STUDIES ON STATIC PROPERTIES OF LITHIUM CHLORIDE

DEEPAK RAWAT

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

ABSTRACT

The static properties of lithium 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

Lithium chloride is an inorganic compound with the formula LiCl. The compound is a bright yellow solid but samples almost always contain impurities of metallic lithium that give a light yellow coloration. The lithium contamination arises because LiCl is highly photosensitive. There are many of the crystal properties which cannot be explained without including the static contributions arising from the potential energy expression. These 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 static properties of solids. The coefficient of first order anharmonic term in the multi-pole interaction potential determines the static 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 (1-7) 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 static properties of lithium 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 –quadrapole attractions is given by

$$W(r) = amZ(Z+6 f(r))/r + [W_1(r) + W_2(r)] e_2 \quad (1)$$

First term is the Coulomb interaction with a am as the Madelung constant, Ze is the ionic charge and e is the electronic charge. Here r (=r0) and r1 (=2r0) are the first and second neighbor distances. f(r) is the three-body

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force parameter dependent on r.W1 and W2 are the short-range interactions defined as

W1(r) =bß/e2ß+- exp(r+ + r- -r)/.+- -C+-/r6 - d+-/r8 (2)

W2(r')=bß/e2 ß++exp (2r+ + r')/.++ + bß--/e2exp (2r- - r')/.-- -(c++ +c--)/r'6 -(d++ +d--)/r'8 (3)

Where ßij =1+(zi/ni)+(zj/nj)   (4)

With ni as the number of electrons in outermost orbit. Here, b and. is the repulsive strength and hardness parameters, respectively. In our calculations value of ionic radii (ri) and van der Waals coefficients (cij and dij)have been taken from Singh(9) and co-workers(11-21).The values of .ij for the lithium chloride have been taken from Hafemeister and Flygare(22).The values of b for them have been evaluated from the equilibrium condition

dW (r) / dr =0 at r=ro   (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(r0)= f0 exp(-r0\.+-) = €+-S+-2   (6)

With f0 =A+- (1-2r+/r0) (7)

Values of overlap integral (S+-) and constants (A+-) are directly taken from (14). Values of parameters (.ij, b and f0) have been given in Table 3.2 together with the equilibrium nearest neighbor distance r0,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 (LiCl)

r0	10-8 cm (a)
r+	10-8 cm (b)
r-	10-8 cm (b)
C11	1011 dyne/cm2 (a)
C12	1011 dyne/cm2 (a)
C44	1011 dyne/cm2 (a)

Table 3.2 Model Parameters for ionic solids

CRYSTAL.	b (in 10-12 erg)		f (r)
LiCl	0.254	0.17	-000016

Table 3.3 Third order elastic constants (TOECs) 1011 dyne/cm2 for ionic crystals.

Crystal	C111	C112	C166	C123	C144	C456
LiCl	-3.23	-1.42	-1.43	-1.31	-1.30	-1.23

Table-3.4 Calculated values of fourth order elastic constants (FOECs) (in 1011 dyne/cm2) for ionic crystals.

Crystal	C1111	C1112	C1166	C1122	C1266	C4444	C1123	C1144	C1244	C1456	C4466
LiCl	33.60	7.90	7.91	8.80	8.80	8.81	8.00	7.20	7.22	7.01	7.01

Table 3.5 Pressure Derivatives of Second Order Elastic Constants (SOECs) (108 dyne /cm2).

Crystal	dc' 44 /dp	ds' /dp	dk'/dp
LiCl	2.38	0.58	6.59

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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

LiCl -76.59 -47.70 -43.59 -44.50 -46.20 -44.12

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions. Ai, Bi, Ci, Di (i=1, 2).Those parameters are the same as those defined by Verma and Coworkers (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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