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Topological structures of tetrahedral (T_d and T) fullerenes with hexagonal and triangular faces and their vibration and NMR spectra*

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Abstract. On analyzing the topological structures of the three types of tetrahedral fullerenes (which consist only of triangles and hexagons), (1) $C_n(T_d, n = 12h^2; h = 1, 2, \ldots)$, (2) $C_n(T_d, n = 4h^2; h = 1, 2, \ldots)$, and (3) $C_n(T, n = 4(h^2 + hk + k^2); h > k, h, k = 1, 2, \ldots)$, we have obtained theoretically the Infrared and Raman active modes by means of the derived formulas for the decomposition of their nuclear motions into irreducible representations, and the ^{13}C NMR spectra with natural abundance for ^{13}C by using the distribution functions for all of the tetrahedral (T_d and T) fullerenes, respectively.

Key words: Fullerenes – Tetrahedral symmetry – IR active – Raman active – NMR

1 Introduction

Since the discovery of C_{60} in 1985 [1], numerous fullerenes have been observed by mass spectrometry with laser vaporizing on graphite. Many theoretical analyses have been done on their structures [2, 3] and their vibration [4–8] and NMR [4, 9, 10] spectra. It is well known that C_{60} with icosahedral symmetry is the structure of a soccer football constituted only by hexagons and pentagons. C_{80}, C_{180}, C_{240}, C_{320}, C_{540}, etc., which are believed to be polyhedrons with hexagonal and pentagonal faces, are considered as fullerenes with icosahedral symmetry. It should be mentioned that Fowler suggested a geometry with tetrahedral group symmetry for C_{28} [11], which is a polyhedron with 12 pentagons and four hexagons. On the other hand, C_{24} is believed to be a polyhedron with six rectangles and eight hexagons and is considered to be the smallest fullerene with octahedral symmetry (O_h). It is interesting to study theoretically those fullerenes with hexagonal faces and non-pentagonal faces. We have also discussed a series of icosahedral (I_h and I), octahedral (O_h and O), and tetrahedral (T_d and T) fullerenes with two kinds of face, one hexagonal and the other pentagonal, rectangular, or triangular, respectively [12].

In fact, by using the Euler equation for a convex polyhedron

$$n + f = l + 2 \qquad (1)$$

where n is the number of vertices, f the number of faces, and l the number of edges of the polyhedron, and by considering that each vertex is connected with three edges for a fullerene polyhedron, or

$$3n = 2l \qquad (2)$$

one has for any fullerene polyhedron

$$l = 3f - 6 \qquad (3)$$

Now we consider a fullerene polyhedron with two kinds of face, a six-side face and a j-side face, of which the numbers are denoted by f_6 and f_j.
Then

$$f_6 + f_j = f \qquad (4)$$

$$6f_6 + jf_j = 2l \qquad (5)$$

and considering Eqs. (3), (4), and (5) we obtain [12]

$$f_j = 12/(6 - j) \qquad (6)$$

Therefore, the j values of the above equation can only be equal to 5, 4, or 3. The highest symmetry group of a polyhedron to which fullerenes with two kinds of face, a six-side face and a j-side face, belong is I_h, O_h, and T_d corresponding to $j = 5$, 4, and 3, respectively.

In present article we have only made a systematic study of the topological geometry structure for the tetrahedral (T_d and T) polyhedron fullerenes which contain only hexagonal and triangular faces and of their vibration spectra and NMR spectra as characteristics to detect and test their existence.

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2 Topological structure of tetrahedral fullerenes

Firstly we determine the carbon counts of tetrahedral fullerenes. If the number of vertices of a polyhedron is equal to the number of faces of another polyhedron, and vice versa, then they are called conjugate polyhedrons. Obviously, a tetrahedron is a self-conjugate polyhedron with the group T_d symmetry:

$$\mathrm{C}_4(n = f = 4)$$

We use the Coxeter method [13] to deduce the carbon counts of tetrahedral fullerenes. Choosing a graphite coordinate system O′HK as shown in Fig. 1, we take a vector O′P with terminal coordinates at (h, k), where h and k are non-negative integers with the restriction $h \geq k, h > 0$, and $k \geq 0$.

