$Ba_5Yb_8Ni_4O_{21}$ Structure: A5B4C21D8_tI76_87_ah_h_bh2i_2h-001

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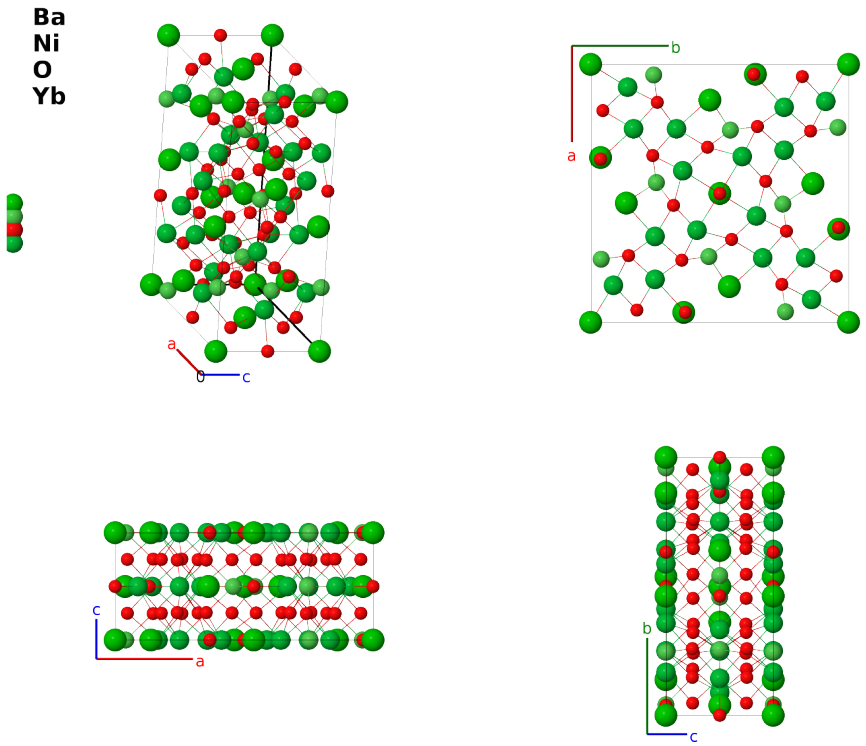
https://aflow.org/prototype-encyclopedia/M4UL

https://aflow.org/prototype-encyclopedia/A5B4C21D8_tI76_87_ah_h_bh2i_2h-001



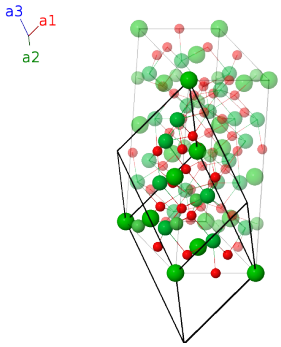
Prototype	$Ba_5Ni_4O_{21}Yb_8$
AFLOW prototype label	A5B4C21D8_tI76_87_ah_h_bh2i_2h-001
ICSD	80614
CCDC	1640819
Pearson symbol	tI76
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A5B4C21D8_tI76_87_ah_h_bh2i_2h-001 --params=`$a, c/a, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7, y_7, x_8, y_8, z_8, x_9, y_9, z_9$

Other compounds with this structure

$Ba_5Dy_8Zn_4O_{21}$, $Ba_5Eu_8Zn_4O_{21}$, $Ba_5Gd_8Mn_4O_{21}$, $Ba_5Gd_8Zn_4O_{21}$, $Ba_5Ho_8Mn_4O_{21}$, $Ba_5Ho_8Zn_4O_{21}$, $Ba_5Lu_8Ni_4O_{21}$, $Ba_5Nd_8Mn_4O_{21}$, $Ba_5Sm_8Mn_4O_{21}$, $Ba_5Tm_8Ni_4O_{21}$

