

**Abstract:** We performed a systematic ab initio study of lanthanide monoxides (La–Lu) under hydrostatic pressure using Density Functional Theory (DFT). At ambient pressure, all compounds are most stable in the B1 (NaCl-type) structure. Upon compression, a pressure-induced B1 → B2 (CsCl-type) structural transition occurs across the whole series, with transition pressures ranging from 29 GPa (YbO) to 209 GPa (LuO). The calculations also provide the equation of state and bulk modulus, which varies smoothly along the lanthanide series (125–152 GPa). These results highlight the relevance of lanthanide monoxides as model systems for understanding high-pressure behavior, with YbO identified as the most suitable candidate for experimental verification.

## Methodology

We performed ab initio calculations within Density Functional Theory (DFT) using the Quantum ESPRESSO code. Ultrasoft pseudopotentials from the SSFP library were employed, treating valence and semicore states explicitly. Calculations were carried out with a plane-wave cutoff of 85 Ry, a 10×10×10 Monkhorst–Pack k-mesh, and using both GGA (PBE) and LDA (Ceperley–Alder) exchange–correlation functionals. After verifying that GGA reproduces experimental lattice parameters more accurately, all high-pressure studies were performed with this functional. For each lanthanide monoxide (La–Lu), we computed total energy vs volume for the B1 (NaCl), B2 (CsCl) and B3 (ZnS type) phases. The resulting data were fitted to a Birch–Murnaghan equation of state to obtain the equilibrium lattice constant, bulk modulus. Curve of enthalpy of B1 and B2 phases versus pressure were built to establish if there is a high pressure structural transition from one to the other, and the value transition pressure.

