

X'Pert HighScore	X'Pert HighScore Report	date: 03/21/25
PANalytical		for internal use only

Fantastic report on CoSbS0.75Se0



Distribution:

Name	Function	0.1	0.5	1.0
N.N.-999	Masterking Group Manager (MGM)	✓		
N.N.-998	Product Ontwikkelt Manager (POM)	✓		
N.N.-1	(AS)			✓
N.N.-2	(DS)			✓
N.N.-3	(BS)			✓
T.P.	Supervisor All Coding			✓

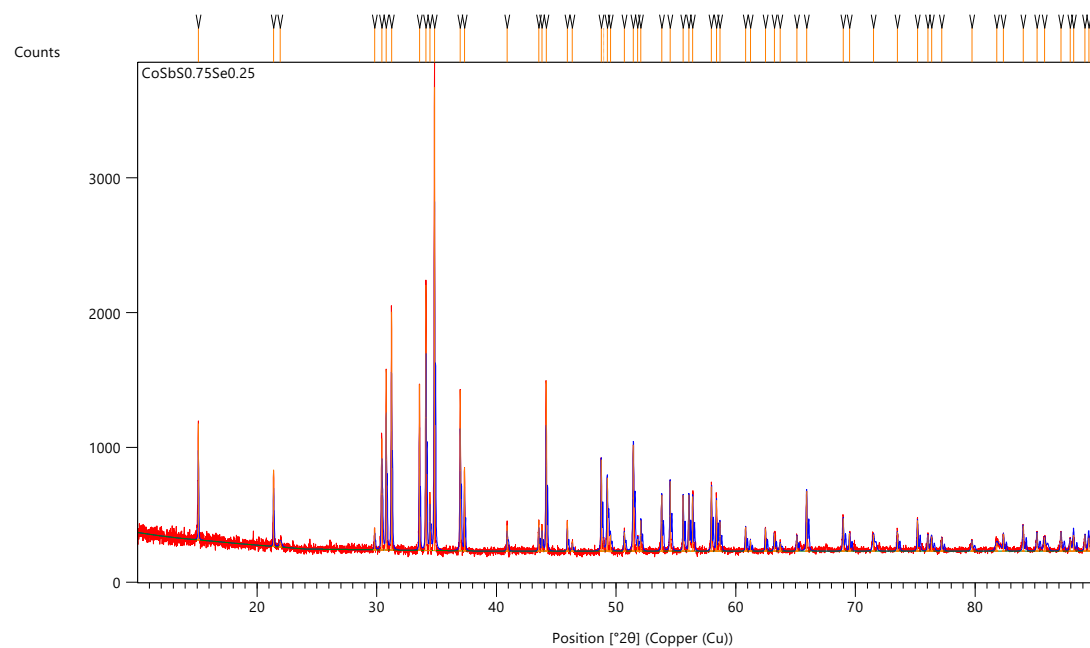
Last saved by XRD	Draft	file: CoSbS0.75Se0	rev: 1
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Anchor Scan Parameters: (Bookmark1)

Dataset Name	CoSbS0.75Se0.25
File name	C:\Users\XRD\Desktop\Material
Characterization	CoSbS0.75Se0.25.ASC
Raw Data Origin	ASCII-2Theta-Intensity (.ASC)
Scan Axis	Gonio
Start Position [$^{\circ}2\theta$]	10,0133
End Position [$^{\circ}2\theta$]	89,9933
Step Size [$^{\circ}2\theta$]	0,0100
Scan Step Time [s]	1,0000
Scan Type	Pre-set time
Offset [$^{\circ}2\theta$]	0,0000
Divergence Slit Type	Fixed
Divergence Slit Size [$^{\circ}$]	1,0000
Specimen Length [mm]	10,00
Receiving Slit Size [mm]	0,1000
Measurement Temperature [$^{\circ}\text{C}$]	25,00
Anode Material	Cu
K-Alpha1 [\AA]	1,54060
K-Alpha2 [\AA]	1,54443
K-Beta [\AA]	1,39225
K-A2 / K-A1 Ratio	0,50000
Generator Settings	0 mA, 0 kV
Diffractionmeter Number	0
Goniometer Radius [mm]	240,00
Dist. Focus-Diverg. Slit [mm]	91,00
Incident Beam Monochromator	No
Spinning	No

Graphics: (Bookmark2)

Peak List: (Bookmark 3)

