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Supplementary materials

Krasnoshteinite, $Al_8[B_2O_4(OH)_2](OH)_{16}Cl_4 \cdot 7H_2O$, a New Microporous Mineral with a Novel Type of Borate Polyanion

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Table S1. Anisotropic displacement parameters of non-hydrogen atoms in the structure of krasnoshteinite.

Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al1	0.0086(7)	0.0132(7)	0.0093(6)	-0.0004(5)	0.0045(5)	-0.0016(5)
Al2	0.0064(7)	0.0142(7)	0.0099(6)	0.0002(5)	0.0049(5)	0.0010(5)
Al3	0.0076(7)	0.0152(7)	0.0081(6)	0.0009(5)	0.0046(5)	0.0013(5)
Al4	0.0062(7)	0.0139(7)	0.0087(6)	0.0000(5)	0.0053(5)	-0.0011(5)
Al5	0.0050(5)	0.0157(6)	0.0109(6)	-0.0014(5)	0.0042(4)	0.0000(4)
Al6	0.0060(6)	0.0158(7)	0.0103(6)	-0.0005(5)	0.0043(5)	-0.0003(5)
Al7	0.0066(7)	0.0138(7)	0.0088(6)	0.0008(5)	0.0039(5)	0.0012(5)
Al8	0.0093(6)	0.0161(7)	0.0103(6)	-0.0011(5)	0.0059(5)	0.0017(5)
B1	0.0053(19)	0.014(2)	0.012(2)	0.005(2)	0.0031(16)	-0.004(2)
B2	0.005(2)	0.015(2)	0.016(2)	0.0003(19)	0.0023(19)	0.0021(18)
Cl1	0.0222(6)	0.0312(7)	0.0437(8)	0.0089(7)	0.0185(5)	0.0043(6)
Cl2	0.0226(6)	0.0181(6)	0.0557(9)	0.0020(7)	0.0131(6)	0.0012(6)
Cl3	0.0253(7)	0.0472(9)	0.0260(7)	0.0109(6)	0.0109(5)	0.0102(6)
Cl4	0.0470(9)	0.0315(7)	0.0269(7)	-0.0014(6)	0.0009(6)	-0.0106(7)
O1	0.0091(16)	0.0120(16)	0.0090(15)	-0.0011(12)	0.0047(12)	0.0001(13)
O2	0.0109(18)	0.024(2)	0.0200(18)	0.0065(15)	0.0077(14)	0.0021(15)
O3	0.0176(15)	0.0164(15)	0.0102(15)	0.0032(14)	0.0050(12)	0.0034(16)
O4	0.0054(16)	0.0150(16)	0.0105(15)	0.0002(13)	0.0023(12)	-0.0046(13)
O5	0.0100(17)	0.0161(17)	0.0167(16)	0.0032(13)	0.0040(13)	-0.0013(13)
O6	0.0117(16)	0.0140(15)	0.0085(15)	0.0011(12)	0.0040(12)	0.0036(13)
O7	0.0085(17)	0.0128(16)	0.0128(15)	-0.0001(12)	0.0054(12)	-0.0020(13)
O8	0.0050(15)	0.0265(19)	0.0126(15)	0.0007(14)	0.0045(12)	0.0022(14)
O9	0.0094(16)	0.0158(16)	0.0074(14)	-0.0003(12)	0.0045(12)	0.0016(13)
O10	0.0093(17)	0.0153(16)	0.0106(15)	-0.0009(13)	0.0022(12)	0.0009(13)
O11	0.0128(17)	0.0140(17)	0.0133(15)	0.0002(13)	0.0083(13)	0.0004(13)
O12	0.0041(15)	0.0145(16)	0.0220(17)	0.0019(13)	0.0061(13)	-0.0009(12)
O13	0.0063(15)	0.0122(16)	0.0106(15)	-0.0021(12)	0.0050(12)	-0.0031(12)
O14	0.0095(16)	0.0168(17)	0.0130(15)	-0.0006(13)	0.0064(12)	-0.0041(13)
O15	0.0167(14)	0.0180(16)	0.0124(15)	-0.0008(14)	0.0111(12)	-0.0021(15)

