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INTERACTION POTENTIAL ENERGIES IN RUBIDIUM IODIDES

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ABSTRACT
The interaction potential energies of rubidium iodide are calculated using a three-body interaction potential. The experimental and theoretical results are in good agreement.

INTRODUCTION

Rubidium iodide is a crystalline salt with a melting point of 647degree centigrade and boiling point is 1300 degree centigrade. Refractive index is 1.6474, formula weight is 212.37 and density is 3.55g/ml at 25 degree centigrade (lit). Storage and sensitivity is hygroscopic at ambient temperature. Its chemical formula is RBI. It can be formed from the reaction of rubidium and iodine. It is 99.9% trace metal basis. It is solubule in water, alcohol and alkali aqueous solution. Solubility is 152g/100g water.

It is used for making metal rubidium and other rubidium salts. It is also used in the production of special glass, miniature high energy battery and crystal scintillation counter. Its crystal structure is cubic face centered cubic lattice, NaCl Fm3m, (100) cleavage, bulk modulus is 11GPa transmission range is 0.3 to 50 micrometer, reflection loss is 10.4% at 10 micrometer covering 2 surfaces, thermal conductivity is 9.9Wm inverse Kelvin inverse, specific heat capacity is 242 joule Kg inverse K inverse at 283K.

Many workers [1-26] have studied the interaction potential energies using both two-body [1-3] and three-body [4-7]) potentials. The latter potentials have given their prediction better than those revealed by other potential [1-3].Elastic constants are measured by Lindquist Potential [8] Singh and Verma [9] Karlsson [10]. In the present paper, we have used three-body potential to explain the interaction potential energies of rubidium iodide.

Calculations have been performed using the expression for the model parameters given by Verma and co-workers [4] and those for the pressure derivatives of SOE constants are given by Garg et al [5] respectively. The essential theory and calculations are given in section 2. The results are presented and discussed in section 3.

THEORY AND METHOD OF CALCULATIONS:

Interaction potential energy of rock salt structure solid with contribution from the long-range coulomb and three-body interactions and the short-range repulsive and van der Waals dipole-dipole and dipole –quadrupole attractions is given by

$$W(r) = \alpha_m Z (Z+6 f(r))/r + [W_1(r)+W_2(r)] e^2 \quad (1)$$

First term is the Coulomb interaction with a α_m as the Madelung constant, Ze is the ionic charge and e is the electronic charge. Here r (=r_0) and r_1 (=$2r_0$) are the first and second neighbor distances. f(r) is the three-body force parameter dependent on r.W_1 and W_2 are the short-range interactions defined as

$$W_1(r) = b\beta/e^2\beta_{+-} \exp(r_+ + r_- - r)/\rho_{+-} - C_{+-}/r^6 - d_{+-}/r^8 \quad (2)$$

$$W_2(r') = b\beta/e^2 \beta_{++}\exp(2r_+ + r')/\rho_{++} + b\beta_{--}/e^2\exp(2r_- - r')/\rho_{--} - (c_{++} + c_{--})/r'^6 - (d_{++} + d_{--})/r'^8 \quad (3)$$

$$\text{Where } \beta_{ij} = 1 + (z_i/n_i) + (z_j/n_j) \quad (4)$$

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With n_i as the number of electrons in outermost orbit. Here, b and ρ are the repulsive strength and hardness parameters, respectively. In our calculations value of ionic radii (r_i) and van der Waals coefficients (c_{ij} and d_{ij})have been taken from Singh[9] and co-workers[11-19].The values of ρ_{ij} for the rubidium iodide have been taken from Hafemeister and Flygare[20].The values of b for them have been evaluated from the equilibrium condition

$$dW(r) / dr = 0 \quad \text{at } r=r_o \qquad (5)$$

Using the values of f(r) obtained from the knowledge of overlap integral and its derivatives from the knowledge of overlap integral (5).

$$f(r_0) = f_0 \exp(-r_0 \backslash \rho_{+-}) = €_{+-} S_{+-}^2 \qquad (6)$$

$$\text{With } f_0 = A_{+-} (1-2r_+/r_0) \qquad (7)$$

Values of overlap integral (S_{+-}) and constants (A_{+-}) are directly taken from[14]. Values of parameters (ρ_{ij} , b and f_0) have been given in Table 1 together with the equilibrium nearest neighbour distance r_0,which is the only input data used for the calculation of the parameter b.

RESULT AND DISCUSSIONS:

TABLE: 3.1 Values of input for ionic crystal.

CRYSTAL	r_0 10^{-8} cm (a)	r_+ 10^{-8} cm (b)	r_- 10^{-8} cm (b)	C_{11} 10^{11} dyne / cm^2 (a)	C_{12} 10^{11} dyne / cm^2 (a)	C_{44} 10^{11} dyne / cm^2 (a)
RbI	2.50	1.49	3.02	3.10	1.00	0.46

Table 3.2 Model Parameters for ionic solids

CRYSTAL	ρ	b (in 10^{-12} erg)	f (r)
RbI	0.203	0.12	-0.00010

Table 3.3 Values of Cohesive Energies In Magnesium Chloride.

CRYSTAL	Experimental Value	Theoretical Value
RbI	**212.32**	200.11

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions. I, Bi, Ci, Di (i=1, 2).Those parameters are the same as those defined by Verma and co-workers[4] except for the difference that we have included the effect of short range Vander Waals attraction and represented the overlap repulsion by the HF potential. With the knowledge of parameters and input data we have calculated the interaction potential energies of Rubidium iodide using their relevant expressions reported (4, 5).

Results obtained in the table are in good agreement with the experimental results which shows that the agreement between experimental and our theoretical results are better.

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