



## Unified Study of Lattice Dynamic of Potassium Iodide (KI)

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### Abstract

A unified description of a series of Phonon properties of potassium iodide (KI) by means of van der Waals three-body force shell model [VTBFSM] is presented. This model includes van der Waals interactions (VWI) and three-body interactions (TBI) in the framework of both ion polarizable rigid shell model (RSM). The present model has revealed much better descriptions of IR/Raman spectra and anharmonic and other dynamical properties of KI. A comparative study of the dynamical behaviour of KI has also been carried out. Agreement between the theoretical and experimental results, indicate the necessity of the adopted unified approach for the complete description of ionic crystals having NaCl structure. We conjecture that the incorporation of van der Waals interactions is essential for the complete harmonic dynamical behavior of KI.

*Keywords:* Phonons; van der Waal's model; Debye temperature; combined density curve; Raman spectra;

### 1. Introduction

During the last two decades, a considerable interest has been shown by theoretical and experimental workers in the investigation of lattice dynamical behavior of potassium Iodide (KI). This solid is an important member of potassium halides and forms a simple class of ionic solids. The knowledge of phonon dispersion curves (PDC), Debye temperature variation, two phonons IR/Raman spectra, third order elastic constants (TOEC), fourth order elastic constants (FOEC) and the pressure derivatives of second order elastic constants (SOEC) and Cauchy discrepancy (C12-C44) have been of fundamental importance. Due to availability of experimental data on elastic constants (Lewis et al., 1967), dielectric constants (Kittel, 1966), vibrational (Buhrer, 1970; Raunio et al., 1969; Krishnan, 1969; Berg et al., 1957; Potts, 1973) and optical properties (Roberts et al., 1970) of this solid, it is quite interesting and encouraging for theoretical workers to predict its lattice dynamical properties. In the recent past some researchers have studied the lattice dynamics of MC60 compounds in FCC (Face centered cubic) phase by using Rigid Shell Model

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(RSM) (Ranjan, 2005; Ranjan et al., 2005; Singh, 1982). The TOEC, FOEC and the pressure derivatives of SOEC and their experimental values were reported independently by Roberts et al. (1970) and Chang (1965). This has motivated us to incorporate the effects of van der Waals interactions and three-body interactions in the framework of ion polarizable (RSM) with short-range interactions effective up to the second neighbour. Therefore, it may be inferred that the most realistic model for complete harmonic dynamical behaviour of the crystals under consideration can be developed by introducing the effect of van der Waals interactions (VWI) and three-body interactions (TBI) in the framework of RSM. The present model is known as van der Waals three-body force shell model (VTBFSM). This model considers all possible interactions for explaining the harmonic properties of potassium iodide.

## 2. Theory

The essential formalism of VTBFSM is the inclusion of VWI and TBI in the framework of RSM. The interactions system of present model thus consists of long-range screened Coulomb, VWI, three-body interactions and short-range overlap repulsion operative up to the second -neighbor's ions in KI. Looking into the adequacy of the interaction system, the present model may hopefully be regarded as a successful approach for the dynamical descriptions of potassium Iodide. The general form of VTBFSM can be derived from the crystal potential energy per unit cell, given by

$$\Phi = \Phi^C + \Phi^R + \Phi^{TBI} + \Phi^{VWI} \quad (1)$$

Where, First term  $\Phi^C$  is Coulomb interaction potential. This interaction potential is long-range in nature. An ionic crystal can be regarded as made up of positive and negative ions separated by a distance  $|\vec{r}_{ij}|$ , where  $\vec{r}_{ij}$  is a vector joining the ions i and j. According to electrostatic theory, the Coulomb energy of interaction of i-th ion with j-th ion is written as  $\Phi^C(\vec{r}_{ij})$ . Thus, total Coulomb energy for the crystal is

$$\Phi^C(r) = \sum_j' \Phi^C(r_{ij}) = \sum_j' \epsilon_{ij} \frac{e^2}{|\vec{r}_{ij}|}$$

where, the prime means summation over all ions except  $i=j$ ,  $\epsilon_{ij}$  will be +1, if i and j are like ions and -1, if they are unlike. If we consider infinite lattice, the Coulomb potential energy for the whole crystal is given as

$$\Phi^C = \alpha_M \frac{Z^2 e^2}{r_0}$$

Where,  $\alpha_m$  is the Modelung constant and  $r_0$  is the equilibrium nearest neighbors distance. Second term  $\Phi^R$  is short-range overlap repulsion potential. In order to prevent the lattice from collapsing under the Coulomb attraction, there must be the overlap repulsion between the ions. These forces have quantum

mechanical origin and arise when further overlap between neighbouring ions is restricted by the Pauli Exclusion Principle.

