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AN EVALUATION OF TRANSITION TEMPERATURE T_c AND EVALUATION OF PRESSURE AND VOLUME DEPENDENT $\left(\frac{dT_c}{dp}\right)$, $\left(\frac{dT_c}{dv}\right)$, ISOTOPE COEFFICIENT (α) AND ENERGY GAP PARAMETER (Δ) FOR ALKALI METAL DOPED FULLERIDE K_3C_{60}

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Abstract: - Using theoretical formalism of *Kresin*(1987& 1991) which is based on the contribution of intermolecular and intermolecular phonon interaction, we have evaluated transition temperature of alkali doped fluoride K_3C_{60} . Our theoretical results matches with the experimental data and with other theoretical workers. We also observed that coulomb repulsive parameter μ^* plays an important role in the evaluation of transition temperature T_c alkali doped fluoride. We have also evaluated pressure and volume dependent transition temperature, isotope coefficient and energy gap parameter for alkali doped fullerenes. Our theoretical results indicate that variation of T_c with pressure depends upon the variation of density of state at the Fermi level, the Coulomb potential and the characteristic phonon frequency. On the other hand for the volume dependent T_c , our theoretical results indicate that it depends upon the three factors (a) screening parameter μ^* (b) intermolecular vibration mode (c) intramolecular phonon coupling strength λ_{ra} .

Keywords: Intermolecular and intermolecular phonons, alkali doped fluorides, transition temperature, T_c renormalized repulsive parameter μ^* , isotope coefficient α , Isotopic mass dependent transition temperature, Soft optical intermolecular phonon, Thermal compressibility, Logarithmic volume derivative.



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INTRODUCTION

Buckminster fullerenes are known to make compounds with alkali metals intensively studied mainly due to superconductivity and the variation of compounds.¹⁻³ Neutron inelastic scattering measurement probes that the vibrational spectrum may be conveniently divided into two regions. One of them belongs to the rotation of C₆₀ molecule and the intermolecular vibrations (~2.5- 2.5meV) and the others are the interamolecular mode. The wide frequency range of phonon spectrum however raises an important issue to clarify which of these molecular phonon modes induce the superconductivity in doped fluoride. The dispersion relation for the interamolecular phonon modes originate due to displacement of C₆₀ molecule or K⁺ ions in doped fluorides. It is evident from the eigen frequencies that these corresponds to the interamolecular acoustic and alkali C₆₀ optical modes in the long wavelength ($q \rightarrow 0$), the mass of three alkali metals (K) is used as 0.17 amu. The interamolecular alkali (C₆₀) optic mode of ω_{er} is 7.84 meV at $q \rightarrow 0$. The electron density η ($= 4/3/a^3$) is estimated⁴ as $4.12 \times 10^{21} \text{ cm}^{-3}$ from the lattice parameters $a=14.28 \text{ \AA}$. The band structure value of mass $=0.3m_e$ is used⁵. Electron parameters as Fermi velocity v_F ($= 1.91 \times 10^7 \text{ cms}^{-1}$) Fermi wave vector ($q_p = 0.496 \text{ \AA}^{-1}$) and plasma frequency ($=1.37\text{eV}$)⁶. The electron phonon coupling strength (λ_{er}) is obtained as 1.2. The dimensionless electron-phonon coupling strength as estimated by Gunnarson⁷ is about 0.5-1.0. Earlier calculations by Zhang *et al*⁸ indicates that the alkali phonons could contribute an attractive interactions of the order of 0.9 eV, which corresponds to $\lambda \cong 2.0$ i.e. strong coupling limit.

The energy scale of the various phonon modes that mediate the electron- phonon Coupling is different because of the isotopic mass dependent transition temperature. The carbon isotopic effect demonstrate $\alpha_c = 0.30 \pm 0.05$, which 100% substitution of ⁶C₁₃ for ⁶C₁₂. This naturally favours the phonon mediated pairing and ruled out electronic in origin. Further investigation shows that it is an alkali metal isotope effect not the carbon isotope effect. This has identified that it is an inter or intra molecular phonon mode that induce the superconductivity in fullerenes⁹.

