



# **CALCULATION OF STRUCTURAL FORCES AND JUMP LIMIT BETWEEN TWO FULLERENE SURFACES IN VARIOUS LIQUIDS**

**A. GUHA<sup>\*</sup> and A. MUKHERJEE<sup>a</sup>**

JIS College of Engineering, KALYANI - 741 235, Dist.: Nadia (W.B.) INDIA

<sup>a</sup>Central Drugs Laboratory, KOLKATA - 700 016 (W.B.) INDIA

## **ABSTRACT**

Structural forces and jump limit between two fullerene surfaces in various liquids have been calculated using Lifshitz theory. Hamaker constant of 15 liquids and jump limits of 5 liquids are reported here.

**Key words:** Fullerene surface, Structural forces, Jump limit.

## **INTRODUCTION**

The carbon nanotubes are important material of study during the last few years considering its application in engineering. This cylindrical carbon molecules have novel properties that make them potentially useful in many applications in nanotechnology, electronics, optics and other fields of materials science. They exhibit extraordinary strength and unique electrical properties, and are efficient conductors of heat. The carbon nanotubes are members of fullerene structure family. Spherical fullerenes are called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of a sheet of linked hexagonal rings, but may also contain pentagonal (or sometimes heptagonal) rings that would prevent a sheet from being planar. One of the most fascinating and unique feature of fullerene is that there is spherical empty space inside the carbon cage. This hollow space, ranges from 0.4 to 1.0 nm in diameter for C<sub>60</sub> to C<sub>240</sub>. Such a characteristic of fullerene implies intuitively an idea of stuffing atoms into its empty space so as to alter the molecular and solid state properties of

---

\* Author for correspondence; E-mail: drasit\_guha@yahoo.co.in; mukherjeeashish@yahoo.co.in

the fullerenes, resulting in the formation of a brand new family- endohedral fullerene. As the novel form of fullerene-based materials, endohedral fullerenes represent a novel type of nanostructure, which are characterized by a robust fullerene cage with atoms, ions, or clusters trapped in its hollow. Because of the electron transfer from the encaged species to the fullerene cage, this new type of molecules has opened many possibilities for research and has been attracting the wide interest not only in the physics and chemistry but also in the area of materials and biological sciences. Considering the above, the behaviour of fluids in between the two fullerene surfaces are to be studied in this paper. The van der Waals forces, which determines the properties of fullerenes, required to be studied. Obviously, the role of Hamaker's constant, which has the major contribution for van der Waals forces requires proper attention.

### **Theory: Dispersion forces between two macroscopic materials –**

#### **Lifshitz approach**

A more accurate approach through a purely macroscopic framework has been constructed by Lifshitz<sup>1</sup>. Lifshitz treated the interacting bodies as continuous media. The dispersion forces in this approach have been derived in terms of the macroscopic properties of interacting bodies, such as their dielectric constants or refractive indexes.

Lifshitz<sup>1</sup> calculated interaction energy using quantum mechanical and electromagnetic approach. The basic idea lies in the fact that oscillation of electrons around a nucleus creates an oscillation of the electromagnetic field around an atom. This electromagnetic field is not only present within any medium due to thermodynamic fluctuations; it is also present to outside of the medium. Maxwell's equations, where the electric and magnetic fields are subjected to fast temporal fluctuations is the origin of Lifshitz's theory of condensed media interactions. In order to accommodate the temporal fluctuations of the fields, Lifshitz has adopted the fluctuation theory developed by Rystov<sup>2</sup>. The derivation of Lifshitz model is beyond the scope of this work. A general expression for the free energy of interaction between two flat surfaces is given by –

$$\Delta G = -\frac{A}{12\pi H^2} \quad \dots(1)$$

Here, 'H' is the distance of separation between two surfaces.

The Hamaker constant,  $A$ , may be designated as  $A_{132}$  and  $A_{131}$  for the interactions between materials 1 and 2 in a medium 3 and materials 1 and 1 in a medium 3, respectively. The Lifshitz theory gives<sup>6</sup>.

$$A_{132} = \frac{3}{4} K_B T \left( \frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right) \left( \frac{\epsilon_2 - \epsilon_3}{\epsilon_2 + \epsilon_3} \right) + \frac{3h\nu_e^{sl}}{8\sqrt{2}} \frac{(n_1^2 - n_3^2)(n_2^2 - n_3^2)}{(n_1^2 + n_3^2)^{\frac{1}{2}}(n_2^2 + n_3^2)^{\frac{1}{2}} \left\{ (n_1^2 + n_3^2)^{\frac{1}{2}} + (n_2^2 + n_3^2)^{\frac{1}{2}} \right\}} \quad \dots(2)$$

and

$$A_{131} = \frac{3}{4} K_B T \left( \frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right)^2 + \frac{3h\nu_e^{sl}}{16\sqrt{2}} \frac{(n_1^2 - n_3^2)^2}{(n_1^2 + n_3^2)^{\frac{3}{2}}} \quad \dots(3)$$

where  $\epsilon_1$ ,  $\epsilon_2$  and  $\epsilon_3$  are the dielectric constants of the three media and  $n_1$ ,  $n_2$  and  $n_3$  are the refractive indexes of the same. In each of Eqs. (2) and (3), the first term on the right hand side gives the zero-frequency energy of the van der Waals energy (which includes the Keesom and Debye interaction energies), while the latter term represents the dispersion energy, which includes London energy contribution.  $\nu_e$  is the absorption frequency in the UV region. In our calculation, we have used ' $\nu_e^{sl}$ ' in place of ' $\nu_e$ ' where  $\nu_e^{sl}$  is the absorption frequency of solid-liquid interaction can be expressed as follows :

$$\nu_e^{sl} = \frac{2\nu_e^{ss}\nu_e^{ll}}{(\nu_e^{ss} + \nu_e^{ll})} \quad \dots(4)$$

Where  $\nu_e^{ss}$  and  $\nu_e^{ll}$  are the absorption frequencies of 'solid-solid' and 'liquid-liquid' interactions and these values has been listed in Table 2.

