Density functional theory study of the magnetic shielding mechanism for ^{11}B in pentaborate minerals: ulexite and probertite

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SUPPORTING INFORMATION

Table S1 Comparison of bond distances (Å) in probertite between XRD and LAPW+LO-optimized structure

Bond	LAPW+LO	XRD[15]	Bond	LAPW+LO	XRD[15]
Ca-O5	2.4096	2.4000	B2-O4	1.4778	1.4617
Ca-O8	2.4265	2.4376	B2-O6	1.4804	1.4685
Ca-O12	2.4306	2.4456	B2-O5	1.4834	1.4867
Ca-O10	2.4340	2.4482	B2-O7	1.4948	1.4856
Ca-O4	2.4650	2.4701	Mean	1.4841	1.4756
Ca-O6	2.4687	2.5074	B4-O11	1.4676	1.4525
Ca-OH1	2.5267	2.5539	B4-O6	1.4730	1.4717
Ca-O6	2.7077	2.6942	B4-O8	1.5015	1.4909
Mean	2.4836	2.4946	B4-O9	1.5056	1.4955
Na-O9	2.3465	2.3474	Mean	1.4869	1.4776
Na-O14	2.3476	2.3574	B3-O8	1.3667	1.358
Na-O11	2.4125	2.4292	B3-O5	1.3770	1.3701
Na-O12	2.4219	2.4297	B3-O3	1.3948	1.3746
Na-OH2	2.4588	2.4702	Mean	1.3795	1.3675
Na-O13	2.6314	2.6528	B5-O9	1.3672	1.352
Mean	2.4364	2.4477	B5-O7	1.3880	1.3699
B1-O4	1.4722	1.4665	B5-O10	1.3993	1.381
B1-OH2	1.4843	1.4644	Mean	1.3848	1.3676
B1-O3	1.4886	1.4771			
B1-OH1	1.4972	1.4807			
Mean	1.4855	1.4721			

Table S2 Comparison of hydrogen bond distances between LAPW+LO and XRD (shown in parentheses) for probertite

Donor (D)	H	Acceptor (A)	D-A (Å)	D-H (Å)	H-A (Å)
OH1	H1	O7	2.9428(2.9856)	0.9850(0.8621)	2.0818(2.2388)
OH2	H2	n.a.		0.9809(0.8205)	
O10	H3	O3	2.6966(2.7328)	1.0058(0.7540)	1.7314(2.0113)
O11	H4	OH1	2.8023(2.8229)	0.9968(0.9162)	1.8167(1.9270)
O*w*12	H5	O7	2.875(2.8772)	0.9989(0.9457)	1.9029(1.9562)
O*w*12	H6	O*w*13	2.7673(2.7806)	1.0031(0.7809)	1.8209(2.0335)
O*w*13	H7	O*w*14	2.7490(2.7666)	1.0073(0.9139)	1.7704(1.8810)
O*w*13	H8	OH2	2.8435(2.8229)	1.0033(0.9218)	1.8696(1.9238)
O*w*14	H9	O3	2.8817(2.9182)	0.9912(0.8402)	1.9187(2.0969)
O*w*14	H10	O4	2.7531(2.7373)	1.0124(0.8390)	1.7445(1.9081)