

Supporting Information

Centrosymmetric to Noncentrosymmetric Structure Transition of the $\text{RbRE}\text{P}_2\text{Se}_6$ ($RE = \text{La} - \text{Nd}$, Sm , $\text{Ho} - \text{Yb}$) Series: Crystal Growth, Magnetic and Optical Properties

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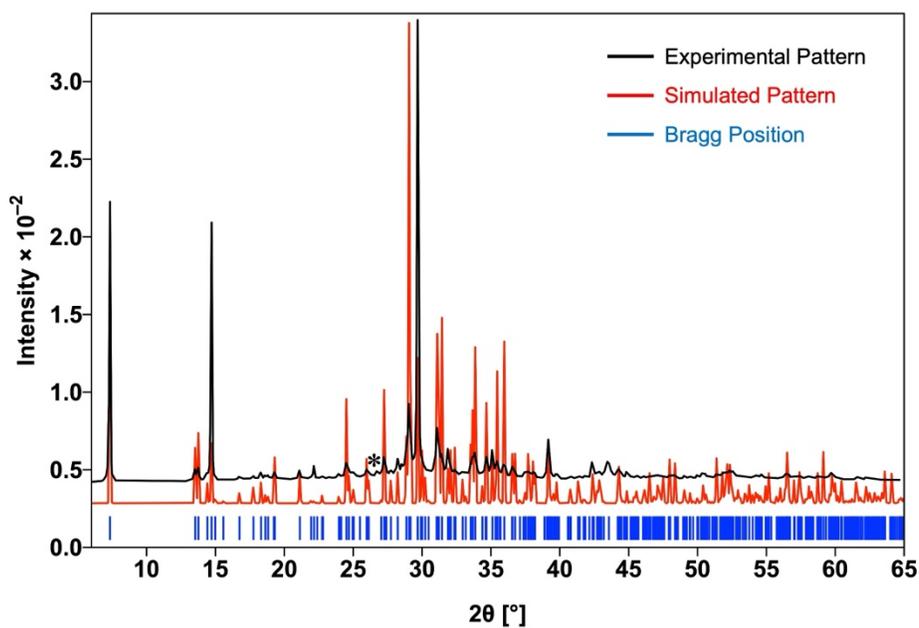


Figure S1: PXRD pattern of polycrystalline RbLaP₂Se₆ (* indicates an unidentified impurity peak).

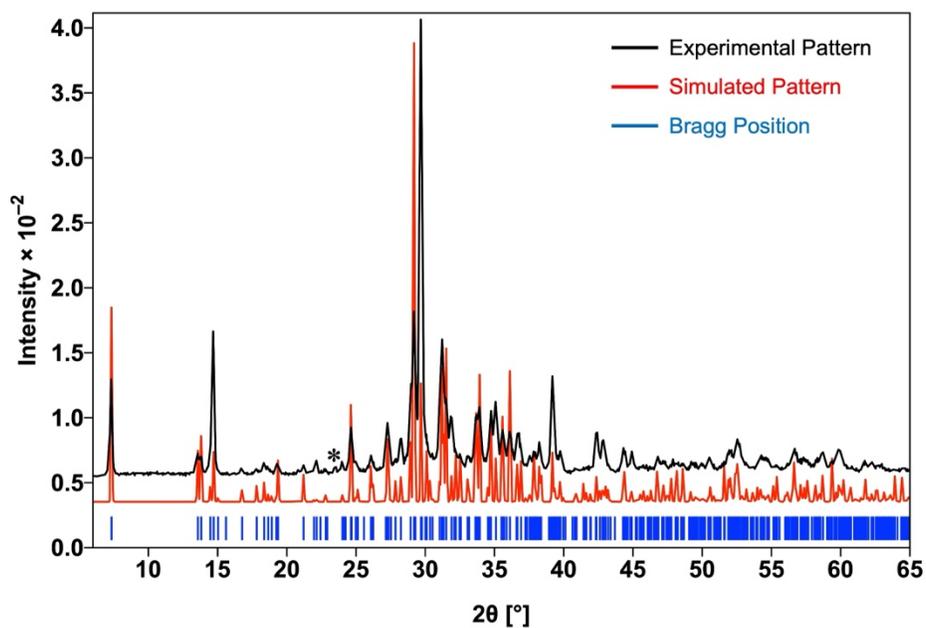


Figure S2: PXRD pattern of polycrystalline RbCeP₂Se₆ (* indicates an unidentified impurity peak).

