Int. J. Chem. Sci.: 10(3), 2012, 1317-1324
ISSN 0972-768X
www.sadgurupublications.com

EVALUATION OF TRANSITION TEMPERATURE T_C AND ISOTOPE EFFECT 'A' IN ALKALI DOPED FULLERIDES

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ABSTRACT

Using the theoretical formalism of Kresin (1991), which includes contribution for both intermolecular and interamolecular phonon coupling, the transition temperature T_C, isotope effect exponent α for K_3C_{60} fulleride was evaluated and theoretical result are in good agreement with the experimental data and also with other theoretical worker's.

Key words: Intermolecular phonon mod, Intramolecular phonon mode, Transition temperature T_C, Isotope effect exponent α, Energy gap parameter.

INTRODUCTION

The fullerenes (C_{60}, C_{70}…) have attracted much interest since their discovery[1]. The interest increased dramatically when it was discovered[2] how to produce C_{60} in large quantities to make solids (fullerites) of a size that allowed traditional solid state experiment. It was also found that interaclation of alkali metal atom in solid C_{60} leads to metallic behaviour. It was also found that some of these alkali doped C_{60} compounds (fullerides) are superconducting with transition temperature T_C around 30-40 K. $RbCs_2C_{60}$ has T_C = 33 K while Cs_3C_{60} under pressure has T_C = 40 K. The great interest of these alkali-doped C_{60} is the question whether or not such a large value of T_C can be caused by coupling to phonons alone. There has been a great effort to characterize and understand both the normal state and the superconducting properties of fullrides[2-4].

C_{60} is a most symmetric molecule. The 60 carbon atoms are all equivalent and form 12 pentagons and 20 hexagons. C_{60} molecule condensed into solid of weekly bond molecule. For an undoped C_{60} solid the h_u band is full and t_{1u} band is empty and this system is

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therefore band insulator. When solid C_{60} is doped by alkali atoms, the alkali atoms denote about one electrons each of the t_{1u} band[5-7].

K_3C_{60} is the subject of renewed interest because of its technological and industrial importance. In close relation the nature of the attracting mechanism with conventional phonon mediated electron pairing unconventional electron mechanism in fullerides (T_C -20-45 K) remains a central point of several experimental studies. Neutron-inelastic scattering measurement[8,9] probes that the vibrational spectrum may be conveniently divided into two region. One of them belongs to the rotation of C_{60} molecule and the intermolecular vibration (≈2.5-25 meV) and the others are the intramolecular mode with frequency 25-200 meV. Raman scattering[10] yields the on-ball C_{60} vibrational mode (~40 meV -0.25eV). Lattice dynamical studies point out that the spectrum consist of mode of C_{60} (26 cm^{-1}), the vibrations of K^+ ions, the translation variation as a whole (45-120 cm^{-1}) and the C_{60} vibrations (~260-1900 cm^{-1}). The wide frequency range of phonon spectrum raises an important issue to clarify which of these molecular phonon modes induce the superconductivity in doped fullerides. The energy scales of the various phonon mode that mediates electron-phonon coupling are different. This differencess was observed because of the dependence of the transition temperature on isotopic mass. It was also pointed out that it is the alkali isotope effect and not the carbon isotope effect that identify whether inter or intramolecular phonon modes induce the superconductivity.

In this paper, taking the theoretical formalism of Kresin[11], we have theoretically evaluated the transition temperature of K_3C_{60} as a function of intramolecular phonon coupling with various values of Coulomb repulsion parameter μ^*. We have also evaluated istope exponent α and energy gap parameter $2\Delta/T_C$.

Mathemtical formulae used in this

In order to calculate transition temperature T_C one uses theoretical formalism given by Kresin[11]. This formalism is developed in the strong coupling theory where $\lambda > 1$, λ is coupling strength.

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

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

μ^* is the renormalized coulomb repulsive parameter and ω_{er} is the characteristic phonon frequency.

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

λ_{er} is the electron-phonon coupling strength. In this formalism both inter or intramolecular phonon modes induces the superconductivity.