In this paper taking the theoretical formalism of Kresin¹⁰, we have theoretically evaluated the transition temperature of alkali doped fulleride particularly K₃C₆₀. Our theoretically evaluated results are in good agreement with the experimental data as well as with the other theoretical workers.¹¹⁻¹³ . We have also evaluated pressure and volume dependent transition temperature isotope coefficient and energy gap parameter for alkali doped fullerenes. Our theoretical result indicates that variation of T_c with pressure depends upon the variation of density of state at Fermi level, the coulomb potential and the

characteristic phonon frequency. On the other hand for the volume dependent T_c , our theoretical results indicates that it depends upon the three factors (a) screening parameter μ^* (b) intermolecular vibration mode (c) intramolecular phonon coupling strength λ_{ra} .

Our theoretical results for isotope coefficient α indicates that it decreases with screening parameter μ^* , energy gap parameter β depends upon the Fermi velocity v_F and a coherence length ξ_0 , alkali metal doped fulleride, the coherence length ξ_0 is small but larger than inverse Fermi momentum.

1.0 MATERIALS AND METHODS

We have taken renormalized coulomb repulsive parameter μ^* , which signifies the role of the intermolecular alkali C_{60} optical phonon frequency. Here the coupling strength ($\lambda > 1$) and $\mu^* = 0.9$, which gives the characteristic phonon frequency ($\omega_{er} = 7.84$)

One takes the theoretical formalism developed by Kresin^{10,11} where transition temperature is written as

$$T_c^{er} = 0.25\omega_{er}[\exp(2/\lambda_{eff}) - 1]^{-1/2} \quad (1)$$

$$\lambda_{eff} = (\lambda_{er} - \mu^*) [1 + 2\mu^* + \lambda_{er}\mu^* t(\lambda_{er})]^{-1} \quad (2)$$

$$t(\lambda_{er}) = 1.5 \exp(-0.28\lambda_{er}) \quad (3)$$

The effective coupling constant, λ_{eff} , deduced as 0.62 for the numerical $t(\lambda_{er})$ value 1.07 with $\lambda_{er} = 1.2$ and T_c^{er} is estimated as $\cong 5$ K which is much lower than reported experimental data of about 18 K. The low value of T_c is due to the fact that the vibrations developed due to lattice deformations, i.e the soft optical intermolecular phonons are considered. The above approach with intermolecular phonons does not explain a medium T_c in K_3C_{60} . It is essential to seek the role of the high energy phonons to assess the reported value.

An analytic result for T_c is employed by incorporating the simultaneous presence of both inter and intra molecular fluorides. Now the above formula given in equation (1) is modified by the simultaneous use of both inter and intramolecular phonon

$$T_c = T_c^{er} [\omega_{ra} / T_c^{er}]^\chi \quad (4)$$

$$\text{with } \chi = \lambda_{ra} [\lambda_{ra} + \lambda_{er}]^{-1}$$

λ_{ra} is the intermolecular coupling constant and is determined from the scattering time¹⁴

$$\lambda_{ra} = \hbar / 2K_{\beta}T_{\tau} \quad (5)$$

$$\tau = 1.2 \times 10^{-4}$$

$$\lambda_{ra} = 0.4$$

To analyze the pressure dependence of T_c in K_3C_{60} systems, one begins with T_c expression (Kresin)^{10,11}

