Chemistry–A European Journal

Supporting Information

$La_3B_6O_{13}(OH)$: The First Acentric High-Pressure Borate Displaying Edge-Sharing BO_4 Tetrahedra

Birgit Fuchs,[a] Gunter Heymann,[a] Xuefei Wang,[b] Abudukadi Tudi,[b] Lkhamsuren Bayarjargal,[c] Renée Siegel,[d] Adrian Schmutzler,[d] Jürgen Senker,[d] Bastian Joachim-Mrosko,[e] Andreas Saxer,[f] Zhihua Yang,[b] Shilie Pan,[b] and Hubert Huppertz*[a]

Supporting Information

$La_3B_6O_{13}(OH)$: The First Acentric High-Pressure Borate Displaying Edge-Sharing BO_4 Tetrahedra

Birgit Fuchs,[a] Gunter Heymann,[a] Xuefei Wang,[b] Abudukadi Tudi,[b] Lkhamsuren Bayarjargal,[c] Renée Siegel,[d] Adrian Schmutzler,[d] Jürgen Senker,[d] Bastian Joachim-Mrosko,[e] Andreas Saxer,[f] Zhihua Yang,[b] Shilie Pan,[b] and Hubert Huppertz*[a]

Table S1. Wyckoff positions, atomic coordinates, and equivalent isotropic displacement parameters U_{eq} /Å^2 (standard deviations in parentheses). All atoms are located at the Wyckoff position 2*a*.

Atom	*x*	*y*	*z*	U_{eq}
La1	0.4415(6)	0.3298(2)	0.7242(3)	0.0031(5)
La2	0.5239(2)	0.5025(4)	0.2729(2)	0.0032(3)
La3	0.5520(9)	0.1737(2)	0.2748(3)	0.0037(6)
B1	0.0553(5)	0.3583(2)	0.4066(3)	0.0035(3)
B2	0.0646(5)	0.6905(2)	0.4109(3)	0.0036(3)
B3	0.0202(8)	0.6832(3)	0.0758(6)	0.0031(6)
B4	0.0643(5)	0.0247(2)	0.4072(3)	0.0036(3)
B5	0.9405(3)	0.0013(4)	0.00627(2)	0.0034(2)
B6	0.0234(8)	0.3188(3)	0.00729(6)	0.0050(6)
O1	0.3534(5)	0.3366(3)	0.3899(4)	0.0043(4)
O2	0.0270(3)	0.4745(2)	0.4245(2)	0.0035(2)
O3	0.8878(5)	0.3300(3)	0.2454(3)	0.0035(4)
O4	0.0544(3)	0.8066(2)	0.4325(2)	0.0036(2)
O5	0.1906(5)	0.7808(2)	0.0604(4)	0.0044(4)
O6	0.1980(6)	0.2221(2)	0.0538(4)	0.0056(4)
O7	0.1075(6)	0.1647(3)	0.7508(4)	0.0038(4)
O8	0.1928(5)	0.5952(2)	0.0154(4)	0.0053(4)
O9	0.3561(3)	0.0000(3)	0.3717(2)	0.0047(2)
O10	0.1232(3)	0.4957(3)	0.7450(2)	0.0037(3)
O11	0.3591(5)	0.6647(3)	0.3913(4)	0.0041(4)
O12	0.2440(2)	0.0027(3)	0.0306(2)	0.0062(2)
O13	0.1929(5)	0.4094(2)	0.0231(4)	0.0042(4)
O14	0.0508(3)	0.1406(2)	0.4280(2)	0.0036(2)
H1	0.3070(60)	0.0080(60)	0.1340(40)	0.015(8)