The repulsive energy is not so well understood as the Coulomb attraction. The most commonly used analytical expressions for the repulsive energy are given by the inverse and exponential power laws such that

$$\Phi^R(r_{ij}) = ar_{ij}^{-n} \quad (\text{Born Potential}), \quad \Phi^R(r_{ij}) = b \exp.(-r_{ij} / \rho) \quad (\text{B-M Potential})$$

Where, a (or b) and n(orρ) are the Born exponents called the strength and hardness parameters, respectively.

Third term  $\Phi^{\text{TBI}}$  is three-body interactions potential. According to quantum-mechanical theory using Heitler-London approximation, the atomic wave-functions are treated rigidly connected with their nuclei and supposed not to change in a deformation of the lattices. This does not mean that the electron-charge density is sum of charge densities for a system of free-ions. The reason for this lies in the fact that when the ions are put in a lattice their electron wave function overlaps and get deformed. These effects lead to the non-orthogonality of the one electron wave function. This non-orthogonality causes the charge distribution to differ from the sum of the densities for free ions, the differences being more pronounced in the regions where the overlap between the atomic wave-functions is large. As a natural consequence of the anti-symmetry requirement on the wave function (Dolling et al, 1966), this alteration in the electronic charge density causes a charge depletion which depends on the inter nuclear separation and interacts with all other charges via Coulomb force law and gives rise to long-range TBI introduced by (Lowdin., 1947) and (Lundqvist, 1952; 1955; 1957; 1962). This interaction potential is expressed as

$$\Phi^{\text{TBI}} = \alpha_m \frac{Z^2 e^2}{r_0} \left[ \frac{2n}{Z} f(r)_0 \right]$$

Where, the term  $f(r)_0$  is a function dependent on the overlap integrals of the electron wave-functions and the subscript zero on the bracket indicates the equilibrium value of the quantities inside.  $\Phi^{\text{TBI}}$  is also long-range in nature hence it is added to the  $\Phi^{\text{C}}$  and last term  $\Phi^{\text{VWI}}$  is van der Waals interaction potential and owes its origin to the correlations of the electron motions in different atoms.

Using the potential energy expression (1) and introducing the effect of VWI and TBI, the secular determinant is given as

$$\left| \underline{D}(\vec{q}) - \omega^2 \underline{MI} \right| = 0 \quad (2)$$

Here  $\underline{D}(\vec{q})$  is the (6 x 6) dynamical matrix for Rigid Shell model expressed as:

$$\underline{D}(\vec{q}) = (\underline{R}' + \underline{Z}_m \underline{C}' \underline{Z}_m) - (\underline{T} + \underline{Z}_m \underline{C}' \underline{Y}_m) \times (\underline{S} + \underline{K} + \underline{Y}_m \underline{C}' \underline{Y}_m)^{-1} (\underline{T}' + \underline{Y}_m \underline{C}' \underline{Z}_m) \quad (3)$$

The numbers of adjustable parameters have been largely reduced by considering all the short-range interactions to act only through the shells. This assumptions leads to  $\underline{R} = \underline{T} = \underline{S}$ .

Where R, T and S are short ranges forces appear in the form of matrices defined by (Woods et al., 1963).

$$\underline{C}' = \underline{C} + (Z_m^{-2} Z_{r_0} f_0') \underline{Y} \quad (4)$$

Where  $f_0'$  is the first –order space derivative and  $Z_m$  modified ionic polarizability

If we consider only the second neighbour dipole-dipole van der Waals interaction energy, then it is expressed as:

$$\Phi_{dd}^{vw}(r) = -S_v \left| \frac{C_{++} + C_{--}}{6r^6} \right| = \Phi^v(r) \quad (5)$$

Where,  $S_v$  is lattice sum and the constants  $C_{++}$  and  $C_{--}$  are the van der Waals coefficients corresponding to the positive-positive and negative-negative ion pairs, respectively.

