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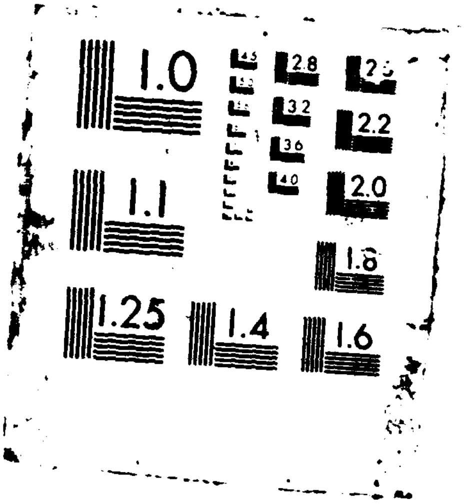
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Vibrational Motions of Buckminsterfullerene

by

Z. C. Wu, Daniel Jelski and Thomas F. George

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BUCKMINSTERFULLERENE,	NON-CARTESIAN COORDINATES
CARBON ~~(60-ATOM)~~ CLUSTER,	FOUR FORCE CONSTANTS
COMPLETE VIBRATIONAL SPECTRUM	180 BY 180 MATRIX

19. ABSTRACT *(Continue on reverse if necessary and identify by block number)*

A non-Cartesian coordinate system is developed which permits the vibrational motions of Buckminsterfullerene (Bucky ball) to be expressed in terms of four force constants. A 180 x 180 matrix is then derived which, when diagonalized, yields the complete vibrational spectrum. These results are compared with those obtained previously via a MNDO calculation.

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VIBRATIONAL MOTIONS OF BUCKMINSTERFULLERENE

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Abstract

A non-Cartesian coordinate system is developed which permits the vibrational motions of Buckminsterfullerene (Bucky ball) to be expressed in terms of four force constants. A 180 × 180 matrix is then derived which, when diagonalized, yields the complete vibrational spectrum. These results are compared with those obtained previously via a MNDO calculation.

I. Introduction

The purpose of this paper is to investigate the vibrational motions of Buckminsterfullerene (Bucky ball) in a way that lends itself toward future application. Hence simplicity, both theoretical and practical, is an important consideration. To this end we can take advantage of the symmetry of the species, and we shall derive a relatively simple procedure for calculating the vibrational normal frequencies. Furthermore, our method lends itself to physical interpretation, and we shall be able to make some statements about the nature of Bucky ball. The experimental literature on Bucky Ball is well known.[1-5] Theoretically much work has been dedicated to determining the most stable structure of C_{60} clusters,[6-10] and to determining some of their optical properties.[11] We continue this work here by assuming that Bucky ball exists and is relatively stable.

In essence our calculation can be described as follows. We express the position of each atom in local coordinates, choosing our coordinate system (non-Cartesian) in a way that simplifies the calculation. This permits us to express the equation of motion of each atom in terms of four force constants, and since all atoms are identical we immediately derive an equation of motion for the entire system. The fundamental principles behind this calculation are found in Ref. 12. While we must input the force constants into our calculation (this is a disadvantage), we generate the correct number of modes, the correct point group properties, and, at least qualitatively, the correct frequencies. This requires only the diagonalization of one 180 × 180 matrix, a procedure which requires only about three minutes CPU on a VAX. Furthermore, since we can vary the force constants and since we can compare our results with those of Stanton,[13] we are able to make some predictions about the structure of Bucky ball as compared to benzene. In the next section we derive our method for calculating the normal mode frequencies, and in Section III we compare our results with those of Stanton[13] and discuss the implications.

