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Crystal Structure and Phase Transition of XeF₂ at High pressures

MINSEOB KIM, Institute for Shock Physics, CHOONG-SHIK YOO, Institute for Shock Physics and Department of Chemistry, STATIC HIGH PRESSURE GROUP IN ISP TEAM — We have investigated the crystal structure and phase transition of solid XeF₂ up to 51 GPa in diamond anvil cells by using Raman and synchrotron x-ray diffraction. The x-ray data indicates the tetragonal-to-orthorhombic phase transition at 7 GPa, which accompanies a small distortion (< 1%) in the ab-plane of the tetragonal structure. The Rietveld refinement further indicates a rapid change of intermolecular F...F contact distance with increasing pressures and, thereby, a rotation of linear symmetric XeF₂ molecules along the c-axis and the observed distortion in the ab-plane. This symmetry lowering tetragonal-to-orthorhombic transition also induces the Davydov splitting of symmetric stretching ν_1 and bending ν_2 modes in the Raman spectrum.

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