

RbAg₅S₃ [1]

Structural features: AgS₃ trigonal units share vertices to form infinite planar nets (large triangular voids), which are interconnected via additional Ag in (approximely) linear coordination (infinite zigzag chains with linear S-Ag-S segments) to form a 3D-framework; Rb in channels parallel to [001].

Wood P.T. et al. (1994) [1]

Ag₅RbS₃

$a = 1.3389$, $c = 0.804$ nm, $c/a = 0.6$, $V = 1.2482$ nm³, $Z = 6$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	6 <i>l</i>	1	0.00003	0.46337	0.2477		non-colinear S ₂
Ag2	6 <i>l</i>	1	0.18413	0.33297	0.2469		non-colinear S ₂
Ag3	6 <i>l</i>	1	0.33353	0.18427	0.2489		non-colinear S ₂
S4	3 <i>k</i>	<i>m</i> ..	0.11073	0.52857	$\frac{1}{2}$		non-coplanar square Ag ₄
S5	3 <i>k</i>	<i>m</i> ..	0.13913	0.22117	$\frac{1}{2}$		non-coplanar square Ag ₄
Ag6	3 <i>k</i>	<i>m</i> ..	0.29503	0.00417	$\frac{1}{2}$		tricapped trigonal prism S ₃ Ag ₆
Ag7	3 <i>k</i>	<i>m</i> ..	0.37043	0.36677	$\frac{1}{2}$		tricapped trigonal prism S ₃ Ag ₆
S8	3 <i>k</i>	<i>m</i> ..	0.44303	0.21847	$\frac{1}{2}$		non-coplanar square Ag ₄
Ag9	3 <i>j</i>	<i>m</i> ..	0.00423	0.29457	0		tricapped trigonal prism S ₃ Ag ₆
S10	3 <i>j</i>	<i>m</i> ..	0.21973	0.44347	0		non-coplanar square Ag ₄
S11	3 <i>j</i>	<i>m</i> ..	0.22063	0.13947	0		non-coplanar square Ag ₄
Ag12	3 <i>j</i>	<i>m</i> ..	0.36693	0.37057	0		tricapped trigonal prism S ₃ Ag ₆
S13	3 <i>j</i>	<i>m</i> ..	0.52843	0.11067	0		non-coplanar square Ag ₄
Rb14	2 <i>i</i>	3..	$\frac{2}{3}$	$\frac{1}{3}$	0.2518		octahedron S ₆
Rb15	2 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.2505		octahedron S ₆
Rb16	2 <i>g</i>	3..	0	0	0.2513		octahedron S ₆

Transformation from published data: $-x, -y, -z$; origin shift $\frac{2}{3}, \frac{1}{3}, 0$

Experimental: single crystal, diffractometer, X-rays, $R = 0.031$, $T = 294$ K

Remarks: We recommend space group (190) *P*-62*c*, rejected by the authors (diffraction symbol *P*---stated), be tested.

References: [1] Wood P.T., Pennington W.T., Kolis J.W. (1994), Inorg. Chem. 33, 1556-1558.