

High-Pressure oP8 Sodium Structure:

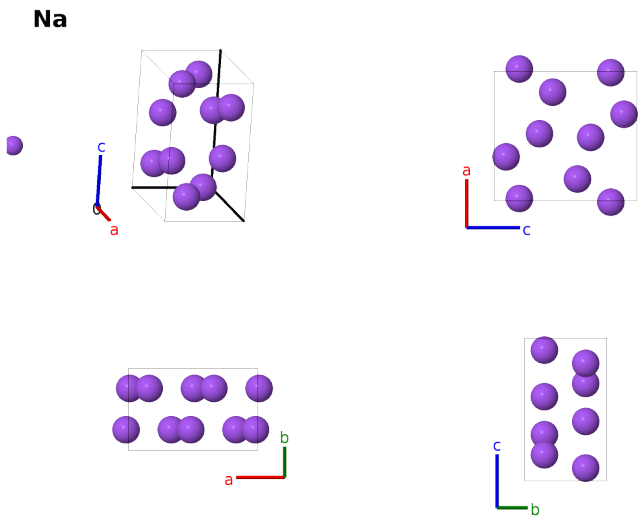
A_oP8_62_2c-002

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<https://aflow.org/prototype-encyclopedia/3BFR>

https://aflow.org/prototype-encyclopedia/A_oP8_62_2c-002



Prototype	Na
AFLOW prototype label	A_oP8_62_2c-002
ICSD	189460
CCDC	1698430
Pearson symbol	oP8
Space group number	62
Space group symbol	$Pnma$
AFLOW prototype command	<code>aflow --proto=A_oP8_62_2c-002</code> <code>--params=a, b/a, c/a, x₁, z₁, x₂, z₂</code>

- 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.

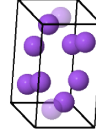
- The data for the current structure was taken at 119 GPa and 300 K.
- oP8 Na and α -Np (A_c) have the same AFLOW prototype label, A_oP8.62.2c. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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.

First cited in

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