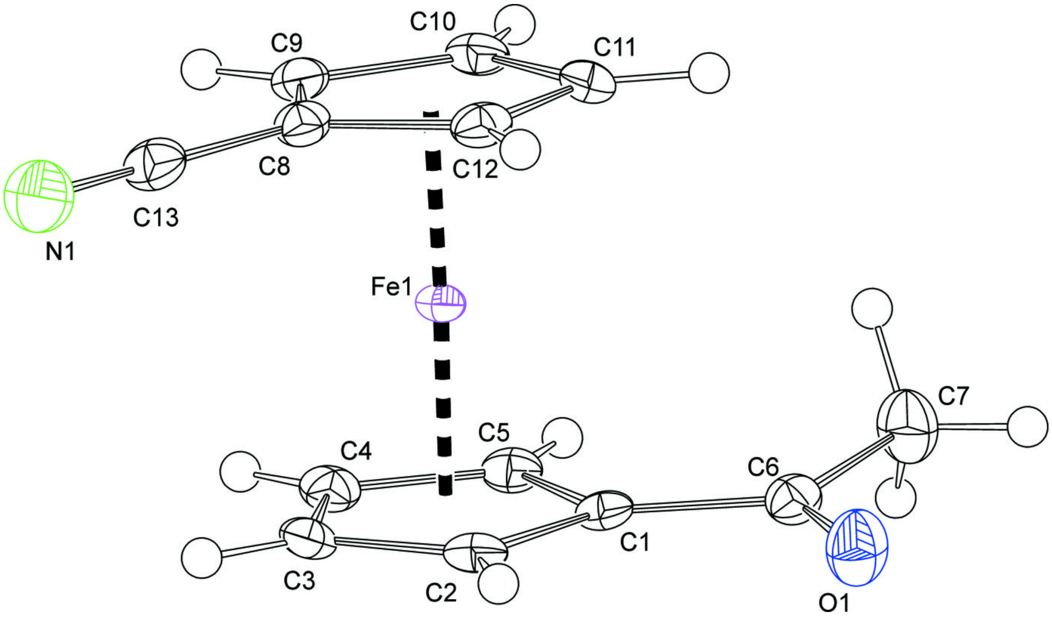
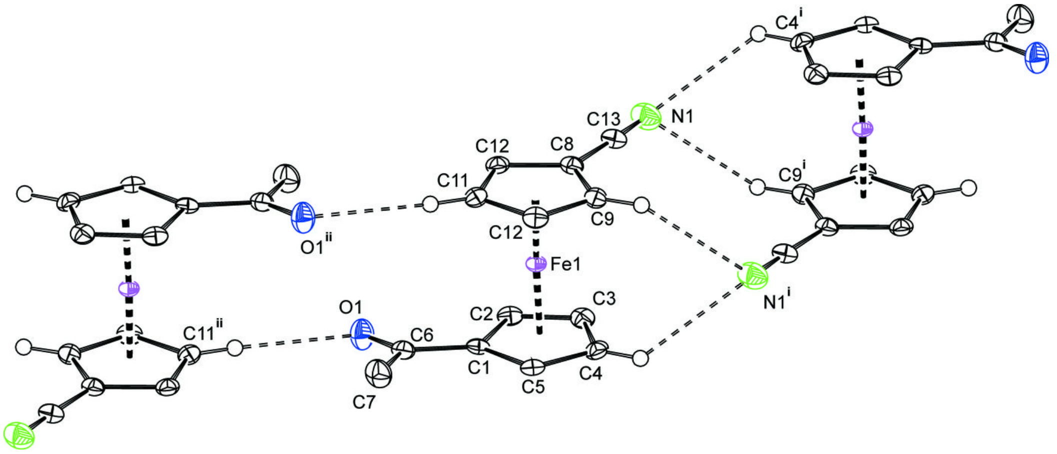


Fig. 2


$C4^{i}$
C13
N1
C12
C8
C11
$C9^{i}$
C12
C9
$O1^{ii}$
Fe1
O1
C2
C3
$C11^{ii}$
C6
C1
C5
C4
C7
$N1^{i}$