Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(3,4-Dichlorobenzoyl)ferrocene

Milan Erben,[a]* Aleš Růžička,[a] Jaromír Vinklárek,[a] Vít Šťáva[b] and David Veselý[b]

[a]Department of General and Inorganic Chemistry, Faculty of Chemical Technology, University of Pardubice, Nám. Čs. legií 565, Pardubice 532 10, Czech Republic, and [b]Department of Paints and Organic Coatings, Faculty of Chemical Technology, University of Pardubice, Nám. Čs. legií 565, Pardubice 532 10, Czech Republic
Correspondence e-mail: milan.erben@upce.cz

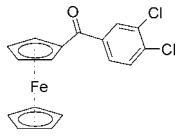
Received 1 October 2007; accepted 26 October 2007

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.101; data-to-parameter ratio = 16.7.

In the title compound, $[Fe(C_5H_5)(C_{12}H_7Cl_2O)]$, the cyclopentadienyl rings are almost parallel and eclipsed as typically found for similar monosubstituted ferrocene derivatives. Weak C—H···O and C—H···Cl hydrogen bonds link molecules into two-dimensional layers parallel to the *ac* plane in the crystal structure.

Related literature

The title complex has been synthesized following a procedure described by Reeves (1977). For related literature dealing with the crystal structures of related ferrocenyl complexes formulated as $FeCp(C_5H_4COAr)$, where Cp = η^5-C_5H_5 and Ar = C_6H_5, 4-$C_6H_4CH_3$, 4-$C_6H_4NH_2$ and 4-C_6H_4OH, see: Butler *et al.* (1988); Figueroa *et al.* (2005); Bényei *et al.* (1997). For the use of derivatives similar to the title complex as catalysts in the drying process of oxidizable paints, see: Šťáva *et al.* (2007).



Experimental

Crystal data

$[Fe(C_5H_5)(C_{12}H_7Cl_2O)]$
M_r = 359.02
Triclinic, $P\overline{1}$
a = 6.1970 (3) Å
b = 10.0720 (5) Å
c = 11.8160 (7) Å
α = 78.098 (4)°
β = 76.452 (4)°
γ = 78.903 (3)°
V = 693.47 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.47 mm^{-1}
T = 150 (1) K
0.40 × 0.30 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
Absorption correction: Gaussian integration (Coppens *et al.*, 1970)
T_{min} = 0.551, T_{max} = 0.916
11098 measured reflections
3169 independent reflections
2773 reflections with $I > 2\sigma(I)$
R_{int} = 0.133

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.102
S = 1.15
3169 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Fe1···*Cg*1	1.6505 (10)	Fe1···*Cg*2	1.6479 (10)
*Cg*1···Fe1···*Cg*2	177.94 (8)		

*Cg*1 and *Cg*2 are the centroids defined by atoms C1–C5 and C6–C10, respectively.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···O1^{i}	0.93	2.56	3.156 (4)	123
C9—H9···Cl2^{ii}	0.93	2.90	3.658 (3)	140

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

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).

The authors thank the Ministry of Education, Youth and Sports of the Czech Republic for financial support of this work within the framework of research project MSM 0021627501.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2140).

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.
Bényei, A. C., Glidewell, C., Lightfoot, P., Royles, B. J. L. & Smith, D. M. (1997). *J. Organomet. Chem.* **539**, 177–186.
Butler, I. R., Cullen, W. R., Rettig, S. J. & Trotter, J. (1988). *Acta Cryst.* C**44**, 1666–1667.
Coppens, P. (1970). *Crystallographic Computing*, edited by F. R. Ahmed, S. R. Hall & C. P. Huber, pp. 255–270. Copenhagen: Munksgaard.
Figueroa, W., Fuentealba, M., Manzur, C., Vega, A. I., Carrillo, D. & Hamon, J.-R. (2005). *C. R. Chim.* **8**, 1268–1275.
Hooft, R. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
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.
Reeves, P. C. (1977). *Org. Synth.* **56**, 28–31.
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.

 doi:10.1107/S1600536807053391

supplementary materials

Acta Cryst. (2007). E**63**, m3067 [**doi:10.1107/S1600536807053391**]

1-(3,4-Dichlorobenzoyl)ferrocene

M. Erben, A. Ruzicka, J. Vinklárek, V. Stáva and D. Veselý

Comment

Ferrocene complexes are widely used in homogenous catalysis, organic or organometallic synthesis and in material science. The use of ferrocene and its derivatives as catalyst in drying process of oxidizable paints was investigated recently (Šťáva *et al.*, 2007) and it was observed that ferrocenes bearing electron-withdrawing substituents show the highest activity. As a part of our investigation of ferrocene derivatives, we have prepared the title compound, (I), and determined its structure in the solid state.

