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Supporting Information

$Na_3B_4O_7X$ (X = Cl, Br): two new borate halides with 1D Na-X (X = Cl, Br) chain formed by the face-sharing XNa_6 octahedra

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Table S1 Selected bond lengths (Å) and angles (deg.) for $Na_3B_4O_7Cl$ [a].

Na(1)-O(2)#1	2.406(6)	Na(2)-Cl(1)#2	3.016(4)
Na(1)-O(1)	2.442(6)	Na(2)-Cl(1)	3.016(4)
Na(1)-O(2)#2	2.443(5)	B(1)-O(4)	1.441(8)
Na(1)-Cl(1)	2.725(3)	B(1)-O(1)	1.465(8)
Na(1)-O(4)#2	2.940(6)	B(1)-O(3)	1.477(8)
Na(2)-O(3)#5	2.283(6)	B(1)-O(2)	1.495(9)
Na(2)-O(3)#3	2.283(6)	B(2)-O(3)#3	1.347(8)
Na(2)-O(4)#3	2.577(5)	B(2)-O(4)#9	1.350(9)
Na(2)-O(4)#5	2.577(5)	B(2)-O(2)	1.386(9)
O(2)#1-Na(1)-O(1)	73.44(14)	O(3)#3-Na(2)-Cl(1)#2	162.32(14)
O(2)#1-Na(1)-O(2)#2	104.35(18)	O(4)#3-Na(2)-Cl(1)#2	105.75(13)
O(1)-Na(1)-O(2)#2	72.80(15)	O(4)#5-Na(2)-Cl(1)#2	94.55(12)
O(2)#1-Na(1)-Cl(1)	158.99(19)	O(3)#5-Na(2)-Cl(1)	162.32(14)
O(1)-Na(1)-Cl(1)	112.56(18)	O(3)#3-Na(2)-Cl(1)	100.05(12)
O(2)#2-Na(1)-Cl(1)	96.63(15)	O(4)#3-Na(2)-Cl(1)	94.55(12)
O(2)#1-Na(1)-O(4)#2	100.7(2)	O(4)#5-Na(2)-Cl(1)	105.75(13)
O(1)-Na(1)-O(4)#2	120.28(17)	Cl(1)#2-Na(2)-Cl(1)	74.63(11)
O(2)#2-Na(1)-O(4)#2	50.69(16)	O(4)-B(1)-O(1)	115.3(5)
Cl(1)-Na(1)-O(4)#2	93.44(14)	O(4)-B(1)-O(3)	107.0(5)
Na(1)#3-Na(1)-O(4)#2	75.57(12)	O(1)-B(1)-O(3)	108.9(5)
O(3)#5-Na(2)-O(3)#3	89.7(3)	O(4)-B(1)-O(2)	106.2(5)
O(3)#5-Na(2)-O(4)#3	103.1(2)	O(1)-B(1)-O(2)	110.5(5)
O(3)#3-Na(2)-O(4)#3	57.34(16)	O(3)-B(1)-O(2)	108.8(5)
O(3)#5-Na(2)-O(4)#5	57.34(16)	O(3)#3-B(2)-O(4)#9	116.8(6)
O(3)#3-Na(2)-O(4)#5	103.1(2)	O(3)#3-B(2)-O(2)	122.0(6)
O(4)#3-Na(2)-O(4)#5	154.5(3)	O(4)#9-B(2)-O(2)	121.2(6)
O(3)#5-Na(2)-Cl(1)#2	100.05(13)		

[a] Symmetry transformations used to generate equivalent atoms:

#1 x-y, -y+1, -z+1, #2 y, -x+y+1, z+1/6, #3 -y+1, -x+1, -z+7/6, #4 x-y+1, -y+2, -z+1, #5 y+1, -x+y+1, z+1/6, #9 x-y+1, -y+1, -z+1

Table S2 Selected bond lengths (Å) and angles (deg.) for $Na_3B_4O_7Br$ [a].

