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Supporting information for article:

Growth, crystal structure and IR luminescence of KSrY1–*x*Er*x*(BO3)2

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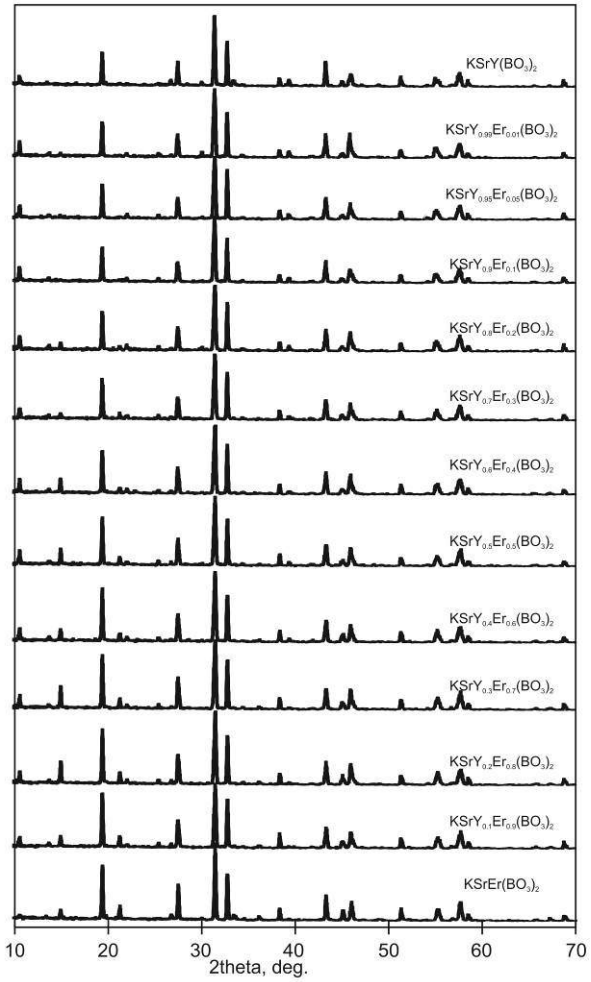

Figure S1. XRD patterns of $KSrY_{1-x}Er_x(BO_3)_2$ syntheses at 950°C.

Table S1. Unit-cell parameters of $KSrY_{1-x}Er_x(BO_3)_2$ syntheses at 950°C .

No.	Composition	a, Å	b	c	δ
1	$KSrY(BO_3)_2$	6.5823(3)	5.3625(7)	8.5242(1)	105.46(6)
2	$KSrY_{0.99}Er_{0.01}(BO_3)_2$	6.5801(9)	5.3614(4)	8.5233(2)	105.46(2)
3	$KSrY_{0.95}Er_{0.05}(BO_3)_2$	6.5800(5)	5.3610(6)	8.5231(5)	105.46(5)
4	$KSrY_{0.9}Er_{0.1}(BO_3)_2$	6.5794(8)	5.3617(4)	8.5224(6)	105.46(2)
5	$KSrY_{0.8}Er_{0.2}(BO_3)_2$	6.5774(2)	5.3608(5)	8.5205(1)	105.44(7)
6	$KSrY_{0.7}Er_{0.3}(BO_3)_2$	6.5742(2)	5.3602 (4)	8.5174(7)	105.42(7)

7	$KSrY_{0.6}Er_{0.4}(BO_3)_2$	6.5729(9)	5.3592(2)	8.5159(9)	105.41(3)
8	$KSrY_{0.5}Er_{0.5}(BO_3)_2$	6.5699(5)	5.3582(5)	8.5125(8)	105.39(9)
9	$KSrY_{0.4}Er_{0.6}(BO_3)_2$	6.5684(2)	5.3576(8)	8.5107(9)	105.38(5)
10	$KSrY_{0.3}Er_{0.7}(BO_3)_2$	6.5650(9)	5.3573(8)	8.5075(8)	105.37(4)
11	$KSrY_{0.2}Er_{0.8}(BO_3)_2$	6.5647(6)	5.3565(9)	8.5056(4)	105.36(4)
12	$KSrY_{0.1}Er_{0.9}(BO_3)_2$	6.5627(5)	5.3557(6)	8.5023(8)	105.36(6)
13	$KSrEr(BO_3)_2$	6.5606(7)	5.3548(7)	8.4983(1)	105.35(5)

