$Zn_{1.685}In_{2.21}S_5$	*hP*18	(186) $P6_3mc$ – b^5a^4

$Zn_{1.685}In_{2.21}S_5$ [1]; $GaInS_3$ IIb [4]
Structural features: Close-packed S layers in h_3c_2 stacking; Zn and (Zn,In) in tetrahedral, In in tetrahedral and octahedral voids. Layer structure with sandwiches consisting of nine sublayers (ignoring vacancies, S-Zn(t)-S-In(o)-S-(Zn,In)(t)-S-In(t)-S).

Gnehm C., Niggli A. (1972) [1]
$In_{2.15}S_5Zn_{1.60}$
a = 0.3851, c = 3.085 nm, c/a = 8.011, V = 0.3962 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0459		tetrahedron $ZnIn_3$
M2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.1229	0.87	tetrahedron S_4
S3	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2529		non-coplanar triangle In_3
Zn4	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.3772		tetrahedron S_4
S5	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.4589		tetrahedron $ZnIn_3$
In6	2*a*	3*m*.	0	0	0.0		octahedron S_6
S7	2*a*	3*m*.	0	0	0.1469		tetrahedron $InZn_3$
In8	2*a*	3*m*.	0	0	0.2226	0.88	tetrahedron S_4
S9	2*a*	3*m*.	0	0	0.3529		non-coplanar triangle Zn_3

M2 = 0.69Zn + 0.31In
Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0 0.2471
Experimental: single crystal, diffractometer, X-rays, R = 0.133

Remarks: Refinement of the occupancies of sites Zn4 and In6 showed no significant deviation from unity. 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. Mixed occupations and partial vacancies on some cation sites are reported also for $GaInS_3$ IIb in [4].

References: [1] Gnehm C., Niggli A. (1972), J. Solid State Chem. 5, 118-125. [2] (1975), Structure Reports 38A, 109-110. [3] 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). [4] Amiraslanov I.R., Asadov Y.G., Valiev R.B., Musaev A.A., Guseinov G.G. (1990), Sov. Phys. Crystallogr. 35, 766-767 (Kristallografiya 35, 1298-1299).