II. Theory

The structure of Buckminsterfullerene, illustrated in Fig. 1, is that of a truncated icosahedron with sixty vertices, twenty hexagonal faces and twelve pentagonal faces. A carbon atom occupies each vertex. The bonds separating a hexagon from a pentagon are found to be more "single" than bonds separating two hexagons.[6,8] The bond lengths are given as 1.41 Å and 1.54 Å, respectively.[8] Since each vertex is at the intersection of two hexagonal and one pentagonal face, it follows that it is joined by one "double" bond and two "single" bonds. This implies that the motion of an atom around it equilibrium position can be decomposed along the three non-coplanar directions of the adjacent bonds (Fig. 2). We can use x_i, y_i and z_i to denote the deviation of atom i from its equilibrium position in these directions (we caution the reader not to confuse our notation with Cartesian coordinates, since ours are not Cartesian). The angle between two adjacent single bonds is $\frac{3\pi}{5}$ and that between a double bond and an adjacent single bond is $\frac{2\pi}{3}$. One can work out the angle between a double bond and its adjacent pentagonal face as $\Psi = \cos^{-1}(\frac{1}{2\cos\frac{3\pi}{5}})$. The angle between two adjacent hexagonal faces is $\Phi = \cos^{-1}[\frac{8}{3}(\sin\frac{3\pi}{10})^2 - 1]$, and the angle betwee adjacent hexagonal and pentagonal faces is

$$\theta = \frac{\pi - \Phi}{2} - \Psi.$$

The variations of the bond length a_{ij}, b_{ik} and $c_{i\ell}$ (see Fig. 2) due to the motion of the atoms are, to first order,

$$\delta a_{ij} = (x_i - \frac{1}{2}y_i - \frac{1}{2}z_i) + (x_j - \frac{1}{2}y_j - \frac{1}{2}z_j),$$

$$\delta b_{ik} = (y_i - \frac{1}{2}x_i - \cos\frac{2\pi}{5}z_i) + (z_k - \frac{1}{2}x_k - \cos\frac{2\pi}{5}y_k), \qquad (1)$$

$$\delta c_{i\ell} = (z_i - \frac{1}{2}x_i - \cos\frac{2\pi}{5}y_i) + (y_\ell - \frac{1}{2}x_\ell - \cos\frac{2\pi}{5}z_\ell).$$

Also, the variations of the angles between bonds α, β and γ are

$$\begin{aligned}\delta\alpha_i = \frac{1}{L}(&-\sin\frac{\pi}{3}\cos\Phi\; y_j + \sin\frac{\pi}{3}\; z_j + \sin\frac{\pi}{3}\; x_k - \sin\frac{2\pi}{5}\cos\theta\; y_k \\ &- \sin\frac{\pi}{3}\; y_i + \sin\frac{\pi}{3}\cos\Phi\; z_i - \sin\frac{\pi}{3}\; x_i + \sin\frac{2\pi}{5}\cos\theta\; z_i),\end{aligned}$$

$$\begin{aligned}\delta\beta_i = \frac{1}{L}(&-\sin\frac{\pi}{3}\cos\Phi\; z_j + \sin\frac{\pi}{3}\; y_j + \sin\frac{\pi}{3}\; x_\ell - \sin\frac{2\pi}{5}\cos\theta\; z_\ell \\ &- \sin\frac{\pi}{3}\; z_i + \sin\frac{\pi}{3}\cos\Phi\; y_i - \sin\frac{\pi}{3}\; x_i + \sin\frac{2\pi}{5}\cos\theta\; y_i), \qquad (2)\end{aligned}$$

$$\begin{aligned}\delta\gamma_i = \frac{1}{L}(&\sin\frac{2\pi}{5}\; y_k - \sin\frac{\pi}{3}\cos\theta\; x_k + \sin\frac{2\pi}{5}\; z_\ell - \sin\frac{\pi}{3}\cos\theta\; x_\ell \\ &+ \sin\frac{\pi}{3}\cos\theta\; x_i - \sin\frac{2\pi}{5}\; y_i + \sin\frac{\pi}{3}\cos\theta\; x_i - \sin\frac{2\pi}{5}\; z_i),\end{aligned}$$

where L refers to the bond lengths which are assumed equal.