One takes[12]

$$\lambda_{eff} = 0.62$$
$$t(\lambda_{er}) = 1.07 \quad \ldots(4)$$
$$\lambda_{er} = 1.2$$

Using Eq. (1) it was found that $T_C^{er} = 5$ K which is much lower than the reported experimental value of K_3C_{60} (20K). Then equation (1) is modified by taking the simultaneous presence of both inter and intramolecular phonon in fullerides.

$$T_c = T_c^{eff}[\omega_{ra} / T_c^{eff}]^{\chi} \quad \ldots(5)$$

$$\text{Where, } \chi = \lambda_{ra} [\lambda_{ra} + \lambda_{er}]^{-1} \quad \ldots(6)$$

λ_{ra} is the intamolecular coupling constant and is obtained from the scattering time[13].

$$\lambda_{ra} = \hbar/(2\pi K_\beta T\zeta) \quad \ldots(7)$$

ζ is the scattering time, [$\zeta = 1.2 \times 10^{-14}$s][13], $\omega_{ra} = 1012$ cm^{-1}

Isotope effect coefficient

The isotope effect coffecient is defined as -

$$\alpha = (0.5)\ (dl_n T_c / d\ l_n m_{red}) \quad \ldots(8)$$

m_{red} is reduced molecular mass. The m_{red} dependence of T_c is introduced in terms of μ^*, then the value of α becomes-

$$\alpha = \{1-\mu^{*2}(1+2\lambda_{er}+\lambda_{er}^2)/\lambda_{eff}(\lambda_{er}-\mu^*)[1+(4T_c/\omega)^2]\}/2 \quad \ldots(9)$$

Here W is the average phonon frerquency for K_3C_{60} Fulleride ($T_c = 20$) one uses

$$\lambda_{er} = 1.2 \text{ and } \lambda_{ra} = 0.4$$

Energy gap parameter-

The energy gap parameter[11] β is given by -

$$B \approx 2\Delta\ (0)/H_s Tc \quad \ldots(10)$$
$$\approx 3.5\ [1+5\ (Tc/\omega_{ra})^2 l_n\ (\omega_{ra}/\ Tc)]$$

Screening parameter

The renormalized coulomb repulsion parameter is defined as -

$$\mu^* = [(1+\mu l_n (\varepsilon_F/\omega_{er})] \quad \ldots(11)$$

The coulomb strength parameter μ is given by -

$$\mu = N(\varepsilon_F)U \quad \ldots(12)$$

Where $N(\varepsilon_F)$ is the density of states at the Fermi energy and U is the static screened interaction, V(q, ω=0) average over the Fermi sphere. One calculate μ from static dielectric funuction.

ε (q) in the long wavelength limit.

$$\varepsilon(q) = (4m_e^2K_F)\,[\pi\hbar^2q^2]^{-1} \quad \ldots(13)$$

Using Eq. (13), μ is calculated as –

$$\mu = 1/2\pi a_b k_\beta \, l_n[1+3\pi a_B k_F/2] \quad \ldots(14)$$

a_B = Bohr radius

K_F = Fermi wave vector

RESULTS AND DISCUSSION

In this paper, we have presented a method of evaluation of Superconducting transition temperature T_c of alkali metal doped fullerides. We have taken the theoretical formalism developed by Kresin[11] to evaluate T_c. T_c was evaluated as function of intramolecular coupling strength λ_{ra}. The result is shown in Table 2. It is clear from the result that T_c is strongly influenced by the Coulomb repulsive parameter μ^*. T_c is higher for smaller values of μ^*. The higher value of the $\mu^*$is the result of the increased electron-phonon repulsive contribution alongwith the intramolecular phonons producing an attractive interaction. This attractive interaction is reduced alone against the phonon attraction and attributes to supress T_c. Higher and positive μ^* implies a constant repulsive interaction that is insufficient to create a superconductivity state despite of coupling of intramolecular phonons. This shows that the Coulombs psudopotential parameter is an important concept in fullerides. It appear from Table 2 that T_c is strongly sensitive to λ_{ra} even for moderate coupling. One can see that for fixed value of λ_{ra} = 0.35 one gets T_c = 30.48 K for μ^* = 0.0, T_c = 23.27 K for μ^* = 0.1 and T_c = 19.29 for μ^* 0.2. Thus, it appears that if one start with a pure inramolecular

