Supplementary information of Pressure-induced order-disorder transitions in β-In_2S_3: an experimental and theoretical study of structural and vibrational properties

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Figure S1. Theoretical pressure dependence of the unit cell volume of β-In_2S_3 and the polyhedral volumes corresponding to the InS_4 and vacancy tetrahedra, $VacS_4$, (8e and 4a sites) and InS_6 octahedra (8c and 16h sites).

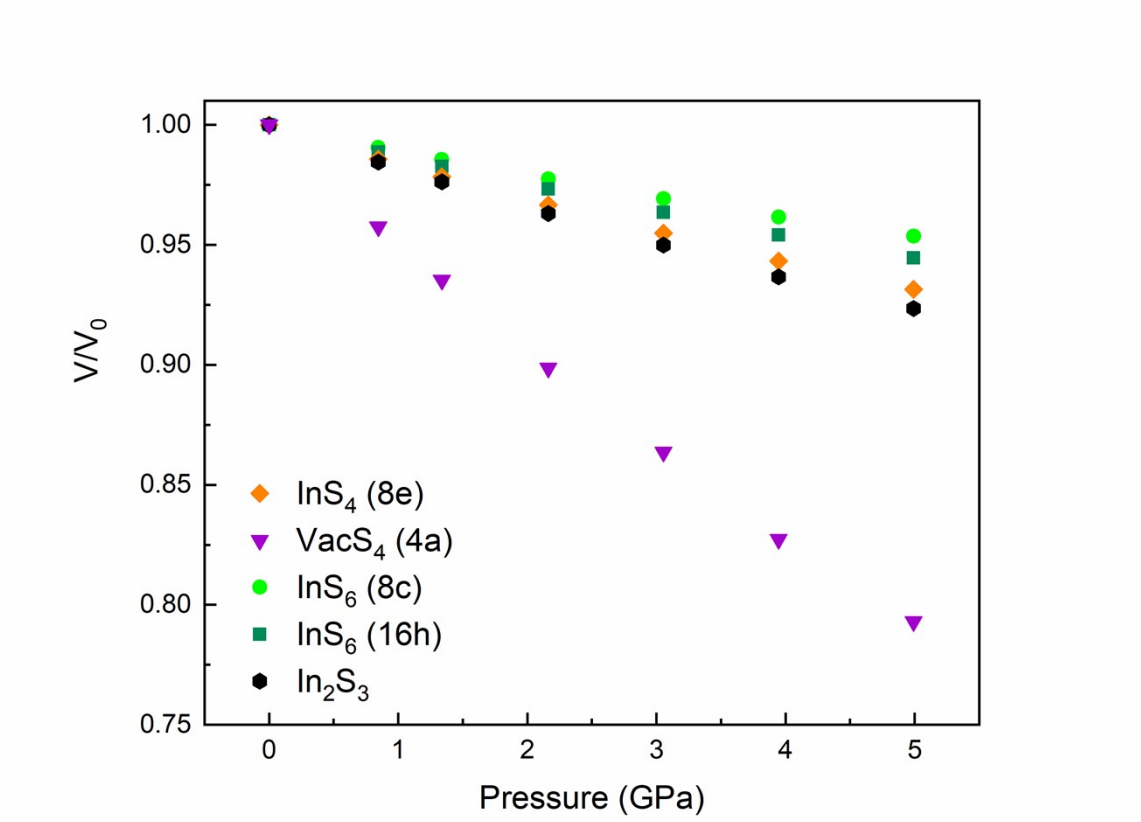

Figure S2. Theoretical pressure dependence of the interatomic distances in β-In_2S_3, corresponding to a) InS_4 and b) vacancy tetrahedra, $VacS_4$, (8e and 4a sites), c) and d) InS_6 octahedra (8c and 16h sites, respectively).

