Name and formula

Reference code:	00-022-0675
Mineral name:	Microcline, intermediate
Compound name:	Potassium Aluminum Silicate
PDF index name:	Potassium Aluminum Silicate
Empirical formula:	$AlKO_8Si_3$
Chemical formula:	$KAlSi_3O_8$
Mineral classification:	Feldspar (Family), orthoclase (Supergroup)

Crystallographic parameters

Crystal system:	Anorthic
Space group:	C-1
Space group number:	2
a (Å):	8.5784
b (Å):	12.9600
c (Å):	7.2112
Alpha (°):	89.7000
Beta (°):	115.9700
Gamma (°):	90.8700
Calculated density (g/cm^3):	2.56
Volume of cell (10^6 pm^3):	360.34
Z:	4.00
RIR::	-

Status, subfiles and quality

Status:	Marked as deleted by ICDD
Subfiles:	Common Phase, Forensic, Inorganic, Mineral, Mineral - Mineral, Mineral - Natural
Quality:	Indexed (I)

Comments

ANX:	ABC3X8
Creation Date:	9/1/1972
Cross-References:	ICDD:04-007-8600
ANX:	ABC3X8
Deleted Or Rejected By:	Deleted by 00-019-0932, calculated confirms experimental, MTG 1992
Additional Diffraction Lines:	Plus 37 additional reflections to 1.271
Warning:	Not enough reflections above the intensity cut off to meet higher quality mark criteria
Unit Cell Data Source:	Powder Diffraction.

References

Primary reference:	Borg, Smith., *Am. Mineral.*, **54**, 163, (1969)
Unit cell:	Bailey, Taylor., *Acta Crystallogr.*, **8**, 621, (1955)

Peak list

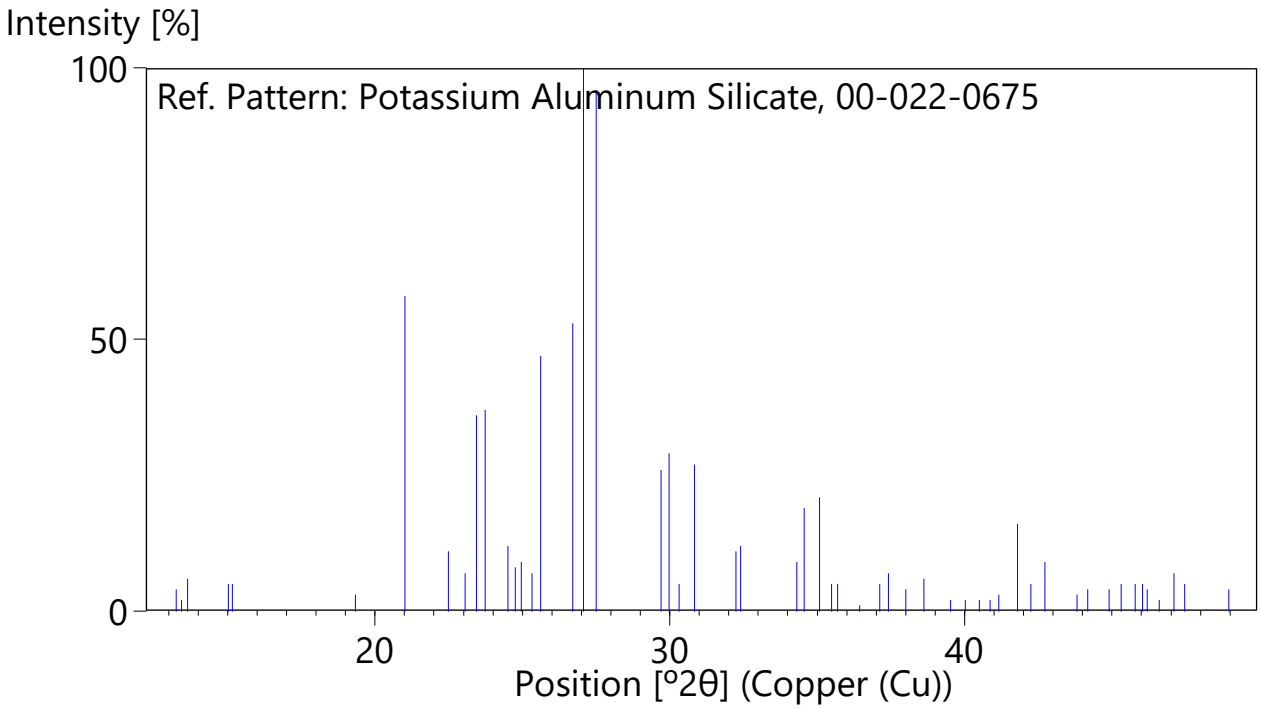
No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	-1	0	6.66900	13.265	4.0
2	1	1	0	6.58500	13.435	2.0
3	0	2	0	6.48100	13.652	6.0
4	-1	1	1	5.89300	15.022	5.0
5	-1	-1	1	5.84200	15.154	5.0
6	0	-2	1	4.58700	19.335	3.0
7	-2	0	1	4.22500	21.010	58.0
8	1	1	1	3.94900	22.497	11.0
9	2	0	0	3.85600	23.047	7.0
10	1	-3	0	3.79200	23.441	36.0
11	1	3	0	3.74600	23.733	37.0
12	-1	3	1	3.62900	24.510	12.0
13	-1	-3	1	3.59300	24.759	8.0
14	-2	2	1	3.56300	24.971	9.0
15	-2	-2	1	3.51500	25.318	7.0
16	-1	1	2	3.47400	25.622	47.0
17	2	-2	0	3.33500	26.709	53.0
18	2	2	0	3.29200	27.064	100.0
19	0	0	2	3.24100	27.499	96.0
20	1	-3	1	3.00500	29.706	26.0
21	1	3	1	2.97900	29.971	29.0
22	-2	2	2	2.94600	30.315	5.0
23	0	2	2	2.89800	30.829	27.0
24	-1	3	2	2.77400	32.244	11.0
25	-1	-3	2	2.76100	32.400	12.0
26	-3	1	2	2.61200	34.304	9.0
27	2	-2	1	2.59300	34.563	19.0
28	1	1	2	2.55600	35.080	21.0
29	3	-1	0	2.52800	35.481	5.0
30	3	1	0	2.51400	35.685	5.0
31	2	4	0	2.46300	36.450	1.0
32	-1	5	1	2.42000	37.121	5.0
33	-3	3	1	2.40100	37.426	7.0
34	-3	-3	1	2.36600	38.000	4.0
35	-1	-1	3	2.32900	38.628	6.0
36	-3	3	2	2.27800	39.528	2.0
37	-3	-3	2	2.25100	40.022	2.0
38	1	3	2	2.22500	40.510	2.0

39	1	-5	1	2.20700	40.855	2.0
40	1	5	1	2.19200	41.148	3.0
41	0	6	0	2.16000	41.786	16.0
42	2	-4	1	2.13700	42.257	5.0
43	2	4	1	2.11500	42.718	9.0
44	3	1	1	2.06500	43.805	3.0
45	0	2	3	2.04900	44.165	4.0
46	-4	2	2	2.01700	44.903	4.0
47	-4	-2	2	2.00000	45.306	5.0
48	2	-2	2	1.98000	45.790	5.0
49	2	2	2	1.97000	46.035	5.0
50	-3	3	3	1.96400	46.184	4.0
51	-3	-3	3	1.94700	46.611	2.0
52	4	0	0	1.92800	47.098	7.0
53	-4	0	3	1.91400	47.463	5.0
54	1	-1	3	1.85900	48.958	4.0

Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	AL1	Al	0.00920	0.18360	0.22790	0.5000	0.2500	4*
2	SI1	Si	0.00950	0.81360	0.22210	0.5000	0.4400	4*
3	AL2	Al	0.70680	0.11590	0.34610	0.5000	0.0700	4*
4	AL3	Al	0.70890	0.88200	0.34270	0.5000	0.0800	4*
5	K1	K	0.28420	0.00330	0.13860	0.5000	1.0000	4*
6	SI2	Si	0.00920	0.18360	0.22790	0.5000	0.7500	4*
7	AL4	Al	0.00950	0.81360	0.22210	0.5000	0.5600	4*
8	SI3	Si	0.70680	0.11590	0.34610	0.5000	0.9300	4*
9	SI4	Si	0.70890	0.88200	0.34270	0.5000	0.9200	4*
10	O1	O	0.00030	0.14520	0.00660	0.5000	1.0000	4*
11	O2	O	0.63890	0.99860	0.28610	0.5000	1.0000	4*
12	O3	O	0.82850	0.14460	0.23520	0.5000	1.0000	4*
13	O4	O	0.82280	0.85520	0.22260	0.5000	1.0000	4*
14	O5	O	0.03740	0.30900	0.26300	0.5000	1.0000	4*
15	O6	O	0.03390	0.68390	0.25480	0.5000	1.0000	4*
16	O7	O	0.17670	0.12640	0.41060	0.5000	1.0000	4*
17	O8	O	0.18390	0.87710	0.40630	0.5000	1.0000	4*

Stick Pattern



Name and formula

Reference code:	01-087-2096
Mineral name:	Quartz, syn
Compound name:	Silicon Oxide
Common name:	α-Si O2
PDF index name:	Silicon Oxide
Empirical formula:	O_2Si
Chemical formula:	SiO_2
Mineral classification:	Quartz (Supergroup), Other members

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	P3221
Space group number:	154
a (Å):	4.9127
b (Å):	4.9127
c (Å):	5.4045
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	120.0000
Volume of cell (10^6 pm^3):	112.96
Z:	3.00
RIR:	2.88

Status, subfiles and quality

Status:	Alternate Pattern
Subfiles:	Alloy, metal or intermetalic, Cement and Hydration Product, Common Phase, Excipient, Forensic, ICSD Pattern, Inorganic, Mineral, Mineral - Mineral, Mineral - Synthetic, Pharmaceutical
Quality:	Star (S)

Comments

ANX:	AX2
ICSD collection code:	83849
Creation Date:	9/1/2000
Modification Date:	9/1/2020
Cross-References:	ICDD:04-008-7651, ICSD:83849
ANX:	AX2
Analysis:	O2 Si1
Formula from original source:	Si O2
ICSD Collection Code:	83849

Calculated Pattern Original Remarks: Structure determination using synchrotron radiation (powder). Structure refinement by Rietveld method. Stable up to 846 K, above P6222, above 1143 K tridymite is stable

Wyckoff Sequence:	c b (P3221)
Unit Cell Data Source:	Powder Diffraction.

References

Primary reference:	Norby, P., *J. Appl. Crystallogr.*, **30**, 21, (1997)
Structure:	Norby, P., *J. Appl. Crystallogr.*, **30**, 21, (1997)

Peak list

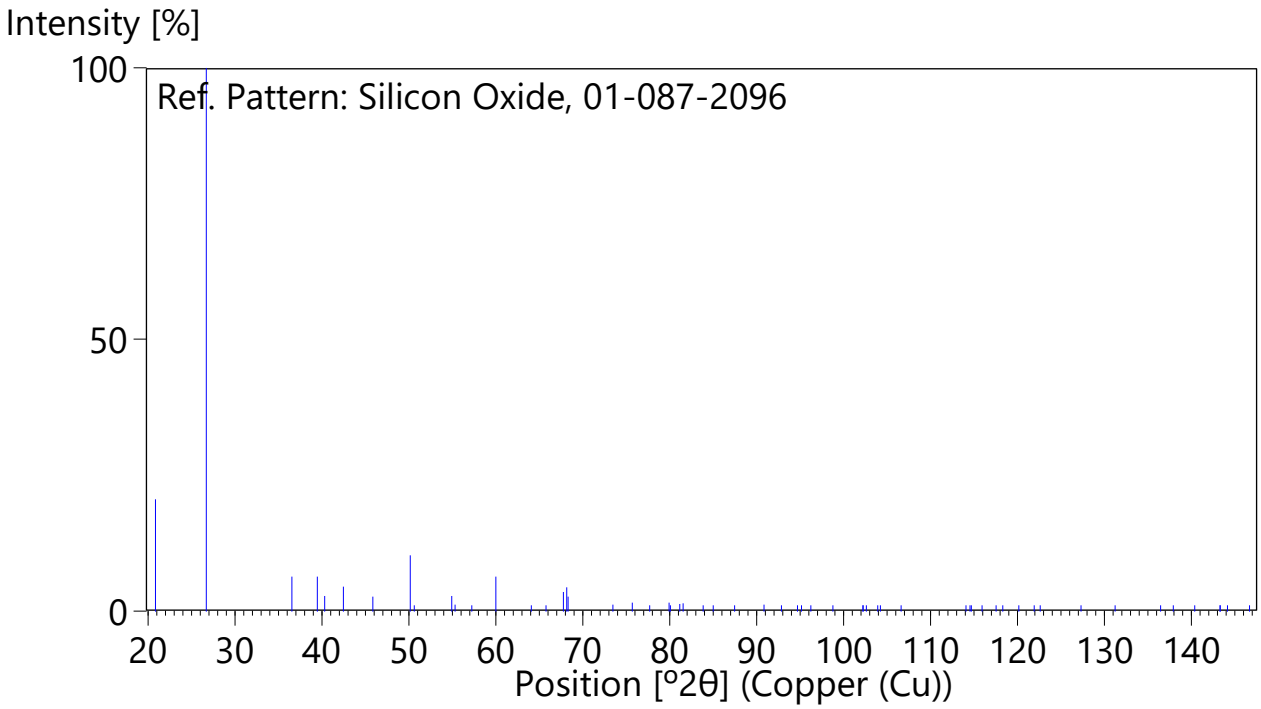
No.	h	k	l	d [Å]	2θ [°]	I [%]
1	1	0	0	4.25452	20.862	20.6
2	0	1	1	3.34296	26.644	100.0
3	1	1	0	2.45635	36.552	6.3
4	1	0	2	2.28104	39.473	6.3
5	1	1	1	2.23622	40.298	2.8
6	2	0	0	2.12726	42.459	4.5
7	2	0	1	1.97944	45.803	2.6
8	1	1	2	1.81763	50.149	10.3
9	0	0	3	1.80150	50.629	0.3
10	0	2	2	1.67148	54.884	2.8
11	0	1	3	1.65891	55.335	1.2
12	2	1	0	1.60806	57.243	0.2
13	1	2	1	1.54128	59.971	6.3
14	1	1	3	1.45269	64.046	1.1
15	3	0	0	1.41817	65.799	0.3
16	1	2	2	1.38189	67.756	3.5
17	2	0	3	1.37476	68.155	4.4
18	0	3	1	1.37173	68.327	2.7
19	1	0	4	1.28775	73.479	1.2
20	3	0	2	1.25575	75.674	1.5
21	2	2	0	1.22818	77.686	0.8
22	2	1	3	1.19965	79.898	1.5
23	2	2	1	1.19764	80.059	0.5
24	1	1	4	1.18385	81.185	1.3
25	3	1	0	1.17999	81.506	1.4
26	1	3	1	1.15283	83.854	0.9
27	2	0	4	1.14052	84.969	0.1
28	3	0	3	1.11432	87.462	0.1
29	1	3	2	1.08139	90.848	1.2
30	4	0	0	1.06363	92.808	0.2
31	0	1	5	1.04762	94.663	0.6
32	4	0	1	1.04361	95.141	0.4
33	2	1	4	1.03445	96.257	0.6
34	2	2	3	1.01478	98.766	0.5
35	0	4	2	0.98935	102.264	0.4
36	1	1	5	0.98935	102.264	0.4
37	1	3	3	0.98709	102.589	0.2
38	0	3	4	0.97824	103.893	0.1