## Calculation

### Calculation of absorption frequency

From definition, we know that ' $h\nu$ ' is approximated by ionisation potential of molecule, ' $I$ '. So,

$$\begin{aligned}
 hv &= I \\
 \therefore v &= \frac{I}{h} \qquad \dots(5)
 \end{aligned}$$

Where, 'h' is Planck's constant ( $\equiv 6.626 \times 10^{-34}$ JS).

So, to calculate the absorption frequency ( $\nu$ ) from Eq. (5), the ionisation potential (I) of the molecule is to be calculated.

### Calculation of ionisation potential

The calculation of ionization potential is based on the hypothesis presented here is that certain molecular properties can be predicted from the sum of the corresponding values of the inert gas atom counterparts of the bonded constituent atoms. It is the same way as the additivity of molar refraction and bond polarizabilities was presented and is accepted.

Molecules may be considered to be composed of bonded atoms that have achieved an inert-gas electronic configuration. So, the electronic properties of molecules are the function of the electronic properties of the inert-gas atoms, whose structures have been achieved. In other words, from an electronic stand-point, each atom of a molecule may be replaced by its inert-gas counterpart. According to Kitaigorodsky<sup>3</sup> 'the patterns of electronic density can be represented as the superposition of spherically symmetric atoms. However, the above mentioned principle may be complicated by the presence of electrons, such as in  $\pi$ -bonds, that cannot be associated with the inert gases and separate discussions must be made for that.

The London<sup>4</sup> dispersion potential ( $3\alpha^2Iz^{-6}/4$ ) has been rewritten as  $\langle m^2 \rangle \alpha z^{-6}/2$ , where the mean-square electric moment,  $\langle m^2 \rangle$ , is given by -

$$\langle m^2 \rangle = \frac{3}{2} \alpha I \times 1.6022 \times 10^{-12} \text{ ergs cc} \qquad \dots(6)$$

where molecular/atomic polarizability,

$$\alpha = \left( \frac{n^2 - 1}{n^2 + 2} \right) \left( \frac{M}{\rho_d} \times \frac{3}{4\pi N_A} \right)$$

Here,  $I$  = First ionization potential in e.V.,  $M$  = Molecular weight,  $\rho_d$  = Density in gm/cc,  $N_A$  = Avogadro number and  $n$  = Refractive index.

According to the hypothesis mentioned above, the mean square moments of the corresponding inert-gas atoms:

$$\langle m^2 \rangle = \sum \langle m^2 \rangle_{\text{inert}} \quad \dots(7)$$

in which the summation is over all  $i$  inert gas atoms corresponding to the bonded-atom constituents of the molecule. In case of polyatomic molecules also, the London's dispersion potential can be extended. Here, it is necessary to specify the anisotropic properties of the bonded species. This problem is overcome in the present approach by representing bonded atoms by the inert-gas atoms, for which only isotropic properties are needed.

Using the values of  $\langle m^2 \rangle_{\text{inert}}$  and with Eq. (7) the mean-square electric dipole moments for an extensive range of molecules has been calculated and are given in Table 1. The agreement between the experimental and calculated mean-square moment values is satisfactory, except in a few cases, which will be discussed now. The majority of molecule listed in Table 1 are essentially saturated and can be represented by the direct replacement of bonded atoms by the corresponding inert gas atoms. In case of ethanol, oxygen (O) and carbon (C) belong the same period of the periodic table. So, 'O' as well as 'C' is assumed to achieve the electronic consideration of neon (Ne), which is present in the same period along with 'C' and 'O'. The calculation of  $\langle m^2 \rangle$  of ethanol has been made by considering three carbon atoms, which has been mentioned in Table 1. Here, we have taken the value of  $\langle m^2 \rangle$  of helium (He) and neon (Ne) as 12.111 ergs cc and 20.450 ergs cc, respectively. However, in case of benzene, in which additional electrons, in this case in the  $\pi$  system, have to be accounted for through the following hypothesis.

According to Eq. (7), the inert-gas atoms only replace the bonded atoms of the sigma skeleton, any additional electrons must be accounted for separately.

In case of  $\pi$ -systems, the each of these extra electrons can be accounted for by assigning to the mean-square molecular moment one quarter of the value for the associated inert-gas atom. In order to accommodate this fact Eq. (7) is extended to Eq. (8).

$$\langle m^2 \rangle_E = \sum \langle m^2 \rangle_{\text{inert}} \pm 0.25 \sum \langle m^2 \rangle_{\text{inert}} \quad \dots(8)$$