The kinetic energy of each atom is

$$T_i = \frac{m}{2}[(\dot{x}_i - \frac{1}{2}\dot{y}_i - \frac{1}{2}\dot{z}_i)^2 + (\dot{y}_i\cos\frac{\pi}{5} - \dot{z}_i\cos\frac{\pi}{5})^2$$
$$+(\dot{y}_i\cos\frac{3\pi}{10}\sin\Psi + \dot{z}_i\cos\frac{3\pi}{10}\sin\Psi)^2], \qquad (3)$$

where m is the mass of each atom. It is assumed that the atoms undergo harmonic oscillations around their equilibrium positions, where the potential is due to the variations of the bond lengths and the angles between them. If atoms j, k and ℓ represent nearest neighbors of atom i, as shown in Fig. 2, then the Lagrangian for this system takes the form

$$L = T - V = \sum_i T_i - \sum_{i>j} \frac{1}{2}k_1\delta a_{ij}^2 - \sum_{i>k} \frac{1}{2}k_2\delta b_{ik}^2 - \sum_{i>\ell} \frac{1}{2}k_2\delta c_{i\ell}^2$$
$$- \sum_i \frac{1}{2}[k_3(\delta\alpha_i^2 + \delta\beta_i^2) + k_4\delta\gamma_i^2], \qquad (4)$$

where k_1, k_2, k_3 and k_4 are all force constants. Equation (4) can be rewritten in the compact form

$$L = \frac{1}{2}\sum_{m,n=1}^{180} (T_{mn}\, \dot{X}^m \dot{X}^n - V_{mn}\, X^m X^n), \qquad (5)$$

and the appropriate Euler-Lagrange equation is

$$\ddot{X}^n = -\sum_{m,\ell=1}^{180} (T^{-1})^{mn}\, V_{m\ell} X^\ell. \qquad (6)$$

By diagonalizing the 180 × 180 matrix $T^{-1}V$, we get the squares of the eigenfrequencies along with their associated eigenvectors.

Several cases are worth discussing:

(a) $k_2 = k_3 = k_4 = 0$. Each double bond with force constant k_1 becomes independent. Then one obtains only one non-zero eigenfrequency, $(k_1/m)^{1/2}$, with a 30-fold degeneracy.

(b) $k_1 = k_3 = k_4 = 0$. The system reduces to 12 independent pentagons. For each pentagon the eigenfrequencies are (with degeneracies) 0.89401 (1), 1.00029 (2) and 1.15166 (2), with $k_2/m = 1$. All other eigenfrequencies are zero.

(c) $k_3 = k_4 = 0$. One obtains 90 non-zero eigenfrequencies corresponding to the 90 bonds. Since there is no force on the angles, Bucky ball can be squished in 90 - 6 = 84 different ways. The remaining 6 degrees of freedom are due to translation and rotation.

(d) In the general case, there are always 6 zero eigenfrequencies corresponding to global translational and rotational motions. There are also three non-degenerate modes.

III. Results and Discussion

Table I contains 180 eigenvalues representing the vibrational frequencies of Buckminsterfullerene. The values of k_1 - k_4 are those that best seem to fit the data of Stanton,[13] which was calculated by the MNDO method with the gradients evaluated at six points around an atom. The best fit was determined by matching the highest and lowest frequencies[6] and also by matching the three non-degenerate frequencies. In addition, we have insisted that the ratio between k_1 and k_2 be approximately equal to the inverse ratio of the bond lengths. Since at this point we have no independent way of determining k_4, we have insisted that it equal k_3.

For benzene the appropriate values would be $k_1 = k_2 = 7.62 \times 10^5$ dynes/cm and $k_3 = .667 \times 10^5$ dynes/cm.[14] Comparing these values with those given in Table I, we see that the force constants for Bucky ball are considerably higher than for benzene. This is physically reasonable since the stretching of a bond in Bucky ball involves a dislocation of the entire molecule, and hence greater resistance. Similarly we expect the stretching constant to be larger.

