ภาคผนวก

ไฟล์มาตรฐานของการเลี้ยวเบนของรังสีเอกซ์

Pattern : 75-107 ***Radiation*** = 1.540600 ***Quality*** : Calculated

Cu In Se_2

Copper Indium Selenide

Lattice : Body-center tetragonal

S.G. : I-42d (122)

a = 5.77300

c = 11.55000

Z = 4

Mol. weight = 336.29

Volume [CD] = 384.93

Dx = 5.803

Dm = 5.650

I/Icor = 11.51

ICSD COLLECTION CODE : 028740

TEST FROM ICSD : Calc. density unusual but tolerable.

TEST FROM ICSD : No R value given.

TEST FROM ICSD : At least one TF missing.

*Calculated from ICSD using POWD-12++, (1997) primary reference:

*Z. Anorg. Allg. Chem., volume 271, page 153, (1953) :

Hahn, H., Frank, W., Meyer, A.D., Stoerger, G.

Radiation : CuKa1

Lambda : 1.54060

Filter : Not specified

d-sp: Calculated spacings

2th	*I*	*h*	*k*	*l*
17.158	3	1	0	1
26.772	100	1	1	2
27.831	5	1	0	3
30.955	1	0	0	4
*30.955	1	2	0	0
34.716	<1	2	0	2
35.603	5	2	1	1
42.107	3	1	0	5
*42.107	3	2	1	3
44.337	58	2	0	4
*44.337	58	2	2	0
47.884	2	3	0	1
49.915	<1	3	1	0
52.531	31	1	1	6
*52.531	31	3	1	2
53.161	1	2	1	5
*53.161	1	3	0	3
55.054	<1	2	2	4
57.499	<1	2	0	6
58.116	<1	1	0	7
*58.116	<1	3	2	1
59.895	<1	3	1	4
62.804	2	3	0	5
*62.804	2	3	2	3
64.515	6	0	0	8
*64.515	6	4	0	0
66.753	<1	4	0	2
67.290	1	2	1	7
*67.290	1	4	1	1
71.115	9	3	1	6
*71.115	9	3	3	2
71.657	2	3	2	5
*71.657	2	4	1	3
73.271	<1	4	0	4
*73.271	<1	4	2	0
75.389	<1	4	2	2
75.899	<1	1	0	9
*75.899	<1	3	0	7
80.080	1	4	1	5
81.633	10	2	2	8
*81.633	10	4	2	4
83.684	<1	4	0	6
84.209	1	5	0	1
85.745	<1	3	1	8
*85.745	<1	5	1	0
87.787	5	3	3	6
*87.787	5	5	1	2
88.296	1	5	0	3

Pattern : 80-535 ***Radiation*** = 1.540600 ***Quality*** : Calculated

Cu In Se_2

Copper Indium Selenide

Lattice : Body-center tetragonal

S.G. : I-42d (122)

a = 5.78400

c = 11.57000

Z = 4

Mol. weight = 336.29

Volume [CD] = 387.07

Dx = 5.771

I/Icor = 11.68

ICSD COLLECTION CODE : 068334

TEST FROM ICSD : Calc. density unusual but tolerable.

TEST FROM ICSD : No R value given.

TEST FROM ICSD : At least one TF missing.

*Calculated from ICSD using POWD-12++, (1997) primary reference:

*Sae Mulli., volume 27, page 456, (1987) :

Lee, D.W., Park, J.Y., Kim, H.S., Chang, B.H., Choi, I.H., Hong, C.Y.

Radiation : CuKa1

Lambda : 1.54060

Filter : Not specified

d-sp: Calculated spacings

2th	*I*	*h*	*k*	*l*
17.125	9	1	0	1
26.672	100	1	1	2
27.780	2	1	0	3
30.895	1	0	0	4
*30.895	1	2	0	0
35.534	2	2	1	1
42.025	2	1	0	5
*42.025	2	2	1	3
44.253	60	2	0	4
*44.253	60	2	2	0
47.787	<1	3	0	1
52.424	33	1	1	6
*52.524	33	3	1	2
53.058	1	2	1	5
*53.058	1	3	0	3
54.944	<1	2	2	4
57.995	1	1	0	7
*57.995	1	3	2	1
62.673	1	3	0	5
*62.673	1	3	2	3
64.378	7	0	0	8
*64.378	7	4	0	0
67.155	1	2	1	7
*67.155	1	4	1	1
70.966	10	3	1	6
*70.966	10	3	3	2
71.505	1	3	2	5
*71.505	1	4	1	3
73.098	<1	2	0	8
*73.098	<1	4	2	0
75.738	<1	1	0	9
*75.738	<1	3	0	7
79.902	<1	4	1	5
81.448	12	2	2	8
*81.448	12	4	2	4
84.012	1	5	0	1
87.578	6	3	3	6
*87.578	6	5	1	2
88.086	<1	4	3	3

Pattern : 47-1698 ***Radiation*** = 1.540600 ***Quality*** : Indexed

Na_2S

Sodium Sulfide

Lattice : Face-centered cubic

S.G. : Fm3m (225)

Mol. weight = 78.04

Volume [CD] = 277.93

a = 6.52600

Z= 4

Dx = 1.865

Dm = 1.880

SAMPLE PREPARATION : Prepared by addition of Na metal to a solution of S in liquid ammonia and annealed for 20-30 hours in vacuum at 120-250 C.

GENERAL COMMENTS : Films used for intensity measurements had a 14mum aluminum foil absorber.

GENERAL COMMENTS : See also 23-441 (calculated pattern).

GENERAL COMMENTS : See also 3-933 (calculated pattern).

ADDITIONAL PATTERN : To replace 3-933.

COLOR : White

CAS: 1313-82-2

*Z. Elektrochem. Angew. Phys. Chem., volume 40, page 588, (1934)

primary reference :

Zintl, E., Harder, A., Dauth, B.

Radiation : CuKa

Lambda : 1.53900

SS/FOM : F23= 18(0.0570,23)

Filter : Beta

d-sp : Debye-Scherrer

Internal standard **:** Ag

2th	*I*	*h*	*k*	*l*
23.389	80	1	1	1
27.155	10	2	0	0
38.963	100	2	2	0
46.102	50	3	1	1
48.294	5	2	2	2
56.422	50	4	0	0
61.909	35	3	3	1
63.717	5	4	2	0
70.693	80	4	2	2
75.734	35	5	1	1
83.794	50	4	4	0
88.511	50	5	3	1
90.229	5	6	0	0
96.562	75	6	2	0
101.333	15	5	3	3
103.099	5	6	2	2
109.681	35	4	4	4
114.869	35	7	1	1
116.679	5	6	4	0
124.153	80	6	4	2
130.212	50	7	3	1
141.669	15	8	0	0
150.093	15	7	3	3