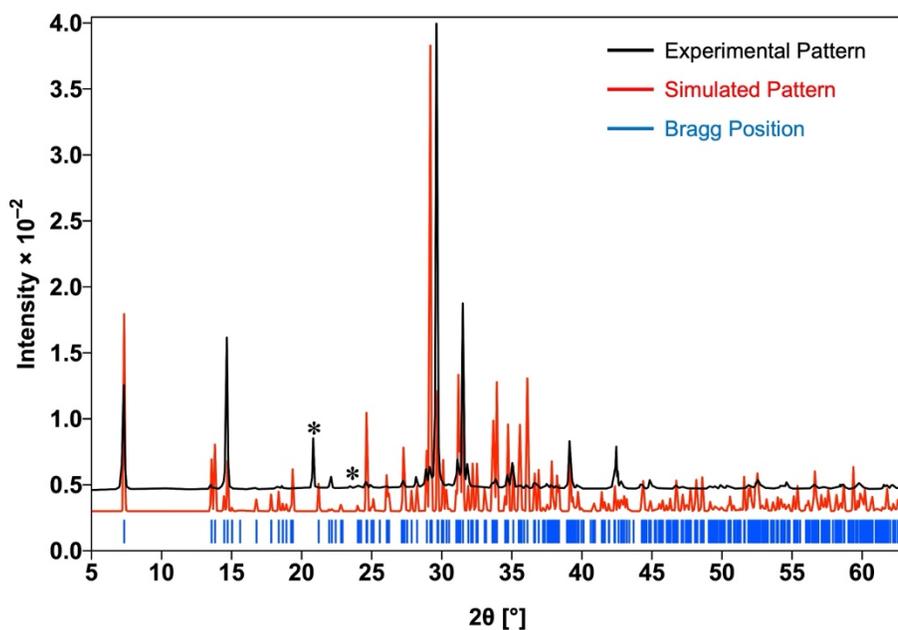


Figure S3: PXRD pattern of polycrystalline $\text{RbPrP}_2\text{Se}_6$ (* indicates an unidentified impurity peak).

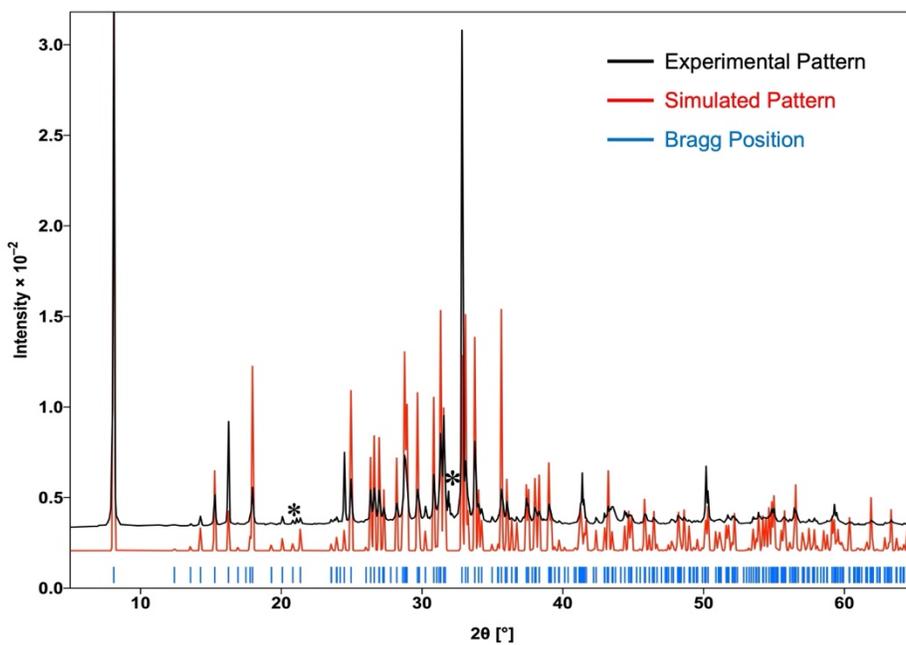


Figure S4: PXRD pattern of polycrystalline $\text{RbNdP}_2\text{Se}_6$ (* indicates an unidentified impurity peak).

