$Fe_2(CO)_9$ ($F4_1$) Structure: A9B2C9_hP40_176_hi_f_hi-001

This structure originally had the label `A9B2C9_hP40_176_hi_f_hi`. Calls to that address will be redirected here.

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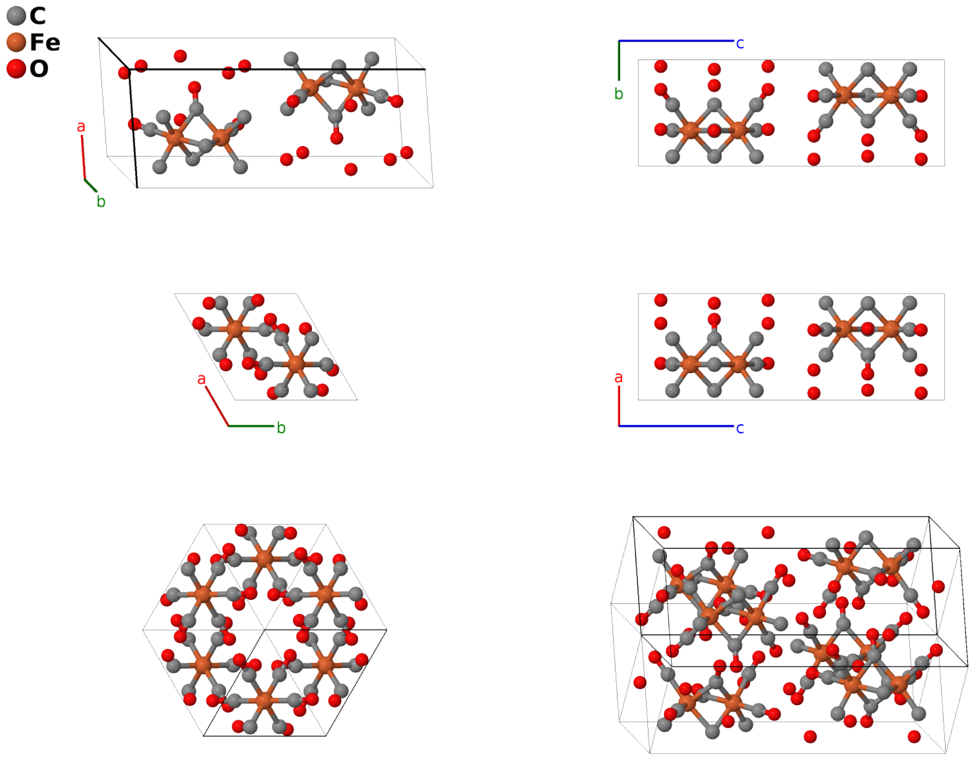
https://aflow.org/p/858V

https://aflow.org/p/A9B2C9_hP40_176_hi_f_hi-001



Prototype $C_9Fe_2O_9$

AFLOW prototype label A9B2C9_hP40_176_hi_f_hi-001

***Strukturbericht* designation** $F4_1$

ICSD 6010

Pearson symbol hP40

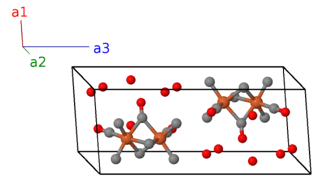
Space group number 176

Space group symbol $P6_3/m$

AFLOW prototype command `aflow --proto=A9B2C9_hP40_176_hi_f_hi-001`
`--params=`$a, c/a, z_1, x_2, y_2, x_3, y_3, x_4, y_4, z_4, x_5, y_5, z_5$

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4f)	Fe I
$\mathbf{B_2}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Fe I
$\mathbf{B_3}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4f)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Fe I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + y_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2 + y_2\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_2 - y_2\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_6}$	=	$-y_2\,\mathbf{a}_1 + \left(x_2 - y_2\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_2 - 2y_2\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_7}$	=	$-\left(x_2 - y_2\right)\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_2 - y_2\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_8}$	=	$-x_2\,\mathbf{a}_1 - y_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_2 + y_2\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_2 - y_2\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_9}$	=	$y_2\,\mathbf{a}_1 - \left(x_2 - y_2\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_2 + 2y_2\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_{10}}$	=	$\left(x_2 - y_2\right)\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_2 - y_2\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_2\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	C I
$\mathbf{B_{11}}$	=	$x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 + y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{12}}$	=	$-y_3\,\mathbf{a}_1 + \left(x_3 - y_3\right)\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_3 - 2y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{13}}$	=	$-\left(x_3 - y_3\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 + \frac{1}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_3 - y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{14}}$	=	$-x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_3 + y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_3 - y_3\right)\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{15}}$	=	$y_3\,\mathbf{a}_1 - \left(x_3 - y_3\right)\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_3 + 2y_3\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{16}}$	=	$\left(x_3 - y_3\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \frac{3}{4}\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_3 - y_3\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_3\,\hat{\mathbf{y}} + \frac{3}{4}c\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{17}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{18}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{19}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{20}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{21}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{22}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + \left(z_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} + c\left(z_4 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{23}}$	=	$-x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{24}}$	=	$y_4\,\mathbf{a}_1 - \left(x_4 - y_4\right)\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_4 + 2y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{25}}$	=	$\left(x_4 - y_4\right)\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{26}}$	=	$x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 + y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_4 - y_4\right)\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{27}}$	=	$-y_4\,\mathbf{a}_1 + \left(x_4 - y_4\right)\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_4 - 2y_4\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{28}}$	=	$-\left(x_4 - y_4\right)\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - \left(z_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_4 - y_4\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}ay_4\,\hat{\mathbf{y}} - c\left(z_4 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(12i)	C II
$\mathbf{B_{29}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 + y_5\right)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	O II
$\mathbf{B_{30}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - 2y_5\right)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}ax_5\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(12i)	O II

$\mathbf{B_{31}}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{32}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{33}}$	=	$y_5\,\mathbf{a}_1 - \left(x_5 - y_5\right)\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{34}}$	=	$\left(x_5 - y_5\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + \left(z_5 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} + c\left(z_5 + \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{35}}$	=	$-x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{36}}$	=	$y_5\,\mathbf{a}_1 - \left(x_5 - y_5\right)\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(-x_5 + 2y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{37}}$	=	$\left(x_5 - y_5\right)\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{38}}$	=	$x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 + y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\left(x_5 - y_5\right)\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{39}}$	=	$-y_5\,\mathbf{a}_1 + \left(x_5 - y_5\right)\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\left(x_5 - 2y_5\right)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II
$\mathbf{B_{40}}$	=	$-\left(x_5 - y_5\right)\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - \left(z_5 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-\frac{1}{2}a\left(2x_5 - y_5\right)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_5\,\mathbf{\hat{y}} - c\left(z_5 - \frac{1}{2}\right)\,\mathbf{\hat{z}}$	(12i)	O II

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