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# STRUCTURAL AND ELASTIC PROPERTIES OF MAGNESIUM OXIDE (MgO) UNDER HIGH PRESSURE

**PURVEE BHARDWAJ, SADHANA SINGH & N. K. GAUR**

**Abstract**

In the present paper we have investigated the high-pressure structural phase transition of barium oxide using the modified three-body potential (TBP) incorporated with covalency effect. Probably this is the first time when oxide has been studied by using three-body potential with including covalency effect. Phase transition pressures are associated with a sudden collapse in volume. The phase transition pressures and associated volume ollapses obtained from TBP show a reasonably good agreement with experimental data. Here, the transition pressure NaCl-CsCl structure increases with decreasing cation to anion radii ratio qualitatively. This compound (MgO) under normal condition crystallize in rock salt structure and show a different phase at high pressure. In addition, the elastic constants and their combinations with pressure are also reported.

**Key Words and Phrases :** *Phase transition, volume collapse,equation of state, three-body Potential, high pressure.*

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