By solving the secular equation (2) the expressions derived for elastic constants ( $C_{11}$ ,  $C_{12}$ ,  $C_{44}$ ) corresponding to VTBFMS are follows as:

$$\frac{4r_0^4}{e^2} C_{11} = \left[ -5.112Z_m^2 + A_{12} + \frac{1}{2}(A_{11} + A_{22}) + \frac{1}{2}(B_{11} + B_{22}) + 9.3204 \xi'^2 \right] \quad (6)$$

$$\frac{4r_0^4}{e^2} C_{12} = \left[ 0.226Z_m^2 - B_{12} + \frac{1}{4}(A_{11} + A_{22}) - \frac{5}{4}(B_{11} + B_{22}) + 9.3204 \xi'^2 \right] \quad (7)$$

$$\frac{4r_0^4}{e^2} C_{44} = \left[ 2.556Z_m^2 + B_{12} + \frac{1}{4}(A_{11} + A_{22}) + \frac{3}{4}(B_{11} + B_{22}) \right] \quad (8)$$

In view of the equilibrium condition  $[(d\Phi/dr)_0=0]$  we obtain

$$B_{11} + B_{22} + B_{12} = -1.165 Z_m^2 \quad (9)$$

Where  $Z_m^2 = Z^2 \left( 1 + \frac{12}{Z} f_0 \right)$  and  $\xi'^2 = Zr_0 f_0'$  (10)

The term  $f_0$  is function dependent on overlap integrals of electron wave functions. Similarly, expressions for two distinct optical vibration frequencies ( $\omega_L$  and  $\omega_T$ ) are obtained as:

$$\left( \mu \omega_L^2 \right)_{q=0} = R'_0 + \frac{(Z'e)^2}{Vf_L} \frac{8\pi}{3} \left( Z_m^2 + 6\xi'^2 \right) \tag{11}$$

$$\left( \mu \omega_T^2 \right)_{q=0} = R'_0 - \frac{(Z'e)^2}{Vf_T} \frac{4\pi}{3} Z_m^2 \tag{12}$$

Where the abbreviations reported by Singh (1982) stand for

$$R'_0 = R_0 - e^2 \left( \frac{d_1^2}{\alpha_1} + \frac{d_2^2}{\alpha_2} \right); Z' = Z_m + d_1 - d_2$$

$$R_0 = \frac{Z^2 e^2}{V} (A_{12} + 2B_{12})$$

$$f_L = 1 + \left( \frac{\alpha_1 + \alpha_2}{V} \right) \frac{8\pi}{3} \left( Z_m^2 + 6\xi'^2 \right)$$

$$f_T = 1 - \left( \frac{\alpha_1}{V} \right) \frac{4\pi}{3} \left( Z_m^2 \right)$$

Where  $\alpha_1, \alpha_2$  electrical polarizabilities and  $Y_1, Y_2$  are shell charge parameters of positive and negative ions.

$$d_1 = \frac{-\alpha_1 R_0}{e^2 Y_1} \quad d_2 = \frac{-\alpha_2 R_0}{e^2 Y_2} \quad \text{and } V = 2r_0^3 \text{ (Unit cell volume for NaCl type lattice)}$$

by solving the dynamical matrix along [.5, .5, .5] directions at L-Point modified expressions for  $\omega_{LO}(L), \omega_{TO}(L), \omega_{LA}(L), \text{ and } \omega_{TA}(L)$  are as follows:

$$m_2 \omega_{LO}^2(L) = R_0 + [(e^2/V) (2A_{22} + B_{22})] + [(e^2/V) Z_m^2 C'_{1L}] \tag{13}$$

$$m_1 \omega_{LA}^2(L) = R_0 + [(e^2/V) (2A_{11} + B_{11})] + [(e^2/V) Z_m^2 C'_{1L}] \tag{14}$$

$$m_2 \omega_{TO}^2(L) = R_0 + [(e^2/2V) (A_{22} + 5B_{22})] + [(e^2/V) Z_m^2 C'_{1T}] \tag{15}$$

$$m_1 \omega_{TA}^2(L) = R_0 + [(e^2/2V) (A_{11} + 5B_{11})] + [(e^2/V) Z_m^2 C'_{1T}] \tag{16}$$