Now

$$\frac{d \ln T_c}{dp} = \left[1 - \frac{\lambda_{ra}}{\lambda_{ra} + \lambda_{er}} \right] \frac{d \ln T_c^{er}}{dp} + [\ln \omega_{ra} - \ln T_c^{er}] \frac{d}{dp} \left[\frac{\lambda_{ra}}{\lambda_{ra} + \lambda_{er}} \right] + \left[\frac{\lambda_{ra}}{\lambda_{ra} + \lambda_{er}} \right] \frac{d \ln \omega_{ra}}{dP} \quad (6)$$

keeping in mind that C_{60} molecules are extremely rigid and hence neglecting the pressure induced effect of intramolecular phonons,

$$\frac{d \ln \omega_{ra}}{dP} = \frac{d \omega_{ra}}{dP} = 0 \quad (7)$$

Then equation (6) assumes the form

$$\frac{d \ln T_c}{dp} = \left[1 - \frac{\lambda_{ra}}{\lambda_{ra} + \lambda_{er}} \right] \frac{d \ln T_c^{er}}{dp} + \frac{1}{(\lambda_{ra} + \lambda_{er})^2} \left[\ln \left(\frac{\omega_{ra}}{T_c^{er}} \right) \right] \left[\lambda_{er} \frac{d \lambda_{ra}}{dp} - \lambda_{er} + \frac{d \lambda_{er}}{dp} \right] \quad (8)$$

Furthermore,

$$\frac{d \ln T_c}{dp} = \frac{\partial \ln T_c^{er}}{\partial \lambda_{er}} \frac{\partial \lambda_{er}}{dp} + \frac{\partial \ln T_c^{er}}{\partial \omega_{er}} \frac{\partial \omega_{er}}{dp} + \frac{\partial \ln T_c^{er}}{\partial \mu^*} \frac{\partial \mu^*}{dp} \quad (9)$$

Now one uses Kresin T_c expression^{10,11}

$$T_c = 0.25 \omega_{er} \left[\exp \left(2 / \pi_{eff} \right) - 1 \right]^{-1/2} \quad (10)$$

where

$$\lambda_{eff} = (\lambda_{eff} - \mu^*) [1 + 2\mu^* + \lambda_{er} \mu^* t(\lambda_{er})]^{-1} \quad (11)$$

and

$$t(\lambda_{er}) = 1.5 \exp. (-0.28\lambda_{er}) \quad (12)$$

$$\lambda_{eff} = 0.62$$

$$\lambda_{er} = 1.2$$

we get the following results

Now

$$\frac{d \ln T_c^{er}}{d \lambda_{er}} \frac{\partial \lambda_{er}}{dP} = D_{11} \frac{d \ln \lambda_{er}}{dP} \quad (13)$$

where

$$D_{11} = \frac{\lambda_{er}(1+2\mu^*+1.07\mu^{*2})}{(\lambda_{er}-\mu^*)^2} \left[1 + \left\{ \exp \left(\frac{2+4\mu^*+2.14\lambda_{er}\mu^*}{\lambda_{er}-\mu^*} \right) \right\}^{-1} \right. \\ \left. + \left\{ \exp \left(\frac{2+4\mu^*+2.14\lambda_{er}\mu^*}{\lambda_{er}-\mu^*} \right) \right\}^{-2} \right] \quad (14)$$

Now ones the following

$$\frac{d \ln T_c^{er}}{\partial \omega_{er}} \frac{\partial \omega_{er}}{dP} = \frac{d \ln \omega_{er}}{dP} \quad (15)$$

and

$$\frac{d \ln T_c^{er}}{\partial \mu^*} \frac{\partial \mu^*}{dP} = D_{12} \frac{d \mu^*}{dP} \quad (16)$$

where

$$D_{12} = \frac{\lambda_{er}(1+2\mu^*+1.07\mu^{*2})}{(\lambda_{er}-\mu^*)^2} \left[1 + \left\{ \exp \left(\frac{2+4\mu^*+2.14\lambda_{er}\mu^*}{\lambda_{er}-\mu^*} \right) \right\}^{-1} \right. \\ \left. + \left\{ \exp \left(\frac{2+4\mu^*+2.14\lambda_{er}\mu^*}{\lambda_{er}-\mu^*} \right) \right\}^{-2} \right] \quad (17)$$

Combining these, one writes

$$\frac{d \ln T_c}{dp} = D_{11} \frac{d \ln \lambda_{er}}{dP} + \frac{d \ln \omega_{er}}{dP} + D_{12} \frac{d \ln \mu^*}{dP} \quad (18)$$

The first and the third terms are dependent on the variation on the with $N(\varepsilon_F)$ pressure.