39	3	2	0	0.97606	104.221	0.3
40	2	3	1	0.96052	106.636	0.5
41	3	2	2	0.91801	114.090	0.2
42	4	0	3	0.91591	114.497	0.4
43	4	1	1	0.91501	114.671	0.5
44	2	2	4	0.90882	115.900	0.2
45	0	0	6	0.90075	117.558	0.1
46	1	2	5	0.89707	118.337	0.3
47	3	1	4	0.88876	120.156	0.3
48	1	0	6	0.88122	121.885	0.1
49	1	4	2	0.87804	122.636	0.2
50	3	0	5	0.85967	127.285	0.1
51	1	1	6	0.84568	131.249	0.1
52	0	2	6	0.82946	136.460	0.3
53	1	4	3	0.82527	137.940	0.4
54	3	3	0	0.81878	140.368	0.1
55	5	0	2	0.81162	143.278	0.4
56	2	2	5	0.81162	143.278	0.4
57	3	3	1	0.80955	144.172	0.1
58	4	2	0	0.80403	146.690	0.2

Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	SI1	Si	0.46800	0.00000	0.33333	0.5000	1.0000	3a
2	O1	O	0.41300	0.26600	0.21300	0.5000	1.0000	6c

Stick Pattern



Name and formula

Reference code:	98-008-7657
Mineral name:	Albite (heat-treated)
Compound name:	Albite (heat-treated)
Common name:	Albite (heat-treated)
Chemical formula:	$Al_1Na_1O_8Si_3$

Crystallographic parameters

Crystal system:	Anorthic
Space group:	P -1
Space group number:	2
a (Å):	7.1320
b (Å):	7.4880
c (Å):	7.6720
Alpha (°):	115.0640
Beta (°):	107.1160
Gamma (°):	100.6130
Calculated density (g/cm^3):	2.63
Volume of cell (10^6 pm^3):	331.36
Z:	4.00
RIR:	0.65

Subfiles and quality

Subfiles:	User Inorganic, User Mineral
Quality:	User From Structure (=)

Comments

Creation Date:	12/16/2000
Cross-References:	ICSD:87657, PANICSD:98-008-7657
Original ICSD space group:	C-1. X-ray diffraction from single crystal

Structure type: Feldspar (TC)-Albite. Temperature factors available
The structure has been assigned a PDF number (calculated powder diffraction data): 01-089-6426
Compound with mineral name: Albite (heat-treated)
Structure type: Feldspar (TC)-Albite
Recording date: 12/16/00
Mineral origin: Stintino, Sardinia, Italy
ANX formula: ABC3X8
Z: 4
Calculated density: 2.63
R value: 0.044
Pearson code: aP26
Wyckoff code: i13
Structure TIDY: Transformed from space group: "C1-" to space group: "P -1".
Structure TIDY: Applied Transformation matrix:
Structure TIDY: -0.5, -0.5, 0
Structure TIDY: 0.5, -0.5, 0
Structure TIDY: 0, 0, 1
Structure TIDY: TRANS c,b,-a origin 0 1/2 1/2
Publication title: Order-disorder process in the tetrahedral sites of albite
ICSD collection code: 87657
Structure: Feldspar (TC)-Albite
Chemical Name: Sodium Tecto-alumotrisilicate
Second Chemical Formula: Na (Al Si3 O8)

References

Structure: Cruciani, G.;Alberti, A.;Meneghinello, E., *American Mineralogist*, **84**, 1144 - 1151, (1999)

Peak list

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	1	-1	6.38020	13.869	8.0
2	1	0	0	6.36761	13.896	9.5
3	0	1	0	6.33656	13.965	4.9
4	0	0	1	6.31271	14.018	2.5
5	1	0	-1	5.87727	15.062	6.0
6	1	-1	0	5.60027	15.812	5.4
7	1	1	-1	4.65717	19.041	0.3
8	1	-1	1	4.37052	20.303	0.2
9	1	-1	-1	4.02895	22.045	100.0
10	1	1	0	3.85608	23.046	17.5
11	1	0	1	3.76451	23.615	40.6
12	0	2	-1	3.67984	24.166	44.9
13	0	1	-2	3.66583	24.260	26.4
14	1	1	-2	3.64791	24.381	15.5
15	0	1	1	3.64100	24.428	0.0
16	2	0	-1	3.48934	25.507	13.9
17	1	0	-2	3.46220	25.710	5.1
18	1	-2	1	3.45133	25.793	0.1
19	2	-1	0	3.36736	26.448	17.0
20	1	-2	0	3.35357	26.558	0.5
21	2	-1	-1	3.20909	27.777	74.7
22	0	2	-2	3.19010	27.946	64.0
23	2	0	0	3.18380	28.003	99.9
24	0	2	0	3.16828	28.143	38.9
25	0	0	2	3.15636	28.251	35.8
26	1	2	-1	2.97387	30.024	24.4
27	2	0	-2	2.93864	30.393	14.7
28	1	2	-2	2.92753	30.511	20.8
29	2	1	-1	2.92388	30.550	12.6
30	1	-1	2	2.85124	31.348	17.3
31	2	1	-2	2.82610	31.634	5.1
32	2	-2	0	2.80013	31.935	0.7
33	1	-2	2	2.78237	32.145	0.8
34	2	-1	1	2.77923	32.182	0.5
35	1	1	1	2.68621	33.328	0.1
36	1	-1	-2	2.65829	33.689	0.5
37	2	-2	1	2.64092	33.917	9.9
38	1	-2	-1	2.63458	34.001	0.0

39	1	1	-3	2.54513	35.234	22.0
40	2	-1	-2	2.53019	35.449	3.9
41	2	1	0	2.50844	35.767	2.0
42	1	2	0	2.50272	35.852	2.1
43	2	-2	-1	2.48540	36.110	1.6
44	1	-3	1	2.45914	36.509	16.0
45	1	0	2	2.44959	36.656	1.9
46	1	2	-3	2.42197	37.090	5.8
47	0	3	-2	2.41175	37.253	1.4
48	0	2	-3	2.40517	37.358	0.0
49	0	3	-1	2.40464	37.367	2.9
50	0	1	-3	2.39422	37.535	5.4
51	0	2	1	2.38649	37.662	3.6
52	0	1	2	2.38266	37.725	2.9
53	3	-1	-1	2.34450	38.362	0.2
54	2	1	-3	2.33362	38.548	0.0
55	2	2	-2	2.32859	38.635	0.5
56	3	0	-1	2.32721	38.659	0.2
57	1	-3	2	2.32402	38.714	2.1
58	1	0	-3	2.30579	39.032	9.6
59	3	-1	0	2.27143	39.647	1.9
60	1	-3	0	2.26015	39.853	3.4
61	3	0	-2	2.25017	40.038	0.3
62	2	0	-3	2.23800	40.265	0.2
63	2	2	-1	2.22705	40.471	1.4
64	2	-3	1	2.19737	41.042	1.7
65	1	3	-2	2.19252	41.137	4.5
66	2	-2	2	2.18526	41.280	2.2
67	3	-2	0	2.15422	41.903	1.4
68	2	-3	0	2.14819	42.026	0.2
69	2	2	-3	2.14466	42.099	0.5
70	3	-1	-2	2.13093	42.383	0.3
71	2	-1	2	2.12753	42.454	0.0
72	0	3	-3	2.12673	42.471	11.7
73	3	0	0	2.12254	42.559	0.7
74	0	3	0	2.11219	42.777	0.4
75	1	-2	3	2.11014	42.821	4.9
76	0	0	3	2.10424	42.947	1.7
77	3	-2	-1	2.08957	43.264	2.5
78	1	3	-1	2.08583	43.345	8.1

79	1	3	-3	2.05679	43.989	0.1
80	3	1	-1	2.05341	44.065	0.2
81	1	-1	3	2.02506	44.715	1.7
82	2	-2	-2	2.01447	44.963	1.9
83	2	-3	2	2.00926	45.086	0.3
84	1	-2	-2	2.00235	45.250	2.0
85	2	1	1	1.99575	45.408	0.9
86	3	-2	1	1.99151	45.510	1.4
87	1	-3	3	1.97981	45.794	4.5
88	3	-1	1	1.97680	45.868	1.2
89	1	2	1	1.97480	45.917	1.0
90	1	1	2	1.96075	46.265	0.6
91	3	0	-3	1.95909	46.307	0.8
92	3	1	-3	1.95289	46.462	0.1
93	2	-1	-3	1.94077	46.770	1.8
94	2	2	0	1.92804	47.097	3.6
95	1	-1	-3	1.91879	47.338	0.1
96	1	2	-4	1.90880	47.601	0.0
97	1	-3	-1	1.90227	47.774	0.1
98	2	-3	-1	1.90182	47.786	10.0
99	2	0	2	1.88226	48.315	7.6
100	1	1	-4	1.87715	48.454	1.8
101	3	-3	0	1.86676	48.742	0.1
102	1	-4	2	1.85396	49.100	0.1
103	2	1	-4	1.84983	49.217	0.1
104	3	-2	-2	1.84820	49.263	11.4
105	2	3	-2	1.84600	49.326	0.1
106	0	4	-2	1.83992	49.500	6.9
107	1	-4	1	1.83623	49.606	0.5
108	0	2	-4	1.83292	49.702	4.2
109	3	-3	1	1.83131	49.748	0.2
110	3	1	0	1.82597	49.904	1.8
111	2	2	-4	1.82396	49.963	1.8
112	2	3	-3	1.82269	50.000	5.9
113	3	2	-2	1.82122	50.043	4.7
114	0	2	2	1.82050	50.064	10.4
115	1	3	0	1.82010	50.076	0.8
116	3	-1	-3	1.79982	50.680	1.1
117	3	0	1	1.79755	50.748	8.1
118	1	0	3	1.78763	51.050	0.4

119	3	2	-3	1.78550	51.115	0.0
120	1	3	-4	1.78192	51.225	0.3
121	4	-1	-1	1.77870	51.325	20.2
122	0	4	-3	1.77017	51.590	1.4
123	0	3	-4	1.76653	51.705	0.4
124	2	-4	1	1.76599	51.721	0.1
125	0	4	-1	1.76269	51.826	0.0
126	0	1	-4	1.75500	52.070	0.0
127	0	3	1	1.75265	52.145	1.1
128	2	-2	3	1.75243	52.152	0.7
129	3	-3	-1	1.75160	52.178	0.5
130	0	1	3	1.74861	52.274	2.5
131	4	0	-2	1.74467	52.401	2.9
132	4	-1	-2	1.73145	52.832	0.0
133	2	0	-4	1.73110	52.844	6.5
134	1	-4	3	1.72650	52.995	0.4
135	2	-4	2	1.72567	53.023	2.9
136	2	3	-1	1.72495	53.047	3.3
137	4	0	-1	1.72394	53.080	0.3
138	2	-3	3	1.71882	53.251	2.5
139	3	-2	2	1.71759	53.292	1.1
140	3	2	-1	1.71625	53.337	2.0
141	1	0	-4	1.70763	53.628	2.1
142	4	-2	-1	1.70130	53.843	0.0
143	4	-1	0	1.69326	54.120	0.7
144	1	4	-2	1.69230	54.153	0.2
145	3	1	-4	1.69029	54.223	1.4
146	1	4	-3	1.68524	54.398	0.5
147	1	-4	0	1.68451	54.424	1.8
148	4	-2	0	1.68368	54.453	2.8
149	2	-4	0	1.67678	54.696	2.2
150	2	3	-4	1.66957	54.952	1.8
151	3	-3	2	1.66764	55.021	0.3
152	2	-1	3	1.66073	55.269	4.2
153	3	-1	2	1.64806	55.731	0.5
154	1	-2	4	1.64359	55.896	0.0
155	4	0	-3	1.64228	55.944	0.5
156	4	1	-2	1.63670	56.152	0.8
157	3	0	-4	1.63564	56.191	0.1
158	1	-3	4	1.63236	56.314	0.6

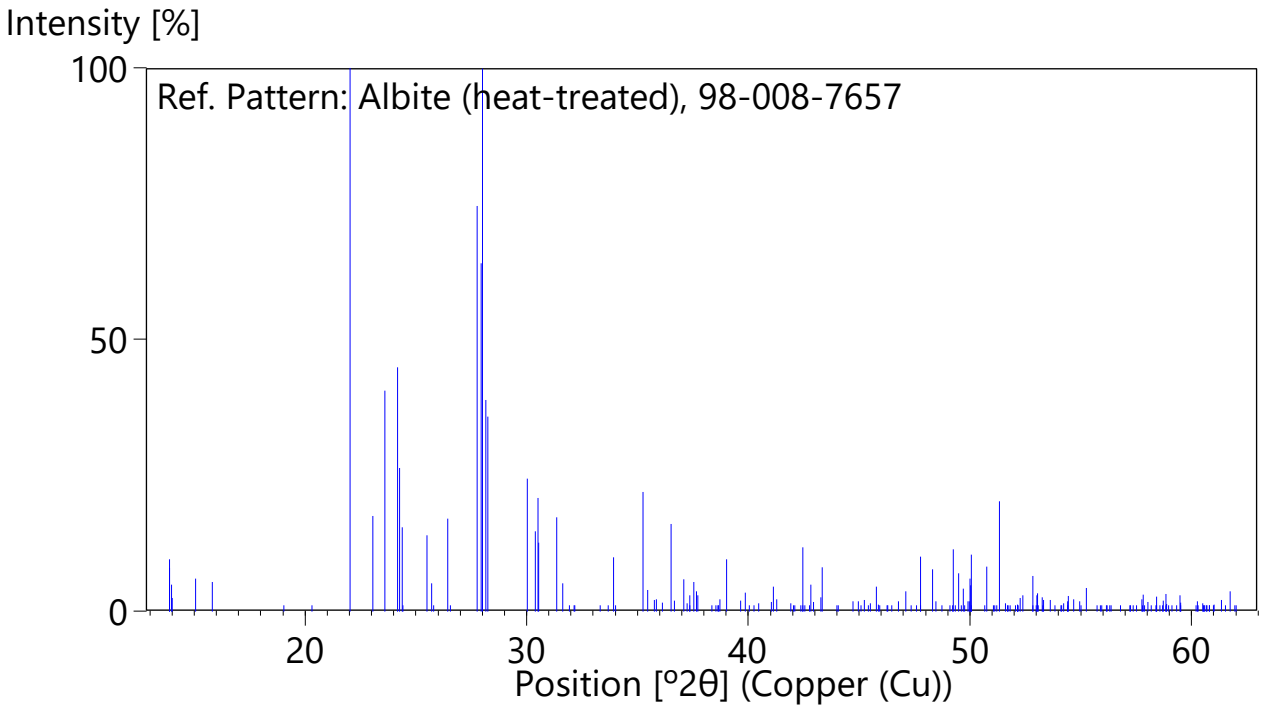
159	3	2	-4	1.63073	56.376	0.3
160	2	-2	-3	1.61978	56.791	0.1
161	2	-3	-2	1.60863	57.221	0.1
162	2	2	1	1.60834	57.232	0.1
163	4	-2	-2	1.60455	57.380	0.0
164	4	1	-3	1.60105	57.517	0.0
165	0	4	-4	1.59505	57.754	2.2
166	2	1	2	1.59436	57.782	0.0
167	3	-4	1	1.59307	57.833	3.0
168	4	0	0	1.59190	57.879	1.0
169	1	4	-1	1.58823	58.026	1.7
170	0	4	0	1.58414	58.190	0.5
171	2	-4	3	1.57886	58.403	0.0
172	4	-1	-3	1.57869	58.410	2.7
173	0	0	4	1.57818	58.431	0.1
174	1	2	2	1.57451	58.580	0.6
175	1	-2	-3	1.57146	58.705	0.7
176	1	4	-4	1.57091	58.727	1.9
177	4	-3	0	1.56834	58.833	0.1
178	4	1	-1	1.56809	58.843	3.2
179	1	-3	-2	1.56725	58.878	1.4
180	3	-4	0	1.56508	58.968	0.3
181	4	-2	1	1.56133	59.124	0.6
182	3	1	1	1.55629	59.334	1.1
183	1	-1	4	1.55252	59.492	2.9
184	3	3	-3	1.55239	59.498	0.0
185	3	-3	-2	1.55212	59.509	1.6
186	1	3	1	1.53562	60.215	0.2
187	4	-3	-1	1.53444	60.266	1.8
188	2	-1	-4	1.53398	60.285	0.5
189	3	2	0	1.52909	60.498	1.5
190	3	3	-2	1.52818	60.538	0.1
191	1	2	-5	1.52742	60.572	0.1
192	2	3	0	1.52693	60.593	0.3
193	3	-4	2	1.52499	60.678	0.5
194	1	-4	4	1.52461	60.695	0.0
195	4	-1	1	1.52204	60.809	0.8
196	1	1	3	1.52177	60.820	0.0
197	2	2	-5	1.51803	60.986	0.6
198	2	4	-3	1.51722	61.022	1.1