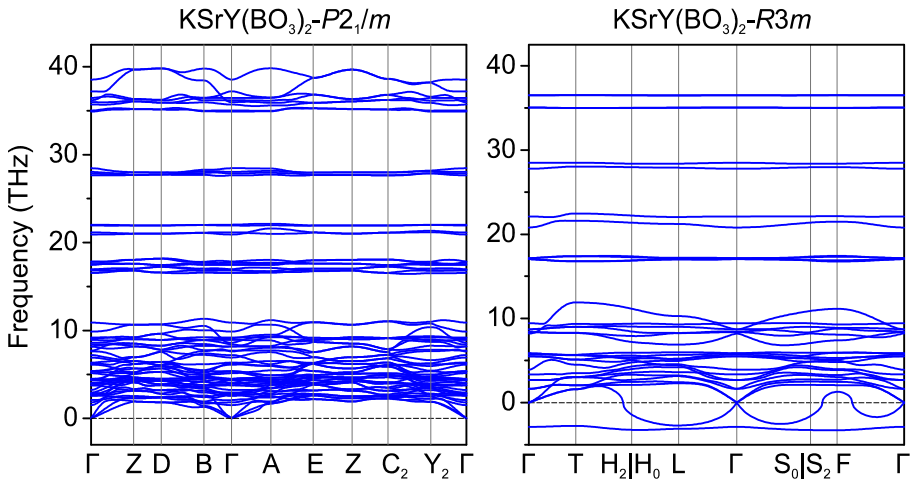

Figure S2. Calculated phonon spectra of $KSrY(BO_3)_2$ polymorphs. The imaginary phonon frequencies are plotted as negative values.

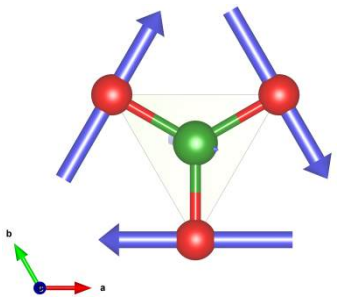

Figure S3. The displacement pattern of the imaginary mode at ~3*i* THz in $KSrY(BO_3)_2$-*R*3*m*.

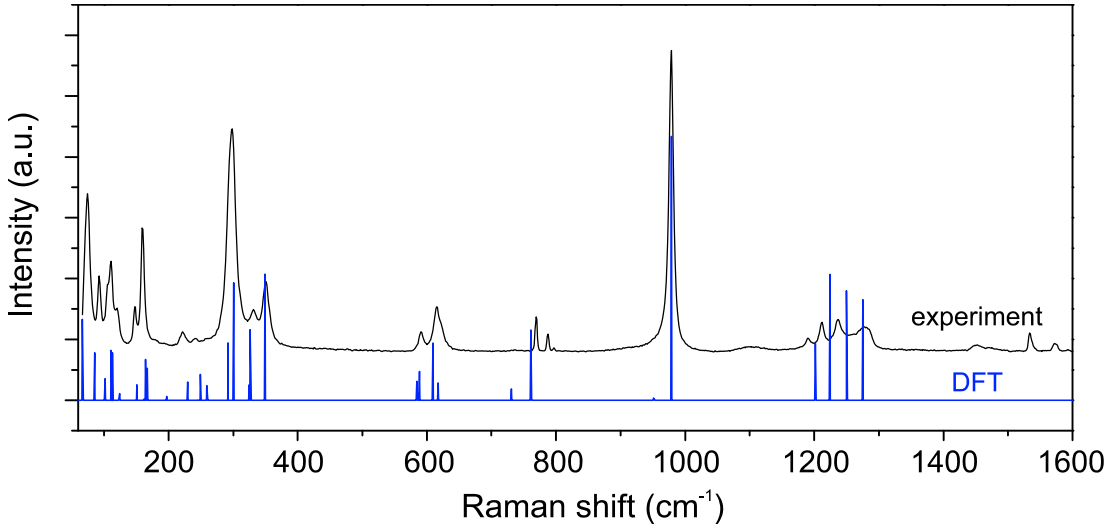

Figure S4. Experimental and calculated (DFT) Raman spectra of $KSrY(BO_3)_2$-$P2_1/m$.

