

**Status** Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K **Phase:**  $\gamma$   
**Chemical Formula:** In Se **Empirical Formula:** In Se **Weight %:** In59.25 Se40.75 **Atomic %:** In50.00 Se50.00  
**Compound Name:** Indium Selenium **Entry Date:** 09/01/2005 **Modification Date:** 09/01/2011  
**Modifications:** Reflections

**Radiation:** CuK $\alpha$ 1 (1.5406 Å) **d-Spacing:** Calculated **Intensity:** Calculated - Peak **I/Ic:** 4.42 **I/Ic - CW ND:** 0.11

**Crystal System:** Rhombohedral **SPGR:** R3m (160)  
**Author's Unit Cell [ a: 4.0046(5) Å c: 24.960(4) Å Volume: 346.65 Å<sup>3</sup> Z: 6.00 MolVol: 57.77 c/a: 6.233 ]**  
**Calculated Density:** 5.569 g/cm<sup>3</sup> **Measured Density:** 5.59 g/cm<sup>3</sup> **Structural Density:** 5.57 g/cm<sup>3</sup>  
**SS/FOM:** F(30) = 389.6(0.0024, 32) **R-factor:** 0.064

**Space Group:** R3m (160) **Molecular Wt:** 193.78 g/mol  
**Crystal Data [ a: 4.005 Å b: 4.005 Å c: 24.960 Å  $\alpha$ : 90.00°  $\beta$ : 90.00°  $\gamma$ : 120.00° XtlCell Vol: 346.65 Å<sup>3</sup>**  
**XtlCell Z: 6.00 c/a: 6.232 a/b: 1.000 c/b: 6.232 ]**  
**Reduced Cell [ a: 4.005 Å b: 4.005 Å c: 8.635 Å  $\alpha$ : 76.59°  $\beta$ : 76.59°  $\gamma$ : 60.00° RedCell Vol: 115.55 Å<sup>3</sup> ]**

**AC Space Group:** R3mH (160)  
**AC Unit Cell [ a: 4.0046(5) Å b: 4.0046(5) Å c: 24.960(4) Å  $\alpha$ : 90°  $\beta$ : 90°  $\gamma$ : 120° ]**

**Space Group Symmetry Operators:**

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator		
1	x,y,z	2	-y,x-y,z	3	-x+y,-x,z	4	-y,-x,z	5	x,x-y,z	6	-x+y,y,z

**ADP Type:** B

**Atomic Coordinates:**

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	Biso	AET
In	1	3a	3m	0.0	0.0	0.0555	1.0	1.2	4-a
In	2	3a	3m	0.0	0.0	-0.0555	1.0	1.2	4-a
Se	3	3a	3m	0.0	0.0	0.7727	1.0	0.65	3#a
Se	4	3a	3m	0.0	0.0	0.5607	1.0	0.65	3#a

**Crystal (Symmetry Allowed):** Non-centrosymmetric - Pyro / Piezo (p), Piezo (2nd Harm.)

**Subfiles:** Inorganic, Metal & Alloy **Pearson Symbol:** hR4.00 **Prototype Structure [Formula Order]:** Ga Se  
**Prototype Structure [Alpha Order]:** Ga Se **LPF Prototype Structure [Formula Order]:** Ga Se,hR12,160  
**LPF Prototype Structure [Alpha Order]:** Ga Se,hR12,160 **ANX:** NO

**Cross-Ref PDF #'s:** 00-029-0676 (Deleted), 00-042-0919 (Deleted), 01-070-2541 (Alternate), 04-003-1009 (Alternate),  
 04-004-4080 (Alternate), 04-004-4621 (Alternate), 04-004-6177 (Alternate), 04-004-6586 (Alternate),  
 04-004-6593 (Alternate), 04-005-1768 (Alternate), 04-005-5113 (Alternate)

**Former PDF Numbers:** 01-071-0447

#### References:

Type	DOI	Reference
Primary Reference Structure		Calculated from LPF using POWD-12++. Nagpal K.C., Ali S.Z. "X-ray Crystallographic Study of Indium Monoselenide". Indian J. Pure Appl. Phys. 1976, 14, 434.

**Database Comments:** ANX: NO. LPF Collection Code: 453335. Sample Preparation: STARTING MATERIALS:In,Se. Compound Preparation: heated at 1193 K for 6 h in evacuated quartz tube with slight excess of Se. Temperature of Data Collection: 298 K. Unit Cell Data Source: Single Crystal.