As Figure 1 shows, the title compound displays a structure typical for monosubstituted acylferrocenes. The cyclopentadienyl (Cp) rings are almost parallel, making a dihedral angle of 2.0 (2)°, and are eclipsed as viewed down the normal of Cp rings. The dihedral angle between a ring C atom, the two ring centroids and the C atom of opposite ring varies from 3.1 (2)° to 3.9 (3)°. The interatomic distances and angles in (I) are very close to those found in benzoylferrocene (Butler *et al.*, 1988), see Table 1.

The angle between the plane defined by ring of 3,4-dichlorobenzoyl group and Cp ring bonded to this group is found to be 39.5 (2)°, validating that Cp and benzene ring π-systems are not conjugated. Carbonyl atom C11 is displaced slightly out of the Cp ring away from the Fe atom, with an angle of 1.3 (2)° between the ring plane and C1—C11 bond.

Geometric parameters of weak intermolecular interactions observed in the crystal of (I) are listed in the Table 2. Atom O1 of the molecule at $(-1+x, 1-y, z)$ serves as an acceptor for atom C17 of the molecule in the asymmetric unit, generating molecular wires along the [100] axis. Atom C9 of the asymmetric unit serves as a donor to atom Cl2 of the molecule at $(-1+x, y, 1+z)$, linking the above mentioned molecular wires into two-dimensional layers parallel to the *ac* plane.

Experimental

The title compound was synthesized from ferrocene and 3,4-dichlorobenzoyl chloride in the presence of $AlCl_3$ following the procedure described by Reeves (1977). Melting point, IR and NMR spectra confirmed identity and purity of prepared compound. Crystals suitable for X-ray diffraction analysis were grown by sublimation in a sealed ampoule at 0.1 Pa and 380 K.

Refinement

All H atoms were positioned geometrically and refined as riding on their parent C atoms, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

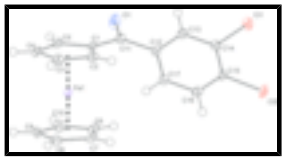


Fig. 1. *ORTEP* view of the title compound with displacement ellipsoids drawn at the 50% probability level.

1-(3,4-Dichlorobenzoyl)ferrocene

Crystal data

$[Fe(C_5H_5)(C_{12}H_7Cl_2O)]$	$Z = 2$
$M_r = 359.02$	$F_{000} = 364$
Triclinic, $P\bar{1}$	$D_x = 1.719$ Mg m^{-3}
Hall symbol: -P 1	Melting point: 426 K
$a = 6.1970$ (3) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 10.0720$ (5) Å	Cell parameters from 11119 reflections
$c = 11.8160$ (7) Å	$\theta = 1$–27.5º
$\alpha = 78.098$ (4)º	$\mu = 1.47$ mm^{-1}
$\beta = 76.452$ (4)º	$T = 150$ (1) K
$\gamma = 78.903$ (3)º	Plate, red
$V = 693.47$ (6) Å^3	0.40 × 0.30 × 0.06 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer	3169 independent reflections
Monochromator: graphite	2773 reflections with $I > 2\sigma(I)$
Detector resolution: 9.091 pixels mm^{-1}	$R_{int} = 0.133$
$T = 150(1)$ K	$\theta_{max} = 27.5$º
φ and ω scans to fill the Ewald sphere	$\theta_{min} = 3.0$º
Absorption correction: integration Gaussian integration (Coppens et al., 1970)	$h = -7 \rightarrow 8$
$T_{min} = 0.551$, $T_{max} = 0.916$	$k = -13 \rightarrow 12$
11098 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.042$	H-atom parameters constrained
$wR(F^2) = 0.102$	$w = 1/[\sigma^2(F_o^2) + (0.0055P)^2 + 0.7487P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.15$	$(\Delta/\sigma)_{max} < 0.001$

