

SUPPLEMENTARY INFORMATION

Quaternary chalcogenides $\text{BaRE}_2\text{In}_2\text{Ch}_7$ ($\text{RE} = \text{La-Nd}$; $\text{Ch} = \text{S, Se}$) containing InCh_5 trigonal bipyramids

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Table S1. EDX analyses of $\text{BaRE}_2\text{In}_2\text{Ch}_7$ ($\text{RE} = \text{La-Nd}$; $\text{Ch} = \text{S, Se}$).

Figure S1. Powder XRD patterns for $\text{BaRE}_2\text{In}_2\text{Ch}_7$ ($\text{RE} = \text{La-Nd}$; $\text{Ch} = \text{S, Se}$).

Figure S2. (a) Density of states (DOS) and (b) crystal orbital Hamilton population (COHP) curves for $\text{BaLa}_2\text{In}_2\text{Se}_7$.

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Table S1. EDX analyses of $\text{BaRE}_2\text{In}_2\text{Ch}_7$ ($RE = \text{La-Nd}$; $Ch = \text{S, Se}$). ^a

Compound	No. of analyses	at. % Ba	at. % <i>RE</i>	at. % In	at. % <i>Ch</i>
$\text{BaLa}_2\text{In}_2\text{S}_7$	6	7(1)	18(2)	17(2)	58(3)
$\text{BaCe}_2\text{In}_2\text{S}_7$	3	10(1)	17(2)	16(2)	58(3)
$\text{BaPr}_2\text{In}_2\text{S}_7$	6	8(1)	18(2)	17(2)	57(3)
$\text{BaNd}_2\text{In}_2\text{S}_7$	5	9(1)	17(2)	16(2)	58(3)
$\text{BaLa}_2\text{In}_2\text{Se}_7$	3	6(1)	18(2)	18(2)	58(3)
$\text{BaCe}_2\text{In}_2\text{Se}_7$	5	10(1)	18(2)	16(2)	56(3)
$\text{BaPr}_2\text{In}_2\text{Se}_7$	6	7(1)	15(2)	15(2)	62(3)
$\text{BaNd}_2\text{In}_2\text{Se}_7$	6	10(2)	20(3)	17(2)	53(5)

^a Expected compositions are 8% Ba, 17% *RE*, 17% In, and 58% *Ch*.