Where

$$\left. \begin{aligned}
 C'_{1L} &= \left[ \underline{C} + Zr_0 f_0 Z^{-2}_m \underline{V} + Z^2 Z^{-2}_m \underline{D} \right]_{xx} \\
 C'_{1T} &= \left[ \underline{C} + Zr_0 f_0 Z^{-2}_m \underline{V} + Z^2 Z^{-2}_m \underline{D} \right]_{yy}
 \end{aligned} \right\} \quad (17)$$

$\underline{C}$  and  $\underline{V}$  is Coulomb and three body force matrices evaluated at L-Point and  $\underline{D}$  is van der Waals contribution. We have used the further expressions for the TOEC, FOEC and pressure derivatives of SOEC and TOEC derived by (Roberts et al., 1970).

Debye's model define the frequency distribution function which is given by

$$\Theta_D = hv_m/K \quad (18)$$

To determine the combined density of states for each polarization is given by

$$D(\omega) = dN/d\omega = (VK^2/2\pi^2) \cdot dK/d\omega \quad (19)$$

Where  $N = (L/2\pi)^3 (4\pi K^3/3)$ ,  $K$  is wave vector and  $L^3=V$ .

### 3. Results and Discussion

The input data and calculated model parameters experimental and theoretical of KI are listed in table 1. We have computed phonon dispersion frequencies for the allowed 48 non - equivalent wave vectors in the first Brillouin zone by using our model parameters. We present the phonon dispersion curves [PDC] only along the three principal symmetry directions Fig. 1. Our phonon dispersion curves for KI agree well with the measured data reported by (Buhner., 1970). It is evident from that our predictions using present model VTBFM are better than those by using other models (Karo et al., 1963; Lynch, 1967).

**Table 1. Input data and model parameters for KI**

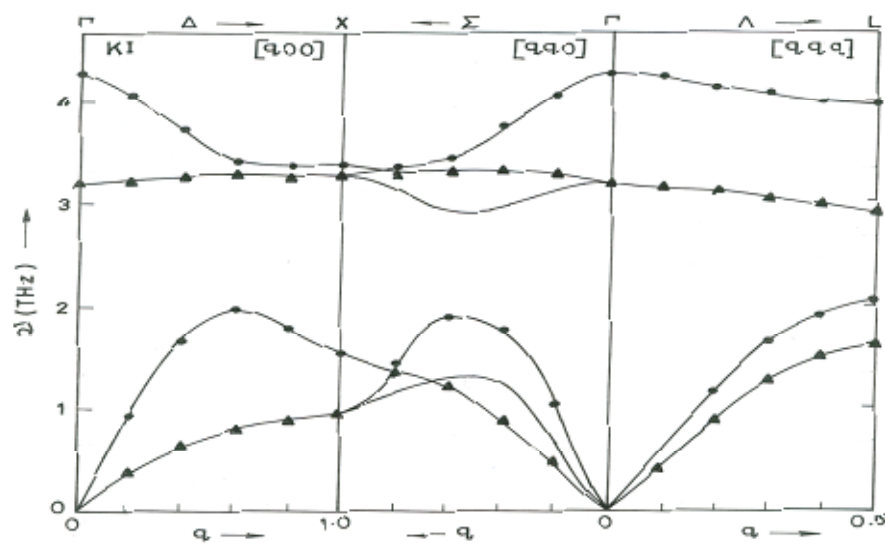
Input data		Model Parameters	
Parameters	Value	Parameters	Value
$C_{11}$ ( $10^{11}$ dyn/cm <sup>2</sup> )	3.380 <sup>[c]</sup>	$A_{12}$	20.6045
$C_{12}$ ( $10^{11}$ dyn/cm <sup>2</sup> )	0.220 <sup>[c]</sup>	$B_{12}$	-3.7923
$C_{44}$ ( $10^{11}$ dyn/cm <sup>2</sup> )	0.368 <sup>[c]</sup>	$A_{11}$	-1.8612
$\nu_L$ (THz)	4.260 <sup>[d]</sup>	$B_{11}$	-2.0391
$\nu_T$ (THz)	3.210 <sup>[d]</sup>	$A_{22}$	3.8319
$r_0$ ( $10^{-8}$ cm)	3.492 <sup>[e]</sup>	$B_{22}$	-1.6938
$\alpha_1$ ( $10^{-24}$ cm <sup>3</sup> )	1.370 <sup>[a]</sup>	$d_1$	0.0452
$\alpha_2$ ( $10^{-24}$ cm <sup>3</sup> )	5.310 <sup>[a]</sup>	$d_2$	0.1855
$C^{++}$ ( $10^{-60}$ erg cm <sup>6</sup> )	64.90 <sup>[b]</sup>	$Y_1$	-4.7047
$C^{--}$ ( $10^{-60}$ erg cm <sup>6</sup> )	1090 <sup>[b]</sup>	$Y_2$	-4.4489
		$r_0 f_0'$	-0.0409

