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STUDIES ON STATIC ELASTIC PROPERTIES OF LITHIUM CARBONATE

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ABSTRACT
The static elastic properties of lithium carbonate 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.3

INTRODUCTION

Lithium Carbonate Li_2CO_3 is an inorganic compound, the lithium salt carbonic acid with the formula Li_2CO_3.This white salt is wide used in processing metal oxides. It is on the world Health Organization list of essential medicines for its efficiency in the treatment of mood disorder, such as bipolar disorder, this medication is used to treat manic depressive disorder, the tablets contain Calcium Stearate, micro crystalline cellulose, povidone, sodium starch glycolate. It has 2D structure, its IUPAC name is dilithium carbonate.

It is soluble in water, its molar mass is 73.891g/mol, its density is 2.11g/Cm3, interactive image is 3D model [JS mole].

I Several investigators [1-28] 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 static elastic properties of lithium Carbonate.

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 are given by

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

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

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

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$W_2(r') = b\beta/e^2\ \beta_{++}\exp(2r_+ + r')/\rho_{++} + b\beta_{--}/e^2\exp(2r_- - r')/\rho_{--} - (c_{++} + c_{--})/r'^6 - (d_{++} + d_{--})/r'^8$ (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 lithium carbonate 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 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)
Li_2CO_3	2.45	2.57	3.05	3.11	1.00	0.52

Table 3.2 Model Parameters for ionic solids

CRYSTAL	ρ	b (in 10^{-12} erg)	f (r)
Li_2CO_3	0.32	0.14	-000014

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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}
Li_2CO_3	-2.15	-1.36	-1.42	-1.23	-1.30	-1.22

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}
Li2C03	32.52	7.82	7.95	8.87	8.86	8.87	8.00	7.26	7.25	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
Li_2CO_3	1.45	0.50	6.30

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 $_{456/dp}$
Li_2CO_3	-75.57	-45.68	-43.67	-44.28	-46.16	-43.11

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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