Table S2. Anisotropic displacement parameters U_{ij} for $La_3B_6O_{13}(OH)$ (standard deviations in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
La1	0.00357(9)	0.00232(2)	0.00327(8)	-0.00009(5)	-0.00020(6)	0.00010(7)
La2	0.00348(4)	0.00287(4)	0.00315(4)	0.00004(8)	0.00040(2)	0.00060(2)
La3	0.00334(8)	0.00469(2)	0.00326(8)	0.00019(5)	-0.00013(6)	0.00074(6)
B1	0.0039(7)	0.0036(8)	0.0031(7)	0.0004(6)	0.0001(6)	0.0000(6)
B2	0.0044(7)	0.0021(8)	0.0042(8)	0.0002(6)	-0.0004(6)	0.0002(6)
B3	0.0050(2)	0.0038(2)	0.0006(2)	0.0008(1)	0.0006(2)	0.0024(1)
B4	0.0036(7)	0.0030(7)	0.0041(7)	-0.0007(5)	0.0000(6)	0.0003(5)
B5	0.0044(5)	0.0035(5)	0.0024(5)	0.0018(2)	0.0009(4)	0.0005(2)
B6	0.0036(2)	0.0049(2)	0.0066(2)	0.0004(2)	-0.0007(2)	0.0018(1)
O1	0.0034(8)	0.0044(1)	0.0050(1)	-0.0005(9)	0.0002(7)	0.0005(8)
O2	0.0050(5)	0.0026(4)	0.0030(5)	0.0002(4)	0.0003(4)	0.0004(4)
O3	0.0036(7)	0.0050(8)	0.0019(8)	0.0004(7)	0.0001(6)	0.0013(7)
O4	0.0052(5)	0.0025(5)	0.0030(5)	-0.0006(4)	0.0013(4)	0.0006(4)
O5	0.0051(8)	0.0029(1)	0.0052(1)	-0.0007(7)	-0.0015(7)	0.0013(7)
O6	0.0045(8)	0.0070(2)	0.0054(1)	-0.0021(8)	-0.0020(7)	0.0012(7)
O7	0.0037(8)	0.0049(8)	0.0028(9)	-0.0004(7)	0.0000(7)	0.0005(6)
O8	0.0050(8)	0.0052(2)	0.0056(1)	0.0026(8)	-0.0005(7)	-0.0005(7)
O9	0.0030(4)	0.0044(5)	0.0067(4)	-0.0001(2)	0.0007(3)	0.0001(1)
O10	0.0036(4)	0.0051(9)	0.0026(4)	0.0001(7)	0.0002(3)	-0.0021(6)
O11	0.0026(9)	0.0035(9)	0.0062(2)	-0.0002(9)	-0.0002(8)	0.0005(8)
O12	0.0043(4)	0.0088(4)	0.0055(4)	0.0000(2)	0.0010(3)	0.0002(2)
O13	0.0045(8)	0.0030(1)	0.0051(1)	-0.0010(8)	0.0009(7)	-0.0001(7)
O14	0.0048(5)	0.0031(5)	0.0029(5)	-0.0004(4)	0.0013(4)	0.0006(4)

Table S3. Interatomic La–O distances /Å for $La_3B_6O_{13}(OH)$ (standard deviations in parentheses).

La1	–O5	2.455(3)	La2	–O11	2.401(3)	La3	–O6	2.434(3)
	–O11	2.486(3)		–O1	2.449(3)		–O1	2.459(3)
	–O9	2.502(4)		–O12	2.521(2)		–O11	2.518(3)
	–O1	2.519(3)		–O2	2.662(2)		–O9	2.532(4)
	–O10	2.629(3)		–O2	2.676(2)		–O3	2.587(3)
	–O4	2.654(2)		–O9	2.690(2)		–O14	2.672(2)
	–O7	2.668(3)		–O13	2.713(3)		–O8	2.683(3)
	–O4	2.702(2)		–O7	2.740(3)		–O14	2.695(2)
	–O13	2.727(3)		–O8	2.750(3)		–O10	2.774(3)
				–O3	2.831(3)			
Ø		**2.594**	**Ø**		**2.643**	**Ø**		**2.595**

Table S4. Charge distributions according to both the bond-length/bond-strength ($\sum V$) and the CHARDI ($\sum Q$) concept.