*a-* (Lowdin, 1947); *b-* (Lundqvist, 1952; 1955; 1957; 1961); *c-*(Woods et al., 1963); *d-* (Karo et al., 1963); *e-* (Lynch,1967)

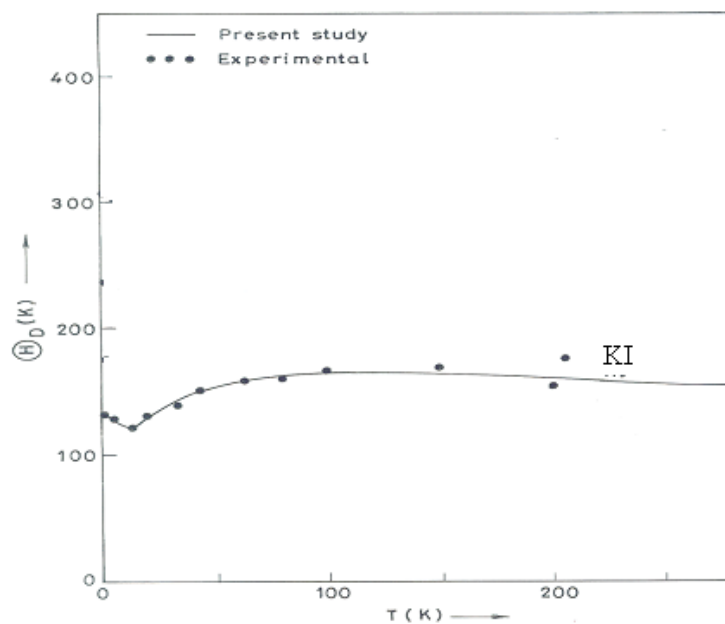
In the present study the variation of Debye temperatures ( $\Theta_D$ ) at different temperatures T have also been calculated and curve has been plotted along with available experimental data (Berg et al., 1957) in Fig 2. Though, the agreement is better with our model, still, there is slight discrepancy between theoretical and experimental results at higher temperatures.

At high temperatures lattice instability develops in which above a certain critical temperature the vibrational and static pressures cannot balance each other at any volume. It is argued that this instability plays a role in causing solids to melt. Anharmonic corrections tend to rise at critical temperatures by about 20%. Debye's theory agrees very well with experiment, especially at low temperatures, because at low temperature and at high temperature it is almost exact. Lattice imperfections are not an important factor for temperatures up to about 90% of the melting temperature.

The present model is also capable to predict the two phonon Raman/IR spectra. The results of these investigations from combined density states (CDS) approach have been shown in figure 3 which shows that the agreement between experimental data (Raunio, 1963; Krishnan, 1969) and our theoretical peaks is generally good for both two phonon Raman/IR spectra for KI.



