

ZnS	<i>hP32</i>	(186) $P6_3mc - b^{10}a^6$
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ZnS 16H [1]

Structural features: Close-packed S layers in hc_7 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

$a = 0.382$, $c = 5.008$ nm, $c/a = 13.11$, $V = 0.6329$ nm³, $Z = 16$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.01563		tetrahedron Zn ₄
Zn2	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0625		tetrahedron S ₄
S3	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.20313		tetrahedron Zn ₄
Zn4	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.25		tetrahedron S ₄
S5	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.39063		tetrahedron Zn ₄
Zn6	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.4375		tetrahedron S ₄
S7	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.64063		tetrahedron Zn ₄
Zn8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.6875		tetrahedron S ₄
S9	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.82813		tetrahedron Zn ₄
Zn10	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.875		tetrahedron S ₄
Zn11	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		tetrahedron S ₄
S12	2 <i>a</i>	3 <i>m</i> .	0	0	0.07813		tetrahedron Zn ₄
Zn13	2 <i>a</i>	3 <i>m</i> .	0	0	0.125		tetrahedron S ₄
S14	2 <i>a</i>	3 <i>m</i> .	0	0	0.26563		tetrahedron Zn ₄
Zn15	2 <i>a</i>	3 <i>m</i> .	0	0	0.3125		tetrahedron S ₄
S16	2 <i>a</i>	3 <i>m</i> .	0	0	0.45313		tetrahedron Zn ₄

Transformation from published data: origin shift 0 0 0.48438

Experimental: single crystal, oscillation photographs, X-rays

Remarks: Zhdanov notation (88). We derived the cell parameters and idealized atom coordinates from the stacking sequence.

References: [1] Mardix S., Alexander E., Brafman O., Steinberger I.T. (1967), Acta Crystallogr. 22, 808-812.