Supporting Information for

Co-substitution Design: A New Glaserite-type Rare-earth Phosphate $K_2RbSc(PO_4)_2$ with High Structural Tolerance

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1. Supplementary figures

Figure S1. Experimental and calculated powder X-ray diffraction patterns of $K_2RbSc(PO_4)_2$.

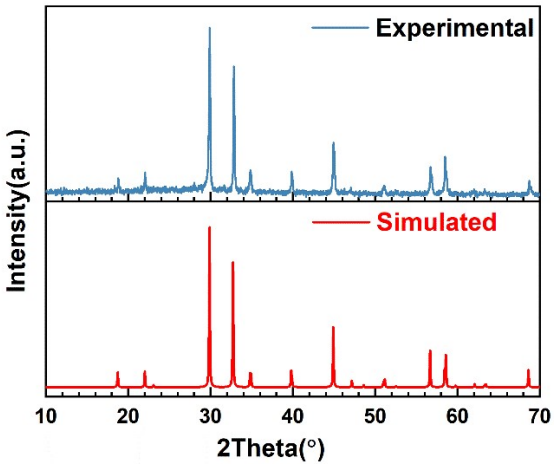


Figure S2. The photograph of $K_2RbSc(PO_4)_2$ crystal.

Figure S3. The elemental analyses of K, Rb, Sc, P and O atoms for $K_2RbSc(PO_4)_2$ by EDS.

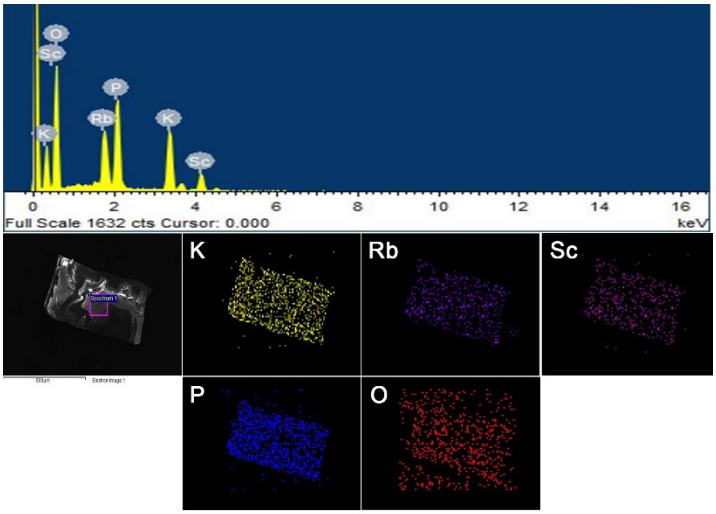


Figure S4. The plot shows $(F(R) \times E)^2$–E of $K_2RbSc(PO_4)_2$, $K_2RbEr(PO_4)_2$ and $K_2RbLu(PO_4)_2$.

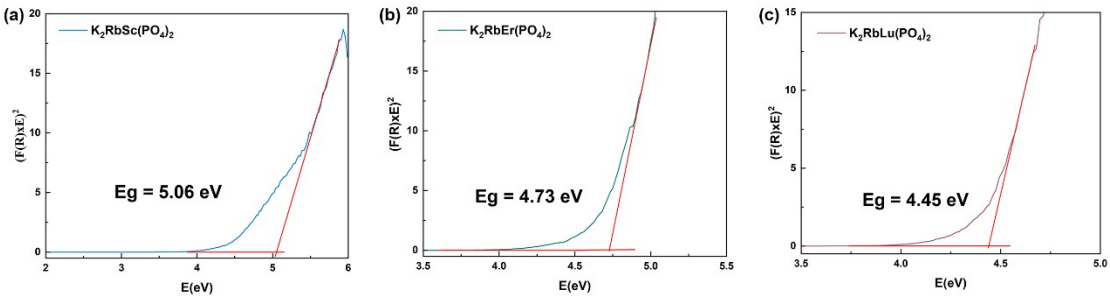


Figure S5. (a)The DSC and TG curves of $K_2RbSc(PO_4)_2$in the temperature range of 50−1000 °C (The inset plot shows the temperature range of 50−150 °C); (b)The DTA and TG curves of $K_2RbEr(PO_4)_2$in the temperature range of 50−1050 °C.

