

Table S1. X-ray powder data of selected samples of gehlenite from Măgurea Vaței (Cerboia Valley).

	Sample P 4			Sample P 49			Sample 2234			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	
1	5.4843	5.4574	6	5.4836	5.4377	6	5.4480	5.4359	4	(110)
2	5.0558	5.0489	11	5.0665	5.0600	8	5.0335	5.0628	10	(001)
3	4.2338	4.2252	8	4.2404	4.2271	8	4.2157	4.2282	5	(101)
4	3.8709	3.8590	3	3.8645	3.8450	2	3.8562	3.8437	4	(200)
5	3.7148	3.7061	22	3.7162	3.7043	18	3.6957	3.7048	24	(111)
6	3.4669	3.4516	4	3.4618	3.4391	4	3.4552	3.4379	12	(210)
7	3.0739	3.0659	28	3.0723	3.0615	23	3.0626	3.0614	24	(201)
8	2.8563	2.8494	100	2.8544	2.8443	100	2.8496	2.8442	100	(211)
9	2.7347	2.7287	8	2.7327	2.7188	5	2.7042	2.7179	9	(220)
10	2.5235	2.5245	12	2.5275	2.5300	10	2.5187	2.5314	8	(002)
11	2.4486	2.4406	15	2.4365	2.4318	21	2.4254	2.4310	11	(310)
12	2.4009	2.4006	25	2.4027	2.3950	5	2.3973	2.3947	24	(221)
13	2.2949	2.2912	14	2.2944	2.2939	16	2.2906	2.2948	12	(112)
14	2.1144	2.1126	2	2.1144	2.1135	2	-	-	-	(202)
15	2.0392	2.0376	19	2.0397	2.0380	16	2.0355	2.0384	18	(212)
16	1.9733	1.9708	5	1.9636	1.9654	3	1.9637	1.9650	8	(321)
17	1.8550	1.8531	5	1.8545	1.8522	4	1.8513	1.8524	6	(222)
18	-	-	-	-	-	-	1.8064	1.8120	2	(330)
19	1.7569	1.7547	34	1.7563	1.7532	32	1.7553	1.7534	24	(312)
20	-	-	-	1.7453	1.7500	2	1.7553	1.7496	24	(411)
21	1.6812	1.6830	8	1.6842	1.6867	5	1.6853	1.6876	3	(003)
22	1.6354	1.6327	4	1.6338	1.6307	4	-	-	-	(322)
23	1.6074	1.6082	5	-	-	-	1.6154	1.6117	4	(113)
24	1.5422	1.5427	3	1.5431	1.5446	3	-	-	-	(203)
25	1.5125	1.5127	18	1.5136	1.5143	14	1.5110	1.5149	12	(213)
26	1.5039	1.5036	2	1.4974	1.5013	4	1.5034	1.5012	3	(412)
27	1.4778	1.4759	3	1.4771	1.4735	3	-	-	-	(332)
28	1.4326	1.4324	8	1.4332	1.4333	9	1.4317	1.4337	6	(223)
29	1.4089	1.4084	3	1.4092	1.4090	3	1.4080	1.4094	4	(303)
30	1.3213	1.3230	4	1.3234	1.3230	2	1.3231	1.3233	5	(323)
31	1.3213	1.3236	2	1.3178	1.3188	3	-	-	-	(530)
32	1.3149	1.3169	2	-	-	-	1.3114	1.3141	2	(432)
33	-	-	-	1.2788	1.2817	2	1.2802	1.2812	3	(600)
34	1.2607	1.2622	8	1.2626	1.2650	2	1.2645	1.2657	3	(004)
35	1.2527	1.2515	7	1.2521	1.2510	5	1.2517	1.2512	6	(413)
36	1.2358	1.2358	3	1.2359	1.2348	2	1.2349	1.2349	5	(333)
37	1.2050	1.2049	2	-	-	-	1.2025	1.2043	13	(423)
38	1.1989	1.2003	1	-	-	-	1.1983	1.1973	2	(442)
39	-	-	-	1.1865	1.1873	2	1.1885	1.1878	2	(214)
40	1.1458	1.1456	2	1.1464	1.1470	3	1.1447	1.1432	4	(224)
41	1.1329	1.1332	2	1.1336	1.1344	2	1.1381	1.1348	3	(304)
43	1.1266	1.1254	4	1.1260	1.1243	3	1.1261	1.1243	4	(513)
44	1.0917	1.0912	2	-	-	-	1.0899	1.0899	3	(523)

Table S2. X-ray powder data for selected samples of grossular I from Măgureaua Vaței.

