

Pressure Induced Structural Phase Transition, Metallization and Superconductivity in KI

Y. Ramola¹, C. Nirmala Louis^{1,*}, A. Amalraj²

¹Research Center of Physics, Holy Cross College, Nagercoil, Tamil Nadu, India

²Associate Professor of Chemistry, St. Jerome's College, Anandhanadarkudy, KK District, Tamil Nadu, India

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Abstract The self-consistent band structure calculation for potassium iodide (KI) performed both in NaCl and CsCl structures using the full potential linear muffin-tin orbital (FP-LMTO) method is reported. The equilibrium lattice constant, bulk modulus and the phase transition pressure at which the compound undergoes structural phase transition from NaCl to CsCl are predicted from the total energy calculations. The band structure, density of states (DOS), electronic charge distributions, metallization and superconducting transition temperature (T_c) of KI are obtained as a function of pressure for both in NaCl and CsCl structures. The density of states at the Fermi level ($N(E_F)$) gets enhanced under pressure, which leads to metallization in KI. It is found that, the charge transfer from s and p states to d state causes structural phase transition and superconductivity in KI. The pressure corresponding to structural phase transition from NaCl structure (B1) to the CsCl structure (B2) is 0.02 Mbar in KI. This value is agreement with the experimental value of 0.019 Mbar. In KI, the metallization occurs through indirect closing of the band gap between Γ and H points at the reduced volume $V/V_0=0.43$ (CsCl structure), the corresponding metallization pressure is 1.228Mbar. Our results completely agree with the experimental observation of 1.31 Mbar. The highest T_c estimated is 2.151 K and the corresponding pressure is 4.945 Mbar in the NaCl structure and 0.107 K in the CsCl structure.

Keywords Band Structure, Metallization, Structural Phase Transition, KI, High Pressure Superconductivity

1. Introduction

Currently there is lot of interest in the study of structural changes and phase stability of materials under pressure [1,2]. Geologists have investigated the behavior of materials under pressure for observing the physico-chemistry of materials near the center of the earth [3,4]. The physical properties of

materials undergo variety of changes when they are subjected to high pressure. With the development of high pressure experimental techniques, research on pressure-induced structural phase transition, insulator – metal transition and superconducting transition are getting the attention of all [4-10]. Various groups of scientists are pursuing this type of work. Systems like Oxygen [5], CsI [3], SnI_4 [7], Selenium [8], Phosphorous [9] and Vanadium [10] are investigated under high pressure and these materials are found to become superconductors at very high pressures. In particular, there is a great interest in the pressure induced insulator – metal transition and superconductivity of simple alkali halides. The alkali iodide KI which crystallizes in NaCl structure under ambient conditions is of great physical interest; since it find application in manufacture of opto-electronic devices and serve as a typical model for other ionic compounds [11]. About twenty new elemental superconductors have already been found at high pressure and this number is increasing [3]. In this list now compounds are being included. One of such compounds is simple ionic salt CsI. This material is a testing ground both for new ideas about compressed matter and new techniques for photo converters [3]. The metallization in CsI is experimentally achieved by Vohra [12]. But Eremets [3] could experimentally find the evidences for the metallization and superconductivity of CsI at high pressure. The ionic salt CsI is a metal under high pressure and as the pressure increases superconductivity sets in CsI [13]. The metallization in CsI is experimentally achieved by Vohra [12]. But Eremets [3] could experimentally find the evidences for the metallization and superconductivity of CsI at high pressure. In KI, Weir et al [11] experimentally reported the structural phase transition and metallization. Experimentally, the metallization pressure of KI as 1.31 Mbar and structural phase transits from NaCl to CsCl structure as 0.019 Mbar [11]. On the theoretical side, the band structure results are used in analyzing metallization and superconductivity of ionic insulators [14]. The metallization of KI under pressure was predicted first by Aidun et al [15] and then by Satpathy et al [16]. Later Asokamani et al [17] predicted metallization in the KI under

high pressure. It is felt that many uncertain parameters are involved in these calculations and further theoretical studies are needed [18-24]. It is also suggested that it would be interesting and useful if one investigates the pressure dependence of T_c which has been observed experimentally [11]. It was felt that many disagreements exist between theory and experiment [13] in the prediction of lattice constant, band gap, phase transition, metallization and superconductivity of KI and this necessitated further theoretical studies in this system. In the present paper, we give more extensive discussion about the band structure, density of states and electronic charge distributions as a function of reduced volume. The structural phase transition, stability of the phases, equilibrium bulk modulus, metallization and superconductivity are reinvestigated and critically analyzed. The pressure dependence of the band gap and enthalpy calculations is performed at various high pressures. We give the details of the calculational procedure and electronic band structure corresponding to various pressures in Section 2. In Section 3, the ground-state properties, structural phase transition and metallization are discussed. Concluding remarks are given in Section 4.

