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Supporting Information for

Bidentate-anionic-group strategy for enhancing electron-phonon coupling and vibronic fluorescence in rare-earth crystals

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1. Experimental Methods

1.1 Crystal growth

$K_3RE(BO_3)_2$ (RE=Pr, Nd, and Gd) single crystals were grown by means of spontaneous crystallization from self-flux system. Specifically, the molar ratios of Gd_2O_3 (or Nd_2O_3): K_2CO_3: H_3BO_3 = 3: 40: 150 and Pr_6O_{11}: K_2CO_3: H_3BO_3 = 1: 40: 150 were employed. The mixture of reagents with high purity was ground thoroughly and put into a platinum crucible with a diameter of 20 mm and a height of 20 mm. The crucible was placed into a vertical programmable temperature furnace. The temperature was raised up to 970 °C and kept for 200 minutes to ensure that the mixture was completely melted and homogeneously mixed, then cooled to 700 °C at a rate of 2 °C/h, and finally cooled to 25 °C at a rate of 30 °C/h. The as-grown transparent crystals were mechanically separated from the platinum crucible for the following measurements of structure and properties.

1.2 Solid state synthesis

1.2.1 $K_3RE(BO_3)_2$ (RE=Pr, Nd, and Gd)

Polycrystalline samples were synthesized through high temperature solid state reaction. The mixture of Gd_2O_3 (or Nd_2O_3), K_2CO_3, and H_3BO_3 with molar ratio of 1: 3: 6 as well as Pr_6O_{11}, K_2CO_3, and H_3BO_3 with molar ratio of 1/3: 3: 6 were ground thoroughly, put into a platinum crucible, and then compressed tightly. Next, the crucible was placed into a programmable temperature furnace. Finally, the mixture was heated to 650 °C within 24 hours, kept at this temperature for 48 hours, and then cooled to room temperature within 2 days. Took out the polycrystalline sample and ground it, and repeated the above steps at 850 °C to ensure a more thorough reaction.

1.2.2 $Li_3K_9Gd_3(BO_3)_7$

The raw materials of synthesizing $Li_3K_9Gd_3(BO_3)_7$ polycrystalline samples are Li_2CO_3, K_2CO_3, Gd_2O_3, and H_3BO_3 with molar ratio of 3: 9: 3: 14. The detailed experimental method was the same as that in "*1.2.1 $K_3RE(BO_3)_2$ (RE=Pr, Nd, and Gd)*".

1.2.3 $K_3Gd(PO_4)_2$

The mixture of Gd_2O_3, K_2CO_3, and $NH_4H_2PO_4$ with molar ratio of 1: 3: 4 were ground thoroughly, put into a platinum crucible, and then compressed tightly. The mixture was heated at 300 °C for 5 hours, then cooled to room temperature, and finally heated at 1000 °C for 24 hours.

1.2.4 $KGd(PO_3)_4$

The mixture of Gd_2O_3, K_2CO_3, and $(NH_4)_2HPO_4$ with molar ratio of 1: 1: 8 were ground thoroughly, put into a platinum crucible, and then compressed tightly. The mixture was heated at 400 °C for 2 days, then cooled to room temperature, and finally heated at 600 °C for 10 hours.

1.3 Single crystal X-ray crystallography

Single Crystal X-ray diffraction data were collected using a Bruker D8 Quest diffractometer (Mo Kα, λ=0.71073 Å). Indexing and data integration were performed using APEX3 (Difference Vectors method). Absorption correction was performed by the multiscan method implemented in SADABS.[S1] Space groups were determined using XPREP implemented in APEX3. Structures were solved using SHELXL-2014 (direct methods) and refined using SHELXL-2014 (full-matrix least-squares on F^2) with anisotropic displacement contained in APEX3 program packages. Hydrogen atoms on carbon and nitrogen were calculated in ideal positions with isotropic placement parameters set to 1.2 × U_{eq} of the attached atoms.[S2]

1.4 Powder X-ray diffraction

X-ray diffraction patterns were obtained on a Bruker D8 focus X-ray diffractometer equipped with a diffracted beam monochromator set for Cu-Kα radiation (λ=1.5418 Å) at room temperature. A scan step width of 0.02° and a fixed counting time of 0.2 s/step were applied to record the patterns in the 2θ range of 5−70°.

1.5 Emission spectra measurements

The fluorescence spectra of Gd-containing crystals were collected by a FLS920 Edinburgh fluorescence spectrometer. The Xenon lamp light of 274−290 nm was used as the incident source. The spectral lines were collected with five repeats.

1.6 UV-vis-NIR diffuse reflectance spectrum

UV-vis-NIR diffuse reflectance data were collected on a Cary 7000 spectrophotometer in the spectral range of 200−2500 nm at room temperature. Fluoroethylene was used as a standard.

1.7 Raman spectroscopy

The Raman spectrum was collected in the range of 50−4000 cm^{-1} using the InVia Reflex Raman spectrometer with a 532 nm laser excitation. Several transparent single crystals with regular shape and flat surface were prepared in advance.