	Sample P 1 ⁽¹⁾			Sample 2159 ⁽²⁾			Sample 2234 ⁽¹⁾			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	
1	3.2168	3.1715*	8	3.1759	3.1796	9	-	-	-	(321)
2	2.9588	2.9667	65	2.9756	2.9742	35	2.9677	2.9670	35	(400)
3	2.6472	2.6535	100	2.6623	2.6602	100	2.6551	2.6538	100	(420)
4	2.5248	2.5300	11	2.5370	2.5364	9	2.5329	2.5303	17	(332)
5	2.4182	2.4223	7	2.4294	2.4285	15	2.4231	2.4226	9	(422)
6	2.3228	2.3272	15	2.3346	2.3332	20	2.3283	2.3275	16	(431)
7	2.1637	2.1665	27	2.1724	2.1721	20	2.1682	2.1668	14	(521)
8	2.0959	2.0977	14	2.1031	2.1031	16	2.0950	2.0980	15	(440)
9	1.9227	1.9250	35	1.9303	1.9299	30	1.9251	1.9252	27	(611)
10	1.8750	1.8763	9	1.8809	1.8811	8	-	-	-	(620)
11	1.7483	1.7496	14	-	-	-	-	-	-	(631)
12	1.7119	1.7128	9	1.7175	1.7172	18	1.1740	1.1730	7	(444)
13	1.6779	1.6782	8	1.6828	1.6825	4	1.6786	1.6784	8	(543)
14	1.6448	1.6456	45	-	-	-	1.6461	1.6458	20	(640)
15	1.6131	1.6148	9	1.6190	1.6190	7	1.6170	1.6150	15	(721)
16	1.5851	1.5857	17	1.5898	1.5898	60	1.5863	1.5859	15	(642)
17	1.5070	1.5071	9	1.5105	1.5109	13	1.5064	1.5072	20	(651)
18	1.4832	1.4833	15	1.4871	1.4871	13	1.4859	1.4835	10	(800)
19	1.4603	1.4607	5	1.4646	1.4644	4	1.4592	1.4609	12	(741)
20	1.4202	1.4194	5	1.4222	1.4220	7	1.4155	1.4165	5	(653)
21	-	-	-	1.4012	1.4021	7	1.4011	1.4023	13	(822)
22	1.3791	1.3795	4	1.3826	1.3830	11	-	-	-	(831)
23	-	-	-	1.3471	1.3471	3	1.3450	1.3438	10	(752)
24	1.3270	1.3267	9	1.3301	1.3301	4	1.3273	1.3269	11	(840)
25	1.2949	1.2948	7	1.2980	1.2981	15	1.2946	1.2949	14	(842)
26	1.2801	1.2796	2	-	-	-	1.2811	1.2798	1	(921)
27	1.2653	1.2650	8	1.2681	1.2682	5	1.2643	1.2651	12	(664)
28	-	-	-	1.2538	1.2540	7	1.2521	1.2510	15	(851)
29	1.2240	1.2240	5	1.2273	1.2271	6	1.2254	1.2241	7	(932)
30	1.1992	1.1987	7	1.2017	1.2018	4	1.1996	1.1989	10	(941)
31	1.1754	1.1750	2	1.1782	1.1780	5	1.1752	1.1751	7	(10.1.1)
32	1.1642	1.1636	2	1.1665	1.1666	6	1.1625	1.1638	4	(10.2.0)
33	1.1527	1.1526	4	1.1553	1.1555	5	1.1540	1.1527	3	(943)
34	1.1319	1.1314	3	-	-	-	1.1290	1.1316	5	(10.3.1)
35	-	-	-	1.1151	1.1143	6	1.1138	1.1115	7	(871)
36	1.1026	1.1018	9	1.1045	1.1046	12	1.1037	1.1019	22	(10.4.0)

(1) Sample from Cerboia Valley; (2) Sample from Crămuț Valley.

