

$\text{Ag}_8\text{V}_2\text{I}_4\text{O}_7$ *hP72*(189) *P-62m - l<sup>2</sup>k<sup>2</sup>i<sup>2</sup>hg<sup>3</sup>f<sup>2</sup>eca***Ag<sub>8</sub>V<sub>2</sub>O<sub>7</sub>I<sub>4</sub>** [1]

Structural features: I forms directly superposed hexagon-mesh layers; units of two vertex-linked VO<sub>4</sub> tetrahedra parallel to [001] center the hexagons of every second layer; Ag in approximately linear (O<sub>2</sub>) voids.

Adams S. (1996) [1]

 $\text{Ag}_{8.01}\text{I}_4\text{O}_7\text{V}_2$  $a = 1.2595$ ,  $c = 0.9119$  nm,  $c/a = 0.724$ ,  $V = 1.2528$  nm<sup>3</sup>,  $Z = 3$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ag1	12 <i>l</i>	1	0.1532	0.3364	0.2243	0.99	non-colinear O <sub>2</sub>
O2	12 <i>l</i>	1	0.3212	0.534	0.256		single atom V
I3	6 <i>k</i>	<i>m</i> ..	0.2707	0.2896	<sup>1</sup> / <sub>2</sub>	0.5	
Ag4	6 <i>k</i>	<i>m</i> ..	0.3078	0.5248	<sup>1</sup> / <sub>2</sub>	0.65	non-colinear O <sub>2</sub>
O5	6 <i>i</i>	.. <i>m</i>	0.1249	0	0.2622		single atom V
Ag6	6 <i>i</i>	.. <i>m</i>	0.5313	0	0.2372	0.96	non-colinear O <sub>2</sub>
V7	4 <i>h</i>	3.. <sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.1951			tetrahedron O <sub>4</sub>
Ag8	3 <i>g</i>	<i>m2m</i>	0.1443	0	<sup>1</sup> / <sub>2</sub>	0.54	non-colinear Ag <sub>2</sub>
I9	3 <i>g</i>	<i>m2m</i>	0.3856	0	<sup>1</sup> / <sub>2</sub>		coplanar triangle Ag <sub>3</sub>
Ag10	3 <i>g</i>	<i>m2m</i>	0.872	0	<sup>1</sup> / <sub>2</sub>	0.29	
I11	3 <i>f</i>	<i>m2m</i>	0.3667	0	0		trigonal prism Ag <sub>6</sub>
I12	3 <i>f</i>	<i>m2m</i>	0.6964	0	0		trigonal prism Ag <sub>6</sub>
V13	2 <i>e</i>	3.. <i>m</i>	0	0	0.1936		tetrahedron O <sub>4</sub>
O14	2 <i>c</i>	-6.. <sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0			colinear V <sub>2</sub>
O15	1 <i>a</i>	-62 <i>m</i>	0	0	0		colinear V <sub>2</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>Experimental: single crystal, diffractometer, X-rays,  $R = 0.040$ ,  $T = 293$  K

Remarks: Cell parameters from [2]. Short interatomic distances for partly occupied site(s).

References: [1] Adams S. (1996), Z. Kristallogr. 211, 770-776. [2] Adams S., Hariharan K., Maier J. (1995), Solid State Ionics 75, 193-201.