199	4	-3	1	1.51000	61.345	2.0
200	2	-4	-1	1.50605	61.524	0.3
201	1	3	-5	1.50130	61.739	3.6
202	1	-5	2	1.49649	61.960	0.0
203	3	0	2	1.49540	62.010	0.1

Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	O1	O	0.28030	0.09750	0.08850	1.0100	1.0000	2i
2	AL1	Al	0.21050	0.34080	0.67700	0.7800	0.7800	2i
3	SI1	Si	0.23480	0.68540	0.32240	0.7400	0.9200	2i
4	AL2	Al	0.23480	0.68540	0.32240	0.7400	0.0800	2i
5	SI2	Si	0.31720	0.08210	0.30210	0.7700	0.9400	2i
6	AL3	Al	0.31720	0.08210	0.30210	0.7700	0.0600	2i
7	SI3	Si	0.35850	0.30300	0.06440	0.7500	0.9200	2i
8	SI4	Si	0.21050	0.34080	0.67700	0.7800	0.2200	2i
9	O2	O	0.02720	0.62740	0.36120	1.3800	1.0000	2i
10	NA1	Na	0.85590	0.22330	0.23590	4.1100	1.0000	2i
11	O3	O	0.19330	0.20440	0.42620	1.4500	1.0000	2i
12	O4	O	0.25460	0.47050	0.17070	1.5600	1.0000	2i
13	O5	O	0.27200	0.21480	0.81320	1.2800	1.0000	2i
14	O6	O	0.22790	0.83170	0.21570	1.2400	1.0000	2i
15	O7	O	0.61180	0.40670	0.18630	1.2600	1.0000	2i
16	O8	O	0.56760	0.18400	0.44760	1.4200	1.0000	2i
17	AL4	Al	0.35850	0.30300	0.06440	0.7500	0.0800	2i

Stick Pattern



Name and formula

Reference code:	98-020-1648
Mineral name:	Anorthite, sodian
Compound name:	Anorthite, sodian
Common name:	Anorthite, sodian
Chemical formula:	$Al_{1.66}Ca_{0.66}Na_{0.34}O_8Si_{2.34}$

Crystallographic parameters

Crystal system:	Anorthic
Space group:	P -1
Space group number:	2
a (Å):	8.1750
b (Å):	8.7850
c (Å):	9.4430
Alpha (°):	89.7650
Beta (°):	83.8200
Gamma (°):	84.1130
Calculated density (g/cm^3):	2.70
Measured density (g/cm^3):	2.70
Volume of cell (10^6 pm^3):	670.66
Z:	8.00
RIR:	0.58

Subfiles and quality

Subfiles:	User Inorganic, User Mineral
Quality:	User From Structure (=)

Comments

Creation Date:	7/17/1985
Modification Date:	2/1/2015

Cross-References: ICSD:201648, ICDD:00-018-1202, PANICSD:98-020-1648
Original ICSD space group: I-1
Mean T-O: 1.640, 1.726, 1.703, 1.625, 1.695, 1.625, 1.626, 1.702, for average structure cf. 100237. X-ray diffraction from single crystal
Structure type: Feldspar.(TC,I1-,i28)-Bytownite. Temperature factors available
The structure has been assigned a PDF number (experimental powder diffraction data): 18-1202
The structure has been assigned a PDF number (calculated powder diffraction data): 01-086-1650
Compound with mineral name: Anorthite, sodian
Structure type: Feldspar.(TC,I1-,i28)-Bytownite
Recording date: 07/17/85
Modification date: 02/01/15
Additional name: Labradorite An66
Mineral origin: Plush, Lake Co., Oregon
ANX formula: AB2C2X8
Z: 8
Authors density: 2.7
Calculated density: 2.7
R value: 0.0293
Pearson code: aP52
Wyckoff code: i28
PDF code: 00-018-1202
Structure TIDY: Transformed from space group: "I1-" to space group: "P -1".
Structure TIDY: Applied Transformation matrix:
Structure TIDY: -1, 0, 0
Structure TIDY: 0.5, -0.5, 0.5
Structure TIDY: 0.5, 0.5, 0.5
Structure TIDY: TRANS -a,c,b origin 1/2 1/2 1/2
Publication title: Analysis of P1-, I1-, and C1- plagioclase structures
ICSD collection code: 201648
Structure: Feldspar.(TC,I1-,i28)-Bytownite
Chemical Name: Calcium Sodium Tecto-alumosilicate *
Second Chemical Formula: Ca0.66 Na0.34 (Al1.66 Si2.34 O8)

References

Structure: Kroll, H.;Wenk, H.R., *Bulletin de Mineralogie (101,1978-)*, **107**, 467 - 487, (1984)

Peak list

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	0	1	9.38789	9.413	0.5
2	0	1	0	8.73845	10.114	0.0
3	1	0	0	8.08450	10.935	0.0
4	1	0	1	6.48124	13.652	8.1
5	0	1	-1	6.41880	13.785	0.1
6	0	1	1	6.37403	13.882	0.2
7	1	1	0	6.26375	14.128	0.2
8	1	0	-1	5.82347	15.202	2.0
9	1	-1	0	5.65198	15.666	0.5
10	1	1	1	5.41018	16.371	0.0
11	1	1	-1	5.03129	17.613	0.9
12	1	-1	1	5.02274	17.644	0.3
13	0	0	2	4.69395	18.890	10.1
14	1	-1	-1	4.67973	18.948	0.0
15	0	2	0	4.36923	20.309	0.0
16	1	0	2	4.26383	20.816	0.4
17	0	1	-2	4.14728	21.408	0.6
18	0	1	2	4.12308	21.535	0.1
19	2	0	0	4.04225	21.971	75.0
20	1	2	0	4.02041	22.092	0.3
21	0	2	-1	3.97190	22.365	0.1
22	0	2	1	3.95063	22.487	0.8
23	1	1	2	3.90629	22.746	16.0
24	1	0	-2	3.88169	22.892	0.5
25	2	0	1	3.86722	22.979	0.0
26	2	1	0	3.82136	23.258	0.1
27	1	-1	2	3.76178	23.632	36.2
28	1	2	1	3.76049	23.640	25.0
29	1	-2	0	3.68857	24.108	0.5
30	2	1	1	3.66825	24.244	0.3
31	1	2	-1	3.63427	24.474	36.1
32	1	1	-2	3.62230	24.556	12.0
33	2	0	-1	3.57534	24.884	0.3
34	2	-1	0	3.53305	25.186	0.0
35	1	-2	1	3.49935	25.433	1.5
36	1	-1	-2	3.47705	25.599	14.0
37	2	1	-1	3.42320	26.009	5.6
38	2	-1	1	3.41780	26.050	0.8

39	1	-2	-1	3.37045	26.423	27.2
40	2	0	2	3.24062	27.502	54.2
41	0	2	-2	3.20940	27.775	59.9
42	2	-1	-1	3.20566	27.808	100.0
43	0	2	2	3.18702	27.974	95.4
44	2	2	0	3.13187	28.477	42.4
45	0	0	3	3.12930	28.500	0.1
46	1	2	2	3.12720	28.520	0.0
47	2	1	2	3.11823	28.604	0.1
48	2	2	1	3.04349	29.322	0.0
49	1	0	3	3.03035	29.452	21.9
50	1	2	-2	2.98474	29.912	0.0
51	1	-2	2	2.98116	29.949	0.1
52	2	-1	2	2.96443	30.122	0.1
53	0	1	-3	2.95267	30.245	28.7
54	0	1	3	2.93955	30.383	19.0
55	0	3	0	2.91282	30.669	0.0
56	2	0	-2	2.91174	30.680	9.9
57	2	2	-1	2.90329	30.772	0.2
58	1	1	3	2.89160	30.899	0.0
59	1	-1	3	2.83538	31.528	0.0
60	1	3	0	2.83481	31.534	24.1
61	2	1	-2	2.82971	31.593	0.0
62	2	-2	0	2.82599	31.635	0.4
63	1	0	-3	2.81784	31.729	8.9
64	0	3	-1	2.78753	32.084	0.2
65	0	3	1	2.77647	32.215	0.1
66	2	-2	1	2.76777	32.319	0.1
67	1	3	1	2.73735	32.688	0.0
68	1	1	-3	2.71547	32.959	0.0
69	2	2	2	2.70509	33.089	0.2
70	2	-1	-2	2.69971	33.157	0.3
71	3	0	0	2.69483	33.218	0.0
72	1	3	-1	2.69082	33.269	0.0
73	3	0	1	2.66761	33.567	0.8
74	1	-3	0	2.65479	33.734	14.8
75	3	1	0	2.65305	33.757	0.4
76	1	-1	-3	2.64945	33.804	0.2
77	2	-2	-1	2.64827	33.820	0.0
78	3	1	1	2.62552	34.122	0.0

79	2	0	3	2.61466	34.268	0.0
80	1	-3	1	2.58303	34.701	0.1
81	0	2	-3	2.55259	35.128	0.1
82	2	1	3	2.54768	35.198	3.8
83	0	2	3	2.53568	35.370	0.1
84	1	2	3	2.52788	35.483	5.7
85	1	-3	-1	2.52710	35.494	0.0
86	3	0	-1	2.51921	35.609	4.5
87	2	2	-2	2.51565	35.661	31.8
88	2	-2	2	2.51137	35.724	20.5
89	3	-1	0	2.50375	35.836	1.7
90	2	3	0	2.48749	36.079	0.0
91	3	1	-1	2.48629	36.097	0.0
92	3	-1	1	2.48319	36.143	0.0
93	0	3	-2	2.48282	36.149	0.0
94	0	3	2	2.46726	36.385	0.1
95	2	-1	3	2.46427	36.430	2.1
96	1	3	2	2.46057	36.487	0.5
97	1	-2	3	2.45389	36.590	0.5
98	2	3	1	2.44126	36.786	3.6
99	3	1	2	2.41998	37.121	4.2
100	1	2	-3	2.41486	37.203	4.1
101	3	2	0	2.40677	37.332	0.1
102	1	3	-2	2.39403	37.539	0.6
103	3	2	1	2.38500	37.686	3.5
104	2	3	-1	2.36937	37.944	3.5
105	3	-1	-1	2.35990	38.102	0.0
106	2	0	-3	2.35464	38.191	0.0
107	1	-3	2	2.35334	38.213	3.3
108	0	0	4	2.34697	38.320	0.0
109	2	-2	-2	2.33987	38.441	0.0
110	1	-2	-3	2.32390	38.716	0.9
111	1	0	4	2.32193	38.750	0.0
112	2	1	-3	2.31168	38.929	0.4
113	3	-1	2	2.30928	38.971	6.2
114	2	2	3	2.30601	39.028	0.1
115	3	2	-1	2.28122	39.470	5.8
116	1	-3	-2	2.27050	39.664	3.8
117	0	1	4	2.26267	39.807	0.1
118	1	1	4	2.25673	39.916	1.5

119	2	-3	0	2.25583	39.933	0.0
120	2	3	2	2.25496	39.949	0.0
121	2	-1	-3	2.23725	40.279	0.0
122	3	0	-2	2.23533	40.315	0.0
123	1	-1	4	2.23160	40.385	4.0
124	2	-3	1	2.22683	40.476	2.6
125	3	1	-2	2.21317	40.737	0.7
126	3	-2	0	2.19511	41.087	0.1
127	1	0	-4	2.19155	41.156	0.1
128	2	-2	3	2.18601	41.265	0.1
129	0	4	0	2.18461	41.293	1.8
130	3	-2	1	2.18210	41.343	0.7
131	1	4	0	2.16574	41.670	0.0
132	2	-3	-1	2.16143	41.757	2.6
133	3	0	3	2.16041	41.777	1.8
134	2	3	-2	2.14503	42.091	0.1
135	1	1	-4	2.14318	42.129	1.3
136	0	3	-3	2.13960	42.203	9.0
137	3	1	3	2.13620	42.273	0.0
138	1	3	3	2.13407	42.317	0.0
139	2	0	4	2.13191	42.362	13.4
140	2	2	-3	2.13158	42.369	0.1
141	0	4	-1	2.13107	42.380	0.0
142	0	3	3	2.12468	42.514	0.4
143	3	-1	-2	2.12098	42.591	0.0
144	1	4	1	2.12052	42.601	0.4
145	1	-1	-4	2.10867	42.852	0.0
146	1	4	-1	2.10025	43.032	9.6
147	3	-2	-1	2.09545	43.136	1.6
148	2	1	4	2.09435	43.160	0.1
149	3	3	0	2.08792	43.300	1.2
150	2	-3	2	2.08738	43.311	0.0
151	0	2	-4	2.07364	43.613	0.1
152	3	3	1	2.07289	43.629	0.0
153	1	2	4	2.06982	43.697	0.1
154	1	3	-3	2.06928	43.709	0.0
155	1	-3	3	2.06750	43.749	0.0
156	3	2	-2	2.06556	43.792	0.0
157	3	-2	2	2.06201	43.872	0.0
158	0	2	4	2.06154	43.882	0.1

159	3	-1	3	2.06039	43.908	0.0
160	1	-4	0	2.05644	43.996	0.0
161	2	-1	4	2.04874	44.171	0.1
162	1	-2	4	2.03148	44.566	0.1
163	1	-4	1	2.02325	44.757	1.3
164	4	0	0	2.02112	44.807	2.8
165	2	-2	-3	2.01863	44.865	0.2
166	4	1	0	2.01511	44.948	0.0
167	4	1	1	2.01448	44.963	3.4
168	2	4	0	2.01021	45.063	0.4
169	2	3	3	2.00713	45.136	0.8
170	3	3	-1	2.00504	45.186	0.0
171	3	2	3	1.99914	45.327	1.8
172	1	-4	-1	1.99468	45.434	2.5
173	1	2	-4	1.98651	45.631	0.0
174	0	4	-2	1.98595	45.645	4.4
175	2	4	1	1.98490	45.670	0.0
176	1	-3	-3	1.98393	45.694	0.0
177	2	-3	-2	1.98307	45.715	0.0
178	0	4	2	1.97532	45.904	0.8
179	3	3	2	1.96586	46.138	1.9
180	2	2	4	1.95315	46.456	2.7
181	1	4	-2	1.95032	46.527	0.1
182	2	4	-1	1.94694	46.612	0.0
183	3	0	-3	1.94116	46.760	1.4
184	2	0	-4	1.94085	46.768	0.9
185	4	0	2	1.93361	46.953	0.1
186	1	-2	-4	1.93248	46.982	0.2
187	4	1	-1	1.92878	47.078	3.8
188	3	1	-3	1.92720	47.119	0.1
189	4	-1	1	1.92685	47.128	10.5
190	4	-1	0	1.92618	47.145	0.1
191	3	-2	-2	1.92220	47.249	0.0
192	2	1	-4	1.91718	47.380	0.0
193	4	2	0	1.91068	47.551	1.2
194	4	2	1	1.90955	47.581	0.1
195	1	-4	2	1.90762	47.632	0.0
196	2	3	-3	1.89240	48.039	1.0
197	2	-3	3	1.88967	48.113	0.1
198	3	-3	0	1.88399	48.267	0.0

199	2	-2	4	1.88089	48.352	5.0
200	2	4	2	1.88025	48.369	7.5
201	3	-2	3	1.87959	48.388	1.3
202	0	0	5	1.87758	48.443	0.0
203	3	-3	1	1.87631	48.477	0.0

