

EFFECT OF PRESSURE ON THE STRUCTURE AND INTERMOLECULAR PHONONS IN SOLID C_{60}

YU.I.PRILUTSKII, V.A.ANDREEV, G.G.SHAPOVALOV

*Kiev Shevchenko University, Dept. of Physics,
64 Volodymyrska St., UA-252017 Kiev, Ukraine*

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The low-temperature orientationally ordered crystalline phase of fullerene C_{60} was investigated in dependence on the external pressure. The vibrational spectrum of C_{60} crystal was calculated using the group theory and atom-atom potentials methods. The frequencies of intermolecular modes as the functions of external pressure were studied. An assumption was made that the energy of the lattice includes two contributions: a Lennard-Jones (12-6) potential and electrostatic interaction of charges located on the single and double bonds of C_{60} molecule. The results obtained are in good agreement with the available experimental data.

1. Introduction

After the discovery of fullerene C_{60} molecules [1] a simple method was developed to condense them to a solid phase [2]. The appearance of superconductivity in alkali-doped fullerenes [3] led to considerable efforts to understand the different physical properties of these compounds as well as pristine C_{60} . The investigations of fullerenes are of great importance for extensive use of multi-atom carbon clusters in technics [4].

In the present paper the low-temperature orientationally ordered crystalline phase of fullerene C_{60} was studied using the atom-atom potentials method [5]. By means of the group theory methods [6] a calculation of the vibrational spectrum of fullerene C_{60} crystal was carried out in the approximation of an intermolecular potential which includes two contributions: a Lennard-Jones (12-6) potential and electrostatic interaction. The dependencies of C_{60} crystal lattice parameter and its intermolecular frequencies on the external pressure were investigated. The study of molecular dynamics under the high pressure give us the essential information about the intermolecular interaction, which is necessary to improve the phonon spectrum calculation for C_{60} crystal.

It is to be pointed out the great interest to the external vibrational spectra of solid fullerenes is due to the following reasons. First of all, they are necessary for the construction of intermolecular potentials which determines the molecular dynamics, elastic constants and thermodynamic properties of these systems [7-18]. Second, the superconductivity models remain actual, in which the low-frequency phonons are considered [19-21]. Besides, the

intermolecular vibrations are to be considered in the investigation of the dynamics of the triplet excited states in organic molecular crystals [22-23].

In the present paper the computer experiment for the investigation of structure and lattice dynamics of C_{60} crystal was analyzed. The results obtained were compared with the available experimental data [24-30].

2. Study of the equilibrium structure of fullerene C_{60} crystal

C_{60} molecule [1] is a basic element of the crystal structure of solid C_{60} . All 60 atoms of carbon are sited in the molecule on the surface of sphere with diameter of about 7 Å. They are arranged in 12 pentagons and 20 hexagons. The experiments on neutron scattering [31] carried out have shown each of 60 single bonds under the temperature $T = 3D4$ K have 1.46 Å in length composing 12 pentagons, and the rest 30 double ones are of 1.381 Å long being common for the neighbouring hexagons. It is to make a note the C_{60} molecule is stable under the hydrostatic pressure up to 200 kbar [32-35].

The solid C_{60} is a molecular crystal. It has fcc lattice at the room temperature and the molecules freely rotate in it. Having temperature decreased below $T_c = 3D250$ K the molecular reorientations cease [36-38] and fcc lattice changes to the simple cubic (sc) one: at $T = 3D4.2 - 5$ K the lattice constant is $a = 3D14.04$ Å, the number of molecules in the unit cell is $Z = 3D4$, the space symmetry group is Pa3 [25].

The orientationally ordered structure of solid C_{60} can be obtained as follows [24]. Start from a fcc crystal in which all molecules have their twofold axes aligned along the [100] crystallographic direction. Then the molecules centered at (0,0,0), (1/2,1/2,0), (0,1/2,1/2) and (1/2,0,1/2) are rotated through an angle $\varphi \neq 3D0^\circ$ about the [111], $[\bar{1}\bar{1}\bar{1}]$, $[\bar{1}\bar{1}1]$ and $[\bar{1}1\bar{1}]$ directions correspondingly. Each of molecules is in a symmetry position 3.

