

$\text{Fe}_2[\text{CO}]_9$ *hP*40(176) $P6_3/m - i^2h^2f$ **Fe₂(CO)₉** [2], Strukturbericht notation F4₁Structural features: Fe₂(CO)₉ units (two face-linked FeC₆ octahedra) in a Mg-type (h.c.p.) arrangement. See Fig. IV.65.

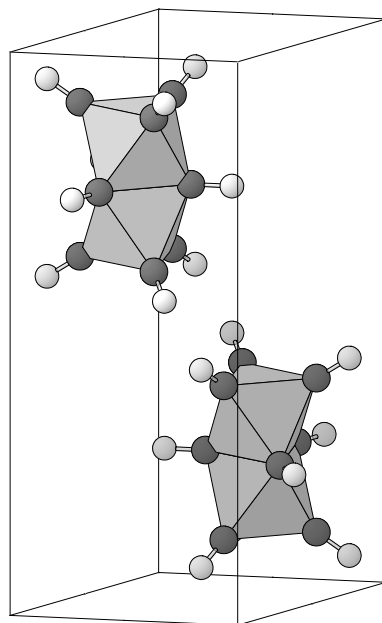
Cotton F.A., Troup J.M. (1974) [1]

C₉Fe₂O₉ $a = 0.6436$, $c = 1.6123$ nm, $c/a = 2.505$, $V = 0.5784$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	12 <i>i</i>	1	0.0863	0.4243	0.1133		single atom O
O2	12 <i>i</i>	1	0.3441	0.0624	0.0747		single atom C
O3	6 <i>h</i>	<i>m</i> ..	0.331	0.2415	$\frac{1}{4}$		single atom C
C4	6 <i>h</i>	<i>m</i> ..	0.332	0.4222	$\frac{1}{4}$		single atom O
Fe5	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.17175		octahedron C ₆

Transformation from published data: $y, x, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.040$, $T = 295$ KRemarks: In the abstract of [1] the number of formula units per cell Z is misprinted as 1 instead of 2.

References: [1] Cotton F.A., Troup J.M. (1974), J. Chem. Soc., Dalton Trans. 1974, 800-802. [2] Powell H.M., Ewens R.V.G. (1939), J. Chem. Soc. 1939, 286-292.

Fig. IV.65. **Fe₂(CO)₉**

Arrangement of Fe(CO)₆ octahedra (C atoms dark, O atoms light). For clarity, atoms located in the cell but belonging to units with the central Fe atom in a neighboring cell are omitted.