Table 2a. Powder X-ray diffraction data for carlsonite*

I_{obs}	d_{obs}	d_{calc}	I_{calc}	*h k l*
100	9.23	9.1020	100	0 0 2
		8.5695	4	0 1 0
40	8.26	8.3939	25	$1\ 0\ 0$
		8.2936	7	$\bar{1}\ 1\ 0$
		8.1161	22	$0\ \bar{1}\ 1$
		8.0439	6	$\bar{1}\ 0\ 1$
43	7.57	7.6129	13	$\bar{1}\ 1\ 1$
		7.4831	17	$1\ \bar{1}\ 1$
		7.4353	22	0 1 1
		7.2612	4	1 0 1
8	6.67	6.6296	9	$\bar{1}\ 0\ 2$
		6.2011	2	$\bar{1}\ 1\ 2$
4	5.83	5.7953	4	$1\ 0\ 2$
5	5.28	5.2642	2	$\bar{1}\ 0\ 3$
		5.2403	4	$0\ \bar{1}\ 3$
23	4.93	4.9453	11	$\bar{1}\ \bar{1}\ 1$
		4.8726	11	$\bar{1}\ 2\ 0$
		4.8448	3	$1\ \bar{1}\ 3$
10	4.74	4.7757	9	$\bar{2}\ 1\ 0$
		4.7682	2	$1\ \bar{2}\ 1$
		4.7069	2	0 1 3
		4.3937	2	$\bar{2}\ 1\ 2$
8	4.302	4.2847	4	0 2 0
		4.2153	5	$\bar{2}\ 0\ 1$
8	4.136	4.1468	3	$\bar{2}\ 2\ 0$
		4.1305	2	$\bar{1}\ \bar{1}\ 3$
		4.0814	2	$2\ \bar{1}\ 2$
		4.0580	2	$0\ \bar{2}\ 2$
		4.0234	2	$2\ \bar{2}\ 1$
6	3.957	3.9746	2	2 0 1
		3.8978	6	$1\ \bar{2}\ 3$
14	3.726	3.7080	10	$\bar{1}\ 2\ 3$
		3.7036	2	$0\ \bar{2}\ 3$
13	3.597	3.5996	2	$2\ \bar{1}\ 3$
		3.5836	12	1 1 3
		3.5168	3	$\bar{1}\ 0\ 5$
9	3.441	3.4524	7	$\bar{2}\ 1\ 4$
		3.4141	3	$1\ \bar{2}\ 4$
		3.3879	3	$2\ \bar{2}\ 3$
20	3.328	3.3269	2	0 2 3
		3.3148	17	$\bar{2}\ 0\ 4$
		3.3061	2	$1\ \bar{1}\ 5$
		3.2693	4	$\bar{1}\ \bar{2}\ 1$
15	3.246	3.2536	5	2 0 3
		3.2443	8	$\bar{1}\ 2\ 4$
		3.2409	3	1 2 0
41	3.144	3.1566	27	$2\ \bar{1}\ 4$
		3.1382	4	$\bar{3}\ 1\ 0$
		3.1332	4	$2\ \bar{3}\ 1$
		3.1280	3	1 1 4
		3.1176	8	1 2 1
		3.1074	3	$\bar{2}\ 3\ 1$
		3.1006	4	$\bar{2}\ 2\ 4$
16	3.035	3.0717	8	$\bar{3}\ 1\ 2$
		3.0376	4	$\bar{1}\ \bar{2}\ 3$
		3.0289	7	$\bar{2}\ 1\ 5$
		3.0142	3	$2\ \bar{3}\ 2$
		2.9907	5	$1\ \bar{2}\ 5$
12	2.943	2.9687	4	$\bar{2}\ 3\ 2$
		2.9590	3	$\bar{1}\ 3\ 2$
		2.9285	3	1 2 2
		2.9203	4	$\bar{3}\ 1\ 3$
		2.8997	2	2 1 2
		2.8944	3	$3\ \bar{2}\ 2$
10	2.849	2.8476	6	$\bar{1}\ \bar{2}\ 5$
		2.8363	2	$2\ \bar{3}\ 3$
		2.8303	3	$\bar{1}\ \bar{2}\ 4$
5	2.758	2.7799	3	$\bar{2}\ 3\ 3$
		2.7465	3	1 1 5
		2.7237	2	$1\ \bar{3}\ 4$
		2.7055	2	$2\ \bar{2}\ 5$
6	2.666	2.6823	3	2 1 3
		2.6713	2	$3\ \bar{1}\ 3$
		2.6592	3	$\bar{3}\ 2\ 4$
		2.6311	2	$0\ 2\ 5$
		2.6286	2	$3\ \bar{3}\ 2$
7	2.463	2.4668	6	2 2 0
		2.4312	3	$2\ \bar{4}\ 1$
6	2.389	2.4010	3	$\bar{1}\ 3\ 1$
		2.3878	2	$\bar{4}\ 2\ 0$
		2.3621	3	$\bar{4}\ 2\ 2$
		2.3534	2	$0\ 2\ 6$
10	2.332	2.3442	3	$0\ \bar{2}\ 7$
		2.3245	3	$\bar{4}\ 1\ 1$
		2.3226	2	$\bar{1}\ \bar{3}\ 3$
		2.3165	3	$\bar{3}\ 4\ 0$
		2.2947	2	$\bar{3}\ 4\ 1$
8	2.268	2.2755	3	0 0 8
		2.2525	3	3 0 4
		2.2388	2	$\bar{3}\ 4\ 2$
5	2.210	2.2263	2	$\bar{3}\ 3\ 5$
		2.2085	2	$0\ \bar{3}\ 6$
		2.1938	2	$4\ \bar{3}\ 2$
2	2.128	2.1402	2	$0\ \bar{4}\ 2$
		2.1254	2	1 0 8
4	1.9225	1.9354	1	$3\ \bar{2}\ 7$
		1.9277	1	$\bar{3}\ 5\ 0$
		1.9241	1	$3\ \bar{5}\ 1$
		1.9195	1	$4\ \bar{2}\ 5$
		1.9179	1	2 2 5
5	1.8628	1.8706	2	$1\ \bar{5}\ 1$
		1.8623	2	$\bar{4}\ \bar{1}\ 1$
8	1.8216	1.8204	4	0 0 10
		1.8039	2	$\bar{5}\ 4\ 1$