**Fig-1 Phonon dispersion curve for KI**  
 Experimental points: ● Longitudinal; ▽ Transverse; — Present study



**Fig -2 Debye Temperature Variation of KI**



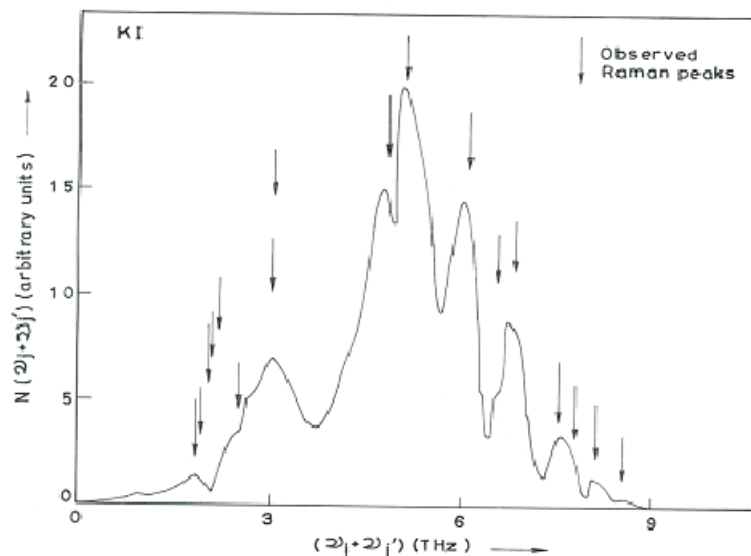


Fig-3 Combined density of States Curve for KI

The assignment made by the critical point analysis, the present study has been listed in Table 2. The interpretation of Raman / IR spectra achieved from both CDS approach and critical point analysis is quite satisfactory.

However, our results are closer to their experimental values reported independently by (Roberts, 1965) and (Chang et al., 1966). To sum up, we can say that the inclusion of VWI and TBI are essential for the description of lattice dynamics of potassium halides (Sharma, 1979). As such this model has been more successfully applied to other alkali halides (Garg et al., 1977; Narwood et al., 1958; Iona, 1941; Heitler et al., 1927; Kushwala et al., 1980; Mohan et al., 1993; Srivastava et al., 2004, 2010).

#### 4. Discussion

In addition of Cauchy discrepancy, and shell model in contrast of used model VTBFMSM is based on more realistic account of the long range interactions by including the contribution of the three-body forces, whose existence in ionic crystals is well founded. There is, however, an important difference between shell model and our model that in shell model the value of  $Z$  less than 1 but in my model value of  $Z$  greater than 1. This model has also predicted zero splitting of optical branches at X-point.

By solving the secular eq. (2) along  $[q\ 0\ 0]$  direction and subjecting the short- and long- range coupling coefficients to the long-wavelength limit, the expression for zone centre optical vibration frequencies are obtained by the phonon anomalies in the longitudinal optical branch along the

(qoo) and (qqo) directions. However our predictions using present model VTBFMSM are better than those by using other models (Garg et al., 1977; Narwood et al., 1958; Iona, 1941; Heitler et al., 1927). The assignment made by the critical point analysis, the present study has been listed in Table 2. The interpretation of Raman / IR spectra achieved from both CDS approach and critical point analysis is quite satisfactory.

**Table 2. Assignment of two phonon Raman and Infra-red peaks for KI**

CDS Peaks (cm <sup>-1</sup> )	Raman Active				Infra-red Active	
	Observed* Peaks (cm <sup>-1</sup> )		Present Study		Present Study	
			Assignments	Values (cm <sup>-1</sup> )	Assignments	Values (cm <sup>-1</sup> )
32			LO-TO(L)	33		
64	64 <sup>a</sup>	65 <sup>b</sup>	2TA(X)	63		
84	85 <sup>a</sup>		LA+TA(X) LO-TA( $\Delta$ )	83 86	LA+TA( $\Delta$ )	93
92	96 <sup>a</sup>	91 <sup>b</sup> 92 <sup>b</sup>	LA+TA( $\Delta$ )	93		
101	101 <sup>a</sup>	101 <sup>b</sup>	2LA(X)	104		
163		163 <sup>b</sup>	TO+LA(X)	140	TO+LA( $\Delta$ )	165
170	170 <sup>a</sup>		LO+LA( $\Delta$ )	180		
200	200 <sup>a</sup>					
220		219 <sup>b</sup>	2TO( $\Delta$ )	220	2TO( $\Delta$ )	220
226		228 <sup>b</sup>	2LO( $\Delta$ )	227	2LO( $\Delta$ )	227
254	250 <sup>a</sup>	256 <sup>b</sup>	2LO(L)	260		
270		271 <sup>b</sup>				
284		284 <sup>b</sup>	2LO( $\Gamma$ )	284		

*a* – (Krishnan, 1969); *b* – (Potts et al., 1973)

It is interesting to note our results on TOEC, FOEC and the pressure derivatives of SOEC are generally better than those of others (Potts et al., 1973; Roberts, 1973) as evident from Table 3.