Table S3. X-ray powder data for selected samples of titanian garnet from Măgureaua Vaței

	Sample 2299 ⁽¹⁾			Sample P 27 ⁽²⁾			Sample P 30 ⁽³⁾			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	
1	4.2155	4.2153	4	4.2730	4.2784	5	4.2629	4.2435	5	(220)
2	-	-	-	3.2399	3.2341	9	-	-	-	(321)
3	2.9800	2.9806	65	3.0274	3.0253	35	3.0049	3.0007	70	(400)
4	2.6643	2.6660	100	2.7081	2.7059	100	2.6866	2.6839	100	(420)
5	2.5439	2.5419	10	2.5817	2.5799	8	2.5618	2.5590	9	(332)
6	2.4338	2.4337	40	2.4723	2.4701	35	2.4515	2.4500	35	(422)
7	2.3367	2.3382	21	2.3742	2.3732	19	2.3547	2.3539	18	(431)
8	2.1795	2.1767	17	2.2101	2.2093	18	2.1912	2.1914	13	(521)
9	2.1095	2.1076	3	2.1419	2.1392	2	2.1212	2.1219	3	(440)
10	-	-	-	1.9633	1.9630	1	1.9461	1.9471	1	(611)
11	1.8890	1.8851	7	-	-	-	-	-	-	(620)
12	1.7495	1.7479	1	1.7800	1.7842	8	-	-	-	(631)
13	1.7188	1.7209	18	1.7462	1.7466	15	1.7311	1.7324	9	(444)
14	1.6771	1.6761	2	-	-	-	1.6947	1.6974	8	(543)
15	1.6531	1.6533	30	1.6798	1.6781	20	1.6630	1.6644	25	(640)
16	1.5960	1.5932	65	1.6167	1.6171	55	-	-	-	(642)
17	-	-	-	1.5382	1.5368	1	1.5255	1.5243	4	(732)
18	1.5143	1.5141	1	-	-	-	-	-	-	(651)
19	1.4917	1.4903	20	1.5124	1.5126	12	1.5039	1.5003	10	(800)
20	1.4697	1.4676	3	1.4898	1.4895	4	1.4788	1.4774	3	(741)
21	1.4437	1.4458	2	-	-	-	1.4549	1.4555	1	(820)
22	-	-	-	1.4256	1.4261	7	1.4119	1.4145	14	(822)
23	1.3518	1.3500	1	1.3715	1.3702	3	-	-	-	(752)
24	-	-	-	1.3526	1.3529	4	-	-	-	(840)
25	1.2994	1.3009	17	-	-	-	1.3114	1.3096	15	(842)
26	1.2698	1.2709	9	1.2898	1.2899	5	1.2769	1.2795	12	(664)
27	-	-	-	1.2353	1.2351	7	-	-	-	(844)
28	1.2040	1.2044	4	1.2223	1.2224	4	-	-	-	(941)
29	1.1799	1.1805	1	1.1905	1.1901	5	1.1878	1.1884	7	(10.1.1)
30	-	-	-	1.1852	1.1866	1	-	-	-	(10.2.0)
31	1.1599	1.1580	1	1.1757	1.1754	5	1.1630	1.1658	3	(943)
32	-	-	-	1.1538	1.1538	2	1.1414	1.1444	2	(765)
33	-	-	-	1.1329	1.1334	6	1.1236	1.1241	5	(871)
34	1.1063	1.1070	3	1.1042	1.1047	4	1.0956	1.0957	1	(10.4.2)
35	1.0976	1.0976	2	-	-	-	-	-	-	(961)

(1) Grossular **II**, Cerboia Valley. (2) Titanian andradite, Crămuț Valley. (3) Grossular **II**, Crămuț Valley.

Table S4. X-ray powder data for a representative sample of monticellite from Măgureaua Vaței (Sample P4, Cerboaia Valley).