One proceeds for further calculations by using the reported value¹³ of B, 13.18 GPA and calculated ε_F , 0.31 eV. The free electron gas results $d \ln(N(\varepsilon_F))/dp = (-2/3) k_T$, where

k_T ($\sim B a^{-1}$) is a thermal compressibility. Deduced value of $d \ln(N(\epsilon_F))/dp$ is about 5.058 % (GPA) $^{-1}$. Kerkoud and coworkers¹⁴ reported a rate of about ~ -10 % (GPA) $^{-1}$ from NMR technique although of limited accuracy.

Now we have electron-phonon coupling strength λ_{er} as

$$\lambda_{er} = \frac{N(\epsilon_F)\langle I^2 \rangle}{M_{red}\langle \omega_{er}^2 \rangle} \quad (19)$$

where $\langle I^2 \rangle$ is a mean square electron ion matrix element M_{red} is the reduced molecular mass and $\langle \omega_{er}^2 \rangle$ is an averaged square molecular vibration frequency.

One has

$$\langle I^2 \rangle = \frac{\int_0^{2k_F} q^3 dq |V(q)|}{\int_0^{2k_F} q dq} \quad (20)$$

$V(q)$ is the screened coulomb potential

From (19) and (20) one has

$$\frac{d \ln \mu^*}{dP} = \frac{d \ln N(\epsilon_F)}{dP} \left(\frac{\mu^*}{\mu} \right) - \mu^* \left[\frac{2 d \ln \omega_p}{dP} - \frac{d \ln N(\epsilon_F)}{dP} - \frac{d \ln \omega_{er}}{dP} \right] \quad (21)$$

$$\frac{d \ln \lambda_{er}}{dP} = \frac{d \ln N(\epsilon_F)}{dP} - \frac{d \ln \langle \omega_{er}^2 \rangle}{dP} \quad (22)$$

Herein the pressure dependence of the quantity $\langle I^2 \rangle$ has been neglected as the mean-square electron-ion matrix element is independent of phonon frequencies. Assuming that delta functions entering the integrals do not vary much under pressure, one neglects the pressure dependence of the quantity $\langle I^2 \rangle$.

Using (21) and (22) into (20), one obtains

$$\begin{aligned} \frac{d \ln T_c^{er}}{dP} = & \left[D_{11} + D_{12} s \left(\frac{\mu^*}{\mu} \right) + D_{12} \mu^* \right] \frac{d \ln N(\epsilon_F)}{dP} \\ & + [1 + D_{12} \mu^* - 2D_{11}] \frac{d \ln \langle \omega_{er} \rangle}{dP} - D_{12} \omega^* \frac{d \ln \omega_p}{dP} \end{aligned} \quad (23)$$

In order to make progress one assumes $d \ln \lambda_{er} / dP \approx d \ln N(\epsilon_F) / dP$, $d \ln \langle \omega_{er} \rangle^2 / dP \approx 2 d \ln \langle \omega_{er} \rangle / dP$ and $d \ln \langle \omega_{er} \rangle / dP \approx d \ln \langle \omega_{er} \rangle / dP$. The free electron estimate for $d \ln \omega_p / dP = 1/2$ yields a value of about 3.79 % (GPA) $^{-1}$. One follows $\gamma_G = +2$ as reported earlier¹⁵. The parameters needed for further calculations are obtained as $D_{11} = 1.7$ and $D_{12} = 0.96$ from the

value of $\lambda=1.2$, $\mu=0.75$ and $\mu^*=0.19$. Using (6) to (23) one finds the value of $(d \ln)\mu^*/dP = -0.78 \%$ (GPa)⁻¹, $d \ln \lambda_{er}/dP = -35.39$ (GPa)⁻¹, $d \ln \lambda_{er}/dp = -5.05 \%$ (GPa)⁻¹, $d \ln T_c^{er}/dP$ is -45.64% (GPa)⁻¹, $d \ln T_c/dP = -39.60$ (GPa)⁻¹, and slope $d t_c/dP = -8.7$ K/ GPa which is consistent with the earlier reported value^{16,17} of -7.8 K/ GPa.

