Electronic Supplementary Information for

Shooting short-wavelength nonlinear optical materials with targeted balance performances in hydroxyborates through first-principles high-throughput screening

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Contents

Table S1 The ICSD code, crystal system, space group, and chemical formula of 222 hydroxyborates crystals with non-centrosymmetric (NCS) structures collected from ICSD.
Table S2 The basic information of hydroxyborates with 0D isolated B-O/OH clusters.
Table S3 The basic information of hydroxyborates with 1D infinite B-O/OH chains.
Table S4 The basic information of hydroxyborates with 2D B-O/OH layered configurations.
Table S5 The basic information of hydroxyborates with 3D B-O/OH frameworks.
Table S6 The ICSD collection numbers, chemical formula, space group, GGA and HSE06 band gaps, second harmonic generation (SHG) coefficients, and birefringence Δn at 1064 nm of 60 screening hydroxyborates crystals. Note that SHG coefficients, and birefringence Δn have been corrected with scissors operators.
Table S7 Calculated band gaps (E_g) by hybrid HSE06, the maximum SHG coefficients (d_{ij}), birefringence at 1064 nm (Δn), UV cutoff wavelengths (λ_{cutoff}), shortest phase-matching wavelengths (λ_{PM}), dimensionality of B−O/OH anionic framework, and (A + OH)/B ratio of screened hydroxyborate crystals.
Table S8 Calculated band gaps (E_g) by hybrid HSE06, the maximum SHG coefficients (d_{ij}), birefringence at 1064 nm (Δn), UV cutoff wavelengths (λ_{cutoff}), shortest phase-matching wavelengths (λ_{PM}), dimensionality of B−O/OH anionic framework, and (A + OH)/B ratio of screened hydroxyborate crystals.
Table S9 The investigation of ratio (A + OH)/B = 0.636, dimensionality of B−O/OH anionic framework, birefringence at 1064 nm (cal.), and [BO_3] & [$B(OH)_3$] & [$BO_2(OH)$] density among hydroxyborates involving the screened compounds.
Table S10 Bonding electron difference ($\Delta\rho$) and contribution percent w (%) of different units in $KCa_4(B_{22}O_{32}(OH)_{10}Cl)\cdot 4H_2O$ calculated by the REDA model.
Figure S1 (a) Band structures by the HSE06 functional. (b) Total and partial density of states (PDOS) and band-resolved NLO coefficients. (c) SHG-weighted density of occupied and unoccupied states in virtual-electron (VE) progress of $KCa_4(B_{22}O_{32}(OH)_{10}Cl)\cdot 4H_2O$. Here, $\chi_{122} = 2d_{12}$.
Notes and references

Table S1 The ICSD code, crystal system, space group, and chemical formula of 222 hydroxyborates crystals with non-centrosymmetric (NCS) structures collected from ICSD.

ICSD code	Crystal system	Space group	Formula
39637	Triclinic	*P*1	$KCa_4(B_{22}O_{32})(OH)_{10}Cl{\cdot}4H_2O$
187776	Triclinic	*P*1	$KCa_4(B_{22}O_{32}(OH)_{10}Cl){\cdot}4H_2O$
172480	Triclinic	*P*1	$Bi(B_4O_6(OH)_2)(OH)$
76888	Triclinic	*P*1	$Ca_9B_{26}O_{34}(OH)_{24}Cl_4{\cdot}13H_2O$
172482	Triclinic	*P*1	$Bi_3(B_6O_{13}(OH))$
174161	Triclinic	*P*1	$Ba_3Na(OH)(B_9O_{16})(B(OH)_4)$
182942	Triclinic	*P*1	$Tl((UO_2)(B_5O_8)(OH)F)$
261299	Triclinic	*P*1	$(NH_4)_8(Co_2B_4P_8O_{30}(OH)_4)$
409327	Triclinic	*P*1	$Mg_2(BP_2O_7(OH)_3)$
420549	Triclinic	*P*1	$Ca_2(B_5O_8(OH))_2B(OH)_3{\cdot}H_2O$
134988	Triclinic	*P*1	$Ca_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$
137621	Triclinic	*P*1	$Na_{0.711}(Al_{1.315}Fe_{1.685})Al_6(BO_3)_3Si_6O_{18}O(OH)_3$
137622	Triclinic	*P*1	$Na_{0.889}(Al_{2.078}Fe_{0.922})Al_6(BO_3)_3Si_6O_{18}O(OH)_3$
42570	Triclinic	*P*1	$Ba_2B_{13}O_{19}(OH)_5{\cdot}5H_2O$
91539	Monoclinic	*P*2	$Ba_5(B_{20}O_{33}(OH)_4){\cdot}H_2O$
28426	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
28427	Monoclinic	$P2_1$	$Ca(B_3O_4(OH)_3){\cdot}H_2O$
171019	Monoclinic	$P2_1$	$CaB_8O_{11}(OH)_4$
250323	Monoclinic	$P2_1$	$Ca(B_8O_{11}(OH)_4)$
256908	Monoclinic	$P2_1$	$Ba_3(B_6O_{10}(OH)_2)(CO_3)$
262502	Monoclinic	$P2_1$	$Ba_2(B_6O_9(OH)_4)$
263504	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263505	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263506	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263507	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263508	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263509	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
263510	Monoclinic	$P2_1$	$CaB_3O_4(OH)_3{\cdot}H_2O$
415082	Monoclinic	$P2_1$	$Ca(B_8O_{11}(OH)_4)$
432814	Monoclinic	$P2_1$	$Ca_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$
4228	Monoclinic	$P2_1$	$Sr(B_8O_{11}(OH)_4)$
20074	Monoclinic	$P2_1$	$Sr_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$
20963	Monoclinic	$P2_1$	$LiNd(BO_3(OH))$
22336	Monoclinic	$P2_1$	$Na(B(OH)_2Si_2O_5)$
28014	Monoclinic	$P2_1$	$Sr_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$
100400	Monoclinic	$P2_1$	$(NH_4)_2(B_4O_5(OH)_4){\cdot}2H_2O$
237586	Monoclinic	$P2_1$	$Eu(B_8O_{11}(OH)_4)$
248128	Monoclinic	$P2_1$	$(UO_2)_2(B_9O_{14}(OH)_4)$
254204	Monoclinic	$P2_1$	$K_5(UO_2)_2(B_2P_3O_{12}(OH))_2(OH){\cdot}2H_2O$
49364	Monoclinic	$P2_1$	$(NH_4)_2B_4O_5(OH)_4(H_2O)_2$
49365	Monoclinic	$P2_1$	$(NH_4)_2B_4O_5(OH)_4(H_2O)_2$
17641	Monoclinic	$P2_1$	$La_3B_6O_{13}(OH)$
19922	Monoclinic	$P2_1$	$Ba_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$