Table 1: Table of ionization potential for some compounds

Compd.	C	H	$\langle m^2 \rangle 10^{-36}$ ergs cc	R. I. (n)	Mol. Wt. (M)	Density ( $\rho_d$ ) gm/cc	Molar Vol. (M/ $\rho_d$ ) cc	I.P.(Calc) (e.V)	I.P.(Expt.) (e.V)	Abs. Freq. $10^{15} \text{ sec}^{-1}$
Pentane	5	12	247.582	1.3575	72.15	0.626	115.219	10.287	10.35	2.487
Hexane	6	14	292.254	1.3749	86.18	0.659	130.695	10.259	10.18	2.480
Heptane	7	16	336.926	1.3877	100.21	0.684	146.549	10.237	10.07	2.475
Octane	8	18	381.598	1.3870	114.23	0.703	162.605	10.466	10.24	2.530
Nonane	9	20	426.27	1.406	128.26	0.718	178.735	10.194	10.21	2.465
Decane	10	22	470.942	1.4120	142.29	0.730	194.891	10.196	9.60	2.465
Benzene	7.5	6	226.041	1.5010	78.11	0.874	89.401	9.010	9.25	2.178
Dodecane	12	26	560.286	1.4110	170.41	0.749	227.517	10.413	-	2.518
Tetradecane	14	30	649.63	1.4180	198.4	0.763	260.128	10.405	-	2.516
Cyclohexane	6	12	268.032	1.4262	84.16	0.779	108.091	10.157	9.90	2.456
Ethanol	3	6	134.016	1.3614	46.07	0.789	58.361	10.886	10.62	2.632
Fullerene	75	0	1533.75	2.2000	720	1.770	406.780	7.051	7.58	1.705
C	=	Number of carbon atoms.				Density	=	Density of molecule (Ref.-13)		
H	=	Number of hydrogen atoms				Mol. Vol	=	Molar volume of molecule		
$m^2$	=	Mean square moment of cor responding inert gas atom (Eq. -7 & 8).				I.P.(Calc)	=	Ionization potential (e.V.) from Equation (Eq.-9)		
R.I	=	Refractive index.(Ref.-12,13)				I.P.(Expt)	=	Ionization potential (e.V.) (Ref.-14)		
Mol.Wt.	=	Molecular weight of molecule (Ref.-13)				Abs. Freq	=	Absorption frequency ( $10^{15} \text{ s}^{-1}$ ) (eq.-5 & 9)		

where the (+) sign accounts for extra electrons as in  $\pi$ -bonds or anions and the (-) sign accounts for the lack of electrons as in cations. For example, in the case of benzene with six 'extra'  $\pi$ -electrons, this molecule is represented by  $\text{Ne}_{7.5}\text{He}_6$ , for which Eq. (8) gives the calculated ( $7.5 \times 20.45 + 6 \times 12.111$ ) value of 226.04, which compares favourably with the molecular value of 230.88 deduced using the experimental molecular parameters.

The ionisation potential,  $I$  in e.V. may be expressed as follows from Eq. (6) :

$$I = \frac{2}{3} \times \frac{1}{1.6022 \times 10^{-12}} \times \left[ \left( \frac{n^2 + 2}{n^2 - 1} \right) \left( \frac{\rho_d}{M} \times \frac{4\pi N_A}{3} \right) \right] \times \langle m^2 \rangle \quad \dots(9)$$

' $n$ ' is the refractive index of materials and ' $N_A$ ' is the Avogadro number. The values of mean square moment,  $\langle m^2 \rangle$  and ionization potential,  $I$  of various compounds have been tabulated in Table 1. It has been noticed that the calculated value of ionization potential is very similar to the experimental value<sup>5</sup>.

So, to calculate the value of absorption frequency from Eq. (5), we put the values of Ionisation potential from Eq. (9). The values of absorption frequency ( $\nu_e$ ) have been tabulated in Table 1.

### Hamaker constant of materials in between fullerene

Lifshitz theory<sup>6</sup> has been applied here to calculate the Hamaker constant of materials in between two fullerene surfaces which is given by, eq. (3)

$$A_{131} = \frac{3}{4} K_B T \left( \frac{\epsilon_1 - \epsilon_3}{\epsilon_1 + \epsilon_3} \right)^2 + \frac{3h\nu_e^{sl}}{16\sqrt{2}} \frac{(n_1^2 - n_3^2)^2}{(n_1^2 + n_3^2)^{3/2}}$$

Where,  $A_{131}$  is the Hamaker constant of materials '3' in between a medium of same compound '1'. ' $K_B$ ' is the Boltzmann constant ( $= 1.38 \times 10^{-23}$  J/K) 'T' is the temperature in 'K'. 'h' is the Planck's constant ( $= 6.626 \times 10^{-34}$  JS),  $\epsilon_1$  and  $\epsilon_3$  are the dielectric constants of materials '1' and '3' and  $n_1$  and  $n_3$  are the refractive indices of materials '1' and '3'. Dielectric constants and refractive indices for some compounds are given in the Table 2. ' $\nu_e^{sl}$ ' is the absorption frequency of solid liquid interactions in u.v. region, which has been calculated from Eq. (4). Where  $\nu_e^{ll}$  and  $\nu_e^{ss}$  are the absorption frequencies of liquid-liquid and solid-solid interactions, those are calculated from Eq. (5) and have been tabulated in Table 2.

In this section, the Hamaker constant of some liquids between two fullerene surfaces has been calculated using Eq. (3). In Eq. (3), '1' represents the fullerene surfaces and '3' represents the liquid taken in between fullerene surfaces. The values of Hamaker constant (A) of different liquids has been tabulated in Table 3 in between fullerene surfaces.

**Table 2: Physical properties of some compounds**

Compound	Dielectric constant	Refractive index	Abs. Freq. ( $\nu$ ) ( $10^{15}\text{s}^{-1}$ )
Pentane	1.8400	1.3575	2.487
Hexane	1.8904	1.3749	2.480
Heptane	1.9265	1.3877	2.475
Octane	1.9500	1.3870	2.530
Nonane	1.9768	1.4060	2.465
Decane	1.9937	1.4120	2.465
Dodecane	2.0100	1.4110	2.518
Tetradecane	2.0300	1.4180	2.516
Hexadecane	2.0500	1.4230	2.900 <sup>12</sup>
Cyclohexane	2.0300	1.4260	2.456
Benzene	2.2800	1.5010	2.178
Carbon tetrachloride	2.2400	1.4600	2.700 <sup>12</sup>
Acetone	21.0000	1.3590	2.900 <sup>12</sup>
Ethanol	26.0000	1.3610	2.632
Water	80.0000	1.3330	3.000 <sup>12</sup>
Fullerenes	4.5000	2.2000	1.705

**Table 3: Hamaker Constant of some compounds between two Fullerene Surfaces**

Compound	Hamaker constant A( $10^{-20}\text{J}$ )	Fig. No.
Pentane	9.2968	1
Hexane	8.8982	2
Heptane	8.6107	3

Cont...



