$Dy_6Fe_{16}O$ Structure: A6B16C_cI46_229_e_ch_a-001

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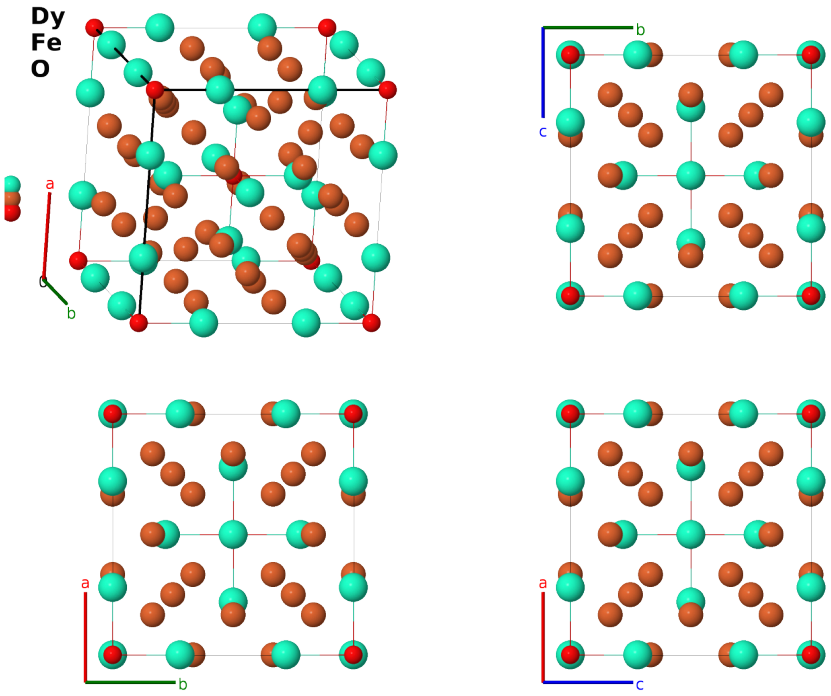
https://aflow.org/prototype-encyclopedia/Y3T5

https://aflow.org/prototype-encyclopedia/A6B16C_cI46_229_e_ch_a-001



Prototype	$Dy_6Fe_{16}O$
AFLOW prototype label	A6B16C_cI46_229_e_ch_a-001
ICSD	9639
CCDC	1594611
Pearson symbol	cI46
Space group number	229
Space group symbol	$Im\bar{3}m$
AFLOW prototype command	`aflow --proto=A6B16C_cI46_229_e_ch_a-001 --params=`a, x_3, y_4

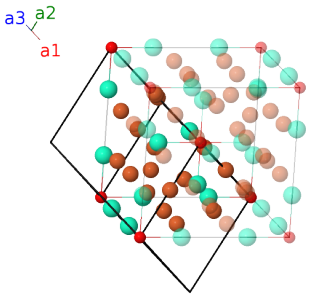
Other compounds with this structure

$Ba_6Na_{16}N$, $Ca_6Ag_{16}N$, $Dy_6Fe_{16}O$, $Dy_6Fe_{16}O$, $Er_6Fe_{16}O$, $Gd_6Fe_{16}O$, $Ho_6Fe_{16}O$, $Tb_6Fe_{16}O$, $Y_6Fe_{16}O$

- 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.*, $Ca_6Ag_{16}N$ was originally thought to be Ag_8Ca_3 (Calvert, 1964), but there is some nitrogen present on the (2a) site. (Villars, 2004)

Body-centered Cubic primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}a\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}a\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	O I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} - \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} - \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_5}$	=	$\frac{1}{2}\,\mathbf{a}_1$	=	$-\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{4}a\,\hat{\mathbf{z}}$	(8c)	Fe I
$\mathbf{B_6}$	=	$x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}}$	(12e)	Dy I
$\mathbf{B_7}$	=	$-x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}}$	(12e)	Dy I
$\mathbf{B_8}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{y}}$	(12e)	Dy I
$\mathbf{B_9}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{y}}$	(12e)	Dy I
$\mathbf{B_{10}}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2$	=	$ax_3\,\hat{\mathbf{z}}$	(12e)	Dy I
$\mathbf{B_{11}}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2$	=	$-ax_3\,\hat{\mathbf{z}}$	(12e)	Dy I
$\mathbf{B_{12}}$	=	$2y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{13}}$	=	$y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{14}}$	=	$-y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{15}}$	=	$-2y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{y}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{16}}$	=	$y_4\,\mathbf{a}_1 + 2y_4\,\mathbf{a}_2 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{17}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{18}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{19}}$	=	$-y_4\,\mathbf{a}_1 - 2y_4\,\mathbf{a}_2 - y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{z}}$	(24h)	Fe II
$\mathbf{B_{20}}$	=	$y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 + 2y_4\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Fe II
$\mathbf{B_{21}}$	=	$y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2$	=	$-ay_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(24h)	Fe II
$\mathbf{B_{22}}$	=	$-y_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2$	=	$ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Fe II
$\mathbf{B_{23}}$	=	$-y_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 - 2y_4\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(24h)	Fe II

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