High-Pressure oP8 Sodium Structure: A_oP8_62_2c-002

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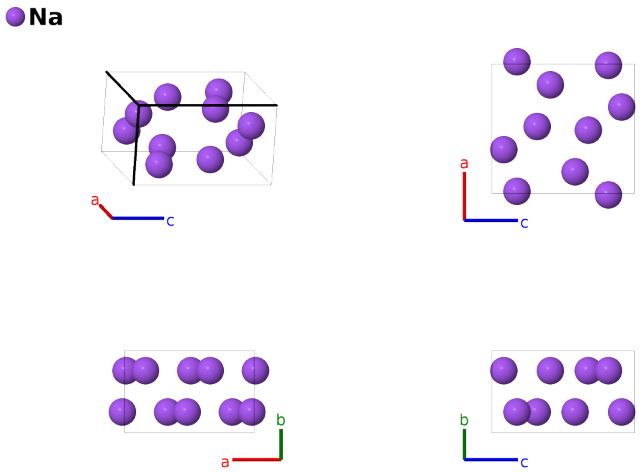
https://aflow.org/p/3BFR

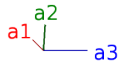
https://aflow.org/p/A_oP8_62_2c-002



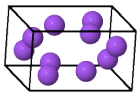
Prototype	Na
AFLOW prototype label	A_oP8_62_2c-002
ICSD	189460
Pearson symbol	oP8
Space group number	62
Space group symbol	*Pnma*
AFLOW prototype command	`aflow --proto=A_oP8_62_2c-002 --params=`$a, b/a, c/a, x_1, z_1, x_2, z_2$

- Pressurized sodium can be found in a wide variety of structures, many of them incommensurate "host-guest" composites (Gregoryanz, 2008):
  - The ground state of sodium is the body-centered cubic lattice ($A2$).
  - Above 78K a metastable hexagonal close-packed ($A3$) phase has been observed. (Donohue, 1974)
  - In the range 100-118 GPa and near room temperature sodium takes on the high pressure cI16 lithium structure.
  - The current oP8 structure is stable in the range 118-125 GPa, again near room temperature.
- The data for the current structure was taken at 119 GPa and 300 K.
- oP8 Na and α-Np (A_c) have the same AFLOW prototype label, A_oP8_62_2c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

Simple Orthorhombic primitive vectors



$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = b\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$x_1\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_1\,\mathbf{a}_3$	=	$ax_1\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_1\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_2}$	=	$-\left(x_1 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_1 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_1 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_1 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_3}$	=	$-x_1\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_1\,\mathbf{a}_3$	=	$-ax_1\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_1\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_4}$	=	$\left(x_1 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_1 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_1 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_1 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Na I
$\mathbf{B_5}$	=	$x_2\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_2\,\mathbf{a}_3$	=	$ax_2\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} + cz_2\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_6}$	=	$-\left(x_2 - \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \left(z_2 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-a\left(x_2 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} + c\left(z_2 + \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_7}$	=	$-x_2\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_2\,\mathbf{a}_3$	=	$-ax_2\,\hat{\mathbf{x}} + \frac{3}{4}b\,\hat{\mathbf{y}} - cz_2\,\hat{\mathbf{z}}$	(4c)	Na II
$\mathbf{B_8}$	=	$\left(x_2 + \frac{1}{2}\right)\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 - \left(z_2 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$a\left(x_2 + \frac{1}{2}\right)\,\hat{\mathbf{x}} + \frac{1}{4}b\,\hat{\mathbf{y}} - c\left(z_2 - \frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4c)	Na II

References

[1] E. Gregoryanz, L. F. Lundegaard, M. I. McMahon, C. Guillaume, R. J. Nelmes, and M. Mezouar, *Structural Diversity of Sodium*, Science **320**, 1054–1057 (2008), doi:10.1126/science.1155715.

[2] J. Donohue, *The Structures of the Elements* (Robert E. Krieger Publishing Company, New York, 1974).

Found in

[1] C. J. Pickard, *Ephemeral data derived potentials for random structure search*, Phys. Rev. B **106**, 014102 (2022), doi:10.1103/PhysRevB.106.014102.

[2] Y. Ma, M. Eremets, A. R. Oganov, Y. Xie, I. Trojan, S. Medvedev, A. O. Lyakhov, M. Valle, and V. Prakapenka, *Transparent dense sodium*, Nature **458**, 182–185 (2009), doi:10.1038/nature07786.