

$\text{Na}_{0.5}(\text{Na}_{0.17}\text{Pb}_{0.83})_3\text{Pb}_3\text{Br}_3\text{F}_9$	<i>hP38</i>	(176) $P6_3/m - h^6b$
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**Na<sub>2</sub>Pb<sub>11</sub>Br<sub>6</sub>F<sub>18</sub>** [1]

Structural features: Infinite columns of base-linked Pb(F<sub>4</sub>Br<sub>2</sub>)F<sub>3</sub> tricapped and (Pb,Na)(F<sub>2</sub>Br<sub>4</sub>)F<sub>2</sub> bicapped trigonal prisms share atoms to form a 3D-framework with WC-type columns (6 prisms in the dented triangular cross-section); Na in channels of hexagonal cross-section parallel to [001] (partial disorder).

Aurivillius B. (1977) [1]

Br<sub>3</sub>F<sub>9</sub>NaPb<sub>5.50</sub>

$a = 1.43421$ ,  $c = 0.40528$  nm,  $c/a = 0.283$ ,  $V = 0.7220$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>h</i>	<i>m</i> ..	0.0165	0.5805	<sup>1</sup> / <sub>4</sub>		8-vertex polyhedron Pb <sub>4</sub> F <sub>4</sub>
F2	6 <i>h</i>	<i>m</i> ..	0.0895	0.179	<sup>1</sup> / <sub>4</sub>		square pyramid Pb <sub>3</sub> Na <sub>2</sub>
Br3	6 <i>h</i>	<i>m</i> ..	0.201	0.48426	<sup>1</sup> / <sub>4</sub>		non-coplanar square Pb <sub>4</sub>
Pb4	6 <i>h</i>	<i>m</i> ..	0.27109	0.22073	<sup>1</sup> / <sub>4</sub>		monocapped trigonal prism F <sub>7</sub>
F5	6 <i>h</i>	<i>m</i> ..	0.3199	0.0645	<sup>1</sup> / <sub>4</sub>		tetrahedron Pb <sub>4</sub>
M6	6 <i>h</i>	<i>m</i> ..	0.51046	0.1242	<sup>1</sup> / <sub>4</sub>		non-coplanar square F <sub>4</sub>
Na7	2 <i>b</i>	-3..	0	0	0	0.5	colinear Na <sub>2</sub>

M6 = 0.833Pb + 0.167Na

Transformation from published data: *y*,*x*,<sup>-</sup>*z*

Experimental: single crystal, diffractometer, X-rays, R = 0.071

Remarks: Homogeneity range Na<sub>2x</sub>Pb<sub>12-x</sub>Br<sub>6</sub>F<sub>18</sub>, 0.25 < *x* < 2. Short interatomic distances for partly occupied site(s).

References: [1] Aurivillius B. (1977), Chem. Scr. 12, 18-22.