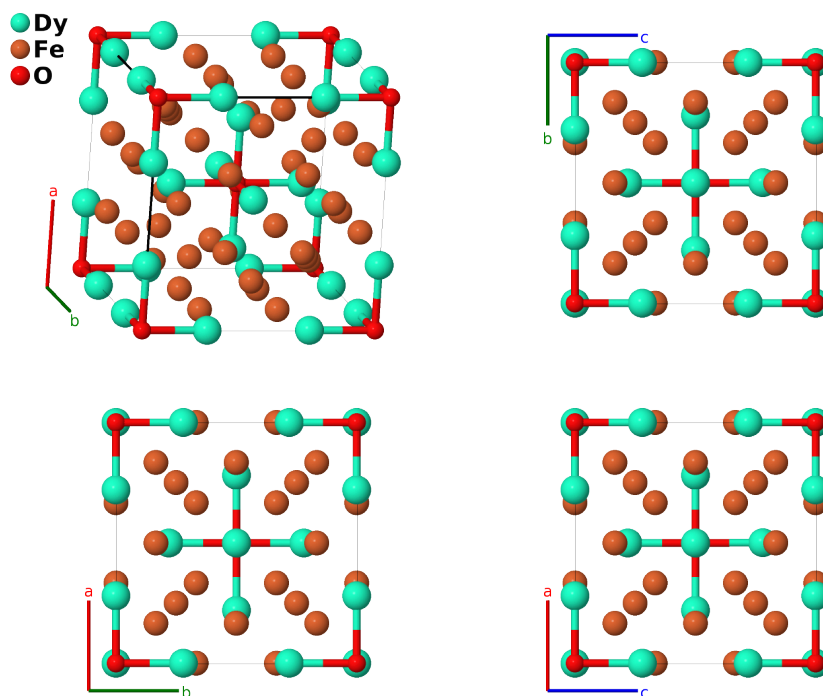


Dy₆Fe₁₆O Structure: A6B16C_cI46_229_e_ch_a-001

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<https://afLOW.org/p/Y3T5>

https://afLOW.org/p/A6B16C_cI46_229_e_ch_a-001



Prototype	Dy ₆ Fe ₁₆ O
AFLOW prototype label	A6B16C_cI46_229_e_ch_a-001
ICSD	9639
Pearson symbol	cI46
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	<code>afLOW --proto=A6B16C_cI46_229_e_ch_a-001 --params=a, x₃, y₄</code>

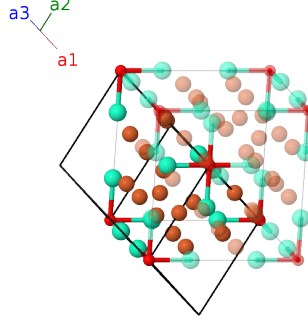
Other compounds with this structure

Ba₆Na₁₆N, Ca₆Ag₁₆N, Dy₆Fe₁₆O, Dy₆Fe₁₆O, Er₆Fe₁₆O, Gd₆Fe₁₆O, Ho₆Fe₁₆O, Tb₆Fe₁₆O, Y₆Fe₁₆O

- This is a body-centered cubic structure with vacancies on the octahedral sites adjacent to the oxygen atoms.
- The (2a) site is often only partially occupied, *e.g.*, Ca₆Ag₁₆N was originally thought to be Ag₈Ca₃ (Calvert, 1964), but there is some nitrogen present on the (2a) site. (Villars, 2004)

Body-centered Cubic primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= -\frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_2 &= \frac{1}{2}a\hat{x} - \frac{1}{2}a\hat{y} + \frac{1}{2}a\hat{z} \\ \mathbf{a}_3 &= \frac{1}{2}a\hat{x} + \frac{1}{2}a\hat{y} - \frac{1}{2}a\hat{z}\end{aligned}$$