The sc structure of fullerene C_{60} crystal in dependence on the external pressure was investigated in experiments [32,39-42]. It was found that the solid C_{60} is stable when the external pressure is below 100 kbar. In the region above about 100 kbar, the C_{60} crystal transforms from a sc structure phase to a low-symmetry insulator phase [32, 39].

Let's write out the free energy of C_{60} crystal which is under the action of uniform external pressure P at the temperature T

$$F = 3DU(a, \varphi) + E - TS + PV, \quad (1)$$

where U is the lattice energy (the potential energy of interaction between the molecules), E is the vibrational part of energy, S is an entropy, $V = 3D\frac{a^3}{4}$ is a volume of the unit cell of cubic crystal per a molecule. At low temperatures the vibrations and entropy factor have not much significance and the equilibrium crystal structure is determined by the minimum of free energy \tilde{F} :

$$\tilde{F} = 3DU(a, \varphi) + \frac{Pa^3}{4}. \quad (2)$$

Within the framework of atom-atom potential method [5] the energy of interaction between the molecules is determined as a sum of pair interactions of atoms i and j which belong to the different molecules μ and μ' :

$$U = 3D \frac{1}{2} \sum_{\mu\mu'} U_{\mu\mu'} (|r_{\mu i} - r_{\mu' j}|). \quad (3)$$

Concerning the choice of the function $U_{\mu\mu'}$ the following should be mentioned. An attempt to use the intermolecular Lennard-Jones (12-6) potential which is known for graphite has shown this potential describes the molecular dynamics of C_{60} crystal insatisfactory [8]. Therefore, a discrimination between single and double bonds was taken into account by locating both additional interaction sites at the centers of the double bonds and charges at these centers and carbon atoms. For the further improvement of this model the authors [16] have proposed to consider Coulomb potential with accounting of the error function. The authors [15] besides the Lennard-Jones potential have taken into consideration the noncentral interaction which can appear due to overlapping the orbitals of neighbouring molecules. To solve the dynamic problem for C_{60} crystal the atom-atom Buckingham (6-exp) potential has been used too [14, 17-18].

In the present paper the function $U_{\mu\mu'}$ includes two contributions [12]: an atom-atom Lennard-Jones (12-6) potential and electrostatic potential of charges located on the single bonds and double ones

$$U_{\mu\mu'} = 3D4\varepsilon \sum_{i,j=3D1}^{60} \left[\left(\frac{\sigma}{|r_{\mu i} - r_{\mu' j}|} \right)^{12} - \left(\frac{\sigma}{|r_{\mu i} - r_{\mu' j}|} \right)^6 \right] + \sum_{m,n=3D1}^{90} \frac{q_m q_n}{|r_{\mu m} - r_{\mu' n}|}, \quad (4)$$

where $r_{\mu i}$ and $r_{\mu m}$ are the coordinates of i th carbon atom and m th bond center in molecule μ respectively, q_m is an effective charge of m th bond: it equals to q in the case of single bond and $-2q$ for the double one.

Minimizing the free energy (2) over parameters a and φ at a constant pressure was carried out in approximation of rigid molecules under the condition of remaining symmetry of the crystal. It was taken into account only twelve nearest neighbours of each C_{60} molecule located within the radius sphere $a/\sqrt{2}$. The contribution of more remote molecules is insignificant.

Our calculations showed that the following values of intermolecular potential parameters $\varepsilon=3D2.935$ meV, $\sigma=3D3.47$ Å and $q = 3D0.27 e$ (e is an elementary charge) give an opportunity to obtain the solid C_{60} structure close to experimental one in the absence of external pressure ($P = 3D0$) [24-25].

The figure 1 exhibits the dependence of the lattice energy U on the setting angle of molecules φ at $P = 3D0$. As we can see the minimum of the lattice energy equals to $U_{min} = 3D - 1911$ meV. It is reached at $\varphi = 3D23.8^\circ$. This minimum is due to the contribution of a Lennard-Jones (12-6) potential on about 90 per cents (the curve 1 on figure 1). The result obtained is in good agreement with the available experimental data: $\varphi = 3D26^\circ$ [24] and $\varphi = 3D22^\circ$ [25] at the temperature $T = 3D4.2 - 5$ K.

