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Di-μ-carbonyl-dicarbonylbis[(2-hydroxyethyl)-η^5-cyclopentadienyl]diiron(*Fe–Fe*)

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Abstract. $C_{18}H_{18}Fe_2O_6$, $M_r = 442.03$, trigonal, $R\bar{3}$, $a = 16.577$ (3), $c = 16.957$ (3) Å, $V = 4035$ (3) Å^3, $Z = 9$, $D_x = 1.637$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, $\mu = 1.65$ mm^{-1}, $F(000) = 2034$, $T = 295$ K, $R_F = 0.039$ for 1173 independent reflections [$I \geq 3\sigma(I)$] and 118 parameters. The compound is the *trans* isomer. The molecules lie on crystallographic inversion centers. Bond lengths include: Fe—Fe 2.534 (1), Fe—CO 1.759 (5), Fe—CO(μ) 1.897, 1.933 (5) Å. Hydrogen bonds between OH groups [all O···O 2.656 (4) Å] link the molecules into nets parallel to the *ab* plane.

Experimental. Preparation: Tenhaeff & Tyler (1991); red-black prism from CH_2Cl_2–hexane, 0.10 × 0.12 × 0.42 mm, mounted on a fiber; Rigaku AFC6R diffractometer, graphite monochromator; orientation matrix and cell dimensions from 20 centered reflections in range $22 \leq 2\theta \leq 26°$; Laue symmetry $\bar{3}$; ω–2θ scans, 8° min^{-1} in ω, width $(1.15 + 0.30\tan\theta)°$; $2\theta_{max} = 50°$; h −16 to 16, k 0 to 19, l 0 to 20; three standard reflections every 300, no change; 1584 independent reflections, 1173 with $I \geq 3\sigma(I)$, $R_{int} = 0.051$ (on F^2); no systematic absences other than for R lattice; relative transmission factors 0.94–1.00 (ψ scans), absorption correction not applied.

Fe position from *MITHRIL E* map (Gilmore, 1984), O and C atoms from *DIRDIF* (Beurskens *et al.*, 1984); Fe, O, C atoms anisotropic; hydroxyl-H atom included at position from difference map without refinement, other H atoms at calculated riding positions, $B(H) = 1.2B_{eq}(C)$; full-matrix refinement on F, 118 parameters, $\sum w(|F_o| - |F_c|)^2$ minimized, $w = 1/\sigma^2(F)$, $\sigma(F)$ from counting statistics + pF^2, $p = 0.03$; $R_F = 0.039$, $wR_F = 0.047$, $S = 1.57$, max. $\Delta/\sigma = 0.02$ in last cycle, max., min. $\Delta\rho + 0.56$ (near origin), −0.37 e Å^{-3}. All calculations from *TEXSAN* (Molecular Structure Corporation, 1989), with atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). Atomic coordinates and equivalent isotropic thermal parameters are given in Table 1, and bond lengths and selected bond angles in Table 2. The molecular structure is shown in Fig. 1 and the hydrogen-bond network in Fig. 2.†

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	B_{eq}
Fe(1)	0·47818 (4)	0·43548 (4)	0·54996 (4)	2·67 (3)
O(1)	0·6433 (2)	0·6122 (2)	0·5870 (2)	4·3 (1)
O(2)	0·3543 (3)	0·4810 (3)	0·6342 (2)	5·8 (2)
O(3)	0·1716 (3)	0·1409 (3)	0·5115 (3)	6·5 (2)
C(1)	0·5790 (3)	0·5631 (3)	0·5466 (3)	3·2 (2)
C(2)	0·4039 (3)	0·4633 (3)	0·6025 (3)	3·7 (2)
C(3)	0·5140 (3)	0·3387 (3)	0·5024 (3)	3·5 (2)
C(4)	0·5836 (3)	0·3990 (3)	0·5562 (3)	4·0 (2)
C(5)	0·5441 (4)	0·3889 (3)	0·6303 (3)	4·2 (2)
C(6)	0·4491 (3)	0·3221 (3)	0·6231 (3)	3·8 (2)
C(7)	0·4297 (3)	0·2890 (3)	0·5442 (3)	3·4 (2)
C(8)	0·3395 (3)	0·2141 (3)	0·5107 (3)	4·2 (2)
C(9)	0·2547 (4)	0·2035 (4)	0·5515 (4)	5·1 (2)

Related literature. The title compound is an intermediate in the synthesis of polymers with Fe—Fe bonds in the backbone (Tenhaeff & Tyler, 1991). The Fe—Co—Fe bridge is slightly asymmetric compared with that in the parent *trans*-Fe$_2$(CO)$_4$(C$_5$H$_5$)$_2$ (Bryan & Greene, 1970), but other dimensions are not significantly affected. Intermolecular hydrogen bonds are also present in Mo$_2$(CO)$_6$(C$_5$H$_4$CH$_2$CH$_2$OH)$_2$ (Tenhaeff, Tyler & Weakley, 1991).