Compound	Hamaker constant A( $10^{-20}$ J)	Fig. No.
Octane	8.7013	4
Nonane	8.2040	5
Decane	8.0772	6
Dodecane	8.1672	7
Tetradecane	8.0164	8
Hexadecane	8.3557	9
Cyclohexane	7.7735	10
Benzene	5.9867	11
Carbon tetrachloride	7.3526	12
Acetone	9.9042	13
Ethanol	9.5275	14
Water	10.7765	15

### Calculation of force

As earlier, it has been mentioned that the Lifshitz theory of van der Waals forces predicts a monotonically attractive force between any two similar bodies in a second medium. Accordingly, the force law as a function of separation between two surfaces is computed without considering the existence of discrete molecules, and interfaces are taken as infinitely sharp. The theoretical, non-retarded continuum van der Waals forces can be calculated from the Lifshitz theory. In a non-retarded approximation, the interaction free energy per unit area,  $E(H)$  between similar half spaces across a second medium is given by Lifshitz theory<sup>7,8</sup>.

$$E(H) = -\frac{A}{12\pi H^2} \quad \dots(10)$$

Where 'A' is the Hamaker constant and 'H' is the surface separation. The energy per unit area between flat surfaces can be related to the force between curved surfaces via the Derjaguin approximation<sup>9</sup>

$$2\pi E(H) = \frac{F(H)}{R} \quad \dots(11)$$

Where 'R' is the mean radius of curvature of the surfaces. From Eqs. (10) and (11), we obtain the standard equation for the force between two fullerene surfaces immersed in different liquids –

$$\frac{F(H)}{R} = -\frac{A}{6H^2} \quad \dots(12)$$

In Eq. (12), we put the value of Hamaker constant calculated from Eq. (3) and get the force curve  $F(H)/R$  (in force curves, we have used  $F/R$  in place of  $F(H)/R$  for simplicity) in mN/m with varying surface separation 'H'.

### Jump limit

#### Introduction

Surface force methods have been reviewed several times over the years. In recent years, much development occurs in instrumental method for surface force measuring techniques<sup>10</sup>. Force measurements can be assorted into various sub-divisions, such as direct and indirect, or according to the nature of the surfaces; solid and liquid surfaces, or macroscopic and colloidal. Three methods for such measurements dominate today, those are SFA (Surface Force Apparatus), MASIF (Measurement and Analysis of Surface Interaction and Forces) and AFM (Atomic Force Microscope).

The normal method of measuring force-distance profiles is to vary the separation continuously, and determine the spring deflection. An alternative method for attractive interactions is to vary the stiffness of the spring and determine the separations at which the two surfaces jump together. The spring is mechanically unstable, when the gradient of the force ( $dF/dH$ ) exceeds the spring stiffness ( $k$ ). For a van der Waals force, whose force law is given by  $F = -AR/6H^2$ , the jump occurs at a separation determined by -

$$k = \frac{dF}{dH} = \frac{AR}{3H_{\text{Jump}}^3} \quad \dots(13)$$

Where, 'k' is the spring constant, 'A' is the Hamaker constant, ' $H_{\text{Jump}}$ ' is the distance where the jump occurs, which is also called the Jump limit and R is the mean radius of the

curvature. Here, we have considered R is the radius of the liquid alkane ( $= \sigma_e/2$ ), where  $\sigma_e$  is the effective hard sphere diameter and has been calculated by Eq. (14)

$$\sigma_e = 1.1532\sigma_{LJ} \left[ 1 + \left( \frac{T^*}{0.527} \right)^{1/2} \right]^{-1/6} \quad \dots(14)$$

and has been tabulated in Table 4. So from Eq. (13), it has been seen that the calculation of jump limit mainly depends on the calculation of spring constant.

**Table 4: Physical parameters of alkanes**

Component	M	N	$\sigma_{LJ}$ (10-10m) <sup>15</sup>	$\epsilon/k$ (K) <sup>15</sup>	$\sigma_e$ (1010m)	T(K)	$\rho_d^{14}$	$\rho^*$	T*
Hexane	86.178	2.021	4.524	199.410	4.429	293	0.660	0.810	1.469
Heptane	100.205	2.085	4.701	205.780	4.610	293	0.684	0.840	1.424
Octane	114.232	2.119	4.892	213.160	4.806	293	0.703	0.872	1.375
Nonane	128.259	2.145	5.072	220.120	4.991	293	0.720	0.902	1.331
Decane	142.286	2.166	5.233	226.460	5.157	293	0.730	0.918	1.294

Where, M = Molecular weight; N = No. of segment of alkanes;  $\sigma_{LJ}$  = Diameter of molecule of each segment;  $\epsilon/K_B$  = Energy parameters ( $K_B$  = Boltzman Constant);  $\sigma_e$  = Effective hard sphere diameter (EHSD); T = Temperature in K;  $\rho$  = Density at g/cc;  $\rho^*$  = Reduced density =  $\frac{\rho X N_A X N X \sigma_e^3}{M X 10}$ , where  $N_A$  = Avogadro number; T\* = Reduced temperature =  $\frac{K_B X T}{\epsilon}$ .”