2. Band Structure and Density of States

2.1. Calculational Procedure

Potassium iodide crystallizes in rocksalt structure under ambient conditions and undergo structural phase transition from NaCl to CsCl structure [25]. The electronic band structure calculations were performed for KI corresponding to different reduced volumes both in NaCl to CsCl structures, by the first-principle linear muffin-tin orbital (FP-LMTO) method [25]. We have used FP-LMTO method with generalized gradient approximation (GGA) [1,2]. It is based on the idea that one electron states of solids can be written as combinations of a small number of states of the constituent atoms. Also the crystal potential is approximated by a series of non-overlapping atomic like spherically symmetric potentials and a constant potential between the spheres. This method has the advantage that the theory and the result are very easy to understand. For this reason most results of the electronic structures computed are interpreted in the light of full potential theory [26]. This full potential model assumes the solution to the time-independent single electron Schrödinger equation Ψ is well approximated by a linear combination of atomic orbitals. In this linear method, functions constructed from partial waves and their first energy derivatives obtained within the muffin-tin approximation are used as fixed basis. The chemical content of this technique acts as a guide to the non-specialist who wants to perform band structure calculations of his own. The problem of electronic structure involves the computation of eigen states for an infinite number of interacting electrons. This leads to the estimation called one electron approximation, which describes each electron as an

independent particle moving in the mean field of the other electrons plus the field of the nuclei [26]. By standard variation technique one can obtain a set of linear equations, in terms of the Hamiltonian \underline{H} and overlap \underline{O} matrices to determine the eigen values \underline{E} and the expansion coefficients \underline{a} . Here the one electron energies are found by a single diagonalisation of the secular matrix $(\underline{H} - \underline{E}\underline{O})$ [1,2].

We give here only the calculational details. The electronic configurations of K and I are $[\text{Ar}] 4s^1$ ($Z=19$) and $[\text{Kr}] 4d^{10} 5s^2 5p^5$ ($Z=53$). The valence electronic configurations chosen in our calculations are $3p^6 4s^1$ for K and $5s^2 5p^5$ for I. There are 14 valence electrons contributing to the valence bands [14]. The final energy convergence is within 10^{-5} Ry. The calculated total energies were fitted to Murnaghan's equation of state (EOS) [2], to determine the bulk modulus and pressure derivative of bulk modulus B_0' . We have obtained,

- (i) normal pressure band structure and density of states of KI (with NaCl structure),
- (ii) high pressure band structure and density of states of KI (with CsCl structure),

Also, we have analyzed the structural phase transition from NaCl to CsCl structure and metallization. The radii of the Wigner-Seitz sphere are chosen according to the criterion for charge transfer from cation to the anion [13]. The entire Brillouin zone is partitioned into 4096 cubical volume elements and $E(k)$ are computed for the k -points located at the center of each volume element. But because of the symmetry considerations this involves only 145 k points for NaCl structure and 165 k -points for KI in CsCl structure, which are uniformly distributed in the 1/48-th of the first Brillouin zone [14]. The calculated total energies are fitted to Murnaghan's equation of state (EOS) [25], to determine the pressure derivative of bulk modulus B_0^1 , phase-transition pressure and other ground-state properties [17,18]. The bulk modulus is a property of the material which defines its resistance to volume change when compressed. The cause for phase transition and the relation between phase transition pressure and atomic radii are deduced from band structure investigation [26-31].

2.2. Band Structure and Density of States of KI under Pressure

The band structures and density of states for KI is computed for various reduced volumes ranging from $V/V_0=1.0$ to 0.3 in steps of 0.05 (Figures 1 to 4). But here we have presented the density of states and band structures along the symmetry directions L- Γ -X-W- K- Γ corresponding to volume compressions $V/V_0=1.0$ and $V/V_0=0.43$ for KI only (Figures 1 and 2). In the bottom of the valence band, a triple band is due to $3p^6$ electrons of potassium and the single band is due to $5s^2$ electrons of iodine (Figures 1 and 2). Below the

Fermi level, the three bands appearing due to the $4s^1$ electrons of potassium and $5p^5$ electrons of iodine (Figure 1). The $5p$, $5d$ states of iodine and $3d$, $4s$ states of potassium produces the empty conduction bands above the Fermi level (Figure 1). The direct band gap at normal pressure is found to be 5.984eV for KI (at Γ point). The increase in the width of the valence band and conduction band due to high pressure, leads to the narrowing of the band gap and finally metallization in KI at $V/V_0=0.43$ ($P_M = 1.228$ Mbar) (Figure 2 and Table.1). Metallization occurs via indirect closing of band gap between Γ and H points (Figure 2). There is appreciable value for density of states at Fermi

energy $N(E_F)$ at the metallization pressure. We have given the DOS histograms of KI corresponding to normal pressure (Figure 3) and metallization pressure (Figure 4). At normal pressure (Figure 3), the long spike near the origin is due to $3p^6$ electrons of K. The short spike near the origin is due to the levels arising from $5s^2$ electrons of I. The short spike near the Fermi energy is due to $5p^5$ electrons of I and $4s^1$ electron of K. The $5p$ and $5d$ state of I and $4p$ and $4d$ state of K produces the short peaks above the Fermi energy E_F . The width of the valence band and the empty conduction band get widened, as the pressure increases. These changes lead to the closing of the band gap under pressure (Figure 4).