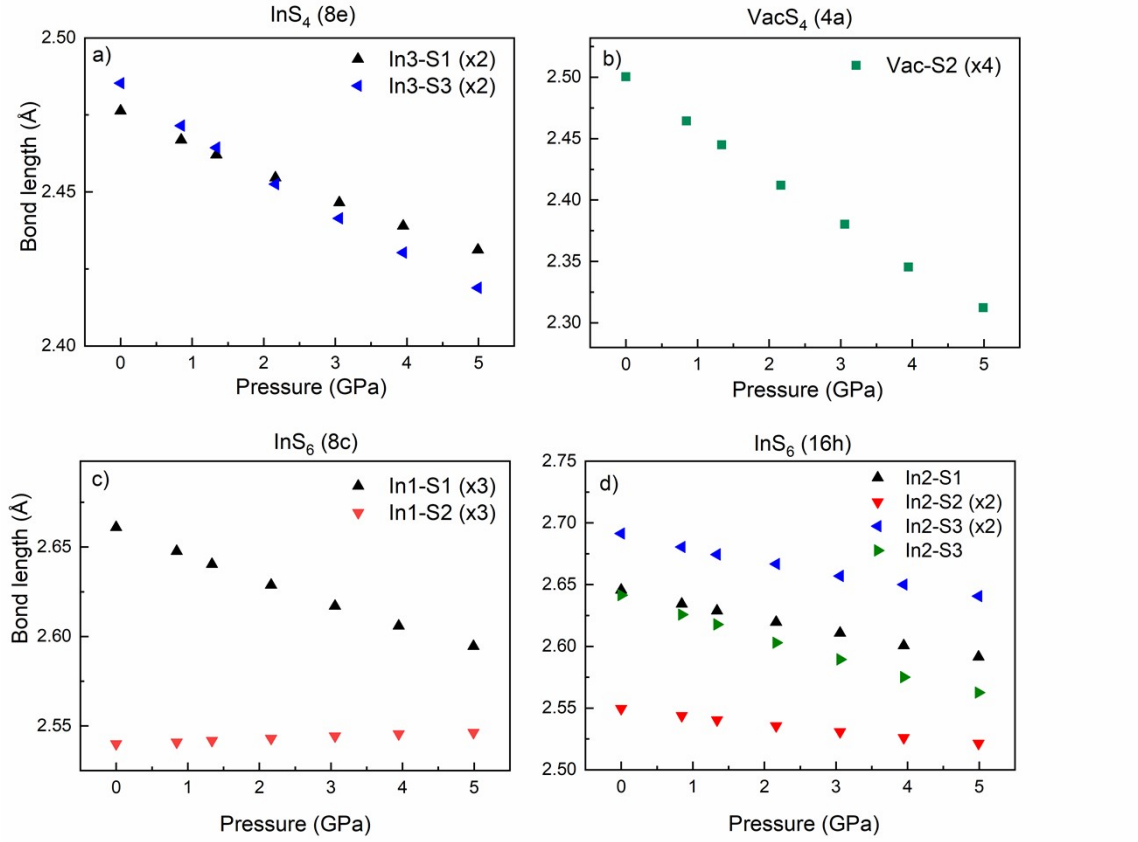

Figure S3. Theoretical pressure dependence of a) the effective coordination number (ECoN), b) bond angle variance (σ^2), c) quadratic elongation (λ) and d) distortion index (D) corresponding to InS_4 and vacancy tetrahedra, $VacS_4$, (8e and 4a sites), and InS_6 octahedra (8c and 16h sites).

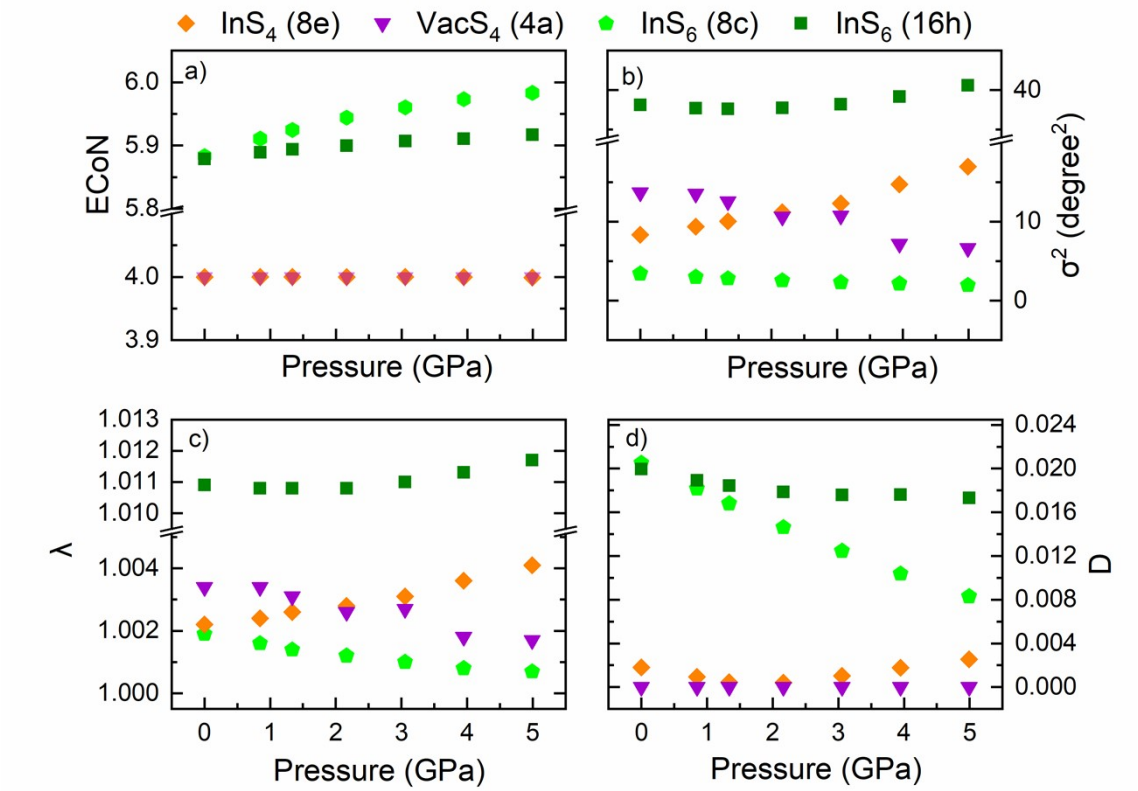

Figure S4. Commercial α-In_2S_3 powders of Sigma Aldrich at room pressure: (a) Le Bail refinement of the XRD pattern with the cubic spinel structure and (b) RS spectrum. Theoretical zero pressure frequencies of Raman-, IR-active, and silent modes of $CdIn_2S_4$ at room pressure are given by ticks.

