Supporting information for: Structure, Vibrational Spectra and ^{11}B-NMR Chemical Shift of $Na_8[AlSiO_4]_6(B(OH)_4)_2$: Comparison of Theory and Experiment

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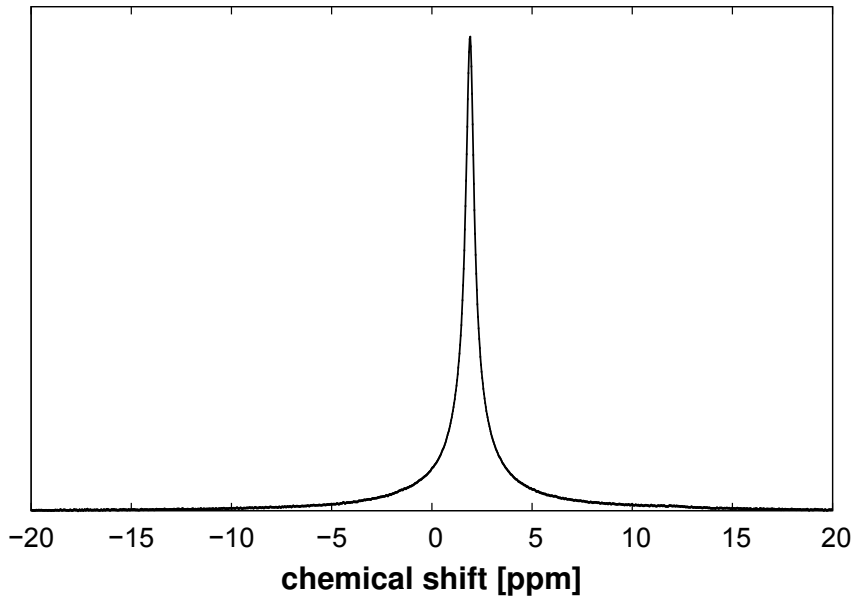

Figure S1: Experimental ^{11}B-NMR spectrum of $Na_8[AlSiO_4]_6(^{11}B(OH)_4)_2$.

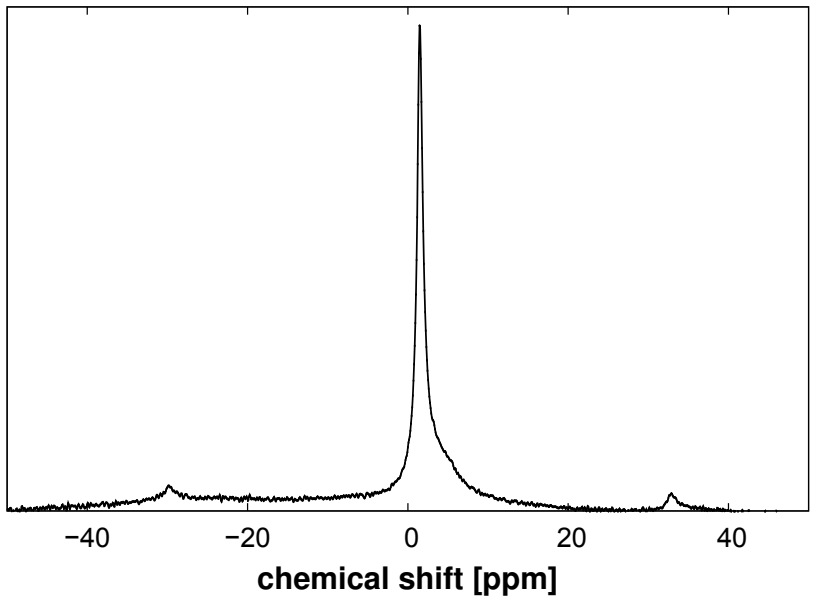

Figure S2: Experimental ^{1}H-NMR spectrum of $Na_8[AlSiO_4]_6(^{11}B(OH)_4)_2$.

