Status Primary **Quality Mark:** Indexed **Environment:** Ambient **Temp:** 298.0 K (Assigned by ICDD editor)
Phase: β **Chemical Formula:** In Se **Empirical Formula:** In Se **Weight %:** In59.25 Se40.75
Atomic %: In50.00 Se50.00 **Compound Name:** Indium Selenide **Entry Date:** 09/01/1984

Radiation: CuKα (1.5418 Å) **d-Spacing:** Diffractometer **Intensity:** Diffractometer - Peak

Crystal System: Hexagonal **SPGR:** P63/mmc (194)
Author's Unit Cell [a: 4.005(5) Å **c:** 16.640(4) Å **Volume:** 231.15 Å³ **Z:** 4.00 **MolVol:** 57.79 **c/a:** 4.155 **]**
Calculated Density: 5.568 g/cm³ **SS/FOM:** F(26) = 5.6(0.0541, 86)

Space Group: P63/mmc (194) **Molecular Wt:** 193.78 g/mol
Crystal Data [a: 4.005 Å **b:** 4.005 Å **c:** 16.640 Å **α:** 90.00° **β:** 90.00° **γ:** 120.00° **XtlCell Vol:** 231.15 Å³
XtlCell Z: 4.00 **c/a:** 4.155 **a/b:** 1.000 **c/b:** 4.155 **]**
Reduced Cell [a: 4.005 Å **b:** 4.005 Å **c:** 16.640 Å **α:** 90.00° **β:** 90.00° **γ:** 120.00° **RedCell Vol:** 231.15 Å³ **]**

Atomic parameters are cross-referenced from PDF entry 04-004-3750 **AC Space Group:** P63/mmc (194)
AC Unit Cell [a: 4.005 Å **b:** 4.005 Å **c:** 16.64 Å **α:** 90° **β:** 90° **γ:** 120° **]**

Space Group Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	6	x-y,x,-z	11	-x+y,y,z	16	-y,x-y,-z+1/2	21	-x,-x+y,z+1/2
2	-x,-y,-z	7	-y,-x,z	12	x-y,-y,-z	17	x-y,x,z+1/2	22	x,x-y,-z+1/2
3	-y,x-y,z	8	y,x,-z	13	-x,-y,z+1/2	18	-x+y,-x,-z+1/2	23	x-y,-y,z+1/2
4	y,-x+y,-z	9	x,x-y,z	14	x,y,-z+1/2	19	y,x,z+1/2	24	-x+y,y,-z+1/2
5	-x+y,-x,z	10	-x,-x+y,-z	15	y,-x+y,z+1/2	20	-y,-x,-z+1/2		

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	IDP	AET
In	1	4f	3m.	0.33333	0.66666	0.17082	1.0		4-a
Se	2	4f	3m.	0.33333	0.66666	0.60191	1.0		3#a

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Inorganic, Metal & Alloy **Pearson Symbol:** hP8.00 **Prototype Structure [Formula Order]:** Ga S
Prototype Structure [Alpha Order]: Ga S **LPF Prototype Structure [Formula Order]:** Ga S-a,hP8,194
LPF Prototype Structure [Alpha Order]: Ga S,hP8,194

Cross-Ref PDF #'s: 04-003-6529 (Primary), 04-004-3750 (Alternate), 04-004-5453 (Alternate), 04-004-6176 (Alternate)

References:

Type	DOI	Reference
Primary Reference		Popovic, S. et al. J. Appl. Crystallogr. 1979, 12, 416.
Crystal Structure		Crystal Structure Source: LPF.

Database Comments: Sample Preparation: Prepared by direct synthesis of the component in stoichiometric ratio in vacuum at 1173 C, then slow cooling to room temperature over two days. Warning: Lines with abs(delta 2Theta)>0.06 DEG.

d-spacings (26) - In Se - 00-034-1431 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
10.624	**8.3200**	16	0	0	2		46.034	1.9700	2	1	0	7		80.922	1.1870	1	0	0	14	
21.290	**4.1700**	100	0	0	4		50.523	1.8050	2	1	1	4		83.569	1.1560	<1	3	0	0	
25.689	3.4650	2	1	0	0		52.944	1.7280	1	2	0	1		85.015	1.1400	3	1	1	12	
26.110	3.4100	3	1	0	1		55.186	1.6630	<1	0	0	10		95.696	1.0390	2	0	0	16	
30.378	2.9400	2	1	0	3		56.667	1.6230	1	1	1	6		97.695	1.0230	<1	1	1	14	
32.255	2.7730	10	0	0	6		60.197	1.5360	<1	2	0	5		100.620	1.0010	<1	2	2	0	
37.441	2.4000	3	1	0	5		64.526	1.4430	1	1	1	8		112.948	0.9240	1	0	0	18	
43.472	2.0800	8	0	0	8		67.526	**1.3860**	12	0	0	12		113.211	0.9226	2	1	1	16	
45.305	2.0000	4	1	1	0		72.222	1.3070	<1	2	1	1								