† Lists of structure factors, full bond angles, anisotropic thermal parameters, H-atom coordinates, intermolecular distances, torsion angles, and mean plane information have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54449 (21 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 2. *Bond lengths* (Å) *and selected bond angles* (°)

Cp denotes the cyclopentadienyl ring centroid.

Fe(1)—Fe(1^i)	2·534 (1)	O(2)—C(2)	1·137 (5)
Fe(1)—C(1)	1·933 (5)	O(3)—C(9)	1·416 (6)
Fe(1)—C(1^i)	1·897 (5)	C(3)—C(4)	1·418 (7)
Fe(1)—C(2)	1·759 (5)	C(3)—C(7)	1·407 (6)
Fe(1)—C(3)	2·128 (4)	C(4)—C(5)	1·388 (7)
Fe(1)—C(4)	2·119 (4)	C(5)—C(6)	1·406 (7)
Fe(1)—C(5)	2·119 (5)	C(6)—C(7)	1·420 (7)
Fe(1)—C(6)	2·097 (5)	C(7)—C(8)	1·499 (6)
Fe(1)—C(7)	2·144 (4)	C(8)—C(9)	1·497 (7)
O(1)—C(1)	1·183 (5)	Fe(1)···Cp	1·771 (4)
O(3)···O(3^{ii})	2·656 (4)		

Fe(1)—Fe(1^i)—C(1)	48·0 (1)	C(4)—C(3)—C(7)	108·0 (4)
Fe(1)—Fe(1^i)—C(1^i)	49·2 (1)	C(3)—C(4)—C(5)	109·2 (4)
C(1)—Fe(1)—C(1^i)	97·2 (2)	C(4)—C(5)—C(6)	107·0 (4)
C(1)—Fe(1)—C(2)	93·6 (2)	C(5)—C(6)—C(7)	109·5 (4)
C(1^i)—Fe(1)—C(2)	90·8 (2)	C(3)—C(7)—C(6)	106·4 (4)
Fe(1)—C(1)—Fe(1^i)	82·8 (2)	C(3)—C(7)—C(8)	125·5 (5)
Fe(1)—C(1)—O(1)	136·4 (4)	C(6)—C(7)—C(8)	128·1 (4)
Fe(1^i)—C(1)—O(1)	140·8 (4)	C(7)—C(8)—C(9)	114·3 (4)
Fe(1)—C(2)—O(2)	177·7 (5)	O(3)—C(9)—C(8)	112·2 (5)

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

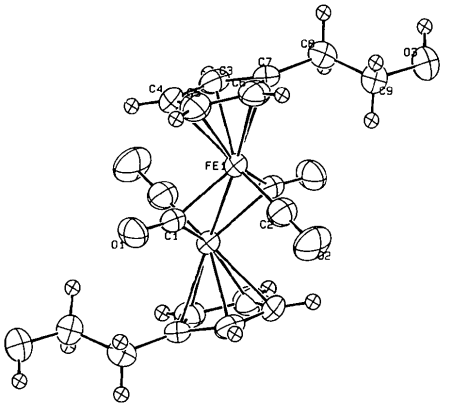

Fig. 1. The molecular structure of $Fe_2(CO)_4(C_5H_4CH_2CH_2OH)_2$ showing thermal ellipsoids and numbering of atoms.

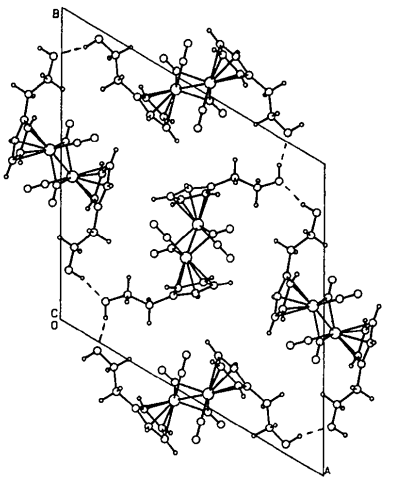

Fig. 2. Part of one hydrogen-bonded net viewed along **c**.

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Structure of Aquabis(2,2′-bipyrimidine-*N*,*N*′)copper(II) Perchlorate Dihydrate

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Abstract. $[Cu(C_8H_6N_4)_2(H_2O)](ClO_4)_2\cdot 2H_2O$, M_r = 632.86, monoclinic, $C2/c$, a = 18.232 (3), b = 7.613 (1), c = 16.842 (4) Å, β = 96.27 (2)°, V = 2323.6 (8) Å^3, Z = 4, D_x = 1.82 g cm^{-3}, Zr-filtered Mo $K\alpha$, λ = 0.71073 Å, μ = 12.54 cm^{-1}, $F(000)$ = 1284, T = 294 (1) K, R = 0.037 for 1211 observed

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