O16	0.0089(17)	0.0176(17)	0.0251(18)	-0.0033(15)	0.0080(14)	-0.0022(13)
O17	0.0112(16)	0.0155(17)	0.0101(15)	0.0001(12)	0.0043(12)	0.0033(13)
O18	0.0205(18)	0.0247(19)	0.0156(17)	0.0040(14)	0.0060(14)	-0.0030(15)
O19	0.0061(15)	0.0125(16)	0.0093(14)	0.0022(12)	0.0028(11)	-0.0008(12)
O20	0.0050(15)	0.0126(15)	0.0101(14)	-0.0022(12)	0.0042(11)	-0.0016(12)
O21	0.0030(15)	0.0188(17)	0.0155(16)	-0.0035(13)	0.0041(12)	-0.0003(13)
O22	0.0130(17)	0.0195(18)	0.0136(16)	0.0012(13)	0.0070(13)	-0.0068(14)
O23	0.0080(17)	0.0143(16)	0.0154(16)	-0.0041(13)	0.0046(12)	-0.0023(13)
O24	0.023(2)	0.0214(18)	0.0202(18)	0.0051(14)	0.0063(15)	0.0102(15)
O25	0.0083(16)	0.0246(18)	0.0095(15)	-0.0004(13)	0.0010(12)	-0.0038(14)
O26	0.0088(17)	0.024(2)	0.0185(17)	-0.0027(15)	0.0029(13)	0.0027(15)
O27	0.025(2)	0.027(2)	0.0218(19)	0.0080(16)	0.0136(16)	0.0097(16)
O28	0.042(3)	0.030(2)	0.037(2)	0.0034(19)	0.017(2)	0.0062(19)
O29	0.043(3)	0.079(4)	0.045(3)	-0.013(3)	0.006(2)	0.022(3)

Table S2. Bond valence calculations for krasnoshteinite. Bond-valence parameters for Al-O and B-O were taken from [14] and for H-bonding from [15,16].

	Al1	Al2	Al3	Al4	Al5	Al6	Al7	Al8	B1	B2		H-bonding	
O1 = OH	0.39	0.49	0.35								1.23	-0.10 (O29) -0.09 (Cl4)	1.04
O2 = H_2O	0.47										0.47	-0.26 (Cl4) -0.17 (Cl1)	0.04
O3 = OH	0.60						0.62				1.22	-0.12 (Cl3)	1.10
O4 = OH		0.43	0.41	0.47							1.31	-0.20(Cl2)	1.11
O5 = OH			0.62		0.54						1.16	-0.08 (Cl1)	1.08
O6 = OH		0.61				0.57					1.18	-0.19 (O15) -0.08 (O18) +0.18 (O16)	1.09
O7 = OH		0.44		0.43		0.40					1.27	-0.24 (Cl2)	1.03
O8 = OH				0.60	0.51						1.11	-0.11 (O26)	1.00
O9 = OH		0.60			0.53						1.13	-0.15 (Cl4)	0.98
O10 = OH	0.54		0.55								1.09	-0.08(Cl2) +0.10 (O23) +0.17(O27)	1.28
O11 = O	0.47	0.52							0.94		1.93		1.93
O12 = OH					0.49					0.70	1.19	-0.14 (Cl2)	1.05
O13 = O				0.53			0.44		0.98		1.95		1.95
O14 = OH	0.59							0.53			1.12	-0.22 (Cl3)	0.90
O15 = O									1.08	0.72	1.80	+0.19 (O6) +0.20 (O16)	2.19
O16 = H_2O					0.46						0.46	-0.20 (O15) -0.18 (O6) -0.14 (Cl2) -0.08(Cl3)	-0.14
O17 = OH			0.61					0.56			1.17	-0.24 (O18)	0.93
O18 = OH										0.79	0.79	+0.08(O6) +0.24(O17) -0.19 (Cl3) +0.18(O29)	1.10
O19 = OH				0.51		0.37	0.44				1.32	-0.22 (O28)	1.10
O20 = O			0.56	0.60						0.81	1.97		1.97
O21 = OH					0.52	0.59					1.11	-0.12 (Cl1)	0.99
O22 = OH						0.61		0.54			1.15	-0.18 (Cl3)	0.97
O23 = OH						0.57	0.58				1.15	-0.11 (Cl1) -0.10 (O10)	0.94

