Investigations of phase transformations in red mercuric iodide under high pressure

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Abstract

We have investigated the behavior of red mercuric iodide (α-Hgl₂) under high pressures using in situ x-ray diffraction and optical absorption measurements. Our experimental results indicate that the tetragonal to orthorhombic phase transformation, observed at 1.4 GPa, is accompanied by an abrupt increase in the band gap while the nature of the gap does not change. In addition we find that all the Raman active mode frequencies increase with pressure up to 1.3 GPa, beyond which the modes of the tetragonal phase disappear and new modes appear supporting the tetragonal → orthorhombic structural transition around this pressure. At still higher pressures, at ~ 7.2 GPa, Hgl₂ undergoes an orthorhombic to hexagonal phase transformation marked by a discontinuous decrease in the band gap as well as its character changes from direct to indirect type. These studies suggest that Hgl₂ may metallize at ~ 40 GPa, if not prevented by any other structural change.