* Calculated lines with $I < 2$ are omitted except those needed to index the observed line at 1.9225 Å.

(*Continued on next page*)

Table 2b. Powder X-ray diffraction data for huizingite-(Al)*

I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\,k\,l$	I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\,k\,l$	I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\,k\,l$
30	10.33	10.2428	45	0 0 1			2.8049	5	3 3 1	7	1.8706	1.8745	6	5 2 0
		9.4581	16	0 1 0			2.7976	5	2 2 2			1.8480	3	4 3 2
60	8.82	8.7110	79	1 0 0	9	2.772	2.7646	10	3 0 2			1.8435	2	1 4 3
11	8.07	8.0581	39	1 1 0			2.7545	2	2 1 2	7	1.8378	1.8385	3	5 1 0
26	7.47	7.4504	8	0 1 1			2.7250	3	3 3 2			1.8350	2	0 4 3
		7.3731	44	1 0 1			2.7194	7	2 3 3			1.8259	2	4 1 3
28	6.55	6.5364	59	0 1 1			2.7166	7	1 3 3			1.8122	2	3 3 1
5	6.14	6.0830	17	1 0 1	20	2.697	2.6973	5	3 2 1			1.8057	2	2 5 4
32	5.60	5.5952	47	1 1 1			2.6860	7	3 3 0			1.8012	2	1 3 4
		5.4788	16	1 1 0			2.6769	5	2 2 1	9	1.7989	1.7995	3	5 1 3
		5.1214	20	0 0 2			2.6664	2	1 3 0			1.7962	2	0 2 5
69	5.037	5.0312	9	1 1 2			2.6623	2	3 0 1			1.7926	2	4 5 0
		5.0122	66	1 2 1			2.6558	2	3 1 3			1.7734	2	3 1 4
		4.9251	10	1 1 1			2.6111	3	0 2 3			1.7705	3	1 4 5
		4.8408	15	1 0 2	9	2.571	2.5764	13	1 4 1	10	1.7656	1.7692	2	1 2 5
32	4.776	4.7573	24	2 1 1			2.5574	2	0 1 4			1.7647	2	5 2 1
		4.7423	7	1 1 1			2.5410	2	1 2 3			1.7598	2	3 0 4
		4.7290	22	0 2 0			2.5324	4	3 1 1			1.7549	5	4 1 5
25	4.521	4.5242	45	0 2 1	8	2.521	2.5129	10	1 2 3			1.7429	8	1 5 4
22	4.337	4.3555	11	2 0 0			2.4664	2	2 0 3	11	1.7411	1.7417	3	5 1 1
		4.3187	20	2 0 1	18	2.458	2.4626	9	2 2 2			1.7359	2	4 1 3
		4.2759	7	0 1 2			2.4563	12	2 1 3			1.7209	4	4 2 3
41	4.122	4.1844	10	2 2 1			2.4313	4	3 3 1	8	1.7141	1.7166	3	3 2 4
		4.1276	14	1 2 2			2.4204	2	2 0 4			1.7134	4	4 4 2
		4.1094	5	1 2 1			2.4090	4	3 1 2			1.6960	2	2 6 0
		4.0949	18	0 2 1			2.3941	3	0 1 4			1.6899	2	3 1 4
		4.0847	32	1 0 2			2.3860	2	0 2 4	7	1.6817	1.6852	2	4 1 4
		4.0290	2	2 2 0			2.3728	2	0 4 1			1.6772	2	0 2 6
		3.8477	3	1 1 2			2.3645	4	0 4 0			1.6689	2	2 6 3
10	3.831	3.8292	16	1 1 2	11	2.369	2.3614	6	1 1 4			1.6671	4	3 6 0