Structure

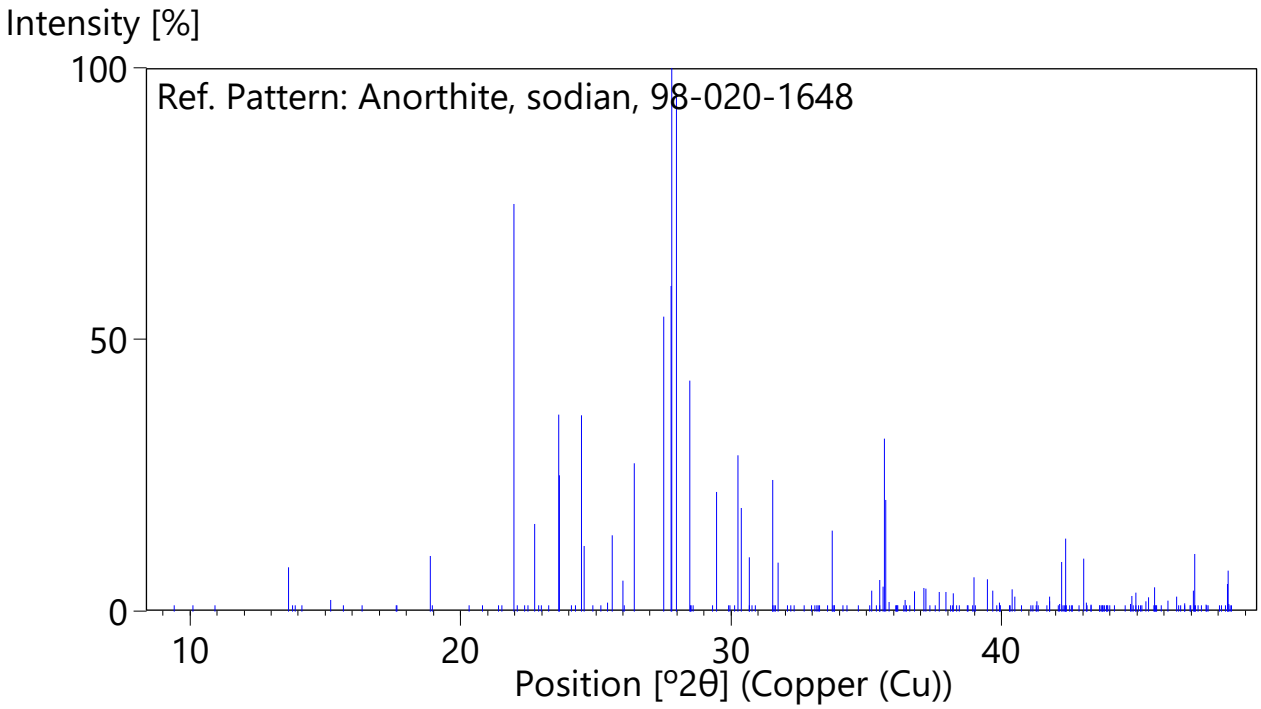
No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	NA1	Na	0.22220	0.07440	0.02040	0.5000	0.2100	2i
2	SI1	Si	0.52218	0.26548	0.05196	0.5000	1.0000	2i
3	SI2	Si	0.02933	0.76933	0.54749	0.5000	0.3000	2i
4	AL1	Al	0.02933	0.76933	0.54749	0.5000	0.7000	2i
5	SI3	Si	0.10871	0.06942	0.70378	0.5000	1.0000	2i
6	SI4	Si	0.61712	0.56652	0.19782	0.5000	0.2000	2i
7	AL2	Al	0.61712	0.56652	0.19782	0.5000	0.8000	2i
8	CA1	Ca	0.31800	0.43190	0.39810	0.5000	0.3200	2i
9	SI5	Si	0.59749	0.23410	0.55568	0.5000	1.0000	2i
10	SI6	Si	0.50607	0.05374	0.30074	0.5000	0.2000	2i
11	CA2	Ca	0.22220	0.07440	0.02040	0.5000	0.4200	2i
12	NA2	Na	0.18690	0.07130	0.08310	0.5000	0.1200	2i
13	CA3	Ca	0.18690	0.07130	0.08310	0.5000	0.2500	2i
14	NA3	Na	0.27221	0.42019	0.48627	0.5000	0.1600	2i
15	CA4	Ca	0.27221	0.42019	0.48627	0.5000	0.3100	2i
16	NA4	Na	0.31800	0.43190	0.39810	0.5000	0.1700	2i
17	AL3	Al	0.10590	0.72535	0.05485	0.5000	1.0000	2i
18	O1	O	0.18470	0.48010	0.77230	0.5000	1.0000	2i
19	O2	O	0.52270	0.41450	0.14990	0.5000	1.0000	2i
20	O3	O	0.00940	0.29730	0.08690	0.5000	1.0000	2i
21	O4	O	0.49600	0.20280	0.41820	0.5000	1.0000	2i
22	O5	O	0.09140	0.20650	0.58750	0.5000	1.0000	2i
23	O6	O	0.59730	0.70870	0.07390	0.5000	1.0000	2i
24	O7	O	0.13080	0.56010	0.14850	0.5000	1.0000	2i
25	SI7	Si	0.00188	0.43878	0.20044	0.5000	1.0000	2i
26	O8	O	0.29810	0.02860	0.73680	0.5000	1.0000	2i
27	AL4	Al	0.50607	0.05374	0.30074	0.5000	0.8000	2i
28	O9	O	0.28980	0.80180	0.00840	0.5000	1.0000	2i
29	O10	O	0.22620	0.69590	0.48970	0.5000	1.0000	2i
30	O11	O	0.43919	0.12990	0.14644	0.5000	1.0000	2i
31	O12	O	0.05983	0.36938	0.35134	0.5000	1.0000	2i
32	O13	O	0.00940	0.11660	0.86080	0.5000	1.0000	2i
33	O14	O	0.51610	0.61940	0.36260	0.5000	1.0000	2i
34	O15	O	0.97310	0.07660	0.34940	0.5000	1.0000	2i
35	O16	O	0.62430	0.07860	0.64680	0.5000	1.0000	2i

Anisotropic Displacement Parameters [10^4 pm^2]

Atom Name	B11	B22	B33	B12	B13	B23

NA1	0.7040(3)	1.602(6)	1.001(6)	0.373(3)	0.165(3)	-0.399(4)
SI1	0.8095(2)	0.745(2)	0.962(2)	0.000(2)	0.303(2)	-0.046(1)
SI2	0.5770(2)	0.600(2)	0.696(2)	0.026(2)	0.187(2)	0.059(1)
AL1	0.5770(2)	0.600(2)	0.696(2)	0.026(2)	0.187(2)	0.059(1)
SI3	0.9106(2)	1.022(2)	0.605(2)	0.301(2)	0.333(2)	0.085(1)
SI4	0.7320(3)	0.877(2)	0.429(2)	0.226(4)	0.224(7)	-0.007(2)
AL2	0.7320(3)	0.877(2)	0.429(2)	0.226(4)	0.224(7)	-0.007(2)
CA1	1.0678(5)	4.858(1)	2.1385(8)	0.0000(5)	0.7743(5)	-2.0685(9)
SI5	0.8697(2)	1.022(2)	0.689(2)	0.000(2)	0.344(2)	-0.013(2)
SI6	0.5920(2)	0.633(2)	0.683(2)	0.026(2)	0.239(2)	0.065(2)
CA2	0.7040(3)	1.602(6)	1.001(6)	0.373(3)	0.165(3)	-0.399(4)
NA2	0.969(6)	0.73(3)	2.34(2)	0.00(1)	0.673(7)	-2.62(2)
CA3	0.969(6)	0.73(3)	2.34(2)	0.00(1)	0.673(7)	-2.62(2)
NA3	0.7815(5)	1.7996(7)	1.2480(7)	0.3202(4)	0.2020(4)	-0.452(5)
CA4	0.7815(5)	1.7996(7)	1.2480(7)	0.3202(4)	0.2020(4)	-0.452(5)
NA4	1.0678(5)	4.858(1)	2.1385(8)	0.0000(5)	0.7743(5)	-2.0685(9)
AL3	0.7556(2)	0.811(2)	0.566(2)	0.000(2)	0.284(2)	0.072(2)
O1	1.92(2)	1.7930(7)	3.2761(8)	0.1168(5)	1.6908(7)	-0.262(7)
O2	1.572(6)	1.628(6)	1.476(6)	0.1092(5)	-0.1721(5)	-0.353(5)
O3	1.442(6)	1.444(6)	1.131(6)	0.0979(5)	0.0337(5)	0.124(5)
O4	1.464(6)	1.470(5)	1.086(5)	0.1507(5)	0.0561(5)	0.177(5)
O5	1.593(6)	1.470(5)	1.268(6)	0.4671(5)	0.3142(5)	-0.046(4)
O6	1.163(6)	1.542(6)	1.242(6)	0.3918(5)	0.2432(5)	-0.1636(9)
O7	1.313(6)	1.325(5)	1.606(6)	0.0000(5)	0.5574(5)	-0.026(5)
SI7	0.7858(2)	0.745(2)	0.930(2)	0.094(2)	0.303(2)	0.157(1)
O8	1.507(6)	1.9644(7)	2.9965(8)	0.264(4)	1.347(7)	-0.262(7)
AL4	0.5920(2)	0.633(2)	0.683(2)	0.026(2)	0.239(2)	0.065(2)
O9	1.636(6)	1.305(5)	2.1645(7)	0.0000(5)	1.1971(6)	-0.157(5)
O10	1.442(6)	1.365(6)	2.0345(7)	0.0000(5)	0.9651(6)	-0.144(5)
O11	1.055(6)	0.995(5)	1.242(6)	0.0000(4)	0.3292(5)	0.065(7)
O12	1.012(6)	0.949(5)	1.099(6)	0.1733(4)	0.3142(5)	0.308(4)
O13	2.433(9)	1.938(6)	0.962(6)	0.4520(5)	1.0624(6)	0.432(5)
O14	2.174(6)	1.846(7)	0.956(6)	0.1243(5)	0.8978(5)	0.111(5)
O15	1.593(6)	2.0566(7)	1.5925(7)	0.2034(5)	-0.2207(6)	-0.308(5)
O16	1.507(6)	1.523(6)	1.573(6)	0.0000(5)	0.7669(5)	0.059(5)

Stick Pattern



Name and formula

Reference code:	98-015-2289
Mineral name:	Birnessite
Compound name:	Birnessite
Common name:	Birnessite
Chemical formula:	$H_{0.8}K_{0.296}Mn_{0.926}O_{2.4}$

Crystallographic parameters

Crystal system:	Hexagonal
Space group:	R -3 m
Space group number:	166
a (Å):	2.8450
b (Å):	2.8450
c (Å):	21.1200
Alpha (°):	90.0000
Beta (°):	90.0000
Gamma (°):	120.0000
Calculated density (g/cm^3):	3.42
Volume of cell (10^6 pm^3):	148.04
Z:	3.00
RIR:	10.54

Subfiles and quality

Subfiles:	User Inorganic, User Mineral
Quality:	User From Structure (=)

Comments

Creation Date:	01-10-2006
Modification Date:	01-02-2008
Cross-References:	ICSD:152289, PANICSD:98-015-2289

Original ICSD space group: R-3MH. Coordinates are given in an orthorhombic cell with cell constants a'=asqrt(3),b'=b,c'=c;the transformation to R3-mh coordinates is given by x=2x',y=x'+y', where x',y' are the coordinates given in Tab.3 in the orthorhombic cell. X-ray diffraction (powder)
Structure type: KxMn1-yO2(H2O)z. Temperature factors available
Temperature in Kelvin: 373. Standard deviation missing in cell constants. Rietveld profile refinement applied. Polytype structure 3R-
Compound with mineral name: Birnessite
Structure type: KxMn1-yO2(H2O)z
Recording date: 10/01/06
Modification date: 02/01/08
Mineral origin: synthetic
ANX formula: AB3X7
Z: 3
Calculated density: 3.42
R value: 0.1224
Pearson code: hR4
Wyckoff code: h2 c a
Publication title: Structure of birnessite obtained from decomposition of permanganate under soft hydrothermal conditions. I. Chemical and structural evolution as a function of temperature
ICSD collection code: 152289
Structure: KxMn1-yO2(H2O)z
Chemical Name: Potassium Manganese Oxide Hydrate (0.3/0.93/2/0.4)
Second Chemical Formula: K0.296 Mn0.926 O2 (H2 O)0.40

References

Structure: Drits, V.A.;Lanson, B.;Gaillot, A.C., *Chemistry of Materials*, **17**, 2959 - 2975, (2005)

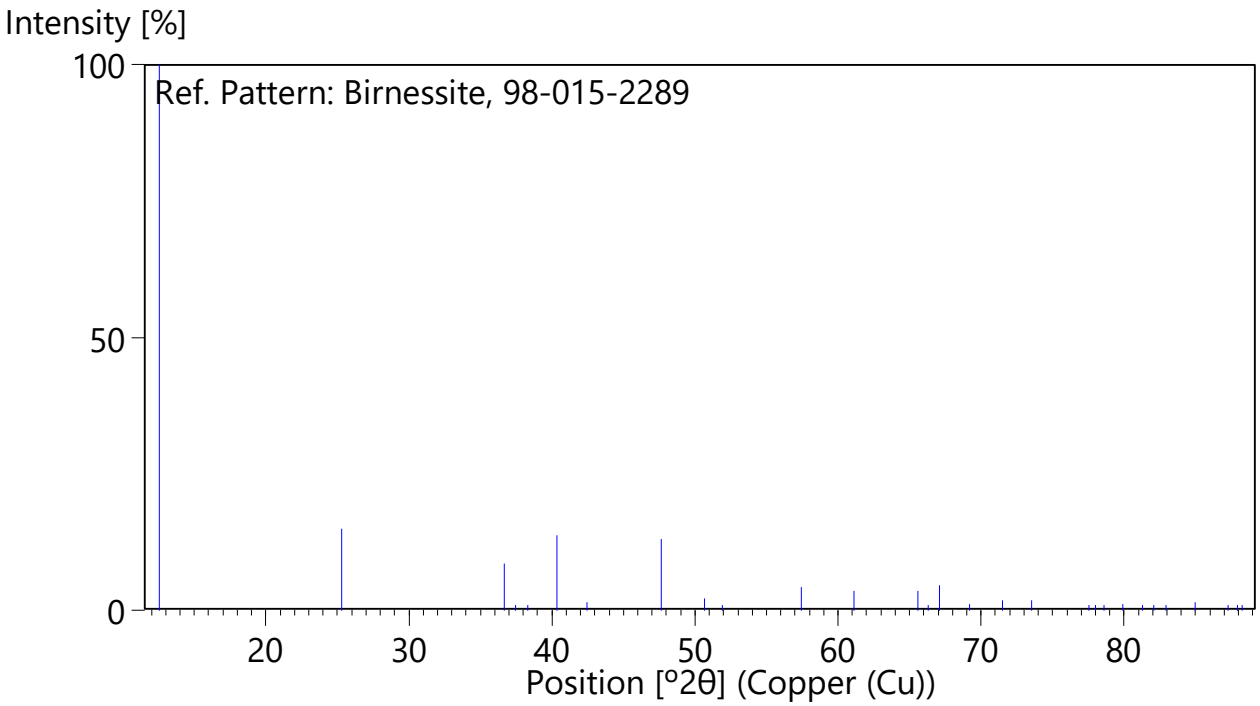
Peak list

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	0	3	7.04000	12.563	100.0
2	0	0	6	3.52000	25.281	15.0
3	1	0	1	2.44725	36.693	8.6
4	0	1	2	2.39940	37.451	1.1
5	0	0	9	2.34667	38.325	0.3
6	1	0	4	2.23272	40.364	13.8
7	0	1	5	2.12825	42.439	1.5
8	1	0	7	1.90837	47.612	13.1
9	0	1	8	1.80126	50.636	2.2
10	0	0	12	1.76000	51.911	0.6
11	1	0	10	1.60351	57.421	4.3
12	0	1	11	1.51446	61.145	3.6
13	1	1	0	1.42250	65.573	3.7
14	0	0	15	1.40800	66.335	0.2
15	1	1	3	1.39432	67.071	4.7
16	1	0	13	1.35630	69.213	1.3
17	1	1	6	1.31888	71.473	2.0
18	0	1	14	1.28656	73.557	2.0
19	0	2	1	1.22983	77.562	0.9
20	2	0	2	1.22362	78.030	0.3
21	1	1	9	1.21645	78.578	0.5
22	0	2	4	1.19970	79.894	1.3
23	2	0	5	1.18265	81.284	0.4
24	0	0	18	1.17333	82.068	0.5
25	1	0	16	1.16354	82.910	0.2
26	0	2	7	1.14051	84.970	1.6
27	2	0	8	1.11636	87.262	0.5
28	0	1	17	1.10931	87.958	1.1
29	1	1	12	1.10633	88.257	0.5

Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	O1	O	0.55000	0.45000	0.01670	2.0000	0.0670	18h
2	K1	K	0.57333	0.42667	0.16667	2.0000	0.0493	18h
3	O2	O	0.00000	0.00000	0.28603	1.0000	1.0000	6c
4	MN1	Mn	0.00000	0.00000	0.00000	0.5000	0.9250	3a

Stick Pattern



Name and formula

Reference code:	98-018-7569
Mineral name:	Muscovite 2M1
Compound name:	Muscovite 2M1
Common name:	Muscovite 2M1
Chemical formula:	$H_8Al_{12}K_4O_{48}Si_{12}$

Crystallographic parameters

Crystal system:	Anorthic
Space group:	P 1
Space group number:	1
a (Å):	5.1870
b (Å):	9.0070
c (Å):	20.1480
Alpha (°):	90.0000
Beta (°):	95.4370
Gamma (°):	90.0000
Calculated density (g/cm^3):	2.82
Volume of cell (10^6 pm^3):	937.07
Z:	1.00
RIR:	0.32

Subfiles and quality

Subfiles:	User Inorganic, User Mineral
Quality:	User From Structure (=)

Comments

Creation Date:	01-08-2013
Cross-References:	ICSD:187569, PANICSD:98-018-7569
Original ICSD space group:	P1. DFT calculation using optimized PP and PBE-GGA with SIESTA code.