The figure 2 represents the dependence of the crystal lattice parameter on the external pressure. When the pressure is increased from 0 to 100 kbar the lattice constant decreases with a rate of 0.004-0.014 Å/kbar. It must be pointed out that at pressure $P = 3D100$ kbar the volume of C_{60} crystal decreases on about 15 per cents in comparison with its initial one.

3. Study of the vibrational spectrum of fullerene C_{60} crystal

Let's calculate the vibrational spectrum of solid C_{60} using the obtained structure. In the harmonic approximation the frequencies and eigenvectors

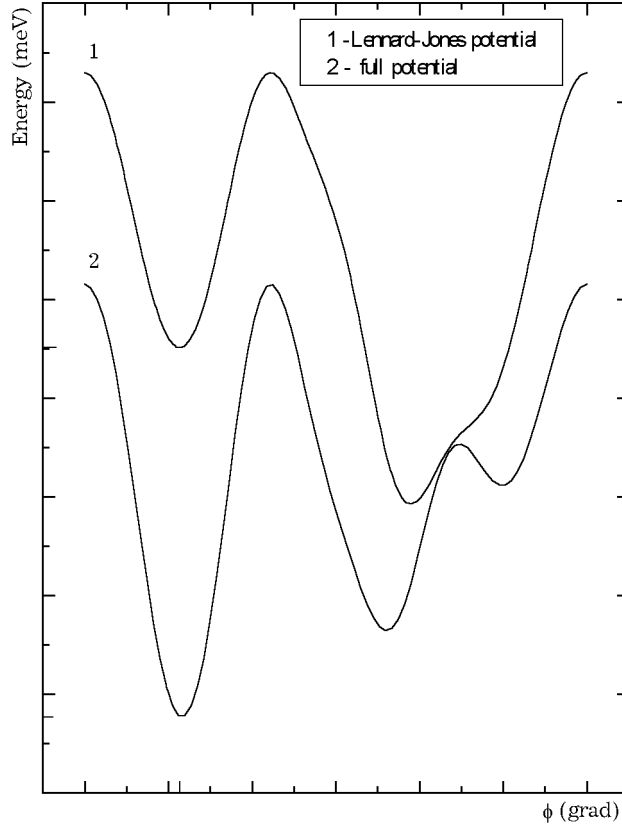


Figure 1. Dependence of the lattice energy on the setting angle of molecules calculated by the atom-atom potentials method at the temperature $T = 3D4.2 - 5$ K and external pressure $P = 3D0$.

of crystal vibrations can be found from the equation [5]

$$\omega^2 e_{\mu s} = 3D \sum_{\mu' s'} D_{\mu s \mu' s'} e_{\mu' s'}, \quad (5)$$

where $e_{\mu s}$ is the s th component of displacement vector of the μ th molecule, $D_{\mu s \mu' s'}$ is a symmetric dynamic matrix which describes the elastic interaction at translational and librational motions of the molecules and their coupling:

$$D_{\mu s \mu' s'} = 3D(M^s M^{s'})^{-1/2} \sum_b \Lambda_{\mu s \mu' s'}^b e^{i\vec{k}\vec{R}_b}. \quad (6)$$

Here the sum is carried out over all units of the C_{60} crystal. M^s means either mass of the C_{60} molecule ($M = 3D720$ a.u.m) if index s corresponds to the translational motions or the inertia moments of this molecule ($I_x = 3DI_y = 3D6.2 \cdot 10^3 \text{ \AA}^2$ a.u.m., $I_z = 3D5.9 \cdot 10^3 \text{ \AA}^2$ a.u.m., $z \parallel C_2$) if index s corresponds to the librational motions. The values of the force constants $\Lambda_{\mu s \mu' s'}^b$ are calculated in the equilibrium state according to the