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
\mathbf{B}_1	0	$=$	0	(2a)	O I
\mathbf{B}_2	$\frac{1}{2}\mathbf{a}_1 + \frac{1}{2}\mathbf{a}_2 + \frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(8c)	Fe I
\mathbf{B}_3	$\frac{1}{2}\mathbf{a}_3$	$=$	$\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} - \frac{1}{4}a\hat{z}$	(8c)	Fe I
\mathbf{B}_4	$\frac{1}{2}\mathbf{a}_2$	$=$	$\frac{1}{4}a\hat{x} - \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(8c)	Fe I
\mathbf{B}_5	$\frac{1}{2}\mathbf{a}_1$	$=$	$-\frac{1}{4}a\hat{x} + \frac{1}{4}a\hat{y} + \frac{1}{4}a\hat{z}$	(8c)	Fe I
\mathbf{B}_6	$x_3\mathbf{a}_2 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{x}$	(12e)	Dy I
\mathbf{B}_7	$-x_3\mathbf{a}_2 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{x}$	(12e)	Dy I
\mathbf{B}_8	$x_3\mathbf{a}_1 + x_3\mathbf{a}_3$	$=$	$ax_3\hat{y}$	(12e)	Dy I
\mathbf{B}_9	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_3$	$=$	$-ax_3\hat{y}$	(12e)	Dy I
\mathbf{B}_{10}	$x_3\mathbf{a}_1 + x_3\mathbf{a}_2$	$=$	$ax_3\hat{z}$	(12e)	Dy I
\mathbf{B}_{11}	$-x_3\mathbf{a}_1 - x_3\mathbf{a}_2$	$=$	$-ax_3\hat{z}$	(12e)	Dy I
\mathbf{B}_{12}	$2y_4\mathbf{a}_1 + y_4\mathbf{a}_2 + y_4\mathbf{a}_3$	$=$	$ay_4\hat{y} + ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{13}	$y_4\mathbf{a}_2 - y_4\mathbf{a}_3$	$=$	$-ay_4\hat{y} + ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{14}	$-y_4\mathbf{a}_2 + y_4\mathbf{a}_3$	$=$	$ay_4\hat{y} - ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{15}	$-2y_4\mathbf{a}_1 - y_4\mathbf{a}_2 - y_4\mathbf{a}_3$	$=$	$-ay_4\hat{y} - ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{16}	$y_4\mathbf{a}_1 + 2y_4\mathbf{a}_2 + y_4\mathbf{a}_3$	$=$	$ay_4\hat{x} + ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{17}	$-y_4\mathbf{a}_1 + y_4\mathbf{a}_3$	$=$	$ay_4\hat{x} - ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{18}	$y_4\mathbf{a}_1 - y_4\mathbf{a}_3$	$=$	$-ay_4\hat{x} + ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{19}	$-y_4\mathbf{a}_1 - 2y_4\mathbf{a}_2 - y_4\mathbf{a}_3$	$=$	$-ay_4\hat{x} - ay_4\hat{z}$	(24h)	Fe II
\mathbf{B}_{20}	$y_4\mathbf{a}_1 + y_4\mathbf{a}_2 + 2y_4\mathbf{a}_3$	$=$	$ay_4\hat{x} + ay_4\hat{y}$	(24h)	Fe II
\mathbf{B}_{21}	$y_4\mathbf{a}_1 - y_4\mathbf{a}_2$	$=$	$-ay_4\hat{x} + ay_4\hat{y}$	(24h)	Fe II
\mathbf{B}_{22}	$-y_4\mathbf{a}_1 + y_4\mathbf{a}_2$	$=$	$ay_4\hat{x} - ay_4\hat{y}$	(24h)	Fe II
\mathbf{B}_{23}	$-y_4\mathbf{a}_1 - y_4\mathbf{a}_2 - 2y_4\mathbf{a}_3$	$=$	$-ay_4\hat{x} - ay_4\hat{y}$	(24h)	Fe II

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