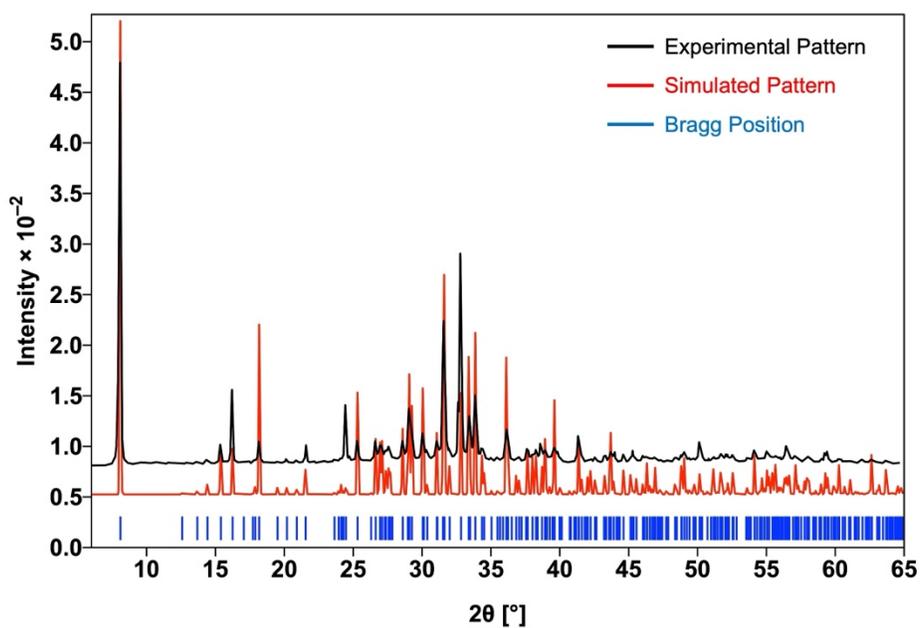


Figure S5: PXRD pattern of polycrystalline $\text{RbSmP}_2\text{Se}_6$.

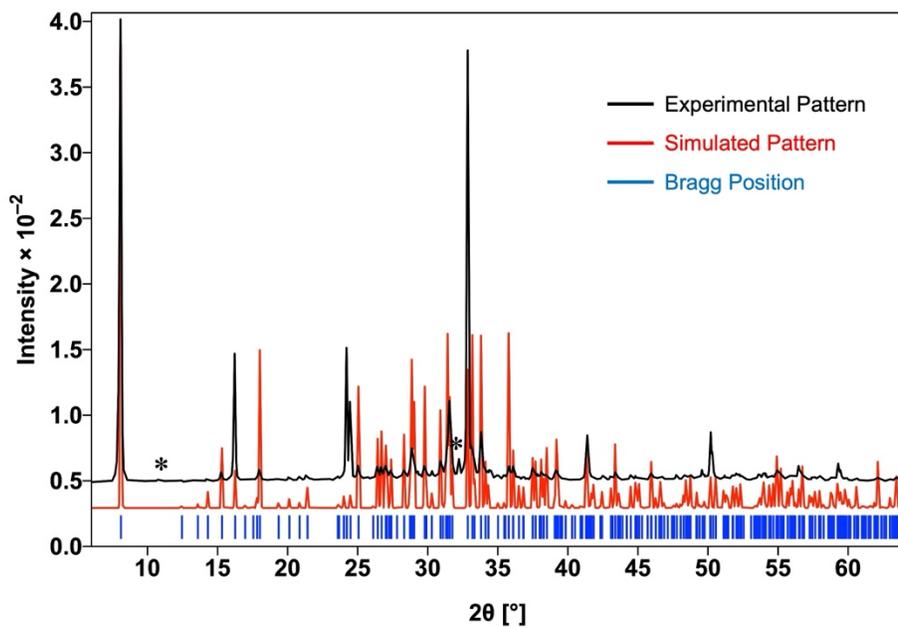


Figure S6: PXRD pattern of polycrystalline $\text{RbHoP}_2\text{Se}_6$ (* indicates an unidentified impurity peak).