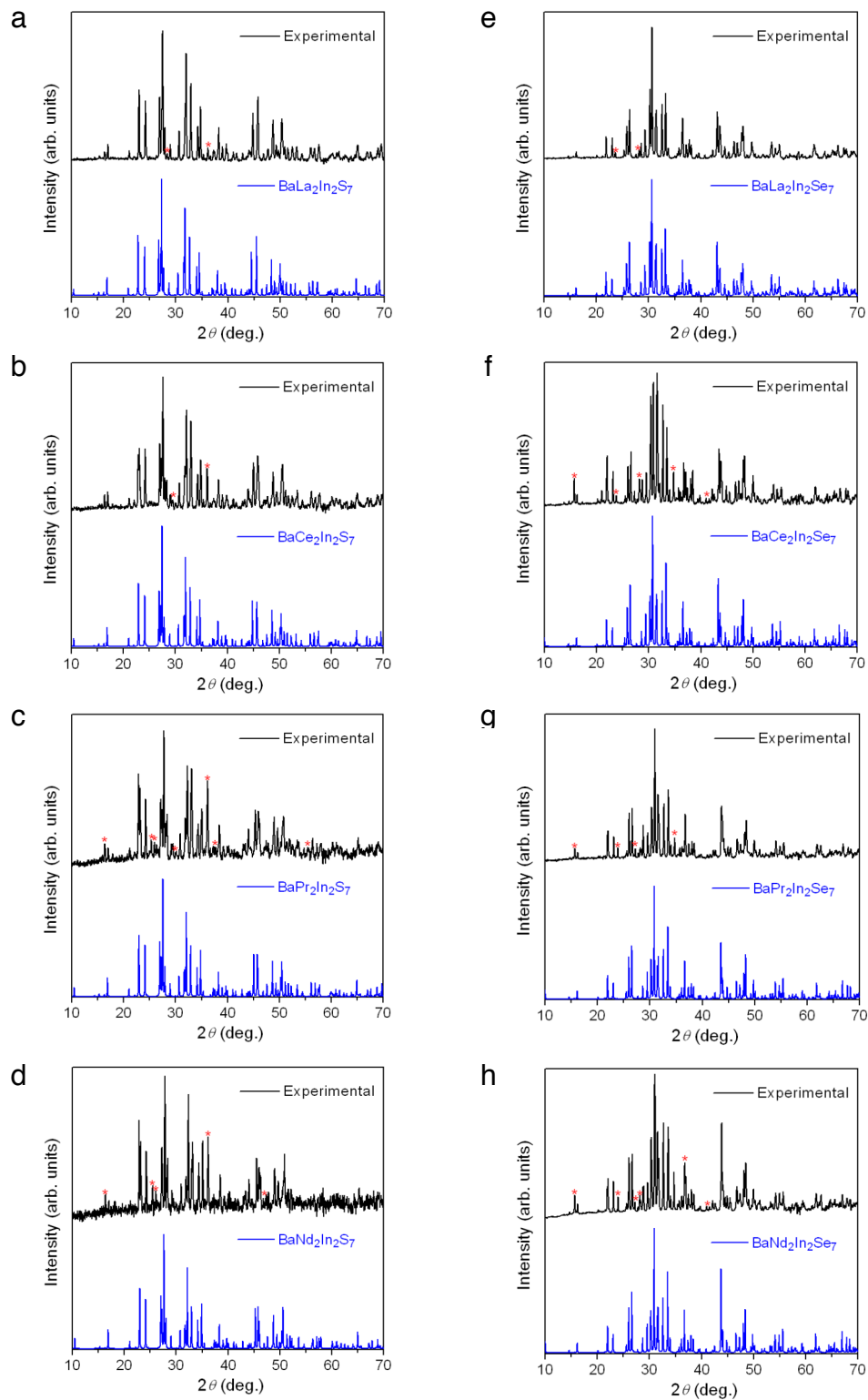


Figure S1. Powder XRD patterns for $\text{BaRE}_2\text{In}_2\text{Ch}_7$ ($\text{RE} = \text{La–Nd}$; $\text{Ch} = \text{S, Se}$).

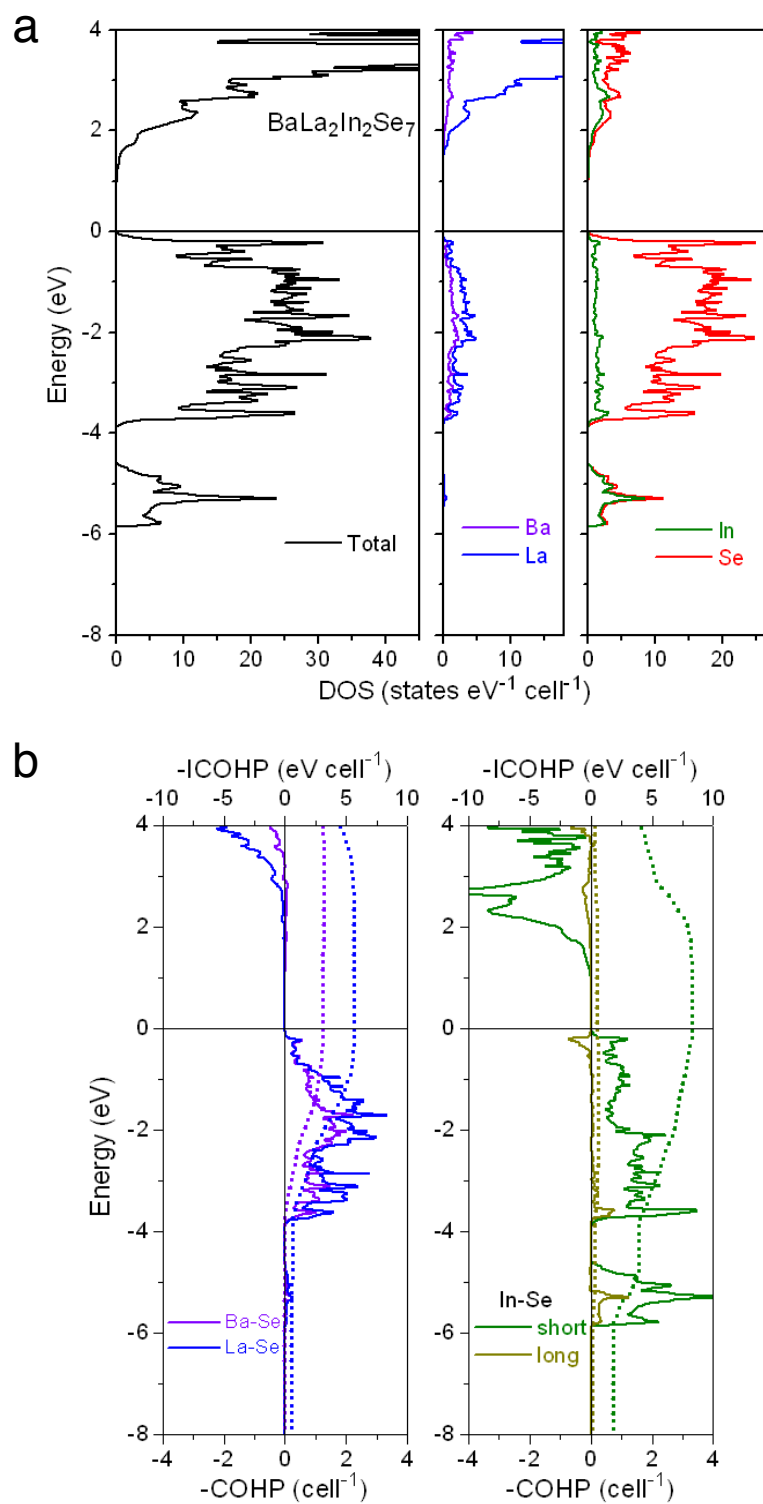


Figure S2. (a) Density of states (DOS) and (b) crystal orbital Hamilton population (–COHP) curves for BaLa₂In₂Se₇.