1.8 Phonon calculations

The atomic-level theoretical calculations for $K_3Gd(BO_3)_2$ and $K_3Gd(PO_4)_2$ crystal were performed by density functional theory[S3] using the Vienna *ab* initio simulation package code,[S4] which has been applied on rare-earth materials successfully.[S5] In all calculations, the 750 eV cutoff energy and (3×3×4) Monkhorst-Pack *k*-point meshes were selected to ensure sufficient accuracy of the simulated results.[S6] The structural lattices and atomic positions were fully optimized. The exchange–correlation functionals were described by generalized gradient density approximation Perdew−Burke−Ernzerhof (PBE) function[S7] and the ion-electron interactions for all elements were modeled by the projector augmented-wave (PAW) potentials.[S8] The lattice vibrations of them were calculated by the Phonopy.[S9]

2. Additional figures

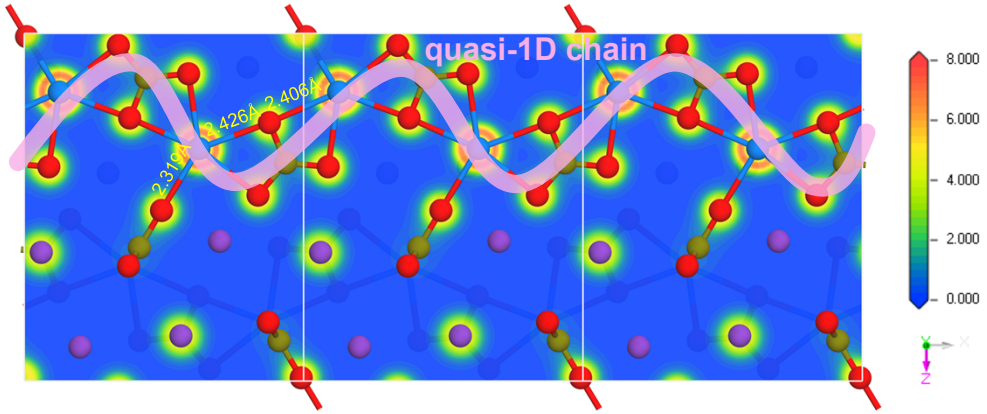

Figure S1. Electronic density distribution of $K_3Gd(BO_3)_2$. The quasi-1D chain was built by Gd^{3+} ion and bidentate-BO_3 groups.

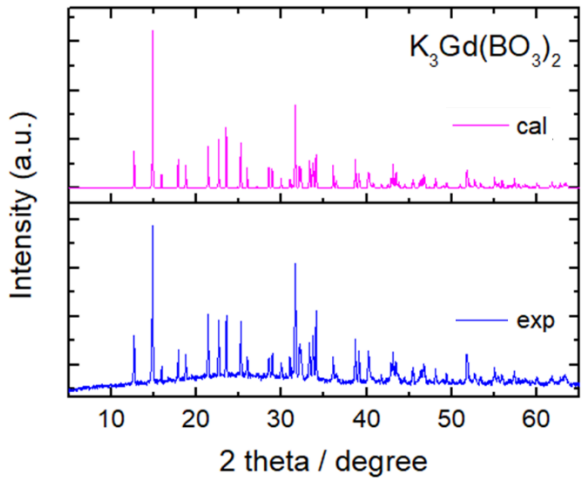

Figure S2. Powder X-ray diffraction pattern of polycrystalline $K_3Gd(BO_3)_2$.

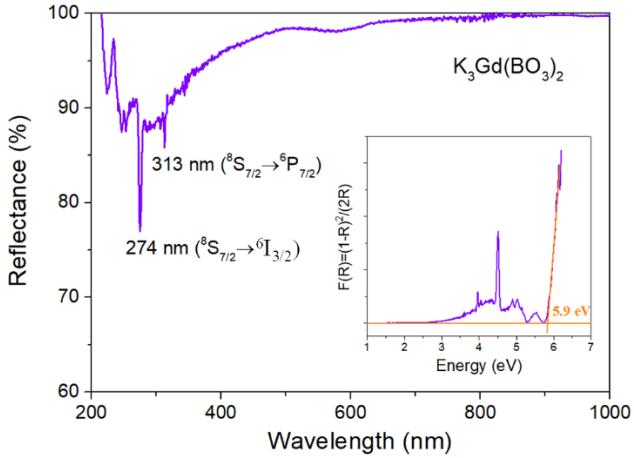

Figure S3. UV-vis-NIR diffuse reflectance spectrum of $K_3Gd(BO_3)_2$. Insert: F(R) versus wavelength.

