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ELASTIC PROPERTIES OF RUBIDIUM CHLORIDE

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ABSTRACT

The elastic properties of rubidium chloride 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

Rubidium chloride is a chemical compound with the formula RbCl,the alkali metalhalide composed of rubidium and chlorine and find diverse uses ranging from electrochemistry to molecular biology.In its gas phase,RbCl is diatomic with a bondlength estimated at 2.7868Angstrom. This distance increases to 3.285Angstrom for cubic RbCl,reflecting the higher coordination number of the ions in the solid phase.Depending on conditions solid RbCl exists in one of three arrangements or polymorphs as determined with holographic imaging.

The most common properties of pure rubidium chloride involve the reaction of its hydroxide with hydrochloric acid followed by re-crystallization because ,RbCl is hygroscopic ,it must be protected from atmospheric moisture e.g desiccator.RbCl is primarily used in laboratories,therefore numerous suppliers produce it in smaller quantities as needed. It is offered in variety of forms for chemical and biomedical research. Rubidium chloride reacts with sulphuric acid to give rubidium hydrogen sulphate.Every 18 mg of rubidium chloride is equivalent to approximately one banana equivalent dose due to large fraction of (27.8%) of naturally occurring radioactive isotope rubidium -87. It is used as a gasoline additive to improve its octane number.It has been shown to modify coupling between circadian oscillators via reduced photaic input to the suprachiasmatic nuclei. The outcome is a more equalized circadian rhythm, even for stressed organisms. Its melting point 718 degree centigrade,molarmass is 120.921g/mol, boiling point is 1,390 degree centigrade,density is 2.8g/centimeter cube.

I 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 Verna [9] Karlsson [10]. In the present paper, we have used three-body potential to explain the elastic properties of rubidium chloride.

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

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

$W_1(r) = b\beta/e^2\beta_{+-} \exp(r_+ + r_- - r)/\rho_{+-} - C_{+-}/r^6 - d_{+-}/r^8$ (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 rubidium chloride 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)
RbCl	2.51	2.67	3.07	3.14	1.00	0.76

Table 3.2 Model Parameters for ionic solids

CRYSTAL	**ρ**	**b (in 10^{-12} erg)**	**f (r)**
RbCl	0.26	0.16	-000017

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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}
RbCl	-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}
RbCl	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
RbCl	1.49	0.60	6.60

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 $_{456/dp}$
RbCl	-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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