

CaZnSO

hP8(186) $P6_3mc - b^2a^2$ **ZnCaOS** [1]

Structural features: Close-packed S and O layers in hc stacking; Ca in octahedral, Zn in tetrahedral voids. Infinite layers of edge-linked $\text{Ca}(\text{S}_3\text{O}_3)$ octahedra and infinite layers of vertex-linked $\text{Zn}(\text{S}_3\text{O})$ tetrahedra share S-S edges and O vertices to form a 3D-framework. Ordering variant of WMnN_2 .

Petrova S.A. et al. (2003) [1]

CaOSZn

 $a = 0.37547$, $c = 1.14014$ nm, $c/a = 3.037$, $V = 0.1392$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.24781		non-coplanar triangle Zn ₃
Ca2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.56095		non-coplanar triangle O ₃
O3	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		tetrahedron ZnCa ₃
Zn4	2 <i>a</i>	3 <i>m.</i>	0	0	0.33125		tetrahedron OS ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.8215Experimental: powder, diffractometer, X-rays, $R_B = 0.065$

References: [1] Petrova S.A., Mar'evich A.P., Zakharov R.G., Selivanov E.N., Chumarev V.M., Udоеva L.Y. (2003), Dokl. Chem. 393, 255-258 (Dokl. Akad. Nauk 393, 52-56).