

$(\text{K}_{0.5}\text{Sr}_{0.5})_{3.5}\text{Sr}_2\text{Bi}_3\text{O}_{12}$  $hP21$ (189)  $P-62m - jg^3fda$ **K<sub>1.75</sub>Sr<sub>3.75</sub>Bi<sub>3</sub>O<sub>12</sub>** [1]

Structural features: Infinite chains of edge-linked BiO<sub>6</sub> octahedra share edges and vertices with (K,Sr)O<sub>6</sub> trigonal prisms (in part monocapped) and SrO<sub>6</sub>O<sub>3</sub> tricapped trigonal prisms to form a 3D-framework. Ordering variant of V<sub>4</sub>P<sub>2</sub>C antitype.

Pshirkov J.S. et al. (2000) [1]

Bi<sub>3</sub>K<sub>1.75</sub>O<sub>12</sub>Sr<sub>3.75</sub> $a = 1.04434$ ,  $c = 0.33793$  nm,  $c/a = 0.324$ ,  $V = 0.3192$  nm<sup>3</sup>,  $Z = 1$ 

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6j	$m..$	0.222	0.438	0		single atom Bi
O2	3g	$m2m$	0.197	0	$\frac{1}{2}$		non-colinear Bi <sub>2</sub>
O3	3g	$m2m$	0.472	0	$\frac{1}{2}$		coplanar triangle Bi <sub>2</sub> K
M4	3g	$m2m$	0.7	0	$\frac{1}{2}$		monocapped trigonal prism O <sub>7</sub>
Bi5	3f	$m2m$	0.3385	0	0		octahedron O <sub>6</sub>
Sr6	2d	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism O <sub>9</sub>
M7	1a	$-62m$	0	0	0	0.5	trigonal prism O <sub>6</sub>

M4 = 0.5K + 0.5Sr; M7 = 0.5K + 0.5Sr

Experimental: powder, diffractometer, X-rays,  $R_B = 0.019$ 

References: [1] Pshirkov J.S., Kazakov S.M., Abakumov A.M., Putilin S.N., Antipov E.V., Bougerol Chaillout C., Lebedev O.I., Van Tendeloo G. (2000), J. Solid State Chem. 152, 492-502.