ICSD code	Crystal system	Space group	Formula
141235	Monoclinic	$P2_1$	$NaRb_3B_6O_9(OH)_3(HCO_3)$
145071	Monoclinic	$P2_1$	$Zn(NH_2CH_2CH_2NH_2)_2Al(B_5O_9(OH))(BO(OH)_2)$
95447	Monoclinic	$C2$	$Na_2Ba_2(B_{10}O_{17}(OH)_2)$
403149	Monoclinic	$C2$	$Ba_3(B_{10}O_{17}(OH)_2)$
92819	Monoclinic	$C2$	$Sr_2(B_5O_9(OH))\cdot H_2O$
182000	Monoclinic	$C2$	$(NH_4)_6(Mn_3B_6P_9O_{36}(OH)_3)\cdot 4H_2O$
250334	Monoclinic	$C2$	$Pb_2(B_4O_5(OH)_6)\cdot H_2O$
261799	Monoclinic	$C2$	$Pb_2(B_4O_5(OH)_4)(OH)_2\cdot H_2O$
131283	Monoclinic	$C2$	$B_5DyH_2O_{10}$
11600	Monoclinic	Pm	$Mn_5(BO_3)_3(OH)$
76661	Monoclinic	Pc	$Ca_3(B_5O_6(OH)_6)(OH)Cl_2\cdot 8H_2O$
89259	Monoclinic	Pc	$Ca_3(B_5O_6(OH)_6)(OH)Cl_2\cdot 8H_2O$
262542	Monoclinic	Pc	$Ba_3B_6O_{11}(OH)_2$
154523	Monoclinic	Pc	$Na_4(B_{10}O_{16}(OH)_2)\cdot 4H_2O$
26380	Monoclinic	Pc	$NH_4(B_5O_6(OH)_4)\cdot 2H_2O$
110994	Monoclinic	Cm	$(Cu(NH_3)_4(H_2O)_2)(B_4O_5(OH)_4)\cdot 2H_2O$
124825	Monoclinic	Cm	$Pr_3Mo_4B_6O_{24}(OH)_3$
2942	Monoclinic	Cc	$Sr_2(B5O8(OH))_2(B(OH)_3)\cdot H_2O$
16921	Monoclinic	Cc	$Sr_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$
251872	Monoclinic	Cc	$La_2(CH_3CO_2)_2(B_5O_9(OH))\cdot H_2O$
251873	Monoclinic	Cc	$Ce_2(CH_3CO_2)_2(B_5O_9(OH))\cdot H_2O$
251874	Monoclinic	Cc	$Pr_2(CH_3CO_2)_2(B_5O_9(OH))\cdot H_2O$
251875	Monoclinic	Cc	$La_2(CH_3CO_2)_2(B_5O_9(OH))$
251876	Monoclinic	Cc	$Ce_2(CH_3CO_2)_2(B_5O_9(OH))$
251877	Monoclinic	Cc	$Pr_2(CH_3CO_2)_2(B_5O_9(OH))$
260879	Monoclinic	Cc	$Na_3(B_3O_4(OH)_4)$
262373	Monoclinic	Cc	$Ce(B_4O_6(OH)_2)Cl$
425058	Monoclinic	Cc	$Cu_3(B_2(PO_4)_3(OH)_3)$
426915	Monoclinic	Cc	$Ca_2(B_5O_9)(OH)\cdot H_2O$
760166	Monoclinic	Cc	$LaB_4O_6(OH)_2Cl$
760167	Monoclinic	Cc	$CeB_4O_6(OH)_2Cl$
95909	Monoclinic	Cc	$Pr(B_4O_6(OH)_2)Cl$
95910	Monoclinic	Cc	$Nd(B_4O_6(OH)_2)Cl$
151307	Monoclinic	Cc	$(Ru_2((CH_3)COO)_4(H_2O)_2)(BF_4)$
182938	Monoclinic	Cc	$Na(UO_2)(B_5O_8)(OH)F\cdot H_2O$
182941	Monoclinic	Cc	$Rb((UO_2)(B_5O_8)(OH)F)$
182943	Monoclinic	Cc	$Na((NpO_2)(B_5O_8)(OH)F)\cdot H_2O$
253445	Monoclinic	Cc	$Co_3(BPO_4)_2(PO_4)(OH)_3$
261402	Monoclinic	Cc	$Ba_3(Ge_2B_7O_{16}(OH)_2)(OH)\cdot H_2O$
261422	Monoclinic	Cc	$(UO_2)(B_8O_{11}(OH)_4)$
261423	Monoclinic	Cc	$(NpO_2)(B_8O_{11}(OH)_4)$
261424	Monoclinic	Cc	$(PuO_2)(B_8O_{11}(OH)_4)$
262913	Monoclinic	Cc	$La(B_4O_6(OH)_2Cl)$
262914	Monoclinic	Cc	$Ce(B_4O_6(OH)_2Cl)$
262918	Monoclinic	Cc	$Pu(B_4O_6(OH)_2Cl)$

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420984	Monoclinic	*Cc*	$Na(UO_2)(B_6O_{10}(OH))\cdot 2H_2O$
420987	Monoclinic	*Cc*	$PuO_2(B_8O_{11}(OH)_4)$
423058	Monoclinic	*Cc*	$Pu(B_4O_6(OH)_2Cl)$
124040	Monoclinic	*Cc*	$Ba_2B_{10}O_{16}(OH)_2(H_3BO_3)\cdot H_2O$
34648	Orthorhombic	$P2_12_12_1$	$K_2(B_4O_5(OH)_4)\cdot 2H_2O$
59278	Orthorhombic	$P2_12_12_1$	$(NH_4)_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
81193	Orthorhombic	$P2_12_12_1$	$(B(C_2H_6N_5))(OH)_2\cdot H_2O$
155932	Orthorhombic	$P2_12_12_1$	$(Mg_2(H_2O))(BP_3O_9(OH)_4)$
425065	Orthorhombic	$P2_12_12_1$	$LiCu_2(BP_2O_8(OH)_2)$
4229	Orthorhombic	$P2_12_12_1$	$Rb_2Sr(B_4O_5(OH)_4)_2\cdot 8H_2O$
35090	Orthorhombic	$P2_12_12_1$	$CaK_2(B_4O_5(OH)_4)_2\cdot 8H_2O$
80648	Orthorhombic	$P2_12_12_1$	$(NH_4)_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
93005	Orthorhombic	$P2_12_12_1$	$K_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
98351	Orthorhombic	$P2_12_12_1$	$Rb_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
99219	Orthorhombic	$P2_12_12_1$	$Cs_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
100670	Orthorhombic	$P2_12_12_1$	$Tl_2(B_4O_6(OH)_2)\cdot 2H_2O$
192187	Orthorhombic	$P2_12_12_1$	$K_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
200950	Orthorhombic	$P2_12_12_1$	$K_2Ca(B_4O_5(OH)_4)_2\cdot 8H_2O$
263926	Orthorhombic	$P2_12_12_1$	$RbSe_3B_2O_9(OH)$
263927	Orthorhombic	$P2_12_12_1$	$CsSe_3B_2O_9(OH)$
57297	Orthorhombic	$P2_12_12_1$	$Ba(BO_2(OH))$
13423	Orthorhombic	*C*222	$Li_2CsB_7O_{10}\cdot 4H_2O$
431106	Orthorhombic	$Pca2_1$	$Na(B_5O_7(OH)_2)\cdot H_2O$
250215	Orthorhombic	*Pnc*2	$CaLi_4(B_5O_8(OH)_2)_2$
36431	Orthorhombic	*Pnc*2	$Li_3(B_5O_8(OH)_2)$
413627	Orthorhombic	$Pmn2_1$	$K_7((BO_3)Mn(B_{12}O_{18}(OH)_6))\cdot H_2O$
70514	Orthorhombic	$Pmn2_1$	$K_7((BO_3)Co(B_{12}O_{18}(OH)_6))\cdot H_2O$
145793	Orthorhombic	$Pmn2_1$	$Tb_3B_{10}O_{17}(OH)_5$
22192	Orthorhombic	$Pna2_1$	$CaB_3O_5(OH)$
23880	Orthorhombic	$Pna2_1$	$CaB_3O_5(OH)$
1973	Orthorhombic	$Pna2_1$	$(Na(H_2O))_2(B_5O_8(OH))$
34700	Orthorhombic	$Pna2_1$	$K_2(B_5O_8(OH))\cdot 2H_2O$
59277	Orthorhombic	$Pna2_1$	$K_2Sr(B_4O_5(OH)_4)_2\cdot 10H_2O$
249876	Orthorhombic	$Pna2_1$	$Na_2B_5O_8(OH)\cdot 2H_2O$
252381	Orthorhombic	$Pna2_1$	$CaB_3O_5(OH)$
426601	Orthorhombic	$Pna2_1$	$Mg(B_6O_9(OH)_2)\cdot 4H_2O$
4220	Orthorhombic	$Pna2_1$	$K_3(B_3O_4(OH)_4)\cdot 2H_2O$
4221	Orthorhombic	$Pna2_1$	$Rb_3(B_3O_4(OH)_4)\cdot 2H_2O$
200266	Orthorhombic	$Pna2_1$	$K_3(B_3O_4(OH)_4)\cdot 2H_2O$
408211	Orthorhombic	$Pna2_1$	$Na_2(BP_2O_7(OH))$
133088	Orthorhombic	$Pna2_1$	$KHC_2O_4B(OH)_3$
117561	Orthorhombic	$Pna2_1$	$La_2B_3O_4(OH)_3(SO_4)_2$
253012	Orthorhombic	$Cmc2_1$	$K_3B_3O_4(OH)_4\cdot 2H_2O$
138088	Orthorhombic	$Cmc2_1$	$Na_8Li_2(B_6O_{10})_4(B(OH)_3)_2(OH)_2$
113334	Orthorhombic	$Cmc2_1$	$(NH_4)_2(B_4O_5(OH)_4)\cdot 2H_2O$