		3.7252	2	0 2 2			2.3515	3	1 4 1	5	1.6550	1.6623	2	1 6 0
		3.6866	2	2 0 2			2.3289	3	3 2 2			1.6429	2	0 1 6
		3.6593	2	1 1 2			2.3225	3	2 1 3			1.6417	2	3 3 3
		3.6320	4	1 2 0			2.3167	3	1 3 2			1.6116	2	5 5 0
38	3.534	3.5321	58	1 1 3	12	2.316	2.3096	5	2 4 3			1.6068	2	4 1 3
		3.4493	3	1 3 1			2.3053	3	4 3 1	8	1.6073	1.6032	2	4 2 2
		3.4449	19	1 2 1			2.2953	2	1 3 4			1.5997	2	3 4 6
		3.4269	100	2 2 1	5	2.212	2.2108	5	3 4 3			1.5974	2	1 6 1
100	3.427	3.4219	6	2 1 1			2.1857	2	2 2 3			1.5907	3	0 3 6
		3.4143	7	0 0 3	10	2.175	2.1735	8	3 1 3			1.5898	9	5 0 4
		3.4018	2	1 2 1			2.1560	3	1 3 3			1.5867	2	1 5 5
		3.3919	14	1 3 0			2.1512	2	4 2 1	12	1.5870	1.5844	2	4 6 0
		3.3543	33	0 1 3	11	2.138	2.1379	10	3 3 2			1.5800	2	1 1 6
		3.2898	17	2 3 1			2.1367	3	3 2 1			1.5700	2	5 4 5
		3.2682	2	0 2 2			2.1128	3	1 2 4			1.5586	2	6 2 0
		3.2167	12	1 2 3			2.0949	8	1 4 0	9	1.5565	1.5573	3	3 4 1
68	3.204	3.2140	3	3 1 1	16	2.087	2.0922	2	4 4 2			1.5564	3	6 1 1
		3.2063	56	2 1 1			2.0861	8	2 2 5			1.5457	3	4 1 4
		3.1979	12	2 1 3			2.0734	2	1 2 4	8	1.5419	1.5441	5	3 1 5
		3.1689	2	2 3 0			2.0601	2	3 1 3			1.5427	2	0 2 6
		3.1585	7	1 3 2			2.0562	12	2 5 2			1.5324	2	5 6 2
		3.1527	31	0 3 0			2.0513	2	4 0 1	5	1.5110	1.5155	2	2 6 2
		3.1172	4	3 1 0	15	2.048	2.0474	2	0 4 2			1.5052	2	1 2 6
		3.0967	11	2 3 2			2.0429	3	1 5 1	8	1.4888	1.4940	3	5 5 5
		3.0854	5	0 1 3			2.0253	7	2 1 4			1.4900	4	4 0 6
		3.0813	3	2 2 3			2.0169	3	4 2 4	8	1.4698	1.4778	2	4 3 4
		3.0420	76	2 1 2	16	2.0097	2.0086	8	2 0 5			1.4769	3	3 3 7
94	3.043	3.0310	9	1 3 1			2.0040	4	3 5 2			1.4693	2	5 6 0
		3.0184	43	3 1 2			1.9985	5	3 2 3			1.4685	2	5 2 0
		3.0010	8	3 2 2			1.9879	2	1 4 2			1.4608	4	3 7 3
		2.9800	2	2 0 3	8	1.9338	1.9346	4	5 2 1			1.4593	5	2 5 2
		2.9586	7	1 1 3			1.9311	3	3 1 4	8	1.4543	1.4588	4	4 5 6
		2.9464	5	3 0 1			1.9095	2	2 5 1			1.4559	2	3 3 4
		2.9350	2	1 2 2			1.9086	2	5 3 2			1.4370	2	1 5 6
		2.8605	4	1 1 3	6	1.8966	1.9051	4	0 5 1	7	1.4207	1.4234	3	6 2 5
5	2.840	2.8564	6	0 3 2			1.8908	2	1 1 5					
							1.8889	2	1 5 3					

* Calculated lines with $I < 2$ are omitted.