	La1	La2	La3	B1	B2	B3	B4	B5	B6	H1
$\sum V$	2.98	2.99	3.00	2.99	2.98	2.97	2.97	3.00	2.97	1.05
$\sum Q$	3.03	2.95	2.99	2.93	2.98	3.13	3.02	2.99	3.02	0.98
	O1	O2	O3	O4	O5	O6	O7	O8	O9	O10
$\sum V$	-2.11	-1.96	-2.05	-1.97	-1.87	-2.00	-2.00	-1.75	-1.82	-1.99
$\sum Q$	-2.02	-2.00	-2.20	-1.99	-1.88	-1.83	-1.93	-2.02	-1.99	-1.98
	O11	O12 (-H)	O12 (+H)	O13	O14					
$\sum V$	-2.15	-1.14	-1.87	-1.95	-1.73					
$\sum Q$	-2.14	-1.18	-2.06	-1.97	-1.98					

Table S5. ^{11}B NMR chemical shift and quadrupolar interactions derived from quantum mechanical calculations.

	δ_{iso} /ppm*	δ_{aniso} /ppm	η_{CS}	C_Q /kHz	η_Q
B1	91.7	2.3	0.32	330	0.89
B2	91.2	-3.3	0.20	363	0.76
B3	91.6	12.6	0.51	503	0.70
B4	91.4	4.0	0.51	388	0.47
B5	91.2	-4.2	0.76	179	0.69
B6	91.7	12.7	0.48	484	0.80

* absolute value: not referenced

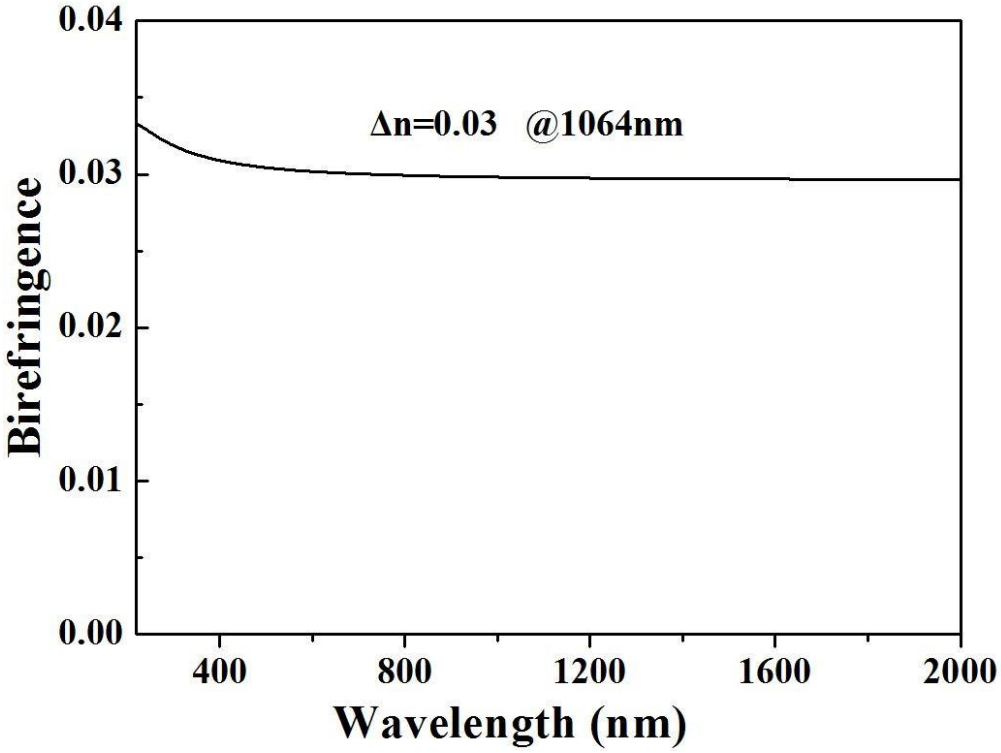

Figure S1. Calculated birefringence of $La_3B_6O_{13}(OH)$.