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63014	Orthorhombic	*Amm*2	$Tl_4Cu(Cu_2B_{18}O_{28}(OH)_8)\cdot 10H_2O$
241953	Orthorhombic	*Ama*2	$K((UO_2)B_6O_{10}(OH))$
6292	Orthorhombic	*Aba*2	$K(B_5O_6(OH)_4)\cdot 2H_2O$
29406	Orthorhombic	*Aba*2	$RbB_5O_6(OH)_4\cdot 2H_2O$
90001	Orthorhombic	*Aba*2	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$
410811	Orthorhombic	*Aba*2	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$
21332	Orthorhombic	*Aba*2	$LiNaRbB_5O_8(OH)_2$
4481	Orthorhombic	*Fdd*2	$K_3B_5O_8(OH)_2$
425727	Orthorhombic	*Fdd*2	$Ba_3Al_2(B_3O_6(OH))_2(B_4O_7(OH)_2)$
425867	Orthorhombic	*Fdd*2	$Ba_3Ga_2(B_3O_6(OH))_2(B_4O_7(OH)_2)$
264389	Orthorhombic	*Fdd*2	$InB_6O_9(OH)_3$
20662	Tetragonal	$P4_2$	$Mg(B_2O(OH)_6)$
24920	Tetragonal	$P4_2$	$Mg(B_2O(OH)_6)$
4222	Tetragonal	$I\bar{4}$	$Cs(B(OH)_4)\cdot 2H_2O$
27527	Tetragonal	$I\bar{4}$	$Ca_2BAsO_4(OH)_4$
142127	Tetragonal	$I\bar{4}$	$H_2Na_2K_2(OCu_4B_{20}O_{32}(OH)_8)\cdot 21H_2O$
142128	Tetragonal	$I\bar{4}$	$H_2Rb_{1.6}K_{2.4}(OCu_4B_{20}O_{32}(OH)_8)\cdot 15H_2O$
20155	Tetragonal	$P4_12_12$	$Li_3(B_5O_8(OH)_2)$
20173	Tetragonal	$P4_12_12$	$Li_3(B_5O_8(OH)_2)$
418166	Tetragonal	$P4_32_12$	$Li_3(B_5O_8(OH)_2)$
34580	Tetragonal	$P\bar{4}2_1c$	$K_6Al_4Si_6BH_4O_{24}Cl$
79472	Trigonal	*P*3	$(Li(H_2O)_4)(B(OH)_4)\cdot 2H_2O$
430533	Trigonal	*P*3	$Li(H_2O)_4B(OH)_4\cdot 2H_2O$
431212	Trigonal	$P3_2$	$Pb_6B_{12}O_{21}(OH)_6$
240324	Trigonal	$P3_121$	$Co(BPO_4(OH)_2)$
416089	Trigonal	$P3_121$	$Mg(BPO_4(OH)_2)$
416129	Trigonal	$P3_121$	$Ni(BPO_4(OH)_2)$
431536	Trigonal	$P3_121$	$Ba_2(B_4O_7(OH)_2)$
240322	Trigonal	$P3_221$	$Mn(BPO_4(OH)_2)$
240323	Trigonal	$P3_221$	$Fe(BPO_4(OH)_2)$
10266	Trigonal	*R*32	$Na_2(B_4O_5(OH)_4)\cdot 3H_2O$
70998	Trigonal	*R*32	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$
70999	Trigonal	*R*32	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$
4493	Trigonal	*P*31*c*	$Pb_3(OH)(B_9O_{16})(B(OH)_3)$
4494	Trigonal	*P*31*c*	$Ba_3(OH)(B_9O_{16})(B(OH)_3)$
428677	Trigonal	*P*31*c*	$LiBa_3(OH)(B_9O_{16})(B(OH)_4)$
94525	Trigonal	*P*31*c*	$Pb_3(OH)(B_9O_{16})(B(OH)_3)$
261808	Trigonal	*P*31*c*	$Pb_3(OH)(B_9O_{16})(B(OH)_3)$
42341	Trigonal	*R*3*m*	$NaAl_9(BO_3)_3(Si_6O_{21})(OH)$
136829	Trigonal	*R*3*m*	$(Na_{0.479}Li_{0.024})Al_{2.976}Al_6(Si_{5.676}B_{0.324}O_{18})(BO_3)_3(OH)_3O$
136830	Trigonal	*R*3*m*	$(Na_{0.617}Li_{0.165})Al_{2.835}Al_6(Si_{5.718}B_{0.282}O_{18})(BO_3)_3(OH)_3O$
112290	Trigonal	*R*3*m*	$(Na_{0.44}Ca_{0.56})(Mg_{1.56}Fe_{1.55}Al_{5.89})(Si_6O_{18})(BO_3)_3(OH)_3O$
112291	Trigonal	*R*3*m*	$(Na_{0.095}Ca_{0.905})(Mg_{2.30}Fe_{0.83}Al_{5.86})(Si_6O_{18})(BO_3)_3(OH)_3O$
137133	Trigonal	*R*3*m*	$Na_{0.768}(Mn_{1.032}Al_{1.878}Fe_{0.09})Al_6(Si_6O_{18})(BO_3)_3(OH)_3O$
127049	Trigonal	*R*3*m*	$Na_{0.824}K_{0.176}Fe_3(Fe_{2.397}Mg_{0.681}Al_{2.922})(Si_6O_{18})(BO_3)_3(OH)_3O$

ICSD code	Crystal system	Space group	Formula
37833	Trigonal	*R*3*m*	$Na_{0.42}(Mn_{1.39}Fe_{0.16}Mg_{0.01}Al_{1.14}Fe_{0.01}Li_{0.28}Ti_{0.01})Al_6((Si_{5.99}Al_{0.01})O_{18})(BO_3)_3(OH)_3((OH)_{0.65}F_{0.03}O_{0.32})$
37834	Trigonal	*R*3*m*	$Na_{0.49}Mn_{0.49}(Mn_{0.90}Fe_{0.50}Al_{1.36}Fe_{0.04}Li_{0.17}Zn_{0.04})(Al_{5.91}Mn_{0.09})((Si_{5.75}B_{0.25})O_{18})(BO_3)_3(OH)_3((OH)_{0.35}F_{0.17}O_{0.48})$
138478	Trigonal	*R*3*m*	$Ca_{0.589}Na_{0.354}Mg_{1.196}Fe_{0.912}Al_{0.892}(Al_5Mg)(Si_6O_{18})(BO_3)_3(OH)_3(OH)_{0.945}F_{0.055}$
112348	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.124})_3(Al_{1.047})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112349	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.173})_3(Al_{1.022})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112350	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.169})_3(Al_{1.024})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112351	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.175})_3(Al_{1.021})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112352	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.176})_3(Al_{1.021})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112353	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.181})_3(Al_{1.018})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112354	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.184})_3(Al_{1.016})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112355	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.185})_3(Al_{1.016})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112356	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.180})_3(Al_{1.019})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112357	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.186})_3(Al_{1.015})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112358	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.183})_3(Al_{1.017})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112359	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.183})_3(Al_{1.017})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112360	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.176})_3(Al_{1.021})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112361	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.175})_3(Al_{1.021})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112362	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.169})_3(Al_{1.024})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112363	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.127})_3(Al_{1.045})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112364	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.109})_3(Al_{1.054})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
112365	Trigonal	*R*3*m*	$Na_{0.854}(Al_{1.109})_3(Al_{1.054})_6Si_6B_3O_{27}(OH)_3(F_{0.58}(OH)_{0.42})$
143071	Trigonal	*R*3*m*	$(Na_{0.40}Ca_{0.26})(Al_{2.04}Li_{0.78}Mn_{0.18})Al_6(Si_{5.5}B_{0.5})O_{18}(BO_3)_3(OH)_3((OH)_{0.38}F_{0.13}O_{0.49})$
120219	Trigonal	*R*3*m*	$Na_{0.781}(Fe_{0.697}Al_{0.303})_3(Al_{0.912}Fe_{0.088})_6(Si_6O_{18})(BO_3)_3(OH)_3((OH)_{0.591}F_{0.409})$
125271	Trigonal	*R*3*m*	$Na_{0.790}Mg_{1.329}Fe_{2.025}Ca_{0.210}Al_{5.646}(Si_6O_{18})(BO_3)_3(OH)_3O$
125066	Trigonal	*R*3*m*	$(Ca_{0.56}Na_{0.44})(Mg_{1.515}Fe_{1.485})Al_6(BO_3)_3(Si_6O_{18})(OH)_3(O_{0.79}F_{0.21})$
125067	Trigonal	*R*3*m*	$(Na_{0.95}Ca_{0.05})(Mg_{1.71}Fe_{1.29})Al_6(Si_6O_{18})(BO_3)_3(OH)_3O$
127050	Trigonal	*R*3*m*	$Na_{0.767}K_{0.233}Fe_3(Fe_{3.786}Mg_{0.336}Al_{1.878})(Si_6O_{18})(BO_3)_3(OH)_3O$
127051	Trigonal	*R*3*m*	$Na_{0.90}K_{0.10}Fe_3(Fe_{3.54}Mg_{0.402}Al_{2.058})(Si_6O_{18})(BO_3)_3(OH)_3O$
127052	Trigonal	*R*3*m*	$Na_{0.85}K_{0.15}Fe_3(Fe_{3.41}Mg_{0.43}Al_{2.17})(Si_6O_{18})(BO_3)_3(OH)_3O$
127053	Trigonal	*R*3*m*	$Na_{0.78}K_{0.22}Fe_3(Fe_{4.002}Mg_{0.276}Al_{1.722})(Si_6O_{18})(BO_3)_3(OH)_3O$
421260	Trigonal	*R*3*c*	$Y(B_2O_3(OH))_3$
250161	Trigonal	*R*3*c*	$Ho(B_6O_9(OH)_3)$
250162	Trigonal	*R*3*c*	$Gd(B_6O_9(OH)_3)$
112337	Hexagonal	$P6_3$	$Ca_3(Si_{0.64}Al_{0.36})((B(OH)_4)_{0.64}(CO_3)_{1.08}(AsO_3)_{0.28})(OH)_6\cdot 12H_2O$
50539	Hexagonal	$P6_3cm$	$Pb_5(B_3O_8(OH)_3)\cdot H_2O$
238716	Hexagonal	$P\bar{6}2m$	$KGd(B_6O_{10}(OH)_2)$
432932	Hexagonal	$P\bar{6}2m$	$Ni_3B_{18}O_{28}(OH)_4\cdot 4H_2O$
403324	Hexagonal	$P\bar{6}2c$	$K_9(B_4O_5(OH)_4)_3(CO_3)Br\cdot 7H_2O$
403325	Hexagonal	$P\bar{6}2c$	$K_9(B_4O_5(OH)_4)_3(CO_3)Cl\cdot 7H_2O$
425207	Hexagonal	$P\bar{6}2c$	$Li_3(B_8O_{12}(OH)_3)$