At least one temperature factor missing in the paper.. No R value given in the paper.
Structure type: Mica_(2M1)-P1. Structure calculated theoretically
Structure type prototype: Mica_(2M1)-P1. Standard deviation missing in cell constants
Compound with mineral name: Muscovite 2M1
Structure type: Mica_(2M1)-P1
Recording date: 08/01/13
ANX formula: AB3C3X12
Z: 1
Calculated density: 2.82
Pearson code: aP84
Wyckoff code: a76
Structure TIDY: TRANS -x,-y,-z origin .72972 .39286 .32871
Publication title: Computational study of the elastic behavior of the 2M1 muscovite-paragonite series
ICSD collection code: 187569
Structure: Mica_(2M1)-P1
Chemical Name: Potassium Aluminosilicate Hydroxide (4/12/8)
Second Chemical Formula: K4 (Al12 Si12 O40 (O H)8)

References

Structure: Hernandez-Laguna, A.;Sainz-Diaz, C.I.;Munoz-Santiburcio, D.;Perez Del Valle, C.;Ortega-Castro, J.;Hernandez-Haro, N., *American Mineralogist*, **98**, 651 - 664, (2013)

Peak list

No.	h	k	l	d [Å]	2θ [°]	I [%]
1	0	0	1	20.05735	4.402	0.0
2	0	0	2	10.02868	8.810	100.0
3	0	1	0	9.00700	9.812	0.1
4	0	1	1	8.21656	10.759	1.2
5	0	1	-2	6.70110	13.202	0.0
6	0	0	3	6.68579	13.232	0.0
7	0	1	3	5.36844	16.499	0.4
8	1	0	0	5.16366	17.158	0.5
9	1	0	-1	5.11909	17.309	0.0
10	0	0	4	5.01434	17.673	33.3
11	1	0	1	4.88999	18.127	0.0
12	1	0	-2	4.77884	18.552	0.1
13	0	2	0	4.50350	19.697	9.2
14	1	1	0	4.47971	19.803	21.6
15	1	-1	-1	4.45051	19.934	42.1
16	1	0	2	4.42344	20.057	0.0
17	0	2	-1	4.39410	20.193	4.7
18	0	1	4	4.38116	20.253	0.0
19	1	1	1	4.29749	20.651	17.2
20	1	0	-3	4.28798	20.698	0.0
21	1	-1	-2	4.22146	21.028	0.1
22	0	2	-2	4.10828	21.614	10.2
23	0	0	5	4.01147	22.142	0.0
24	1	-1	2	3.97046	22.373	4.4
25	1	0	3	3.91135	22.716	0.0
26	1	-1	-3	3.87163	22.952	40.0
27	1	0	-4	3.78080	23.511	0.3
28	0	2	-3	3.73515	23.803	39.0
29	0	1	5	3.66447	24.269	0.1
30	1	1	3	3.58767	24.797	1.8
31	1	-1	-4	3.48612	25.531	57.5
32	1	0	4	3.43817	25.893	0.5
33	1	-2	0	3.39402	26.236	0.1
34	1	-2	-1	3.38126	26.337	0.1
35	0	2	-4	3.35055	26.583	32.5
36	0	0	6	3.34289	26.645	87.8
37	1	0	-5	3.32413	26.798	0.0
38	1	-2	1	3.31268	26.892	0.0

39	1	-2	-2	3.27747	27.187	0.9
40	1	1	4	3.21211	27.751	55.9
41	1	2	2	3.15577	28.256	0.4
42	0	1	6	3.13400	28.457	0.1
43	1	1	-5	3.11853	28.601	3.4
44	1	-2	-3	3.10546	28.724	0.1
45	1	0	5	3.03175	29.438	0.0
46	0	3	0	3.00233	29.733	0.0
47	0	2	-5	2.99545	29.803	60.4
48	0	3	-1	2.96925	30.072	0.2
49	1	2	3	2.95306	30.241	0.2
50	1	0	-6	2.93595	30.421	0.1
51	1	-2	-4	2.89565	30.855	0.0
52	0	3	2	2.87621	31.069	0.0
53	1	-1	5	2.87334	31.101	36.1
54	0	0	7	2.86534	31.190	0.0
55	1	-1	-6	2.79139	32.038	29.2
56	0	3	3	2.73885	32.670	0.0
57	1	-2	4	2.73280	32.744	0.7
58	0	1	-7	2.73050	32.772	0.0
59	1	0	6	2.69221	33.252	0.3
60	0	2	-6	2.68422	33.354	0.2
61	1	-2	-5	2.67448	33.479	0.0
62	1	0	-7	2.61268	34.295	0.0
63	1	3	0	2.59549	34.529	3.9
64	2	0	-1	2.59199	34.577	0.0
65	1	3	-1	2.58978	34.608	22.6
66	2	0	0	2.58183	34.717	31.8
67	1	1	6	2.57945	34.751	10.3
68	0	3	4	2.57590	34.800	0.0
69	2	0	-2	2.55954	35.030	77.0
70	1	-3	1	2.55857	35.043	69.3
71	1	3	-2	2.54225	35.276	0.2
72	2	0	1	2.53052	35.445	0.0
73	1	2	5	2.51496	35.671	0.0
74	1	1	-7	2.50924	35.755	6.0
75	0	0	8	2.50717	35.786	9.7
76	2	1	-1	2.49090	36.027	0.0
77	2	0	-3	2.48905	36.055	0.0
78	1	3	2	2.48417	36.128	0.5

79	2	-1	0	2.48188	36.163	0.0
80	2	1	-2	2.46206	36.464	0.0
81	1	-3	-3	2.45941	36.505	24.1
82	2	0	2	2.44499	36.728	20.4
83	2	-1	1	2.43620	36.865	0.1
84	0	2	7	2.41750	37.161	3.0
85	0	1	8	2.41534	37.195	0.0
86	1	0	7	2.41042	37.274	0.0
87	0	3	5	2.40367	37.382	0.0
88	2	-1	-3	2.39912	37.456	0.1
89	2	0	-4	2.38942	37.614	16.3
90	1	-3	3	2.38160	37.742	18.1
91	2	-1	2	2.35960	38.107	0.0
92	1	3	-4	2.35118	38.249	0.3
93	1	0	-8	2.34434	38.365	0.1
94	2	0	3	2.33528	38.520	0.0
95	1	-1	7	2.32848	38.637	0.2
96	1	-2	6	2.31079	38.944	0.0
97	2	1	-4	2.30953	38.966	0.0
98	2	0	-5	2.27118	39.652	0.0
99	1	1	-8	2.26875	39.696	0.4
100	1	-3	4	2.26146	39.829	0.0
101	2	1	3	2.26053	39.846	0.0
102	1	2	-7	2.25991	39.858	0.0
103	0	4	0	2.25175	40.008	1.2
104	2	2	-1	2.24648	40.106	6.1
105	2	-2	0	2.23986	40.230	2.2
106	0	4	-1	2.23769	40.271	2.0
107	0	3	6	2.23370	40.346	0.1
108	0	0	9	2.22860	40.442	0.0
109	1	3	-5	2.22808	40.452	4.9
110	2	-2	-2	2.22526	40.505	0.1
111	2	0	4	2.21172	40.764	5.5
112	2	2	1	2.20611	40.873	6.1
113	2	1	-5	2.20224	40.948	0.0
114	0	4	2	2.19705	41.049	4.8
115	0	2	-8	2.19058	41.175	0.0
116	2	2	-3	2.17846	41.415	8.0
117	1	0	8	2.17582	41.468	0.0
118	0	1	9	2.16336	41.718	0.0

119	2	-2	2	2.14874	42.015	2.4
120	2	-1	4	2.14791	42.032	0.1
121	2	0	-6	2.14399	42.112	34.3
122	0	4	-3	2.13397	42.320	3.5
123	1	-3	5	2.13329	42.334	32.9
124	1	-2	7	2.12516	42.503	0.0
125	1	0	-9	2.12056	42.600	0.0
126	1	-1	8	2.11499	42.718	0.0
127	2	-2	-4	2.11073	42.808	0.0
128	1	3	-6	2.09911	43.057	0.6
129	2	-1	-6	2.08571	43.348	0.0
130	2	0	5	2.08307	43.405	0.0
131	1	-2	-8	2.07946	43.485	0.0
132	2	-2	3	2.07313	43.624	6.0
133	0	3	-7	2.07284	43.631	0.0
134	1	-1	-9	2.06413	43.824	0.5
135	1	-4	-1	2.06116	43.891	0.1
136	0	4	4	2.05414	44.048	9.3
137	1	-4	1	2.04532	44.248	0.1
138	1	-4	-2	2.03695	44.440	0.0
139	2	1	5	2.02950	44.612	0.7
140	2	2	-5	2.02789	44.649	3.2
141	2	0	-7	2.01536	44.942	0.0
142	1	4	2	2.00671	45.146	0.1
143	0	0	10	2.00574	45.169	51.4
144	1	3	6	2.00438	45.201	0.1
145	0	2	-9	1.99741	45.368	0.4
146	1	4	-3	1.99359	45.460	0.2
147	2	2	4	1.98523	45.662	0.6
148	1	0	9	1.97907	45.812	0.0
149	1	-3	-7	1.97091	46.013	18.7
150	2	1	-7	1.96673	46.116	0.0
151	0	4	5	1.96355	46.195	0.4
152	2	-3	-1	1.96198	46.234	0.0
153	1	-2	8	1.95915	46.305	0.0
154	0	1	10	1.95778	46.339	0.0
155	2	3	0	1.95756	46.345	0.2
156	2	0	6	1.95567	46.392	15.2
157	1	-4	3	1.95147	46.498	0.1
158	2	3	-2	1.94779	46.591	0.4

159	2	-2	-6	1.93581	46.896	2.1
160	2	-3	1	1.93491	46.920	0.0
161	1	4	-4	1.93463	46.927	0.0
162	1	1	9	1.93296	46.970	0.2
163	1	0	-10	1.93246	46.983	0.0
164	0	3	-8	1.92441	47.191	0.0
165	1	2	-9	1.91852	47.345	0.0
166	2	-3	-3	1.91618	47.406	0.0
167	2	-1	6	1.91114	47.539	0.0
168	2	-3	2	1.89586	47.946	0.0
169	2	-2	5	1.89062	48.087	0.2
170	2	0	-8	1.89040	48.093	2.8
171	1	-1	-10	1.88946	48.119	0.3
172	1	4	4	1.88371	48.275	0.0
173	1	3	7	1.87961	48.387	1.6
174	2	-3	-4	1.86960	48.663	0.0
175	0	4	6	1.86758	48.719	1.1
176	1	4	-5	1.86429	48.810	0.0
177	2	-1	-8	1.85009	49.210	0.0
178	1	3	-8	1.84776	49.276	1.6
179	2	-3	3	1.84332	49.403	0.0
180	2	2	-7	1.83956	49.510	0.1
181	2	0	7	1.83360	49.682	0.0
182	0	2	-10	1.83223	49.722	0.8
183	0	0	11	1.82340	49.979	0.0
184	1	0	10	1.81258	50.298	0.1
185	1	2	9	1.81184	50.320	0.0
186	2	-3	-5	1.81130	50.336	0.0
187	1	-4	5	1.80769	50.443	0.0
188	0	5	0	1.80140	50.632	0.0
189	2	1	7	1.79675	50.773	0.0
190	0	5	1	1.79418	50.850	0.2
191	2	-2	6	1.79384	50.861	0.4
192	0	3	9	1.78948	50.994	0.0
193	0	1	11	1.78714	51.065	0.0
194	1	4	-6	1.78675	51.077	0.0
195	2	-3	4	1.78071	51.263	0.1
196	1	-1	10	1.77695	51.379	0.0
197	1	-2	-10	1.77587	51.413	0.0
198	0	5	2	1.77302	51.501	0.0

199	2	0	-9	1.77213	51.529	0.0
200	0	4	-7	1.77047	51.581	0.7
201	1	-3	8	1.76181	51.853	0.4
202	2	-3	-6	1.74478	52.398	0.1
203	2	-2	-8	1.74306	52.453	2.2

