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ELASTIC PROPERTIES OF POTTASSIUM IODIDE

DEEPAK RAWAT
Department of Physics, Saifia P.G College of Science and Education,
Bhopal-462001(INDIA)

ABSTRACT

The elastic properties of pottassium iodide are calculated using a three-body interaction potential. This includes the prediction of third order elastic constant (TOEC), Fourth order elastic constant (FOEC) and pressure derivatives second order elastic constant (SOEC) and third order elastic constant (TOEC).The experimental and theoretical results are in good agreement.

INTRODUCTION

Pottassium iodide is a chemical compound, medication and dietary supplement .As a medication it is used to treat hyperthyroidism in radiation emergencies and to protect the thyroid gland when certain types of radio pharmaceuticals are used in the developing world it is also used to treat skin sporotrichosis and phycomycosis.As a supplement it is used in those who have low intake of iodine in the diet. It is given by mouth. Its chemical formula is KI. It consists of one potassium (K positive ion) and one iodide (I negative ion).Its molecular weight is 166.0028 g/mol. It is a metal iodide composed of potassium and iodide. Pottassium maintains intracellular tonicity is required for nerve conduction, cardiac, skeletal and smooth muscle contraction, production of energy, the synthesis of nucleic acids, maintenance of blood pressure and normal reval function. Common side effects include vomiting, diarrhea, abdominalpain, rash and swelling of the salivary glands.other side effects include allergic reactions, headache, goiter and depression.while using during pregnancy may harm the baby, its use is still recommended in radiation emergencies. The crystal properties are the thermal expansion, the specific heat beyond 3R(R is the gas constant) the thermal conductivity and higher order elastic constants and their pressure and temperature variations among them are of special interest because they are related to all the elastic properties of solids. The coefficient of first order elastic term in the multi-pole interaction potential determines the elastic properties such as thermal expansion pressure dependence of SOECS etc. The thermal expansion produces the difference between the adiabatic and isothermal elastic constant which provide physical insights into the nature of bonding and interatomic forces in solids.

Several investigators [1-26] have studied the Third order elastic constant (TOEC) and pressure derivatives second order elastic constant (SOEC) 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 Lundqvist Potential [8] Singh and Verma [9] Karlsson [10]. In the present paper, we have used three-body potential to explain the elastic properties of potassium iodide.

Calculations have been performed using the expression for the third and fourth order elastic constant

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.

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

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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

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

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

Where $\beta_{ij} = 1+(z_i/n_i) + (z_j/n_j)$ (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 cesium bromide have been taken from Hafemeister and Flygare[20].The values of b for them have been evaluated from the equilibrium condition

$dW(r) / dr = 0$ 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 neighbour 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)
KI	2.62	2.69	3.07	3.24	1.00	0.86

Table 3.2 Model Parameters for ionic solids

CRYSTAL	ρ	b (in 10^{-12} erg)	f (r)
KI	0.26	0.18	-000018

Table 3.3 Third order elastic constants (TOECs) 10^{11} dyne/cm^2 for ionic crystals.

Crystal	C_{111}	C_{112}	C_{166}	C_{123}	C_{144}	C_{456}
KI	-2.16	-1.36	-1.46	-1.24	-1.30	-1.24

Table-3.4 Calculated values of fourth order elastic constants (FOECs) (in 10^{11} dyne/cm$^{2)}$ for ionic crystals.

Crystal	C_{1111}	C_{1112}	C_{1166}	C_{1122}	C_{1266}	C_{4444}	C_{1123}	C_{1144}	C_{1244}	C_{1456}	C_{4466}
KI	32.62	7.92	7.95	8.88	8.88	8.89	8.00	7.27	7.29	7.01	7.01

Table 3.5 Pressure Derivatives of Second Order Elastic Constants (SOECs) (10^8 dyne /cm^2).

Crystal	dc' $_{44}$ /dp	ds' /dp	dk'/dp
KI	1.49	0.60	6.60

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Table 3.6: Calculated values of pressure derivatives of third order elastic constants (TOECs).

Crystals	$dc_{111/dp}$	$dc_{112/dp}$	$dc_{116/dp}$	$dc_{123/dp}$	$dc_{144/dp}$	$dc_{456/dp}$
KI	-75.67	-45.78	-43.67	-44.58	-46.26	-44.11

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions.A_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 values of third, fourth order elastic constants 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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Corresponding Author : email :