It is also instructive to look at the three non-degenerate modes. Stanton[13] has calculated their frequencies (in cm^{-1}) as 611 (for the A_g mode), 973 (A_u) and 1667 (A_g). Our calculation reveals frequencies at 548, 970, and 1627 cm^{-1}, respectively. We have found that the two A_g modes depend only on constants k_1 and k_2. The first is a "breathing" motion whereas the second involves oscillation between the "single" and "double" bonds. In both cases angles can be expected to play no role. The A_u motion, on the other hand, involves a twisting (angle-dependent) motion of the pentagons. When k_3 and k_4 are zero, the eigenfrequency of this motion becomes zero. All other modes must be degenerate according to the point group of Buckminsterfullerene.[13]

Our method is well suited to elucidating this sort of physical description of the motions since the k's have obvious physical significance. This is a big advantage of this calculation, along with the numerical simplicity. We intend to use this method to further investigate the vibrational spectrum of Buckminsterfullerene.

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References

1. H.W. Kroto, J.R. Heath, S.C. O'Brien, R.F. Curl and R.E. Smalley, Nature 318, 162 (1985). For a review of the experimental techniques involved, see A. Kaldor, D.M. Cox, D.J. Trevor and M.R. Zakin, Z. Phys. D 3, 195 (1986).