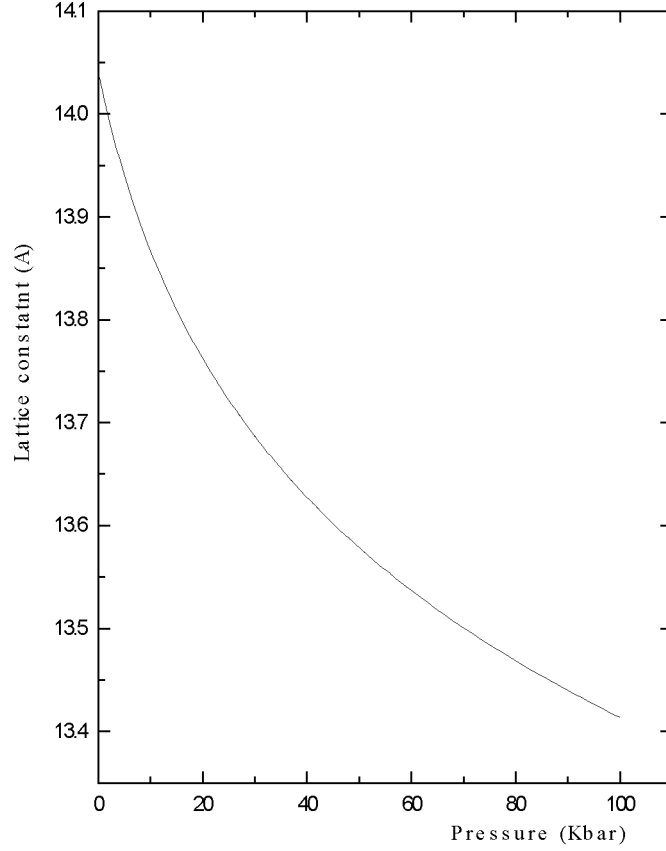


Figure 2. Calculated dependence of the lattice constant on the external pressure at the temperature $T = 3D4.2-5$ K.

formulas [43]. At the value of wave vector $\vec{k} = 3D0$ the dynamic problem (5) is solved for translational and librational motions of the molecules in a crystal separately.

The symmetry analysis of the dynamic matrix of solid C_{60} [11] has shown that for the pure librational vibrations of the lattice of C_{60} crystal its symmetry dynamic matrix of order 12×12 consists of eight independent components only:

$$\begin{aligned} d_1 &= 3DD_{1x1x}; & d_2 &= 3DD_{1x1y}; & d_3 &= 3DD_{1x2x}; & d_4 &= 3DD_{1x2y}; \\ d_5 &= 3DD_{1x2z}; & d_6 &= 3DD_{1x3x}; & d_7 &= 3DD_{1x3z}; & d_8 &= 3DD_{1x4x}. \end{aligned} \quad (7)$$

For the pure translational vibrations of the lattice of C_{60} crystal its symmetry dynamics matrix of order 12×12 includes only five independent components (the additional conditions on the dynamic matrix elements appear owing to the existence of threefold degenerated acoustic mode) [11]:

$$d_1 + d_3 + d_6 + d_8 = 3D0; \quad d_7 = 3D - d_2; \quad d_5 = 3Dd_4. \quad (8)$$

The classification of intermolecular modes at $\vec{k}=3D0$ can be found by a positional symmetry method [6]

$$= 83 = 3DA_g + E_g + 3F_g + A_u + E_u + 3F_u, \quad (9)$$

where the even (g) representations are related to the librational modes and odd (u) ones to the translational modes of C_{60} molecule in a crystal. All even modes are Raman active, one of the F_u modes is acoustic and only two modes F_u are infrared active.

Finally, for undegenerated modes A_g and A_u the frequencies are equal to [11]:

$$\begin{aligned} \omega^2(A_g) &= 3D \quad d_1 + 2d_2 + d_3 - 2d_4 - 2d_5 - d_6 - 2d_7 - d_8, \\ \omega^2(A_u) &= 3D \quad 2(d_1 + 2d_2 + d_3 - 2d_4). \end{aligned} \quad (10)$$

For twofold degenerated modes E_g and E_u the frequencies are equal to [11]:

$$\begin{aligned} \omega^2(E_g) &= 3D \quad d_1 - d_2 + d_3 + d_4 + d_5 - d_6 + d_7 - d_8, \\ \omega^2(E_u) &= 3D \quad 2(d_1 - d_2 + d_3 + d_4). \end{aligned} \quad (11)$$

