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Octacarbonylbis[μ-(pentacarbonylmanganio)indium(III)]-diiron

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Abstract. $Fe_2(CO)_8[InMn(CO)_5]_2$, $M_r = 955{\cdot}40$, tetragonal, $I4_1/a$, $a = 13{\cdot}283\ (2)$, $c = 30{\cdot}123\ (3)$ Å, $U = 5314{\cdot}8$ Å^3, $Z = 8$, $D_c = 2{\cdot}387$ Mg m^{-3}, $F(000) = 3616$, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, μ(Mo $K\alpha$) = 3·56 mm^{-1}. The structure was refined with 2821 unique reflections ($I > 3\sigma$) to $R = 0{\cdot}027$. No Fe–Fe bond is present in the four-membered In_2Fe_2 ring.

Introduction. We have prepared a number of compounds of the type $M''(CO)_8[\mu\text{-}MM'(CO)_5]$ [M = Ge, X = Br, $M' = M''$ = Mn (Preut & Haupt, 1979); M = Sn, X = Cl, Br, $M' = M''$ = Mn (Preut & Haupt, 1976; Haupt, Preut & Wolfes, 1978)] and of the type $M''_2(CO)_8[\mu\text{-}MM'(CO)_5]_2$ [M = Ga, $M' = M''$ = Mn; M = In, $M' = M''$ = Mn, Re (Preut & Haupt, 1974, 1975)] and we now report on the similar compound $Fe_2(CO)_8[InMn(CO)_5]_2$, which has been prepared in a bomb tube by reaction of $Fe(CO)_5$, In metal and $Hg[Mn(CO)_5]$ in the presence of xylene at a temperature of 443–453 K.

Data were collected from a crystal 0·30 [100] × 0·23 [010] × 0·30 [001] mm. Cell parameters were determined by least squares from the positions of 11 reflexions on a Hilger & Watts Y 290 four-circle diffractometer with graphite-monochromated Mo $K\alpha$ radiation and a scintillation counter. The intensities of 5817 reflexions ($I > 3\sigma$) with $2 \le \theta \le 30{\cdot}0°$ were measured by the $\omega/2\theta$ scan technique, with a scan width $\Delta 2\theta = (1{\cdot}34 + 0{\cdot}34 \tan\theta)°$ from background to background and a scan speed of 0·02° s^{-1} in 2θ. Backgrounds were measured at either end of the scan range for 8 s. Five standard reflexions were measured every fifty reflexions, and showed only random deviations from their mean intensities. Lp but no absorption corrections were applied, and after averaging of equivalent reflexions the data set contained 2821 reflexions for the analysis. The structure was solved by Patterson and Fourier methods and refined by full-matrix least

Table 1. *Positional parameters* ($\times 10^4$) *with e.s.d.'s in parentheses*

	x	y	z
In(1)	4552 (0)	6362 (0)	2814 (0)
Mn(1)	4034 (0)	4446 (0)	2813 (0)
Fe(1)	5000 (0)	7500 (0)	2114 (0)
Fe(2)	5000 (0)	7500 (0)	3514 (0)
C(1)	3697 (3)	3111 (3)	2811 (2)
C(2)	3074 (4)	4743 (3)	2380 (2)
C(3)	5021 (4)	4349 (4)	2385 (2)
C(4)	3102 (4)	4812 (4)	3241 (2)
C(5)	4982 (4)	4301 (4)	3256 (2)
C(6)	4676 (5)	6538 (4)	3902 (2)
C(7)	6252 (4)	7060 (4)	3397 (2)
C(8)	6203 (4)	6992 (3)	2225 (2)
C(9)	5397 (4)	8461 (3)	1733 (1)
O(1)	3516 (4)	2279 (3)	2800 (2)
O(2)	2486 (3)	4892 (3)	2125 (3)
O(3)	5620 (3)	4282 (4)	2115 (1)
O(4)	2543 (4)	5038 (4)	3511 (3)
O(5)	5534 (3)	4189 (4)	3534 (2)
O(6)	4493 (4)	5943 (4)	4160 (2)
O(7)	7055 (3)	6781 (4)	3346 (2)
O(8)	6998 (3)	6623 (3)	2270 (2)
O(9)	5646 (3)	9085 (3)	1497 (1)

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squares with *SHELX* (Sheldrick, 1976). The refinement converged with anisotropic temperature factors to $R = \sum \Delta / \sum F_o = 0{\cdot}027$, $R' = \sum w^{1/2} \Delta / \sum w^{1/2} F_o = 0{\cdot}028$.* Complex neutral-atom scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Positional parameters are given in Table 1, bond lengths and angles in Table 2.

Discussion. The nucleus of the molecule is the planar metal ring In_2Fe_2 of a similar type as in $M_2''(CO)_8[\mu\text{-}M(X)M'(CO)_5]$ [M = Ge, X = Br, M' = M'' = Mn (Preut & Haupt, 1979); M = Sn, X = Cl, Br, M' = M'' = Mn (Preut & Haupt, 1976; Haupt, Preut & Wolfes, 1978)] and $M_2''(CO)_8[\mu\text{-}MM'(CO)_5]_2$ [M = Ga, M' = M'' = Mn; M = In, M' = M'' = Mn, Re (Preut & Haupt, 1974, 1975)], whose inner metal rings show bonds between the transition elements Mn and Re across the ring. The compound $Fe_2(CO)_8[InMn(CO)_5]_2$ which we have now analysed does not have this bond, as the acute angles at the two Fe atoms indicate. Fig. 1 shows the structure of such a molecule with the numbering scheme of its atoms and Fig. 2 shows a stereoscopic view of the molecule.

