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High Pressure Phase Transition of Copper Halides

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Abstract: The structural changes within copper halides induced by pressure from zinc-blend to rock-salt passing through an intermediate tetragonal structure have been investigated using an effective interionic interaction potential. The values of the phase transition pressures obtained by us for the copper halides are in good agreement with their available experimental data. We have also investigated the equation of state, which shows an appreciable volume collapses at the phase transition pressures.

Key Words: High Pressure, Structural Phase Transition, Gibbs free energy, Volume Collapses, Cohesive Energy

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