

Pressure-induced ferroelastic phase transition in LuLiF₄ compound

Petrova A., Nedopekin O., Minisini B., Tayurskii D.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

© 2015 Taylor & Francis. The behavior of LuLiF₄ sheelite (I41/a, Z = 4) under hydrostatic pressure was investigated by means of first principles calculations. The ferroelastic phase transition from the tetragonal structure of LuLiF₄ to the fergusonite structure (C12/c1, Z = 4) has been found at 10.5 GPa. It has been determined that this is the second-order phase transition.

<http://dx.doi.org/10.1080/01411594.2014.1000578>

Keywords

ab initio calculations, fluorides, high pressure, phase transitions