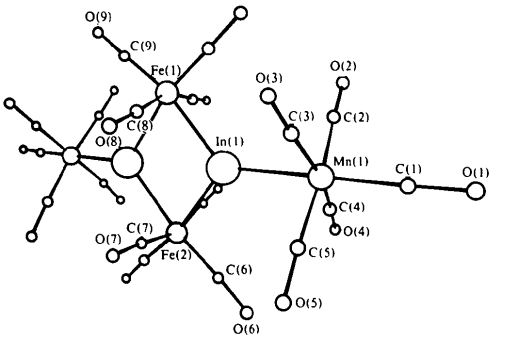

Fig. 1. General view of the molecule (*ORTEP* plot, Johnson, 1965). A twofold axis runs through Fe(1) and Fe(2).

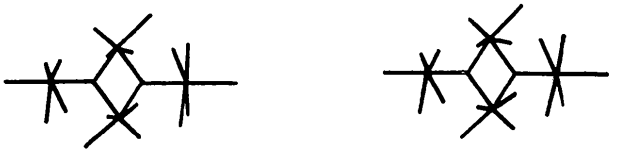

Fig. 2. Stereoscopic view of the molecule.

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* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34470 (16 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

In(1)–Fe(1)	2·662 (1)	Fe(1)–C(8)	1·767 (10)
In(1)–Fe(2)	2·663 (1)	Fe(1)–C(9)	1·795 (9)
In(1)–In(1^i)	3·250 (1)	C(1)–O(1)	1·13 (1)
Fe(1)–Fe(2)	4·218 (1)	C(2)–O(2)	1·11 (2)
In(1)–Mn(1)	2·635 (1)	C(3)–O(3)	1·14 (1)
Mn(1)–C(1)	1·830 (9)	C(4)–O(4)	1·14 (1)
Mn(1)–C(2)	1·867 (9)	C(5)–O(5)	1·12 (1)
Mn(1)–C(3)	1·844 (9)	C(6)–O(6)	1·14 (1)
Mn(1)–C(4)	1·851 (9)	C(7)–O(7)	1·14 (1)
Mn(1)–C(5)	1·844 (9)	C(8)–O(8)	1·17 (1)
Fe(2)–C(6)	1·785 (9)	C(9)–O(9)	1·14 (1)
Fe(2)–C(7)	1·797 (9)		

Fe(1)–In(1)–Fe(2)	104·8 (0)	C(8)–Fe(1)–C(8^i)	158·1 (2)
Fe(1)–In(1)–Mn(1)	127·3 (0)	C(8)–Fe(1)–C(9)	97·3 (2)
Fe(2)–In(1)–Mn(1)	127·3 (0)	C(8)–Fe(1)–C(9^i)	96·6 (2)
In(1)–Mn(1)–C(1)	179·0 (3)	C(9)–Fe(1)–C(9^i)	100·7 (2)
In(1)–Mn(1)–C(2)	88·5 (3)	In(1)–Fe(2)–In(1^i)	75·2 (0)
In(1)–Mn(1)–C(3)	83·3 (3)	In(1)–Fe(2)–C(7)	82·4 (2)
In(1)–Mn(1)–C(4)	85·5 (3)	In(1)–Fe(2)–C(7^i)	79·8 (2)
In(1)–Mn(1)–C(5)	85·6 (3)	In(1)–Fe(2)–C(6)	93·4 (3)
C(1)–Mn(1)–C(2)	92·0 (5)	In(1)–Fe(2)–C(6^i)	168·4 (2)
C(1)–Mn(1)–C(3)	95·9 (5)	C(7)–Fe(2)–C(7^i)	157·5 (5)
C(1)–Mn(1)–C(4)	95·4 (5)	C(7)–Fe(2)–C(6)	96·8 (5)
C(1)–Mn(1)–C(5)	93·9 (5)	C(7)–Fe(2)–C(6^i)	97·9 (5)
C(2)–Mn(1)–C(3)	90·6 (4)	C(6)–Fe(2)–C(6^i)	98·1 (4)
C(2)–Mn(1)–C(4)	88·5 (4)	Mn(1)–C(1)–O(1)	177·7 (11)
C(2)–Mn(1)–C(5)	173·8 (5)	Mn(1)–C(2)–O(2)	177·8 (9)
C(3)–Mn(1)–C(4)	168·7 (5)	Mn(1)–C(3)–O(3)	178·9 (9)
C(3)–Mn(1)–C(5)	90·7 (5)	Mn(1)–C(4)–O(4)	178·5 (9)
C(4)–Mn(1)–C(5)	88·9 (5)	Mn(1)–C(5)–O(5)	177·3 (9)
In(1)–Fe(1)–In(1^i)	75·2 (0)	Fe(2)–C(6)–O(6)	177·5 (11)
In(1)–Fe(1)–C(8)	80·5 (2)	Fe(2)–C(7)–O(7)	176·5 (9)
In(1)–Fe(1)–C(8^i)	82·2 (2)	Fe(1)–C(8)–O(8)	175·2 (9)
In(1)–Fe(1)–C(9)	167·3 (2)	Fe(1)–C(9)–O(9)	178·7 (9)
In(1)–Fe(1)–C(9^i)	92·1 (2)		

Symmetry code: (i) $1-x$, $1{\cdot}5-y$, z.

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