

ZnIn ₂ S ₄	<i>hP</i> 14	(186) <i>P</i> 6 ₃ <i>mc</i> – b ⁴ a ³
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ZnIn₂S₄ form IIb [1]

Structural features: Close-packed S layers in h₃c stacking; Zn in tetrahedral, In in tetrahedral and octahedral voids. Layer structure with sandwiches consisting of seven sublayers (S-Zn(t)-S-In(o)-S-In(t)-S).

Donika F.G. et al. (1972) [1]

In₂S₄Zn

$a = 0.385$, $c = 2.468$ nm, $c/a = 6.410$, $V = 0.3168$ 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> .	1/3	2/3	0.212		tetrahedron In ₄
In2	2 <i>b</i>	3 <i>m</i> .	1/3	2/3	0.312		tetrahedron S ₄
S3	2 <i>b</i>	3 <i>m</i> .	1/3	2/3	0.468		non-coplanar triangle Zn ₃
In4	2 <i>b</i>	3 <i>m</i> .	1/3	2/3	0.656		octahedron S ₆
Zn5	2 <i>a</i>	3 <i>m</i> .	0	0	0.0		tetrahedron S ₄
S6	2 <i>a</i>	3 <i>m</i> .	0	0	0.1		tetrahedron ZnIn ₃
S7	2 <i>a</i>	3 <i>m</i> .	0	0	0.344		non-coplanar triangle In ₃

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 0.094

Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.164

References: [1] Donika F.G., Radautsan S.I., Semiletov S.A., Kiosse G.A., Mustya I.G. (1972), Sov. Phys. Crystallogr. 17, 575-577 (Kristallografiya 17, 663-665).