### Calculation of jump limit

It has been discussed earlier that the calculation of jump limit from Eq. (13) mainly depends on the spring constant value. If spring constant is known, then we can easily calculate the jump limit of various liquids in between two surfaces.

To calculate the spring constant of fullerene surfaces, it has been used here that the known value of jump limit of hexane in between two mica surfaces<sup>11</sup> is 5 nm. From that we can easily calculate the spring constant of mica surfaces immersed in hexane from Eq. (13).

The value of spring constant thus calculated for hexane in between two mica surfaces is  $0.00733 \times 10^{-3}$  N/mt.

The spring constant, calculated in the above mentioned way, has been used to calculate the jump limit of various liquids in between two fullerene surfaces (Tables 5).

**Table 5: Jump limit of some linear alkane between fullerene surfaces for spring constant  $0.00733 \times 10^{-3}$  N/m**

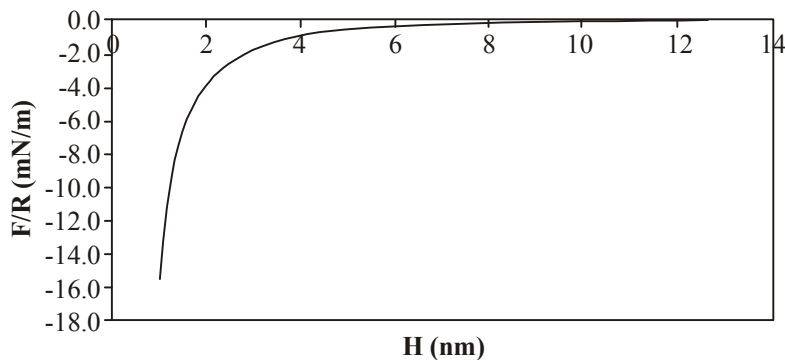
Compound	Effective diameter ( $\sigma_e$ ) (Å)	Hamaker constant (A) ( $10^{-20}$ J)	Jump limit (nm)
Hexane	4.429	8.8982	9.6409
Heptane	4.610	8.6107	9.6641
Octane	4.806	8.7013	9.8334
Nonane	4.991	8.2040	9.7646
Decane	5.157	8.0772	9.8205

## RESULTS AND DISCUSSION

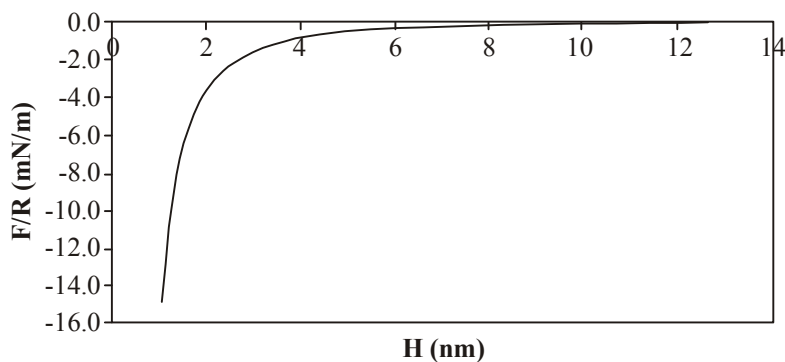
Previously, the force,  $F$  is measured as a function of surface separation  $H$  between two molecularly smooth surfaces immersed in the liquid in interest by using surface force apparatus. The description of apparatus and measuring techniques are stated in the paper of Horn and Israelachvili<sup>9</sup> and Christenson<sup>11</sup>, where we see an important term i.e. 'Jump Limit'. Here, the jump limit has also been calculated as per Eq. (13) for some linear alkanes in between fullerene surfaces.

**Pentane:** The force curve between two fullerene surfaces in pentane has been presented in Fig. 1. The Hamaker constant has also been calculated, which is 9.2968 in the order of  $10^{-20}$ J.

**Hexane:** The force curve between fullerene surfaces in hexane are presented in Fig. 2. The Hamaker constant has also been calculated, which is 8.8982 in the order of  $10^{-20}$ J. The jump limit has been calculated for hexane in between fullerene surface, which is 9.6409 nm.

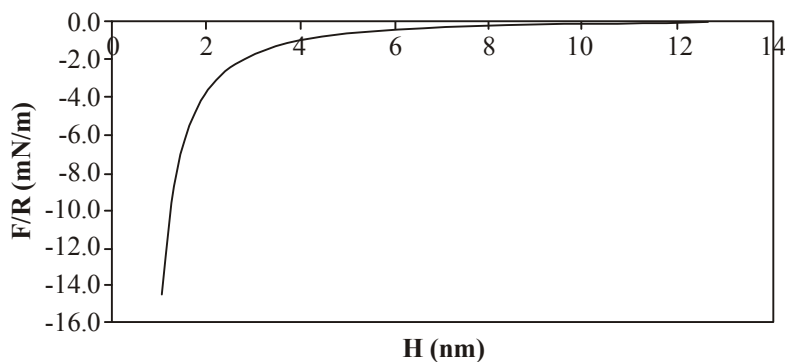


**Fig. 1: Force as a function of separation between fullerene surface in pentane**



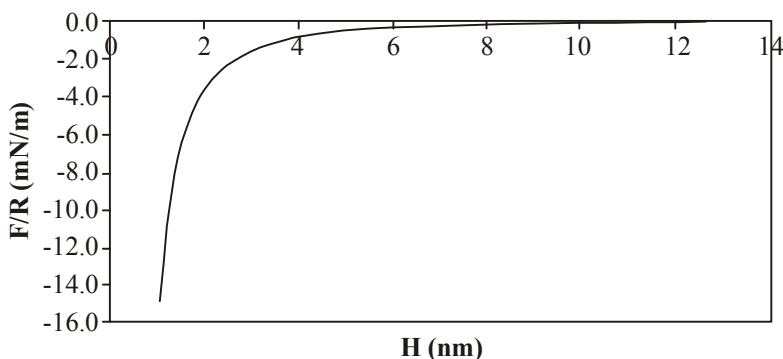
**Fig. 2: Force as a function of separation between fullerene surfaces in hexane**

**Heptane:** The force curve between fullerene surface is presented in Fig. 3. The Hamaker constant has also been calculated, which is  $8.6107$  in the order of  $10^{-20}$ J. We have also calculated the jump limit from Eq. (13), which is  $9.6641$  nm.