Reflection No.	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	(hkl)	Reflection No.	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	(hkl)
1	4.2038	4.1950	35	(021)	26	1.4778	1.4749	3	(330)
2	3.8709	3.8479	14	(101)	27	1.4540	1.4556	2	(252)
3	3.6399	3.6442	70	(120)	28	1.4326	1.4327	8	(261)
4	3.6399	3.6367	70	(111)	29	1.3923	1.3918	14	(340)
5	3.1950	3.1922	13	(002)	30	1.3923	1.3901	14	(322)
6	2.9416	2.9404	47	(130)	31	1.3680	1.3650	5	(172)
7	2.6680	2.6708	100	(131)	32	1.3594	1.3599	4	(341)
8	2.5872	2.5888	65	(112)	33	1.3594	1.3593	4	(081)
9	2.4086	2.4100	19	(140)	34	1.3213	1.3215	7	(214)
10	2.4009	2.4013	19	(122)	35	1.2358	1.2343	1	(105)
11	2.2159	2.2123	11	(220)	36	1.2050	1.2065	4	(352)
12	2.2159	2.2106	11	(211)	37	1.2050	1.2055	4	(400)
13	1.8550	1.8550	3	(060)	38	1.2050	1.2050	4	(280)
14	1.7569	1.7522	9	(241)	39	1.1989	1.2006	6	(244)
15	1.7309	1.7313	6	(160)	40	1.1753	1.1773	2	(191)
16	1.6354	1.6355	2	(250)	41	1.1753	1.1735	2	(164)
17	1.6074	1.6039	12	(062)	42	1.1599	1.1605	3	(045)
18	1.5964	1.5961	6	(004)	43	1.1599	1.1586	3	(421)
19	1.5901	1.5908	7	(310)	44	1.1458	1.1465	1	(430)
20	1.5617	1.5587	1	(301)	45	1.1266	1.1268	2	(314)
21	1.5422	1.5442	7	(320)	46	1.1266	1.1274	2	(282)
22	1.5422	1.5436	7	(311)	47	1.1266	1.1262	2	(273)
23	1.5125	1.5100	16	(170)	48	1.1210	1.1227	3	(215)
24	1.5039	1.5014	8	(114)	49	1.1210	1.1220	3	(412)
25	1.5039	1.5009	8	(321)	50	1.1210	1.1215	3	(192)

Table S5. X-ray powder data for selected samples of vesuvianite from Măgureaua Văței (Cerboia Valley).