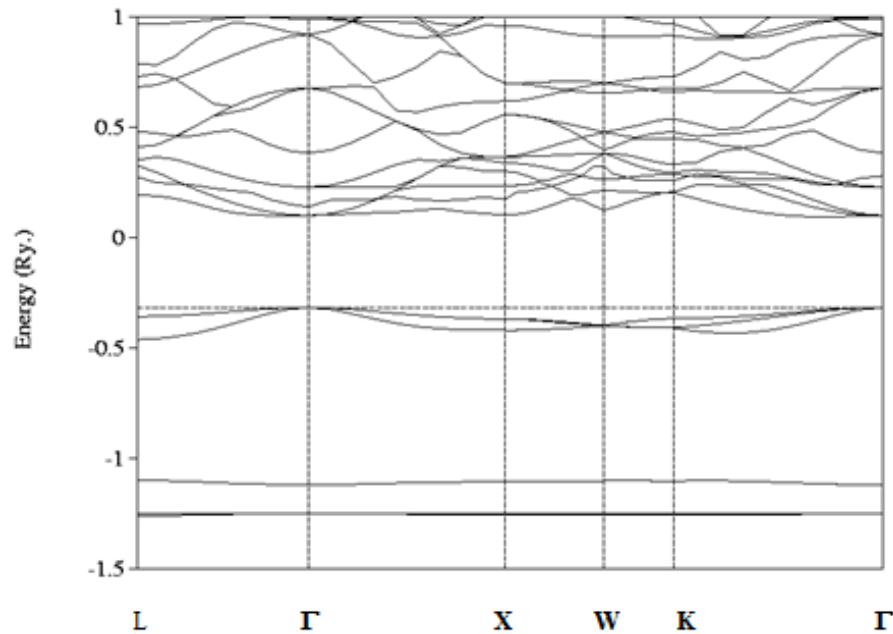


Figure 1. Normal pressure band structure of KI (NaCl structure)

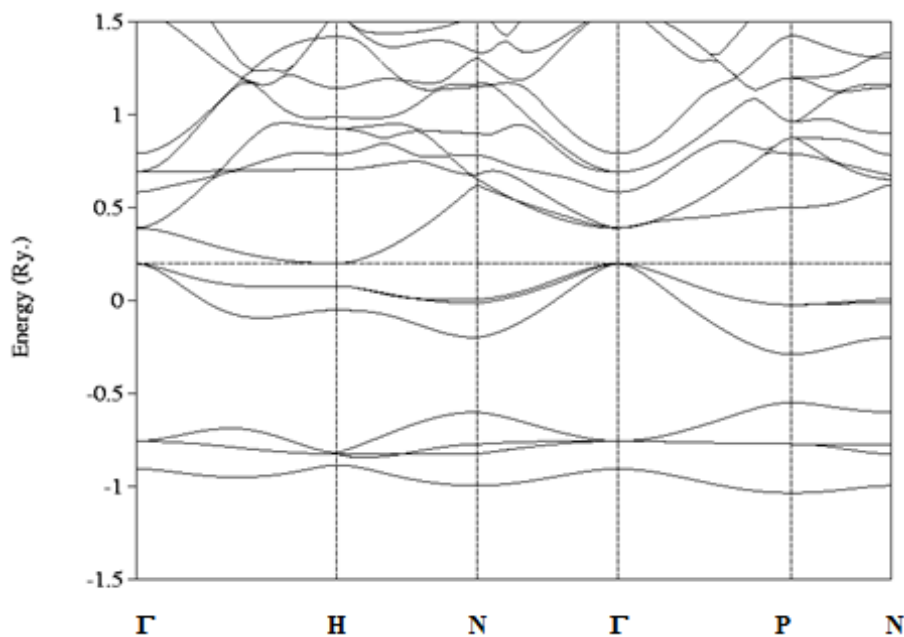


Figure 2. Metallization pressure band structure of KI (CsCl structure)