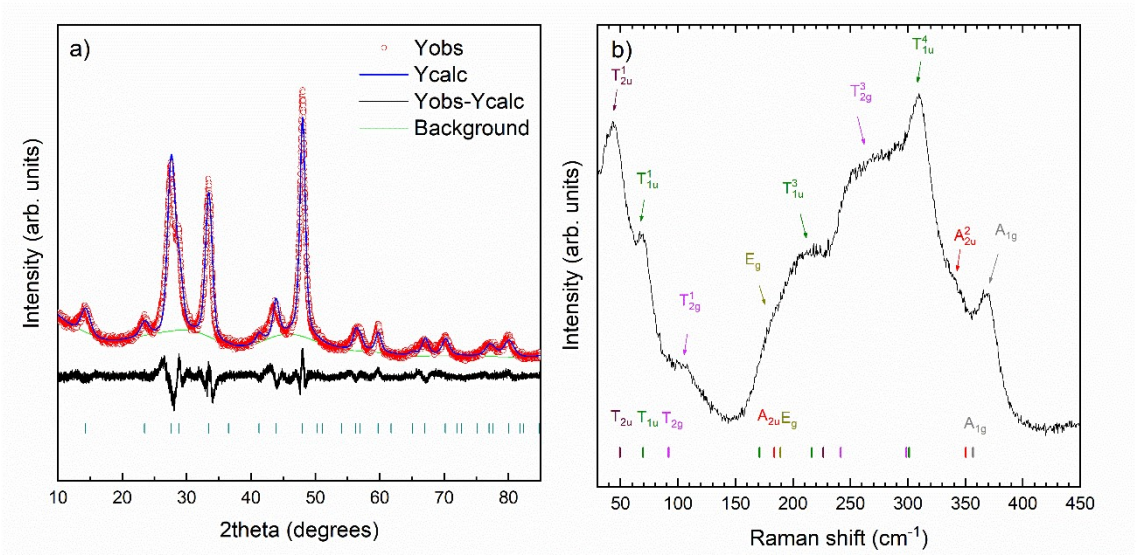

Figure S5. Theoretical one-phonon density of states of a) β-In_2S_3 and b) $CdIn_2S_4$ at room pressure.

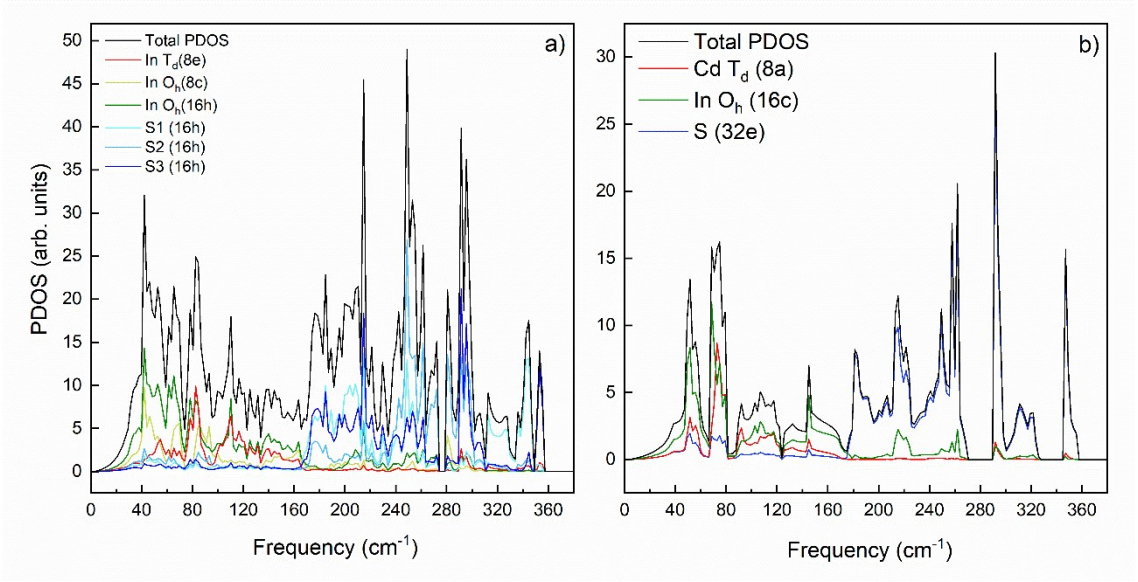

Figure S6. a) Theoretical volume dependence of the energy of β and ϕ-In_2S_3 and b) theoretical pressure dependence of the enthalpy difference between β and ϕ-In_2S_3. Enthalpy of β-In_2S_3 is taken as reference.