To sum up, we can say that the inclusion of VWI and TBI are essential for the description of lattice dynamics of potassium halides (Lynch, 1967; Sharma, 1979; Garg et al., 1977; Narwood, 1958; Iona, 1941). We have also investigated the anharmonic properties of KI by use of this model.

**Table 3. TOEC and FOEC ( $10^{12}$  dyn/cm<sup>2</sup>), pressure derivatives of SOEC and TOEC (dimensionless) and Cauchy discrepancy (in  $10^{12}$  dyn/cm<sup>2</sup>) for KI.**

Property	KI	Property	KI		Property	KI
	Present		Present	Expt.		Present
C <sub>111</sub>	-5.339	dk <sup>1</sup> /dp	5.087	5.470 <sup>a</sup>	C <sub>112</sub> -C <sub>166</sub>	0.46835
C <sub>112</sub>	-0.336	ds <sup>1</sup> /dp	5.571	6.030 <sup>a</sup>	C <sub>123</sub> -C <sub>456</sub>	-0.02650
C <sub>123</sub>	0.058	dc <sup>1</sup> <sub>44</sub> /dp	-0.610	-0.244 <sup>a</sup>	C <sub>144</sub> -C <sub>456</sub>	-0.00883
C <sub>144</sub>	0.076	dc <sup>1</sup> <sub>111</sub> /dp	30.765		C <sub>123</sub> -C <sub>144</sub>	-0.01767
C <sub>166</sub>	-0.124	dc <sup>1</sup> <sub>112</sub> /dp	0.075		C <sub>1112</sub> -C <sub>1166</sub>	-1.58388
C <sub>456</sub>	0.085	dc <sup>1</sup> <sub>166</sub> /dp	1.055		C <sub>1122</sub> -C <sub>4444</sub>	-5.54924
C <sub>1111</sub>	1.884	dc <sup>1</sup> <sub>123</sub> /dp	0.678		C <sub>1123</sub> -C <sub>1144</sub>	0.06225
C <sub>1112</sub>	2.534	dc <sup>1</sup> <sub>144</sub> /dp	-1.038		C <sub>1123</sub> -C <sub>1244</sub>	0.53561
C <sub>1166</sub>	0.984	dc <sup>1</sup> <sub>456</sub> /dp	0.989		C <sub>1123</sub> -C <sub>1456</sub>	0.56633
C <sub>1122</sub>	-1.046				C <sub>1123</sub> -C <sub>4466</sub>	-0.41042
C <sub>1266</sub>	0.482				C <sub>1122</sub> -C <sub>1266</sub>	-4.61456
C <sub>4444</sub>	1.503					
C <sub>1123</sub>	0.350					
C <sub>1144</sub>	0.288					
C <sub>1244</sub>	-0.185					
C <sub>1456</sub>	-0.215					
C <sub>4466</sub>	0.760					

a- (Roberts et al., 1970)

## 5. Conclusion

From the above discussion, it may be concluded that our model provides a good agreement between theoretical and experimental results. Therefore, it may be inferred that the inclusion of van der Waals interaction is very essential for the complete description of the phonon dynamical behavior of crystal structure.

- The calculated phonon dispersion curves (In Fig.1) after inclusion of van der waals interaction have improved the agreement between experimental data (Buhrer, 1970) and our calculated results.
- Another striking feature of present model is noteworthy from the excellent reproduction of almost all branches hence the prediction of (PDC) for KI using (VTSM) may be considered more satisfactory than from other models (Singh,1982).
- It is evident from Fig.2 our results for Debye temperature curve is good with measured experimental data (Berg et al.,1957) and generally better than of breathing shell model (BSM).
- The combined density of states for KI has plotted in Fig.3 the basic aim of the study of two phonon IR/Raman scattering spectra is to correlate the neutron and optical experimental data of KI .
- We have also investigated the anharmonicity properties of KI by using VTBFMS this includes the predictions of third and fourth order elastic constants.
- In this paper for (KI) we have systematically reported phonon dispersion curves, Debye temperature, combined density of states and anharmonicity property of KI .on the basis of overall fair agreement , it may be concluded that the present model van der waals three body force shell model (VTBFMS) is adequately capable to describe the crystal dynamic of KI.

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