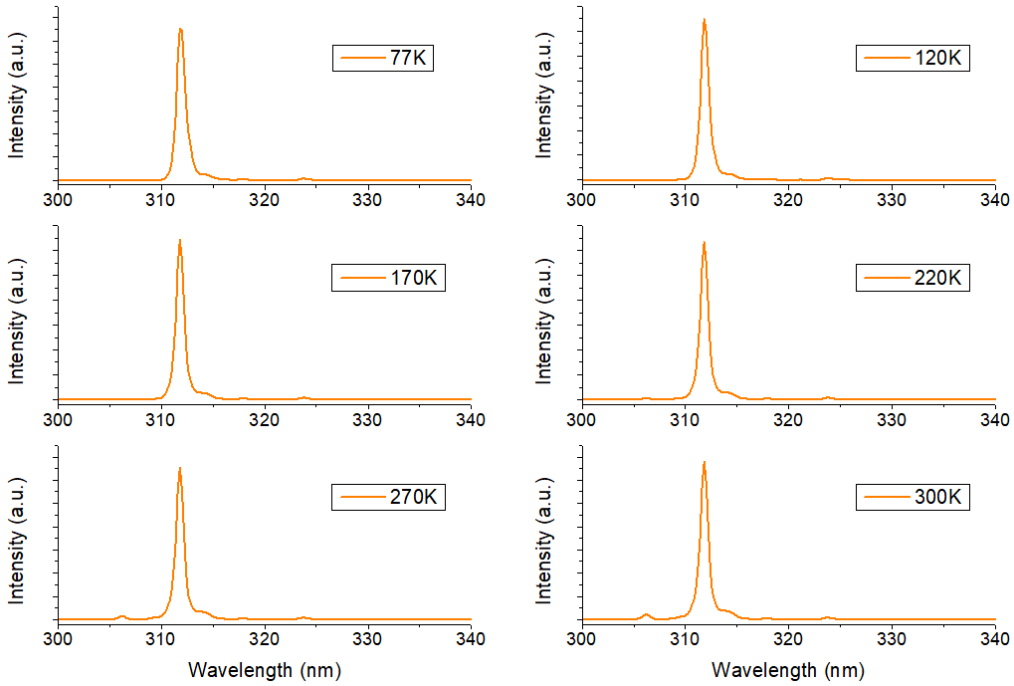

Figure S4. Fluorescence emission of $K_3Gd(BO_3)_2$ under different temperatures.

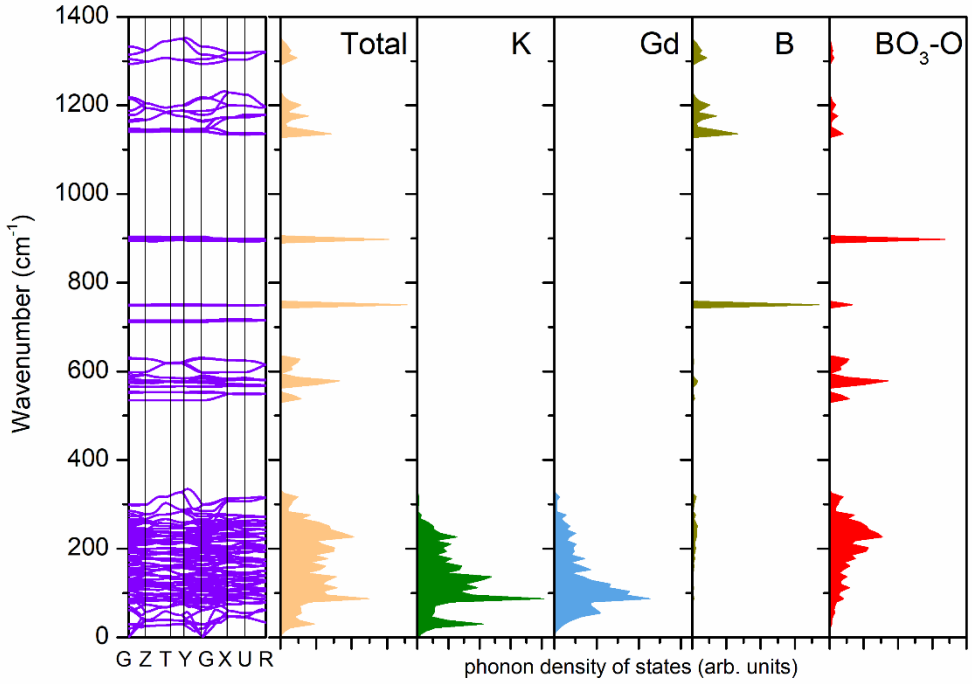

Figure S5. Phonon dispersion and phonon projected density of states of $K_3Gd(BO_3)_2$.

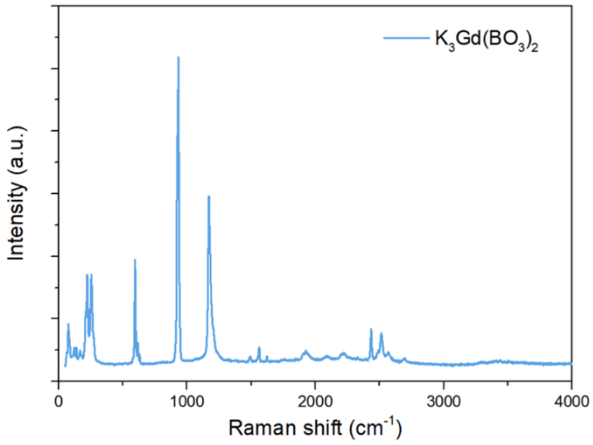

Figure S6. Raman spectrum of $K_3Gd(BO_3)_2$.

