## **Supporting Information**

## Rare earth indates (RE: La-Yb): Influence of synthesis route and heat treatment on crystal structure

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 $\begin{array}{c} 1.0 \\ 0.8 \\ 0.6 \\ 0.4 \\ 0.2 \\ 0.0 \\ 200 \\ \end{array} \begin{pmatrix} (a) \\ (a) \\ (b) \\ (b) \\ (b) \\ (b) \\ (b) \\ (c) \\ ($ 

Figure S1: DR-UV plot for (a) hexagonal SmInO<sub>3</sub> and (b) orthorhombic SmInO<sub>3</sub>.



Figure S2: Spin polarised total and projected density of states (DOS) of (a) Hexagonal and (b) orthorhombic SmInO<sub>3</sub> calculated using HSE06 method.



Figure S3. Variation of energy with volume fitted to Birh-Murnaghan equation of state for (a) Orthorhombic and (b) Hexagonal SmInO<sub>3</sub>.



Figure S4. Variation of free energy with respect to volume at different temperatures from 0 K to 2000 K for (a) Orthorhombic and (b) Hexagonal SmInO<sub>3</sub>.