$Ba_4NbRu_3O_{12}$ Structure: A4BC12D3_hR20_166_2c_a_2h_bc-001

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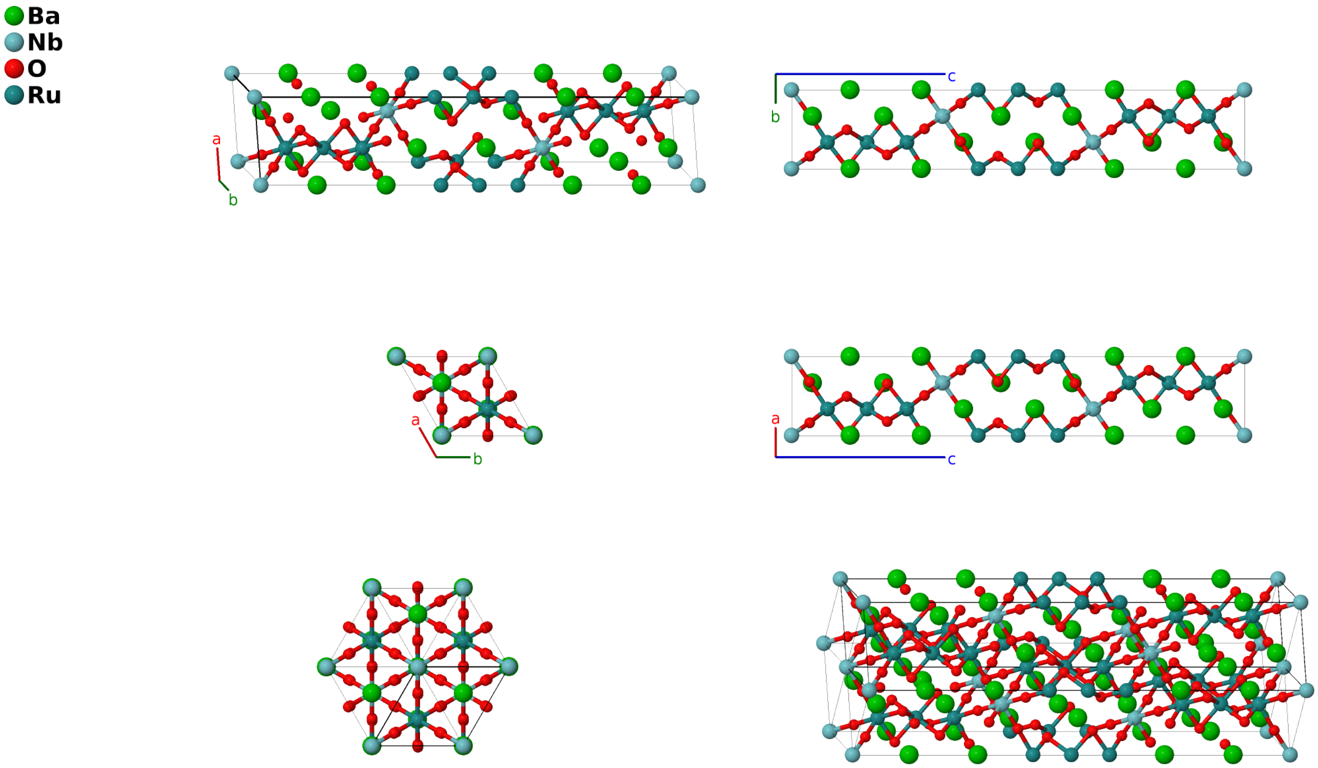
https://aflow.org/p/9CFG

https://aflow.org/p/A4BC12D3_hR20_166_2c_a_2h_bc-001



Prototype	$Ba_4NbO_{12}Ru_3$
AFLOW prototype label	A4BC12D3_hR20_166_2c_a_2h_bc-001
ICSD	none
Pearson symbol	hR20
Space group number	166
Space group symbol	$R\bar{3}m$
AFLOW prototype command	`aflow --proto=A4BC12D3_hR20_166_2c_a_2h_bc-001 --params=`$a, c/a, x_3, x_4, x_5, x_6, z_6, x_7, z_7$

Other compounds with this structure

$Ir_4NbRu_3O_{12}$, $Mn_4NbRu_3O_{12}$, $Rh_4NbRu_3O_{12}$

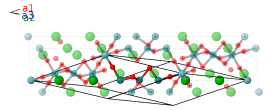
- Hexagonal settings of this structure can be obtained with the option `--hex`.

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

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Nb I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(1b)	Ru I
$\mathbf{B_3}$	=	$x_3\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + x_3\,\mathbf{a}_3$	=	$cx_3\,\hat{\mathbf{z}}$	(2c)	Ba 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)	Ba I
$\mathbf{B_5}$	=	$x_4\,\mathbf{a}_1 + x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$cx_4\,\hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B_6}$	=	$-x_4\,\mathbf{a}_1 - x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-cx_4\,\hat{\mathbf{z}}$	(2c)	Ba II
$\mathbf{B_7}$	=	$x_5\,\mathbf{a}_1 + x_5\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$cx_5\,\hat{\mathbf{z}}$	(2c)	Ru II
$\mathbf{B_8}$	=	$-x_5\,\mathbf{a}_1 - x_5\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-cx_5\,\hat{\mathbf{z}}$	(2c)	Ru II
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{10}}$	=	$z_6\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{11}}$	=	$x_6\,\mathbf{a}_1 + z_6\,\mathbf{a}_2 + x_6\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_6 - z_6)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{12}}$	=	$-z_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{13}}$	=	$-x_6\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 - z_6)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{14}}$	=	$-x_6\,\mathbf{a}_1 - z_6\,\mathbf{a}_2 - x_6\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_6 - z_6)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_6 + z_6)\,\hat{\mathbf{z}}$	(6h)	O I
$\mathbf{B_{15}}$	=	$x_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + z_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{16}}$	=	$z_7\,\mathbf{a}_1 + x_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{17}}$	=	$x_7\,\mathbf{a}_1 + z_7\,\mathbf{a}_2 + x_7\,\mathbf{a}_3$	=	$-\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} + \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{18}}$	=	$-z_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{19}}$	=	$-x_7\,\mathbf{a}_1 - x_7\,\mathbf{a}_2 - z_7\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_7 - z_7)\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II
$\mathbf{B_{20}}$	=	$-x_7\,\mathbf{a}_1 - z_7\,\mathbf{a}_2 - x_7\,\mathbf{a}_3$	=	$\frac{1}{\sqrt{3}}a\,(x_7 - z_7)\,\hat{\mathbf{y}} - \frac{1}{3}c\,(2x_7 + z_7)\,\hat{\mathbf{z}}$	(6h)	O II

References

[1] L. T. Nguyen, T. Halloran, W. Xie, T. Kong, C. L. Broholm, and R. J. Cava, *Geometrically frustrated trimer-based Mott insulator*, Phys. Rev. Mater. **2**, 054414 (2018), doi:10.1103/PhysRevMaterials.2.054414.

Found in

[1] E. V. Komleva, D. I. Khomskii, and S. V. Streltsov, *Three-site transition-metal clusters: Going from localized electrons to molecular orbitals*, Phys. Rev. B **102**, 174448 (2020), doi:10.1103/PhysRevB.102.174448.