ICSD code	Crystal system	Space group	Formula
429622	Hexagonal	$P\bar{6}2c$	$K_9(B_4O_5(OH)_4)_3(CO_3)(BH_4)\cdot 7H_2O$
14601	Hexagonal	$P\bar{6}2c$	$NaK_{15}(B_4O_5(OH)_4)_6(NO_2)_2(CO_3)\cdot 7H_2O$
56497	Cubic	$P\bar{4}3m$	$Na_8(Al_6Si_6O_{24})(B(OH)_4)_2$
428956	Cubic	$F\bar{4}3c$	$Na_4Ga_3B_4O_{12}(OH)$

Table S2 The basic information of hydroxyborates with 0D isolated anionic clusters.

No.	ICSD code	Compounds	(*A*+OH)/B ratio	Anionic units	FBB units	Anionic cluster
1	100400	$(NH_4)_2(B_4O_5(OH)_4)\cdot 2H_2O$	1.5	$[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
2	49364	$(NH_4)_2B_4O_5(OH)_4\cdot 2H_2O$	1.5	$[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
3	49365	$(NH_4)_2B_4O_5(OH)_4\cdot 2H_2O$	1.5	$[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
4	26380	$NH_4(B_5O_6(OH)_4)\cdot 2H_2O$	1	$[BO_2(OH)]$, $[BO_4]$	$[B_5O_6(OH)_4]$	$[B_5O_6(OH)_4]$
5	260879	$Na_3(B_3O_4(OH)_4)$	2.333	$[BO_3]$, $[BO_2(OH)_2]$	$[B_3O_4(OH)_4]$	$[B_3O_4(OH)_4]$
6	34648	$K_2(B_4O_5(OH)_4)\cdot 2H_2O$	1.5	$[BO_2(OH)]$, $[BO_4]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
7	57297	$Ba(BO_2(OH))$	2	$[BO_2(OH)]$	$[BO_2(OH)]$	$[BO_2(OH)]$
8	253012	$K_3B_3O_4(OH)_4\cdot 2H_2O$	2.333	$[BO_3]$, $[BO_2(OH)_2]$	$[B_3O_4(OH)_4]$	$[B_3O_4(OH)_4]$
9	113334	$(NH_4)_2(B_4O_5(OH)_4)\cdot 2H_2O$	1.5	$[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
10	6292	$K(B_5O_6(OH)_4)\cdot 2H_2O$	1	$[BO_2(OH)]$, $[BO_4]$	$[B_5O_6(OH)_4]$	$[B_5O_6(OH)_4]$
11	29406	$RbB_5O_6(OH)_4\cdot 2H_2O$	1	$[BO_2(OH)]$, $[BO_4]$	$[B_5O_6(OH)_4]$	$[B_5O_6(OH)_4]$
12	90001	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$	1	$[BO_2(OH)]$, $[BO_4]$	$[B_5O_6(OH)_4]$	$[B_5O_6(OH)_4]$
13	410811	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$	1	$[BO_2(OH)]$, $[BO_4]$	$[B_5O_6(OH)_4]$	$[B_5O_6(OH)_4]$
14	4481	$K_3B_5O_8(OH)_2$	1	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_5O_8(OH)_2]$	$[B_5O_8(OH)_2]$
15	20662	$Mg(B_2O(OH)_6)$	3.5	$[BO(OH)_3]$	$[B_2O(OH)_6]$	$[B_2O(OH)_6]$
16	24920	$Mg(B_2O(OH)_6)$	3.5	$[BO(OH)_3]$	$[B_2O(OH)_6]$	$[B_2O(OH)_6]$
17	10266	$Na_2(B_4O_5(OH)_4)\cdot 3H_2O$	1.5	$[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$	$[B_4O_5(OH)_4]$
18	70998	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$	1.462	$[BO_2]$, $[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$, $[BO_2]$	$[B_4O_5(OH)_4]$, $[BO_2]$
19	70999	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$	1.462	$[BO_2]$, $[BO_2(OH)]$, $[BO_3(OH)]$	$[B_4O_5(OH)_4]$, $[BO_2]$	$[B_4O_5(OH)_4]$, $[BO_2]$

Table S3 The basic information of hydroxyborates with 1D infinite anionic chains.

No.	ICSD code	Compounds	(*A*+OH)/B ratio	Anionic units	FBB units	Anionic chain
1	172480	$Bi(B_4O_6(OH)_2)(OH)$	0.75	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_4O_7(OH)_2]$	$^1[B_4O_6(OH)_2]_\infty$
2	28426	$CaB_3O_4(OH)_3 \cdot H_2O$	1.333	$[BO_3]$, $[BO_3(OH)]$, $[BO_2(OH)_2]$	$[B_3O_5(OH)_3]$	$^1[B_3O_4(OH)_3]_\infty$
3	28427	$CaB_3O_4(OH)_3 \cdot H_2O$	1.333	$[BO_3]$, $[BO_3(OH)]$, $[BO_2(OH)_2]$	$[B_3O_5(OH)_3]$	$^1[B_3O_4(OH)_3]_\infty$
4	141235	$NaRb_3B_6O_9(OH)_3(HCO_3)$	1.167	$[BO_2(OH)]$, $[BO_4]$	$[B_6O_{11}(OH)_3]$	$^1[B_6O_9(OH)_3]_\infty$
5	262542	$Ba_3B_6O_{11}(OH)_2$	0.833	$[BO_3]$, $[BO_4]$, $[BO_2(OH)_2]$	$[B_6O_{13}(OH)_2]$	$^1[B_6O_{11}(OH)_2]_\infty$
6	431106	$Na(B_5O_7(OH)_2) \cdot H_2O$	0.6	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_5O_8(OH)_2]$	$^1[B_5O_7(OH)_2]_\infty$
7	431536	$Ba_2(B_4O_7(OH)_2)$	1	$[BO_3]$, $[BO_4]$, $[BO_2(OH)_2]$	$[B_4O_9(OH)_2]$	$^1[B_4O_7(OH)_2]_\infty$

Table S4 The basic information of hydroxyborates with 2D anionic layered configurations.

