Status Primary **Quality Mark:** Star **Environment:** Ambient **Temp:** 298.0 K (Assigned by ICDD editor)
Chemical Formula: In4 Se3 **Empirical Formula:** In4 Se3 **Weight %:** In65.97 Se34.03 **Atomic %:** In57.14 Se42.86
Compound Name: Indium Selenium **Entry Date:** 09/01/2005 **Modification Date:** 09/01/2011
Modifications: Reflections

Radiation: CuKα1 (1.5406 Å) **d-Spacing:** Calculated **Intensity:** Calculated - Peak **I/Ic:** 5.48 **I/Ic - CW ND:** 0.13

Crystal System: Orthorhombic **SPGR:** Pnnm (58)
Author's Unit Cell [a: 15.297(1) Å **b:** 12.308(1) Å **c:** 4.081(1) Å **Volume:** 768.35 Å³ **Z:** 4.00
MolVol: 192.09 **c/a:** 0.267 **a/b:** 1.243 **c/b:** 0.332 **] Calculated Density:** 6.018 g/cm³
Structural Density: 6.02 g/cm³ **Color:** Black **SS/FOM:** F(30) = 376.6(0.0023, 34) **R-factor:** 0.06

Space Group: Pnnm (58) **Molecular Wt:** 696.15 g/mol
Crystal Data [a: 12.308 Å **b:** 15.297 Å **c:** 4.081 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **XtlCell Vol:** 768.35 Å³
XtlCell Z: 4.00 **c/a:** 0.332 **a/b:** 0.805 **c/b:** 0.267 **]**
Reduced Cell [a: 4.081 Å **b:** 12.308 Å **c:** 15.297 Å **α:** 90.00° **β:** 90.00° **γ:** 90.00° **RedCell Vol:** 768.35 Å³ **]**

AC Space Group: Pnnm (58)
AC Unit Cell [a: 15.297(1) Å **b:** 12.308(1) Å **c:** 4.081(1) Å **α:** 90° **β:** 90° **γ:** 90° **]**

Space Group Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	3	-x,-y,z	5	x+1/2,-y+1/2,-z+1/2	7	-x+1/2,y+1/2,-z+1/2
2	-x,-y,-z	4	x,y,-z	6	-x+1/2,y+1/2,z+1/2	8	x+1/2,-y+1/2,z+1/2

ADP Type: U

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	Uiso	AET
In	1	4g	..m	0.7111	0.3393	0.0	1.0	0.01107	4-a
In	2	4g	..m	0.8157	0.5236	0.0	1.0	0.0154	4-a
In	3	4g	..m	0.9675	0.6442	0.0	1.0	0.01063	4-a
In	4	4g	..m	0.4238	0.3974	0.0	1.0	0.0231	6-a
Se	5	4g	..m	0.9033	0.8493	0.0	1.0	0.01357	3#a
Se	6	4g	..m	0.7688	0.1386	0.0	1.0	0.0143	5-a
Se	7	4g	..m	0.4239	0.156	0.0	1.0	0.01387	3#a

Anisotropic Displacement Parameters:

Atom	Num	Uani11	Uani22	Uani33	Uani12	Uani13	Uani23
In	1	0.0148	0.0102	0.0082	0.00305	0.0	0.0
In	2	0.0145	0.0151	0.0166	0.0055	0.0	0.0
In	3	0.0113	0.0129	0.0077	0.0016	0.0	0.0
In	4	0.0226	0.0224	0.0243	-0.0037	0.0	0.0
Se	5	0.016	0.0139	0.0108	-4.5E-4	0.0	0.0
Se	6	0.017	0.0139	0.012	6.0E-4	0.0	0.0
Se	7	0.0133	0.0177	0.0106	-3.5E-4	0.0	0.0

Crystal (Symmetry Allowed): Centrosymmetric

Subfiles: Inorganic, Metal & Alloy **Pearson Symbol:** oP28.00 **Prototype Structure [Formula Order]:** In4 Se3
Prototype Structure [Alpha Order]: In4 Se3 **LPF Prototype Structure [Formula Order]:** In4 Se3,oP28,58
LPF Prototype Structure [Alpha Order]: In4 Se3,oP28,58 **ANX:** N3O4

Cross-Ref PDF #'s: 00-048-1575 (Deleted), 00-051-0808 (Primary), 01-082-4581 (Alternate), 01-082-4582 (Alternate), 01-082-4583 (Alternate), 01-082-4584 (Alternate), 04-004-4084 (Alternate), 04-004-4616 (Alternate), 04-004-4622 (Alternate), 04-005-9724 (Alternate), 04-007-0793 (Alternate), 04-007-3037 (Alternate)

Former PDF Numbers: 01-071-0521

References:

Type	DOI	Reference
Primary Reference		Calculated from LPF using POWD-12++.
Structure	10.1107/S0567740873005108	Hogg J.H.C., Sutherland H.H., Williams D.J. "The Crystal Structure of Tetraindium Triselenide". Acta Crystallogr., Sect. B: Struct. Crystallogr. Cryst. Chem. 1973, 29, 1590.

