$M(B(SeO_3)_3)H_2O(M=Al,Ga)$:The first boroselenites with a unique sandwich like double-layer structure

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Supporting information

Content

Table S1. Crystal data and structure refinements for Al(B(SeO$_3$)$_3$)H$_2$O and Ga(B(SeO$_3$)$_3$)H$_2$O.

Formula	Al(B(SeO$_3$)$_3$)H$_2$O	Ga(B(SeO$_3$)$_3$)H$_2$O
Formula weight	434.80	479.43
Temperature	293(2)K	293(2)K
Wavelength	0.71073	0.71073
Space group	*Pbca*	*Pbca*
a (Å)	8.4650(5)	8.5773(5)
b (Å)	8.7788(7)	8.8445(5)
c (Å)	21.9237(14)	22.0195(13)
Volume (Å^3)	1629.21(19)	1670.44(17)
Z, Calculated density(g/cm^3)	8, 3.545	8, 3.813
Absorption coefficient(mm^{-1})	13.695	16.409
F(000)	1601.0	1760.0
Theta range for data collection	3.716 to 54.206 deg	6.022 to 54.202 deg
Limiting indices	$-10 \leq h \leq 10$, $-11 \leq k \leq 8$, $-28 \leq 1 \leq 27$	$-10 \leq h \leq 10$, $-11 \leq k \leq 11$, $-28 \leq 1 \leq 27$
Reflections collected	11735	20265
Independent reflections	1794 [R_{int} = 0.0482, R_{sigma} = 0.0283]	1843 [R_{int} = 0.0835, R_{sigma} = 0.0328]
Refinement method	Full-matrix least-squares on $F_0{}^2$	Full-matrix least-squares on $F_0{}^2$
Goodness-of-fit on F2	1.130	1.069
Final R indices [I>2sigma(I)]	R_1 = 0.0275, wR_2 = 0.0542	R_1 = 0.0240, wR_2 = 0.0575
R indices (all data)[a]	R_1 = 0.0335, wR_2 = 0.0569	R_1 = 0.0281, wR_2 = 0.0597
Largest diff. peak and hole	0.62/-1.00 e.A^{-3}	0.73/-1.06 e.A^{-3}

[a]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ and $wR_2 = [\Sigma w(F_o{}^2 - F_c{}^2)^2 /\Sigma wF_o{}^4]$ 1/2 for $F_o{}^2 > 2\sigma(F_o{}^2)$.

Table S2. Selected bond lengths (Å) for $Al(B(SeO_3)_3)H_2O$ and $Ga(B(SeO_3)_3)H_2O$.

Al(B(SeO₃)₃)H₂O		Ga(B(SeO₃)₃)H₂O	
Atom- Atom	**Length/Å**	**Atom- Atom**	**Length/Å**
Al1-O1	1.893(3)	Ga1-O1	1.973(3)
Al1-O4	1.880(3)	Ga1-O4	1.944(2)
Al1- O5#1	1.908(3)	Ga1- O5#1	1.956(2)
Al1- O7	1.876(3)	Ga1- O7	1.939(2)
Al1- O9#2	1.895(3)	Ga1- O9#2	1.954(2)
Al1-O1w	1.917(3)	Ga1- O1w	1.997(3)
B1- O2#3	1.463(5)	B1- O2#3	1.470(4)
B1- O3	1.483(5)	B1- O3	1.479(4)
B1- O6	1.460(5)	B1- O6	1.453(5)
B1- O8#2	1.476(5)	B1- O8#2	1.478(5)
Se1- O1	1.660(3)	Se1- O1	1.662(3)
Se1- O2	1.714(3)	Se1- O2	1.709(3)
Se1-O3	1.730(3)	Se1-O3	1.732(2)
Se2-O4	1.689(3)	Se2-O4	1.687(2)
Se2-O5	1.682(3)	Se2-O5	1.687(2)
Se2-O6	1.739(3)	Se2-O6	1.737(3)
Se3-O7	1.683(3)	Se3-O7	1.682(2)
Se3-O8	1.744(3)	Se3-O8	1.737(2)
Se3-O9	1.674(3)	Se3-O9	1.674(2)

Symmetry transformations used to generate equivalent atoms: #1 3/2-x,1/2+y,+z; #2 1/2-x,-1/2+y,+z; #3 1-x,-1/2+y,1/2-z;

Table S3 Selected bond angles (°) for Al(B(SeO$_3$)$_3$)H$_2$O and Ga(B(SeO$_3$)$_3$)H$_2$O.