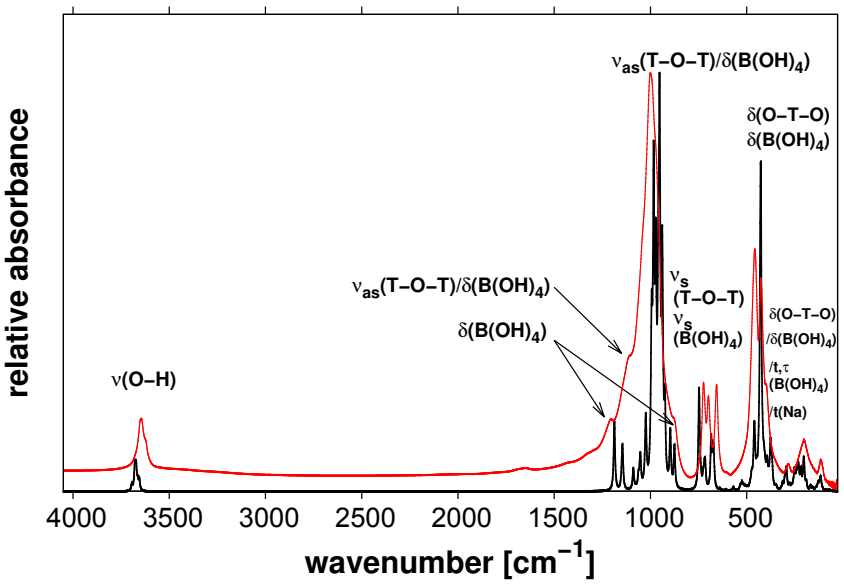

Figure S3: Measured (red) and calculated (black) IR vibrational spectrum (relative absorbance) of $Na_8[AlSiO_4]_6(^{11}B(OH)_4)_2$.

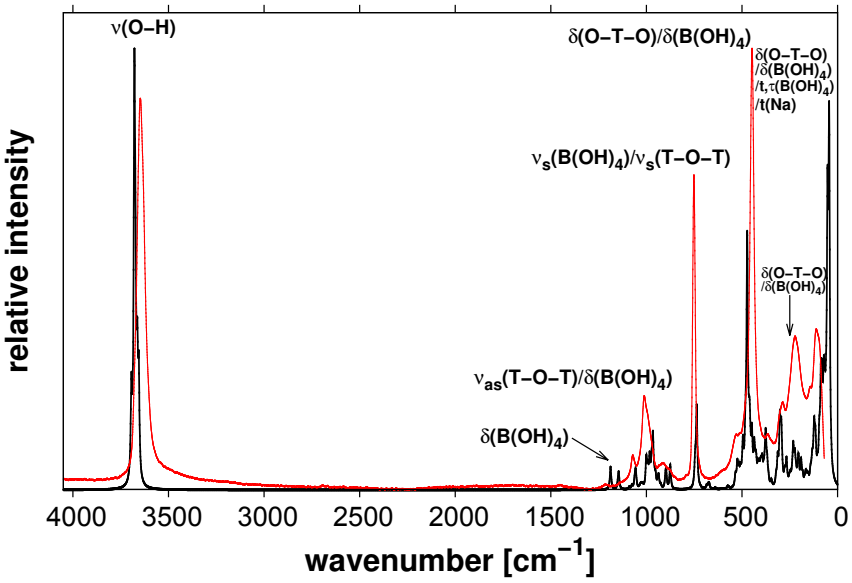

Figure S4: Measured (red) and calculated (black) Raman vibrational spectrum (relative intensity) of $Na_8[AlSiO_4]_6(^{11}B(OH)_4)_2$.

Table S1: Experimental atomic positions of $NaB(OH)_4$-SOD at 295 K in fractional units.

