

Na₁₃Pb₅ (γ -NaPb) Structure: A13B5_hP36_194_a2e4f_b2f-001

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<https://aflow.org/prototype-encyclopedia/G1KV>

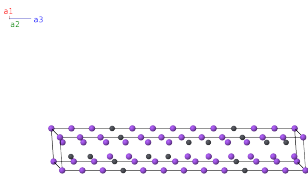
https://aflow.org/prototype-encyclopedia/A13B5_hP36_194_a2e4f_b2f-001

Prototype	Na ₁₃ Pb ₅
AFLOW prototype label	A13B5_hP36_194_a2e4f_b2f-001
Pearson symbol	hP36
Space group number	194
Space group symbol	$P6_3/mmc$
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- (Weston, 1957) determined the space group, lattice constants, and positions of the lead atoms in Na₁₃Pb₅, 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 no further experimental study of Na₁₃Pb₅ has taken place.
- There is no ICSD entry for this structure, but (Ward, 2015) provide the CIF for this structure in their supplementary material.

Hexagonal primitive vectors

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



Basis vectors

	Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
B₁	=	0	=	0	(2a) Na I

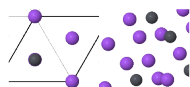
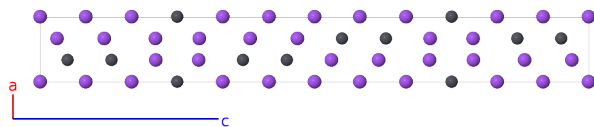
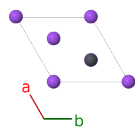
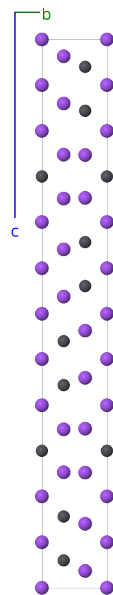
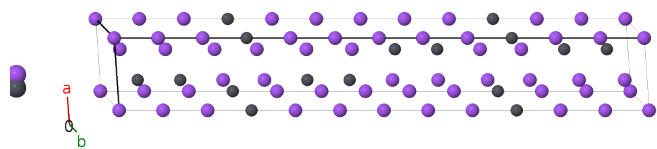
$\mathbf{B}_2$	$=$	$\frac{1}{2} \mathbf{a}_3$	$=$	$\frac{1}{2} c \hat{\mathbf{z}}$	(2a)	Na I
$\mathbf{B}_3$	$=$	$\frac{1}{4} \mathbf{a}_3$	$=$	$\frac{1}{4} c \hat{\mathbf{z}}$	(2b)	Pb I
$\mathbf{B}_4$	$=$	$\frac{3}{4} \mathbf{a}_3$	$=$	$\frac{3}{4} c \hat{\mathbf{z}}$	(2b)	Pb I
$\mathbf{B}_5$	$=$	$z_3 \mathbf{a}_3$	$=$	$cz_3 \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_6$	$=$	$(z_3 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_3 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_7$	$=$	$-z_3 \mathbf{a}_3$	$=$	$-cz_3 \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_8$	$=$	$-(z_3 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_3 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B}_9$	$=$	$z_4 \mathbf{a}_3$	$=$	$cz_4 \hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B}_{10}$	$=$	$(z_4 + \frac{1}{2}) \mathbf{a}_3$	$=$	$c(z_4 + \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B}_{11}$	$=$	$-z_4 \mathbf{a}_3$	$=$	$-cz_4 \hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B}_{12}$	$=$	$-(z_4 - \frac{1}{2}) \mathbf{a}_3$	$=$	$-c(z_4 - \frac{1}{2}) \hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B}_{13}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_5 \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{14}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_5 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_5 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{15}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_5 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_5 \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{16}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_5 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_5 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na IV
$\mathbf{B}_{17}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_6 \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{18}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_6 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_6 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{19}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_6 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_6 \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{20}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_6 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_6 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na V
$\mathbf{B}_{21}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_7 \hat{\mathbf{z}}$	(4f)	Na VI
$\mathbf{B}_{22}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_7 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_7 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na VI
$\mathbf{B}_{23}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_7 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_7 \hat{\mathbf{z}}$	(4f)	Na VI
$\mathbf{B}_{24}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_7 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_7 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na VI
$\mathbf{B}_{25}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_8 \hat{\mathbf{z}}$	(4f)	Na VII
$\mathbf{B}_{26}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_8 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_8 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na VII
$\mathbf{B}_{27}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_8 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_8 \hat{\mathbf{z}}$	(4f)	Na VII
$\mathbf{B}_{28}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_8 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_8 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Na VII
$\mathbf{B}_{29}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_9 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_9 \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{30}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_9 + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_9 + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{31}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_9 \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_9 \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{32}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_9 - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_9 - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb II
$\mathbf{B}_{33}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 + z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + cz_{10} \hat{\mathbf{z}}$	(4f)	Pb III
$\mathbf{B}_{34}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 + (z_{10} + \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} + c(z_{10} + \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb III
$\mathbf{B}_{35}$	$=$	$\frac{2}{3} \mathbf{a}_1 + \frac{1}{3} \mathbf{a}_2 - z_{10} \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} - \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - cz_{10} \hat{\mathbf{z}}$	(4f)	Pb III
$\mathbf{B}_{36}$	$=$	$\frac{1}{3} \mathbf{a}_1 + \frac{2}{3} \mathbf{a}_2 - (z_{10} - \frac{1}{2}) \mathbf{a}_3$	$=$	$\frac{1}{2} a \hat{\mathbf{x}} + \frac{\sqrt{3}}{6} a \hat{\mathbf{y}} - c(z_{10} - \frac{1}{2}) \hat{\mathbf{z}}$	(4f)	Pb III

References

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- [2] N. E. Weston and D. P. Shoemaker, *The crystal structures of three phases in the Na-Pb system*, Acta Cryst. **10**, 775 (1957), doi:10.1107/S0365110X57002649. International Union of Crystallography Abstracts, pp. 735-863.

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Na
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