	Sample P 6			Sample 1513			Sample 2293			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	
1	5.9364	5.9232	9	5.9384	5.9162	5	5.9434	5.9187	3	(002)
2	4.0432	4.0393	10	4.0204	4.0324	6	4.0480	4.0309	8	(222)
3	3.4994	3.4969	18	3.4924	3.4905	25	3.5031	3.4886	10	(322)
4	3.4994	3.4930	18	3.4924	3.4853	25	3.5031	3.4816	10	(420)
5	3.2602	3.2604	8	3.2580	3.2543	7	-	-	-	(402)
6	-	-	-	3.0796	3.0796	6	3.0784	3.0791	7	(313)
7	3.0686	3.0635	15	3.0534	3.0568	6	3.0504	3.0536	14	(510)
8	2.9650	2.9616	35	2.9616	2.9581	70	2.9651	2.9594	35	(004)
9	2.9200	2.9185	17	2.9160	2.9137	8	2.9207	2.9130	9	(323)
10	2.7623	2.37634	100	2.7601	2.7579	100	2.7622	2.7559	100	(432)
11	2.6725	2.6790	9	2.6709	2.6731	5	2.6732	2.6703	18	(530)
12	2.6070	2.6051	8	2.6041	2.6063	10	2.6089	2.5979	7	(522)
13	-	-	-	2.4994	2.5044	4	2.5013	2.5019	6	(611)
14	2.4682	2.4699	40	2.4671	2.4645	60	2.4652	2.4619	35	(620)
15	2.3053	2.3077	12	2.3054	2.3041	4	2.3087	2.3037	8	(334)
16	2.2442	2.2437	7	-	-	-	2.2416	2.2493	7	(542)
17	2.2182	2.2169	6	2.2113	2.2128	4	2.2054	2.2115	5	(533)
18	2.2082	2.2092	11	-	-	-	2.2054	2.2020	5	(710)
19	2.1705	2.1672	11	2.1681	2.1627	8	-	-	-	(632)
20	2.1345	2.1363	15	2.1307	2.1333	11	2.1353	2.1337	10	(315)
21	2.0946	2.0940	11	2.0911	2.0900	4	2.0884	2.0887	3	(623)
22	2.0728	2.0754	7	2.0695	2.0715	13	-	-	-	(543)
23	2.0728	2.0699	7	2.0695	2.0656	13	2.0614	2.0638	11	(712)
24	2.0500	2.0511	9	2.0461	2.0467	15	2.0424	2.0445	16	(730)
25	-	-	-	2.0299	2.0303	5	2.0279	2.0285	9	(642)
26	-	-	-	2.0175	2.0167	4	2.0169	2.0147	5	(731)
27	2.0049	2.0058	15	2.0026	2.0020	9	2.0042	2.0006	9	(633)
28	1.9726	1.9722	9	1.9684	1.9679	8	1.9600	1.9659	9	(651)
29	1.9402	1.9402	6	1.9331	1.9368	4	1.9346	1.9360	6	(614)
30	1.9175	1.9142	9	1.9128	1.9118	26	1.9132	1.9125	11	(206)
31	1.7708	1.7708	15	1.7675	1.7675	13	1.7678	1.7666	13	(714)
32	-	-	-	1.7449	1.7433	5	1.7423	1.7417	4	(832)
33	1.7208	1.7251	8	1.7201	1.7213	8	-	-	-	(910)
34	1.6684	1.6690	23	1.6663	1.6666	11	1.6672	1.6666	14	(436)
35	1.6289	1.6290	24	1.6268	1.6256	64	1.6273	1.6240	30	(922)
36	-	-	-	1.5891	1.5913	4	1.5865	1.5898	14	(852)
37	1.5641	1.5653	7	1.5613	1.5628	5	1.5614	1.5626	16	(616)
38	1.5353	1.5385	10	1.5361	1.5397	4	1.5396	1.5395	16	(626)
39	1.5353	1.5369	10	1.5361	1.5378	4	1.5396	1.5362	16	(10.1.1)
40	1.5175	1.5173	13	1.5121	1.5139	17	1.5114	1.5123	17	(950)
41	1.5029	1.5034	13	1.5016	1.5002	17	1.5023	1.5058	14	(10.1.2)
42	1.4807	1.4808	15	1.4794	1.4790	10	1.4805	1.4797	15	(008)
43	1.4584	1.4592		1.4551	1.4568	6	1.4581	1.4565	15	(646)
44	-	-	-	-	-	-	1.4093	1.4097	7	(11.1.0)

Table S6. X-ray powder data for selected samples of “hibschite” (H₄O₄-substituted grossular) from Măgureaua Vaței.

	Sample 2161			Sample 2301			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	d _{meas.} (Å)	d _{calc.} (Å)	I/I ₀	
1	4.2011	4.2111	4	4.2046	4.2261	5	(220)
2	2.9829	2.9908	65	2.9816	2.9883	35	(400)
3	2.6679	2.6750	100	2.6697	2.6728	100	(420)
4	2.5494	2.5506	10	2.5464	2.5484	8	(332)
5	2.4365	2.4420	40	2.4375	2.4399	35	(422)
6	2.1842	2.1842	17	2.1824	2.1824	18	(521)
7	1.9386	1.9407	5	-	-	-	(611)
8	1.7254	1.7267	18	1.7271	1.7253	15	(444)
9	1.6901	1.6918	2	1.6871	1.6905	5	(543)
10	1.6585	1.6590	30	1.6579	1.6576	20	(640)
11	1.6302	1.6280	2	-	-	-	(721)
12	1.5973	1.5986	65	1.5982	1.5973	55	(642)
13	1.4979	1.4954	20	1.4951	1.4941	12	(800)
14	1.4706	1.4726	3	1.4752	1.4713	4	(741)
15	1.4515	1.4507	2	1.4513	1.4495	-	(820)
16	1.4285	1.4299	7	1.4315	1.4287	3	(653)
17	1.4091	1.4099	1	1.4069	1.4087	7	(822)
18	-	-	-	1.3535	1.3534	3	(752)
19	1.3388	1.3375	3	1.3374	1.3364	4	(840)
20	1.3033	1.3053	17	1.3058	1.3042	-	(842)
21	-	-	-	1.2875	1.2889	-	(655)
22	-	-	-	1.2733	1.2742	5	(664)
23	1.2355	1.2339	9	1.2341	1.2329	7	(932)
24	1.2053	1.2085	4	1.2091	1.2074	4	(941)
25	1.1645	1.1620	1	1.1590	1.1610	5	(943)
26	1.1112	1.1108	3	-	-	-	(10.4.0)
27	-	-	-	1.0995	1.1003	-	(961)

Table S7. X-ray powder data for selected samples of secondary calcite from Măgureaua Vaței.

