$(NH_4)Pb_2Br_5$ ($K3_4$) Structure (*Erroneous*): A5BC2_tI32_140_bl_a_h-001

This structure originally had the label `A5BC2_tI32_140_bl_a_h`. Calls to that address will be redirected here.

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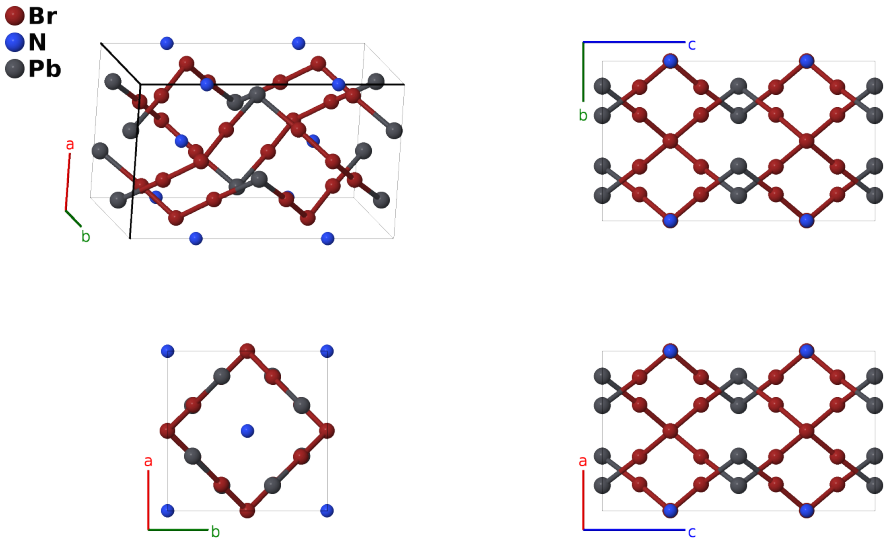
https://aflow.org/p/HL9W

https://aflow.org/p/A5BC2_tI32_140_bl_a_h-001

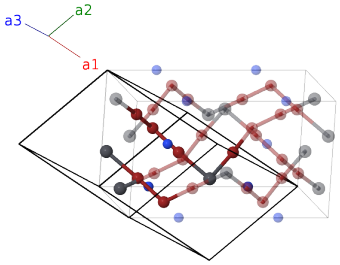


Prototype	$Br_5(NH_4)Pb_2$
AFLOW prototype label	A5BC2_tI32_140_bl_a_h-001
***Strukturbericht* designation**	$K3_4$
ICSD	26662
Pearson symbol	tI32
Space group number	140
Space group symbol	$I4/mcm$
AFLOW prototype command	`aflow --proto=A5BC2_tI32_140_bl_a_h-001 --params=`$a, c/a, x_3, x_4, z_4$

- (Powell, 1937) gives the first bromine site a (2b) label, but gives the position as (000), which corresponds to the (2c) Wyckoff position. We (Hicks, 2021) and (Gottfried, 1940) chose to place this atom on the (2b) site. Unfortunately, the interatomic distances given in (Powell, 1937) are consistent with the (2c) site. Accordingly, we have labeled this structure as being incorrect. The proper structure can be found on the corrected $K3_4$ page.
- The positions of the hydrogen atoms in the NH_4 ions were not determined, so we only provide the positions of the nitrogen atoms (labeled as NH_4).
- The ICSD entry refers to the correct structure.

Body-centered Tetragonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}a\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}} \\
\mathbf{a_3} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}a\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\hat{\mathbf{z}}$	(4a)	N I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{y}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Br I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{1}{4}c\,\hat{\mathbf{z}}$	(4b)	Br I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\hat{\mathbf{x}} + a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Pb I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\hat{\mathbf{x}} - a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{y}}$	(8h)	Pb I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_3\,\hat{\mathbf{y}}$	(8h)	Pb I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_3\,\hat{\mathbf{y}}$	(8h)	Pb I
$\mathbf{B_9}$	=	$\left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + z_4\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{10}}$	=	$\left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - z_4\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{11}}$	=	$\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{12}}$	=	$-\left(x_4 - z_4\right)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{13}}$	=	$\left(x_4 - z_4\right)\,\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{x}} + ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{14}}$	=	$-\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{x}} - ax_4\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{15}}$	=	$\left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 - z_4\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}} + a\left(x_4 + \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Br II
$\mathbf{B_{16}}$	=	$-\left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 + z_4\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}} - a\left(x_4 - \frac{1}{2}\right)\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(16l)	Br II

References

[1] H. M. Powell and H. S. Tasker, *The valency angle of bivalent lead: the crystal structure of ammonium, rubidium, and potassium pentabromodiplumbites*, J. Chem. Soc. p. 119 (1937), doi:10.1039/JR9370000119.

[2] D. Hicks, M. J.Mehl, M. Esters, C. Oses, O. Levy, G. L. W. Hart, C. Toher, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 3*, Comput. Mater. Sci. **199**, 110450 (2021), doi:10.1016/j.commatsci.2021.110450.

[3] C. Gottfried, ed., *Strukturbericht Band V 1937* (Akademische Verlagsgesellschaft M. B. H., Leipzig, 1940).