American Mineralogist, Volume 110, pages 1072–1081, 2025

Structural mechanisms of pressure-induced isosymmetric second-order phase transitions

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Abstract

Pressure-induced polymorphic phase transitions are important in fundamental physics, chemistry, materials science, and geoscience. The isosymmetric phase transition is unique in that it retains crystal symmetry through the transition and exhibits either first- or second-order characteristics. However, the underlying mechanisms of the isosymmetric second-order phase transition have not been well constrained under high pressures. Here, we report a novel case of pressure-induced isosymmetric phase transition in cerite, a rare earth element (REE) mineral, using a diamond-anvil cell combined with in situ synchrotron single-crystal X-ray diffraction. This phase transition is triggered by an increase in coordination number (CN) and exhibits the second-order characteristics. By combining our findings with previous studies, we identify five distinct types of pressure-induced isosymmetric phase transitions. Furthermore, we propose an explanation for the nature (first- or second-order) of phase transitions triggered by increases in coordination number under pressure. The complexity of a mineral structure plays a crucial role in determining the type of isosymmetric phase transition observed. Crystal structures composed of single-building units tend to exhibit first-order transitions, while those with multiple building units exhibit greater flexibility and are more prone to second-order transitions. This study provides new evidence for isosymmetric second-order phase transitions triggered by pressure and an increase in coordination number, while offering valuable insights into the mechanisms governing such transitions.

Keywords: Isosymmetric phase transition, coordination number increase, high pressure, second-order phase transition, phase transition mechanisms