	Sample 2158 ⁽¹⁾			Sample 2292 ⁽²⁾			Sample 2299 ⁽²⁾			(hkl)
	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	
1	3.8541	3.8533	15	3.8494	3.8555	27	3.8312	3.8536	7	(012)
2	3.0348	3.0345	100	3.0411	3.0369	100	3.0301	3.0359	100	(104)
3	2.8433	2.8427	5	2.8471	2.8460	4	2.8426	2.8458	4	(006)
4	2.4940	2.4938	12	2.4978	2.4948	23	2.4956	2.4933	11	(110)
5	2.2838	2.2838	16	2.2863	2.2849	25	2.2827	2.2838	34	(113)
6	2.0935	2.0936	16	2.0954	2.0946	27	2.0902	2.0933	32	(202)
7	1.9263	1.9267	7	1.9285	1.9278	10	1.9301	1.9268	3	(024)
8	1.9120	1.9118	13	1.9143	1.9138	18	1.9173	1.9134	16	(018)
9	1.8748	1.8747	16	1.8762	1.8760	20	1.8795	1.8753	18	(116)
10	1.6249	1.6251	5	1.6264	1.6258	8	1.6244	1.6248	2	(211)
11	1.6034	1.6035	14	1.6046	1.6042	13	1.6042	1.6032	5	(122)
12	1.5864	1.5864	3	1.5883	1.5881	2	-	-	-	(1.0.10)
13	1.5246	1.5247	5	1.5257	1.5254	8	1.5257	1.5246	3	(214)
14	1.5171	1.5173	6	1.5182	1.5185	5	1.5167	1.5179	13	(208)
15	1.5089	1.5089	4	1.5100	1.5102	4	-	-	-	(119)
16	1.4727	1.4726	3	1.4729	1.4734	5	1.4712	1.4727	2	(125)
17	1.4397	1.4398	6	1.4403	1.4404	9	-	-	-	(300)
18	1.4214	1.4214	4	1.4231	1.4230	3	-	-	-	(0.0.12)
19	1.3564	1.3563	2	-	-	-	-	-	-	(217)
20	1.3384	1.3385	4	1.3392	1.3397	3	1.3381	1.3393	2	(0.2.10)
21	1.2965	1.2962	4	1.2975	1.2971	3	1.2983	1.2966	4	(128)
22	1.2838	1.2844	3	1.2804	1.2852	3	-	-	-	(306)
23	1.2472	1.2469	3	1.2474	1.2474	3	1.2466	1.2466	2	(220)
24	1.2348	1.2349	3	1.2327	1.2361	2	1.2350	1.2358	2	(1.1.12)
25	1.1860	1.1863	2	1.1832	1.1868	1	-	-	-	(312)
26	1.1793	1.1794	3	1.1802	1.1803	3	1.1759	1.1799	3	(2.1.10)
27	1.1533	1.1533	3	1.1535	1.1539	6	1.1525	1.1532	4	(134)
28	1.1421	1.1418	3	1.1423	1.1425	3	1.1469	1.1419	3	(226)
29	1.1256	1.1243	2	1.1275	1.1252	1	-	-	-	(1.2.11)
30	-	-	-	1.0666	1.0622	1	-	-	-	(2.0.14)
31	-	-	-	1.0463	1.0473	4	1.0449	1.0467	3	(404)
32	-	-	-	1.0463	1.0450	3	1.0449	1.0445	3	(318)

(1) Sample from Crămuț Valley; (2) Sample from Cerboia Valley.

Table S8. X-ray powder data for selected samples of kaolinite from Măgureaua Vaței (sample 1519).