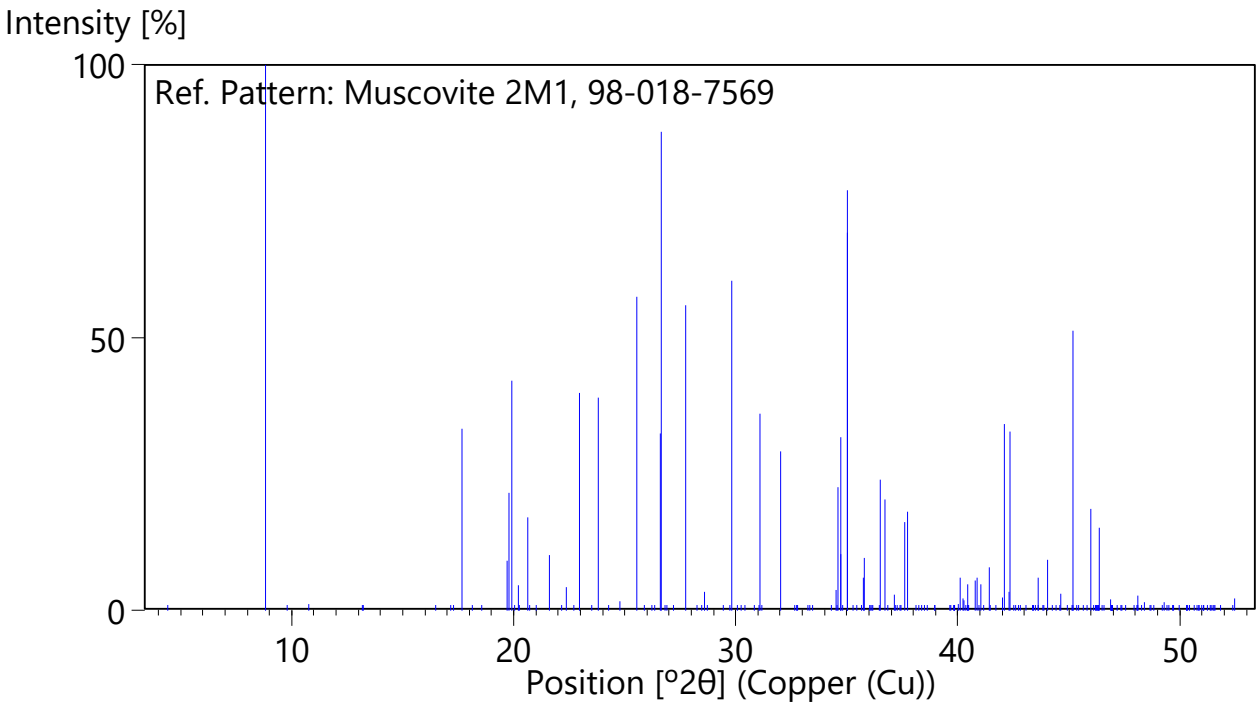
Structure

No.	Name	Element	X	Y	Z	Biso	sof	Wyck.
1	AL1	Al	0.02267	0.52175	0.67027	0.5000	1.0000	1a
2	H1	H	0.90934	0.94882	0.61833	0.5000	1.0000	1a
3	SI1	Si	0.73085	0.67642	0.30683	0.5000	1.0000	1a
4	AL2	Al	0.73430	0.34610	0.30761	0.5000	1.0000	1a
5	O1	O	0.73081	0.66718	0.22512	0.5000	1.0000	1a
6	O2	O	0.65405	0.35740	0.22072	0.5000	1.0000	1a
7	O3	O	0.72588	0.04185	0.22208	0.5000	1.0000	1a
8	O4	O	0.68129	0.52165	0.34346	0.5000	1.0000	1a
9	O5	O	0.52048	0.80114	0.33014	0.5000	1.0000	1a
10	K1	K	0.77027	0.00356	0.42129	0.5000	1.0000	1a
11	H2	H	0.63123	0.94883	0.22425	0.5000	1.0000	1a
12	H3	H	0.63125	0.26542	0.72425	0.5000	1.0000	1a
13	SI2	Si	0.80970	0.67641	0.53576	0.5000	1.0000	1a
14	AL3	Al	0.80627	0.34610	0.53498	0.5000	1.0000	1a
15	O6	O	0.80975	0.66717	0.61747	0.5000	1.0000	1a
16	O7	O	0.88651	0.35739	0.62186	0.5000	1.0000	1a
17	O8	O	0.81470	0.04184	0.62050	0.5000	1.0000	1a
18	O9	O	0.85926	0.52165	0.49913	0.5000	1.0000	1a
19	O10	O	0.02008	0.80113	0.51245	0.5000	1.0000	1a
20	K2	K	0.77029	0.21072	0.92129	0.5000	1.0000	1a
21	O11	O	0.01753	0.73954	0.33978	0.5000	1.0000	1a
22	AL4	Al	0.51790	0.69251	0.67232	0.5000	1.0000	1a
23	AL5	Al	0.02266	0.69252	0.17027	0.5000	1.0000	1a
24	SI3	Si	0.80971	0.53786	0.03575	0.5000	1.0000	1a
25	AL6	Al	0.80627	0.86818	0.03497	0.5000	1.0000	1a
26	O12	O	0.80975	0.54709	0.11746	0.5000	1.0000	1a
27	O13	O	0.88651	0.85688	0.12186	0.5000	1.0000	1a
28	O14	O	0.81468	0.17242	0.12050	0.5000	1.0000	1a
29	O15	O	0.85926	0.69262	0.99912	0.5000	1.0000	1a
30	O16	O	0.02008	0.41314	0.01244	0.5000	1.0000	1a
31	AL7	Al	0.51790	0.52176	0.17231	0.5000	1.0000	1a
32	H4	H	0.90933	0.26545	0.11833	0.5000	1.0000	1a
33	K3	K	0.27029	0.70594	0.92129	0.5000	1.0000	1a
34	SI4	Si	0.73085	0.53786	0.80683	0.5000	1.0000	1a
35	AL8	Al	0.73431	0.86817	0.80761	0.5000	1.0000	1a
36	O17	O	0.73081	0.54708	0.72512	0.5000	1.0000	1a
37	O18	O	0.65407	0.85687	0.72072	0.5000	1.0000	1a
38	O19	O	0.72590	0.17240	0.72208	0.5000	1.0000	1a

39	O20	O	0.68130	0.69262	0.84346	0.5000	1.0000	1a
40	O21	O	0.52048	0.41314	0.83014	0.5000	1.0000	1a
41	O22	O	0.01753	0.47473	0.83978	0.5000	1.0000	1a
42	O23	O	0.52303	0.47474	0.00280	0.5000	1.0000	1a
43	AL9	Al	0.52451	0.02365	0.67187	0.5000	1.0000	1a
44	O24	O	0.52303	0.73954	0.50280	0.5000	1.0000	1a
45	SI5	Si	0.25272	0.17720	0.30776	0.5000	1.0000	1a
46	SI6	Si	0.22021	0.85093	0.30567	0.5000	1.0000	1a
47	O25	O	0.23508	0.16007	0.22538	0.5000	1.0000	1a
48	O26	O	0.17032	0.85642	0.22466	0.5000	1.0000	1a
49	O27	O	0.22709	0.55053	0.22291	0.5000	1.0000	1a
50	O28	O	0.17498	0.01357	0.33967	0.5000	1.0000	1a
51	O29	O	0.06083	0.30673	0.32942	0.5000	1.0000	1a
52	K4	K	0.27028	0.50833	0.42129	0.5000	1.0000	1a
53	H5	H	0.14457	0.46089	0.23777	0.5000	1.0000	1a
54	H6	H	0.14457	0.75338	0.73777	0.5000	1.0000	1a
55	SI7	Si	0.28785	0.17719	0.53482	0.5000	1.0000	1a
56	SI8	Si	0.32035	0.85093	0.53692	0.5000	1.0000	1a
57	O30	O	0.30550	0.16007	0.61720	0.5000	1.0000	1a
58	O31	O	0.37026	0.85642	0.61793	0.5000	1.0000	1a
59	O32	O	0.31347	0.55052	0.61968	0.5000	1.0000	1a
60	O33	O	0.36558	0.01356	0.50292	0.5000	1.0000	1a
61	O34	O	0.47974	0.30673	0.51316	0.5000	1.0000	1a
62	O35	O	0.00001	0.21428	0.50000	0.5000	1.0000	1a
63	O36	O	0.54056	0.21428	0.34258	0.5000	1.0000	1a
64	AL10	Al	0.01609	0.19060	0.67071	0.5000	1.0000	1a
65	AL11	Al	0.52449	0.19061	0.17187	0.5000	1.0000	1a
66	SI9	Si	0.28785	0.03708	0.03482	0.5000	1.0000	1a
67	SI10	Si	0.32035	0.36335	0.03691	0.5000	1.0000	1a
68	O37	O	0.30549	0.05420	0.11720	0.5000	1.0000	1a
69	O38	O	0.37025	0.35785	0.11792	0.5000	1.0000	1a
70	O39	O	0.31347	0.66375	0.11967	0.5000	1.0000	1a
71	O40	O	0.36558	0.20071	0.00291	0.5000	1.0000	1a
72	O41	O	0.47973	0.90755	0.01316	0.5000	1.0000	1a
73	AL12	Al	0.01607	0.02366	0.17071	0.5000	1.0000	1a
74	H7	H	0.39599	0.75339	0.10481	0.5000	1.0000	1a
75	H8	H	0.39599	0.46088	0.60481	0.5000	1.0000	1a
76	SI11	Si	0.25273	0.03707	0.80777	0.5000	1.0000	1a
77	SI12	Si	0.22022	0.36334	0.80567	0.5000	1.0000	1a
78	O42	O	0.23509	0.05420	0.72539	0.5000	1.0000	1a

79	O43	O	0.17032	0.35784	0.72467	0.5000	1.0000	1a
80	O44	O	0.22709	0.66375	0.72291	0.5000	1.0000	1a
81	O45	O	0.17498	0.20070	0.83967	0.5000	1.0000	1a
82	O46	O	0.06085	0.90754	0.82942	0.5000	1.0000	1a
83	O47	O	0.54058	0.99999	0.84259	0.5000	1.0000	1a
84	O48	O	0.00000	0.00000	0.00000	0.5000	1.0000	1a

Stick Pattern

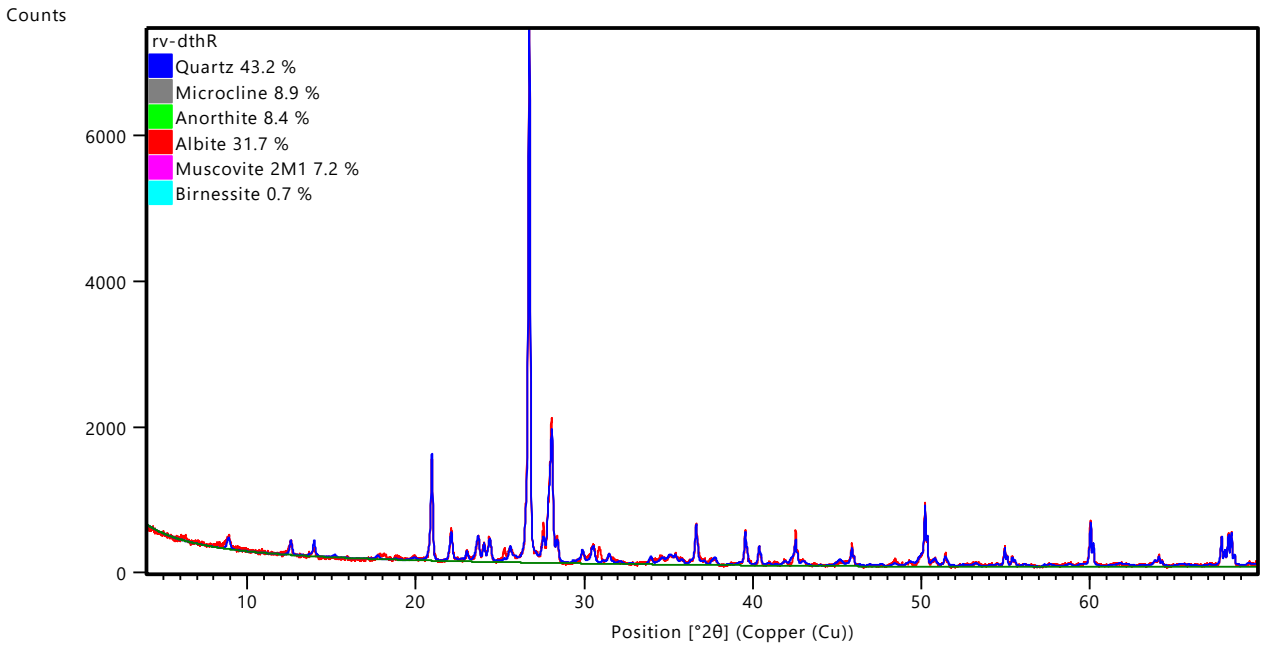


Anchor Scan Parameters

Dataset Name	rv-dthR
File name	D:\Mangesh\Application Support\Post Sales\Birbal Sahni, Lucknow\New folder\rv-dthR.xrdml
Comment	Configuration=Multi Purpose Sample Stage, Owner=User-1, Creation date=3/27/2015 3:44:05 PM
Goniometer=PW3050/60 (Theta/Theta); Minimum step size 2Theta:0.001; Minimum step size Omega:0.001	
Sample stage=Multi purpose sample stage; Minimum step size Phi:2.5	
Diffractometer system=XPERT-3	
Measurement program=C:\PANalytical\Data Collector\Programs**Bulk Powder_BBHD_MPPS_1D.xrdmp**, Identifier={FA755B84-DF04-41AA-8AD7-C4E850FAC733}	
MPSS stage	
Measurement Start Date/Time	12-03-2021 13:21:15
Operator	User
Raw Data Origin	XRD measurement (*.XRDML)
Scan Axis	Gonio
Start Position [°2θ]	4.0076
End Position [°2θ]	69.9956
Step Size [°2θ]	0.0130
Scan Step Time [s]	29.0700
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [°2θ]	3.35
Offset [°2θ]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [°]	0.2177
Specimen Length [mm]	10.00
Measurement Temperature [°C]	25.00
Anode Material	Cu
Intended Wavelength Type	K-α1
K-α1 [Å]	1.54060
K-α2 [Å]	1.54443
K-β1 [Å]	1.39225
K-β2 [Å]	1.38113
K-β3 [Å]	1.39261
K-A2 / K-A1 Ratio	0.50000
K-Alpha2 Line Shift	0.00000
K Absorption Edge	1.37868
Generator Settings	30 mA, 40 kV
Diffractometer Type	0000000011166139

Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	100.00
Incident Beam Monochromator	No
Spinning	No

Graphics



Peak List

Pos. [°2θ]	Height [cts]	FWHM Left [°2θ]	d-spacing [Å]	Rel. Int. [%]
4.476	0.00	0.2001	19.72350	0.00
8.874	109.63	0.2001	9.95656	2.59
9.401	0.57	0.1342	9.40013	0.01
9.867	0.06	0.2001	8.95697	0.00
10.170	0.02	0.1342	8.69122	0.00
10.812	0.12	0.2001	8.17624	0.00
10.812	0.12	0.2001	8.17624	0.00
10.989	0.02	0.1342	8.04459	0.00
12.567	135.01	0.1696	7.03777	3.19
13.224	3.15	0.2600	6.68962	0.07
13.250	0.00	0.2001	6.67678	0.00
13.250	0.00	0.2001	6.67678	0.00
13.285	0.00	0.2001	6.65917	0.00
13.300	1.35	0.2600	6.65151	0.03
13.699	2.71	0.2600	6.45884	0.06

13.713	9.45	0.1342	6.45238	0.22
13.726	3.69	0.2600	6.44642	0.09
13.733	0.09	0.1342	6.44286	0.00
13.899	5.32	0.1556	6.36656	0.13
13.926	0.26	0.1342	6.35394	0.01
13.942	52.64	0.1556	6.34692	1.24
13.976	110.89	0.1556	6.33167	2.62
14.083	0.20	0.1342	6.28360	0.00
14.135	15.04	0.1556	6.26083	0.36
14.988	4.61	0.2600	5.90610	0.11
15.142	2.35	0.1342	5.84628	0.06
15.180	24.51	0.1555	5.83206	0.58
15.275	3.68	0.2600	5.79567	0.09
15.786	0.62	0.1342	5.60939	0.01
15.854	4.09	0.1555	5.58561	0.10
16.385	0.03	0.1342	5.40567	0.00
16.540	0.00	0.2001	5.35521	0.00
16.540	0.00	0.2001	5.35521	0.00
17.284	0.42	0.2001	5.12642	0.01
17.433	0.00	0.2001	5.08309	0.00
17.449	1.05	0.1342	5.07823	0.02
17.715	37.09	0.2001	5.00254	0.88
17.723	0.37	0.1342	5.00045	0.01
18.247	0.00	0.2001	4.85813	0.00
18.666	0.00	0.2001	4.74985	0.00
18.778	12.04	0.1342	4.72171	0.28
18.999	0.03	0.1342	4.66749	0.00
19.040	2.11	0.1554	4.65751	0.05
19.229	0.29	0.2600	4.61208	0.01
19.575	1.47	0.2600	4.53134	0.03
19.721	7.42	0.2001	4.49816	0.18
19.908	11.86	0.2001	4.45632	0.28
19.908	11.86	0.2001	4.45632	0.28
20.037	2.22	0.2001	4.42779	0.05
20.037	2.22	0.2001	4.42779	0.05
20.166	0.00	0.2001	4.39987	0.00
20.215	1.36	0.2001	4.38923	0.03
20.215	1.36	0.2001	4.38923	0.03
20.285	0.00	0.2001	4.37427	0.00
20.285	0.00	0.2001	4.37427	0.00
20.333	0.02	0.1342	4.36415	0.00

