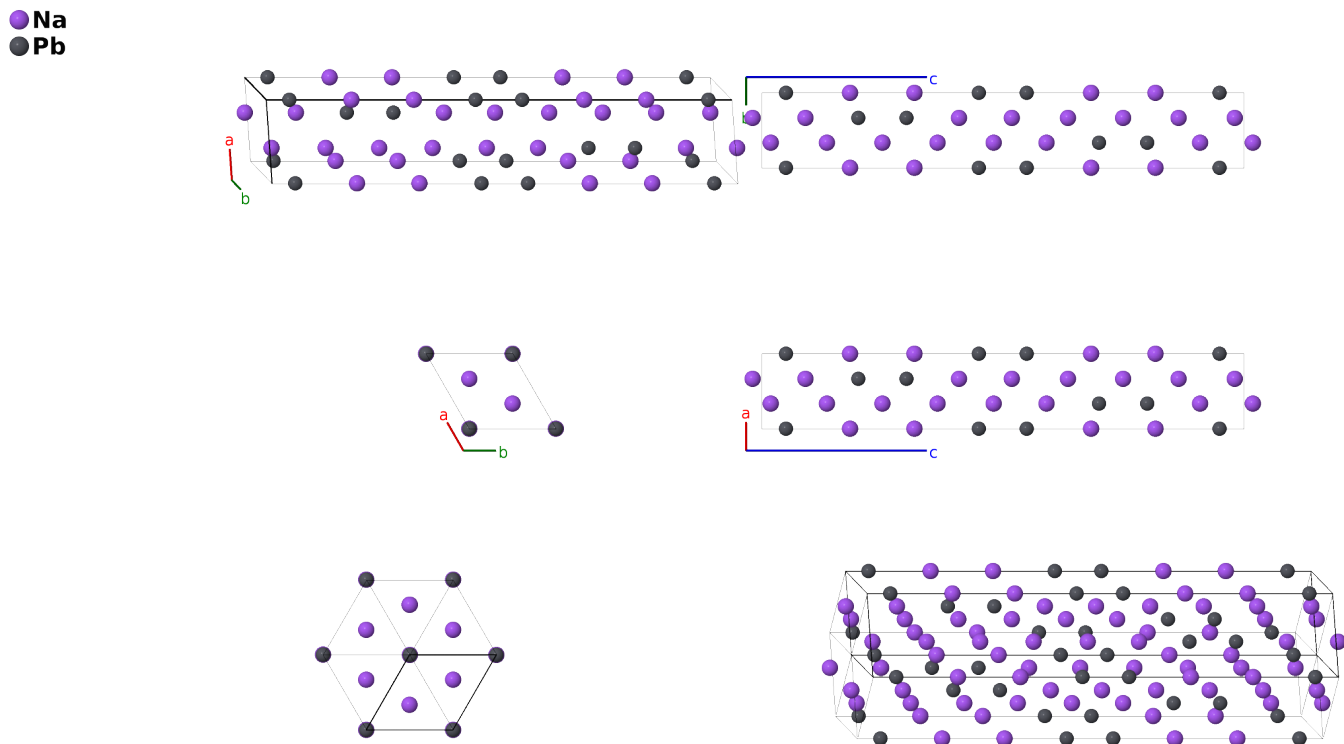


# Na<sub>9</sub>Pb<sub>4</sub> ( $\delta'$ -NaPb) Structure: A9B4\_hP26\_194\_ce3f\_ef-001

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<https://aflow.org/p/J5ST>

[https://aflow.org/p/A9B4\\_hP26\\_194\\_ce3f\\_ef-001](https://aflow.org/p/A9B4_hP26_194_ce3f_ef-001)



<b>Prototype</b>	Na <sub>9</sub> Pb <sub>4</sub>
<b>AFLOW prototype label</b>	A9B4_hP26_194_ce3f_ef-001
<b>ICSD</b>	none
<b>Pearson symbol</b>	hP26
<b>Space group number</b>	194
<b>Space group symbol</b>	$P6_3/mmc$
<b>AFLOW prototype command</b>	<code>aflow --proto=A9B4_hP26_194_ce3f_ef-001 --params=a, c/a, z<sub>2</sub>, z<sub>3</sub>, z<sub>4</sub>, z<sub>5</sub>, z<sub>6</sub>, z<sub>7</sub></code>

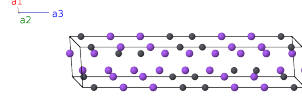
- (Weston, 1957) determined the space group, lattice constants, and positions of the lead atoms in Na<sub>9</sub>Pb<sub>4</sub> but were unable to place the sodium atoms. Using the First-Principles Assisted Structure Solution (FPASS) method, (Ward, 2015) determined a set of positions for the sodium atoms consistent with the available experimental data. To our knowledge further experimental study of Na<sub>9</sub>Pb<sub>4</sub> has taken place.
- We have shifted the origin of the  $\hat{z}$  axis by  $c/2$  from that chosen by (Weston, 1957), changing the Na-I site from the (2d) Wyckoff position to (2c).

- There is no ICSD entry for this structure, but (Ward, 2015) provide the CIF for this structure in their supplementary material.

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### Hexagonal primitive vectors

$$\begin{aligned}\mathbf{a}_1 &= \frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_2 &= \frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a \hat{\mathbf{y}} \\ \mathbf{a}_3 &= c \hat{\mathbf{z}}\end{aligned}$$




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### Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B}_1$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + \frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{1}{4}c \hat{\mathbf{z}}$	(2c)	Na I
$\mathbf{B}_2$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + \frac{3}{4} \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + \frac{3}{4}c \hat{\mathbf{z}}$	(2c)	Na I
$\mathbf{B}_3$	$= z_2 \mathbf{a}_3$	$=$	$cz_2 \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_4$	$= (z_2 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_2 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_5$	$= -z_2 \mathbf{a}_3$	$=$	$-cz_2 \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_6$	$= -(z_2 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_2 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_7$	$= z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_8$	$= (z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_9$	$= -z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_{10}$	$= -(z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Pb I
$\mathbf{B}_{11}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_4 \hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B}_{12}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B}_{13}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_4 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_4 \hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B}_{14}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na III
$\mathbf{B}_{15}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{16}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{17}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{18}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{19}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{20}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{21}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{22}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{23}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{24}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{25}$	$= \frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{26}$	$= \frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2}a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb II

### References

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