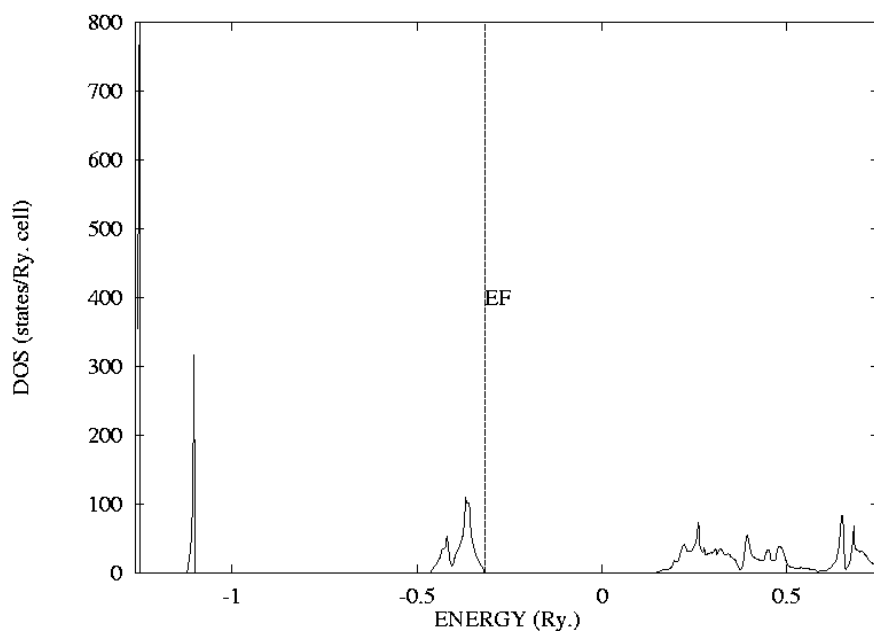


Figure 3. Normal pressure density of states of KI (NaCl structure)

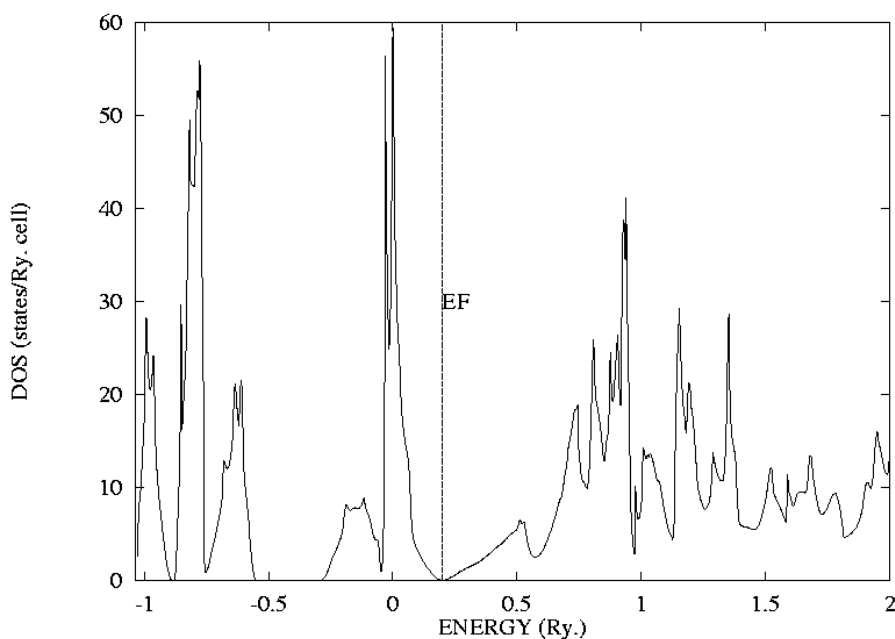


Figure 4. Metallization pressure Density of states of KI (CsCl structure)

Table 1. Equilibrium lattice constant , bulk modulus and band gap

Compound	Present work			Experiment [11]			Previous theory [30]		
	a_0 a.u	B_0 Mbar	E_g eV	a_0 a.u	B_0 Mbar	E_g eV	a_0 a.u	B_0 Mbar	E_g eV
KI	13.406	0.115	5.984	13.356	0.116	6.00	13.056	0.148	5.307

When pressure increases (reduced volume decreases)the value of the DOS at Fermi energy, E_F ($N(E_F)$) increases [2].The normal pressure DOS trend is changed under high pressure. The increase of pressure leads to the broadening of

bands and decrease of density of states value in most of the energy regions. It also increases the width of the valence band and empty conduction bands [1, 2]. When pressure increases, the value of E_F increases, whereas no density of

states is available at the Fermi level up to metallization pressure. Further increase in pressure leads to enhanced density of states at the Fermi level which induces superconductivity [4].