Al(B(SeO$_3$)$_3$)H$_2$O		Ga(B(SeO$_3$)$_3$)H$_2$O	
Atom-Atom-Atom	**Angle/°**	**Atom-Atom-Atom**	**Angle/°**
O1-Al1-O5#1	91.00(14)	O1-Ga1- O5#1	92.20(11)
O1-Al1-O9#2	90.94(14)	O1-Ga1- O9#2	89.72(11)
O1-Al1-O1W	176.33(13)	O1-Ga1-O1W	175.08(11)
O1-Al1-O4	96.11(13)	O1-Ga1-O4	96.68(11)
O1-Al1-O7	88.50(13)	O1-Ga1-O7	87.43(11)
O4-Al1-O5#1	90.81(13)	O4-Ga1-O5#1	90.66(10)
O4-Al1-O9#2	89.36(13)	O4-Ga1-O9#2	89.20(10)
O4-Al1-O1W	87.26(13)	O4-Ga1-O1W	87.13(11)
O4-Al1-O7	175.34(13)	O4-Ga1-O7	175.58(11)
O5#1-Al1-O1W	90.41(13)	O5#1-Ga1-O1W	90.86(11)
O5#1- Al1-O7	89.74(13)	O5#1-Ga1-O7	90.79(10)
O5#1- Al1-O9#2	178.03(13)	O5#1-Ga1-O9#2	178.08(11)
O7-Al1-O9#2	89.94(13)	O7-Ga1- O9#2	89.21(10)
O7-Al1-O1W	88.11(12)	O7-Ga1-O1W	88.68(10)
O9#2-Al1-O1W	87.63(13)	O9#2-Ga1-O1W	87.22(11)
O2#3-B1-O3	109.6(3)	O2#3-B1-O3	109.6(3)
O2#3-B1-O6	105.0(3)	O2#3-B1-O6	106.0(3)
O2#3-B1-O8^2	109.1(3)	O2#3-B1-O8^2	107.2(3)
O3-B1-O6	110.0(3)	O3-B1-O6	109.8(3)
O3-B1-O8#2	108.5(3)	O3-B1-O8#2	109.3(3)
O6-B1-O8#2	114.5(3)	O6-B1-O8#2	114.8(3)
O1-Se1-O2	98.99(14)	O1-Se1-O2	98.61(13)
O1-Se1-O3	99.79(15)	O1-Se1-O3	99.62(13)
O2-Se1-O3	91.84(14)	O2-Se1-O3	92.98(12)
O4-Se2-O5	98.56(13)	O4-Se2-O5	97.10(11)
O4-Se2-O6	98.44(14)	O4-Se2-O6	98.47(12)
O5-Se2-O6	97.50(13)	O5-Se2-O6	98.06(12)
O7-Se3-O8	96.22(14)	O7-Se3-O8	96.39(11)
O7-Se3-O9	96.89(13)	O7-Se3-O9	96.16(12)
O8-Se3-O9	99.36(14)	O8-Se3-O9	99.59(12)

Symmetry transformations used to generate equivalent atoms: #1 3/2-x,1/2+y,+z; #2 1/2-x,-1/2+y,+z; #3 1-x,-1/2+y,1/2-z;
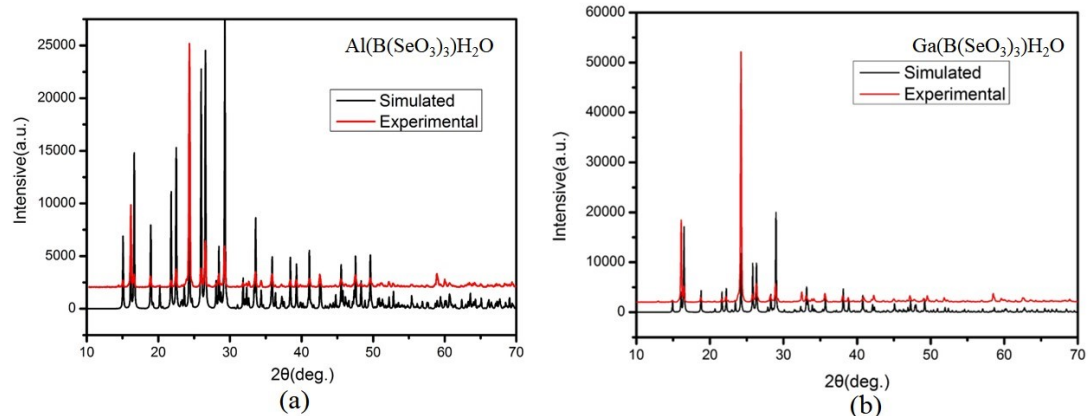
Table S4 Hydrogen bonds in $Al(B(SeO_3)_3)H_2O$ and $Ga(B(SeO_3)_3)H_2O$.