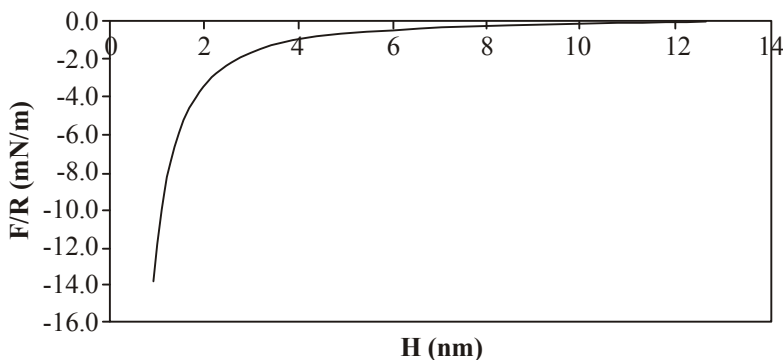
**Fig. 3: Force as a function of separation between fullerene surfaces in heptane**

**Octane:** The force curve between two fullerene surfaces is presented in Fig. 4. The Hamaker constant has also been calculated, which is  $8.7013$  in the order of  $10^{-20}\text{J}$ . We have also calculated the jump limit from Eq. (13), which is  $9.8334$  nm.



**Fig. 4: Force as a function of separation between fullerene surfaces in heptane**

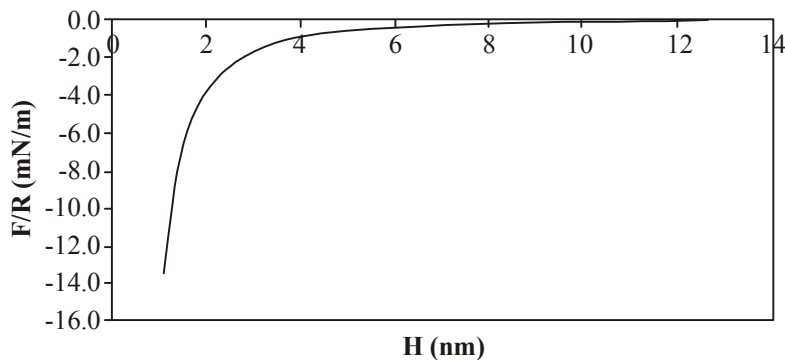
**Nonane:** The force curve between two fullerene surfaces in nonane is presented in Fig. 5. The Hamaker constant has also been calculated, which is  $8.2040$  in the order of  $10^{-20}\text{J}$ . The jump limit has been calculated from Eq. (13), which is  $9.7646$  nm.



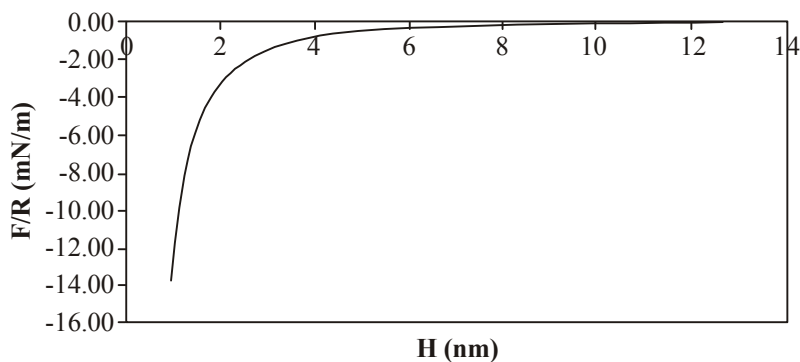
**Fig. 5: Force as a function of separation between fullerene surfaces in nonane**

**Decane:** The force curve between two fullerene surfaces is presented in Fig. 6. The Hamaker constant has also been calculated, which is  $8.0772$  in the order of  $10^{-20}\text{J}$ . We have also calculated the jump limit from Eq. (13), which is  $9.8205$  nm.

**Dodecane:** The force curve between two fullerene surfaces is presented in Fig. 7. The Hamaker constant has also been calculated, which is  $8.1672$  in the order of  $10^{-20}\text{J}$ .

