

## ELASTIC PROPERTIES OF POTTASSIUM FLOURIDE

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### ABSTRACT

The elastic properties of potassium fluoride 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

Potassium fluoride is the chemical compound with the formula KF, after hydrogen fluoride HF is the primary sources of the fluoride ion for application in manufacturing and in chemistry. It is an alkali halide and occurs naturally as the rare mineral carborbite. It is an ideal reagent for fluorination because it is safe, easy to handle and lowcost. It is colorless or white crystalline compound with no odour. Solutions of KF will etch glass due to the formation of soluble fluorosilicates, although HF is more effective.

KF can be used for conversion of chlorocarbons into fluorocarbons via the alkali halides and Hell-Volhard-Zelinsky reactions (aryl chlorides). Like other sources of fluoride ion, KF is poisonous, although lethal doses approach gram levels for humans. It is harmful by inhalation and ingestion. It is highly corrosive and skin contact may cause severe burns. Its Molar mass is 58.0967 gram/mole, Melting point is 858 degree centigrade, Boiling point is 1505 degree centigrade, Density is 2.48 gram/centimeter cube. It is soluble in HF, insoluble in alcohol, its molecular weight is 58.0967, and structure is cubic.

It appears as a white powder or crystal with a sharp saline taste, shipped as solid or aqueous solutions, strongly irritates skin, eyes.

Several investigators<sup>(1-28)</sup> have studied the Third order elastic constant (TOEC) and pressure derivatives second order elastic constant (SOEC) using both two-body<sup>(1-3)</sup> and three-body<sup>(4-7)</sup> potentials. The latter potentials have given their prediction better than those revealed by other potential<sup>(1-3)</sup>. Elastic constants are measured by Lundqvist Potential<sup>(8)</sup> Singh and Verna<sup>(9)</sup> Karlsson<sup>(10)</sup>. In the present paper, we have used three-body potential to explain the elastic properties of Potassium fluoride.

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

Given by Verma and co-workers<sup>(4)</sup> and those for the pressure derivatives of SOE constants are given by Garg et al<sup>(5)</sup> 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  $\alpha_m$  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

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

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

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

With  $n_i$  as the number of electrons in outermost orbit. Here, b and p 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<sup>(9)</sup> and co-workers<sup>(11-19)</sup>. The values of  $\rho_{ij}$  for the rubidium chloride have been taken from Hafemeister and Flygare<sup>(20)</sup>. The values of b for them have been evaluated from the equilibrium condition

$$dW(r) / dr = 0 \quad \text{at } r=r_0 \quad (5)$$

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

$$f(r_0) = f_0 \exp(-r_0/\rho_+) = \epsilon_+ S_+^{-2} \quad (6)$$

$$\text{with } f_0 = A_+ (1 - 2r_+/r_0) \quad (7)$$

Values of overlap integral ( $S_{+-}$ ) and constants ( $A_{+-}$ ) are directly taken from<sup>(14)</sup>. Values of parameters ( $\rho_{ij}$ ,  $b$  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	$r_0$	$r_+$	$r_-$	$C_{11}$ 10 <sup>11</sup> dyne/ cm <sup>2</sup> (a)	$C_{12}$ 10 <sup>11</sup> dyne/ cm <sup>2</sup> (a)	$C_{44}$ 10 <sup>11</sup> dyne/ cm <sup>2</sup> (a)
KF	2.41 10 <sup>-8</sup> cm (a)	2.57 10 <sup>-8</sup> cm (b)	3.07 10 <sup>-8</sup> cm (b)	3.14	1.00	0.66

**Table 3.2: Model Parameters for ionic solids**

CRYSTAL	$\rho$	$b$ (in 10 <sup>-12</sup> erg)	$f(r)$
KF	0.26	0.16	-000016

**Table 3.3: Third order elastic constants (TOECs) 10<sup>11</sup> dyne/cm<sup>2</sup> for ionic crystals.**

Crystal	$C_{111}$	$C_{112}$	$C_{166}$	$C_{123}$	$C_{144}$	$C_{456}$
KF	-2.06	-1.26	-1.36	-1.24	-1.30	-1.14

**Table-3.4: Calculated values of fourth order elastic constants (FOECs) (in 10<sup>11</sup> dyne/cm<sup>2</sup>) for ionic crystals.**

Crystal	$C_{1111}$	$C_{1112}$	$C_{1166}$	$C_{1122}$	$C_{1266}$	$C_{4444}$	$C_{1123}$	$C_{1144}$	$C_{1244}$	$C_{1456}$	$C_{4466}$
KF	32.52	7.92	7.85	8.78	8.88	8.89	8.00	7.17	7.19	7.01	7.01

**Table 3.5: Pressure Derivatives of Second Order Elastic Constants (SOECs) ( $10^8$  dyne /cm<sup>2</sup>).**

Crystal	$dc'_{44}/dp$	$ds'/dp$	$dk'/dp$
KF	1.39	0.50	6.50

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

Crystals	$dc_{111}/dp$	$dc_{112}/dp$	$dc_{116}/dp$	$dc_{123}/dp$	$dc_{144}/dp$	$dc_{456}/dp$
KF	-75.57	-45.68	-43.57	-44.48	-46.16	-44.11

The model parameters listed in Table 3.1 have been used to evaluate the various –order derivatives of the short-range interactions.  $A_i, B_i, C_i, D_i$  ( $i=1, 2$ ). Those parameters are the same as those defined by Verma and co-workers<sup>4</sup> 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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