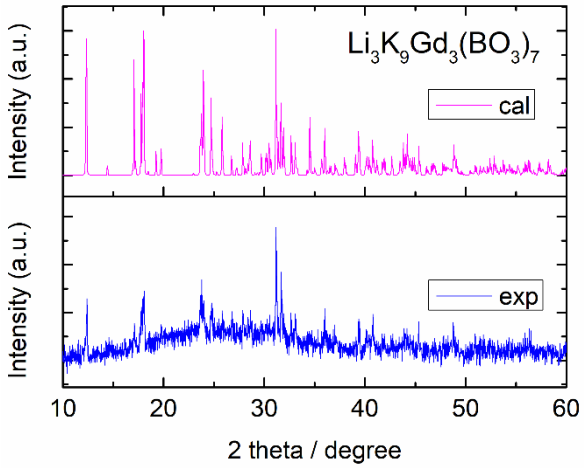

Figure S7. Powder X-ray diffraction pattern of polycrystalline $Li_3K_9Gd_3(BO_3)_7$.

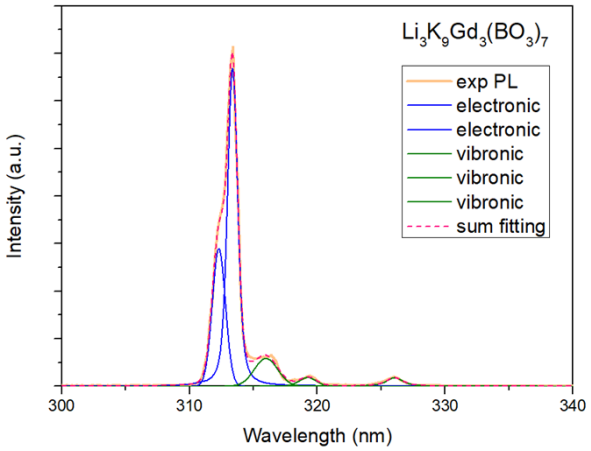

Figure S8. Peak fitting results of fluorescence spectra of $Li_3K_9Gd_3(BO_3)_7$ at 77 K.

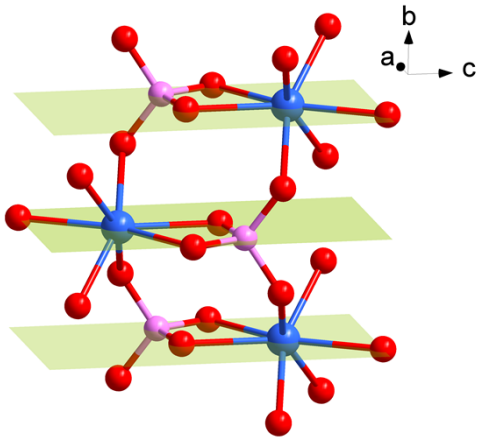

Figure S9. Coordination environment of $K_3Gd(PO_4)_2$.

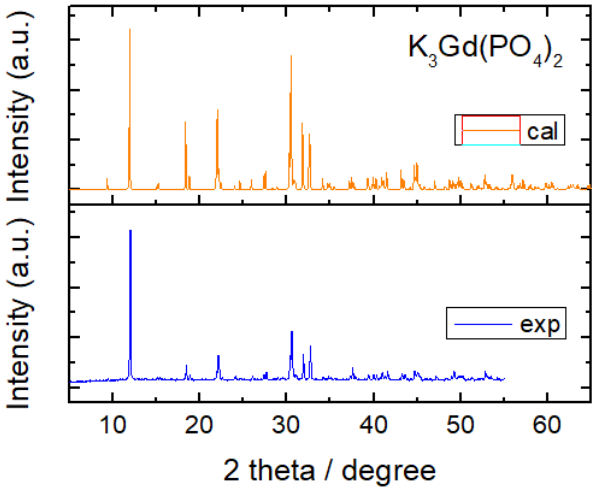

Figure S10. Powder X-ray diffraction pattern of $K_3Gd(PO_4)_2$.

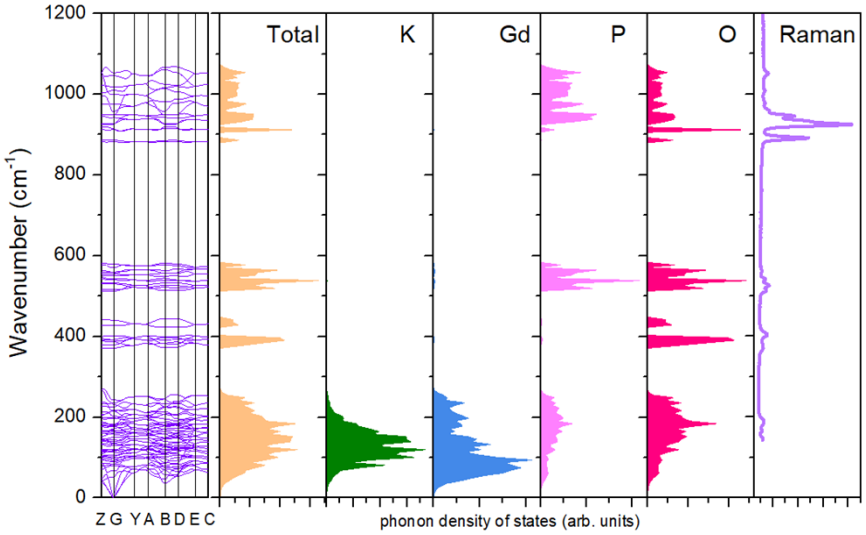

Figure S11. Phonon dispersion and phonon projected density of states of $K_3Gd(PO_4)_2$. Raman spectrum is also plotted.