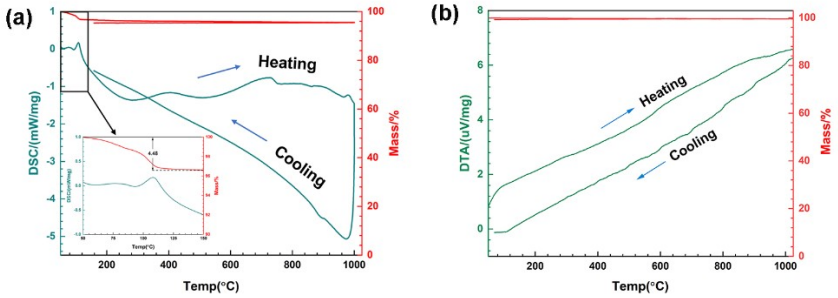
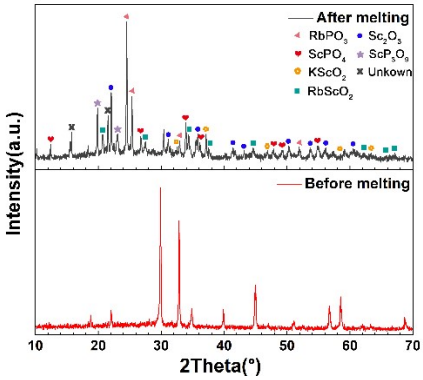


Figure S6. The powder XRD patterns of $K_2RbSc(PO_4)_2$ before and after melting.



2. Supplementary tables

Table S1 Atomic coordinates and equivalent isotropic temperature factors of $K_2RbSc(PO_4)_2$.

Atom	Wyckoff	x/a	y/b	z/c	U(eq)/(Å²)
K1	2d	0.0113(11)	0.0113(11)	0.0183(16)	0.0056(5)
Rb1	1b	0.0315(11)	0.0315(11)	0.0208(13)	0.0157(6)
Sc1	1a	0.0045(12)	0.0045(12)	0.025(2)	0.0023(6)
P1	2d	0.0078(12)	0.0078(12)	0.0054(16)	0.0039(6)
O1	2d	0.082(6)	0.082(6)	0.026(6)	0.041(3)
O2	6i	0.012(2)	0.009(3)	0.059(5)	0.0043(16)

Table S2. Selected bond lengths (Å) for $K_2RbSc(PO_4)_2$.

Atom	Length/Å
Sc1—O2 × 6	2.104(7)
P1—O2 × 3	1.526(6)
P1—O1	1.480(16)
K1—O2 × 6	2.822(2)
K1—O1	2.592(16)
Rb1—O1 × 6	3.223(3)
Rb1—O2 × 6	3.138(8)

Table S3. Selected bond angles (°) for $K_2RbSc(PO_4)_2$.

Atom	angle/°	Atom	angle/°

O2—Sc1—O2	89.7(3)	O2—Rb1—O2	123.57(19)
O2—Sc1—O2	90.3(3)	O2—Rb1—O2	180.0
O2—Sc1—O2	180.0(3)	O2—Rb1—O1	84.4(2)
O2—Sc1—O2	180.0	O2—Rb1—O1	134.8(3)
O1—P1—O2	109.0(3)	O2—Rb1—O1	45.2(3)
O1—K1—O2	104.17(16)	O2—Rb1—O1	95.6(2)
O1—K1—O1	67.8(2)	O1—Rb1—O1	116.00(18)
O1—K1—O1	106.7(3)	O1—Rb1—O1	64.00(18)
O2—Rb1—O2	56.43(19)	O1—Rb1—O1	180.0

Table S4. The element compositions of $K_2RbSc(PO_4)_2$ by EDS.

Element	Weight%	Atomic%	Atomic ratio
O K	60.89	79.45	
P K	12.84	8.94	
K K	10.30	5.69	1.96
Sc K	4.07	2.91	1
Rb L	11.91	3.01	1.03
Totals	100.00	100	

Table S5. The bond valence sums (BVS) of $K_2RbSc(PO_4)_2$.

Element	BVS
K1	1.2343
Rb1	0.8692
Sc1	2.9215
P1	5.1546
O1	-2.1210
O2	-1.9216