

Match! Phase Analysis Report

Sample: ThuyDHD 06

Sample Data

File name	ThuyDHD 06.UXD
File path	E:/Syn/DANG BAO/Bai bao dang sua de dang/2020 T11 sulfinat Molbank/Upload/Spectra
Data collected	Oct 31, 2020 16:14:39
Data range	2.000° - 60.000°
Original data range	2.000° - 60.000°
Number of points	2901
Step size	0.020
Rietveld refinement converged	No
Alpha2 subtracted	No
Background subtr.	No
Data smoothed	No
Radiation	X-rays
Wavelength	1.541874 Å

Candidates

<i>Name</i>	<i>Formula</i>	<i>Entry No.</i>	<i>FoM</i>
Ba45 Cu28 Al17 F197	Al17 Ba45 Cu28 F197	96-153-6586	0.8871
	Mo3 O22.5 P6	96-430-3254	0.8869
	Mo3 O22.5 P6	96-711-1395	0.8869
Na2 (C O3)	C Na2 O3	96-210-6756	0.8725
	Mo3 O22.5 P6	96-430-3256	0.8702
	Mo2 O15 P4	96-430-3255	0.8701
Cu47.18 Si91.22 P144	Cu47.18 P144 Si91.22	96-152-6073	0.8697
	C4 Cl2 F N2 O2 S5	96-411-6447	0.8619
Metakirchheimerite	As2 Co H16 O20 U2	96-900-4898	0.8614
	As8 Eu3 Ga6	96-412-7424	0.8610
Na[N(SO2F)2]	F2 N Na O4 S2	96-433-3524	0.8602
Nb8 W9 O47	Nb8 O32 W9	96-210-6864	0.8589
Calcium catena-polyphosphate	Ca O6 P2	96-400-1395	0.8581
	C9 B Br6.13 Cl0.87 F2 N2	96-715-5228	0.8569
	As2 H16 Mn O20 U2	96-900-4896	0.8553
	F36 P4 Sr2 Xe6	96-430-8199	0.8552
	Bi Cl O3 Se	96-451-0600	0.8547
	Na13 Nb35 O94	96-153-4377	0.8530
(S Br3) (Sb F6)	Br3 F6 S Sb	96-154-1090	0.8524
	Al Cs2 O10 P3	96-700-9288	0.8522
	C4 Cl3 N2 O4 S4	96-411-6448	0.8513
	As2 Fe H16 O20 U2	96-900-4897	0.8512
Metakahlerite	Na2 O5 Si2	96-810-3802	0.8511
	O7 P2 Ti	96-201-1793	0.8506
1,10-octachlorophenanthroline	C14 Cl4 F6 N4	96-402-7315	0.8506
	C16 Al Cl N16 S4	96-430-9965	0.8506
	C12 Cl8 N2	96-432-3462	0.8505
Monoclinic titanium metaphosphate	O27 P9 Ti3	96-201-0156	0.8501
	C9 B Br4 Cl3 F2 N2	96-715-5229	0.8501
Mn (P4 O11)	Mn O11 P4	96-153-5800	0.8492
[Me3HN][Ni(dmise)2]2	C15 H10 N Ni2 S16 Se4	96-432-3670	0.8492
	Br0.17 I1.67 O3.17 Pb3.83	96-433-6645	0.8484
	C19 H29 N S Si	96-200-0263	0.8481
	C16 N16 O S4 V	96-432-7835	0.8480
VOTDPPz	C9 Ca9 O27	96-150-8972	0.8473
Vaterite	I10 Nb2 O32 Sr2	96-712-3508	0.8464
	Gd O9 P3	96-430-7098	0.8463
gadolinium metaphosphate	H2 K O3 P	96-202-0165	0.8460
	Cs2 Ga O10 P3	96-700-9289	0.8460
Cesium disulfate	Cs2 O7 S2	96-210-4417	0.8457
K (H Se O4) (H2 Se O4)	H3 K O8 Se2	96-152-2052	0.8456
(Mg0.87 Fe0.13) (Mo1.87 V0.13) O7	Fe0.13 Mg0.87 Mo1.87 O7 V0.13	96-153-6199	0.8456
Cannizzarite	Bi54 Pb46 S127	96-901-1203	0.8456
Me3NH[Ni(dmise)2]2	C13 H6 N Ni2 S16 Se4	96-432-3672	0.8455
	Cr F10 Xe	96-432-2838	0.8452
	C9 H15.5 N3 O4.25	96-155-7589	0.8449
L-Glutamic Acid.2-Methylimidazole	Ba2 Sn Te5	96-400-0471	0.8449
	As39.51 Pb6.13 S136 Sb41.51 Ti16.85	96-231-0155	0.8448
	Ce H2 I4 O13	96-231-0606	0.8447
Potassium tecto-vanadatophosphate *	K O17 P4 V3	96-100-1594	0.8444
	Mo15.39 O47	96-154-0783	0.8444