Na(1)-O(2)#1	2.387(4)	Na(2)-Br(1)	3.145(4)
Na(1)-O(1)	2.449(5)	Na(2)-Br(1)#8	3.145(4)
Na(1)-O(2)#2	2.449(5)	B(1)-O(4)#10	1.356(6)
Na(1)-Br(1)#3	2.822(3)	B(1)-O(2)	1.366(7)
Na(1)-O(4)#2	2.928(5)	B(1)-O(3)#4	1.370(7)
Na(1)-Br(1)#5	3.346(4)	B(2)-O(4)	1.451(6)
Na(2)-O(3)#7	2.282(5)	B(2)-O(1)	1.456(6)
Na(2)-O(3)	2.282(5)	B(2)-O(3)	1.483(6)
Na(2)-O(4)	2.659(4)	B(2)-O(2)	1.501(6)
Na(2)-O(4)#7	2.659(4)	O(3)-Na(2)-O(4)#7	105.90(16)
O(2)#1-Na(1)-O(1)	74.20(12)	O(4)-Na(2)-O(4)#7	156.6(2)
O(2)#1-Na(1)-O(2)#2	105.80(15)	O(3)#7-Na(2)-Br(1)	160.97(11)
O(1)-Na(1)-O(2)#2	73.13(11)	O(3)-Na(2)-Br(1)	100.35(11)
O(2)#1-Na(1)-Br(1)#3	160.45(14)	O(4)-Na(2)-Br(1)	93.02(10)
O(1)-Na(1)-Br(1)#3	112.54(12)	O(4)#7-Na(2)-Br(1)	106.04(10)
O(2)#2-Na(1)-Br(1)#3	93.75(12)	O(3)#7-Na(2)-Br(1)#8	100.35(11)
O(2)#1-Na(1)-O(4)#2	102.49(16)	O(3)-Na(2)-Br(1)#8	160.97(11)
O(1)-Na(1)-O(4)#2	121.54(14)	O(4)-Na(2)-Br(1)#8	106.04(10)
O(2)#2-Na(1)-O(4)#2	51.17(13)	O(4)#7-Na(2)-Br(1)#8	93.02(10)
Br(1)#3-Na(1)-O(4)#2	89.64(10)	Br(1)-Na(2)-Br(1)#8	71.78(11)
O(2)#1-Na(1)-Br(1)#5	88.08(13)	O(4)#10-B(1)-O(2)	122.8(5)
O(1)-Na(1)-Br(1)#5	99.61(11)	O(4)#10-B(1)-O(3)#4	116.0(4)
O(2)#2-Na(1)-Br(1)#5	161.36(15)	O(2)-B(1)-O(3)#4	121.2(4)
Br(1)#3-Na(1)-Br(1)#5	72.86(8)	O(4)-B(2)-O(1)	115.5(4)
O(4)#2-Na(1)-Br(1)#5	138.84(11)	O(4)-B(2)-O(3)	106.6(4)
O(3)#7-Na(2)-O(3)	92.0(2)	O(1)-B(2)-O(3)	109.5(4)
O(3)#7-Na(2)-O(4)	105.90(16)	O(4)-B(2)-O(2)	106.3(4)
O(3)-Na(2)-O(4)	56.22(12)	O(1)-B(2)-O(2)	110.9(4)
O(3)#7-Na(2)-O(4)#7	56.22(12)	O(3)-B(2)-O(2)	107.8(4)

[a] Symmetry transformations used to generate equivalent atoms:

#1 x-y+1, -y+1, -z, #2 y, -x+y, z+1/6, #3 x-1, y-1, z, #5 x-y, x-1, z-1/6, #7 x-y+1, -y+2, -z, #8 x-y+1, x, z-1/6, #9 y, -x+y+1, z+1/6, #10 x-y, -y+1, -z

Table S3 The element analysis of $Na_3B_4O_7X$ (X = Cl, Br).

	$Na_3B_4O_7Cl$		$Na_3B_4O_7Br$	
Element	Cal.	Exp.	Cal.	Exp.
Na	26.56	26.71	22.68	22.82
B	16.65	16.75	14.22	14.34

Table S4 The assignment of infrared spectra for $Na_3B_4O_7X$ (X = Cl, Br).

$Na_3B_4O_7Cl$ (cm^{-1})	$Na_3B_4O_7Br$ (cm^{-1})	Assignment
1338	1346	asymmetric stretching vibrations of BO_3
1140	1140	asymmetric stretching vibrations of BO_4
950	950	symmetric stretching vibrations of BO_3
853, 808, 753	862, 807, 763	symmetric stretching vibrations of BO_4
654	663	out-of-plane bending of BO_3
519	520	bending of BO_3 and BO_4
465	475	bending of BO_4

Captions for Figures:

Figure S1. Infrared spectra of $Na_3B_4O_7X$ (X = Cl, Br).

Figure S2. The coordination environments of the cations in $Na_3B_4O_7Br$.

Figure S3. The boron-oxygen framework in the crystal structure of $Na_3B_4O_7Br$ in *bc* plane (BO_3 triangles and BO_4 tetrahedra are shown in rose and green, respectively).