Database Comments: ANX: N3O4. LPF Collection Code: 451600. Sample Preparation: Compound Preparation: crystals grown by directional freezing method. Unit Cell Data Source: Powder Diffraction.

d-spacings (198) - In4 Se3 - 04-003-0988 (Stick, Fixed Slit Intensity) - Cu Kα1 1.54056 Å

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
9.215	9.58937	11	1	1	0		51.622	1.76912	35m	6	5	0	
11.560	7.64850	2	2	0	0		52.332	1.74678	10	1	7	0	
13.619	6.49633	22	2	1	0		52.428	1.74380	8	7	3	1	
14.381	6.15400	1	0	2	0		52.690	1.73575	15	5	5	1	
15.508	5.70930	1	1	2	0		52.776	1.73313	12	8	3	0	
18.490	4.79468	30	2	2	0		52.949	1.72785	6	4	2	2	
18.822	4.71075	2	3	1	0		53.212	1.71993	102	3	3	2	
22.530	3.94309	11	1	0	1		53.391	1.71460	63m	2	7	0	
22.628	3.92635	13	3	2	0		53.391	1.71460	63m	8	1	1	
22.940	3.87362	281	0	1	1		53.757	1.70379	26	5	6	0	
23.240	3.82425	25	4	0	0		53.867	1.70056	67	0	4	2	
23.674	3.75509	8	1	1	1		54.226	1.69015	37	1	4	2	
24.352	3.65202	46	4	1	0		54.451	1.68369	21	9	1	0	
24.603	3.61538	5	2	3	0		54.523	1.68165	21	5	1	2	
25.759	3.45570	1	2	1	1		55.050	1.66677	4	8	2	1	
26.831	3.32004	1	1	2	1		55.214	1.66223	14	3	7	0	
27.436	3.24817	13	4	2	0		55.293	1.66002	18	2	4	2	
27.889	**3.19646**	381	3	3	0		55.556	1.65280	2	4	6	1	
28.923	**3.08450**	1000m	0	4	0		55.712	1.64854	10	4	3	2	
28.923	**3.08450**	1000m	3	1	1		56.090	1.63833	21	9	2	0	
29.589	3.01658	127	1	4	0		56.160	1.63645	20	5	2	2	
30.073	2.96905	59	5	1	0		56.295	1.63285	31m	7	4	1	
30.880	2.89333	10	0	3	1		56.295	1.63285	31m	7	5	0	
31.309	2.85465	56	2	4	0		56.609	1.62452	21m	6	5	1	
31.441	2.84293	40	1	3	1		56.609	1.62452	21m	8	4	0	
31.595	2.82944	131	3	2	1		57.042	1.61321	3m	0	7	1	
31.966	2.79741	33	4	3	0		57.042	1.61321	3m	3	4	2	
32.660	2.73954	40	5	2	0		57.327	1.60586	1	1	7	1	
32.884	2.72144	14	4	1	1		57.655	1.59752	4m	4	7	0	
33.074	2.70618	36	2	3	1		57.655	1.59752	4m	6	6	0	
34.001	2.63449	9	3	4	0		57.830	1.59309	12m	6	0	2	
35.171	2.54950	43	6	0	0		57.830	1.59309	12m	8	3	1	
35.286	2.54144	101	4	2	1		58.359	1.57991	8m	2	7	1	
35.649	2.51644	159	3	3	1		58.359	1.57991	8m	6	1	2	
35.943	2.49650	19	6	1	0		58.753	1.57025	16	9	3	0	
36.610	2.45256	44	5	3	0		58.821	1.56859	17m	5	3	2	
36.682	2.44791	53	5	0	1		58.821	1.56859	17m	9	0	1	
36.956	2.43033	26m	1	4	1		59.064	1.56273	9	1	5	2	
36.956	2.43033	26m	1	5	0		59.327	1.55643	3	9	1	1	
37.427	2.40088	29m	4	4	0		59.435	1.55385	6	4	4	2	
37.427	2.40088	29m	5	1	1		59.928	1.54225	8	6	2	2	
38.177	2.35537	19	6	2	0		60.089	1.53850	8m	0	8	0	
38.452	2.33917	17m	2	4	1		60.089	1.53850	8m	2	5	2	
38.452	2.33917	17m	2	5	0		60.470	1.52970	5m	1	8	0	
39.004	2.30736	72	4	3	1		60.470	1.52970	5m	10	0	0	
39.589	2.27457	65	5	2	1		60.985	1.51802	12m	7	5	1	
40.732	2.21336	72m	3	4	1		60.985	1.51802	12m	10	1	0	
40.732	2.21336	72m	3	5	0		61.389	1.50898	6m	2	8	0	
41.675	2.16544	1	6	3	0		61.389	1.50898	6m	8	4	1	
41.955	2.15163	24	7	1	0		61.737	1.50131	3	3	5	2	
42.409	2.12963	42	6	1	1		62.361	1.48778	44m	4	7	1	
42.991	2.10215	10	5	3	1		62.361	1.48778	44m	9	4	0	
43.294	2.08811	46	1	5	1		62.699	1.48058	12	7	1	2	
43.757	2.06707	21m	4	4	1		63.063	1.47291	8	3	8	0	
43.757	2.06707	21m	4	5	0		63.418	1.46551	9	9	3	1	
43.931	2.05930	25	7	2	0		64.023	1.45312	4	4	5	2	
44.111	2.05133	69	0	6	0		64.204	1.44945	14	7	2	2	
44.357	**2.04050**	408m	0	0	2		64.342	1.44667	37m	0	6	2	
44.357	**2.04050**	408m	6	2	1		64.342	1.44667	37m	6	7	0	
44.551	2.03208	100m	1	6	0		64.664	1.44024	1	1	6	2	
44.551	2.03208	100m	2	5	1		65.018	1.43326	5m	1	8	1	
45.405	1.99582	2	1	1	2		65.018	1.43326	5m	10	3	0	
45.756	1.98131	11	2	6	0		65.284	1.42807	6m	4	8	0	
46.204	1.96317	75	6	4	0		65.284	1.42807	6m	5	7	1	
46.585	1.94796	254m	2	1	2		65.625	1.42146	6m	2	6	2	
46.585	1.94796	254m	3	5	1		65.625	1.42146	6m	10	1	1	
47.078	1.92874	45	7	3	0		65.978	1.41472	67m	2	8	1	
47.136	1.92647	45	7	0	1		65.978	1.41472	67m	6	4	2	
47.512	1.91212	36m	6	3	1		66.672	1.40167	19	7	3	2	
47.512	1.91212	36m	8	0	0		66.881	1.39779	12m	5	5	2	
47.746	1.90330	7m	3	6	0		66.881	1.39779	12m	9	4	1	
47.746	1.90330	7m	7	1	1		67.027	1.39509	42m	8	0	2	
48.117	1.88946	4	8	1	0		67.027	1.39509	42m	10	2	1	
48.442	1.87755	4	2	2	2		67.505	1.38637	3m	3	8	1	
48.584	1.87239	1	3	1	2		67.505	1.38637	3m	8	1	2	
49.325	1.84600	6	4	5	1		67.757	1.38184	1	11	1	0	
49.539	1.83850	5	7	2	1		68.169	1.37449	2	5	8	0	
49.901	1.82601	8	8	2	0		68.428	1.36991	2m	7	7	0	
50.083	1.81980	27	1	6	1		68.428	1.36991	2m	10	4	0	
50.442	1.80769	8m	3	2	2		68.756	1.36418	28	6	7	1	
50.442	1.80769	8m	4	6	0		68.955	1.36072	5	8	2	2	
50.665	1.80027	5	4	0	2		69.203	1.35644	2	11	2	0	
51.243	1.78131	15m	4	1	2		69.457	1.35210	12m	0	1	3	
51.243	1.78131	15m	7	4	0		69.457	1.35210	12m	10	3	1	
51.622	1.76912	35m	6	4	1		69.805	1.34621	7m	1	1	3	