Search-Match

Settings	
Reference database used	COD-Inorg REV254652 2020.07.29
Automatic zeropoint adaptation	Yes
Downgrade entries with low scaling factors	Yes
Minimum figure-of-merit (FoM)	0.60
2theta window for peak corr.	0.30 deg.
Minimum rel. int. for peak corr.	0
Parameter/influence 2theta	0.50
Parameter/influence intensities	0.50
Parameter multiple/single phase(s)	0.50

Peak List

No.	2theta [°]	d [Å]	I/I0	FWHM
1	9.10	9.7182	26.15	0.2000
2	10.14	8.7237	150.70	0.2000
3	13.44	6.5882	122.54	0.2000
4	14.82	5.9777	328.29	0.3600
5	14.98	5.9142	214.49	0.2400
6	15.72	5.6374	29.00	0.4400
7	16.98	5.2218	32.71	0.6800
8	17.64	5.0279	185.70	0.2000
9	18.58	4.7756	26.28	0.8400
10	18.94	4.6857	170.20	0.2000
11	19.28	4.6038	27.76	2.1200
12	19.56	4.5385	30.25	2.6800
13	20.08	4.4221	53.10	0.4400
14	20.46	4.3409	71.63	0.4400
15	20.94	4.2424	122.11	0.2000
16	21.22	4.1871	43.09	3.6000
17	21.44	4.1446	53.63	3.2000
18	21.92	4.0549	322.93	0.2400
19	22.22	4.0009	77.92	1.8400
20	22.44	3.9621	63.61	5.2800
21	22.80	3.9004	565.28	0.2400
22	23.06	3.8570	154.09	0.2400
23	23.60	3.7699	113.15	0.3600
24	23.92	3.7202	204.88	0.2000
25	24.22	3.6748	1000.00	0.2000
26	24.56	3.6247	71.30	0.2000
27	25.02	3.5591	40.68	6.9200
28	25.42	3.5040	56.05	5.6000
29	25.62	3.4771	45.68	5.2800
30	25.88	3.4428	44.34	5.1600
31	26.50	3.3636	218.34	0.2400
32	27.14	3.2857	56.87	2.1200
33	27.50	3.2435	325.10	0.2400
34	28.00	3.1867	40.70	0.9200
35	28.38	3.1449	28.91	0.2400
36	28.62	3.1191	30.95	0.2400
37	28.84	3.0958	28.91	7.1200
38	29.44	3.0340	52.01	0.5200
39	29.58	3.0200	49.01	0.9600
40	29.98	2.9806	155.54	0.3600
41	30.36	2.9442	245.44	0.2800
42	30.64	2.9179	120.55	0.2400
43	31.68	2.8244	67.27	0.2400
44	32.32	2.7700	34.70	0.1200
45	33.04	2.7112	55.85	0.2800
46	33.58	2.6689	31.19	0.2000
47	34.72	2.5838	63.23	0.2400
48	35.26	2.5454	168.29	0.2800
49	35.82	2.5069	44.99	0.2000
50	36.48	2.4631	121.31	0.1600
51	37.32	2.4095	41.08	0.3200
52	37.70	2.3861	35.40	0.2800
53	38.24	2.3537	30.31	0.2400
54	38.44	2.3419	45.94	0.4400
55	38.68	2.3279	32.43	0.2400
56	39.10	2.3039	37.32	0.2000

57	39.86	2.2617	85.09	0.2400
58	40.68	2.2179	50.72	0.2000
59	44.48	2.0369	76.37	0.2400
60	45.32	2.0011	40.35	0.4400
61	45.60	1.9894	34.43	0.4000
62	46.56	1.9506	31.94	0.1600
63	48.48	1.8778	36.09	0.2400

Integrated Profile Areas

Based on calculated profile

Profile area	Counts	Amount
Overall diffraction profile	85122	100.00%
Background radiation	36398	42.76%
Diffraction peaks	48724	57.24%
Peak area belonging to selected phases	0	0.00%
Unidentified peak area	48724	57.24%

Peak Residuals

Peak data	Counts	Amount
Overall peak intensity	2392	100.00%
Peak intensity belonging to selected phases	1343	56.18%
Unidentified peak intensity	1048	43.82%

Diffraction Pattern Graphics