20.384	1.40	0.1554	4.35326	0.03
20.752	5.75	0.2001	4.27680	0.14
20.752	5.75	0.2001	4.27680	0.14
20.796	0.43	0.1342	4.26787	0.01
20.798	0.00	0.2001	4.26749	0.00
20.847	54.15	0.2600	4.25772	1.28
20.950	1155.31	0.1518	4.23686	27.30
21.124	0.01	0.2001	4.20241	0.00
21.124	0.01	0.2001	4.20241	0.00
21.241	0.74	0.1342	4.17950	0.02
21.494	0.09	0.1342	4.13091	0.00
21.634	1.01	0.2001	4.10456	0.02
21.634	1.01	0.2001	4.10456	0.02
21.993	88.09	0.1342	4.03821	2.08
21.995	0.31	0.1342	4.03784	0.01
22.111	273.84	0.1554	4.01709	6.47
22.172	0.00	0.2001	4.00600	0.00
22.293	0.10	0.1342	3.98466	0.00
22.298	7.30	0.2600	3.98374	0.17
22.403	10.20	0.2600	3.96526	0.24
22.466	0.62	0.2001	3.95432	0.01
22.466	0.62	0.2001	3.95432	0.01
22.534	0.91	0.1342	3.94249	0.02
22.714	0.57	0.1342	3.91165	0.01
22.726	19.05	0.1342	3.90964	0.45
22.733	5.11	0.2600	3.90840	0.12
22.810	0.00	0.2001	3.89538	0.00
23.021	75.24	0.1554	3.86030	1.78
23.038	13.31	0.2001	3.85743	0.31
23.038	13.31	0.2001	3.85743	0.31
23.045	0.02	0.1342	3.85620	0.00
23.166	0.09	0.1342	3.83637	0.00
23.491	31.81	0.2600	3.78411	0.75
23.596	0.00	0.2001	3.76738	0.00
23.605	42.90	0.1342	3.76600	1.01
23.612	29.71	0.1342	3.76490	0.70
23.621	32.80	0.2600	3.76347	0.78
23.709	196.92	0.1554	3.74968	4.65
23.818	2.95	0.2001	3.73280	0.07
23.818	2.95	0.2001	3.73280	0.07
24.039	182.33	0.1554	3.69894	4.31

24.226	0.33	0.1342	3.67091	0.01
24.227	0.60	0.1342	3.67076	0.01
24.261	43.52	0.1342	3.66567	1.03
24.277	14.71	0.1342	3.66324	0.35
24.291	0.00	0.2001	3.66114	0.00
24.291	0.00	0.2001	3.66114	0.00
24.380	196.10	0.1555	3.64797	4.63
24.405	9.67	0.2600	3.64430	0.23
24.456	0.29	0.1555	3.63692	0.01
24.471	59.57	0.1555	3.63474	1.41
24.791	6.91	0.2600	3.58851	0.16
24.798	0.34	0.1342	3.58751	0.01
24.878	0.12	0.2001	3.57615	0.00
24.878	0.12	0.2001	3.57615	0.00
24.943	5.73	0.2600	3.56696	0.14
25.200	20.53	0.1696	3.53113	0.49
25.227	3.35	0.2600	3.52744	0.08
25.300	0.05	0.1342	3.51748	0.00
25.498	1.84	0.1342	3.49061	0.04
25.535	16.58	0.1342	3.48553	0.39
25.568	26.69	0.2600	3.48122	0.63
25.604	20.98	0.2001	3.47639	0.50
25.604	20.98	0.2001	3.47639	0.50
25.606	65.62	0.1555	3.47606	1.55
25.742	0.49	0.1555	3.45796	0.01
25.797	6.73	0.1342	3.45074	0.16
25.872	13.02	0.1556	3.44094	0.31
25.872	22.13	0.2600	3.44091	0.52
25.972	0.01	0.2001	3.42786	0.00
26.174	0.91	0.1342	3.40193	0.02
26.301	0.01	0.2001	3.38580	0.00
26.301	0.01	0.2001	3.38580	0.00
26.400	0.06	0.2001	3.37325	0.00
26.400	0.06	0.2001	3.37325	0.00
26.476	1.16	0.1556	3.36377	0.03
26.518	31.59	0.1342	3.35862	0.75
26.531	168.48	0.1556	3.35698	3.98
26.539	47.72	0.2600	3.35590	1.13
26.592	0.00	0.2001	3.34944	0.00
26.592	0.00	0.2001	3.34944	0.00
26.663	98.61	0.2001	3.34058	2.33

26.695	46.97	0.2600	3.33672	1.11
26.732	4231.90	0.1520	3.33220	100.00
26.732	1918.50	0.1520	3.33220	45.33
26.867	0.00	0.2001	3.31575	0.00
26.955	0.00	0.2001	3.30511	0.00
26.955	0.00	0.2001	3.30511	0.00
27.079	50.40	0.2600	3.29029	1.19
27.246	1.09	0.2001	3.27046	0.03
27.246	1.09	0.2001	3.27046	0.03
27.509	69.69	0.2600	3.23978	1.65
27.537	63.70	0.1342	3.23652	1.51
27.563	25.66	0.2600	3.23353	0.61
27.579	71.69	0.1342	3.23174	1.69
27.819	5.60	0.2001	3.20438	0.13
27.819	5.60	0.2001	3.20438	0.13
27.839	117.49	0.1342	3.20208	2.78
27.875	404.21	0.1557	3.19803	9.55
27.917	40.94	0.1557	3.19335	0.97
27.974	112.28	0.1342	3.18700	2.65
28.005	400.59	0.1557	3.18347	9.47
28.075	1112.68	0.1557	3.17580	26.29
28.284	0.10	0.1342	3.15277	0.00
28.294	50.92	0.1342	3.15161	1.20
28.314	0.07	0.2001	3.14947	0.00
28.314	0.07	0.2001	3.14947	0.00
28.400	208.13	0.1558	3.14016	4.92
28.468	0.00	0.2001	3.13275	0.00
28.468	0.00	0.2001	3.13275	0.00
28.491	0.01	0.1342	3.13033	0.00
28.591	0.12	0.1342	3.11955	0.00
28.660	1.22	0.2001	3.11226	0.03
28.660	1.22	0.2001	3.11226	0.03

Document History

Insert Measurement:

- File name = "Rvdth-airdried complete angle.xrdml"
- Modification time = "8/19/2021 7:14:43 AM"
- Modification editor = "Sandeep Nagar"

Default properties:

- Measurement step axis = "None"

- Internal wavelengths used from anode material: Copper (Cu)
- Original K-Alpha1 wavelength = "1.54060"
- Used K-Alpha1 wavelength = "1.54060"
- Original K-Alpha2 wavelength = "1.54443"
- Used K-Alpha2 wavelength = "1.54443"
- Original K-Beta wavelength = "1.39225"
- Used K-Beta wavelength = "1.39225"
- Irradiated length = "10.00000"
- Spinner used = "No"
- KBeta filter material = "Ni"
- KBeta filter thickness = "0.02000"
- Receiving slit size = "0.10000"
- Step axis value = "0.00000"
- Offset = "0.00000"
- Sample length = "10.00000"
- Modification time = "8/19/2021 7:14:43 AM"
- Modification editor = "Sandeep Nagar"

Interpolate Step Size:
- Initial Scan Range = 3.00257 - 69.99330
- Initial Step Size = 0.01313
- Derived Step Size = 0.01300
- Use Derived Step Size = "Yes"
- Parameterset name = "Default"
- PANalytical factory default
- Modification time = "8/19/2021 7:14:43 AM"
- Modification editor = "Sandeep Nagar"

Clip Range:
- Old/New start = "3.0026/5.2650"
- Old/New end = "69.9916/69.9920"
- Modification time = "8/19/2021 7:15:08 AM"
- Modification editor = "Sandeep Nagar"

Determine Background:
- Add to net scan = "Nothing"
- User defined intensity = "0"
- Correction method = "Automatic"
- Bending factor = "0"
- Minimum significance = "1"
- Minimum tip width = "0.01"
- Maximum tip width = "1"

- Peak base width = "2"
- Use smoothed input data = "Yes"
- Granularity = "100"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:15:32 AM"
- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:15:58 AM"
- Modification editor = "Sandeep Nagar"

Search Peaks:
- Minimum significance = "1"
- Minimum tip width = "0.01"
- Maximum tip width = "1"
- Peak base width = "2"
- Method = "Minimum 2nd derivative"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/5/2021 9:09:30 AM"
- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:16:07 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = 5.278 - 69.992
- Step No. 1
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 2
- Title = "More background"
- Switch off after usage = "No"
- No. additional parameters = "2"
- Use 1/X background too = "Yes"
- Step No. 3
- Title = "Peak Position"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- Step No. 4
- Title = "Peak Area"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- Step No. 5
- Title = "Peak FWHM"
- Switch off after usage = "No"

- Minimum Irelative % = "-1"
- Step No. 6
- Title = "Peak Shape"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- No. of refined parameters = 192
- Chi Square = 1.22437312181155
- Rp = 0.07094
- Rwp = 0.09384
- Rexp = 0.07664
- Modification time = "8/19/2021 7:16:24 AM"
- Modification editor = "Sandeep Nagar"

Insert Peak:
- Peak position Gonio = "30.7887"
- Modification time = "8/19/2021 7:17:01 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = 5.278 - 69.992
- Step No. 1
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 2
- Title = "More background"
- Switch off after usage = "No"
- No. additional parameters = "2"
- Use 1/X background too = "Yes"
- Step No. 3
- Title = "Peak Position"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- Step No. 4
- Title = "Peak Area"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- Step No. 5
- Title = "Peak FWHM"
- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- Step No. 6
- Title = "Peak Shape"

- Switch off after usage = "No"
- Minimum Irelative % = "-1"
- No. of refined parameters = 196
- Chi Square = 1.17091361832959
- Rp = 0.06731
- Rwp = 0.08970
- Rexp = 0.07661
- Modification time = "8/19/2021 7:17:41 AM"
- Modification editor = "Sandeep Nagar"

Search & Match:
- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Profile and peak list"
- Demote unmatched strong = "Yes"
- 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"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:18:49 AM"
- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:19:53 AM"
- Modification editor = "Sandeep Nagar"

Search & Match:
- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Profile and peak list"
- Demote unmatched strong = "Yes"
- 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"

- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:22:01 AM"
- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:22:07 AM"
- Modification editor = "Sandeep Nagar"

Search & Match:
- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Profile and peak list"
- Demote unmatched strong = "Yes"
- 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"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:23:19 AM"

- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:23:26 AM"
- Modification editor = "Sandeep Nagar"

Search & Match:
- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Profile and peak list"
- Demote unmatched strong = "Yes"
- 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"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:24:28 AM"
- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:24:32 AM"

- Modification editor = "Sandeep Nagar"

Convert Ref. Pattern to Phase:
- Modification time = "8/19/2021 7:24:49 AM"
- Modification editor = "Sandeep Nagar"

Search & Match:
- Allow pattern shift = "No"
- Auto residue = "Yes"
- Data source = "Profile and peak list"
- Demote unmatched strong = "Yes"
- 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"
- Parameterset name = "Untitled"
- Parameterset modification time = "8/19/2021 7:25:46 AM"

- Parameterset modification editor = "Sandeep Nagar"
- Modification time = "8/19/2021 7:25:54 AM"
- Modification editor = "Sandeep Nagar"

Delete All Phases:
- Modification time = "8/19/2021 7:26:53 AM"
- Modification editor = "Sandeep Nagar"

Convert Ref. Pattern to Phase:
- Modification time = "8/19/2021 7:27:00 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = 5.278 - 69.992
- Step No. 1
- Title = "Scale Factor"
- Switch off after usage = "No"
- Step No. 2
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 3
- Title = "More background"
- Switch off after usage = "No"
- No. additional parameters = "2"
- Use 1/X background too = "Yes"
- Step No. 4
- Title = "Specimen Displacement"
- Switch off after usage = "No"
- Step No. 5
- Title = "Lattice Parameters"
- Switch off after usage = "No"
- Minimum weight % = "5"
- Step No. 6
- Title = "Caglioti W"
- Switch off after usage = "No"
- Minimum weight % = "5"
- No. of refined parameters = 36
- Chi Square = 1.66442755486243
- Rp = 0.09940
- Rwp = 0.12962
- Rexp = 0.07788
- Modification time = "8/19/2021 7:28:09 AM"

- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:28:33 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:36 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:37 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y43p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:38 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:38 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y63p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:39 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:39 AM"
- Modification editor = "Sandeep Nagar"

Edit Method:
- Old Value = "Polynomial"
- Modification time = "8/19/2021 7:28:51 AM"
- Modification editor = "Sandeep Nagar"

Edit Use Extended Background Terms:
- Old Value = "False"
- Modification time = "8/19/2021 7:28:52 AM"
- Modification editor = "Sandeep Nagar"

Change Flat background Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:04 AM"
- Modification editor = "Sandeep Nagar"

Change 1/X Background Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:05 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 1 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:06 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 2 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:07 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 3 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:07 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 4 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:08 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 5 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:09 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 6 Refinement Flag:
- Old Value = "False"

- Modification time = "8/19/2021 7:29:09 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 7 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:10 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 8 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:11 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 9 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:14 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 10 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:15 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 11 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:15 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 12 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:16 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 13 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:17 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 14 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:17 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 15 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:21 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 16 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:22 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 17 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:23 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 18 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:23 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 19 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:24 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:24 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 21 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:25 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 22 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:29:26 AM"
- Modification editor = "Sandeep Nagar"

Change Coefficient 23 Refinement Flag:

- Old Value = "False"
- Modification time = "8/19/2021 7:29:28 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "63"
- Chi Square = "1.38017091062857"
- Rp = "0.08074"
- Rwp = "0.10719"
- Rexp = "0.07767"
- Modification time = "8/19/2021 7:29:53 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Profile Caglioti V Left Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:30:09 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "64"
- Chi Square = "1.37956857548839"
- Rp = "0.08067"
- Rwp = "0.10713"
- Rexp = "0.07766"
- Modification time = "8/19/2021 7:30:21 AM"
- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Asymmetry Type:
- Old Value = "No Asymmetry Function"
- Modification time = "8/19/2021 7:30:32 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn S/L Asymmetry Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:30:35 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn D/L Asymmetry Refinement Flag:

- Old Value = "False"
- Modification time = "8/19/2021 7:30:36 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Peak Shape 1 Left Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:30:36 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "67"
- Chi Square = "1.35820700644622"
- Rp = "0.07946"
- Rwp = "0.10544"
- Rexp = "0.07763"
- Modification time = "8/19/2021 7:30:56 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn Peak Shape 2 Left Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:30:58 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "68"
- Chi Square = "1.33809032483275"
- Rp = "0.07861"
- Rwp = "0.10387"
- Rexp = "0.07763"
- Modification time = "8/19/2021 7:31:10 AM"
- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Preferred Orientation Model:
- Old Value = "Spherical Harmonics"
- Modification time = "8/19/2021 7:31:54 AM"
- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Direction h:

- Old Value = "0"
- Modification time = "8/19/2021 7:31:56 AM"
- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Direction l:
- Old Value = "1"
- Modification time = "8/19/2021 7:32:00 AM"
- Modification editor = "Sandeep Nagar"

Edit Quartz, syn Parameter (March/Dollase) 1:
- Old Value = "1"
- Modification time = "8/19/2021 7:32:03 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "62"
- Chi Square = "1.56178032982541"
- Rp = "0.08689"
- Rwp = "0.12131"
- Rexp = "0.07767"
- Modification time = "8/19/2021 7:32:36 AM"
- Modification editor = "Sandeep Nagar"