Pos. [°2 θ]	Height [cts]	FWHM Left [°2 θ]	d-spacing [Å]	Rel. Int. [%]	Tip Width	Matched by
15,0958	862,52	0,0394	5,86913	25,09	0,0472	
21,3779	570,23	0,0492	4,15651	16,59	0,0590	
21,9428	45,69	0,2362	4,05077	1,33	0,2834	
29,8307	163,00	0,0590	2,99519	4,74	0,0708	
30,4218	826,78	0,0886	2,93833	24,05	0,1063	
30,8001	1336,91	0,0590	2,90310	38,89	0,0708	
31,2372	1768,23	0,0590	2,86346	51,44	0,0708	
33,5739	1231,36	0,0492	2,66933	35,82	0,0590	
34,1176	1969,14	0,0590	2,62802	57,29	0,0708	
34,4461	431,02	0,0590	2,60371	12,54	0,0708	
34,8295	3437,39	0,0590	2,57592	100,00	0,0708	
36,9821	1191,43	0,0689	2,43078	34,66	0,0827	
37,3348	619,52	0,0492	2,40862	18,02	0,0590	
40,9038	193,97	0,0886	2,20633	5,64	0,1063	
43,5416	231,73	0,0689	2,07859	6,74	0,0827	
43,8111	196,55	0,0590	2,06643	5,72	0,0708	
44,1606	1264,21	0,0590	2,05088	36,78	0,0708	
45,9286	227,53	0,0689	1,97597	6,62	0,0827	
46,3477	74,49	0,0590	1,95907	2,17	0,0708	
48,7603	679,78	0,0720	1,86609	19,78	0,0864	
48,9660	99,90	0,0960	1,86334	2,91	0,1152	
49,2626	544,45	0,0960	1,84823	15,84	0,1152	
49,5289	122,13	0,0840	1,83891	3,55	0,1008	
50,6894	141,13	0,0960	1,79950	4,11	0,1152	
51,4461	789,50	0,0960	1,77479	22,97	0,1152	
51,8117	90,51	0,0720	1,76313	2,63	0,0864	
52,0740	229,26	0,0840	1,75486	6,67	0,1008	
53,8143	418,18	0,0840	1,70215	12,17	0,1008	
54,5153	520,89	0,0840	1,68190	15,15	0,1008	
55,6124	416,82	0,0720	1,65129	12,13	0,0864	
56,0843	418,98	0,0720	1,63851	12,19	0,0864	
56,4042	406,87	0,0720	1,62998	11,84	0,0864	
57,9710	482,25	0,0720	1,58959	14,03	0,0864	
58,3832	378,13	0,0600	1,57935	11,00	0,0720	
58,6744	217,72	0,0840	1,57220	6,33	0,1008	
60,8204	180,84	0,0720	1,52177	5,26	0,0864	
61,2281	84,21	0,0720	1,51261	2,45	0,0864	
62,4827	170,28	0,0720	1,48522	4,95	0,0864	
63,2199	132,48	0,0960	1,46966	3,85	0,1152	
63,7111	60,86	0,1440	1,45951	1,77	0,1728	
65,1030	116,86	0,0960	1,43163	3,40	0,1152	
65,9220	446,70	0,0960	1,41581	13,00	0,1152	
68,9805	244,39	0,0960	1,36031	7,11	0,1152	
69,5196	135,83	0,0960	1,35108	3,95	0,1152	
71,5090	124,34	0,1680	1,31830	3,62	0,2016	
73,5054	144,31	0,0960	1,28735	4,20	0,1152	
75,1905	229,98	0,0960	1,26262	6,69	0,1152	
76,0498	119,61	0,0960	1,25048	3,48	0,1152	

76,3712	109,03	0,1200	1,24601	3,17	0,1440
77,2093	101,91	0,0960	1,23457	2,96	0,1152
79,7351	79,07	0,1440	1,20169	2,30	0,1728
81,8192	65,84	0,2880	1,17627	1,92	0,3456
82,3672	128,56	0,0960	1,16982	3,74	0,1152
84,0166	191,85	0,0960	1,15101	5,58	0,1152
85,1698	137,41	0,1200	1,13835	4,00	0,1440
85,8063	103,85	0,1920	1,13153	3,02	0,2304
87,1838	141,07	0,1200	1,11716	4,10	0,1440
87,9464	90,86	0,1440	1,10943	2,64	0,1728
88,2266	120,61	0,0960	1,10662	3,51	0,1152
89,1856	122,74	0,1200	1,09719	3,57	0,1440
89,5068	99,85	0,1200	1,09409	2,90	0,1440

Identified Patterns List: (Bookmark4)

Plot of Identified Phases: (Bookmark 5)

Document History: (Bookmark 6)

Insert Measurement:

- File name = CoSbS0.75Se0.25.ASC
- Modification time = "21.3.2025 15.07.26"
- Modification editor = "XRD"

Search Peaks:

- Minimum significance = "2"
- Minimum tip width = "0,01"
- Maximum tip width = "3"
- Peak base width = "7"
- Method = "Minimum 2nd derivative"
- Modification time = "21.3.2025 15.07.53"
- Modification editor = "XRD"

Search & Match:

- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Peak list"
- Demote unmatched strong = "No"
- Multi phase = "Yes"
- Restriction set = "Untitled"
- Restriction = "Restriction set"
- Subset name = ""
- Match intensity = "Yes"
- Two theta shift = "0"
- Identify = "No"
- Max. no. of accepted patterns = "5"
- Minimum score = "50"
- Min. new lines / total lines = "60"
- Search depth = "10"
- Minimum new lines = "5"
- Minimum scale factor = "0,1"
- Intensity threshold = "0"
- Use line clustering = "Yes"
- Line cluster range = "1,5"
- Search sensitivity = "1,8"
- Use adaptive smoothing = "Yes"
- Smoothing range = "1,5"
- Threshold factor = "3"
- Match Threshold = "0"
- N * Esds = "-1"
- Raw Weight = "-1"
- Peak Shape = "-1"
- Accepted Shape = "-1"
- Peak Power = "-1"
- New Peak Power = "-1"
- Intensity Power = "-1"
- N Peaks Power = "-1"
- Modification time = "21.3.2025 13.32.26"
- Modification editor = "XRD"

Search & Match:

- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Peak list"
- Demote unmatched strong = "No"
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- Peak Power = "-1"
- New Peak Power = "-1"
- Intensity Power = "-1"
- N Peaks Power = "-1"
- Modification time = "21.3.2025 15.23.23"
- Modification editor = "XRD"