$Zn_2In_2S_5$	$hP18$	(186) $P6_3mc$ – b^8a

$Zn_2In_2S_5$ form IIa [1]
Structural features: Close-packed S layers in h stacking; Zn in tetrahedral, In in tetrahedral and octahedral voids. Layer structure with sandwiches consisting of nine sublayers (S-Zn(t)-S-In(o)-S-Zn(t)-S-In(t)-S).

Donika F.G. et al. (1972) [1]
$In_2S_5Zn_2$
$a = 0.385$, $c = 3.085$ nm, $c/a = 8.013$, $V = 0.3960$ nm^3, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.044		tetrahedron $ZnIn_3$
Zn2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.121		tetrahedron S_4
S3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.252		non-coplanar triangle In_3
Zn4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.377		tetrahedron S_4
S5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.456		tetrahedron $ZnIn_3$
S6	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.643		tetrahedron Zn_3In
In7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.722		tetrahedron S_4
S8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.847		non-coplanar triangle Zn_3
In9	2*a*	3*m*.	0	0	0.0		octahedron S_6

Transformation from published data: origin shift 0 0 0.693
Experimental: single crystal, Weissenberg and rotation photographs, X-rays, R = 0.167

Remarks: We took the *x*- and *y*-coordinates for the atom sites in Wyckoff position 2*b* from fig. 1. A different model in the same space group is proposed for $Zn_2In_2S_5$ IIa in [3]. In [2] a large number of atom coordinates and Wyckoff positions are wrongly interpreted and, contrary to what is stated, the structure proposals in [1] and [3] do not differ only in the distribution of the metal atoms.

References: [1] Donika F.G., Radautsan S.I., Semiletov S.A., Donika T.V., Mustya I.G. (1972), Sov. Phys. Crystallogr. 17, 578-579 (Kristallografiya 17, 666-667). [2] (1975), Structure Reports 38A, 109-110. [3] Gnehm C., Niggli A. (1972), J. Solid State Chem. 5, 118-125.