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Scientific Journals Home Page Second Order Elastic Constants and Some Thermoelastic Properties of Alkali Halides Using WOODCOCK Potential

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Abstract: Second Order Elastic Constants (S.O.E.C) of NaCI-type crystals have been calculated using the Woodcock potential. Short-range repulsive interactions have been included up to second-nearest neighbors. This potential form represents the composite form of the inverse power dependence and exponential dependence of the repulsive energy on interionic distance. Some thermoelastic and thermodynamic properties such as Anderson-Grüneisen parameters δ_T, and δ_S, Volume thermal expansion coefficient β and Grüneisen gama γ_G have been calculated in terms of calculated values of S.O.E.C and Third Order Elastic Constant (T.O.E.C).

Key Words: Second order elastic constant, NaCl-type crystal, Anderson-Grüneisen.

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