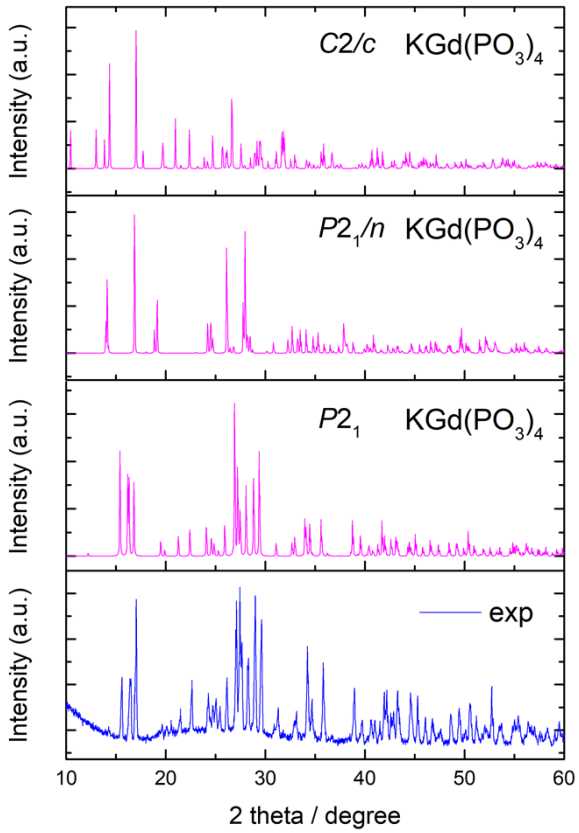

Figure S12. Powder X-ray diffraction pattern of $KGd(PO_3)_4$.

3. Additional tables

Table S1. Crystal data and structure refinements.

Empirical formula	$K_3Pr(BO_3)_2$	$K_3Nd(BO_3)_2$	$K_3Gd(BO_3)_2$
CCDC code	2169921	2169922	2169923
Formula weight	375.83	379.16	392.17
Temperature/K	296(2)	296(2)	296(2)
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic
Space group	*Pnma*	*Pnma*	*Pnma*
a/Å	9.0940(12)	9.0605(17)	8.9588(13)
b/Å	7.1721(11)	7.1533(15)	7.0621(10)
c/Å	11.2310(16)	11.213(2)	11.1427(14)
α/°	90	90	90
β/°	90	90	90
γ/°	90	90	90
Volume/Å^3	732.52(18)	704.98(17)	704.98(17)
Z	4	4	4
ρ_{calc} g/cm^3	3.408	3.465	3.695
μ/mm^{-1}	8.332	8.838	11.154
F(000)	696.0	700.0	716.0
Radiation	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)	Mo Kα (λ = 0.71073)
2θ range for data collection/°	5.764 to 61.032	6.756 to 50.418	5.834 to 61.022
Index ranges	$-12 \le h \le 9$, $-6 \le k \le 10$, $-16 \le l \le 15$	$-10 \le h \le 10$, $-7 \le k \le 8$, $-11 \le l \le 13$	$-12 \le h \le 11$, $-9 \le k \le 9$, $-12 \le l \le 15$
Reflections collected	8219	7562	5042
Independent reflections	1192 [R_{int} = 0.0929]	707 [R_{int} = 0.1364]	1139 [R_{int} = 0.0837]
Data/restraints/parameters	1192/0/67	707/12/67	1139/0/68
Goodness-of-fit on F^2	1.051	1.016	1.043
Final *R* indexes [$I>=2\sigma(I)$]	R_1 = 0.0414, wR_2 = 0.0778	R_1 = 0.0405, wR_2 = 0.0658	R_1 = 0.0368, wR_2 = 0.0617
Final *R* indexes [all data]	R_1 = 0.0652, wR_2 = 0.0866	R_1 = 0.0738, wR_2 = 0.0757	R_1 = 0.0571, wR_2 = 0.0694
Largest diff. peak/hole / e Å^{-3}	1.51/-2.02	1.16/-1.35	1.75/-2.28

Table S2. Fractional atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$).

