Title Ca2C4O10H2.57 (**Whewellite**)

Lattice type P
Space group name P 21/c
Space group number 14
Setting number 1

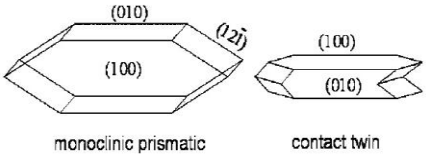
Lattice parameters

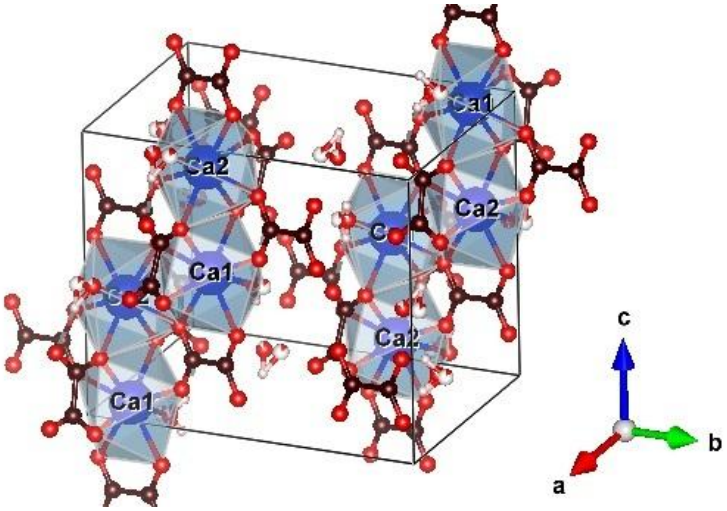
a	b	c	alpha	beta	gamma
6.29000	**14.58300**	**10.11600**	90.0000	109.4600	90.0000

Unit-cell volume = 874.903501 Å^3

Structure parameters

			x	y	z	Occ.	U	Site	Sym.
1	Ca	Ca1	0.96760	0.12430	0.05460	1.000	0.008	4e	1
2	Ca	Ca2	0.99680	0.12360	0.43570	1.000	0.008	4e	1
3	C	C1	0.98320	0.32010	0.24520	1.000	0.010	4e	1
4	C	C2	0.00090	0.42700	0.24920	1.000	0.010	4e	1
5	C	C3	0.51890	0.12660	0.18120	1.000	0.014	4e	1
6	C	C4	0.45050	0.11730	0.31310	1.000	0.014	4e	1
7	O	O1	0.97560	0.28260	0.13220	1.000	0.015	4e	1
8	O	O2	0.00660	0.46590	0.13950	1.000	0.014	4e	1
9	O	O3	0.97990	0.28190	0.35500	1.000	0.015	4e	1
10	O	O4	0.00730	0.46580	0.36140	1.000	0.015	4e	1
11	O	O5	0.36140	0.14180	0.06900	1.000	0.028	4e	1
12	O	O6	0.72450	0.12270	0.19740	1.000	0.015	4e	1
13	O	O7	0.24380	0.12290	0.29570	1.000	0.017	4e	1
14	O	O8	0.60730	0.10680	0.42640	1.000	0.028	4e	1
15	H	H11	0.48700	0.37200	0.05100	0.850	0.063	4e	1
16	H	H21	0.51000	0.36400	0.42600	0.860	0.063	4e	1
17	H	H22	0.53000	0.36700	0.32000	0.860	0.063	4e	1
18	O	OW1	0.39320	0.34590	0.10220	0.850	0.023	4e	1
19	O	OW2	0.59130	0.38290	0.39080	0.860	0.057	4e	1
20	O	OW10	0.38800	0.39600	0.09900	0.150	0.023	4e	1
21	O	OW20	0.58400	0.40900	0.39200	0.140	0.057	4e	1