Atom	Wyckoff Pos.	x/a	y/a	z/a	occ.
Na	8e	0.1827	0.1827	0.1827	0.499
Na	8e	0.2038	0.2038	0.2038	0.152
Na	8e	0.2274	0.2274	0.2274	0.18
Na	8e	0.1963	0.1963	0.1963	0.113
Al	6d	0.25	0	0.5	1
Si	6c	0.25	0.5	0	1
O(cage)	24i	0.1422	0.4523	0.1522	1
B	24i	-0.0755	0.0028	-0.0256	0.0702
O(molecule)	24i	0.0363	0.1592	-0.0462	0.0702
O(molecule)	24i	0.0503	-0.0868	0.8503	0.0702
O(molecule)	24i	0.8292	0.0080	-0.0219	0.0702
O(molecule)	24i	0.0541	-0.053	0.1154	0.0702
O(water)	24i	0.431	0.423	0.395	0.0821

Table S2: Results of the structure optimization of $Na_8[AlSiO_4]_6(B(OH)_4)_2$ (PWGGA, CRYSTAL basis sets): Atomic positions in fractional units of the lattice constant $a = 8.94$.

atom	x/a	y/a	z/a	atom	x/a	y/a	z/a
Na(1)	0.1652	0.1898	0.1626	O(12)	0.4392	0.8654	0.8248
Na(2)	0.7977	0.8336	0.1656	O(13)	0.9337	0.6611	0.6286
Na(3)	0.1937	0.8132	0.8029	O(14)	0.0582	0.3607	0.6282
Na(4)	0.8117	0.1821	0.7959	O(15)	0.0617	0.6705	0.3427
Na(5)	0.6738	0.7097	0.6656	O(16)	0.9370	0.3684	0.3478
Na(6)	0.3175	0.3422	0.6626	O(17)	0.6469	0.6528	0.9279
Na(7)	0.3253	0.6956	0.2959	O(18)	0.6341	0.9633	0.6310
Na(8)	0.6942	0.3137	0.3030	O(19)	0.3444	0.3678	0.9232
Al(1)	0.2453	1.0146	0.4924	O(20)	0.6419	0.0682	0.3248
Al(2)	0.7468	0.0141	0.4804	O(21)	0.3438	0.6507	0.0420
Al(3)	0.4927	0.2620	0.9925	O(22)	0.3476	0.0803	0.6473
Al(4)	1.0003	0.5162	0.2376	O(23)	0.6441	0.3711	0.0566
Al(5)	0.4933	0.7606	0.9804	O(24)	0.3585	0.9486	0.3476
Al(6)	0.9911	0.5071	0.7376	B(1)	0.9959	0.0138	0.9919
Si(1)	0.2438	0.5078	0.9846	O(1-1)	0.1320	0.9255	0.0225
Si(2)	0.7442	0.5106	0.9880	H(1-1)	0.1155	0.8485	0.0981
Si(3)	0.9996	0.2636	0.4846	O(1-2)	0.9330	0.0612	0.1380
Si(4)	0.4905	1.0119	0.2375	H(1-2)	0.8465	0.1265	0.1252
Si(5)	0.9968	0.7632	0.4880	O(1-3)	0.0431	0.1499	0.9096
Si(6)	0.4955	1.0169	0.7375	H(1-3)	0.1266	0.1346	0.8408
O(1)	0.1467	0.4491	0.1282	O(1-4)	0.8728	0.9311	0.9156
O(2)	0.8462	0.5736	0.1286	H(1-4)	0.9029	0.8714	0.8292
O(3)	0.1389	0.5704	0.8478	B(2)	0.4935	0.5115	0.4919
O(4)	0.8369	0.4457	0.8427	O(2-1)	0.4462	0.5744	0.6381
O(5)	0.1395	0.1630	0.4232	H(2-1)	0.3809	0.6609	0.6252
O(6)	0.4271	0.1598	0.1473	O(2-2)	0.5819	0.3754	0.5225
O(7)	0.8546	0.8604	0.4279	H(2-2)	0.6589	0.3919	0.5981
O(8)	0.5587	0.1488	0.8476	O(2-3)	0.5763	0.6346	0.4156
O(9)	0.1363	0.8633	0.5566	H(2-3)	0.6360	0.6045	0.3292
O(10)	0.5441	0.8733	0.1309	O(2-4)	0.3575	0.4642	0.4096
O(11)	0.8567	0.1636	0.5420	H(2-4)	0.3729	0.3808	0.3408