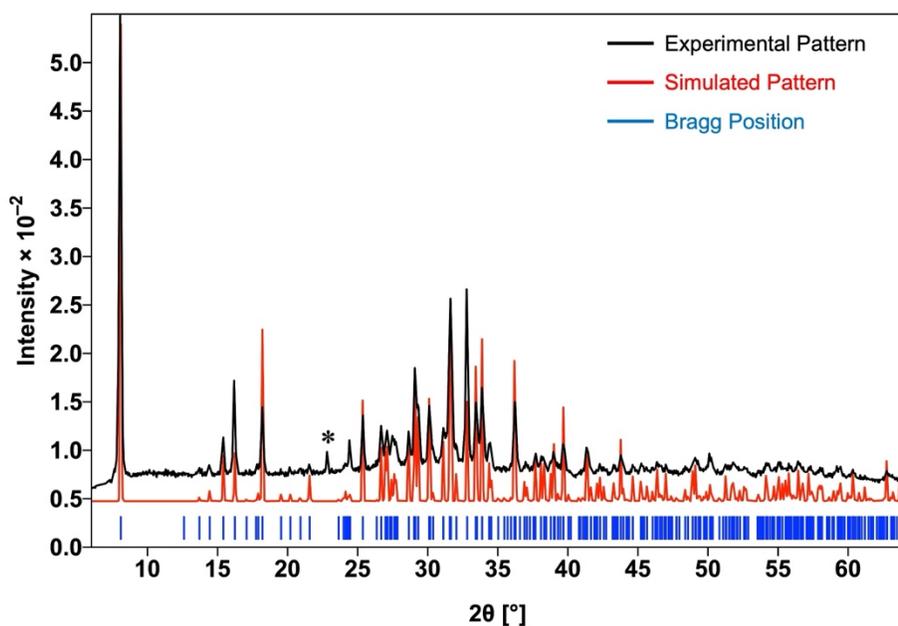


Figure S7: PXRD pattern of polycrystalline RbErP₂Se₆ (* indicates an unidentified impurity peak).

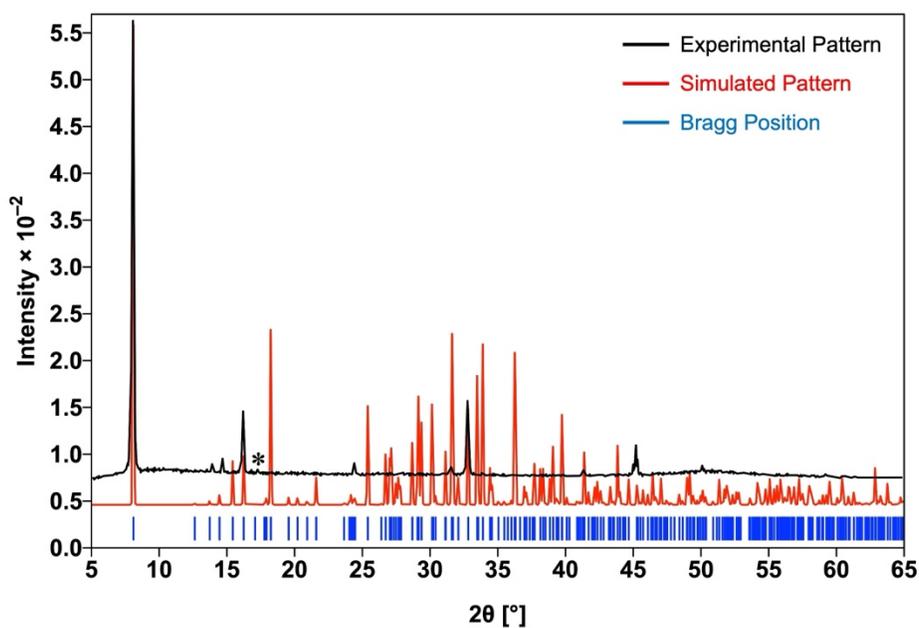


Figure S8: PXRD pattern of polycrystalline RbTmP₂Se₆ (* indicates an unidentified impurity peak).