3169 reflections	$\Delta\rho_{max} = 0.72$ e Å^{-3}
190 parameters	$\Delta\rho_{min} = -0.74$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. Melting point: 426–427 K. Spectroscopic analysis: ^{1}H NMR (benzene-d_6, δ, p.p.m.): 3.84 (s, 5H), 4.09 (m, 2H), 4.66 (m, 2H), 6.95 (m, 1H), 7.44 (m, 1H), 8.04 (d, 1H). ^{13}C NMR (benzene-d_6, δ, p.p.m.): 67.0, 71.1, 72.3, 77.8, 129.5, 130.2, 132.3, 135.4, 139.3, 184.5. Uv-Vis (cyclohexane, maxima at nm): 473, 369, 284 (sh). IR (KBr disc, cm^{-1}): 3108 (*m*), 1625 (*s*), 1581 (*m*), 1555 (*m*), 1533 (w), 1455 (*m*), 1445 (*s*), 1385 (*s*), 1289 (*s*), 1246 (*m*), 1172 (*m*), 1131 (w), 1106 (*m*), 1054 (*m*), 1028 (*m*), 1002 (w), 969 (*m*), 907 (*m*), 877 (w), 848 (w), 829 (*s*), 767 (*m*), 752 (*m*), 678 (*m*), 667 (w), 579 (w), 538 (*m*), 501 (*m*), 486 (*m*), 442 (w).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.83358 (6)	0.22818 (4)	0.27185 (4)	0.01123 (12)
Cl2	0.33933 (12)	0.18553 (8)	0.93854 (7)	0.02494 (19)
Cl1	0.76392 (12)	0.31674 (8)	0.92710 (7)	0.02464 (19)
O1	1.1551 (3)	0.3333 (3)	0.4841 (2)	0.0256 (5)
C4	0.9628 (5)	0.3893 (3)	0.1563 (3)	0.0178 (6)
H4	1.0332	0.3891	0.0776	0.021*
C13	0.8399 (4)	0.3279 (3)	0.6918 (3)	0.0138 (6)
H13	0.9690	0.3638	0.6888	0.017*
C1	0.9018 (4)	0.3649 (3)	0.3600 (3)	0.0133 (6)
C15	0.5085 (4)	0.2371 (3)	0.8039 (3)	0.0138 (6)
C16	0.4526 (4)	0.2223 (3)	0.7020 (3)	0.0149 (6)
H16	0.3223	0.1873	0.7056	0.018*
C7	0.6071 (5)	0.0945 (3)	0.3417 (3)	0.0181 (6)
H7	0.4651	0.1143	0.3879	0.022*
C11	0.9590 (4)	0.3365 (3)	0.4761 (3)	0.0149 (6)
C14	0.6996 (4)	0.2925 (3)	0.7995 (3)	0.0140 (6)
C12	0.7887 (4)	0.3099 (3)	0.5885 (3)	0.0129 (6)
C17	0.5904 (4)	0.2596 (3)	0.5934 (3)	0.0139 (6)
H17	0.5513	0.2512	0.5241	0.017*
C5	1.0691 (5)	0.3524 (3)	0.2539 (3)	0.0173 (6)
H5	1.2222	0.3245	0.2502	0.021*
C10	0.9866 (5)	0.0274 (3)	0.2838 (3)	0.0198 (7)
H10	1.1371	−0.0044	0.2858	0.024*
C2	0.6896 (4)	0.4111 (3)	0.3241 (3)	0.0153 (6)
H2	0.5507	0.4278	0.3740	0.018*
C9	0.8939 (5)	0.0678 (3)	0.1809 (3)	0.0191 (6)
H9	0.9731	0.0672	0.1037	0.023*
C8	0.6603 (5)	0.1094 (3)	0.2159 (3)	0.0181 (6)
H8	0.5591	0.1410	0.1657	0.022*
C3	0.7291 (5)	0.4269 (3)	0.1992 (3)	0.0186 (6)
H3	0.6206	0.4568	0.1531	0.022*