3. Results and Discussion

3.1. Ground State Properties

From the total energies obtained from our calculation, the ground state properties and structural phase transition of KI is studied. Relation connecting reduced volume and lattice constant of KI is given in Figure 5. In this figure, when the volume decreases lattice constant also decreases. Relation connecting reduced volume and pressure of KI is given in Figure 6. In this figure, when the volume decreases pressure increases. Relation connecting lattice constant and pressure of KI is given in Figure 7. In this figure, when the lattice constant decreases pressure increases. The total energy versus reduced volume curve is given in Figure 8. The total energy is calculated as a function of reduced volume (V/V_0)

for both NaCl and CsCl phases of KI. Here, V_0 is the experimental equilibrium volume corresponding to the experimental equilibrium lattice constant. The calculated total energies were fitted to Murnaghan's equation of state [1]

$$P = 1.5B_0 \left[\left(\frac{V_0}{V} \right)^{7/3} - \left(\frac{V_0}{V} \right)^{5/3} \right] \left[1 + 0.75 (B_0 - 4) \left\{ \left(\frac{V_0}{V} \right)^{2/3} - 1 \right\} \right] \quad (1)$$

to obtain the pressure derivative of bulk modulus B_0' [2]. The calculated reduced volumes, lattice constant and pressure values of KI for different pressure are given in Figures 5, 6 and 7 respectively. The equilibrium lattice constant, bulk modulus and band gap values are given in Table.1 along with experimental [11] and previous theoretical values [30]. From the total energy as a function of reduced volume curve (Figure 8), it is found that, in KI, up to $V/V_0 = 0.875$ ($P_T = 0.02$ Mbar), NaCl structure has the lowest energy and on further reduction of volume CsCl structure becomes more stable in energy than the NaCl structure (Table 2).

