MS16-P08 | Lattice Constants Prediction And Thermochemistry Of Hexahalometallate A_2MX_6

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In this study we describes the attention of lattice parameters of hexahalometallate A_2MX_6 salts in cubic structure Fm3m. Mail parameters received from recent experimental studies are investigated for 87 compounds to obtain a linear prediction formula depending on ionic radius and electronegativity of constituents. A good agreement between the experimental and predicted lattice constants is found with an average error less than 1.6 % only. First principles calculations of enthalpies of formation is presented using GGA approximations.

It was shown that the lattice constant is a linear function of the Enthalpy of formation