Change Quartz, syn March-Dollase Factor Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:32:38 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "63"
- Chi Square = "1.32365171825994"
- Rp = "0.07733"
- Rwp = "0.10280"
- Rexp = "0.07767"
- Modification time = "8/19/2021 7:33:00 AM"
- Modification editor = "Sandeep Nagar"

Edit Albite (heat-treated) Preferred Orientation Model:

- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:33:21 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:27 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y21p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:28 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y21m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:29 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y22p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:29 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y22m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:30 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:30 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y41p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:31 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y41m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:31 AM"

- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y42p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:32 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y42m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:35 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y43p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:36 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y43m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:36 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y44p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:37 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y44m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:37 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:38 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y61p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:38 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y61m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:39 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y62p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:42 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y62m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:42 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y63p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:43 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y63m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:44 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y64p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:44 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y64m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:45 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y65p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:45 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y65m Refinement Flag:
- Old Value = "False"

- Modification time = "8/19/2021 7:33:46 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:49 AM"
- Modification editor = "Sandeep Nagar"

Change Albite (heat-treated) Coefficient Y66m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:33:50 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "90"
- Chi Square = "1.20193345748222"
- Rp = "0.06998"
- Rwp = "0.09309"
- Rexp = "0.07745"
- Modification time = "8/19/2021 7:34:08 AM"
- Modification editor = "Sandeep Nagar"

Edit Microcline, intermediate Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:34:56 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:34:59 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y21p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:00 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y21m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:00 AM"

- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y22p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:01 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y22m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:02 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:02 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y41p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:05 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y41m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:05 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y42p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:06 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y42m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:07 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y43p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:07 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y43m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:08 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y44p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:09 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y44m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:09 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:12 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y61p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:13 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y61m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:14 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y62p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:14 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y62m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:15 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y63p Refinement Flag:
- Old Value = "False"

- Modification time = "8/19/2021 7:35:16 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y63m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:16 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y64p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:17 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y64m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:18 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y65p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:19 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y65m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:21 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:22 AM"
- Modification editor = "Sandeep Nagar"

Change Microcline, intermediate Coefficient Y66m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:35:23 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "117"

- Chi Square = "1.16671320109024"
- Rp = "0.06765"
- Rwp = "0.09011"
- Rexp = "0.07724"
- Modification time = "8/19/2021 7:35:41 AM"
- Modification editor = "Sandeep Nagar"

Edit Annite-siderophyllite Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:35:59 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:02 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y22p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:03 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y22m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:04 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:04 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y42p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:05 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y42m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:09 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y44p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:10 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y44m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:10 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:11 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y62p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:12 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y62m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:13 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y64p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:13 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y64m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:14 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:14 AM"
- Modification editor = "Sandeep Nagar"

Change Annite-siderophyllite Coefficient Y66m Refinement Flag:
- Old Value = "False"

- Modification time = "8/19/2021 7:36:17 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "132"
- Chi Square = "1.1610419981818"
- Rp = "0.06717"
- Rwp = "0.08954"
- Rexp = "0.07712"
- Modification time = "8/19/2021 7:36:30 AM"
- Modification editor = "Sandeep Nagar"

Edit Anorthite, sodian Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:36:38 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:42 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y21p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:42 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y21m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:43 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y22p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:43 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y22m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:46 AM"

- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:47 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y41p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:47 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y41m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:48 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y42p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:48 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y42m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:49 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y43p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:49 AM"
- Modification editor = "Sandeep Nagar"

Change Anorthite, sodian Coefficient Y43m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:36:50 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "144"
- Chi Square = "1.15582182555383"

- Rp = "0.06672"
- Rwp = "0.08903"
- Rexp = "0.07702"
- Modification time = "8/19/2021 7:37:04 AM"
- Modification editor = "Sandeep Nagar"

Edit Ferromerrillite Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:37:21 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:25 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:25 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y43p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:26 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:29 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y63p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:29 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:30 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:

- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "150"
- Chi Square = "1.14978473936602"
- Rp = "0.06633"
- Rwp = "0.08851"
- Rexp = "0.07698"
- Modification time = "8/19/2021 7:37:42 AM"
- Modification editor = "Sandeep Nagar"

Edit Greenalite Preferred Orientation Model:
- Old Value = "March/Dollase Model"
- Modification time = "8/19/2021 7:37:50 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y20 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:55 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y22p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:55 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y22m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:56 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y40 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:57 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y42p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:57 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y42m Refinement Flag:
- Old Value = "False"

- Modification time = "8/19/2021 7:37:58 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y44p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:37:59 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y44m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:00 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y60 Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:00 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y62p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:01 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y62m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:04 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y64p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:05 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y64m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:05 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y66p Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:06 AM"
- Modification editor = "Sandeep Nagar"

Change Greenalite Coefficient Y66m Refinement Flag:
- Old Value = "False"
- Modification time = "8/19/2021 7:38:07 AM"
- Modification editor = "Sandeep Nagar"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "165"
- Chi Square = "1.11020168590623"
- Rp = "0.06395"
- Rwp = "0.08533"
- Rexp = "0.07686"
- Modification time = "8/19/2021 7:38:21 AM"
- Modification editor = "Sandeep Nagar"

Change Ferromerrillite Use Flag:
- Old Value = "True"
- Modification time = "25-08-2021 18:45:02"
- Modification editor = "mangesh.mahajan"

Change Greenalite Use Flag:
- Old Value = "True"
- Modification time = "25-08-2021 18:45:02"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "5.278 - 69.992"
- Refinement Mode = "Manual"
- No. of refined parameters = "142"
- Chi Square = "1.1633276122015"
- Rp = "0.06623"
- Rwp = "0.08962"
- Rexp = "0.07704"
- Modification time = "25-08-2021 18:45:11"
- Modification editor = "mangesh.mahajan"

Insert Measurement:
- File name = "rv-dthR.xrdml"
- Modification time = "26-08-2021 13:49:06"
- Modification editor = "mangesh.mahajan"

Default properties:
- Measurement step axis = "None"
- Internal wavelengths used from anode material: Copper (Cu)
- Original K-Alpha1 wavelength = "1.54060"
- Used K-Alpha1 wavelength = "1.54060"
- Original K-Alpha2 wavelength = "1.54443"
- Used K-Alpha2 wavelength = "1.54443"
- Original K-Beta wavelength = "1.39225"
- Used K-Beta wavelength = "1.39225"
- Irradiated length = "10.00000"
- Spinner used = "No"
- KBeta filter material = "Ni"
- KBeta filter thickness = "0.02000"
- Receiving slit size = "0.10000"
- Step axis value = "0.00000"
- Offset = "0.00000"
- Sample length = "10.00000"
- Modification time = "26-08-2021 13:49:06"
- Modification editor = "mangesh.mahajan"

Interpolate Step Size:
- Initial Scan Range = 3.00657 - 69.99730
- Initial Step Size = 0.01313
- Derived Step Size = 0.01300
- Use Derived Step Size = "Yes"
- Parameterset name = "Default"
- PANalytical factory default
- Modification time = "26-08-2021 13:49:06"
- Modification editor = "mangesh.mahajan"

Clip Range:
- Old/New start = "3.0066/4.0000"
- Old/New end = "69.9956/69.9956"
- Modification time = "26-08-2021 20:28:04"
- Modification editor = "mangesh.mahajan"

Delete Selected Phase:
- Modification time = "26-08-2021 20:37:38"
- Modification editor = "mangesh.mahajan"

Delete Selected Phase:

- Modification time = "26-08-2021 20:37:43"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = 4.008 - 69.996
- Step No. 1
- Title = "Scale Factor"
- Switch off after usage = "No"
- Step No. 2
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 3
- Title = "More background"
- Switch off after usage = "No"
- No. additional parameters = "3"
- Use 1/X background too = "Yes"
- Step No. 4
- Title = "Specimen Displacement"
- Switch off after usage = "No"
- Step No. 5
- Title = "Lattice Parameters"
- Switch off after usage = "No"
- Minimum weight % = "5"
- No. of refined parameters = 31
- Chi Square = 2.05351972904851
- Rp = 0.10323
- Rwp = 0.13555
- Rexp = 0.06601
- Modification time = "26-08-2021 20:38:53"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = 4.008 - 69.996
- Step No. 1
- Title = "Scale Factor"
- Switch off after usage = "No"
- Step No. 2
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 3
- Title = "More background"
- Switch off after usage = "No"

- No. additional parameters = "3"
- Use 1/X background too = "Yes"
- Step No. 4
- Title = "Specimen Displacement"
- Switch off after usage = "No"
- Step No. 5
- Title = "Lattice Parameters"
- Switch off after usage = "No"
- Minimum weight % = "5"
- Step No. 6
- Title = "Caglioti W"
- Switch off after usage = "No"
- Minimum weight % = "5"
- Step No. 7
- Title = "Preferred Orientation"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Toggle directions = "No"
- Step No. 8
- Title = "Caglioti U"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Step No. 9
- Title = "Caglioti V"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Step No. 10
- Title = "Peak Shape Parameter 1"
- Switch off after usage = "No"
- Minimum weight % = "20"
- No. of refined parameters = 82
- Chi Square = 1.71999569666898
- Rp = 0.08210
- Rwp = 0.11296
- Rexp = 0.06567
- Modification time = "26-08-2021 20:39:28"
- Modification editor = "mangesh.mahajan"

Delete Selected Phase:
- Modification time = "26-08-2021 21:32:01"
- Modification editor = "mangesh.mahajan"

Insert Phase: Muscovite 2M1:
- Modification time = "26-08-2021 21:34:12"
- Modification editor = "mangesh.mahajan"

Insert Phase: Birnessite:
- Modification time = "26-08-2021 21:34:18"
- Modification editor = "mangesh.mahajan"

Edit Anorthite, sodian Display Color:
- Old Value = "Aqua"
- Modification time = "26-08-2021 21:34:28"
- Modification editor = "mangesh.mahajan"

Fix all parameters:
- Modification time = "26-08-2021 21:34:39"
- Modification editor = "mangesh.mahajan"

Initialize Global Parameters:
- Modification time = "26-08-2021 21:34:42"
- Modification editor = "mangesh.mahajan"

Initialize All Phases:
- Modification time = "26-08-2021 21:34:46"
- Modification editor = "mangesh.mahajan"

Edit Muscovite 2M1 Spherical Harmonics Order:
- Old Value = "6"
- Modification time = "26-08-2021 21:35:13"
- Modification editor = "mangesh.mahajan"

Edit Muscovite 2M1 Spherical Harmonics Order:
- Old Value = "8"
- Modification time = "26-08-2021 21:35:16"
- Modification editor = "mangesh.mahajan"

Edit Birnessite Spherical Harmonics Order:
- Old Value = "6"
- Modification time = "26-08-2021 21:35:33"
- Modification editor = "mangesh.mahajan"

Edit Birnessite Spherical Harmonics Order:
- Old Value = "8"

- Modification time = "26-08-2021 21:35:36"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = 4.008 - 69.996
- Step No. 1
- Title = "Scale Factor"
- Switch off after usage = "No"
- Step No. 2
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 3
- Title = "More background"
- Switch off after usage = "No"
- No. additional parameters = "3"
- Use 1/X background too = "Yes"
- Step No. 4
- Title = "Specimen Displacement"
- Switch off after usage = "No"
- Step No. 5
- Title = "Lattice Parameters"
- Switch off after usage = "No"
- Minimum weight % = "5"
- No. of refined parameters = 32
- Chi Square = 2.31670692402768
- Rp = 0.11370
- Rwp = 0.15290
- Rexp = 0.06600
- Modification time = "26-08-2021 21:36:21"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = 4.008 - 69.996
- Step No. 1
- Title = "Scale Factor"
- Switch off after usage = "No"
- Step No. 2
- Title = "Flat Background"
- Switch off after usage = "No"
- Step No. 3
- Title = "More background"
- Switch off after usage = "No"

- No. additional parameters = "3"
- Use 1/X background too = "Yes"
- Step No. 4
- Title = "Specimen Displacement"
- Switch off after usage = "No"
- Step No. 5
- Title = "Lattice Parameters"
- Switch off after usage = "No"
- Minimum weight % = "5"
- Step No. 6
- Title = "Caglioti W"
- Switch off after usage = "No"
- Minimum weight % = "5"
- Step No. 7
- Title = "Preferred Orientation"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Toggle directions = "No"
- Step No. 8
- Title = "Caglioti U"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Step No. 9
- Title = "Caglioti V"
- Switch off after usage = "No"
- Minimum weight % = "15"
- Step No. 10
- Title = "Peak Shape Parameter 1"
- Switch off after usage = "No"
- Minimum weight % = "20"
- No. of refined parameters = 83
- Chi Square = 1.78327458434042
- Rp = 0.08518
- Rwp = 0.11710
- Rexp = 0.06567
- Modification time = "26-08-2021 21:36:50"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "4.008 - 69.996"
- Refinement Mode = "Manual"
- No. of refined parameters = "110"

- Chi Square = "1.72053549553991"
- Rp = "0.08177"
- Rwp = "0.11267"
- Rexp = "0.06549"
- Modification time = "26-08-2021 21:37:17"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Profile Caglioti W Left Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:37:25"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "4.008 - 69.996"
- Refinement Mode = "Manual"
- No. of refined parameters = "111"
- Chi Square = "1.70182529133982"
- Rp = "0.08082"
- Rwp = "0.11144"
- Rexp = "0.06548"
- Modification time = "26-08-2021 21:37:30"
- Modification editor = "mangesh.mahajan"

Change Birnessite Profile Caglioti W Left Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:37:43"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "4.008 - 69.996"
- Refinement Mode = "Manual"
- No. of refined parameters = "112"
- Chi Square = "1.68123932606876"
- Rp = "0.07977"
- Rwp = "0.11008"
- Rexp = "0.06547"
- Modification time = "26-08-2021 21:37:48"
- Modification editor = "mangesh.mahajan"

Change Birnessite Cell a [Å] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:37:57"

- Modification editor = "mangesh.mahajan"

Change Birnessite Cell c [Å] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:37:58"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Profile Caglioti W Left Refinement Flag:
- Old Value = "True"
- Modification time = "26-08-2021 21:38:29"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Cell a [Å] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:38:35"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Cell b [Å] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:38:36"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Cell c [Å] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:38:38"
- Modification editor = "mangesh.mahajan"

Change Muscovite 2M1 Cell beta [°] Refinement Flag:
- Old Value = "False"
- Modification time = "26-08-2021 21:38:40"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "4.008 - 69.996"
- Refinement Mode = "Manual"
- No. of refined parameters = "117"
- Chi Square = "1.65025803520023"
- Rp = "0.07801"
- Rwp = "0.10800"
- Rexp = "0.06544"
- Modification time = "26-08-2021 21:38:48"
- Modification editor = "mangesh.mahajan"

Profile/Rietveld fitting:
- Angular range Gonio = "4.008 - 69.996"
- Refinement Mode = "Manual"
- No. of refined parameters = "117"
- Chi Square = "1.65549750515656"
- Rp = "0.07812"
- Rwp = "0.10834"
- Rexp = "0.06544"
- Modification time = "26-08-2021 21:40:00"
- Modification editor = "mangesh.mahajan"

Edit Quartz, syn Title:
- Old Value = "Quartz, syn"
- Modification time = "26-08-2021 21:40:46"
- Modification editor = "mangesh.mahajan"

Edit Microcline, intermediate Title:
- Old Value = "Microcline, intermediate"
- Modification time = "26-08-2021 21:40:54"
- Modification editor = "mangesh.mahajan"

Edit Anorthite, sodian Title:
- Old Value = "Anorthite, sodian"
- Modification time = "26-08-2021 21:41:02"
- Modification editor = "mangesh.mahajan"

Edit Albite (heat-treated) Title:
- Old Value = "Albite (heat-treated)"
- Modification time = "26-08-2021 21:41:10"
- Modification editor = "mangesh.mahajan"