2. Q.L. Zhang, S.C. O'Brien, J.R. Heath, Y. Liu, H.W. Kroto and R.E. Smalley, J. Phys. Chem. 90, 525 (1986).

3. A. O'Keefe, M.M. Ross and A.P. Baronavski, Chem. Phys. Lett. 130, 17 (1986).

4. M.Y. Hahn, E.C. Honea, A. J. Paguia, K.E. Schriver, A.M. Camarena and R.L. Whetten, Chem. Phys. Lett. 130, 12 (1986).

5. S.C. O'Brien, J.R. Heath, H.W. Kroto, R.F. Curl and R.E. Smalley, Chem. Phys. Lett. 132, 99 (1986).

6. M.D. Newton and R.E. Stanton, J. Am. Chem. Soc. 108, 2469 (1986).

7. T.G. Schmalz, W.A. Seitz, D.J. Klein and G.E. Hite, Chem. Phys. Lett. 130, 203 (1986).

8. S. Satpathy, Chem. Phys. Lett. 130, 545 (1986).

9. R.C. Haddon, L.E. Brus and K. Raghavachari, Chem. Phys. Lett. 131, 165 (1986).

10. P.W. Fowler, Chem. Phys. Lett. 131, 444 (1986).

11. D.A. Jelski and T.F. George, J. Phys. Chem., submitted.

12. E.B. Wilson, J.C. Decius and P.C. Cross, Molecular Vibrations (McGraw-Hill, New York, 1955).

13. R.E. Stanton, private communication.

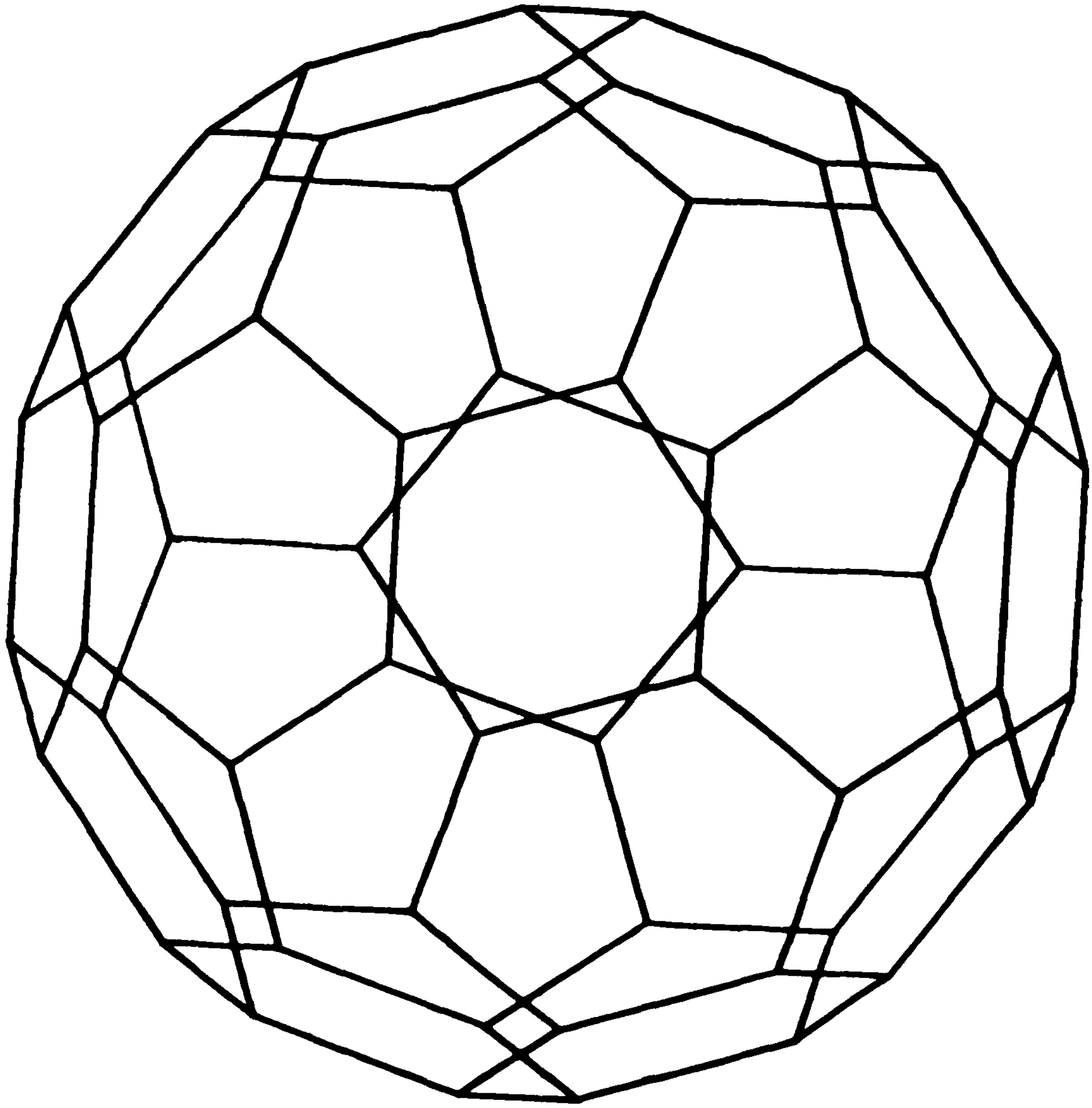
14. B.L. Crawford and F.A. Miller, J. Chem. Phys. 17, 249 (1949).