2θ (°)	d (Å)	I	h	k	l	*	2θ (°)	d (Å)	I	h	k	l	*
69.805	1.34621	7m	2	9	0		72.759	1.29867	22m	9	1	2	
70.052	1.34207	1	7	4	2		72.759	1.29867	22m	10	4	1	
70.330	1.33744	2	6	5	2		73.046	1.29427	3	8	7	0	
70.969	1.32697	6	1	7	2		73.192	1.29205	2m	0	3	3	
71.208	1.32310	5m	8	6	1		73.192	1.29205	2m	1	9	1	
71.208	1.32310	5m	9	5	1		73.411	1.28874	8m	3	7	2	
71.341	1.32095	10m	3	9	0		73.411	1.28874	8m	4	9	0	
71.341	1.32095	10m	8	3	2		73.513	1.28720	5m	1	3	3	
71.586	1.31703	3m	11	0	1		73.513	1.28720	5m	11	2	1	
71.586	1.31703	3m	11	3	0		73.635	1.28537	8	3	2	3	
71.888	1.31224	14	2	7	2		74.164	1.27751	15m	2	9	1	
72.226	1.30693	48m	3	1	3		74.164	1.27751	15m	9	2	2	
72.226	1.30693	48m	5	6	2		74.296	1.27556	6m	4	1	3	
72.505	1.30259	8	5	8	1		74.296	1.27556	6m	7	5	2	