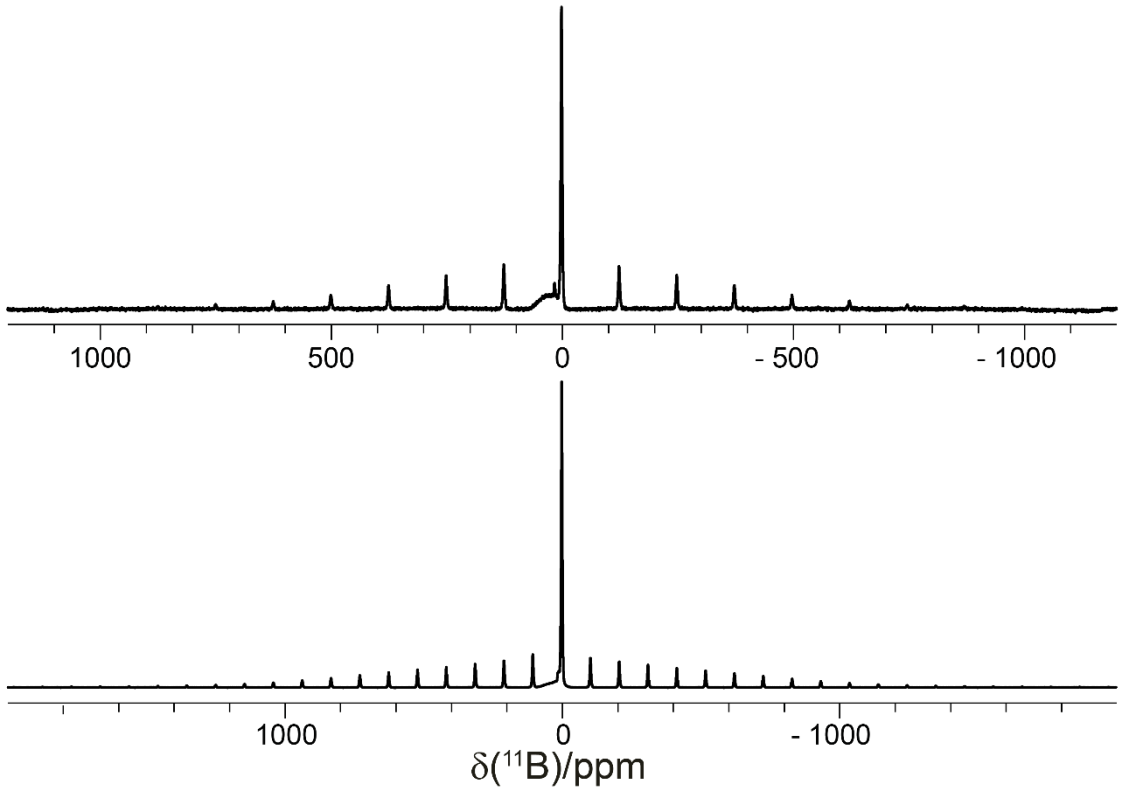

Figure S2. ^{11}B MAS NMR spectra acquired at B_0 field of 23.4 T with a spinning speed of 40 kHz (top) and 14.1 T with a spinning speed of 20 kHz (bottom).