For threefold degenerated modes F_g and F_u the frequencies can be found from the following characteristic equation:

$$\begin{vmatrix} C_{11} - \omega^2 & C_{12} & C_{13} \\ C_{12} & C_{22} - \omega^2 & C_{23} \\ C_{13} & C_{23} & C_{33} - \omega^2 \end{vmatrix} = 3D0, \quad (12)$$

where for the librational vibrations

$$\begin{aligned} C_{11} &= 3Dd_1 + d_3 + d_6 + d_8; & C_{22} &= 3Dd_1 - d_3 + d_6 - d_8; \\ C_{12} &= 3Dd_2 - d_4 + d_5 + d_7; & C_{23} &= 3Dd_2 + d_4 + d_5 - d_7; \\ C_{13} &= 3Dd_2 + d_4 - d_5 + d_7; & C_{33} &= 3Dd_1 - d_3 - d_6 + d_8, \end{aligned} \quad (13)$$

and for the translational vibrations with account of expression (8) we have:

$$\begin{aligned} C_{11} &= 3DC_{12} = 3DC_{13} = 3D0; & C_{22} &= 3D2(d_1 + d_6); \\ C_{23} &= 3D2(d_2 + d_4); & C_{33} &= 3D - 2(d_3 + d_6). \end{aligned} \quad (14)$$

The obtained expressions (13) and (14) differ from the result [11] owing to multiple choice of the normal vibrations forms for the C_{60} crystal [44]. They have more simple form in our case.

The obtained above parameters for the potential (4) turned out to be unsatisfactory for the calculation of intermolecular frequencies being compared with the experimental data [27]. By means of potential simulation the following values were received: $\varepsilon = 3D0.059$ meV and $q = 3D0.03$ e (the value of σ was remained constant).

The calculated intermolecular frequencies of C_{60} crystal in the Brillouin zone center at $T = 3D4.2 - 5$ K and $P = 3D0$ are represented in table 1. It is seen that all translational modes are located higher then the librational ones. The values obtained for the frequencies are distinguished from the experimental data [26-29] up to 7 percents.

The analysis of formulas (10),(11),(12) and (14) has shown the frequencies of translational modes satisfy the following expressions:

Table 1. Frequencies (in cm^{-1}) of intermolecular modes $\vec{k} = 3D0$ calculated by the atom-atom potentials method at the temperature $T = 3D4.2 - 5$ K and external pressure $P = 3D0$.

symmetry	theory	experiment
	$T = 3D4.2 - 5K$	[27] $T = 3D10K$
A_u	35.0	
E_u	46.7	
F_u	42.9	40.8
F_u	51.0	54.8
A_g	18.6	18.5
E_g	18.5	
F_g	17.1	
F_g	17.5	
F_g	22.0	21.8

$$\begin{aligned} \{3[\omega_1^2(F_u) + \omega_2^2(F_u)] + 2\omega^2(E_u) + \omega^2(A_u)\} / 12 &= 3D \quad d_1, \\ \{2\omega^2(E_u) + \omega^2(A_u) - 3[\omega_1^2(F_u) + \omega_2^2(F_u)]\} / 12 &= 3D \quad d_3. \end{aligned} \quad (15)$$

$$\begin{aligned} [\omega_1^2(F_u) - \omega_2^2(F_u)]^2 &= 3D \quad 4[(d_6 - d_8)^2 + 4(d_2 + d_4)^2], \\ \omega^2(E_u) - \omega^2(A_u) &= 3D \quad 6(d_4 - d_2). \end{aligned} \quad (16)$$

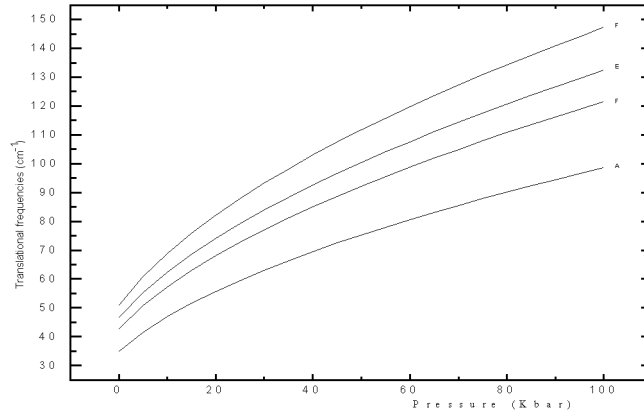


Figure 3. Calculated dependence of the translational frequencies on the external pressure at the temperature $T = 3D4.2 - 5$ K.

