$Na_2BaNi(PO_4)_2$ Structure: AB2CD8E2_hP14_147_a_d_b_dg_d-001

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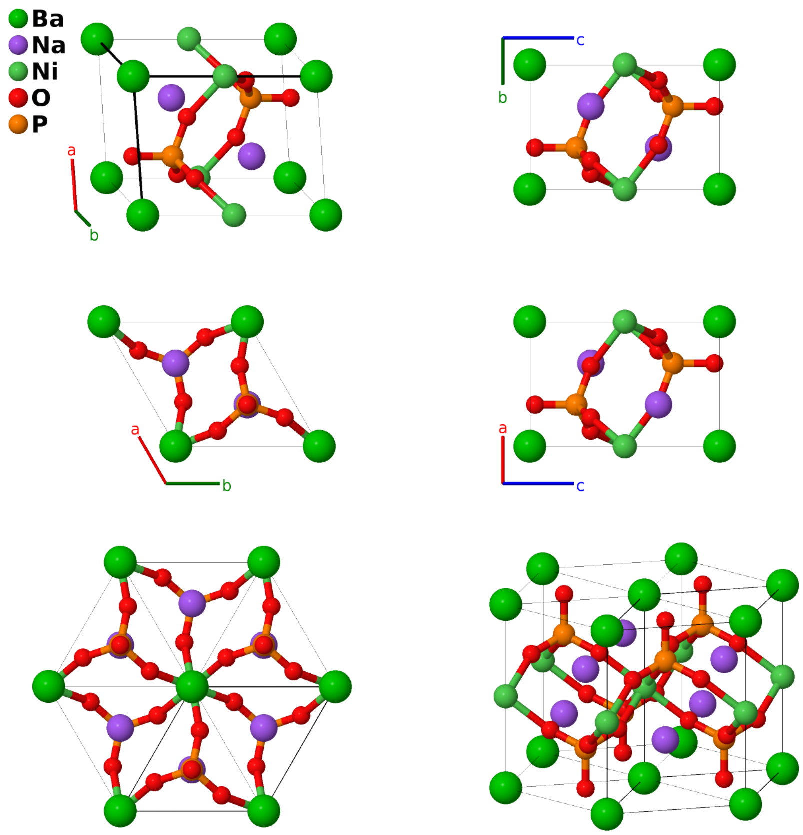
https://aflow.org/p/B64B

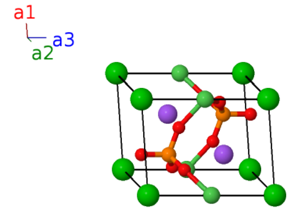
https://aflow.org/p/AB2CD8E2_hP14_147_a_d_b_dg_d-001



Prototype	$BaNa_2NiO_8P_2$
AFLOW prototype label	AB2CD8E2_hP14_147_a_d_b_dg_d-001
ICSD	none
Pearson symbol	hP14
Space group number	147
Space group symbol	$P\bar{3}$
AFLOW prototype command	`aflow --proto=AB2CD8E2_hP14_147_a_d_b_dg_d-001` `--params=`$a, c/a, z_3, z_4, z_5, x_6, y_6, z_6$

Trigonal (Hexagonal) primitive vectors

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(1a)	Ba I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}c\,\mathbf{\hat{z}}$	(1b)	Ni I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_3\,\mathbf{\hat{z}}$	(2d)	Na I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - cz_3\,\mathbf{\hat{z}}$	(2d)	Na I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(2d)	O I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(2d)	O I
$\mathbf{B_7}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} + cz_5\,\mathbf{\hat{z}}$	(2d)	P I
$\mathbf{B_8}$	=	$\frac{2}{3}\,\mathbf{a}_1 + \frac{1}{3}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{6}a\,\mathbf{\hat{y}} - cz_5\,\mathbf{\hat{z}}$	(2d)	P I
$\mathbf{B_9}$	=	$x_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 + y_6)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\mathbf{\hat{y}} + cz_6\,\mathbf{\hat{z}}$	(6g)	O II
$\mathbf{B_{10}}$	=	$-y_6\,\mathbf{a}_1 + (x_6 - y_6)\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(x_6 - 2y_6)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ax_6\,\mathbf{\hat{y}} + cz_6\,\mathbf{\hat{z}}$	(6g)	O II
$\mathbf{B_{11}}$	=	$-(x_6 - y_6)\,\mathbf{a}_1 - x_6\,\mathbf{a}_2 + z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(2x_6 - y_6)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ay_6\,\mathbf{\hat{y}} + cz_6\,\mathbf{\hat{z}}$	(6g)	O II
$\mathbf{B_{12}}$	=	$-x_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$-\frac{1}{2}a\,(x_6 + y_6)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}a\,(x_6 - y_6)\,\mathbf{\hat{y}} - cz_6\,\mathbf{\hat{z}}$	(6g)	O II
$\mathbf{B_{13}}$	=	$y_6\,\mathbf{a}_1 - (x_6 - y_6)\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(-x_6 + 2y_6)\,\mathbf{\hat{x}} - \frac{\sqrt{3}}{2}ax_6\,\mathbf{\hat{y}} - cz_6\,\mathbf{\hat{z}}$	(6g)	O II
$\mathbf{B_{14}}$	=	$(x_6 - y_6)\,\mathbf{a}_1 + x_6\,\mathbf{a}_2 - z_6\,\mathbf{a}_3$	=	$\frac{1}{2}a\,(2x_6 - y_6)\,\mathbf{\hat{x}} + \frac{\sqrt{3}}{2}ay_6\,\mathbf{\hat{y}} - cz_6\,\mathbf{\hat{z}}$	(6g)	O II

References

[1] N. Li, Q. Huang, A. Brassington, X. Y. Yue, W. J. Chu, S. K. Guang, X. H. Zhou, P. Gao, E. X. Feng, H. B. Cao, E. S. Choi, Y. Sun, Q. J. Li, X. Zhao, H. D. Zhou, and X. F. Sun, *Quantum spin state transitions in spin-1 equilateral triangular lattice antiferromagnet $Na_2BaNi(PO_4)_2$*, Phys. Rev. B **104**, 104403 (2021), doi:10.1103/PhysRevB.104.104403.