O24 = H_2O								0.42			0.42	-0.13 (Cl1) -0.20 (O29)	0.09
O25 = OH							0.56	0.50			1.06	-0.14(Cl4)	0.92
O26 = H_2O							0.43				0.43	+0.11 (O8) -0.20(Cl1) -0.24(Cl4)	0.10
O27 = H_2O								0.48			0.48	-0.17 (O10) -0.07(Cl1) -0.26(O28)	-0.02
O28 = H_2O											0	+0.22 (O19) +0.26 (O27) -0.23 (Cl3) -0.21(O29)	0.04
O29 = H_2O											0	+0.10 (O1) +0.20 (O24) +0.21 (O28) -0.16 (Cl2) -0.18(O18)	0.17
Cl1											0	+0.17(O2) +0.08(O5) +0.12(O21) +0.11(O23) +0.13(O24) +0.20 (O26)+0.07(O27)	0.88
Cl2											0	+0.20 (O4) +0.24(O7) +0.08 (O10) +0.14 (O12) +0.14 (O16) +0.16 (O29)	0.96
Cl3											0	+0.12 (O3) +0.22(O14) +0.08(O16) +0.19 (O18) +0.18 (O22) +0.23 (O28)	1.02
Cl4											0	+0.09 (O1) +0.26 (O2) +0.15 (O9) +0.14(O25) +0.24(O26)	0.88
	3.06	3.09	3.10	3.14	3.05	3.11	3.07	3.03	3.00	3.02			

Table S3. Powder X-ray diffraction data (*d* in Å) of krasnoshteinite.

I_{obs}	d_{obs}	I_{calc}*	d_{calc}**	*h k l*
41	**10.81**	98	10.831	001
26	**8.65**	43	8.659	011
67	**8.38**	67	8.373	100
100	**7.22**	100	7.206	020
5	6.85	8	6.855	-111
9	5.995	11	6.000	021
5	5.863	5	5.861	101
22	**5.452**	37, 11	5.462, 5.429	120, 111
12	5.288	8, 8	5.292, 5.291	-102, -121
2	5.063	1	5.070	012
2	4.967	1	4.967	-112
2	4.548	1	4.547	121
6	4.385	6	4.392	031
11	4.330	13	4.329	022
5	4.266	5	4.265	-122
9	4.165	14, 2	4.167, 4.161	130, -211
6	4.086	10	4.090	-131
8	3.759	12	3.762	-212
19	3.720	14, 15	3.722, 3.715	-221, 131
21	**3.610**	27, 10, 1	3.620, 3.610, 3.608	220, 003, -113
4	3.504	4	3.502	013
19	3.421	14, 26	3.428, 3.419	-222, 041
7	3.310	6, 5	3.310, 3.310	-123, 140
5	3.270	9	3.271	-141
18	3.225	11, 6	3.228, 3.223	023, -231
13	3.206	23	3.203	221
2	3.155	1, 1	3.156, 3.152	230, -213
2	3.099	1	3.096	132
22	**3.019**	2, 18	3.026, 3.016	-232, 103
8	2.977	8	2.978	-142
11	2.948	5, 9	2.948, 2.945	-223, -133
2	2.885	2	2.886	033
22	**2.826**	16	2.824	-104
12	2.774	19, 1, 3, 3, 9	2.791, 2.786, 2.780, 2.774, 2.772	300, 051, -312, -241, -114
2	2.724	1	2.726	150
5	2.697	5, 6	2.700, 2.692	-321, 142
6	2.646	6, 1	2.646, 2.646	-204, -242
10	2.590	6, 9	2.590, 2.587	-143, 151
4	2.552	5, 2, 3	2.557, 2.554, 2.550	-313, 133, 043