Figure S4. UV–Vis–NIR diffuse-reflectance spectra of $Na_3B_4O_7X$ (X = Cl, Br).

Figure S5. Calculated band structure of $Na_3B_4O_7Br$.

Figure S6. The total and partial densities of states of $Na_3B_4O_7Br$.

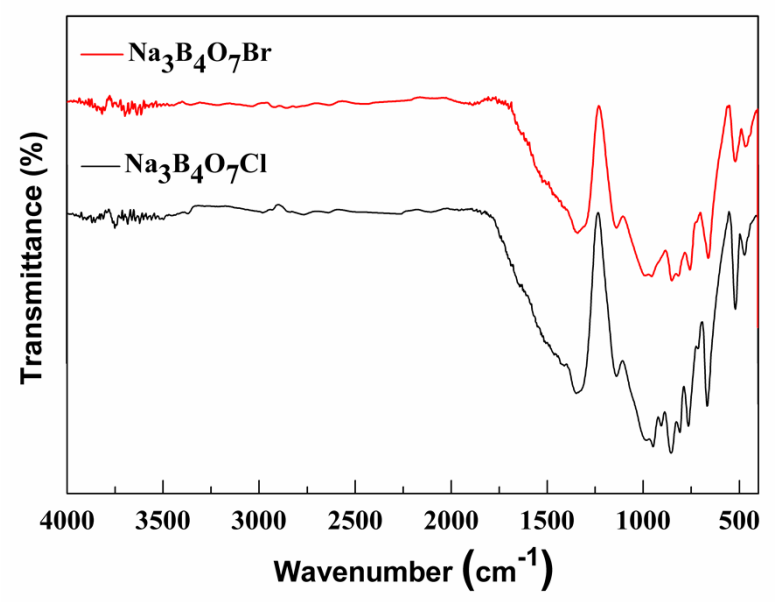

Figure S1. Infrared spectra of $Na_3B_4O_7X$ (X = Cl, Br).

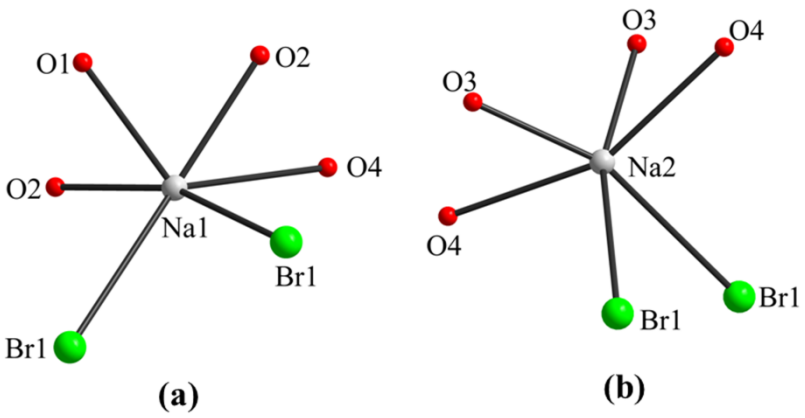

Figure S2. The coordination environments of the cations in $Na_3B_4O_7Br$.

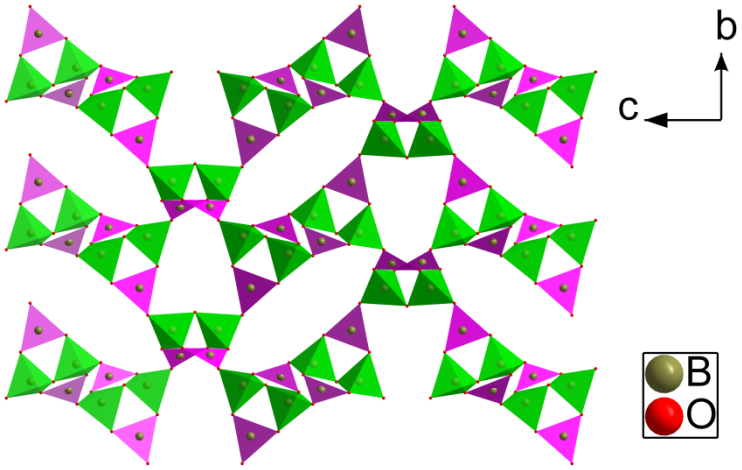

Figure S3. The boron-oxygen framework in the crystal structure of $Na_3B_4O_7Br$ in *bc* plane (BO_3 triangles and BO_4 tetrahedra are shown in rose and green, respectively).