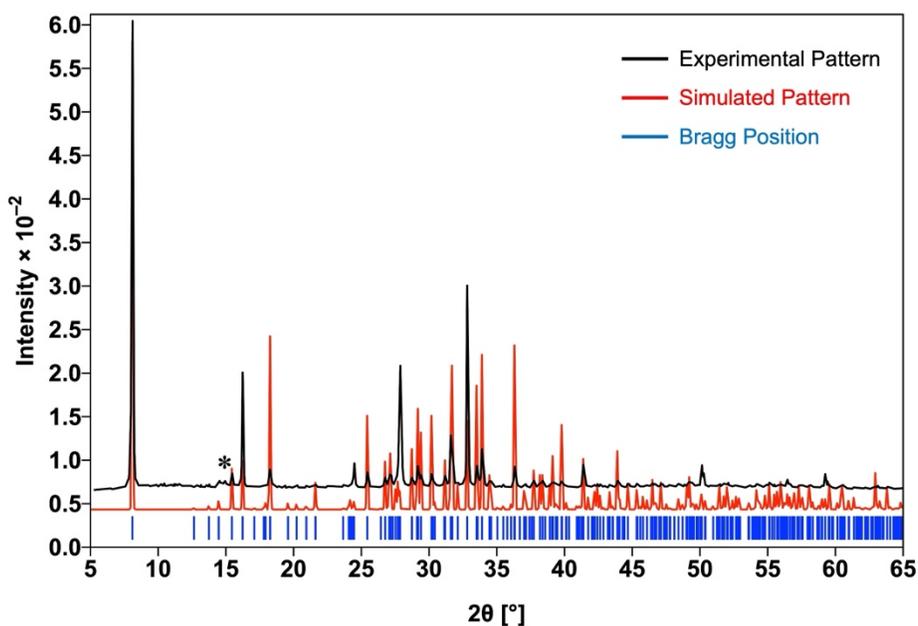


Figure S9: PXRD pattern of polycrystalline $\text{RbYbP}_2\text{Se}_6$ (* indicates an unidentified impurity peak).

Table S1: Comparison of lattice parameters of the reported $\text{RbRE}P_2\text{Se}_6$ ($RE = \text{Gd} - \text{Dy}$) with our synthesized $\text{RbRE}P_2\text{Se}_6$ ($RE = \text{Nd}, \text{Sm}, \text{Ho} - \text{Yb}$) analogues.

	$\text{RbNdP}_2\text{Se}_6$	$\text{RbSmP}_2\text{Se}_6$	$\text{RbGdP}_2\text{Se}_6$	$\text{RbTbP}_2\text{Se}_6$	$\text{RbDyP}_2\text{Se}_6$	$\text{RbHoP}_2\text{Se}_6$	$\text{RbErP}_2\text{Se}_6$	$\text{RbTmP}_2\text{Se}_6$	$\text{RbYbP}_2\text{Se}_6$
crystal system	Orthorhombic								
space group	$P2_12_12_1$								
a (Å)	6.8411(10)	6.81850(10)	6.8025(3)	6.7987(5)	6.7760(4)	6.7682(2)	6.7564(3)	6.7452(2)	6.7364(10)
b (Å)	7.5436(10)	7.5083(2)	7.4780(3)	7.4702(5)	7.4388(4)	7.4233(3)	7.4097(3)	7.3970(2)	7.3865(10)
c (Å)	21.8006(4)	21.7858(4)	21.7875(9)	21.7805(15)	21.7913(12)	21.801(7)	21.812(10)	21.8094(4)	21.815(3)
V (Å ³)	1125.05(3)	1115.33(4)	1108.31(8)	1106.18(13)	1098.40(11)	1095.35(7)	1091.98(8)	1088.16(5)	1085.52(3)
Z	4								
R_1 ($I > 2\sigma(I)$)	0.0219	0.0271	0.0235	0.0362	0.0314	0.0386	0.0167	0.0452	0.0203

Table S2: Elemental composition percentages measured by EDS.

$\text{RbLaP}_2\text{Se}_6$			$\text{RbCeP}_2\text{Se}_6$			$\text{RbPrP}_2\text{Se}_6$		
Element	Atom %	Error %	Element	Atom %	Error %	Element	Atom %	Error %
Rb	8.42	0.55	Rb	8.11	0.52	Rb	9.97	0.50
La	9.78	0.17	Ce	7.31	0.14	Pr	10.77	0.15
P	28.06	0.63	P	11.35	0.44	P	22.02	0.51
Se	53.74	0.77	Se	73.22	0.88	Se	57.23	0.71

RbNdP₂Se₆			RbSmP₂Se₆			RbHoP₂Se₆		
Element	Atom %	Error %	Element	Atom %	Error %	Element	Atom %	Error %
Rb	8.61	0.38	Rb	10.32	0.49	Rb	15.20	0.42
Nd	12.31	0.13	Sm	9.58	0.14	Ho	8.98	0.10
P	23.50	0.41	P	18.08	0.46	P	29.10	0.45
Se	55.58	0.55	Se	62.02	0.71	Se	46.72	0.47

RbErP₂Se₆			RbTmP₂Se₆			RbYbP₂Se₆		
Element	Atom %	Error %	Element	Atom %	Error %	Element	Atom %	Error %
Rb	9.45	0.37	Rb	10.29	0.55	Rb	10.14	0.55
Er	9.54	0.10	Tm	8.64	0.15	Yb	9.19	0.15
P	24.33	0.41	P	22.68	0.56	P	18.36	0.54
Se	57.69	0.53	Se	58.39	0.76	Se	62.30	0.82