C6	0.8093 (5)	0.0440 (3)	0.3838 (3)	0.0198 (7)
H6	0.8235	0.0252	0.4624	0.024*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0107 (2)	0.00976 (18)	0.0112 (2)	−0.00165 (14)	0.00060 (14)	−0.00050 (15)
Cl2	0.0214 (4)	0.0346 (4)	0.0160 (4)	−0.0112 (3)	0.0055 (3)	−0.0020 (3)
Cl1	0.0274 (4)	0.0353 (4)	0.0144 (4)	−0.0120 (3)	−0.0057 (3)	−0.0030 (3)
O1	0.0101 (9)	0.0460 (14)	0.0210 (14)	−0.0065 (9)	−0.0018 (8)	−0.0056 (11)
C4	0.0257 (14)	0.0134 (12)	0.0114 (16)	−0.0076 (11)	0.0017 (11)	0.0025 (11)
C13	0.0099 (11)	0.0157 (12)	0.0152 (16)	−0.0029 (10)	−0.0030 (10)	−0.0001 (11)
C1	0.0139 (12)	0.0111 (12)	0.0138 (16)	−0.0039 (10)	0.0005 (10)	−0.0015 (11)
C15	0.0117 (12)	0.0131 (12)	0.0140 (16)	−0.0013 (10)	0.0015 (10)	−0.0017 (11)
C16	0.0104 (12)	0.0154 (12)	0.0182 (17)	−0.0022 (10)	−0.0019 (10)	−0.0023 (11)
C7	0.0173 (13)	0.0173 (13)	0.0197 (17)	−0.0099 (11)	0.0000 (11)	−0.0009 (12)
C11	0.0120 (12)	0.0155 (12)	0.0171 (16)	−0.0025 (10)	−0.0027 (11)	−0.0023 (11)
C14	0.0153 (12)	0.0147 (12)	0.0125 (16)	−0.0006 (10)	−0.0057 (10)	−0.0020 (11)
C12	0.0103 (12)	0.0122 (12)	0.0137 (16)	0.0001 (10)	−0.0009 (10)	0.0002 (10)
C17	0.0099 (11)	0.0163 (12)	0.0155 (16)	−0.0012 (10)	−0.0028 (10)	−0.0034 (11)
C5	0.0158 (13)	0.0180 (13)	0.0163 (16)	−0.0069 (11)	0.0039 (11)	−0.0029 (11)
C10	0.0189 (13)	0.0099 (12)	0.027 (2)	0.0023 (10)	−0.0034 (12)	−0.0010 (12)
C2	0.0149 (12)	0.0089 (11)	0.0212 (17)	0.0003 (10)	−0.0038 (11)	−0.0020 (11)
C9	0.0263 (15)	0.0162 (13)	0.0133 (16)	−0.0060 (12)	0.0045 (12)	−0.0065 (11)
C8	0.0225 (14)	0.0163 (13)	0.0173 (17)	−0.0063 (11)	−0.0053 (11)	−0.0020 (12)
C3	0.0228 (14)	0.0115 (12)	0.0203 (18)	−0.0002 (11)	−0.0054 (12)	−0.0009 (11)
C6	0.0271 (15)	0.0122 (12)	0.0182 (17)	−0.0069 (11)	−0.0023 (12)	0.0025 (12)

Geometric parameters (Å, °)

Fe1—C2	2.037 (3)	C15—C16	1.372 (4)
Fe1—C8	2.043 (3)	C15—C14	1.390 (4)
Fe1—C1	2.045 (3)	C16—C17	1.389 (4)
Fe1—C5	2.046 (3)	C16—H16	0.9300
Fe1—C7	2.047 (2)	C7—C6	1.421 (4)
Fe1—C9	2.049 (3)	C7—C8	1.428 (5)
Fe1—C4	2.053 (2)	C7—H7	0.9300
Fe1—C6	2.053 (3)	C11—C12	1.502 (4)
Fe1—C10	2.053 (3)	C12—C17	1.402 (3)
Fe1—C3	2.053 (3)	C17—H17	0.9300
Cl2—C15	1.728 (3)	C5—H5	0.9300
Cl1—C14	1.720 (3)	C10—C9	1.417 (5)
O1—C11	1.235 (3)	C10—C6	1.426 (4)
C4—C5	1.409 (4)	C10—H10	0.9300
C4—C3	1.422 (4)	C2—C3	1.419 (5)
C4—H4	0.9300	C2—H2	0.9300
C13—C12	1.384 (4)	C9—C8	1.414 (4)
C13—C14	1.385 (4)	C9—H9	0.9300
C13—H13	0.9300	C8—H8	0.9300