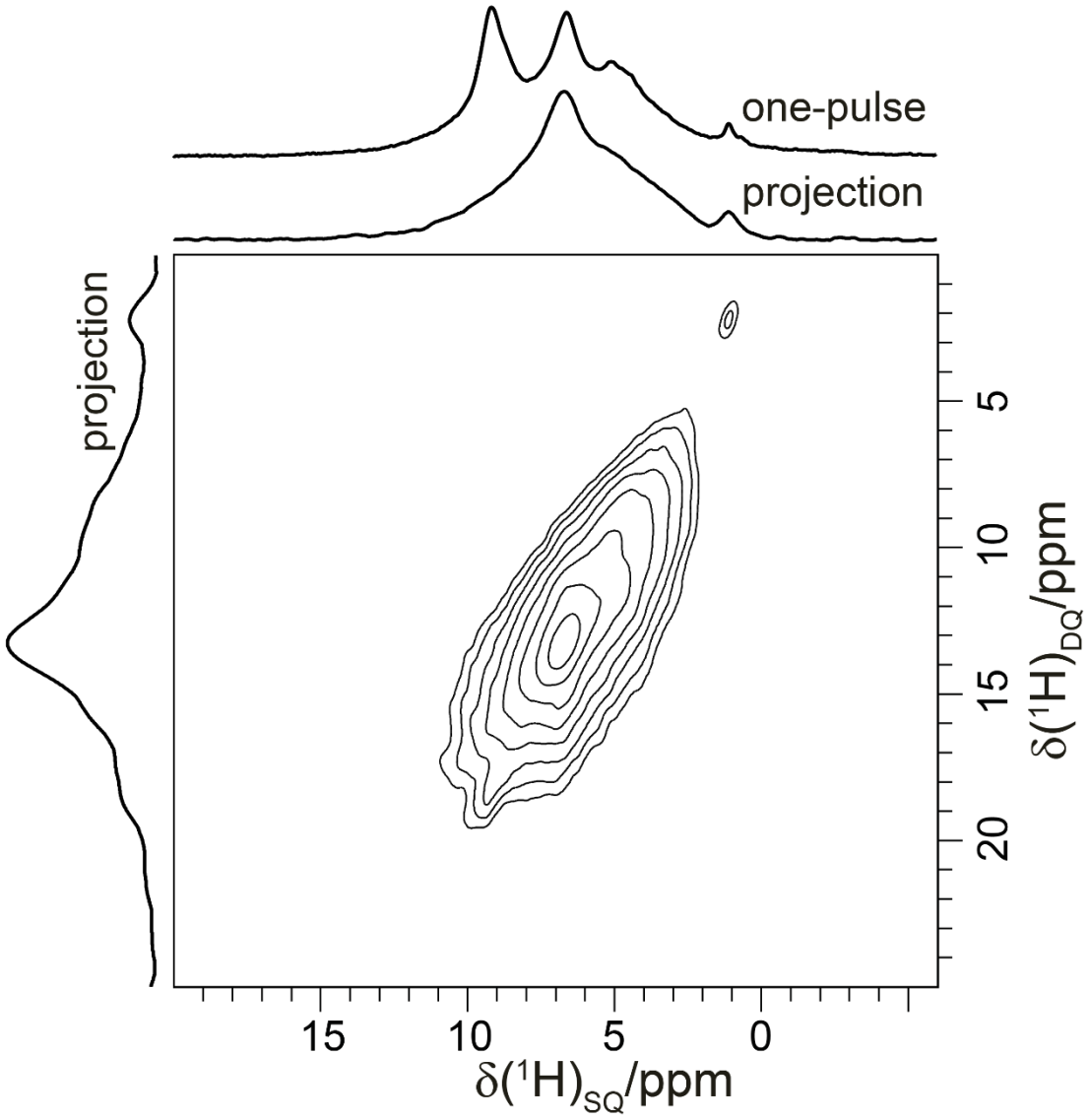

Figure S3. ^{1}H-^{1}H DQ-SQ NMR spectrum acquired at B_0 field 14.1 T, with a spinning speed of 62.5 kHz using the $R12_2^5$ sequence with a DQ excitation and recoupling of 64.0 μs.