$Na_{13}Pb_5$ (γ-NaPb) Structure: A13B5_hP36_194_a2e4f_b2f-001

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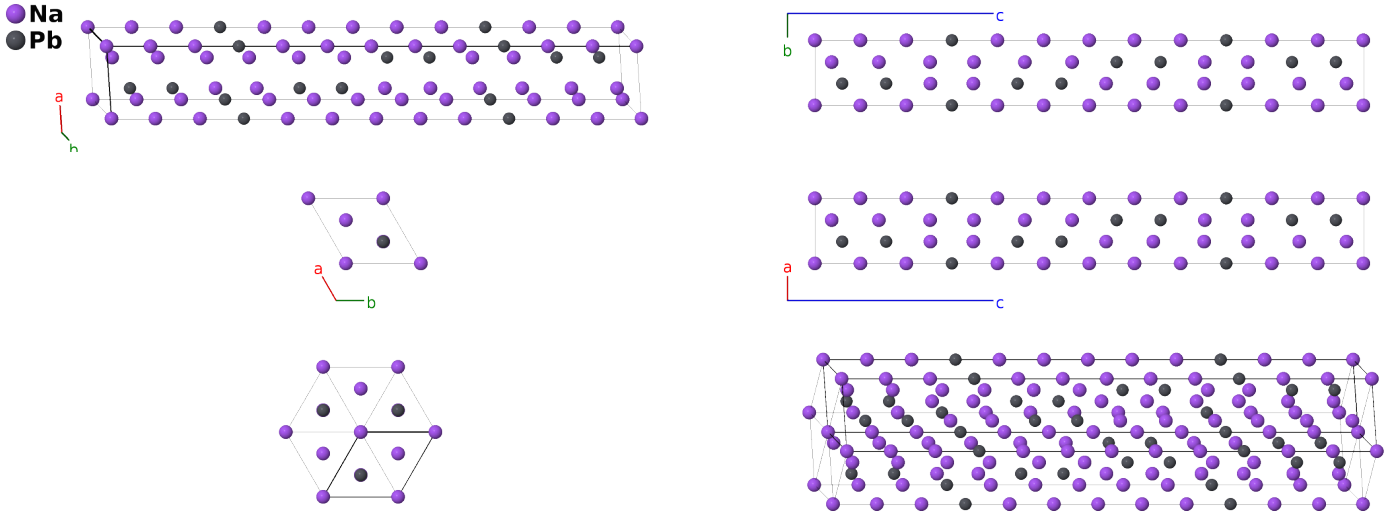
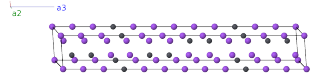


Prototype	$Na_{13}Pb_5$
AFLOW prototype label	A13B5_hP36_194_a2e4f_b2f-001
ICSD	none
Pearson symbol	hP36
Space group number	194
Space group symbol	$P6_3/mmc$
AFLOW prototype command	`aflow --proto=A13B5_hP36_194_a2e4f_b2f-001 --params=`$a, c/a, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}$

- (Weston, 1957) determined the space group, lattice constants, and positions of the lead atoms in $Na_{13}Pb_5$, 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 $Na_{13}Pb_5$ 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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	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
$\mathbf{B_6}$	=	$\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_7}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_8}$	=	$-\left(z_3-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_3-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Na II
$\mathbf{B_9}$	=	$z_4\,\mathbf{a}_3$	=	$cz_4\,\hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B_{10}}$	=	$\left(z_4+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_4+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B_{11}}$	=	$-z_4\,\mathbf{a}_3$	=	$-cz_4\,\hat{\mathbf{z}}$	(4e)	Na III
$\mathbf{B_{12}}$	=	$-\left(z_4-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$-c\left(z_4-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{14}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_5+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_5+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{16}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_5-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_5-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{18}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_6+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_6+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{20}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_6-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_6-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{22}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_7+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_7+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{24}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_7-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_7-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{26}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_8+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_8+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{28}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_8-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_8-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{30}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_9+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_9+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{32}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_9-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_9-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{34}}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_{10}+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_{10}+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(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
$\mathbf{B_{36}}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2-\left(z_{10}-\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}-c\left(z_{10}-\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(4f)	Pb III

References

[1] L. Ward, K. Michel, and C. Wolverton, *Three new crystal structures in the Na-Pb system: solving structures without additional experimental input*, Acta Crystallogr. Sect. A **71**, 542–548 (2015), doi:10.1107/S2053273315012516.

[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.