C1—C5	1.439 (4)	C3—H3	0.9300
C1—C2	1.439 (4)	C6—H6	0.9300
C1—C11	1.454 (4)		
C2—Fe1—C8	122.72 (11)	C15—C16—C17	120.0 (2)
C2—Fe1—C1	41.27 (11)	C15—C16—H16	120.0
C8—Fe1—C1	160.73 (11)	C17—C16—H16	120.0
C2—Fe1—C5	68.79 (11)	C6—C7—C8	108.0 (3)
C8—Fe1—C5	155.61 (13)	C6—C7—Fe1	69.95 (14)
C1—Fe1—C5	41.17 (11)	C8—C7—Fe1	69.44 (14)
C2—Fe1—C7	107.01 (11)	C6—C7—H7	126.0
C8—Fe1—C7	40.86 (12)	C8—C7—H7	126.0
C1—Fe1—C7	124.75 (12)	Fe1—C7—H7	126.2
C5—Fe1—C7	162.75 (13)	O1—C11—C1	119.5 (3)
C2—Fe1—C9	159.04 (13)	O1—C11—C12	117.7 (3)
C8—Fe1—C9	40.44 (12)	C1—C11—C12	122.8 (2)
C1—Fe1—C9	158.00 (12)	C13—C14—C15	119.7 (3)
C5—Fe1—C9	121.68 (12)	C13—C14—Cl1	119.8 (2)
C7—Fe1—C9	68.28 (12)	C15—C14—Cl1	120.5 (2)
C2—Fe1—C4	68.58 (12)	C13—C12—C17	119.6 (3)
C8—Fe1—C4	119.76 (13)	C13—C12—C11	117.6 (2)
C1—Fe1—C4	68.83 (12)	C17—C12—C11	122.7 (3)
C5—Fe1—C4	40.22 (12)	C16—C17—C12	119.8 (3)
C7—Fe1—C4	155.46 (13)	C16—C17—H17	120.1
C9—Fe1—C4	106.74 (12)	C12—C17—H17	120.1
C2—Fe1—C6	122.28 (13)	C4—C5—C1	108.8 (2)
C8—Fe1—C6	68.47 (12)	C4—C5—Fe1	70.13 (15)
C1—Fe1—C6	108.89 (12)	C1—C5—Fe1	69.37 (14)
C5—Fe1—C6	126.45 (12)	C4—C5—H5	125.6
C7—Fe1—C6	40.56 (12)	C1—C5—H5	125.6
C9—Fe1—C6	68.30 (13)	Fe1—C5—H5	126.5
C4—Fe1—C6	162.02 (12)	C9—C10—C6	108.2 (3)
C2—Fe1—C10	158.73 (14)	C9—C10—Fe1	69.63 (16)
C8—Fe1—C10	68.11 (12)	C6—C10—Fe1	69.67 (16)
C1—Fe1—C10	123.20 (12)	C9—C10—H10	125.9
C5—Fe1—C10	109.30 (12)	C6—C10—H10	125.9
C7—Fe1—C10	68.18 (11)	Fe1—C10—H10	126.4
C9—Fe1—C10	40.41 (13)	C3—C2—C1	108.1 (2)
C4—Fe1—C10	124.55 (12)	C3—C2—Fe1	70.31 (17)
C6—Fe1—C10	40.65 (12)	C1—C2—Fe1	69.65 (16)
C2—Fe1—C3	40.58 (13)	C3—C2—H2	125.9
C8—Fe1—C3	105.76 (12)	C1—C2—H2	125.9
C1—Fe1—C3	68.74 (12)	Fe1—C2—H2	125.7
C5—Fe1—C3	67.95 (12)	C8—C9—C10	108.2 (3)
C7—Fe1—C3	120.48 (11)	C8—C9—Fe1	69.58 (17)
C9—Fe1—C3	122.75 (14)	C10—C9—Fe1	69.96 (18)
C4—Fe1—C3	40.52 (11)	C8—C9—H9	125.9
C6—Fe1—C3	156.78 (12)	C10—C9—H9	125.9
C10—Fe1—C3	159.99 (14)	Fe1—C9—H9	126.2
C5—C4—C3	108.0 (3)	C9—C8—C7	108.0 (3)