Volume Dependent Transition Temperature

One now explore one's efforts in studying the volume derivative of T_c or dT_c/dV . One notes that due to extreme rigidity of C_{60} the compression contracts the weak intermolecular bonds and high- energy intramolecular bonds are unaffected.

Now one uses equations for T_c given in equation (1) and (2) and obtained $\frac{dT_c}{dV}$ as

$$\frac{dT_c}{dV} = T_c^{er} \frac{d}{dV} \left[\frac{\omega_{ra}}{T_c^{er}} \right]^\chi + \left[\frac{\omega_{ra}}{T_c^{er}} \right]^\chi \frac{dT_c^{er}}{dV} \quad (24)$$

One further writes

$$\frac{dT_c}{dV} = (1 - \chi) \left[\frac{\omega_{ra}}{T_c^{er}} \right]^\chi T_c^{er} \quad (25)$$

Herein, it is assumed that intramolecular phonons are independent in any change of the volume

$$\frac{d \ln \omega_{ra}}{dV} = \frac{d \omega_{ra}}{dV} = 0 \quad (26)$$

Following eq.(8) ones write

$$\begin{aligned} \frac{dT_c^{er}}{dV} &= \frac{0.25}{[\exp(2/\lambda_{eff})-1]^{1/2}} \times \frac{d\omega_{ra}}{dV} + \\ &\frac{\exp(2/\lambda_{eff})}{[\exp(2/\lambda_{eff})-1]^{3/2}} \times \left(\frac{0.25 d\omega_{er}}{\lambda_{eff}^2} \right) \frac{\lambda_{eff}}{dV} \end{aligned} \quad (27)$$

where

$$\begin{aligned} \frac{\lambda_{eff}}{dV} &= (1 + 2\mu^* + \mu^{*2} t(\lambda_{er})) \frac{\lambda_{er}}{dV} + \\ &(\mu^* \lambda_{er} - \mu^* \lambda_{er}^2) \frac{dt(\lambda_{er})}{dV} - \\ &(1 + 2\lambda_{er} + 2\lambda_{er}^2 t(\lambda_{er})) \frac{d\mu^*}{dV} \end{aligned} \quad (28)$$

Using (27) and (28), one writes

$$\frac{dT_c}{dV} = D_{21} \frac{d\omega_{er}}{dV} + D_{22} \frac{d\lambda_{er}}{dV} + D_{23} \frac{dt(\lambda_{er})}{dV} - D_{24} \frac{d\mu^*}{dV} \quad (29)$$

Here one defines,

$$D_{21} = V_{00} \left\{ \frac{0.25}{[\exp(2/\lambda_{eff}) - 1]^{1/2}} \right\} \quad (30)$$

$$D_{22} = V_{00} \left\{ \frac{\exp(2/\lambda_{eff})}{[\exp(2/\lambda_{eff}) - 1]^{3/2}} \times \frac{0.25 d\omega_{er}}{\lambda_{eff}^2} \right\} \quad (31)$$

$$(1 + 2\mu^* + \mu^{*2} t(\lambda_{er}))$$

$$D_{23} = V_{00} \left\{ \frac{\exp(2/\lambda_{eff})}{[\exp(2/\lambda_{eff}) - 1]^{3/2}} \times \frac{0.25 d\omega_{er}}{\lambda_{eff}^2} \right\} \quad (32)$$

$$(\mu^* \lambda_{er} - \mu^* \lambda_{er}^2)$$

$$D_{24} = V_{00} \left\{ \frac{\exp(2/\lambda_{eff})}{[\exp(2/\lambda_{eff}) - 1]^{3/2}} \times \frac{0.25 d\omega_{er}}{\lambda_{eff}^2} \right\} \quad (33)$$

$$(1 + 2\lambda_{er} + 2\lambda_{er}^2 t(\lambda_{er}))$$

where

$$V_{00} = (\omega_{ra}/T_c^{er}) \frac{\lambda_{ra}}{\lambda_{er} + \lambda_{ra}} \left(1 - \frac{\lambda_{ra}}{\lambda_{er} + \lambda_{ra}} \right) \quad (34)$$