Reflection No.	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	(hkl)	Reflection no.	d _{meas.} (Å)	d _{calc.} (Å)	I/I _o	(hkl)
1	7.0601	7.1379	100	(002)	44	1.4914	1.4941	7	(029)
2	4.3829	4.4038	32	(110)	45	1.4834	1.4862	9	(154)
3	4.3829	4.4027	32	(-111)	46	1.4834	1.4859	9	(-155)
4	3.7901	3.7758	18	(022)	47	1.4696	1.4679	3	(330)
5	3.5914	3.5690	8	(004)	48	1.4696	1.4676	3	(-333)
6	2.5345	2.5340	5	(200)	49	1.4503	1.4521	2	(062)
7	2.5345	2.5332	5	(-202)	50	1.4385	1.4379	9	(331)
8	2.4701	2.4816	5	(131)	51	1.4385	1.4374	9	(-334)
9	2.4701	2.4816	5	(-132)	52	1.4254	1.4243	3	(119)
10	2.2097	2.2014	8	(-222)	53	1.4254	1.4236	3	(-1.1.10)
11	2.1683	2.1749	9	(133)	54	1.4101	1.4118	2	(155)
12	2.1683	2.1740	9	(-134)	55	1.4101	1.4114	2	(-156)
13	2.1325	2.1275	2	(221)	56	1.3952	1.3924	3	(-229)
14	2.1325	2.1266	2	(-223)	57	1.3952	1.3920	3	(048)
15	2.0137	2.0186	4	(222)	58	1.3031	1.3007	3	(1.1.10)
16	2.0137	2.0153	4	(043)	59	1.3031	1.3002	3	(-1.1.11)
17	2.0004	1.9975	4	(134)	60	1.2952	1.2978	11	(-248)
18	2.0004	1.9966	4	(-135)	61	1.2952	1.2970	11	(-1.3.10)
19	1.9664	1.9706	6	(116)	62	1.2653	1.2670	5	(400)
20	1.9664	1.9694	6	(-117)	63	1.2653	1.2666	5	(-404)
21	1.9058	1.9128	4	(204)	64	1.2595	1.2586	4	(066)
22	1.9058	1.9111	4	(-206)	65	1.2359	1.2365	7	(-422)
23	1.8550	1.8539	5	(027)	66	1.2301	1.2318	8	(-423)
24	1.8261	1.8267	2	(135)	67	1.2301	1.2300	8	(-338)
25	1.8261	1.8259	2	(-136)	68	1.2244	1.2239	7	(171)
26	1.7568	1.7560	45	(-226)	69	1.2244	1.2239	7	(-172)
27	1.7568	1.7548	45	(045)	70	1.2205	1.2185	5	(420)
28	1.7568	1.7510	45	(117)	71	1.2205	1.2182	5	(-424)
29	1.6813	1.6832	8	(-241)	72	1.2087	1.2105	4	(-406)
30	1.6813	1.6823	8	(-311)	73	1.2087	1.2089	4	(-265)
31	1.6813	1.6791	8	(-151)	74	1.1888	1.1891	4	(-3.1.10)
32	1.6150	1.6159	9	(-314)	75	1.1888	1.1887	4	(158)
33	1.6150	1.6134	9	(-153)	76	1.1839	1.1826	2	(352)
34	1.5955	1.5993	11	(206)	77	1.1735	1.1721	2	(264)
35	1.5955	1.5979	11	(-208)	78	1.1735	1.1717	2	(-266)
36	1.5867	1.5872	29	(242)	79	1.1358	1.1350	1	(423)
37	1.5867	1.5866	29	(-244)	80	1.1358	1.1343	1	(-427)
38	1.5297	1.5299	7	(137)	81	1.1321	1.1326	6	(404)
39	1.5297	1.5293	7	(-138)	82	1.1321	1.1317	6	(-408)
40	1.5210	1.5228	5	(243)	83	1.1204	1.1211	3	(-2.2.12)
41	1.5210	1.5221	5	(-245)	84	1.1204	1.1210	3	(0.4.11)
42	1.5021	1.5050	4	(226)	85	1.1119	1.1123	2	(080)
43	1.5021	1.5033	4	(047)	86	1.1119	1.1123	2	(-3.3.10)