$YbFe_2O_4$ Structure: A2B4C_hR7_166_c_2c_a-001

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

https://aflow.org/prototype-encyclopedia/A2B4C_hR7_166_c_2c_a-001

Prototype	Fe_2O_4Yb
AFLOW prototype label	A2B4C_hR7_166_c_2c_a-001
ICSD	4192
CCDC	1592877
Pearson symbol	hR7
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A2B4C_hR7_166_c_2c_a-001 --params=`$a, c/a, x_2, x_3, x_4$

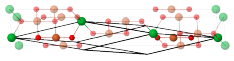
Other compounds with this structure

$LuFe_2O4$, $TmFe_2O4$, $InAlCuO_4$, $InFe_2O_4$, $InGaMgO_4$, $InGaMnO_4$, $InGaZnO_4$, $InMgMnO_4$, $LuGaMgO_4$, $ScAlCuO_4$, $ScGaCuO_4$, $ScGaZnO_4$, $TmGaMgO_4$, $YbGaMgO_4$

- Compounds such as $InGaMnO_4$ have the second and third atoms evenly distributed on the Fe (2c) site.
- Hexagonal settings of this structure can be obtained with the option `--hex`.

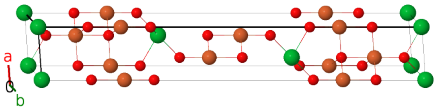
Rhombohedral primitive vectors

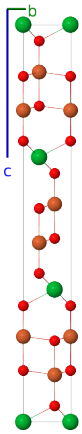
$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \frac{1}{\sqrt{3}}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = -\frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{3}c\,\hat{\mathbf{z}}$$

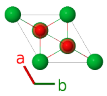


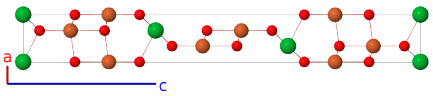
Basis vectors

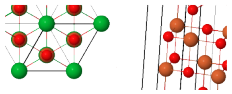
Fe
O
Yb











		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Yb I
$\mathbf{B_2}$	=	$x_2\,\mathbf{a}_1 + x_2\,\mathbf{a}_2 + x_2\,\mathbf{a}_3$	=	$cx_2\,\hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B_3}$	=	$-x_2\,\mathbf{a}_1 - x_2\,\mathbf{a}_2 - x_2\,\mathbf{a}_3$	=	$-cx_2\,\hat{\mathbf{z}}$	(2c)	Fe I
$\mathbf{B_4}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_5}$	=	$-x_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - x_3\,\mathbf{a}_3$	=	$-cx_3\,\hat{\mathbf{z}}$	(2c)	O I
$\mathbf{B_6}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	O II
$\mathbf{B_7}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	O II

References

[1] K. Kato, I. Kawada, N. Kimizuka, and T. Katsura, *Die Kristallstruktur von $YbFe_2O_4$*, Z. Kristallog. **141**, 314–320 (1975), doi:10.1524/zkri.1975.141.16.314.

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