$(NH_4)Pb_2Br_5$ ($K3_4$) Structure (*Revised*): A5BC2_tI32_140_cl_a_h-001

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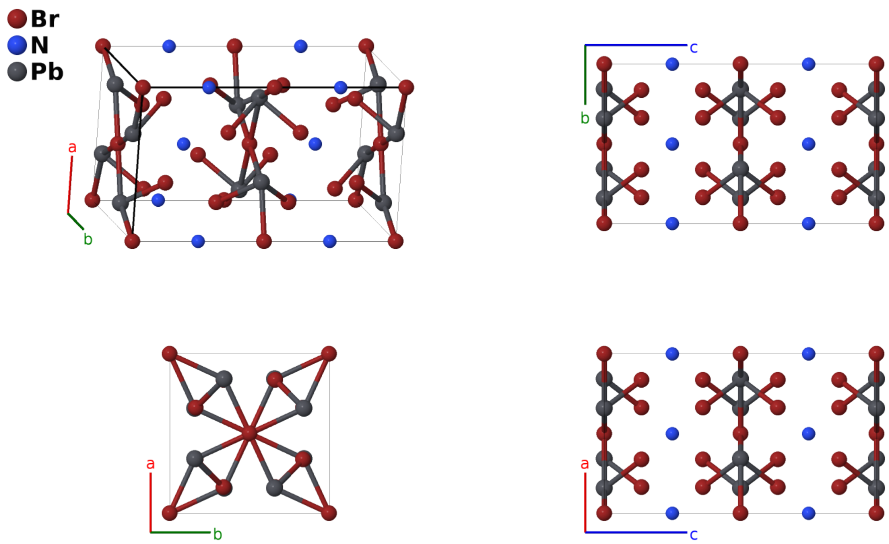
https://aflow.org/p/REV7

https://aflow.org/p/A5BC2_tI32_140_cl_a_h-001



Prototype	$Br_5(NH_4)Pb_2$
AFLOW prototype label	A5BC2_tI32_140_cl_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_cl_a_h-001` `--params=`$a, c/a, x_3, x_4, z_4$

Other compounds with this structure

$CsPb_2Br_5$, $CsSn_2Br_5$, ISe_2Tl_5, $InPb_2I_5$, $InSn_2Br_5$, $InSn_2I_5$, KPb_2Br_5, KSn_2Br_5, KSn_2I_5, $RbPb_2Br_5$, $RbSn_2Br_5$, $TlSn_2Br_5$

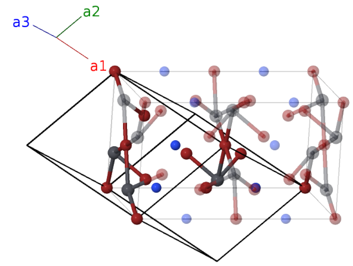
- (Powell, 1937) gives the first bromine site a (2b) label, but gives the position as (000), which corresponds to the (2c) Wyckoff position. In our previous attempt at presenting this structure we followed the first choice, but the second choice is the correct one. See the previous $K3_4$ page for more information.
- 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).

Body-centered Tetragonal primitive vectors

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

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

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



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}c\,\mathbf{\hat{z}}$	(4a)	N I
$\mathbf{B_2}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}c\,\mathbf{\hat{z}}$	(4a)	N I
$\mathbf{B_3}$	=	0	=	0	(4c)	Br I
$\mathbf{B_4}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\mathbf{\hat{z}}$	(4c)	Br I
$\mathbf{B_5}$	=	$\left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_1 + x_3\,\mathbf{a}_2 + \left(2x_3 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_3\,\mathbf{\hat{x}} + a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{y}}$	(8h)	Pb I
$\mathbf{B_6}$	=	$-\left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_1 - x_3\,\mathbf{a}_2 - \left(2x_3 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_3\,\mathbf{\hat{x}} - a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{y}}$	(8h)	Pb I
$\mathbf{B_7}$	=	$x_3\,\mathbf{a}_1 - \left(x_3 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_3 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_3\,\mathbf{\hat{y}}$	(8h)	Pb I
$\mathbf{B_8}$	=	$-x_3\,\mathbf{a}_1 + \left(x_3 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_3 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_3\,\mathbf{\hat{y}}$	(8h)	Pb I
$\mathbf{B_9}$	=	$\left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 + z_4\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{10}}$	=	$\left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 - z_4\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{11}}$	=	$\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(-x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{12}}$	=	$-\left(x_4 - z_4\right)\,\mathbf{a}_1 + \left(x_4 + z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_4\,\mathbf{\hat{y}} + cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{13}}$	=	$\left(x_4 - z_4\right)\,\mathbf{a}_1 - \left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$-a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{x}} + ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{14}}$	=	$-\left(x_4 + z_4\right)\,\mathbf{a}_1 + \left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{x}} - ax_4\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{15}}$	=	$\left(x_4 - z_4 + \frac{1}{2}\right)\,\mathbf{a}_1 + \left(x_4 - z_4\right)\,\mathbf{a}_2 + \left(2x_4 + \frac{1}{2}\right)\,\mathbf{a}_3$	=	$ax_4\,\mathbf{\hat{x}} + a\left(x_4 + \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(16l)	Br II
$\mathbf{B_{16}}$	=	$-\left(x_4 + z_4 - \frac{1}{2}\right)\,\mathbf{a}_1 - \left(x_4 + z_4\right)\,\mathbf{a}_2 - \left(2x_4 - \frac{1}{2}\right)\,\mathbf{a}_3$	=	$-ax_4\,\mathbf{\hat{x}} - a\left(x_4 - \frac{1}{2}\right)\,\mathbf{\hat{y}} - cz_4\,\mathbf{\hat{z}}$	(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.