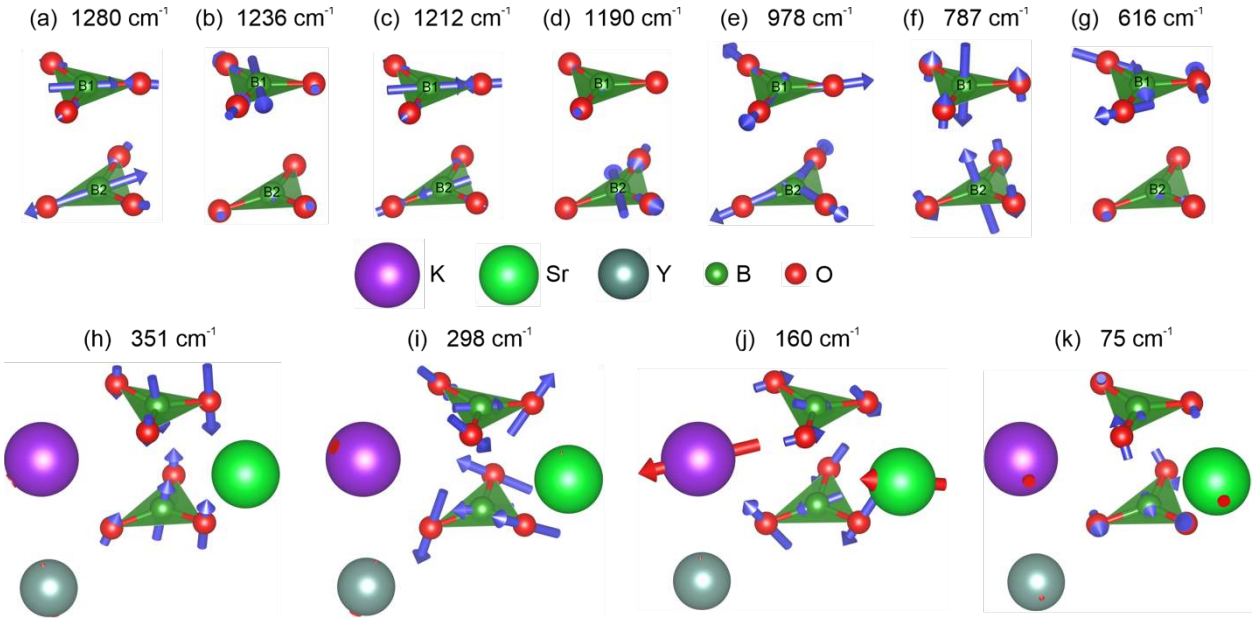

Figure S5. The eigenvectors of the Raman-active vibrational modes according to density functional theory (DFT) calculations.

Table S2. Observed and calculated Raman-active modes of $KSrY(BO_3)_2$-$P2_1/m$.

Observed	Calculated	Mulliken symbol	Observed	Calculated	Mulliken symbol
1280	1275	A_g	332	327	B_g

1236	1250	B_g	298	301	A_g
1212	1224	A_g	241	249	A_g
1190	1201	B_g	222	230	B_g
978	978	A_g	160	164	A_g
787	761	A_g	148	151	B_g
616	609	B_g	110	115	A_g
591	589	A_g	92	85	A_g
351	350	A_g	75	66	B_g

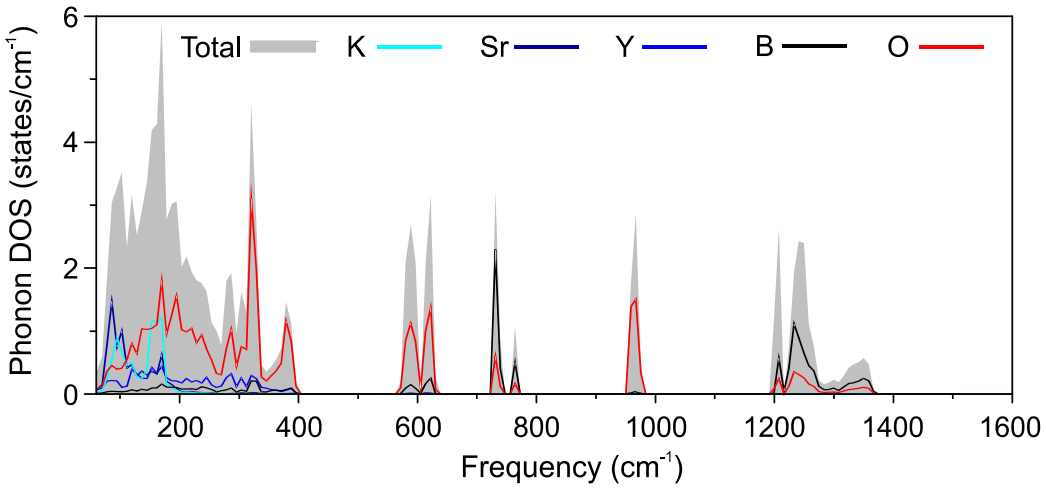

Figure S6. Total and partial phonon density of states of $KSrY(BO_3)_2$-$P2_1/m$.