Furthermore the logarithmic volume derivative of the coupling constant parameter λ_{er} follows

$$\Phi = \frac{d \ln \lambda_{er}}{d \ln V} = B \frac{d \ln(\epsilon_F)}{dP} + 2\gamma_G$$

With the value of $B, \ln N(\epsilon_F)/dP, \ln(\omega)/dP$ discussed earlier, one finds $\Phi=3.3$ for K_3C_{60} . To ascertain the physical significance of the volume derivative of T_c one estimates the parameter as $D_{21}= 0.16, D_{22}= 70.6, D_{23}= - 2.7$ and $D_{24}= - 323$ from the earlier mentioned values of various coupling strengths. Looking to (27), dT_c/dV is being influenced by (a) volume dependence of screening parameter and (b) volume dependence of intermolecular vibrational mode as well as intramolecular phonons coupling strength. Because of the difficulties in determining the

volume derivative of molecular phonon frequency, one is only able to provide some suggestive formal argument below.

Usually, the compression increases the bandwidth and hence ϵ_F resulted in the reduction of renormalized screening parameter. One notes that the Coulomb repulsion suppresses T_c . Henceforth, the condition dT_c/dV proportional to $d\mu^*/dV$ is negative. The logarithmic dependence of μ^* of ϵ_F points to the fact that volume derivative of μ^* is small in magnitude. A natural argument follows that the volume derivative of $t(\lambda_{er})$ and of μ^* is small in comparison to $d\lambda_{er}/dV$, henceforth, one neglects these two terms in (29)

we have

$$\frac{d \ln T_c}{d \ln V} = - \frac{d \ln T_c}{d \ln P} B \quad (35)$$

As dT_c/dP is negative, one finds the volume derivative of T_c is positive and large in fullerenes.

Isotope effect coefficient

Isotope effect coefficient is defined as

$$\alpha = (0.5)(d \ln T_c / d \ln M_{red}) \quad (36)$$

The M_{red} dependence of T_c is introduced in terms of μ^* , leading to the following result

$$\alpha = \{1 - \mu^{*2}(1 + 2\lambda_{er} + \lambda_{er}^2) / \lambda_{eff}(\lambda_{er} - \mu^*) [1 + (4T_c/\omega)^2]\} / 2$$

with ω as the average phonon frequency. (37)

Equation (37) yields $\alpha \cong 0.24$ which is slightly lower than the reported value¹⁸ of $\alpha = 0.30 \pm 0.06$ with 100% substitution of ^{13}C for ^{12}C and consistent with results of Fuhrer et al.¹⁹. It is noticed that the BCS one half value is recovered for $\mu^* = 0.0$. With the increase in μ^* values the isotope effect exponent decreases for $\lambda_{er} = 1.2$ and $\lambda_{ra} = 0.4$.

Energy gap parameter

The energy gap parameter is

$$\beta = 2\Delta(0) / k_B T_c = 3.25 [1 + 5(T_c / \omega_{ra})^2 \ln(\omega_{ra} / T_c)] \quad (38)$$

where $\Delta(0)$ is the energy gap at zero temperature. The gap parameter when intramolecular phonons are alone considered in the pairing mechanism is estimated as 3.54 which is close to the BCS limit where the values, $\omega_{ra} = 1012^{-1}$ cm and $T_c = 22$ K, are used. This implies that, the intramolecular phonons require moderate interaction with the conduction electrons and is consistent with infrared spectroscopy²⁰, muon spin relaxation measurements²¹ and nuclear spin relaxation measurements²², which strongly favour the participation of intramolecular phonons in the pairing mechanism. Furthermore, the absolute reflectivity measurements²³, on K_3C_{60} reports $\beta = 3.6$ 4.0, which is similar to BCS weak coupling limit and the electron-phonon coupling strength cannot be as large as 2.