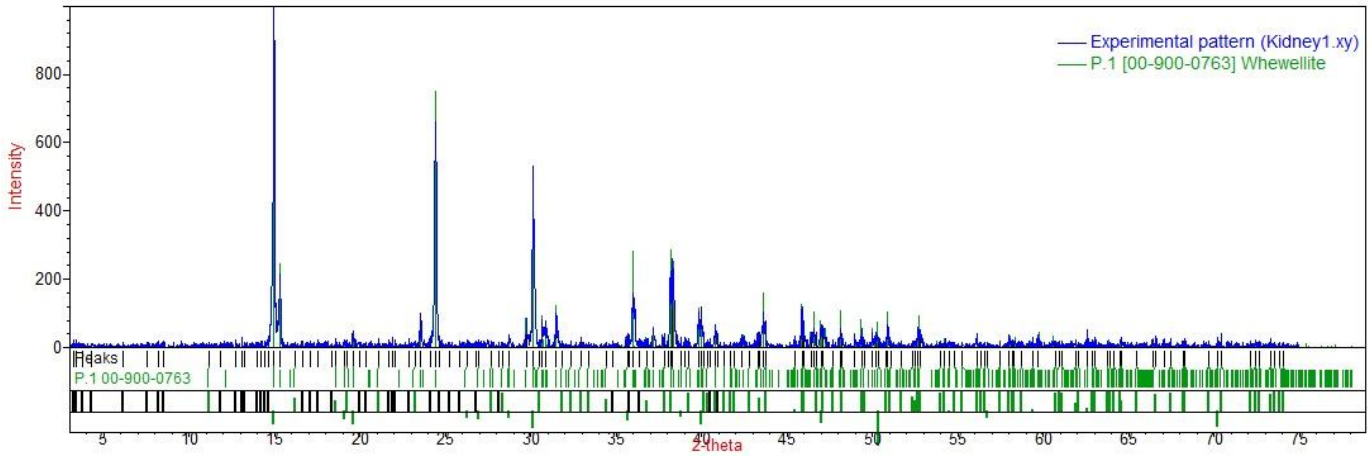


Whewellite
Tazzoli V, Domeneghetti M C
American Mineralogist 65 (1980) 327-334
The crystal structures of whewellite and weddellite: re-examination and comparison
_database_code_amcsd 0000776

CELL PARAMETERS: 6.2900 14.5830 10.1160 90.000 109.460 90.000
SPACE GROUP: P2_1/c
X-RAY WAVELENGTH: 1.541838
Cell Volume: 874.904
Density (g/cm3): 2.207
MAX. ABS. INTENSITY / VOLUME**2: 7.578285835
RIR: 1.118
RIR based on corundum from Acta Crystallographica A38 (1982) 733-739

2-THETA	INTENSITY	D-SPACING	H	K	L	Multiplicity
14.94	**100.00**	**5.9307**	**1**	**0**	**0**	**2**
15.30	29.53	5.7927	0	2	1	4
19.13	1.69	4.6397	-1	2	1	4
19.62	4.55	4.5249	-1	0	2	2
23.54	10.49	3.7794	1	2	1	4
24.42	**88.48**	**3.6458**	**0**	**4**	**0**	**2**
26.18	1.68	3.4043	0	3	2	4
26.92	1.77	3.3120	-1	3	2	4
28.74	3.24	3.1058	1	4	0	4
29.74	9.48	3.0038	-1	2	3	4
30.14	**53.43**	**2.9653**	**2**	**0**	**0**	**2**
30.68	10.01	2.9144	0	2	3	4
30.77	2.59	2.9059	2	1	0	4
30.87	8.07	2.8964	0	4	2	4
31.51	13.58	2.8389	-1	4	2	4
35.59	2.94	2.5223	-1	0	4	2
36.01	30.06	2.4939	-2	2	3	4
36.74	3.31	2.4464	2	2	1	4
37.20	6.48	2.4169	1	4	2	4
37.73	3.08	2.3845	0	0	4	2
38.21	31.26	2.3552	0	6	1	4
38.35	27.23	2.3472	1	2	3	4
38.82	1.96	2.3199	-2	4	2	4
39.16	2.92	2.3005	2	4	0	4
39.84	11.77	2.2624	-2	0	4	2
40.01	10.61	2.2535	-1	6	1	4
40.84	6.85	2.2097	2	0	2	2
42.44	4.08	2.1297	1	6	1	4
43.31	4.00	2.0889	-3	0	2	2
43.64	17.22	2.0742	-1	4	4	4
45.45	1.02	1.9956	0	4	4	4
45.48	1.69	1.9944	1	0	4	2
45.90	14.13	1.9769	3	0	0	2
46.42	4.63	1.9563	-1	6	3	4
46.59	11.01	1.9494	-1	2	5	4
47.01	8.40	1.9331	-3	2	3	4
47.06	5.45	1.9309	0	6	3	4
47.27	5.82	1.9229	-2	6	1	4
48.15	11.65	1.8897	2	4	2	4
49.02	4.08	1.8584	-2	2	5	4
49.38	8.37	1.8455	0	2	5	4