	Al(B(SeO₃)₃)H₂O			
D-H…A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O1W-H1WB…O7#1	0.86	2.17	2.912(4)	144.7
O1W-H1WA…O5#2	0.86	1.93	2.757(4)	161.6
	Ga(B(SeO₃)₃)H₂O			
D-H…A	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O1W-H1WB…O7#1	0.87	2.10	2.849(3)	143.2
O1W-H1WA…O5#2	0.87	1.92	2.753(3)	159.5

Symmetry transformations used to generate equivalent atoms: #1 1/2+x,3/2-y,-z; #2 -1/2+x,3/2-y,-z

**Table S5** Bond valence calculations for oxygen atoms in $Al(B(SeO_3)_3)H_2O$ and $Ga(B(SeO_3)_3)H_2O$.

Al(B(SeO₃)₃)H₂O		Ga(B(SeO₃)₃)H₂O	
Atom	Bond valence	**Atom**	Bond valence
O1	2.02	O1	2.02
O2	2.09	O2	2.07
O3	1.98	O3	1.98
O4	1.91	O4	1.94
O5	1.92	O5	1.91
O6	1.99	O6	2.01
O7	1.96	O7	1.98
O8	1.95	O8	1.95
O9	1.97	O9	2.01
O1w	0.48	O1w	0.48