Body-centered Tetragonal primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	O I
$\mathbf{B_3}$	=	$y_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + (x_3+y_3)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + ay_3\,\hat{\mathbf{y}}$	(8h)	Ba II
$\mathbf{B_4}$	=	$-y_3\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - (x_3+y_3)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - ay_3\,\hat{\mathbf{y}}$	(8h)	Ba II
$\mathbf{B_5}$	=	$x_3\,\mathbf{a}_1 - y_3\,\mathbf{a}_2 + (x_3-y_3)\,\mathbf{a}_3$	=	$-ay_3\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Ba II
$\mathbf{B_6}$	=	$-x_3\,\mathbf{a}_1 + y_3\,\mathbf{a}_2 - (x_3-y_3)\,\mathbf{a}_3$	=	$ay_3\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Ba II
$\mathbf{B_7}$	=	$y_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + (x_4+y_4)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + ay_4\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_8}$	=	$-y_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - (x_4+y_4)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - ay_4\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_9}$	=	$x_4\,\mathbf{a}_1 - y_4\,\mathbf{a}_2 + (x_4-y_4)\,\mathbf{a}_3$	=	$-ay_4\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_{10}}$	=	$-x_4\,\mathbf{a}_1 + y_4\,\mathbf{a}_2 - (x_4-y_4)\,\mathbf{a}_3$	=	$ay_4\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}}$	(8h)	Ni I
$\mathbf{B_{11}}$	=	$y_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + (x_5+y_5)\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + ay_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{12}}$	=	$-y_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - (x_5+y_5)\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} - ay_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{13}}$	=	$x_5\,\mathbf{a}_1 - y_5\,\mathbf{a}_2 + (x_5-y_5)\,\mathbf{a}_3$	=	$-ay_5\,\hat{\mathbf{x}} + ax_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{14}}$	=	$-x_5\,\mathbf{a}_1 + y_5\,\mathbf{a}_2 - (x_5-y_5)\,\mathbf{a}_3$	=	$ay_5\,\hat{\mathbf{x}} - ax_5\,\hat{\mathbf{y}}$	(8h)	O II
$\mathbf{B_{15}}$	=	$y_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + (x_6+y_6)\,\mathbf{a}_3$	=	$ax_6\,\hat{\mathbf{x}} + ay_6\,\hat{\mathbf{y}}$	(8h)	Yb I
$\mathbf{B_{16}}$	=	$-y_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - (x_6+y_6)\,\mathbf{a}_3$	=	$-ax_6\,\hat{\mathbf{x}} - ay_6\,\hat{\mathbf{y}}$	(8h)	Yb I
$\mathbf{B_{17}}$	=	$x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 + (x_6-y_6)\,\mathbf{a}_3$	=	$-ay_6\,\hat{\mathbf{x}} + ax_6\,\hat{\mathbf{y}}$	(8h)	Yb I
$\mathbf{B_{18}}$	=	$-x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 - (x_6-y_6)\,\mathbf{a}_3$	=	$ay_6\,\hat{\mathbf{x}} - ax_6\,\hat{\mathbf{y}}$	(8h)	Yb I
$\mathbf{B_{19}}$	=	$y_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + (x_7+y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + ay_7\,\hat{\mathbf{y}}$	(8h)	Yb II
$\mathbf{B_{20}}$	=	$-y_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - (x_7+y_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - ay_7\,\hat{\mathbf{y}}$	(8h)	Yb II
$\mathbf{B_{21}}$	=	$x_7\,\mathbf{a}_1 - y_7\,\mathbf{a}_2 + (x_7-y_7)\,\mathbf{a}_3$	=	$-ay_7\,\hat{\mathbf{x}} + ax_7\,\hat{\mathbf{y}}$	(8h)	Yb II
$\mathbf{B_{22}}$	=	$-x_7\,\mathbf{a}_1 + y_7\,\mathbf{a}_2 - (x_7-y_7)\,\mathbf{a}_3$	=	$ay_7\,\hat{\mathbf{x}} - ax_7\,\hat{\mathbf{y}}$	(8h)	Yb II
$\mathbf{B_{23}}$	=	$(y_8+z_8)\,\mathbf{a}_1 + (x_8+z_8)\,\mathbf{a}_2 + (x_8+y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{24}}$	=	$-(y_8-z_8)\,\mathbf{a}_1 - (x_8-z_8)\,\mathbf{a}_2 - (x_8+y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16i)	O III

$$\mathbf{B_{25}} = (x_8 + z_8)\,\mathbf{a}_1 - (y_8 - z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{26}} = -(x_8 - z_8)\,\mathbf{a}_1 + (y_8 + z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{27}} = -(y_8 + z_8)\,\mathbf{a}_1 - (x_8 + z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3 = -ax_8\,\hat{\mathbf{x}} - ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{28}} = (y_8 - z_8)\,\mathbf{a}_1 + (x_8 - z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3 = ax_8\,\hat{\mathbf{x}} + ay_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{29}} = -(x_8 + z_8)\,\mathbf{a}_1 + (y_8 - z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3 = ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{30}} = (x_8 - z_8)\,\mathbf{a}_1 - (y_8 + z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3 = -ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}} \quad (16i) \quad \text{O III}$$

$$\mathbf{B_{31}} = (y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{32}} = -(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{33}} = (x_9 + z_9)\,\mathbf{a}_1 - (y_9 - z_9)\,\mathbf{a}_2 + (x_9 - y_9)\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{34}} = -(x_9 - z_9)\,\mathbf{a}_1 + (y_9 + z_9)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{35}} = -(y_9 + z_9)\,\mathbf{a}_1 - (x_9 + z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3 = -ax_9\,\hat{\mathbf{x}} - ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{36}} = (y_9 - z_9)\,\mathbf{a}_1 + (x_9 - z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3 = ax_9\,\hat{\mathbf{x}} + ay_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{37}} = -(x_9 + z_9)\,\mathbf{a}_1 + (y_9 - z_9)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3 = ay_9\,\hat{\mathbf{x}} - ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

$$\mathbf{B_{38}} = (x_9 - z_9)\,\mathbf{a}_1 - (y_9 + z_9)\,\mathbf{a}_2 + (x_9 - y_9)\,\mathbf{a}_3 = -ay_9\,\hat{\mathbf{x}} + ax_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}} \quad (16i) \quad \text{O IV}$$

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[1] A. Jain, S. Ping, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, *Commentary: The Materials Project: A materials genome approach to accelerating materials innovation*, APL Materials **1**, 011002 (2013), doi:10.1063/1.4812323.

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