$K_3Pr(BO_3)_2$:

Atom	*x*	*y*	*z*	U(eq)
B1	5618(10)	7500	1245(8)	9.8(18)
B2	5910(10)	7500	6181(8)	9.8(19)
K1	4392(3)	7500	-1308(2)	50.7(9)
K2	8001.9(14)	5033(2)	-976.8(11)	17.3(3)
O1	6588(5)	7500	319(5)	15.5(14)
O2	6196(5)	7500	2397(5)	15.9(14)
O3	4117(6)	7500	1127(5)	16.6(14)
O4	5096(6)	7500	5135(5)	11.8(12)
O5	6291(4)	9172(6)	6699(4)	20.6(11)
Pr1	3737.9(5)	7500	3321.9(4)	7.34(14)

$K_3Nd(BO_3)_2$:

Atom	*x*	*y*	*z*	U(eq)
B1	5637(18)	7500	6278(15)	19(4)
B2	9095(17)	2500	6184(16)	20(4)
K1	8004(2)	9963(3)	4020(2)	23.2(6)
K2	4391(4)	7500	3696(3)	54.7(13)
Nd1	8739.3(8)	7500	6680.4(7)	12.7(2)
O1	4115(9)	7500	6144(8)	16(2)
O2	6203(10)	7500	7409(8)	18(2)
O3	6593(9)	7500	5316(8)	18(2)
O4	8714(7)	4174(8)	6703(6)	23.9(15)
O5	9910(9)	2500	5138(9)	16(2)

$K_3Gd(BO_3)_2$:

Atom	*x*	*y*	*z*	U(eq)
B1	643(11)	2500	6272(8)	9.6(19)
B2	5878(10)	2500	3840(8)	13(2)
Gd1	3745.7(4)	2500	6688.2(3)	7.51(16)
K1	-609(3)	2500	3700.7(18)	44.9(7)
K2	3003.8(15)	4946.1(19)	4022.0(10)	17.5(3)
O1	-882(6)	2500	6162(5)	13.4(13)
O2	1225(5)	2500	7434(4)	12.7(13)
O3	1631(6)	2500	5347(5)	16.1(13)
O4	5085(6)	2500	4907(5)	11.2(12)
O5	6267(4)	798(6)	3307(3)	16.8(10)

Table S3. Anisotropic displacement parameters ($Å^2 \times 10^3$).

$K_3Pr(BO_3)_2$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	11(4)	14(5)	4(4)	0	0(4)	0
B2	12(5)	12(5)	5(4)	0	5(3)	0
K1	20.1(12)	119(3)	12.9(10)	0	-1.6(9)	0
K2	17.0(7)	14.8(7)	20.1(7)	-8.4(6)	-0.1(5)	-1.4(6)
O1	10(3)	29(4)	8(3)	0	0(2)	0
O2	6(3)	33(4)	9(3)	0	-2(2)	0
O3	9(3)	30(4)	11(3)	0	-1(2)	0
O4	9(3)	14(3)	12(3)	0	-2(2)	0
O5	34(3)	6(2)	22(2)	-1.9(18)	-12.1(18)	-1(2)
Pr1	7.0(2)	9.3(2)	5.7(2)	0	-0.41(16)	0

$K_3Nd(BO_3)_2$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	19(4)	18(4)	19(4)	0	-0.2(10)	0
B2	16(9)	14(9)	31(11)	0	6(8)	0
K1	19.0(11)	19.4(12)	31.2(14)	6.6(12)	0.2(10)	1.2(11)
K2	22.6(19)	115(4)	26(2)	0	-1.7(17)	0
Nd1	10.0(4)	11.2(4)	16.8(4)	0	0.2(4)	0
O1	16(2)	17(2)	16(2)	0	-0.5(10)	0
O2	10(4)	28(5)	17(5)	0	-1(4)	0
O3	14(5)	22(5)	18(6)	0	8(4)	0
O4	30(4)	20(4)	22(4)	-4(3)	6(4)	-2(3)
O5	6(4)	18(5)	25(6)	0	-5(4)	0

$K_3Gd(BO_3)_2$:

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	6(5)	10(5)	14(4)	0	5(4)	0
B2	9(5)	15(6)	15(4)	0	1(3)	0
Gd1	6.4(2)	8.8(3)	7.3(2)	0	0.34(14)	0
K1	20.0(12)	99(2)	15.6(9)	0	-3.0(9)	0
K2	15.7(7)	15.3(7)	21.3(6)	7.5(6)	0.7(5)	0.5(6)
O1	6(3)	22(4)	12(3)	0	0(2)	0
O2	8(3)	21(3)	8(2)	0	-2(2)	0
O3	7(3)	29(4)	12(2)	0	5(2)	0
O4	11(3)	10(3)	13(3)	0	-1(2)	0
O5	28(3)	7(2)	15(2)	-0.9(16)	7.8(17)	-0.1(19)

Table S4. Selected bond lengths.