5	2.540	5, 3, 1	2.545, 2.538, 2.535	052, 241, 024
2	2.486	2	2.484	-224
2	2.441	5	2.441	-332
3	2.406	3	2.405	-243
4	2.376	1, 7	2.380, 2.374	213, 250
6	2.352	2, 5	2.352, 2.348	114, 152
3	2.314	4	2.313	143
3	2.296	2, 2, 2	2.301, 2.296, 2.288	-304, -161, 223
4	2.272	5	2.272	-314
3	2.255	1, 5	2.263, 2.253	124, 053
4	2.225	3, 1, 3	2.227, 2.223, 2.223	-342, -144, 161
6	2.197	2, 7	2.198, 2.196	-205, 062
10	2.173	3, 12	2.175, 2.173	-401, -215
5	2.159	3, 4	2.165, 2.157	044, -125
7	2.104	7	2.103	-225
4	2.083	1, 2, 9	2.084, 2.084, 2.082	153, 260, -421
8	2.068	7, 11	2.071, 2.066	410, 162
8	2.047	12, 1	2.045, 2.045	-135, -262
3	2.018	3, 2	2.019, 2.017	-163, -154
3	2.000	4, 1	2.000, 1.999	063, -235
3	1.995	1, 3	1.994, 1.988	-315, 144
3	1.977	2, 4	1.980, 1.975	-432, 035
2	1.950	3, 1, 2	1.953, 1.949, 1.949	401, -254, 224
6	1.925	14	1.925	072
5	1.918	5, 7	1.919, 1.915	-172, -145
2	1.898	1, 2	1.903, 1.896	351, 125
2	1.889	3, 2	1.886, 1.885	323, 421
3	1.861	3, 3, 4	1.865, 1.861, 1.858	234, -442, 262
2	1.851	2, 1	1.853, 1.848	-361, -216
5	1.834	1, 7	1.835, 1.832	172, -362
3	1.822	3	1.820	-272
4	1.806	1, 4, 1, 1, 3	1.810, 1.810, 1.806, 1.805, 1.804	333, 431, -434, 006, -226
3	1.792	3, 2, 1	1.791, 1.789, 1.788	016, 073, 402
2	1.781	1, 3	1.782, 1.778	-405, -264
2	1.765	2, 1	1.769, 1.761	-415, 180
3	1.752	1, 2, 1	1.755, 1.750, 1.748	-181, -136, -255
1	1.738	1	1.737	-236
2	1.724	5	1.722	181
2	1.668	2, 2, 3	1.672, 1.667, 1.666	-523, 324, -146
2	1.657	1, 1, 2	1.658, 1.656, 1.655	116, -336, -246
1	1.633	4	1.631	520
2	1.619	1, 2, 1, 2	1.622, 1.618, 1.617, 1.617	-183, -533, 353, 451

3	1.601	6, 2	1.601, 1.598	442, 371
2	1.584	4, 2, 1	1.584, 1.581, 1.581	091, 530, 423
5	1.575	4, 4	1.574, 1.573	-156, -283
3	1.565	2, 2	1.568, 1.565	-127, -256
3	1.549	1, 2, 1, 2	1.551, 1.550, 1.547, 1.547	-543, -515, 007, 183
1	1.538	1	1.535	433
3	1.524	1, 5, 2, 3	1.526, 1.523, 1.523, 1.519	-237, -525, -137, 452
2	1.479	1, 1, 1, 3	1.483, 1.482, 1.480, 1.478	-535, 325, -337, 443
2	1.470	2, 2, 1, 6, 1	1.473, 1.471, 1.469, 1.467, 1.467	037, -193, -247, -147, -473
1	1.436	1, 3	1.435, 1.434	-293, 462
1	1.423	2, 1, 2	1.427, 1.424, 1.422	-622, -526, 047
2	1.406	2, 1, 1, 1	1.409, 1.409, 1.409, 1.405	-621, -456, -185, -218
2	1.398	5	1.396	345

*For the calculated pattern, only reflections with intensities ≥1 are given; **for the unit-cell parameters calculated from single-crystal data; the strongest reflections are marked in boldtype.