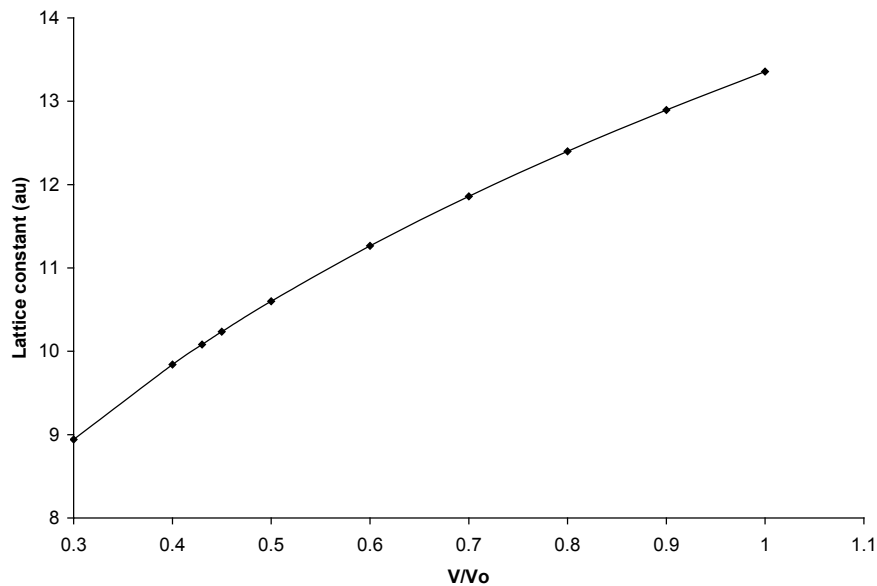


Figure 5. Relation connecting reduced volume and lattice constant of KI

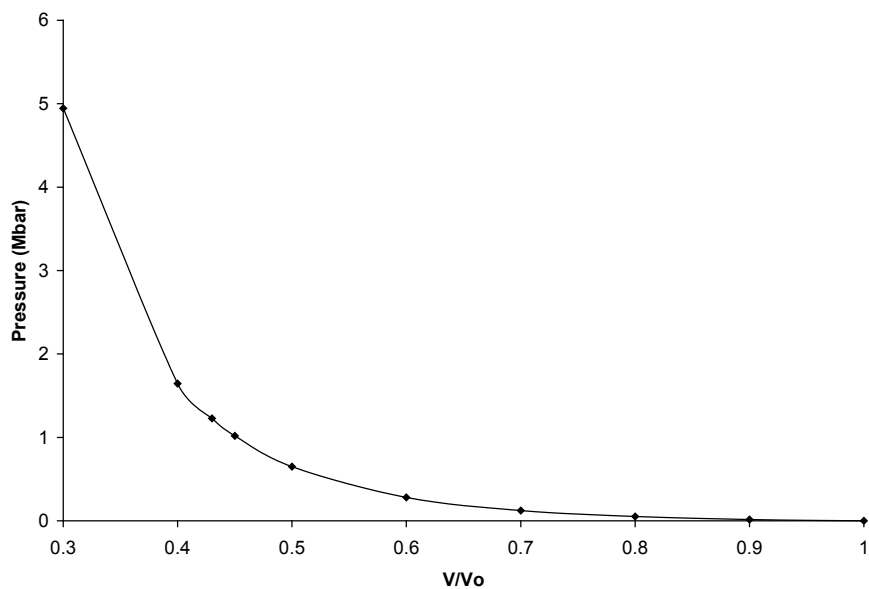


Figure 6. Relation connecting reduced volume and pressure of KI

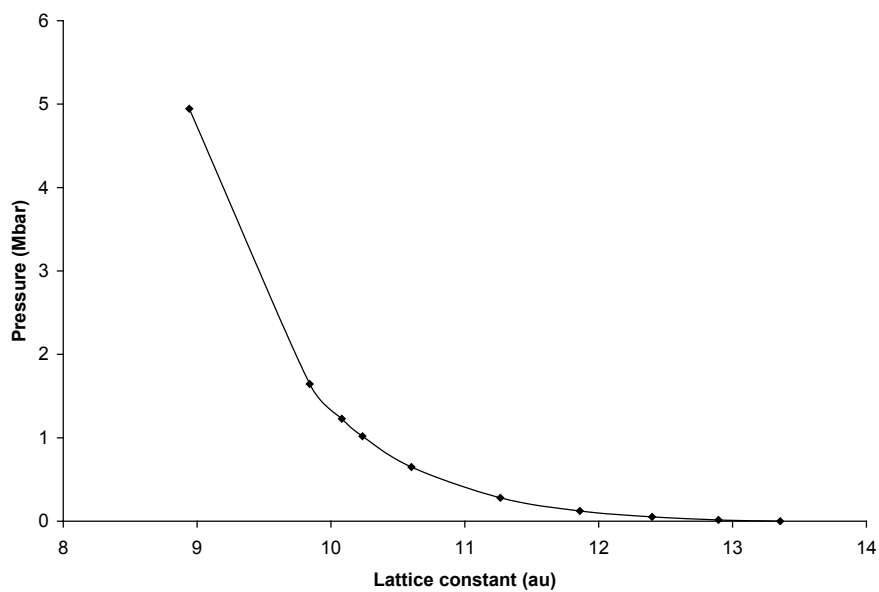


Figure 7. Relation connecting lattice constant and pressure of KI

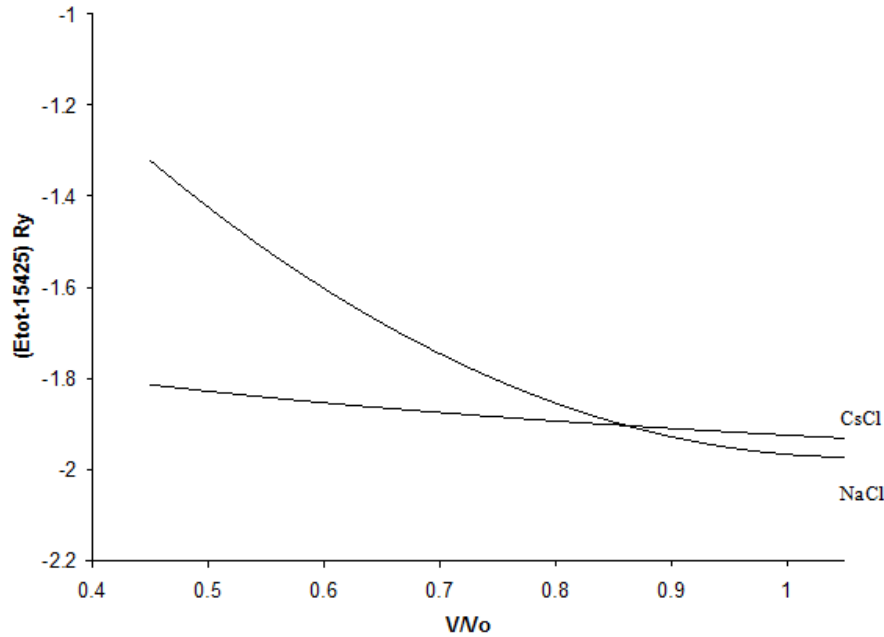


Figure 8. Relation connecting reduced volume and total energy of KI

Table 2. Metallization and phase transition pressures in KI

Alkali iodide	Metallization		Phase transition	
	P M Mbar	(V/Vo) M	P T Mbar	(V/Vo) T
KI	1.228	0.430	0.02	0.875

3.2. Structural Phase Transition

At ambient pressure KI is in the NaCl structure. The phase stability of the B1 (NaCl) and B2 (CsCl) structures of KI is analyzed using the enthalpy calculation [17,18]. The enthalpy $H(P)$ is defined by

$$H(P) = E_{\text{tot}}(P) + PV(P) \quad (2)$$

where $E_{\text{tot}}(P)$ is the total energy of KI as a function of pressure P and V is the volume of KI at pressure P .

The transition pressure corresponding to the phase transition from B1 to B2 is obtained from the relation

$$H_{B1}(P) = H_{B2}(P) \quad (3)$$

where H_{B1} and H_{B2} are the enthalpies of the B1 and B2 phases respectively. The pressure versus enthalpy curve for KI is given in Fig.9. From the enthalpy calculation, the phase transition pressure ($P_T=0.02$ Mbar) and the corresponding reduced volume ($(V/Vo)_T = 0.875$) are estimated for KI (Table.2). Our calculated phase transition pressure of KI supports the experimental value of 0.019 Mbar [11]). The mechanism for the phase transition is a geometric effect involving a change in the coordination number from 6 in the NaCl phase to 8 in the CsCl phase [30].