## Results

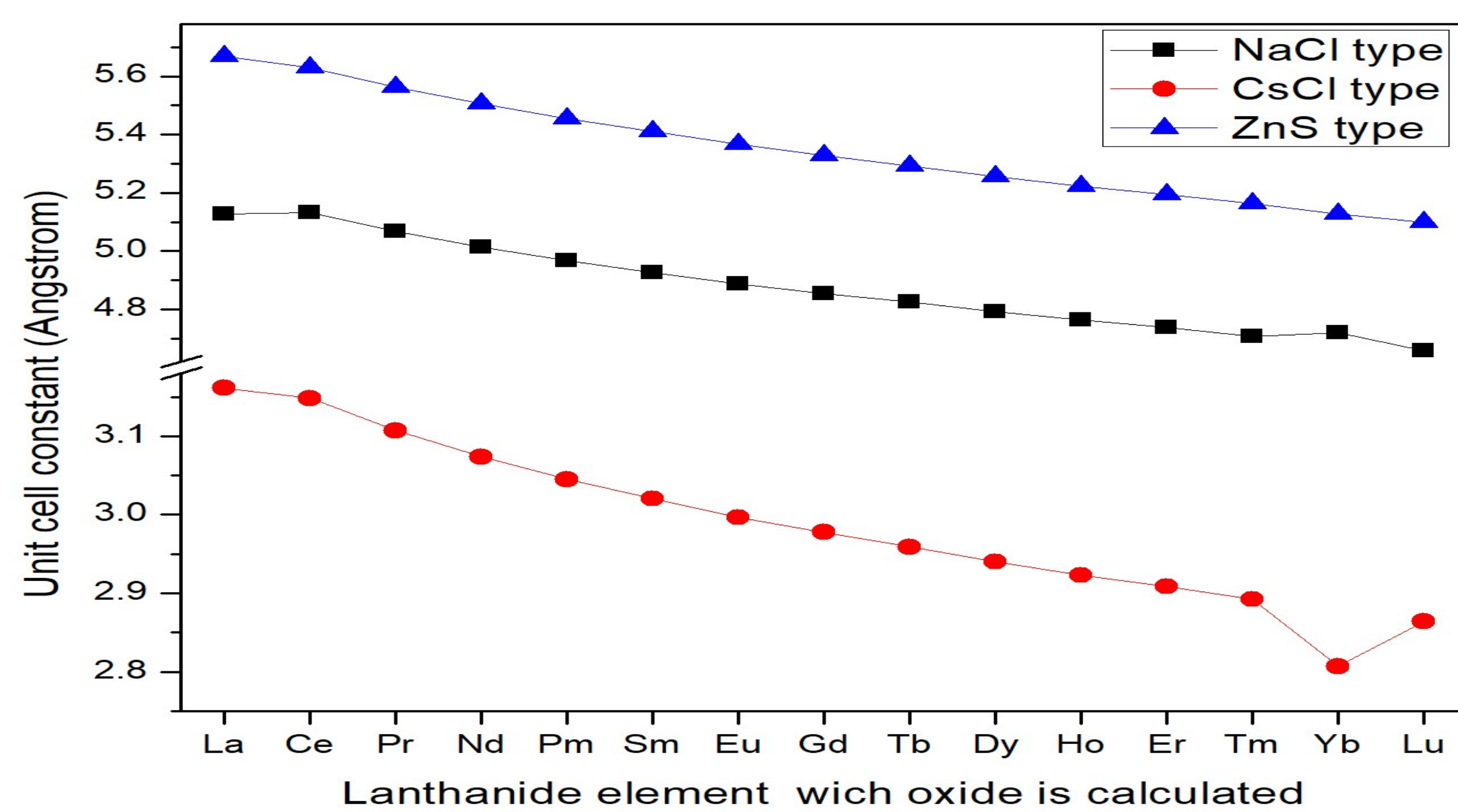


Fig. 1. Equilibrium lattice constant of lanthanide monoxide for the different structures.