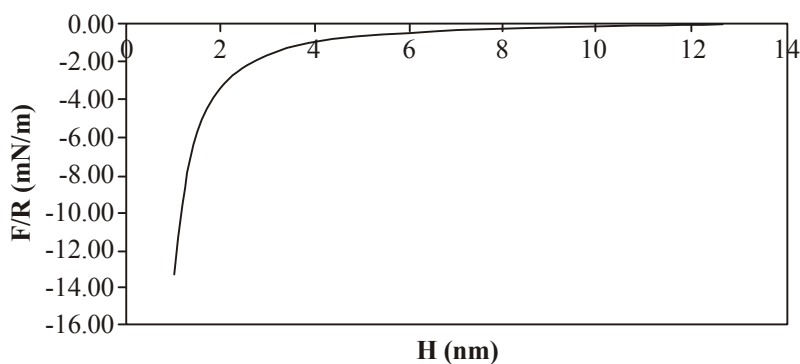


**Fig. 6: Force as a function of separation between fullerene surfaces in decane**



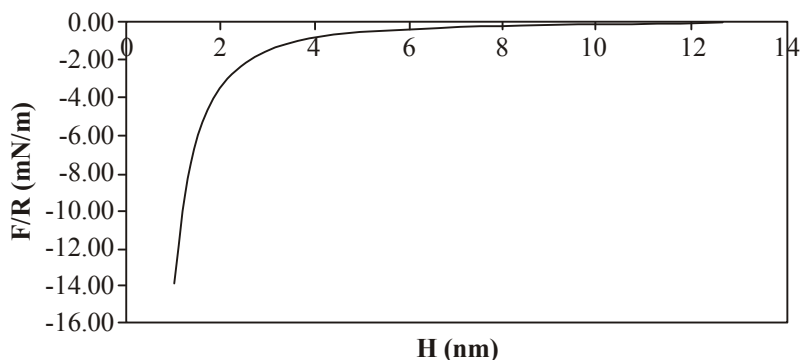
**Fig. 7: Force as a function of separation between fullerene surfaces in dodecane**

**Tetradecane:** The force curve between two fullerene surfaces is presented in Fig. 8. The Hamaker constant has also been calculated, which is  $8.0164$  in the order of  $10^{-20}$ J.



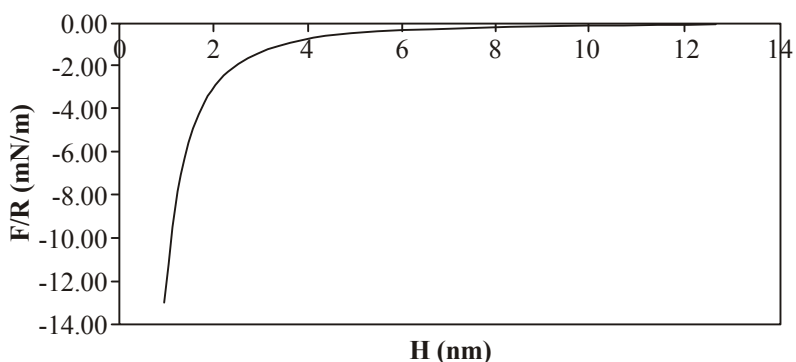
**Fig. 8: Force as a function of separation between fullerene surfaces in tetradecane**

**Hexadecane:** The force curve between two fullerene surfaces is presented in Fig. 9. The Hamaker constant has also been calculated, which is  $8.3557$  in the order of  $10^{-20}\text{J}$ .



**Fig. 9: Force as a function of separation between fullerene surfaces in hexadecane**

**Cyclohexane:** The force curve between two fullerene surfaces is presented in Fig. 10. The Hamaker constant has also been calculated, which is  $7.7735$  in the order of  $10^{-20}\text{J}$ .



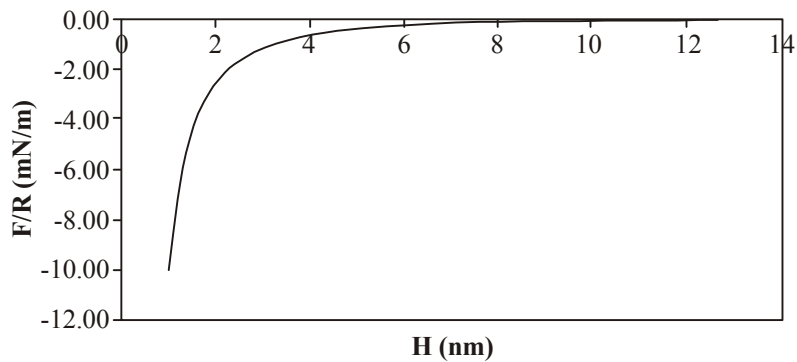
**Fig. 10: Force as a function of separation between fullerene surfaces in cyclohexane**

**Benzene:** The force curve between two fullerene surfaces is presented in Fig. 11. The Hamaker constant has also been calculated, which is  $5.9867$  in the order of  $10^{-20}\text{J}$ .

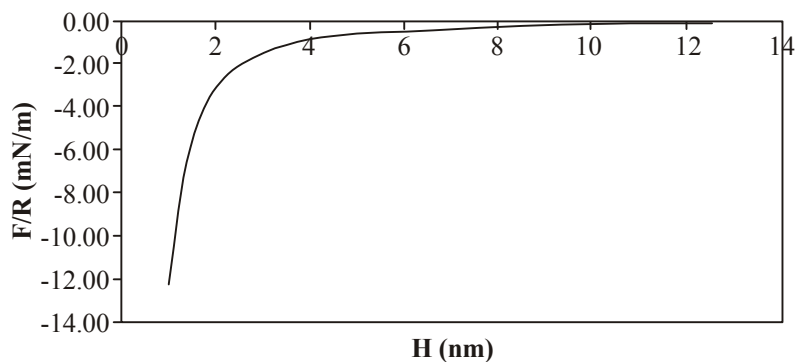
**Carbon tetrachloride:** The force curve between two fullerene surfaces is presented in Fig. 12. The Hamaker constant has also been calculated, which is  $7.3526$  in the order of  $10^{-20}\text{J}$ .

**Acetone:** The force curve between two fullerene surfaces is presented in Fig. 13. The Hamaker constant has also been calculated, which is  $9.9042$  in the order of  $10^{-20}\text{J}$ .

