$Ba_5Yb_8Ni_4O_{21}$ Structure: A5B4C21D8_tI76_87_ah_h_bh2i_2h-001

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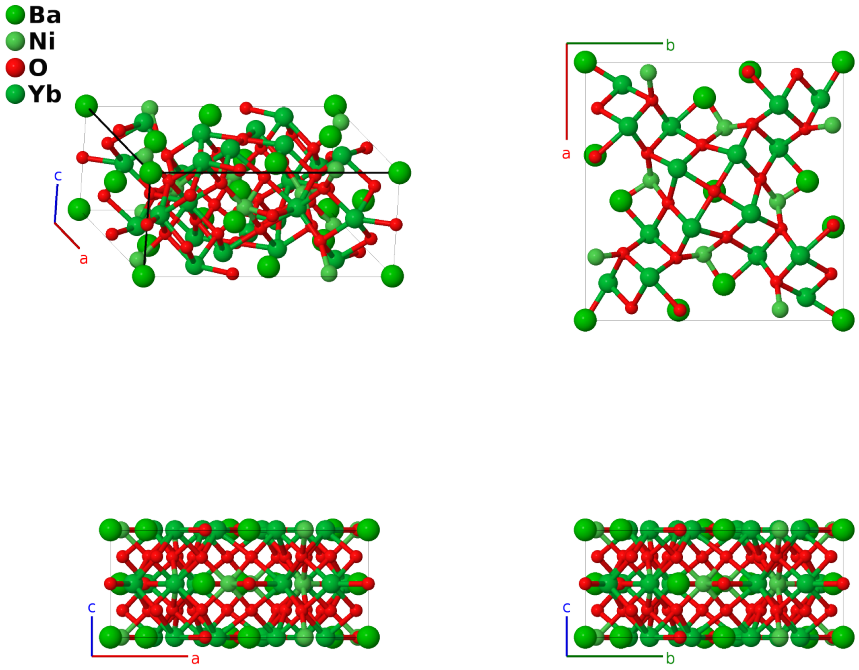
https://aflow.org/p/M4UL

https://aflow.org/p/A5B4C21D8_tI76_87_ah_h_bh2i_2h-001



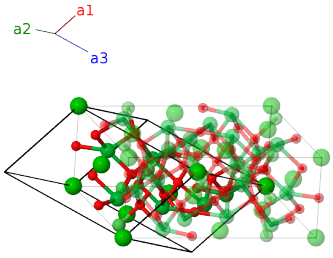
Prototype	$Ba_5Ni_4O_{21}Yb_8$
AFLOW prototype label	A5B4C21D8_tI76_87_ah_h_bh2i_2h-001
ICSD	80614
Pearson symbol	tI76
Space group number	87
Space group symbol	$I4/m$
AFLOW prototype command	`aflow --proto=A5B4C21D8_tI76_87_ah_h_bh2i_2h-001 --params=`$a, c/a, x_3, y_3, x_4, y_4, x_5, y_5, x_6, y_6, x_7,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

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
$\mathbf{B_{25}}$	=	$(x_8+z_8)\,\mathbf{a}_1 - (y_8-z_8)\,\mathbf{a}_2 + (x_8-y_8)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}} + ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{26}}$	=	$-(x_8-z_8)\,\mathbf{a}_1 + (y_8+z_8)\,\mathbf{a}_2 - (x_8-y_8)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}} - ax_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(16i)	O III

$\mathbf{B_{27}}$	=	$-(y_8+z_8)\,\mathbf{a}_1-(x_8+z_8)\,\mathbf{a}_2-(x_8+y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}}-ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{28}}$	=	$(y_8-z_8)\,\mathbf{a}_1+(x_8-z_8)\,\mathbf{a}_2+(x_8+y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}}+ay_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{29}}$	=	$-(x_8+z_8)\,\mathbf{a}_1+(y_8-z_8)\,\mathbf{a}_2-(x_8-y_8)\,\mathbf{a}_3$	=	$ay_8\,\hat{\mathbf{x}}-ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{30}}$	=	$(x_8-z_8)\,\mathbf{a}_1-(y_8+z_8)\,\mathbf{a}_2+(x_8-y_8)\,\mathbf{a}_3$	=	$-ay_8\,\hat{\mathbf{x}}+ax_8\,\hat{\mathbf{y}}-cz_8\,\hat{\mathbf{z}}$	(16i)	O III
$\mathbf{B_{31}}$	=	$(y_9+z_9)\,\mathbf{a}_1+(x_9+z_9)\,\mathbf{a}_2+(x_9+y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{32}}$	=	$-(y_9-z_9)\,\mathbf{a}_1-(x_9-z_9)\,\mathbf{a}_2-(x_9+y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-ay_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{33}}$	=	$(x_9+z_9)\,\mathbf{a}_1-(y_9-z_9)\,\mathbf{a}_2+(x_9-y_9)\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{x}}+ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{34}}$	=	$-(x_9-z_9)\,\mathbf{a}_1+(y_9+z_9)\,\mathbf{a}_2-(x_9-y_9)\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{x}}-ax_9\,\hat{\mathbf{y}}+cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{35}}$	=	$-(y_9+z_9)\,\mathbf{a}_1-(x_9+z_9)\,\mathbf{a}_2-(x_9+y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}}-ay_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{36}}$	=	$(y_9-z_9)\,\mathbf{a}_1+(x_9-z_9)\,\mathbf{a}_2+(x_9+y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}}+ay_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{37}}$	=	$-(x_9+z_9)\,\mathbf{a}_1+(y_9-z_9)\,\mathbf{a}_2-(x_9-y_9)\,\mathbf{a}_3$	=	$ay_9\,\hat{\mathbf{x}}-ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16i)	O IV
$\mathbf{B_{38}}$	=	$(x_9-z_9)\,\mathbf{a}_1-(y_9+z_9)\,\mathbf{a}_2+(x_9-y_9)\,\mathbf{a}_3$	=	$-ay_9\,\hat{\mathbf{x}}+ax_9\,\hat{\mathbf{y}}-cz_9\,\hat{\mathbf{z}}$	(16i)	O IV

References

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