

ZnS	<i>hP28</i>	(186) $P6_3mc - b^{10}a^4$
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**ZnS 14H** [1], wurtzite-14H

Structural features: Close-packed S layers in  $hc_6$  stacking; Zn in tetrahedral voids (same stacking position as the preceding S layer).  $ZnS_4$  tetrahedra share vertices to form a 3D-framework.

Mardix S. et al. (1967) [1]

SZn

$a = 0.382$ ,  $c = 4.382$  nm,  $c/a = 11.471$ ,  $V = 0.5538$  nm<sup>3</sup>,  $Z = 14$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Zn1	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.07143		tetrahedron S <sub>4</sub>
S2	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.125		tetrahedron Zn <sub>4</sub>
Zn3	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.28571		tetrahedron S <sub>4</sub>
S4	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.33929		tetrahedron Zn <sub>4</sub>
Zn5	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.42857		tetrahedron S <sub>4</sub>
S6	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.48214		tetrahedron Zn <sub>4</sub>
Zn7	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.64286		tetrahedron S <sub>4</sub>
S8	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.69643		tetrahedron Zn <sub>4</sub>
Zn9	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.85714		tetrahedron S <sub>4</sub>
S10	2 <i>b</i>	3 <i>m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.91071		tetrahedron Zn <sub>4</sub>
Zn11	2 <i>a</i>	3 <i>m.</i>	0	0	0.0		tetrahedron S <sub>4</sub>
S12	2 <i>a</i>	3 <i>m.</i>	0	0	0.05357		tetrahedron Zn <sub>4</sub>
Zn13	2 <i>a</i>	3 <i>m.</i>	0	0	0.21429		tetrahedron S <sub>4</sub>
S14	2 <i>a</i>	3 <i>m.</i>	0	0	0.26786		tetrahedron Zn <sub>4</sub>

Transformation from published data ( $P6_3mc$  \*): origin shift  $\frac{1}{3} \frac{2}{3} 0.07143$

Experimental: single crystal, photographs, X-rays

Remarks: Zhdanov notation (77); idealized atom coordinates. We deduced the space group from the coordinates of all the atoms in the unit cell. In [1] the origin of the cell is shifted by  $\frac{1}{3} \frac{2}{3} 0$  from the description in the International Tables for Crystallography.

References: [1] Mardix S., Brafman O., Steinberger I.T. (1967), Acta Crystallogr. 22, 805-807.