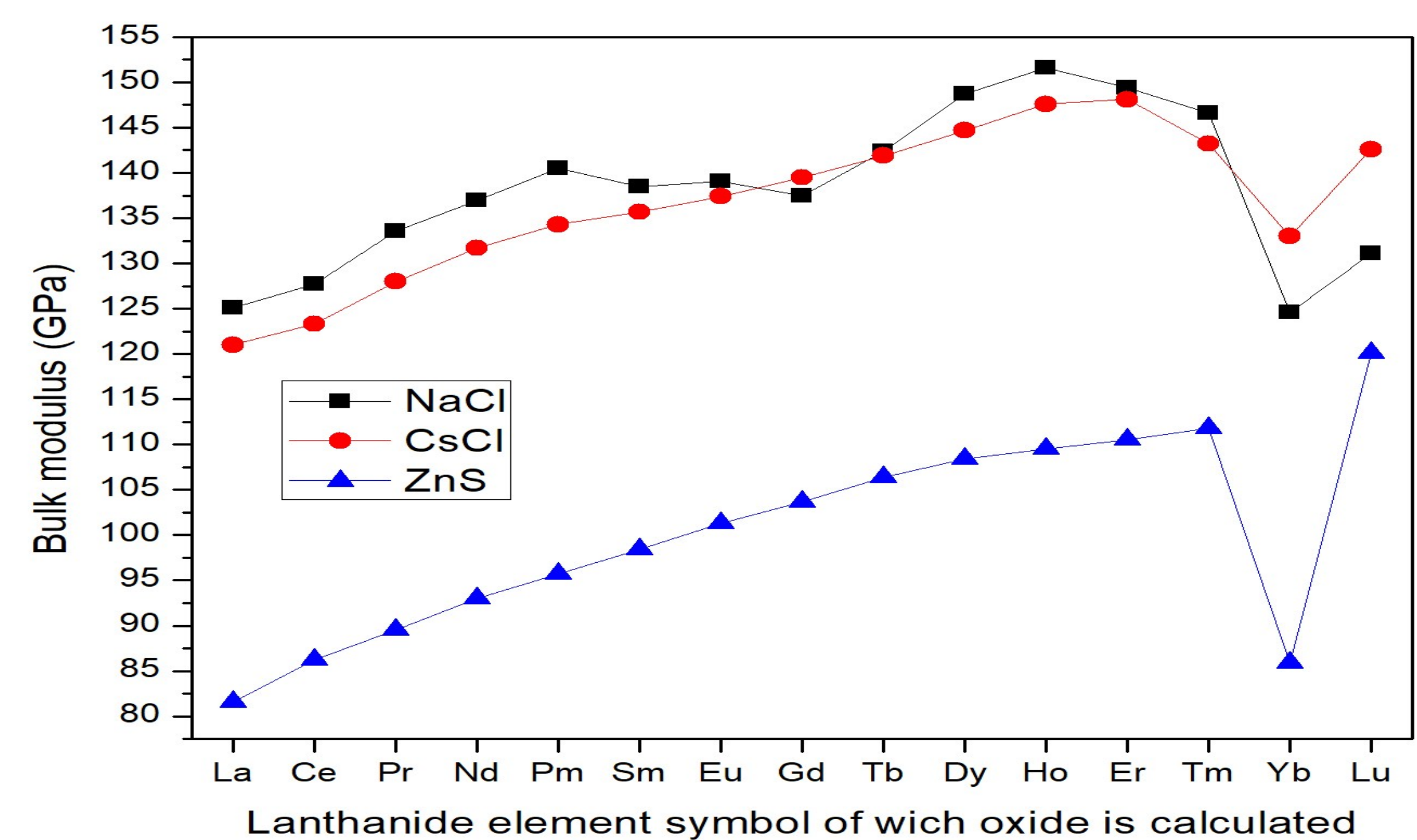


Fig. 2. Obtained bulk modulus from Birch-Murghanam EoS fit of data Energy (from DFT calculus) vs Volume