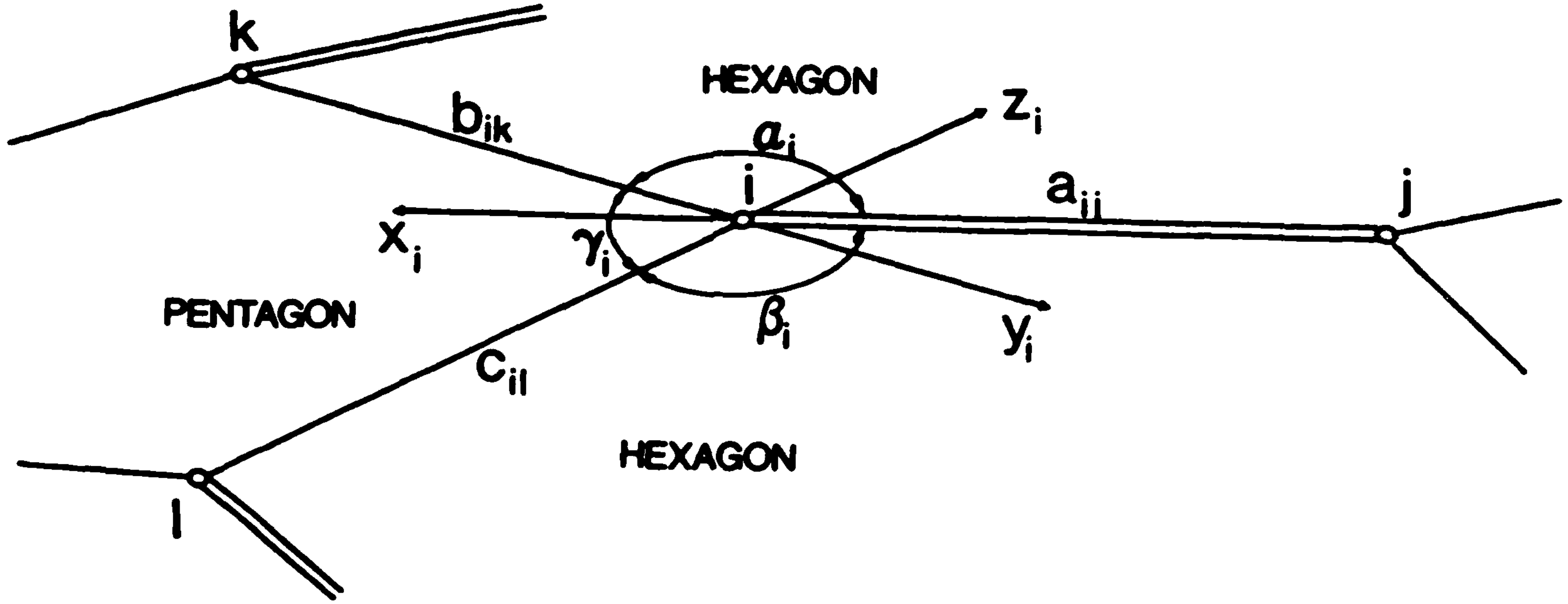
Frequency	Symmetry	Frequency	Symmetry
0.0	-	272.0	Hg
354.7	Hu	361.8	F2u
373.7	Gu	427.9	Hg
455.8	Gg	491.3	F1u
491.6	Hu	525.2	F2g
530.2	Gg	547.6	Ag
550.9	F1u	552.4	Hg
566.8	F1g	577.7	Hu
626.6	F2u	672.7	Gg
701.9	Gu	726.4	F2g
755.8	Gu	770.3	Hu
779.8	Hg	810.9	F1g
926.6	F2g	958.3	Gu
1019.0	F2u	1084.3	Au
1160.0	Hg	1173.5	Gg
1289.7	Hu	1309.4	F2u
1374.1	F1u	1398.5	Hg
1463.8	F2g	1578.5	Hu
1590.0	Gg	1620.4	Gu
1627.4	Ag	1655.3	F1u
1665.1	F2g	1688.2	Hg
1720.1	F2u	1764.4	Gu
1765.4	Gg	1830.0	Hu
1830.7	Hg		

Table 1. Frequencies in cm^{-1} and their degeneracies for the vibrational modes of Buckminsterfullerene. $k_1 = 1.1 \times 10^6$, $k_2 = 1.0 \times 10^6$, $k_3 = 1.0 \times 10^5$ and $k_4 = 1.0 \times 10^5$ dynes/cm.

FIGURE CAPTIONS

Figure 1.	The C_{60} cluster, better known as Buckminsterfullerene, is a truncated icosahedron with 20 hexagonal faces and 12 pentagonal faces.
Figure 2.	A diagram of the local coordinate system used in the calculation.

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