

1 **Table S1.** Bond-valence sums (in valence units, v.u.) in batoniite.

	Al(1)	Al(2)	Al(3)	Al(4)	Al(5)	Al(6)	Al(7)	Al(8)	S(1)	S(2)	S(3)	S(4)	S(5)	Σ_{anions}	Σ_{anions}^*
O(1)	0.49													0.49	0.04
O(2)	0.58	0.53												1.11	0.94
O(3)	0.57		0.58											1.15	1.00
O(4)	0.44													0.44	0.00
O(5)	0.51													0.51	-0.02
O(6)	0.53													0.53	0.00
O(7)		0.45	0.42											1.29	1.13
O(8)		0.55	0.42	0.58										1.13	0.96
O(9)		0.54	0.55											1.09	0.98
O(10)		0.58	0.57											1.15	0.96
O(11)		0.50												0.50	0.15
O(12)			0.56	0.58										1.14	0.98
O(13)				0.44										0.44	0.09
O(14)				0.53										0.53	0.07
O(15)				0.50										0.50	0.10
O(16)				0.43										0.43	0.04
O(17)					0.47									0.47	-0.02
O(18)					0.57	0.57								1.14	0.97
O(19)					0.59		0.56							1.15	0.98
O(20)					0.47									0.47	0.02
O(21)					0.49									0.49	0.06
O(22)					0.50									0.50	0.09
O(23)						0.58		0.57						1.15	0.94
O(24)						0.56	0.54							1.10	1.00
O(25)						0.42	0.47							1.30	1.09
O(26)						0.41									
O(27)						0.55	0.48							1.03	0.93
O(28)							0.55							0.55	0.03
O(29)							0.52	0.57						1.09	0.94
O(30)								0.50						0.50	0.05
O(31)								0.45						0.45	0.05
O(32)								0.50						0.50	-0.01
O(33)								0.45						0.45	0.00
O(34)									1.50					1.50	2.04
O(35)									1.57					1.57	1.98
O(36)									1.53					1.53	2.00
O(37)									1.48					1.48	2.05
O(38)										1.54				1.54	2.04
O(39)										1.45				1.45	1.83 ¹
O(40)											1.52			1.52	1.96
O(41)											1.63			1.63	2.04
O(42)												1.49			2.18 ¹
O(43)												1.49		1.49	1.99
O(44)												1.66		1.66	2.13
O(45)												1.57		1.57	1.99
O(46)												1.58		1.58	2.15
O(47)													1.49	1.49	2.16
O(48)													1.62	1.62	2.06
O(49)													1.57	1.57	2.10
O(50)													1.56	1.56	2.08
O(51)														1.53	2.11
O(52)														1.55	2.07
Ow(1)														1.52	2.08
Ow(2)														1.60	2.01
Ow(3)														-	0.15
Ow(4)														-	-0.07
Ow(5)														-	0.12
														-	0.06
														-	0.07

Σ_{cations}	3.12	3.15	3.10	3.06	3.09	3.09	3.12	3.04	6.08	6.14	6.30	6.24	6.20
Theor.	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	6.00	6.00	6.00	6.00	6.00
Note: * corrected for H-bonds (see Table 5). ¹ if acceptor of H-bond from O(15).													

3 **Table S2.** X-ray powder diffraction data (d in Å) for batoniite.

