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INTERACTION POTENTIAL ENERGIES IN POTTASSIUM BROMIDE

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ABSTRACT
The interaction potential energies of potassium bromide are calculated using a three-body interaction potential. The experimental and theoretical results are in good agreement.
Keywords: b, ρi f(r) are model parameters.

1.INTRODUCTION

Pottassium bromide (KBr) is a salt, widely used as an anticonvulsant and a sedative in the late nineteenth and early twentieth century's, with over the counter use extending to 1975 in the US. Its action is due to the bromide ion (sodium bromide is equally effective).

Melting point of potassium bromide is 734 degree centigrade .It has been used in human and veterinary medicine as an anti-seizure medication. Phenobarbital or PB has also been used for years to treat seizures. Despite both drugs long history of common use, neither is approved by FDA to treat seizures. In people or animals. The lack of FDA approval means that no drug company has presented information to the agency to prove that KBr or PB is safe and effective to treat seizures. It also means that no drug company has proven to FDA that either drug can be consistently manufactured according to quality standards. Without FDA approval, veterinarians' and pet owners may be unaware of the risks of these drugs.

Co-workers [1-27] 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 potassium bromide.

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 Second order elastic 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.

2. 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 neighbour distances. f(r) is the three-body force parameter dependent on r.W_1 and W_2 are the short-range interactions defined as

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

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

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

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 potassium bromide have been taken from Hafemeister and Flygare[20].The

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values of b for them have been evaluated from the equilibrium condition

$dW(r) / dr = 0$ at $r=r_o$ (5)

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

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

With $f_0 = A_{+-} (1-2r_+/r_0)$ (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 neighbor distance r_0, which is the only input data used for the calculation of the parameter b.

3. 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)
KBr	2.03	1.30	3.00	3.12	1.00	0.13

Table 3.2 Model Parameters for ionic solids

CRYSTAL	ρ	b (in 10^{-12} erg)	f (r)
KBr	0.112	0.12	-0.00001

Table 3.3 Values of Interaction potential energies of Pottassium Bromide in (KJ/Mol)

CRYSTAL	Experimental Value	Theoretical Value
KBr	**1908**	1901

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions. ı, 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 pottassium bromide 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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