C5—C4—Fe1	69.65 (15)	C9—C8—Fe1	69.98 (16)
C3—C4—Fe1	69.76 (14)	C7—C8—Fe1	69.70 (16)
C5—C4—H4	126.0	C9—C8—H8	126.0
C3—C4—H4	126.0	C7—C8—H8	126.0
Fe1—C4—H4	126.2	Fe1—C8—H8	125.9
C12—C13—C14	120.2 (2)	C2—C3—C4	108.4 (3)
C12—C13—H13	119.9	C2—C3—Fe1	69.11 (16)
C14—C13—H13	119.9	C4—C3—Fe1	69.72 (15)
C5—C1—C2	106.6 (3)	C2—C3—H3	125.8
C5—C1—C11	122.2 (2)	C4—C3—H3	125.8
C2—C1—C11	131.2 (3)	Fe1—C3—H3	127.0
C5—C1—Fe1	69.46 (17)	C7—C6—C10	107.6 (3)
C2—C1—Fe1	69.07 (16)	C7—C6—Fe1	69.49 (15)
C11—C1—Fe1	127.36 (18)	C10—C6—Fe1	69.68 (15)
C16—C15—C14	120.6 (3)	C7—C6—H6	126.2
C16—C15—Cl2	119.39 (19)	C10—C6—H6	126.2
C14—C15—Cl2	120.0 (2)	Fe1—C6—H6	126.2

Selected geometric parameters (Å, °)

Fe1···*Cg*1	1.6505 (10)
Fe1···*Cg*2	1.6479 (10)
*Cg*1···Fe1···*Cg*2	177.94 (8)

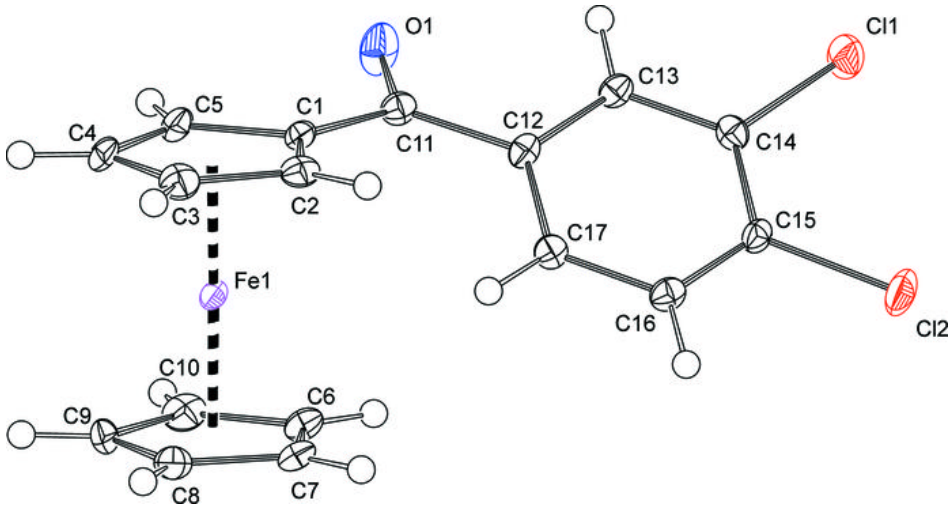
*Cg*1 and *Cg*2 are the centroids defined by atoms C1–C5 and C6–C10, respectively.

Hydrogen-bond geometry (Å, °)

D—H···A	D—H	H···A	D···A	D—H···A
C17—H17···O1^{i}	0.93	2.56	3.156 (4)	123
C9—H9···Cl2^{ii}	0.93	2.90	3.658 (3)	140

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

Fig. 1


O1
Cl1
C13
C5
C1
C12
C4
C11
C14
C3
C2
C17
C15
Fe1
C16
Cl2
C10
C6
C9
C8
C7