No.	ICSD code	Compounds	(*A*+OH)/B ratio	Anionic units	FBB units	Anionic layered configuration
1	39637	$KCa_4(B_{22}O_{32})(OH)_{10}Cl \cdot 4H_2O$	0.682	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
2	187776	$KCa_4(B_{22}O_{32}(OH)_{10}Cl) \cdot 4H_2O$	0.682	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
3	420549	$Ca_2(B_5O_8(OH))_2 B(OH)_3 \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
4	134988	$Ca_2(B_5O_8(OH))_2 (B(OH)_3) \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_{10}O_{20}(OH)_2]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
5	42570	$Ba_2B_{13}O_{19}(OH)_5 \cdot 5H_2O$	0.539	$[BO_3]$, $[BO_2(OH)]$, $[BO(OH)_2]$, $[BO_4]$, $[BO_3(OH)]$	$[B_{13}O_{25}(OH)_5]$	$^2[B_{13}O_{19}(OH)_5]_\infty$
6	171019	$CaB_8O_{11}(OH)_4$	0.625	$[BO_3]$, $[BO_2(OH)]$, $[BO(OH)_2]$, $[BO_4]$	$[B_8O_{13}(OH)_4]$	$^2[B_8O_{11}(OH)_4]_\infty$
7	250323	$CaB_8O_{11}(OH)_4$	0.625	$[BO_3]$, $[BO_2(OH)]$, $[BO(OH)_2]$, $[BO_4]$	$[B_8O_{13}(OH)_4]$	$^2[B_8O_{11}(OH)_4]_\infty$
8	262502	$Ba_2(B_6O_9(OH)_4)$	1	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$, $[BO_2(OH)_2]$	$[B_6O_{13}(OH)_4]$	$^2[B_6O_9(OH)_4]_\infty$
9	415082	$Ca(B_8O_{11}(OH)_4)$	0.625	$[BO_3]$, $[BO_2(OH)]$, $[BO(OH)_2]$, $[BO_4]$	$[B_8O_{13}(OH)_4]$	$^2[B_8O_{11}(OH)_4]_\infty$
10	432814	$Ca_2(B_5O_8(OH))_2 (B(OH)_3) \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$,	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
11	4228	$Sr(B_8O_{11}(OH)_4)$	0.625	$[BO_3]$, $[BO_2(OH)]$, $[BO(OH)_2]$, $[BO_4]$	$[B_8O_{13}(OH)_4]$	$^2[B_8O_{11}(OH)_4]_\infty$
12	20074	$Sr_2(B_5O_8(OH))_2 (B(OH)_3)(H_2O)$	0.636	$[BO_3]$,$[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
13	28014	$Sr_2(B_5O_8(OH))_2 (B(OH)_3) \cdot H_2O$	0.636	$[BO_3]$,$[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
14	19922	$Ba_2(B_5O_8(OH))_2 (B(OH)_3) \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
15	95447	$Na_2Ba_2(B_{10}O_{17}(OH)_2)$	0.6	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_{10}O_{21}(OH)_2]$	$^2[B_{10}O_{17}(OH)_2]_\infty$
16	403149	$Ba_3(B_{10}O_{17}(OH)_2)$	0.5	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_{10}O_{23}(OH)_2]$	$^2[B_{10}O_{17}(OH)_2]_\infty$
17	154523	$Na_4(B_{10}O_{16}(OH)_2) \cdot 4H_2O$	0.6	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_5O_{10}(OH)]$	$^2[B_5O_8(OH)]_\infty$
18	2942	$Sr_2(B_5O_8(OH))_2 (B(OH)_3) \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$
19	262913	$La(B_4O_6(OH)_2Cl)$	0.75	$[BO_3]$, $[BO_3(OH)]$	$[B_4O_{10}(OH)_2]$	$^2[B_4O_6(OH)_2]_\infty$
20	124040	$Ba_2B_{10}O_{16}(OH)_2(H_3BO_3) \cdot H_2O$	0.636	$[BO_3]$, $[BO_2(OH)]$, $[B(OH)_3]$, $[BO_4]$	$[B(OH)_3]$, $[B_5O_{10}(OH)]$	$[B(OH)_3]$, $^2[B_5O_8(OH)]_\infty$

No.	ICSD code	Compounds	(*A*+OH)/B ratio	Anionic units	FBB units	Anionic layered configuration
21	13423	$Li_2CsB_7O_{10}(OH)_4$	1	$[BO_3]$, $[BO_4]$, $[BO_2(OH)_2]$	$[B_7O_{12}(OH)_4]$	$^2[B_7O_{10}(OH)_4]_\infty$
22	250215	$CaLi_4(B_5O_8(OH)_2)_2$	0.9	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_5O_{10}(OH)_2]$	$^2[B_5O_8(OH)_2]_\infty$
23	36431	$Li_3(B_5O_8(OH)_2)$	1	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_5O_{10}(OH)_2]$	$^2[B_5O_8(OH)_2]_\infty$
24	22192	$CaB_3O_5(OH)$	0.667	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_3O_7(OH)]$	$^2[B_3O_5(OH)]_\infty$
25	23880	$CaB_3O_5(OH)$	0.667	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_3O_7(OH)]$	$^2[B_3O_5(OH)]_\infty$
26	1973	$(Na(H_2O))_2(B_5O_8(OH))$	0.6	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_5O_{10}(OH)]$	$^2[B_5O_8(OH)]_\infty$
27	249876	$Na_2B_5O_8(OH)\cdot 2H_2O$	0.6	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$	$[B_5O_{10}(OH)]$	$^2[B_5O_8(OH)]_\infty$
28	252381	$CaB_3O_5(OH)$	0.667	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_3O_9(OH)]$	$^2[B_3O_5(OH)]_\infty$
29	425207	$Li_3(B_8O_{12}(OH)_3)$	0.75	$[BO_2(OH)]$, $[BO_4]$	$[B_8O_{18}(OH)_3]$	$^2[B_8O_{12}(OH)_3]_\infty$

Table S5 The basic information of hydroxyborates with 3D anionic frameworks.

No.	ICSD code	Compounds	(*A*+OH)/B ratio	Anionic units	FBB units	Anionic framework
1	76888	$Ca_9B_{26}O_{34}(OH)_{24}Cl_4 \cdot 13H_2O$	1.269	$[BO_3]$, $[BO_2(OH)]$, $[BO_4]$, $[BO_2(OH)_2]$, $[BO_3(OH)]$	$[B_{26}O_{47}(OH)_2]$	$^3[B_{26}O_{34}(OH)_{24}]_\infty$
2	20155	$Li_3(B_5O_8(OH)_2)$	1	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_5O_{10}(OH)_2]$	$^3[B_5O_8(OH)_2]_\infty$
3	20173	$Li_3(B_5O_8(OH)_2)$	1	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_5O_{10}(OH)_2]$	$^3[B_5O_8(OH)_2]_\infty$
4	418166	$Li_3(B_5O_8(OH)_2)$	1	$[BO_3]$, $[BO_4]$, $[BO_3(OH)]$	$[B_5O_{10}(OH)_2]$	$^3[B_5O_8(OH)_2]_\infty$
5	421260	$Y(B_2O_3(OH))_3$	0.667	$[BO_3]$, $[BO_3(OH)]$	$[B_2O_5(OH)]$	$^3[B_2O_3(OH)]_\infty$

Table S6 The ICSD collection numbers, chemical formula, space group, GGA and HSE06 band gaps, second harmonic generation (SHG) coefficients, and birefringence Δ*n* at 1064 nm of 60 screening hydroxyborates crystals. Note that SHG coefficients, and birefringence Δ*n* have been corrected with scissors operators.