The Fermi velocity v_F , along with a T_c of 22 K leads to a BCS coherence length of 12.9 nm using the precise definition

$$\xi_0 \cong \hbar v_F / 1.76 \pi k_B T_c \quad (39)$$

which is consistent with the value²⁴ of 12.0, 13.0 \pm 0.15 and 15.0 nm for K_3C_{60} fullerenes²⁵.

In the case of alkali metal doped fullerides the coherence length is small but larger than the inverse Fermi momentum. One further estimates the zero temperature mean free path $\ell = v_{FT} = 3.4$ nm. The small value of ℓ is mainly attributed to the disorder which is present in the doped fulleride samples of single crystals. The effective coherence length following $\xi_{00} = \xi_{10} + \ell^{-1}$ leads to a value of about 2.7 nm consistent with the earlier estimates of

2.6- 4.5 nm²⁶. It shows that the alkali metal doped fullerides are dirty superconductor doped by $\ell \leq \xi_0 < \xi_{00}$.

The magnetic penetration depth at $T = 0$ K as $\lambda_{10} = [m^* c^2 / 4\pi n e^2]^{1/2}$ is estimated as 143.6 nm which is slightly smaller than the values²⁷ of 156 nm in K_3C_{60} . The consistency is attributed to the proper choice of transport parameters as effective mass and carrier density. The effective penetration depth $\lambda_{1.00} = \lambda_{1.0} \{1 + \xi_{00} \ell^{-1}\}$ is about 192 nm consistent from the earlier estimate of 240 nm, 600 nm and 800 nm. Given the numbers that emerge from the analysis it seems fair to conclude that fullerides belong to conventional s-wave superconductor^{28,29}.

RESULTS AND DISCUSSION:

In this paper, using the theoretical formalism of Kresin^{10,11}, we have evaluated the superconducting transition temperature T_c as a function of intramolecular phonon coupling

constant (λ_{ra}) for fixed value of coulomb repulsion parameter μ^* . The results are shown in table T₂. We have compared our theoretical results with experimental data of K₃C₆₀. Our evaluated results shows that for set of values ($\lambda_{ra} = 0.25$ & $\mu^* = 0$), ($\lambda_{ra} = 0.35$ & $\mu^* = 0.1$), ($\lambda_{ra} = 0.40$ & $\mu^* = 0.2$) and ($\lambda_{ra} = 0.50$ & $\mu^* = 0.3$) the theoretical result matches with experimental data 20K for K₃C₆₀ fluoride. It indicates that coulomb repulsive parameter μ^* is a very important parameter along with λ_{ra} . In table T₁, we have shown the transition temperature T_c of various alkali metal doped compounds which varies from 20K to 45K. Some recent observations shown superconductivity above 30K in alkali doped hydrocarbon and hole doped C₆₀. Superconductivity³⁰ at 33K is obtained in K-doped dibenzopentacium (C₃₀H₁₈) and superconductivity³¹ at 52K is observed in hole-doped C₆₀. We have also evaluated the pressure dependent and volume dependent transition temperature isotope effect exponent and energy gap parameter for alkali metal doped fullerenes (K₃C₆₀). For pressure dependent transition temperature we have used equation (16) in which the first and third terms depends upon the variation of density of state N(E_F) with pressure. The result is showing in **table T₃** along with experimental data. We have used empirical relation

