

ZnS	<i>hP40</i>	(186) $P6_3mc - b^{14}a^6$
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ZnS 20H [1]

Structural features: Close-packed S layers in hc_9 stacking; Zn in tetrahedral voids (same stacking position as the preceding S layer). ZnS_4 tetrahedra share vertices to form a 3D-framework.

Kiflawi I. et al. (1969) [1]

SZn

$a = 0.382$, $c = 6.26$ nm, $c/a = 16.387$, $V = 0.7911$ nm³, $Z = 20$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.05		tetrahedron Zn ₄
Zn2	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.0875		tetrahedron S ₄
S3	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2		tetrahedron Zn ₄
Zn4	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2375		tetrahedron S ₄
S5	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.35		tetrahedron Zn ₄
Zn6	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.3875		tetrahedron S ₄
S7	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.45		tetrahedron Zn ₄
Zn8	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.4875		tetrahedron S ₄
S9	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6		tetrahedron Zn ₄
Zn10	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.6375		tetrahedron S ₄
S11	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.75		tetrahedron Zn ₄
Zn12	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.7875		tetrahedron S ₄
S13	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.9		tetrahedron Zn ₄
Zn14	<i>2b</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.9375		tetrahedron S ₄
S15	<i>2a</i>	<i>3m.</i>	0	0	0.0		tetrahedron Zn ₄
Zn16	<i>2a</i>	<i>3m.</i>	0	0	0.0375		tetrahedron S ₄
S17	<i>2a</i>	<i>3m.</i>	0	0	0.15		tetrahedron Zn ₄
Zn18	<i>2a</i>	<i>3m.</i>	0	0	0.1875		tetrahedron S ₄
S19	<i>2a</i>	<i>3m.</i>	0	0	0.3		tetrahedron Zn ₄
Zn20	<i>2a</i>	<i>3m.</i>	0	0	0.3375		tetrahedron S ₄

Experimental: single crystal, oscillation photographs, X-rays

Remarks: Zhdanov notation (10 10). We derived idealized atom coordinates from the stacking sequence.

References: [1] Kiflawi I., Mardix S., Steinberger I.T. (1969), Acta Crystallogr. B 25, 1581-1586.