No.	ICSD code	Compounds	Space group	Band gap (eV)		SHG coefficients (pm/V)	Δ*n* at 1064 nm
				GGA	HSE06		
1	39637	$KCa_4(B_{22}O_{32})(OH)_{10}Cl{\cdot}4H_2O$	*P*1	5.49	7.02	d_{11} = 0.54, d_{12} = −0.57 d_{16} = 0.48, d_{22} = −0.56	0.064
2	187776	$KCa_4(B_{22}O_{32}(OH)_{10}Cl){\cdot}4H_2O$	*P*1	5.48	7.08	d_{11} = −0.55, d_{12} = 0.59 d_{16} = 0.50, d_{22} = −0.55	0.065
3	172480	$Bi(B_4O_6(OH)_2)(OH)$	*P*1	4.69	5.59	*0*	0.110
4	76888	$Ca_9B_{26}O_{34}(OH)_{24}Cl_4{\cdot}13H_2O$	*P*1	5.36	6.65	d_{11} = −0.09, d_{15} = 0.41, d_{23} = 0.12, d_{24} = −0.41, d_{33} = 0.09	0.031
5	420549	$Ca_2(B_5O_8(OH))_2B(OH)_3{\cdot}H_2O$	*P*1	5.52	7.08	d_{11} = −0.59, d_{12} = 0.67, d_{13} = 0.12, d_{14} = −0.14, d_{16} = −0.56, d_{22} = 0.51, d_{24} = −0.17, d_{33} = 0.10	0.060
6	134988	$Ca_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$	*P*1	5.90	7.38	d_{11} = 0.66, d_{12} = −0.67, d_{16} = 0.60, d_{22} = −0.55	0.071
7	42570	$Ba_2B_{13}O_{19}(OH)_5{\cdot}5H_2O$	*P*1	5.15	6.58	d_{16} = −0.29, d_{22} = −0.49, d_{23} = 0.65	0.035
8	28426	$CaB_3O_4(OH)_3{\cdot}H_2O$	$P2_1$	5.59	7.28	d_{11} = 0.13	0.011
9	28427	$Ca(B_3O_4(OH)_3){\cdot}H_2O$	$P2_1$	5.67	7.20	d_{22} = 0.15, d_{23} = −0.05	0.028
10	171019	$CaB_8O_{11}(OH)_4$	$P2_1$	5.56	6.71	d_{22} = 0.65, d_{23} = −0.66	0.091
11	250323	$CaB_8O_{11}(OH)_4$	$P2_1$	5.59	6.81	d_{14} = −0.07, d_{16} = 0.10, d_{22} = 0.62, d_{23} = −0.64	0.061
12	262502	$Ba_2(B_6O_9(OH)_4)$	$P2_1$	5.22	7.14	d_{16} = −0.43, d_{22} = 1.07	0.037
13	415082	$Ca(B_8O_{11}(OH)_4)$	$P2_1$	5.58	6.80	d_{14} = −0.07, d_{16} = 0.12, d_{22} = 0.63, d_{23} = −0.64	0.091
14	432814	$Ca_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$	$P2_1$	5.89	7.54	d_{16} = −0.06, d_{22} = 0.13, d_{23} = −0.08	0.076
15	4228	$Sr(B_8O_{11}(OH)_4)$	$P2_1$	5.06	6.45	d_{16} = −0.88, d_{22} = 0.57, d_{23} = 0.47	0.076
16	20074	$Sr_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$	$P2_1$	5.85	7.36	d_{22} = 0.08, d_{23} = −0.07	0.040
17	28014	$Sr_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$	$P2_1$	5.35	6.77	d_{22} = 0.21, d_{23} = −0.03	0.050
18	100400	$(NH_4)_2(B_4O_5(OH)_4){\cdot}2H_2O$	$P2_1$	4.97	6.30	d_{14} = 0.18, d_{16} = 0.32, d_{22} = −0.62, d_{23} = 0.25	0.014
19	49364	$(NH_4)_2B_4O_5(OH)_4{\cdot}2H_2O$	$P2_1$	5.18	6.68	d_{14} = −0.20, d_{16} = −0.37, d_{22} = 0.80, d_{23} = −0.42	0.016
20	49365	$(NH_4)_2B_4O_5(OH)_4{\cdot}2H_2O$	$P2_1$	5.17	6.47	d_{14} = −0.10, d_{16} = −0.24, d_{22} = 0.55, d_{23} = −0.28	0.041
21	19922	$Ba_2(B_5O_8(OH))_2(B(OH)_3){\cdot}H_2O$	$P2_1$	5.83	6.76	d_{16} = −0.07, d_{22} = −0.16, d_{23} = 0.10	0.070
22	141235	$NaRb_3B_6O_9(OH)_3(HCO_3)$	$P2_1$	4.19	5.40	d_{14} = 0.08, d_{16} = 0.06, d_{22} = 0.11, d_{23} = 0.16	0.017

No.	ICSD code	Compounds	Space group	Band gap (eV)		SHG coefficients (pm/V)	Δ*n* at 1064 nm
				GGA	HSE06		
23	95447	$Na_2Ba_2(B_{10}O_{17}(OH)_2)$	*C*2	4.70	6.12	$d_{16} = 0.38$, $d_{22} = -1.08$	0.027
24	403149	$Ba_3(B_{10}O_{17}(OH)_2)$	*C*2	4.62	5.95	$d_{22} = 0.33$, $d_{23} = -0.18$	0.033
25	262542	$Ba_3B_6O_{11}(OH)_2$	*Pc*	4.76	6.12	$d_{11} = -0.67$, $d_{33} = 0.33$	0.010
26	154523	$Na_4(B_{10}O_{16}(OH)_2)\cdot 4H_2O$	*Pc*	4.79	6.42	$d_{11} = 0.65$, $d_{12} = -0.25$, $d_{13} = -0.38$, $d_{15} = -0.08$, $d_{33} = 0.21$	0.030
27	26380	$NH_4(B_5O_6(OH)_4)\cdot 2H_2O$	*Pc*	4.98	6.47	$d_{11} = 0.29$, $d_{12} = -0.39$, $d_{13} = 0.06$, $d_{15} = 0.10$, $d_{33} = 0.07$	0.050
28	2942	$Sr_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$	*Cc*	5.91	7.49	$d_{11} = 0.07$, $d_{13} = 0.06$, $d_{24} = -0.08$, $d_{33} = 0.12$	0.005
29	260879	$Na_3(B_3O_4(OH)_4)$	*Cc*	4.64	5.92	$d_{15} = 0.26$, $d_{24} = -0.34$	0.037
30	262913	$La(B_4O_6(OH)_2Cl)$	*Cc*	6.17	7.14	$d_{11} = -0.79$, $d_{12} = 0.77$, $d_{13} = 0.34$, $d_{15} = -0.38$, $d_{24} = -0.39$, $d_{33} = 0.93$	0.030
31	124040	$Ba_2B_{10}O_{16}(OH)_2(H_3BO_3)\cdot H_2O$	*Cc*	5.48	7.29	$d_{24} = 0.10$, d33 = −0.11	0.069
32	34648	$K_2(B_4O_5(OH)_4)\cdot 2H_2O$	$P2_12_12_1$	5.12	6.67	$d_{14} = -0.13$	0.008
33	57297	$Ba(BO_2(OH))$	$P2_12_12_1$	4.10	5.88	$d_{14} = 0.07$	0.082
34	13423	$Li_2CsB_7O_{10}(OH)_4$	*C*222	5.20	7.26	$d_{14} = 0.70$	0.023
35	431106	$Na(B_5O_7(OH)_2)\cdot H_2O$	$Pca2_1$	5.79	7.29	$d_{24} = -0.14$, $d_{33} = -0.09$	0.059
36	250215	$CaLi_4(B_5O_8(OH)_2)_2$	*Pnc*2	5.08	6.75	$d_{24} = -0.11$, $d_{33} = 0.29$	0.033
37	36431	$Li_3(B_5O_8(OH)_2)$	*Pnc*2	5.60	6.26	$d_{24} = -0.05$	0.037
38	22192	$CaB_3O_5(OH)$	$Pna2_1$	5.50	6.36	$d_{15} = -0.65$, $d_{24} = 0.48$, $d_{33} = 0.82$	0.043
39	23880	$CaB_3O_5(OH)$	$Pna2_1$	5.50	6.96	$d_{15} = 0.41$, $d_{24} = -0.57$, $d_{33} = 0.72$	0.040
40	1973	$(Na(H_2O))_2(B_5O_8(OH))$	$Pna2_1$	5.00	6.47	$d_{15} = 0.34$, $d_{24} = 0.33$, $d_{33} = -0.68$	0.023
41	249876	$Na_2B_5O_8(OH)\cdot 2H_2O$	$Pna2_1$	5.00	6.62	$d_{15} = -0.35$, $d_{24} = -0.34$, $d_{33} = 0.70$	0.023
42	252381	$CaB_3O_5(OH)$	$Pna2_1$	5.74	7.15	$d_{15} = -0.50$, $d_{24} = 0.70$, $d_{33} = -0.77$	0.037
43	253012	$K_3B_3O_4(OH)_4\cdot 2H_2O$	$Cmc2_1$	4.45	5.77	$d_{15} = 0.01$, $d_{24} = -0.39$, $d_{33} = 0.33$	0.036
44	113334	$(NH_4)_2(B_4O_5(OH)_4)\cdot 2H_2O$	$Cmc2_1$	5.19	6.71	$d_{15} = 0.61$, $d_{24} = -0.20$, $d_{33} = -0.50$	0.016
45	6292	$K(B_5O_6(OH)_4)\cdot 2H_2O$	*Aba*2	*5.57*	7.02	$d_{15} = 0.116$, $d_{24} = -0.085$, $d_{33} = 0.082$	0.050
46	29406	$RbB_5O_6(OH)_4\cdot 2H_2O$	*Aba*2	5.50	7.22	$d_{15} = 0.08$, $d_{24} = -0.08$, $d_{33} = 0.07$	0.050
47	90001	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$	*Aba*2	5.58	6.91	$d_{15} = -0.18$, $d_{24} = 0.15$, $d_{33} = 0.26$	0.049