$K_3Pr(BO_3)_2$:

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	K1	3.077(9)	K2	O4[3]	2.766(4)
B1	K1[1]	3.5868(6)	K2	O4[13]	2.802(4)
B1	K1[2]	3.5868(6)	K2	O5[14]	3.152(4)
B1	O1	1.364(10)	K2	O5[15]	3.135(4)
B1	O2	1.397(10)	K2	O5[12]	3.091(4)
B1	O3	1.372(11)	K2	Pr1[3]	3.5311(13)
B1	Pr1[3]	2.878(9)	O1	K2[9]	2.627(4)
B1	Pr1	2.892(9)	O1	Pr1[3]	2.481(5)
B2	K1[3]	3.170(9)	O2	K2[5]	2.677(4)
B2	K1[4]	3.140(9)	O2	K2[7]	2.677(4)
B2	K2[5]	3.187(7)	O2	Pr1[3]	2.448(5)
B2	K2[6]	3.190(8)	O2	Pr1	2.465(5)
B2	K2[7]	3.187(7)	O3	K2[2]	2.654(4)
B2	K2[8]	3.190(8)	O3	K2[16]	2.654(4)
B2	O4	1.389(10)	O3	Pr1	2.489(6)
B2	O5	1.378(6)	O4	K2[8]	2.766(4)
B2	O5[9]	1.378(6)	O4	K2[6]	2.766(4)
K1	B1[2]	3.5868(6)	O4	K2[7]	2.802(4)
K1	B1[1]	3.5868(6)	O4	K2[5]	2.802(4)
K1	B2[6]	3.170(9)	O4	Pr1	2.381(5)
K1	B2[10]	3.140(9)	O5	K1[3]	3.095(4)
K1	K2[11]	3.745(2)	O5	K1[4]	3.071(5)
K1	O1	2.707(6)	O5	K2[7]	3.135(4)
K1	O3	2.747(6)	O5	K2[17]	3.091(4)
K1	O5[12]	3.071(5)	O5	K2[8]	3.152(4)
K1	O5[8]	3.095(4)	O5	Pr1[18]	2.387(4)
K1	O5[10]	3.071(5)	Pr1	B1[6]	2.878(9)
K1	O5[6]	3.095(4)	Pr1	K2[8]	3.5311(13)
K2	B2[3]	3.190(8)	Pr1	K2[6]	3.5311(13)
K2	B2[13]	3.187(7)	Pr1	K2[7]	3.5653(14)
K2	K2[9]	3.539(3)	Pr1	O1[6]	2.481(5)
K2	O1	2.627(4)	Pr1	O2[6]	2.448(5)
K2	O2[13]	2.677(4)	Pr1	O5[18]	2.387(4)
K2	O3[2]	2.654(4)	Pr1	O5[19]	2.387(4)

[1]1-X,2-Y,-Z; [2]1-X,1-Y,-Z; [3]1/2+X,+Y,1/2-Z; [4]+X,+Y,1+Z; [5]3/2-X,1-Y,1/2+Z; [6]-1/2+X,+Y,1/2-Z; [7]3/2-X,1/2+Y,1/2+Z; [8]-1/2+X,3/2-Y,1/2-Z; [9]+X,3/2-Y,+Z; [10]+X,+Y,-1+Z; [11]-1/2+X,+Y,-1/2-Z; [12]+X,3/2-Y,-1+Z; [13]3/2-X,1-Y,-1/2+Z; [14]1/2+X,3/2-Y,1/2-Z; [15]3/2-X,-1/2+Y,-1/2+Z; [16]1-X,1/2+Y,-Z; [17]+X,3/2-Y,1+Z; [18]1-X,2-Y,1-Z; [19]1-X,-1/2+Y,1-Z

$K_3Nd(BO_3)_2$:

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	K2	3.108(17)	K2	O1	2.757(10)
B1	K2[1]	3.5769(8)	K2	O3	2.698(9)
B1	K2[2]	3.5769(8)	K2	O4[1]	3.091(7)
B1	Nd1	2.847(16)	K2	O4[14]	3.062(7)
B1	Nd1[3]	2.863(17)	K2	O4[15]	3.091(7)
B1	O1	1.387(18)	K2	O4[12]	3.062(7)
B1	O2	1.368(18)	Nd1	B1[16]	2.863(17)
B1	O3	1.383(18)	Nd1	K1[17]	3.552(2)
B2	K1[4]	3.188(15)	Nd1	K1[7]	3.528(2)
B2	K1[5]	3.172(13)	Nd1	O1[16]	2.463(9)
B2	K1[6]	3.172(13)	Nd1	O2	2.439(10)
B2	K1[7]	3.188(15)	Nd1	O2[16]	2.455(10)
B2	K2[8]	3.132(18)	Nd1	O3	2.474(9)
B2	K2[1]	3.162(16)	Nd1	O4[7]	2.380(6)
B2	O4	1.375(10)	Nd1	O4	2.380(6)
B2	O4[9]	1.375(10)	Nd1	O5[6]	2.378(9)
B2	O5	1.386(19)	O1	K1[2]	2.648(6)
K1	B2[6]	3.172(13)	O1	K1[18]	2.648(6)
K1	B2[10]	3.188(15)	O1	Nd1[3]	2.463(9)
K1	K1[7]	3.523(5)	O2	K1[19]	2.660(7)
K1	Nd1	3.528(2)	O2	K1[20]	2.660(7)
K1	O1[2]	2.648(6)	O2	Nd1[3]	2.455(9)
K1	O2[11]	2.660(7)	O3	K1[7]	2.617(7)
K1	O3	2.617(7)	O4	K1[5]	3.133(7)
K1	O4[7]	3.138(7)	O4	K1[20]	3.081(7)
K1	O4[12]	3.081(7)	O4	K1[7]	3.137(7)
K1	O4[13]	3.133(7)	O4	K2[8]	3.062(7)
K1	O5[10]	2.801(7)	O4	K2[1]	3.091(7)
K1	O5[6]	2.751(7)	O5	K1[4]	2.801(7)
K2	B1[2]	3.5769(8)	O5	K1[7]	2.801(7)
K2	B1[1]	3.5769(8)	O5	K1[6]	2.751(7)
K2	B2[14]	3.132(18)	O5	K1[5]	2.751(7)
K2	B2[1]	3.162(16)	O5	Nd1[6]	2.378(9)