I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\ k\ l$	I_{obs}	d_{obs}	d_{calc}	I_{calc}	$h\ k\ l$
s	11.1	10.97	91	0 1 1	-	-	3.370	6	-1 -3 2
mw	10.5	10.37	35	0 0 2			3.324	5	2 -2 2
vw	9.3	9.16	5	1 0 0	vw	3.318	3.298	14	-1 2 5
s	8.5	8.50	86	1 0 1			3.290	9	0 -3 3
m	8.3	8.25	30	-1 0 1	w	3.220	3.231	2	1 3 4
s	7.5	7.45	100	1 1 0			3.219	3	0 -1 6
		7.41	9	0 -1 2			3.082	8	2 3 0
vw	6.9	6.82	5	-1 1 1			3.077	9	1 -3 3
vw	6.4	6.33	6	0 1 3			3.061	5	1 -1 6
w	6.0	5.98	10	-1 1 2	w	3.055	3.057	6	2 3 2
		5.95	10	0 2 1			3.054	12	1 -2 5
mw	5.79	5.76	7	-1 -1 2			3.042	10	-1 -2 5
-	-	5.63	7	1 0 3			3.002	6	-3 0 1
mw	5.46	5.48	18	0 2 2			2.997	10	-2 -3 1
		5.41	7	-1 0 3	-	-	2.936	6	-1 2 6
-	-	5.36	7	1 1 3	vw	2.895	2.887	8	2 -3 1
ms	5.20	5.19	42	0 0 4			2.835	12	-1 3 4
-	-	4.986	6	0 1 4	vw	2.835	2.835	6	3 0 3
-	-	4.935	14	0 -2 2			2.821	5	-1 4 1
-	-	4.909	10	1 -2 0			2.808	5	1 -4 0
		4.862	36	-1 2 1	w	2.796	2.808	9	-3 1 2
ms	4.87	4.845	6	1 2 2			2.803	5	2 3 4
		4.835	58	-1 -2 1			2.699	9	-1 4 3
		4.828	13	0 2 3	w	2.699	2.697	5	-2 -3 3
vw	4.58	4.562	10	0 -1 4			2.673	6	3 1 4
		4.490	13	1 1 4	w	2.594	2.593	5	0 0 8
w	4.46	4.436	18	-1 0 4	vw	2.527	2.538	6	-3 1 4
w	4.34	4.325	59	2 1 1			2.454	7	1 -2 7
w	4.29	4.252	56	2 0 2	w	2.461	2.444	5	-1 4 5
		4.131	9	-2 1 1	vw	2.421	2.411	5	3 2 5
		4.127	5	-2 0 2	w	2.372	2.370	6	-1 -1 8
vs	4.08	4.055	43	-1 -1 4	vw	2.341	2.331	7	2 -3 5
		4.014	36	0 3 1	vw	2.316	2.290	6	-1 5 2
		3.994	6	0 3 0	vw	2.243	2.245	6	0 2 9
vw	3.884	3.889	10	0 3 2	vw	2.221	2.226	4	3 -2 5
		3.863	9	1 -2 3	vw	2.198	2.196	8	4 1 3
		3.838	19	1 0 5	vw	2.121	2.132	7	4 -1 3
ms	3.793	3.804	16	1 1 5			2.085	2	1 3 9
		3.781	25	0 -1 5	vw	2.073	2.083	2	2 -5 0
-	-	3.726	5	1 3 0			2.069	2	1 5 6
-	-	3.723	5	2 2 0			2.063	2	-4 0 4
-	-	3.712	6	-1 2 4	w	2.017	2.027	6	-2 -2 8
w	3.646	3.661	19	1 3 2	vw	1.976			
		3.623	12	0 2 5	vw	1.944			
		3.605	13	-2 1 3	w	1.896			
s	3.563	3.600	14	1 -3 0	w	1.864			
		3.558	18	2 -2 0	vw	1.832			
		3.550	40	-2 -1 3	w	1.763			
		3.531	7	-2 2 1	vw	1.735			
mw	3.457	3.445	23	1 2 5	vw	1.722			
		3.408	12	-2 2 2	vw	1.685			

Intensity and d_{hkl} were calculated using the software *PowderCell* 2.3 (Kraus and Nolze, 1996) on the basis of the structural model given in Table 3. For $d_{\text{obs}} > 2$ Å, observed and calculated X-ray lines are compared, showing only the reflections with $I_{\text{calc}} > 5$. I_{obs} were visually estimated: vs = very strong; s = strong; ms = medium-strong; m = medium; mw = medium-weak; w = weak; and vw = very weak. The eight strongest reflections are given in bold.