No.	ICSD code	Compounds	Space group	Band gap (eV)		SHG coefficients (pm/V)	Δ*n* at 1064 nm
				GGA	HSE06		
48	410811	$(NH_4)(B_5O_6(OH)_4)\cdot 2H_2O$	*Aba*2	5.59	6.88	$d_{15} = -0.17$, $d_{24} = 0.13$, $d_{33} = 0.26$	0.049
49	4481	$K_3B_5O_8(OH)_2$	*Fdd*2	4.84	6.26	$d_{15} = 0.21$, $d_{24} = 0.26$	0.042
50	20662	$Mg(B_2O(OH)_6)$	$P4_2$	5.44	7.15	0	0.004
51	24920	$Mg(B_2O(OH)_6)$	$P4_2$	4.30	5.86	$d_{33} = -0.39$	0.002
52	20155	$Li_3(B_5O_8(OH)_2)$	$P4_12_12$	6.37	7.82	0	0.004
53	20173	$Li_3(B_5O_8(OH)_2)$	$P4_12_12$	5.97	7.53	0	0.004
54	418166	$Li_3(B_5O_8(OH)_2)$	$P4_32_12$	5.96	7.81	0	0.004
55	431536	$Ba_2(B_4O_7(OH)_2)$	$P3_121$	4.13	5.15	$d_{11} = 0.57$, $d_{12} = -0.57$	0.014
56	10266	$Na_2(B_4O_5(OH)_4)\cdot 3H_2O$	*R*32	5.23	6.60	$d_{11} = 0.10$, $d_{12} = -0.10$	0.007
57	70998	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$	*R*32	4.75	5.83	$d_{11} = 0.02$, $d_{12} = -0.02$	0.010
58	70999	$NaRb_6(B_4O_5(OH)_4)_3(BO_2)$	*R*32	4.73	5.82	$d_{11} = 0.09$, $d_{12} = -0.09$	0.010
59	421260	$Y(B_2O_3(OH))_3$	*R*3*c*	6.25	7.60	$d_{21} = -0.78$, $d_{22} = 0.78$, $d_{15} = 0.20$, $d_{24} = 0.20$	0.037
60	425207	$Li_3(B_8O_{12}(OH)_3)$	$P\bar{6}2c$	5.72	6.84	$d_{16} = 0.20$, $d_{22} = -0.20$	0.036

Table S7 Calculated band gaps (E_g) by hybrid HSE06, the maximum SHG coefficients (d_{ij}), birefringence at 1064 nm (Δn), UV cutoff wavelengths (λ_{cutoff}), shortest phase-matching wavelengths (λ_{PM}), dimensionality of B−O/OH anionic framework, and (A + OH)/B ratio of screened hydroxyborate crystals.

No.	ICSD code	Compounds	Space group	E_g (eV)	d_{ij} (pm/V)	Δn	λ_{cutoff} (nm)	λ_{PM} (nm)	Dimmension / Ration
1	42570	$Ba_2B_{13}O_{19}(OH)_5\cdot 5H_2O$	$P1$	6.58	d_{23} = 0.65	0.04	189	298	2/0.539
1a[1]			$P1$	> 6.2	$d_{<powder>} \approx$ 1.0 × KDP	---	<200	---	
1b[1]			$P1$	5.41 GGA	d_{23} = 0.87	0.042	230	270	
2	171019	$CaB_8O_{11}(OH)_4$	$P2_1$	6.71	d_{23} = −0.66	0.091	185	199	2/0.625
2a[2]			$P2_1$	> 6.3	$d_{<powder>} \approx$ 1.4 × KDP	---	<200	---	
2b[2]			$P2_1$	7.43 PBE0	d_{23} = −0.41	0.093	165	174	
3	4228	$Sr(B_8O_{11}(OH)_4)$	$P2_1$	6.45	d_{16} = −0.88	0.076	193	211	2/0.625
3a[2]			$P2_1$	>6.30	$d_{<powder>} \approx$ 1.4 × KDP	0.109	<200	---	
3b[2]			$P2_1$	7.02 PBE0	d_{16} = 0.39	0.087	176	185	
4	13423	$Li_2CsB_7O_{10}(OH)_4$	$C222$	7.26	d_{14} = 0.70	0.023	171	321	2/1
4a[3]			$C222$	6.35	$d_{<powder>} \approx$ 2.5 × KDP	---	196	---	
4b[3]			$C222$	4.56 GGA	d_{14} = −0.76	---	273	---	
5	249876	$Na_2B_5O_8(OH)\cdot 2H_2O$	$Pna2_1$	6.62	d_{33} = 0.70	0.023	188	348	2/0.6
5a[4]			$Pna2_1$	> 6.5	$d_{<powder>} \approx$ 0.5 × KDP	---	<190	---	
6	253012	$K_3B_3O_4(OH)_4\cdot 2H_2O$	$Cmc2_1$	5.77	d_{24} = −0.39	0.036	216	295	0/2.333
6a[5]			$Cmc2_1$	6.1	$d_{<powder>} \approx$ 0.8 × KDP	---	204	---	
6b[5]			$Cmc2_1$	4.8 GGA	d_{24} = 0.37	---	256	---	

[a] Experimentally measured data in references. [b] Theoretically calculated data in references.

Table S8 Predicted band gaps (E_g) by hybrid HSE06, largest SHG coefficients (d_{ij}), birefringence at 1064 nm (Δn), UV cutoff wavelengths (λ_{cutoff}), shortest phase-matching wavelengths (λ_{PM}), dimensionality of B−O/OH anionic framework, and (A + OH)/B ratio of screened hydroxyborate crystals.

No.	ICSD code	Compounds	Space group	E_g (eV)	d_{ij} (pm/V)	Δn	λ_{cutoff} (nm)	λ_{PM} (nm)	Dimmension / Ration
1	187776	$KCa_4(B_{22}O_{32})(OH)_{10}Cl{\cdot}4H_2O$	$P1$	7.08	d_{12} = 0.59	0.065	176	235	2/0.682
2	76888	$Ca_9B_{26}O_{34}(OH)_{24}Cl_4{\cdot}13H_2O$	$P1$	6.65	d_{24} = −0.41	0.031	187	336	3/1.269
3	95447	$Na_2Ba_2(B_{10}O_{17}(OH)_2)$	$C2$	6.12	d_{22} = −1.08	0.027	203	368	2/0.6
4	154523	$Na_4(B_{10}O_{16}(OH)_2){\cdot}4H_2O$	Pc	6.42	d_{11} = 0.65	0.03	194	318	2/0.6
5	1973	$(Na(H_2O))_2(B_5O_8(OH))$	$Pna2_1$	6.47	d_{33} = −0.68	0.023	192	346	2/0.6
6	134988	$Ca_2(B_5O_8(OH))_2B(OH)_3{\cdot}H_2O$	$P1$	7.38	d_{12} = −0.67	0.071	170	229	2/0.636
6a[6]			$P1$	>5.75	$d_{<powder>} \approx$ 1.8 × KDP	---	<216	---	
7	262502	$Ba_2(B_6O_9(OH)_4)$	$P2_1$	7.14	d_{22} = 1.07	0.037	174	302	2/1
7a[7]			$P2_1$	>6.5	$d_{<powder>} \approx$ 3 × KDP	---	<190	---	
8	26380	$NH_4(B_5O_6(OH)_4){\cdot}2H_2O$	Pc	6.47	d_{12} = −0.39	0.05	192	240	0/1
8a[8]			Pc	6.91	---	0.058	≈180	---	
9	252381	$CaB_3O_5(OH)$	$Pna2_1$	7.15	d_{33} = −0.77	0.037	174	327	2/0.667
9a[9]			$Pna2_1$	---	$d_{<powder>} \approx$ 1 × KDP	---	---	---	

[a] Experimentally measured data in references.