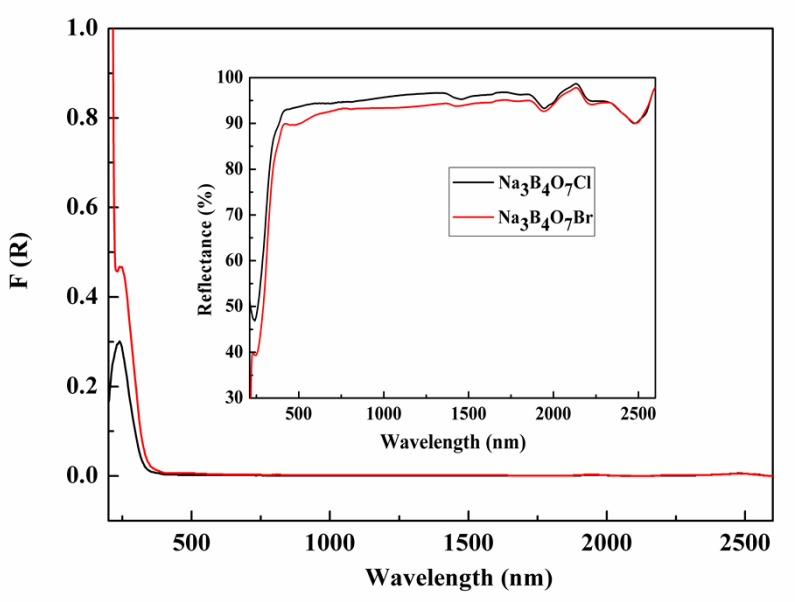

Figure S4. UV–Vis–NIR diffuse-reflectance spectra of $Na_3B_4O_7X$ (X = Cl, Br).

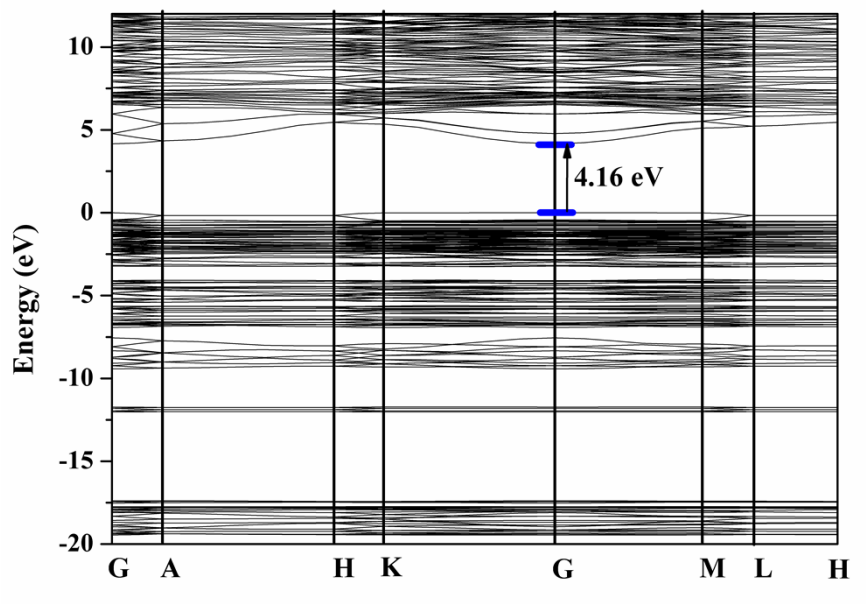

Figure S5. Calculated band structure of $Na_3B_4O_7Br$.

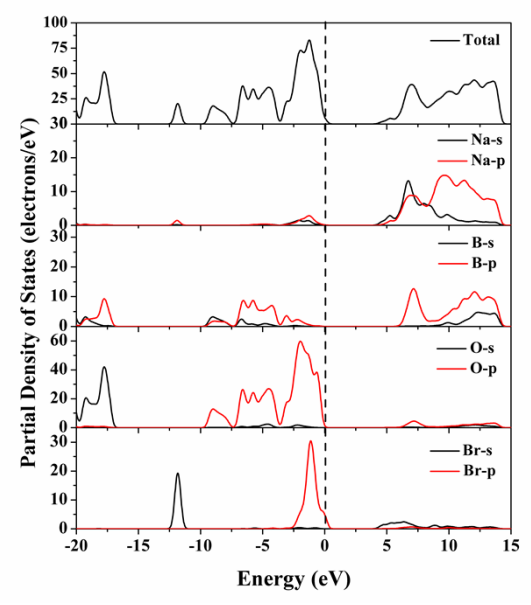

Figure S6. The total and partial densities of states of $Na_3B_4O_7Br$.