phonon mechanism and later on adding a correction term with moderetly coupled a inramolecular phonons. One can easily inhance T_c value. In table 1, we shown the transition temperature T_c of some alkali metal doped C_{60} compound using equation (9), we have evaluated the isotope effect exponent 'α' for K_3C_{60} as a function of μ^* keeping, the fixed value of $\lambda_{er} = 1.2$ and $\lambda_{ra} = 0.4$. The result are shown in Table 3. Our theoretically evaluated results show that isotope exponent α decreases with increase value of μ^*. Our theoretically obtained result is in agreement with the experimental data[14] and also with other theoretical workers[15,16]. In table 4, we have given the values of energy gap parameter $2\Delta/T_c$ obtained with various experimental studies[17-26] for Rb_6C_{60} and K_3C_{60} compounds.

Table 1: Transition temperature T_C of some alkali metal doped C_{60} compounds

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

Table 2: An evaluated result of superconducting transition temperature T_C as a function of λ_{ra} (intramolecular coupling constant) for different values of coulomb repulsive parameter μ^*. The result are compared with alkali doped C_{60} (K_3C_{60})

λ_{er}	Theory T_c (K)				Expt. T_c (K)
	$\mu^* = 0.0$	$\mu^* = 0.1$	$\mu^* = 0.2$	$\mu^* = 0.3$	
0.00	11.25	6.78	4.78	3.25	20.0
0.10	13.68	9.49	7.16	5.10	20.0
0.20	16.38	12.58	10.24	6.28	20.0
0.25	21.59	16.16	12.59	8.46	20.0
0.30	24.26	18.25	15.56	10.29	20.0

Cont…

λ_{er}	Theory T_c (K)				Expt. T_c (K)
	$\mu^* = 0.0$	$\mu^* = 0.1$	$\mu^* = 0.2$	$\mu^* = 0.3$	
0.35	30.48	20.16	17.18	12.50	20.0
0.40	35.12	23.27	19.29	14.56	20.0
0.45	38.46	27.18	21.86	16.29	20.0
0.50	42.56	31.56	24.28	18.58	20.0
0.55	48.29	33.29	27.47	22.25	20.0
0.60	52.18	37.54	31.26	25.18	20.0
0.65	58.29	43.56	34.18	29.56	20.0
0.70	62.17	48.28	38.56	31.48	20.0
0.75	67.29	54.62	40.14	35.29	20.0
0.80	70.18	59.10	44.25	40.15	20.0

Table 3: An evaluated result of isotope effect exponent α as a function of Coulomb pseudopotential parameter μ^* for K_3C_{60} Fulleride, $\lambda_{er} = 1.2$, $\lambda_{ra} = 0.4$

μ^*	Isotope exponent α
0.00	0.525
0.025	0.517
0.050	0.502
0.075	0.476
0.10	0.457
0.12	0.405
0.14	0.386
0.15	0.325
0.16	0.305
0.18	0.269
0.20	0.248
0.22	0.207
0.24	0.196
0.25	0.108

Table 4: An experimental result of energy gap parameter $2\Delta/T_C$ for various alkali doped fulloride

Fulleride	$2\Delta/T_C$	References	
Rb_6C_{60}	5.3	Z. Zang et al.	1991
	5.4	Jess et al.	1994
	2.0-4.0	Jess et al.	1996
	4.3	Tycho et al.	1992
	3.6	Kiefl et al.	1993
	3.48	Degorgi et al.	1995
	4.1	Gu et al.	1994
K_3C_{60}	3.0	Tycko et al.	1992
	4.7	Sasaki et al.	1994
	3.4 ± 0.4	Ausen-Sinzie et al.	1993
	3.44	Degiorgi et al.	1994
$(2\Delta/T_C)_{BCS} = 4.2$			

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Revised : 13.06.2012 *Accepted : 14.06.2012*