[1]1-X,1-Y,1-Z; [2]1-X,2-Y,1-Z; [3]-1/2+X,+Y,3/2-Z; [4]+X,-1+Y,+Z; [5]2-X,-1/2+Y,1-Z; [6]2-X,1-Y,1-Z; [7]+X,3/2-Y,+Z; [8]3/2-X,1-Y,1/2+Z; [9]+X,1/2-Y,+Z; [10]+X,1+Y,+Z; [11]3/2-X,2-Y,-1/2+Z; [12]3/2-X,1/2+Y,-1/2+Z; [13]2-X,1/2+Y,1-Z; [14]3/2-X,1-Y,-1/2+Z; [15]1-X,1/2+Y,1-Z; [16]1/2+X,+Y,3/2-Z; [17]2-X,2-Y,1-Z; [18]1-X,-1/2+Y,1-Z; [19]3/2-X,2-Y,1/2+Z; [20]3/2-X,-1/2+Y,1/2+Z

$K_3Gd(BO_3)_2$:

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	Gd1	2.818(10)	K1	O1	2.753(6)
B1	Gd1[1]	2.838(9)	K1	O3	2.718(6)
B1	K1[2]	3.5313(5)	K1	O5[14]	3.045(4)
B1	K1[3]	3.5313(5)	K1	O5[13]	3.045(4)
B1	K1	3.077(9)	K1	O5[15]	3.077(4)
B1	O1	1.373(10)	K1	O5[12]	3.077(4)
B1	O2	1.396(10)	K2	B2[8]	3.152(8)
B1	O3	1.358(10)	K2	K2[6]	3.455(3)
B2	K1[4]	3.152(9)	K2	O1[2]	2.628(4)
B2	K1[5]	3.128(9)	K2	O2[16]	2.619(4)
B2	K2[6]	3.107(8)	K2	O3	2.584(4)
B2	K2[7]	3.152(8)	K2	O4	2.726(4)
B2	K2	3.107(8)	K2	O4[8]	2.759(4)
B2	K2[8]	3.152(8)	K2	O5[6]	3.076(4)
B2	O4	1.385(10)	K2	O5[11]	3.106(4)
B2	O5[6]	1.385(6)	K2	O5[14]	3.071(4)
B2	O5	1.385(6)	O1	Gd1[1]	2.419(5)
Gd1	B1[9]	2.838(9)	O1	K2[17]	2.628(4)
Gd1	K2[6]	3.5002(12)	O1	K2[2]	2.628(4)
Gd1	K2	3.5002(12)	O2	Gd1[1]	2.427(5)
Gd1	K2[8]	3.5156(14)	O2	K2[18]	2.619(4)
Gd1	O1[9]	2.419(5)	O2	K2[19]	2.619(4)
Gd1	O2[9]	2.427(5)	O3	K2[6]	2.584(4)
Gd1	O2	2.406(5)	O4	K2[8]	2.759(4)
Gd1	O3	2.413(5)	O4	K2[6]	2.726(4)
Gd1	O4	2.319(5)	O4	K2[7]	2.759(4)
Gd1	O5[10]	2.329(4)	O5	Gd1[10]	2.329(4)
Gd1	O5[11]	2.329(4)	O5	K1[4]	3.077(4)
K1	B1[2]	3.5313(5)	O5	K1[5]	3.045(4)
K1	B1[3]	3.5313(5)	O5	K2[6]	3.076(4)
K1	B2[12]	3.152(9)	O5	K2[7]	3.106(4)
K1	B2[13]	3.128(9)	O5	K2[20]	3.071(4)
K1	K2	3.686(2)			

[1]-1/2+X,+Y,3/2-Z; [2]-X,1-Y,1-Z; [3]-X,-Y,1-Z; [4]1+X,+Y,+Z; [5]1/2+X,+Y,1/2-Z; [6]+X,1/2-Y,+Z; [7]1-X,-1/2+Y,1-Z; [8]1-X,1-Y,1-Z; [9]1/2+X,+Y,3/2-Z; [10]1-X,-Y,1-Z; [11]1-X,1/2+Y,1-Z; [12]-1+X,+Y,+Z; [13]-1/2+X,+Y,1/2-Z; [14]-1/2+X,1/2-Y,1/2-Z; [15]-1+X,1/2-Y,+Z; [16]1/2-X,1-Y,-1/2+Z; [17]-X,-1/2+Y,1-Z; [18]1/2-X,1-Y,1/2+Z; [19]1/2-X,-1/2+Y,1/2+Z; [20]1/2+X,1/2-Y,1/2-Z

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