The numerical calculations carried out for the pure translational vibrations have shown that $d_6 \approx d_8$. Then we can found from equations (8) and

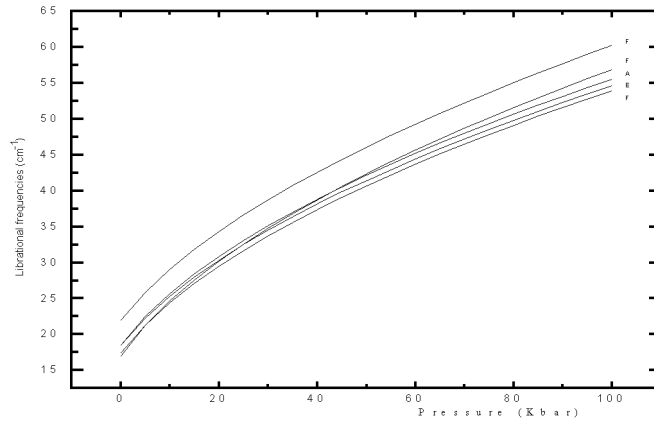


Figure 4. Calculated dependence of the librational frequencies on the external pressure at the temperature $T = 3D4.2 - 5$ K.

(16):

$$d_6 = 3D - \frac{1}{2}(d_1 + d_3)$$

$$\begin{aligned} \{3[\omega_2^2(F_u) - \omega_1^2(F_u)] + 2[\omega^2(A_u) - \omega^2(E_u)]\} / 24 &= 3D - d_2, \\ \{2[\omega^2(E_u) - \omega^2(A_u)] - 3[\omega_1^2(F_u) - \omega_2^2(F_u)]\} / 24 &= 3D - d_4. \end{aligned} \quad (17)$$

Thus, all components of the translational dynamic matrix of fullerene C_{60} crystal can be determined from expressions (15) and (17) if the experimental values of frequencies are known. It makes feasible suability to define the parameters of intermolecular potential (4) more precise by.

Figures 3 and 4 depict the dependencies of frequencies for translational modes and librational ones on the external pressure correspondingly. When the pressure is increased from 0 to 100 kbar the librational modes and translational ones shift toward higher frequencies with a rate of 0.35-0.65 $\text{cm}^{-1}/\text{kbar}$ and 0.77-1.38 $\text{cm}^{-1}/\text{kbar}$ respectively. This results is in good agreement with the experimentally observed values for the librational modes [30]: the strongest libron mode A_g shifts at a rate of 0.37 $\text{cm}^{-1}/\text{kbar}$, while a weaker, higher energy libron mode F_g shifts at a rate of 0.52 $\text{cm}^{-1}/\text{kbar}$.

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ВПЛИВ ТИСКУ НА СТРУКТУРУ ТА КОЛИВНИЙ СПЕКТР КРИСТАЛУ ФУЛЕРЕНУ C_{60}

Ю.І.Прилуцький, В.О.Андрєєв, Г.Г.Шаповалов

У залежності від зовнішнього тиску досліджена низькотемпературна орієнтаційно впорядкована кристалічна фаза фулерену C_{60} . З використанням методів теорії груп та атом-атомних потенціалів розраховано колильний спектр цього кристалу. Частоти зовнішніх фононних мод вивчені як функції тиску. Припускалось, що енергія ґратки містить два вклади: потенціал Ленарда-Джонса (12-6) та електростатичну взаємодію зарядів, локалізованих на одинарних і подвійних зв'язках молекули C_{60} . Отримані результати добре узгоджуються з існуючими експериментальними даними.