Figure S1. Powder X-ray diffraction patterns of Al(B(SeO$_3$)$_3$)H$_2$O (a) and Ga(B(SeO$_3$)$_3$)H$_2$O (b).
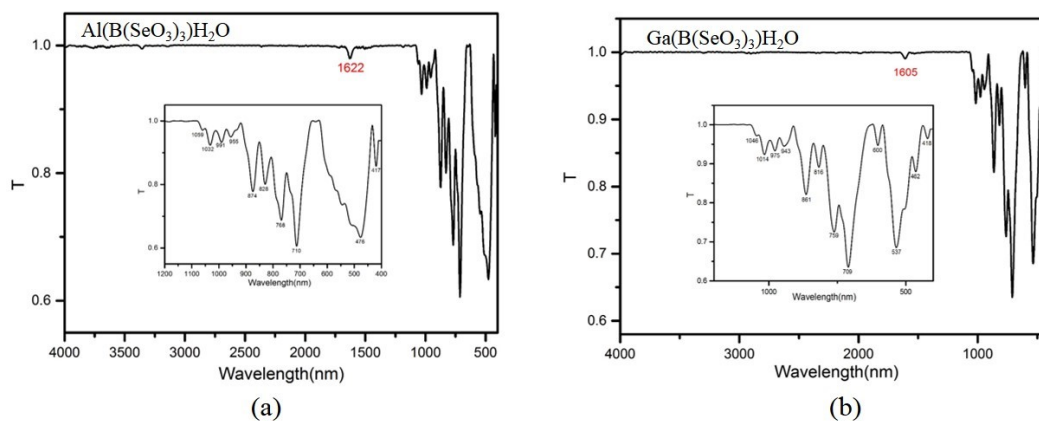
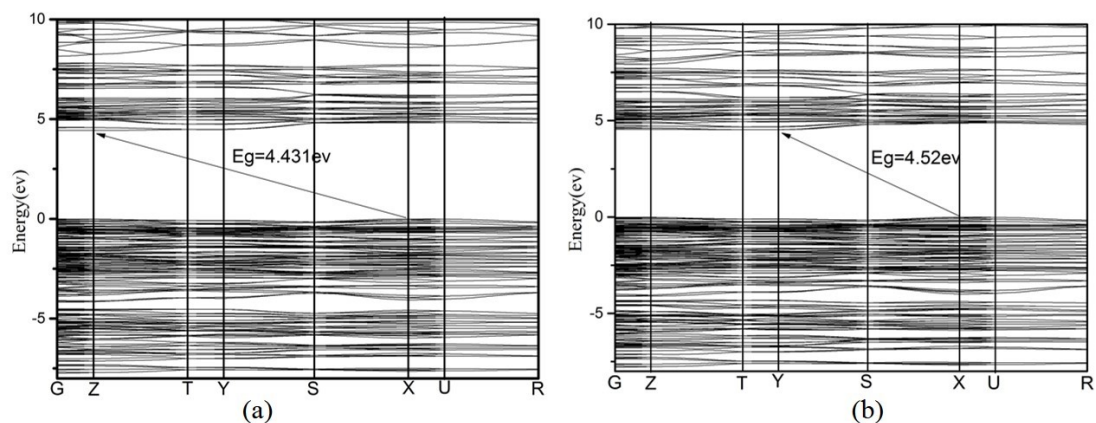**Figure S2.** IR spectra of Al(B(SeO$_3$)$_3$)H$_2$O (a) and Ga(B(SeO$_3$)$_3$)H$_2$O (b).
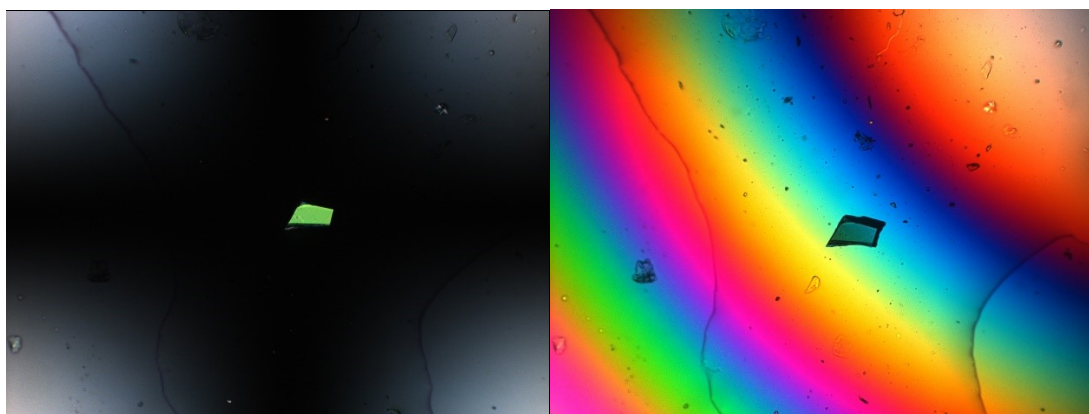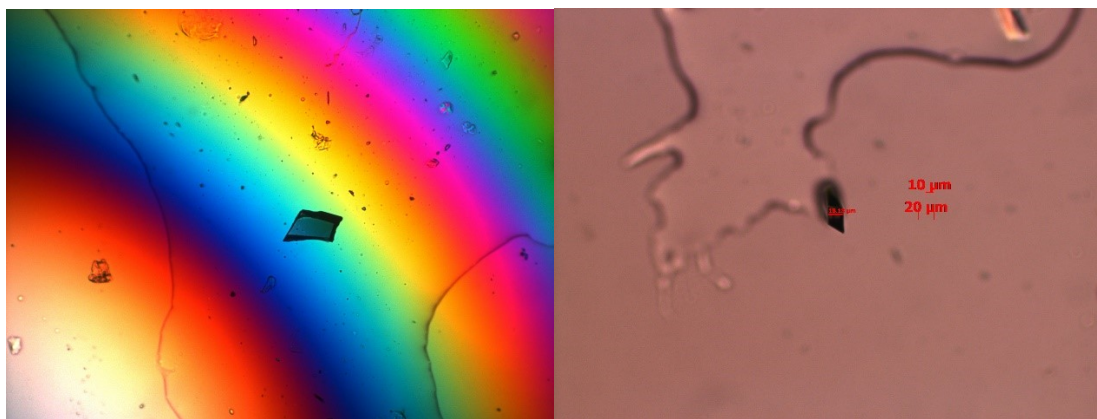
Figure S3. Photograph of $Al(B(SeO_3)_3)H_2O$ for the measurement of birefringence.