$$T_c(P) = T_c(0) \exp[0.3\gamma_G \cdot P] \quad (40)$$

Hence the value of the γ_G has been taken +2, from the paper¹⁵ and for the evaluation of $\frac{dT_c}{dP}$ and $\frac{dT_c}{dV}$, we have taken the value of the parameter D₂₁ = 0.16, D₂₂ = 17.6, D₂₃ = - 2.7, D₂₄ = - 323, using various coupling strength³². For the evaluation of isotope coefficient α , we have used the equation (36) and (37). Here ω is the average phonon frequency we get the value of $\alpha = 0.24$, which is slightly lower than the reported values^{18,19} of 0.30 ± 0.06 . In this evaluation we have taken the value of $\lambda_{er} = 1.2$, $\lambda_{ra} = 0.4$ and the result is shown in **table T₄**. From our evaluated results it appears that isotope exponent α decreases with increasing μ^* . This result is consistent with BCS results and also with other theoretical workers^{33,34}. There is some recent calculations³⁵⁻⁴² which also reveals the similar behaviour.

CONCLUSION:

From the above investigations and theoretical analysis, we have come across the following conclusions:

- (i) The theoretical formalism of Kresin which includes both intermolecular and intramolecular phonons works quite well in order to calculate T_c of doped alkali fluoride.

- (ii) Our theoretical results indicate that variation of T_c with pressure depends upon the variation of density of state at the Fermi level, Coulomb Potential and characteristic phonon frequency
- (iii) Our theoretical results for volume dependence T_c depends on three factors (a) screening parameter μ^* (b) intermolecular Vibration mode (c) intramolecular coupling strength
- (iv) Our theoretical results for isotopic coefficient α decreases with screening parameter μ^* .

Table T1: Transition temperature T_c of some alkali doped C_{60} full rides.

Compounds	Transition temperature T_c (K)
K_3C_{60}	20
K_2RbC_{60}	22
Rb_2KC_{60}	25
Rb_3C_{60}	29
Rb_2CsC_{60}	31
Cs_2RbC_{60}	33
Cs_3C_{60}	47
$Rb_{2.7}Tl_{2.2}C_{60}$	45

Table T2: An evaluated results of superconducting transition temperature T_c as a function of λ_{ra} (intramolecular coupling constant) for different values of Coulomb repulsive parameter μ^* . The results were compared with doped alkali metal K_3C_{60} .

λ_{ra}	T_c (K) Cal.				EXPT 20K
	$\mu^*=0.0$	$\mu^*=0.10$	$\mu^*=0.20$	$\mu^*=0.30$	
0.0	11.25	6.78	4.78	3.25	
0.10	13.68	9.49	7.17	5.10	
0.20	16.38	12.58	10.25	6.28	
0.30	24.26	18.25	15.87	10.29	
0.40	35.12	23.27	19.35	14.56	
0.50	44.56	31.52	24.28	18.59	
0.60	53.18	37.63	31.27	25.23	
0.70	62.17	48.28	38.65	32.45	
0.75	67.29	54.62	40.14	37.21	
0.80	70.18	59.10	44.29	39.34	

Table T3: An evaluated result of pressure dependent transition temperature T_c , The results were compared with K_3C_{60} fluoride.

Pressure P(GPa)	Theory T_c (K)	EXPT T_c (K)
0.00	20.25	19.26
0.20	18.16	17.57
0.40	16.30	16.89
0.60	14.86	15.22
0.80	12.20	14.56
1.00	10.58	12.32
1.20	9.88	10.49
1.40	8.72	9.78
1.60	7.46	8.17
1.80	6.15	7.29
2.00	5.05	6.59

Table T4: An evaluated result of isotope effect exponent α as a function of pseudo potential parameter μ^* for K_3C_{60} fluoride taking $\lambda_{er}=1.2$ and $\lambda_{ra}=0.4$.

μ^*	Isotope exponent α
0.00	0.525
0.025	0.517
0.050	0.502
0.075	0.476
0.100	0.457
0.120	0.405
0.140	0.386
0.150	0.325
0.180	0.269
0.200	0.248
0.220	0.207
0.240	0.196
0.250	0.108

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