50.04	7.13	1.8229	0	8	0	2
50.14	1.62	1.8193	2	2	3	4
50.34	7.81	1.8125	-3	4	2	4
50.95	11.23	1.7924	-2	6	3	4
51.50	1.34	1.7746	2	6	1	4
52.67	1.91	1.7378	3	4	0	4
52.74	10.11	1.7356	1	6	3	4
53.84	1.89	1.7027	0	8	2	4
54.25	2.91	1.6908	-1	8	2	4
54.56	1.08	1.6820	-1	0	6	2
56.16	2.44	1.6378	-3	2	5	4
56.82	1.22	1.6202	1	2	5	4
58.11	3.45	1.5873	1	8	2	4
58.43	3.20	1.5795	-3	6	1	4
59.28	1.71	1.5588	-2	8	2	4
59.45	1.54	1.5549	-1	6	5	4
59.53	1.13	1.5529	2	8	0	4
59.80	4.79	1.5466	-3	6	3	4
60.63	3.59	1.5273	-1	4	6	4
60.83	1.76	1.5227	-4	2	3	4
61.77	1.97	1.5019	-2	4	6	4
62.48	1.65	1.4864	2	6	3	4
62.66	2.88	1.4827	4	0	0	2
62.98	2.03	1.4759	2	4	4	4
63.88	2.14	1.4572	0	4	6	4
64.54	1.49	1.4439	3	2	3	4
66.49	3.10	1.4061	2	8	2	4
67.16	2.59	1.3937	-3	4	6	4
67.92	1.61	1.3800	2	2	5	4
68.29	2.04	1.3735	-3	8	2	4
70.28	2.41	1.3394	0	2	7	4
72.03	1.23	1.3111	-4	6	3	4
72.48	2.52	1.3040	-4	6	1	4
75.46	1.07	1.2598	3	6	3	4
78.75	1.75	1.2153	0	12	0	2
80.71	1.15	1.1905	1	12	0	4
81.01	1.40	1.1869	-5	2	5	4
81.07	1.25	1.1861	5	0	0	2
81.34	3.51	1.1830	-1	10	5	4
82.13	1.67	1.1735	3	2	5	4
83.15	1.52	1.1617	-2	10	5	4
83.43	2.23	1.1586	0	10	5	4
83.90	2.16	1.1532	-3	4	8	4
85.73	2.30	1.1332	0	4	8	4
86.56	1.07	1.1245	2	12	0	4
88.84	1.52	1.1015	-3	10	5	4
89.12	2.22	1.0987	-5	4	6	4
89.39	1.16	1.0961	1	10	5	4



QualX Phase Identification Results

General Informations

Filename	Kidney1.qlx
Data range	3.000° to 75.000°
Number of points	3601
Step size	3601
Alpha2 subtracted	No
Background subtr.	Yes
Radiation Wavelength	Cu: 1.540560Å

Peak List

Serial	2theta [°]	d [Å]	I/I0
1	3.22	27.4159	24.279

2	3.34	26.4312	24.208
3	3.76	23.4796	11.585
4	4.24	20.8226	11.451
5	6.12	14.4297	15.811
6	7.56	11.6841	14.880
7	8.22	10.7474	18.293
8	8.46	10.4430	18.100
9	11.12	7.9502	15.512
10	11.82	7.4809	14.577
11	12.74	6.9427	21.651
12	13.08	6.7630	29.512
13	13.24	6.6816	16.842
14	13.96	6.3386	14.783
15	14.16	6.2495	18.247
16	14.42	6.1374	17.587
17	14.64	6.0456	33.853
18	14.96	5.9170	1000.000
19	15.30	5.7863	215.651
20	16.22	5.4601	16.251
21	16.62	5.3296	17.390
22	17.06	5.1931	18.159
23	17.56	5.0464	22.257
24	18.38	4.8230	12.735
25	18.60	4.7665	24.748
26	19.08	4.6476	23.768
27	19.22	4.6141	23.608
28	19.60	4.5255	48.096
29	19.98	4.4403	15.342
30	20.32	4.3667	15.845
31	21.10	4.2070	25.211
32	21.70	4.0920	21.456
33	21.90	4.0551	29.524
34	22.04	4.0297	21.155
35	22.90	3.8803	27.531
36	23.20	3.8308	18.401
37	23.56	3.7730	99.946
38	24.16	3.6807	33.415
39	24.44	3.6391	661.374
40	24.64	3.6100	34.452
41	25.26	3.5228	15.429
42	25.86	3.4424	17.335
43	26.24	3.3934	21.904
44	26.80	3.3238	17.885
45	26.92	3.3092	22.057
46	27.68	3.2201	17.666
47	28.14	3.1685	16.770
48	28.32	3.1487	16.405
49	28.74	3.1037	35.563
50	29.76	2.9996	87.219