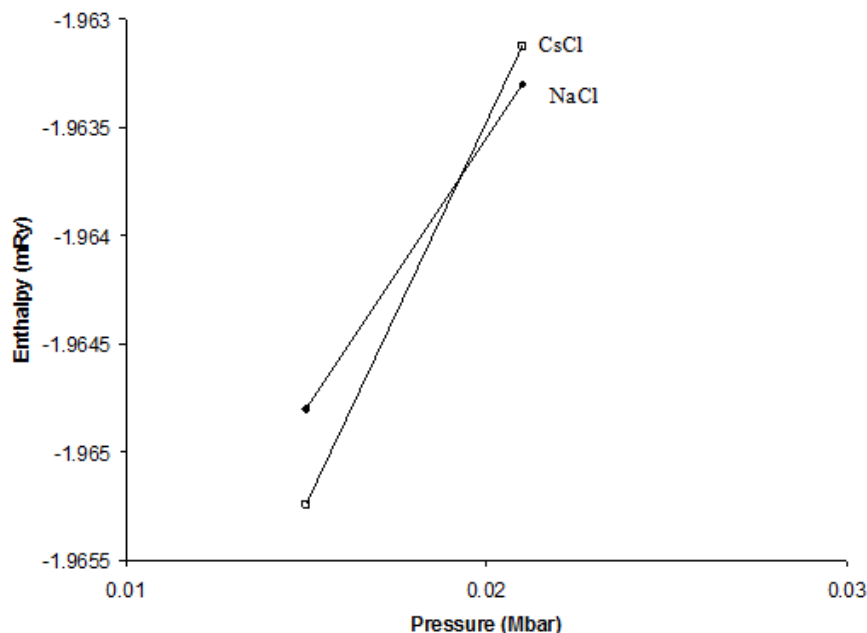


Figure 9. Relation connecting pressure and enthalpy of KI

Table 3. Metallization pressure for KI

Compound	Lattice constant a.u	Present study		Experiment [11]		Previous theory[30]	
		$(V/V_0)_M$	P_M Mbar	$(V/V_0)_M$	P_M Mbar	$(V/V_0)_M$	P_M Mbar
KI	13.356		1.228	0.424	1.31	0.350	1.549

3.3. Metallization

The electronic band structure calculations on alkali halides suggest that the insulator – metal transitions are due to the reordering of the energy bands [11] with the empty d-like band dropping in energy below the top of the filled p-like bands. We felt that it would be interesting to investigate the pressure dependence of metallization and superconductivity in ionic solid KI. At normal pressure, KI is a direct band gap insulator [17]. The band gap decreases with the increase of the pressure and at a particular pressure, there is a closing of the band gap. The band structure corresponding to metallization of KI is shown in Figure 2. In KI, the metallization occurs through indirect closing of the band gap between Γ and H points (Figure 2). In KI, closure of the band gap takes place at the reduced volume $V/V_0=0.43$ (CsCl structure), the corresponding metallization pressure is 1.228Mbar (Table.2). The comparisons of metallization volume $(V/V_0)_M$ and the corresponding pressure (P_M) with experimental measurement and previous theoretical works are done in Table.3. Our results completely agree with the experimental observation of Weir et al [11]. At normal pressure (Figure 1), the fundamental energy gap at Γ -point is between the filled p-like valence band and empty d-like conduction band [14,17]. The band gap is 5.984 eV (Table 1). With increase of pressure the band gap decreases and at a particular pressure, there is a closing of band gap. As the pressure is increased, a fraction of 4s and 3p electrons of K is

transferred to 3d states of K as well as 5p, 5d states of I. Also a small fraction of 5s electrons of I is promoted to the 5d state of I. Thus there is a continuous s, p states to d state transition of electron in KI, which leads to the increase in d-electron number [13] and increase in the width of the valence band and conduction bands. All these lead to the decrease in the energy gap and finally metallization in KI. The metallization occurs because of the closure of band gap between I-5p like valence band and K- 3d like conduction band [14]. In the present case, metallization occurs via closing of indirect band gap (Figure 2) as reported by others [14,30]. The values for density of states at Fermi energy $N(E_F)$ are very small, at the metallization pressures, which indicate that metallization has just set in KI (Figure 4). Thereafter $N(E_F)$ increases slowly with pressure and becomes fairly large at a particular value of V/V_0 [20]. The values of E_F and $N(E_F)$ corresponding to different V/V_0 are used in studying the pressure variation of superconducting transition temperature [31].

3.4. Superconductivity and its Pressure Variation

The continuous promotion of s, p electron to d shell in solids under pressure is one of the factors which will induce superconductivity [13]. The theory of Gaspari and Gyoffy in conjunction with McMillan's formula is used to calculate T_c [32].