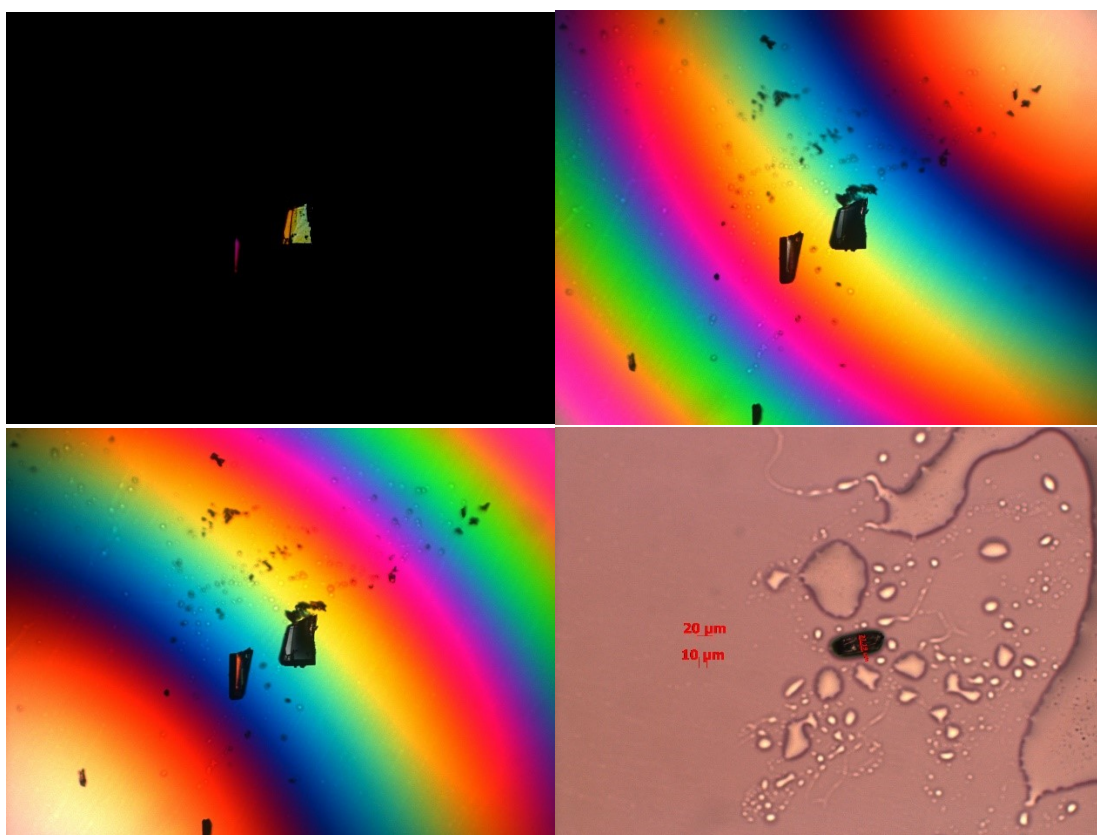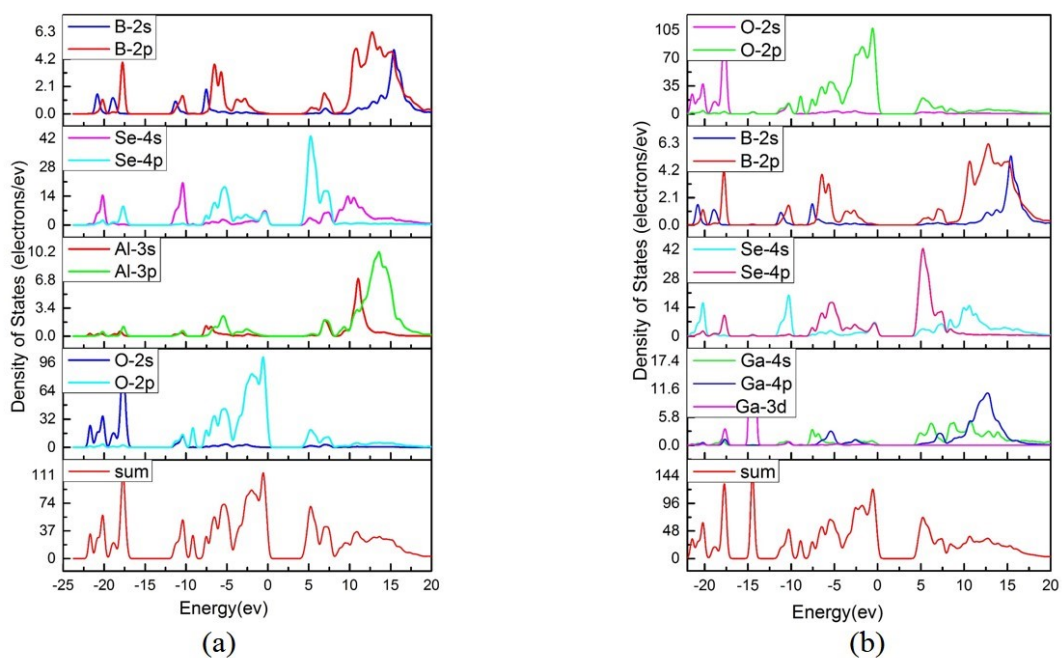

Figure S4. Photograph of $Ga(B(SeO_3)_3)H_2O$ for the measurement of birefringence.

Figure S5. The calculated band structure of $Al(B(SeO_3)_3)H_2O$ (a) and $Ga(B(SeO_3)_3)H_2O$ (b).

Figure S6. The graphs of scissor-added partial density of states and the largest tensors for $Al(B(SeO_3)_3)H_2O$ (a) and $Ga(B(SeO_3)_3)H_2O$ (b).