Table S9 The investigation of ratio (A + OH)/B = 0.636, dimensionality of B−O/OH anionic framework, birefringence at 1064 nm (cal.), and $[BO_3]$ & $[B(OH)_3]$ & $[BO_2(OH)]$ density among hydroxyborates involving the screened compounds.

No.	ICSD code	Compounds	Space group	Dimension	Number of $[BO_3]$ & $[B(OH)_3]$ & $[BO_2(OH)]$ in cell	Cell volume (Å^3)	Birefringence at 1064 nm (cal.)	Density of $[BO_3]$ & $[B(OH)_3]$ & $[BO_2(OH)]$ groups(Å^{-3})
1	420549	$Ca_2(B_5O_8(OH))_2B(OH)_3\cdot H_2O$-I	*P*1	2D	6.5	386.3	0.06	0.0168
2	134988	$Ca_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-II	*P*1	2D	7	385.7	0.071	0.0181
3	432814	$Ca_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-III	$P2_1$	2D	14	773.2	0.076	0.0181
4	20074	$Sr_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-I	$P2_1$	2D	13	802.5	0.040	0.0162
5	28014	$Sr_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-II	$P2_1$	2D	13	802.5	0.050	0.0162
6	2942	$Sr_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-III	*Cc*	2D	18	1627.7	0.005	0.0111
7	19922	$Ba_2(B_5O_8(OH))_2(B(OH)_3)\cdot H_2O$-I	$P2_1$	2D	14	857.1	0.070	0.0163
8	124040	$Ba_2B_{10}O_{16}(OH)_2(H_3BO_3)\cdot H_2O$-II	*Cc*	2D	30	1717.0	0.069	0.0174

Table S10 Bonding electron difference ($\Delta\rho$) and contribution percent w (%) of different units in $KCa_4(B_{22}O_{32}(OH)_{10}Cl)\cdot 4H_2O$ calculated by the REDA model.

Compounds	units	$\Delta\rho$	w (%)
$KCa_4(B_{22}O_{32}(OH)_{10}Cl)\cdot 4H_2O$	$[BO_3]$	0.0106	52.46
	$[BO_2(OH)]$	0.0054	26.55
	$[B(OH)_3]$	0.0029	14.28
	$[BO_4]$	0.0008	4.04
	$[KO_4]$	0.0001	0.73
	$[CaO_9]$	0.0003	1.45
	$[CaO_8Cl]$	0.0001	0.49

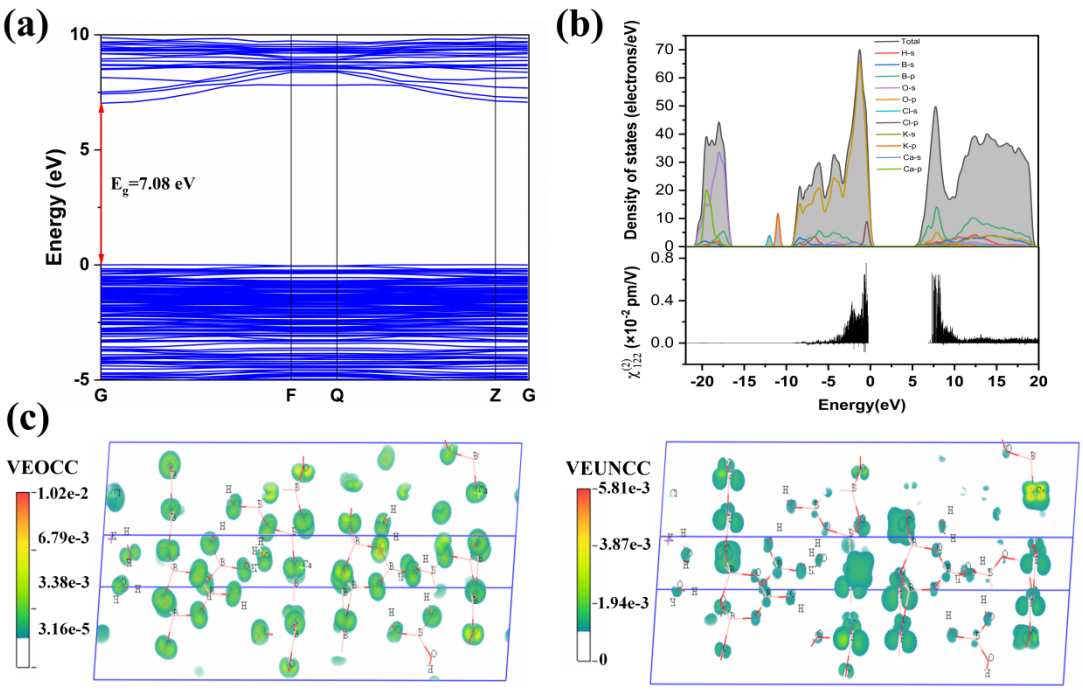

Figure S1. (a) Band structures by the HSE06 functional. (b) Total and partial density of states (PDOS) and band-resolved NLO coefficients. (c) SHG-weighted density of occupied and unoccupied states in virtual-electron (VE) progress of $KCa_4(B_{22}O_{32}(OH)_{10}Cl)\cdot 4H_2O$. Here, $\chi_{122} = 2d_{12}$.

Notes and references

1 K. Liu, J. Han, F. Li, C. Jin, Z. Yang, M. Mutailipu and S. Pan, $Ba_2B_{13}O_{19}(OH)_5 \cdot 5H_2O$: A promising nonlinear optical material with a unique $^2[B_{13}O_{19}(OH)_5]_\infty$ two-dimensional layer, J. Alloys Compd., 2022, **897**, 163194.

2 P. Gong, L. Kang and Z. Lin, Realizing deep-ultraviolet second harmonic generation by first-principles-guided materials exploration in hydroxyborates, J. Am. Chem. Soc., 2020, **142**, 15157–15163.

3 J.-H. Huang, C.-C. Jin, P.-L. Xu, P. Gong, Z. Lin, J.-W. Cheng and G.-Y. Yang, $Li_2CsB_7O_{10}(OH)_4$: A deep-ultraviolet nonlinear-optical mixed-alkaline borate constructed by unusual heptaborate anions, Inorg. Chem., 2019, **58**, 1755–1758.

4 Y. Wang, S. Pan, X. Tian, Z. Zhou, G. Liu, J. Wang and D. Jia, Synthesis, structure, and properties of the noncentrosymmetric hydrated borate $Na_2B_5O_8(OH) \cdot 2H_2O$, Inorg. Chem., 2009, **48**, 7800–7804.

5 Q. Liu, X. Zhang, Z. Yang, F. Zhang, L. Liu, J. Han, Z. Li and S. Pan, $K_3B_3O_4(OH)_4 \cdot 2H_2O$: A UV nonlinear optical crystal with isolated $[B_3O_4(OH)_4]^{3-}$ anion groups, Inorg. Chem., 2016, **55**, 8744–8749.

6 Q.-M. Qiu, X.-Y. Li, C.-A. Chen, K.-N. Sun and G.-Y. Yang, Polar polymorphism: β-$Ca_2[B_5O_8(OH)]_2[B(OH)_3] \cdot H_2O$-synthesis, structure and nonlinear optical property, J. Solid State Chem., 2021, **299**, 122193.

7 L. Wang, S. Pan, L. Chang, J. Hu and H. Yu, UV nonlinear optical crystal $Ba_2[B_6O_9(OH)_4]$ featuring unique chiral layers with a new $B_{18}O_{42}$ circle based on BO_3 and BO_4 units, Inorg. Chem., 2012, **51**, 1852–1858.

8 P. Becker, P. Held and L. Bohatý, Crystal growth and optical properties of the polar hydrated pentaborates $Rb[B_5O_6(OH)_4] \cdot 2H_2O$ and $NH_4[B_5O_6(OH)_4] \cdot 2H_2O$ and structure redetermination of the ammonium compound, Cryst. Res. Technol., 2000, **35**, 1251–1262.

9 N. A. Yamnova, S. M. Aksenov, S. Y. Stefanovich, A. S. Volkov and O. V. Dimitrova, Synthesis, crystal structure refinement, and nonlinear-optical properties of $CaB_3O_5(OH)$: Comparative crystal chemistry of calcium triborates, Crystallogr. Rep., 2015, **60**, 649–655.