#### d-spacings (104) - In Se - 04-003-2450 (Stick, Fixed Slit Intensity) - Cu K $\alpha$ 1 1.54056 Å

2 $\theta$ (°)	d (Å)	I	h	k	l	*	2 $\theta$ (°)	d (Å)	I	h	k	l	*
10.624	8.320000	203	0	0	3		53.292	1.717540	78	2	0	2	
21.341	<b>4.160000</b>	723	0	0	6		54.589	1.679760	26	1	0	13	
25.916	<b>3.435090</b>	1000	1	0	1		54.909	1.670730	68	0	2	4	
26.656	3.341460	683	0	1	2		56.101	1.638030	45	2	0	5	
29.441	3.031360	504	1	0	4		56.651	1.623410	35	1	1	9	
31.381	2.848200	298	0	1	5		58.129	1.585610	66	0	1	14	
32.251	2.773330	39	0	0	9		59.201	1.559420	59	0	2	7	
36.099	2.486100	329	1	0	7		61.089	1.515680	130	2	0	8	
38.791	2.319500	647	0	1	8		64.549	1.442530	54	1	1	12	
43.472	2.080000	39	0	0	12		65.488	1.424100	146m	0	2	10	
44.695	2.025870	536	1	0	10		65.488	1.424100	146m	1	0	16	
45.250	<b>2.002300</b>	775	1	1	0		67.489	1.386670	52	0	0	18	
46.617	1.946720	28	1	1	3		67.983	1.377790	59	2	0	11	
47.866	1.898780	221	0	1	11		69.460	1.352060	41	0	1	17	
50.547	1.804190	330	1	1	6		72.093	1.309010	65	2	1	1	
52.883	1.729870	108	0	2	1		72.437	1.303640	48	1	2	2	

**04-003-2450**

Oct 30, 2019 5:45 PM (shl12)

$2\theta$ (°)	$d$ (Å)	I	h	k	l	*	$2\theta$ (°)	$d$ (Å)	I	h	k	l	*
73.534	1.286890	9	0	2	13		108.454	0.949392	4m	0	2	22	
73.806	1.282810	45	2	1	4		108.454	0.949392	4m	0	3	15	
74.826	1.267830	31	1	2	5		109.282	0.944500	10	3	1	5	
76.584	1.243050	23	2	0	14		109.769	0.941671	3	2	2	9	
77.524	1.230310	43	2	1	7		112.082	0.928678	16	1	3	7	
77.660	1.228500	30	1	0	19		112.225	0.927898	20	2	1	19	
79.195	1.208490	96	1	2	8		112.723	0.925208	12	0	1	26	
80.793	1.188570	4	0	0	21		113.149	0.922931	34	1	1	24	
81.985	1.174280	14	0	1	20		113.860	0.919183	35	3	1	8	
83.172	1.160510	116m	0	2	16		116.906	0.903859	11	1	2	20	
83.172	1.160510	116m	2	1	10		117.272	0.902094	9	2	2	12	
83.567	1.156030	81	3	0	0		118.234	0.897535	44	1	3	10	
84.554	1.145030	4	0	3	3		120.337	0.887937	57	3	0	18	
85.016	1.139980	131	1	1	18		120.869	0.885592	23	3	1	11	
85.475	1.135030	51	1	2	11		125.485	0.866499	8	4	0	1	
86.854	1.120520	18	2	0	17		125.888	0.864936	9m	0	2	25	
87.508	1.113820	43	0	3	6		125.888	0.864936	9m	0	4	2	
90.718	1.082580	8	2	1	13		126.298	0.863364	22	1	0	28	
91.178	1.078310	4	1	0	22		127.193	0.859990	5	1	3	13	
92.421	1.067040	5	3	0	9		127.522	0.858771	6	4	0	4	
93.667	1.056090	24	1	2	14		127.773	0.857847	6m	2	1	22	
94.719	1.047120	13	0	2	19		127.773	0.857847	6m	2	2	15	
95.574	1.040000	8	0	0	24		128.770	0.854233	4	0	4	5	
96.100	1.035700	6	0	1	23		130.990	0.846530	14	3	1	14	
97.816	1.022060	13	1	1	21		132.215	0.842474	6	4	0	7	
99.006	1.012940	8	2	0	20		133.020	0.839880	10	2	0	26	
99.337	1.010450	12	0	3	12		133.200	0.839309	7	1	1	27	
100.268	1.003560	27	2	1	16		134.472	0.835349	30m	0	1	29	
100.599	1.001150	46	2	2	0		134.472	0.835349	30m	0	4	8	
101.600	0.993980	2	2	2	3		135.584	0.832000	1	0	0	30	
103.952	0.977822	21	1	2	17		136.715	0.828702	7	0	3	21	
104.626	0.973359	26	2	2	6		140.270	0.819016	28m	1	3	16	
106.529	0.961160	19	1	3	1		140.270	0.819016	28m	4	0	10	
106.871	0.959029	16m	1	0	25		143.233	0.811704	50	2	2	18	
106.871	0.959029	16m	3	1	2		144.004	0.809911	10	0	4	11	
108.245	0.950646	14	1	3	4		146.416	0.804588	13	3	1	17	