The electron –phonon mass enhancement factor, λ is

$$\lambda = N(E_F) \langle I^2 \rangle / M \langle \omega^2 \rangle \quad (3)$$

where M is the atomic mass, $\langle \omega^2 \rangle$ is an average of the phonon frequency square and $\langle I^2 \rangle$ is the square of the electron – phonon matrix element averaged over the Fermi surface. $\langle I^2 \rangle$ (in Rydbergs) can be written as [13]

$$\langle I^2 \rangle = 2 \sum_l \{ (l+1)/((2l+1)(2l+3)) \} M_{l,l+1}^2 \{ (N_l(E_F) N_{l+1}(E_F)) / N(E_F)^2 \} \quad (4)$$

Where,

$$M_{l,l+1} = \phi_l \phi_{l+1} [(D_l(E_F)-1)(D_{l+1}(E_F)+l+2) + (E_F-V(S))S^2]$$

and in this,

ϕ_l is the radial wave function at the Muffin-Tin sphere radius corresponding to the Fermi energy.

D_l is the logarithmic derivative of the radial wave function at the sphere boundary.

$V(S)$ is the Muffin-Tin potential at the sphere boundary.

S is the radius of the Muffin-Tin sphere.

The above quantities to calculate $M_{l,l+1}$ are taken from the band structure results [13,31]. We have calculated λ separately for K and I atoms and for the Tc calculation (Eq. (7)) the mean value of λ is used [9].

The average of the phonon frequency square is

$$\langle \omega^2 \rangle = 0.5 \theta_D^2 \quad (5)$$

The variation of Debye temperature with pressure $\theta_D(P)$ is given by [13]

$$\theta_D(P) = \theta_D^0 (a_0/a) (\sqrt{E_F} / \sqrt{E_F^0}) \quad (6)$$

where θ_D^0 , a_0 and E_F^0 are normal pressure quantities.

McMillan's formula,

$$T_c = (\theta_D / 1.45) \exp \{ -1.04(1+\lambda) / [\lambda - \mu^*(1+0.62\lambda)] \} \quad (7)$$

gives the good estimate of the T_c value [31]. Here μ^* is the electron-electron interaction parameter which is estimated using the relation [33],

$$\mu^* = 0.26 N(E_F) / (1+N(E_F)) \quad (8)$$

where $N(E_F)$ is the density of levels per atom per eV at E_F .

The Fermi energy E_F (Ry) and density of states $N(E_F)$ (states/Ry.cell) are obtained from the self-consistent calculation and we have calculated the variation of θ_D , λ and T_c with pressure using Eqs.(5 - 8) [31]. The value of T_c is determined at higher pressures also. The calculated values for θ_D , λ and T_c under various pressures are given in Table 4 (for NaCl structure) and Table.5 (for CsCl structure). The onset of superconductivity occurs at 2.77 Mbar. The calculated T_c value is 0.03 K at 2.77 Mbar in NaCl structure and 0.003 K at 2.77 Mbar in CsCl structure. From Tables 4 and 5, it is seen that in both structures T_c increases with increase of pressure. In our calculation the highest T_c obtained is 2.151 K at 4.945 Mbar in NaCl structure and 0.107 K at 4.945 Mbar in CsCl structure. The calculated T_c values depends more sensitively on λ rather than θ_D [31] . For KI, no experimental T_c value available for comparison.

Table 4. T_c as a function of pressure for KI (NaCl structure)

Pressure P Mbar	λ	θ_D K	μ^*	T_c Te K
2.770	0.162	210.8	0.018	0.030
3.890	0.186	247.6	0.020	0.091
4.380	0.228	260.8	0.021	0.344
4.945	0.337	275.1	0.022	2.151

Table 5. T_c as a function of pressure for KI (CsCl structure)

Pressure P Mbar	λ	θ_D K	μ^*	T_c Te K
2.770	0.123	291.5	0.016	0.003
3.890	0.158	314.4	0.025	0.021
4.380	0.188	325.7	0.028	0.085
4.945	0.214	341.0	0.044	0.107

4. Conclusions

In the present investigation, the pressure dependent band structures and density of states of KI are computed and the results are used to study the structural phase transition, metallization and superconductivity under pressure. Our calculation confirms the structural phase transition from NaCl structure to CsCl structure in KI under pressure [11]. The calculated metallization pressure P_M is in better agreement with the experimental observation [11] than the previous theoretical calculations [30]. In KI, both NaCl and CsCl structures give increasing of T_c with increase of pressure. In our calculation the highest T_c obtained is 2.151 K at 4.945 Mbar in NaCl structure and 0.107 K at 4.945 Mbar in CsCl structure. The calculated T_c values depend more sensitively on λ rather than θ_D . So KI comes under an electron-phonon mediated superconductor. For KI, no experimental T_c value available for comparison. The structural phase transition (0.02 Mbar), metallization (1.228 Mbar) and onset of superconductivity (2.77 Mbar) do not occur simultaneously in ionic salts [13] is confirmed in the simple ionic salt KI.

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