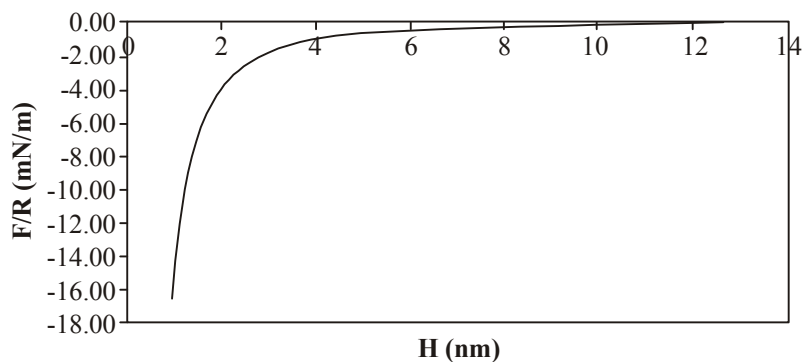




**Fig. 11: Force as a function of separation between fullerene surfaces in benzene**

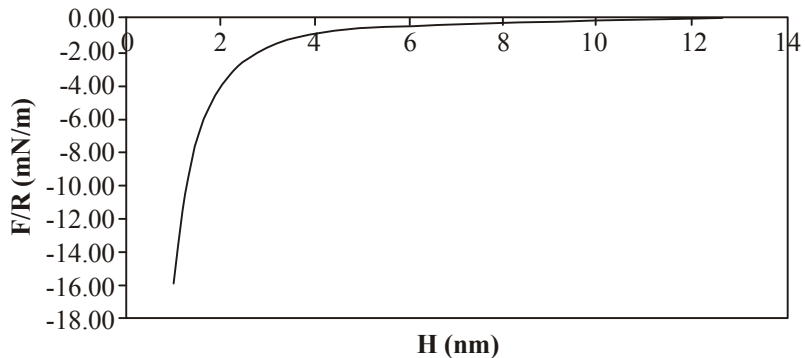


**Fig. 12: Force as a function of separation between fullerene surfaces in carbon tetrachloride**



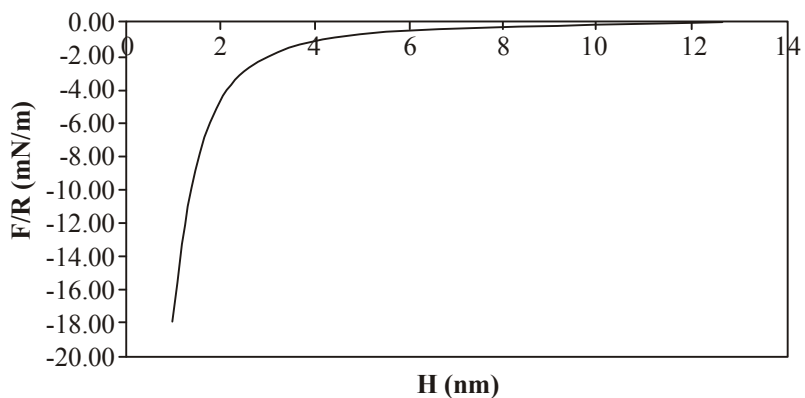
**Fig. 13: Force as a function of separation between fullerene surfaces in acetone**

**Ethanol:** The force curve between two fullerene surfaces is presented in Fig. 14. The Hamaker constant has also been calculated, which is 9.5275 in the order of  $10^{-20}$ J.



**Fig. 14: Force as a function of separation between fullerene surfaces in ethanol**

**Water:** The force curve between two fullerene surfaces is presented in Figure- 15. The Hamaker constant has also been calculated, which is  $10.7765$  in the order of  $10^{20}$ J.



**Fig. 15: Force as a function of separation between fullerene surfaces in water**

### REFERENCES

1. E. M. J. Lifshitz, *Exp. Theor. Phys.*, **29**, 94. (1955).
2. S. M. Rystov, *Theory of Electric Fluctuations and Thermal Radiations*, Moscow Academy of Science Press, Moscow (1953).
3. A. I. Kitaigorodsky, *Mol. Cryst. And Molecules* Academic Press, New York (1973).
4. F. London, *Trans. Faraday Soc.*, **33**, 8 (1937).
5. C. R. C. *Handbook of Chemistry and Physics*, CRC Press, Boca Raton, U.S.A, 71<sup>st</sup> Edition (1990-91).

6. J. N. Israelachvill, *Intermolecular and Surface Forces*, 2<sup>nd</sup> Edition, Academic Press, London (1991).
7. D. B. Hough and I. R. White, *Adv. Colloid Interface Sci.*, **14**, 3 (1980).
8. B. W. Ninham and V. A. Parsegian, *Biophys. J.*, **10**, 646 (1970).
9. R. G. Horn and J. N. J. Israelachvili, *Chem. Phys.*, **75**, 1400 (1981).
10. V. S. J. Craig, *Colloids and Surfaces A*, 129-130, 75 (1997).
11. H. K. Christenson, R. G. Gruendwr Horn and J. N. J. Israelachvili, *Chem. Phys.*, **87**, 1834 (1987).
12. J. N. Israelachvill, *Intermolecular and Surface Forces*, 2<sup>nd</sup> Edition, Academic Press, London (1991).
13. *Lange's Handbook of Chemistry*, McGraw-Hill Inc, New York (1985).
14. *C. R. C. Handbook of Chemistry and Physics*, 71<sup>st</sup> Edition, CRC Press, Boca Raton, U.S.A (1990-91).
15. Y. X. Yu and G. H. Gao, *Int. J. Thermophys.*, **21**, 57 (2000).

*Revised : 29.09.2009*

*Accepted : 03.10.2009*