51	30.12	2.9645	531.702
52	30.46	2.9322	23.293
53	30.68	2.9117	80.786
54	30.86	2.8951	77.042
55	31.48	2.8395	100.009
56	31.86	2.8065	19.589
57	32.32	2.7676	17.384
58	32.96	2.7153	28.198
59	33.42	2.6790	16.730
60	34.40	2.6049	16.297
61	34.76	2.5787	19.496
62	35.68	2.5143	41.346
63	35.78	2.5075	36.889
64	36.00	2.4927	160.256
65	36.32	2.4714	27.161
66	36.76	2.4429	26.767
67	37.14	2.4187	55.182
68	37.82	2.3768	41.755
69	38.02	2.3648	25.101
70	38.20	2.3540	223.351
71	38.30	2.3481	260.580
72	38.80	2.3190	29.737
73	39.02	2.3064	30.009
74	39.26	2.2929	26.678
75	39.82	2.2619	102.805
76	39.98	2.2532	119.642
77	40.12	2.2457	45.920
78	40.32	2.2350	22.010
79	40.48	2.2265	26.379
80	40.82	2.2088	68.523
81	40.94	2.2026	40.016
82	41.32	2.1832	16.007
83	41.68	2.1652	16.375
84	41.88	2.1553	16.672
85	42.38	2.1310	37.042
86	42.82	2.1101	15.885
87	43.30	2.0878	44.584
88	43.40	2.0833	44.608
89	43.62	2.0733	102.682
90	43.74	2.0679	78.111
91	45.44	1.9944	35.233
92	45.88	1.9763	119.315
93	45.98	1.9722	77.395
94	46.40	1.9553	46.423
95	46.58	1.9482	54.493
96	46.70	1.9434	46.059
97	47.00	1.9317	66.968
98	47.12	1.9271	63.015
99	47.70	1.9050	22.867

100	48.12	1.8894	56.863
101	48.24	1.8849	36.451
102	48.98	1.8582	36.721
103	49.38	1.8441	57.194
104	49.52	1.8392	24.039
105	50.00	1.8226	44.495
106	50.24	1.8145	44.839
107	50.38	1.8098	28.710
108	50.78	1.7965	29.526
109	50.90	1.7925	66.936
110	51.06	1.7873	30.274
111	51.66	1.7679	19.678
112	52.32	1.7471	17.116
113	52.54	1.7403	17.494
114	52.66	1.7367	58.945
115	52.80	1.7324	50.876
116	53.98	1.6973	19.416
117	54.22	1.6903	15.480
118	54.54	1.6812	19.759
119	54.82	1.6732	15.822
120	55.28	1.6604	15.893
121	56.10	1.6381	40.761
122	56.34	1.6316	16.002
123	56.58	1.6253	16.073
124	56.72	1.6216	16.129
125	57.46	1.6025	19.727
126	58.02	1.5883	35.619
127	58.18	1.5843	23.100
128	58.28	1.5819	18.808
129	58.76	1.5701	18.085
130	59.40	1.5547	30.459
131	59.72	1.5471	38.652
132	60.70	1.5245	18.672
133	60.94	1.5190	18.927
134	61.10	1.5154	19.079
135	61.90	1.4978	23.683
136	62.10	1.4934	15.429
137	62.60	1.4827	52.941
138	62.86	1.4772	24.044
139	63.02	1.4738	28.173
140	63.78	1.4581	19.889
141	63.92	1.4552	15.904
142	64.14	1.4507	11.805
143	64.50	1.4435	24.212
144	64.62	1.4411	28.372
145	65.48	1.4243	16.483
146	66.44	1.4060	20.840
147	66.62	1.4026	33.255
148	67.10	1.3938	20.883

149	67.48	1.3868	25.094
150	68.20	1.3739	17.372
151	68.32	1.3718	25.725
152	69.72	1.3476	17.671
153	70.24	1.3389	29.891
154	70.44	1.3356	42.356
155	72.14	1.3083	18.324
156	72.44	1.3036	18.451
157	72.68	1.2999	18.631
158	73.30	1.2904	27.252
159	73.56	1.2865	15.058
160	73.82	1.2826	15.302
161	74.06	1.2790	15.443

Plausible phases

Name	Formula	PDF Number	FoM
[Whewellite]	**C4 H2.57 Ca2 O10**	**00-900-0763**	**0.744**