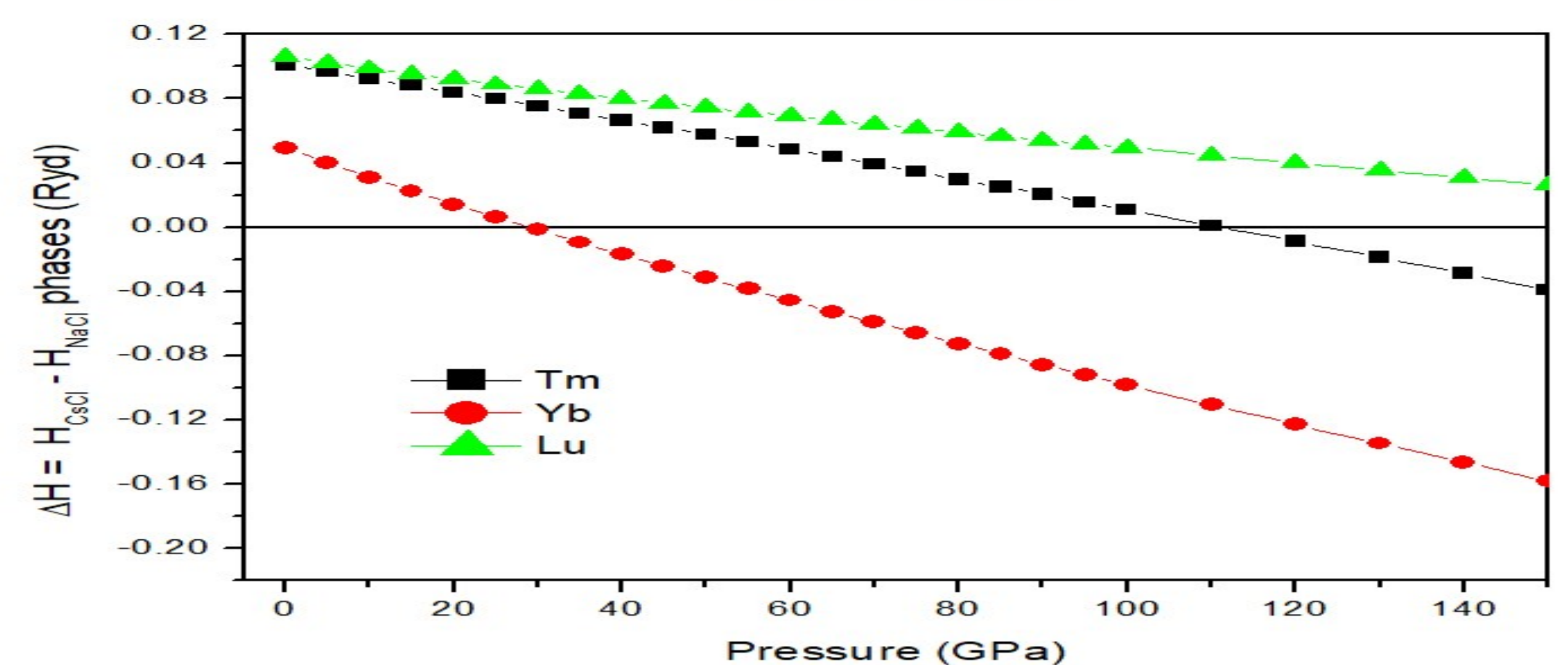
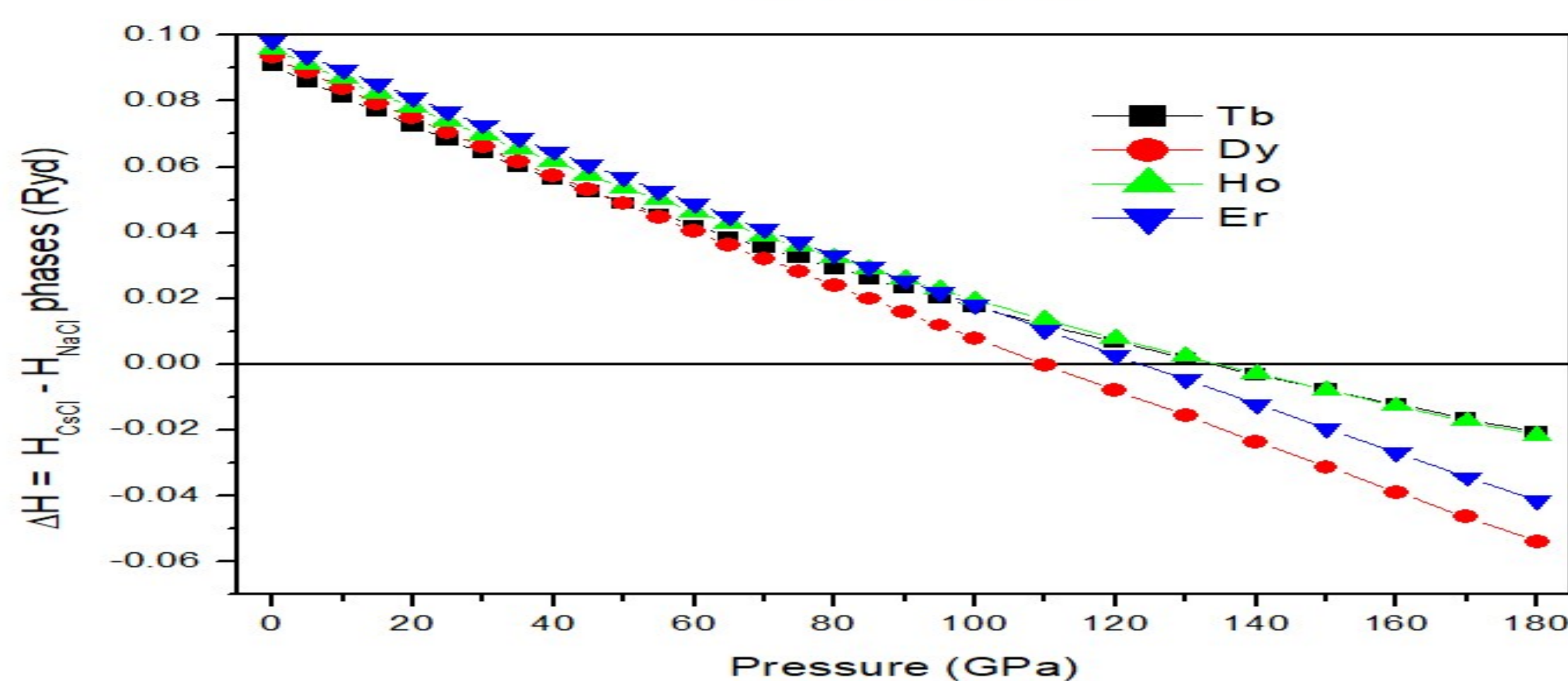
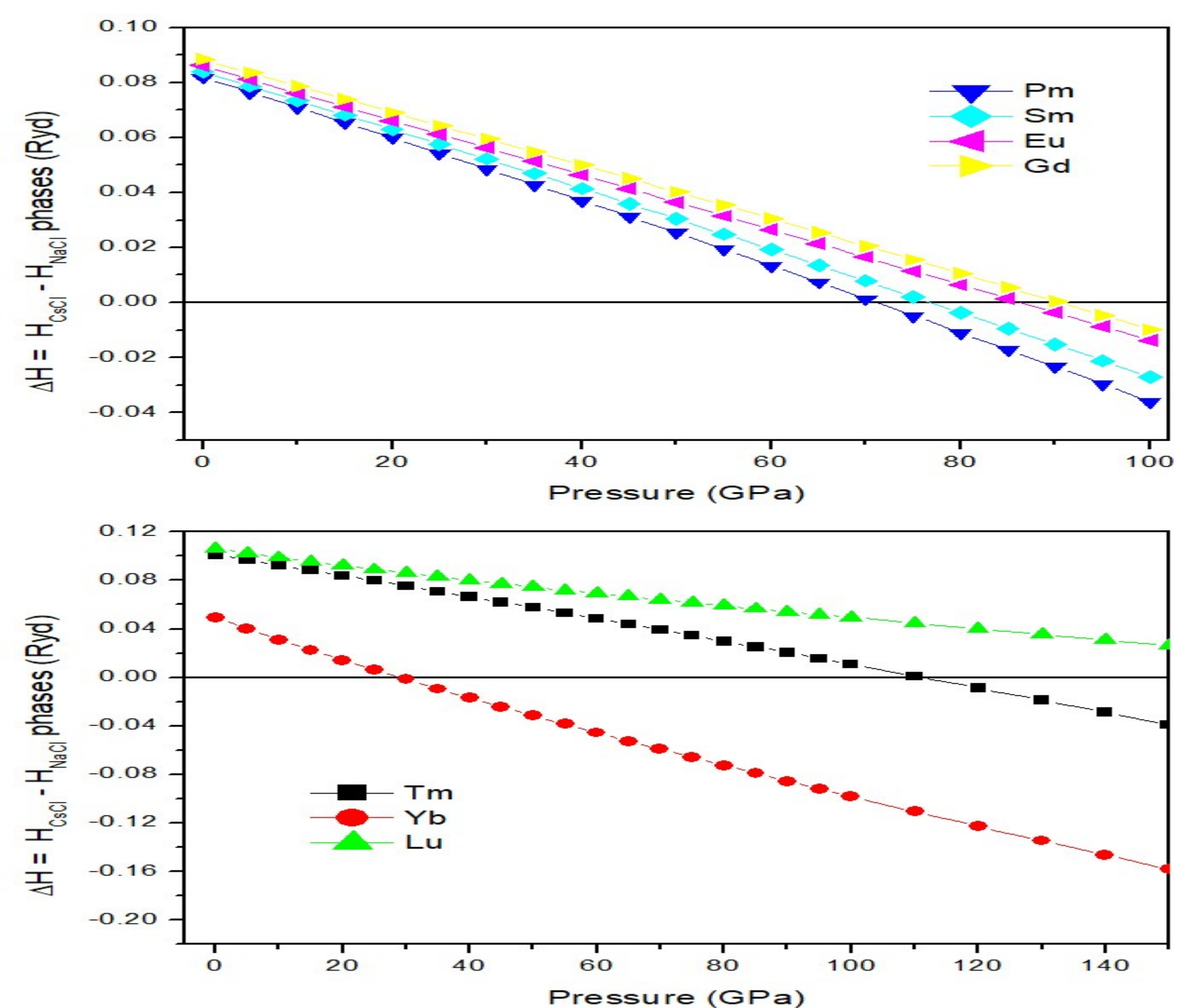
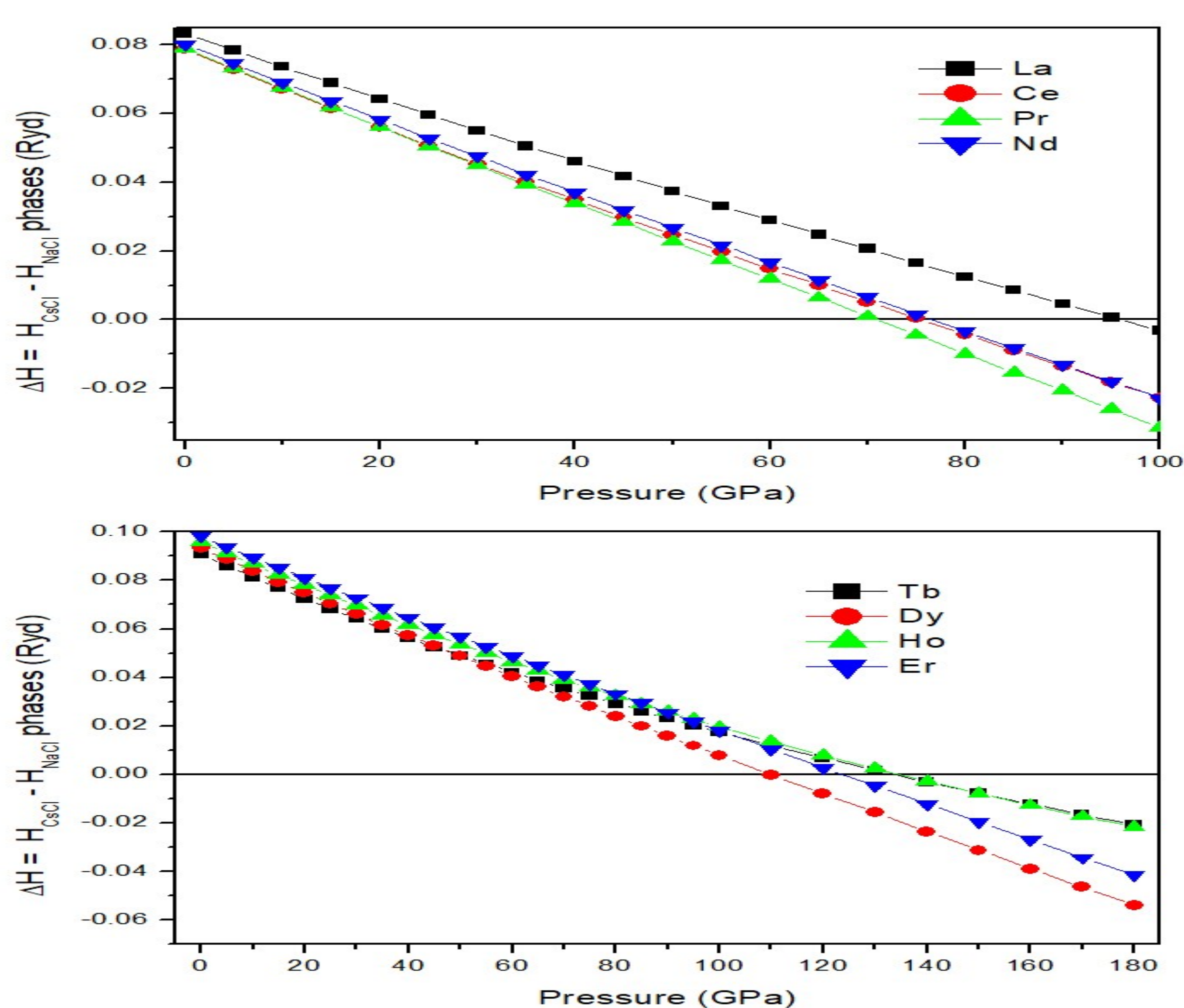


Fig. 3. Difference of enthalpy of phase B2 with phase B1 vs pressure. Crossing zero implies transition from B1 to B2

## Conclusions

- All lanthanide monoxides (La–Lu) are most stable in the B1 (NaCl-type) structure at ambient pressure.
- Under compression, all compounds undergo a B1 → B2 (CsCl-type) structural transition.
- The equilibrium lattice constant decreases progressively with increasing atomic number, following the lanthanide contraction.
- The bulk modulus increases toward the end of the series, showing a smooth variation across La–Lu.
- The transition pressure ranges from 29 GPa (YbO) to 209 GPa (LuO), confirming YbO as the best experimental candidate.
- These results provide the first systematic DFT description of structural stability and compressibility in lanthanide monoxides under pressure.