Any tetrahedral fullerene corresponds to four equivalent triangles with each edge equal to the length of O′P; then we can deduce the carbon counts as $\mathrm{C}_n : n = 4(h^2 + hk + k^2)$. When O′P is along the bisector of HO′K, or along the O′H axis, the tetrahedral fullerene has symmetry planes; then we have

$$\mathrm{C}_n(T_d, n = 12h^2, h = 1, 2, \ldots)$$

$$\mathrm{C}_n(T_d, n = 4h^2, h = 1, 2, \ldots)$$

$$\mathrm{C}_n(T, n = 4(h^2 + hk + k^2), \quad h > k, k = 1, 2, \ldots) \tag{7}$$

Let us consider a fullerene C_n with point group G as its symmetry, and G is denoted as

$$G = \{\hat{e} = \hat{g}_1, \hat{g}_2, \ldots, \hat{g}_q\}$$

With respect to group G the n carbon atoms in C_n are divided into l sets, each of which contains q carbon atoms. Starting with the carbon atoms $1, 2, \ldots, l$, we can obtain the l sets by the operations of G on them in turn as follows:

$$\left(\hat{g}_1\omega, \hat{g}_2\omega, \ldots, \hat{g}_q\omega\right), \omega = 1, 2, \ldots, l$$

The aggregates of C atoms in C_n are divided into sets called patches which are expressed as follows:

$$(\hat{g}_t 1, \hat{g}_t 2, \ldots, \hat{g}_t l), t = 1, 2, \ldots, q$$

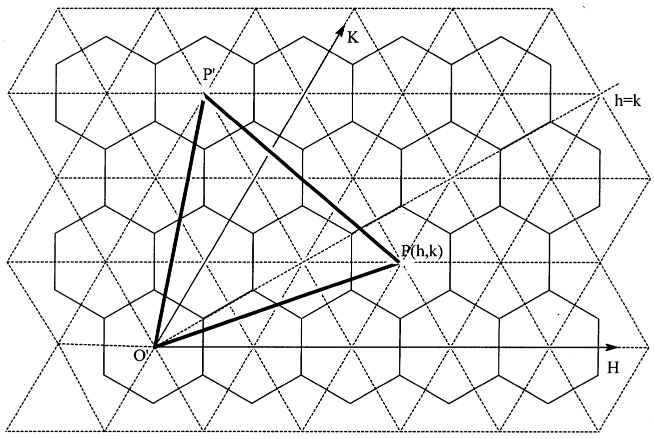

Fig. 1. The graphite coordinate system

If we choose the first patch $(1, 2, \ldots, l)$ as the representative patch, all the other patches can be obtained by the successive applications of group operation $\hat{g}_t(t = 2, 3, \ldots, q)$ on it. As all the q patches are equivalent, we only need to consider the representative patch and its surrounding atoms instead of the whole C_n in discussing many properties of the fullerenes.

In order to simplify the following discussion, we only use the T symmetry group to treat the structures of tetrahedral (T_d and T) fullerenes with hexagonal and triangular faces. Therefore, on the circumsphere of any tetrahedral fullerene, we may take one of the 12 equivalent patches as the representative patch, from which all the other patches can be obtained by operations of the tetrahedral group T.

Since the tetrahedral fullerenes consist of three types as Eq. (7), the corresponding patches and the distribution functions are also different. This is discussed below.

2.1 $\mathrm{C}_n(T_d, n = 12h^2; h = 1, 2, \ldots)$

The representative patch is characterized by the presence of three threefold axes ($\mathrm{OP}_3, \mathrm{OP}'_3$, and OP''_3) and one twofold axis (OP_2) at the boundaries, and a symmetry plane σ_d determined by OP_3 and OP_2 passing through the medium of the patch as shown in Fig. 2. Inside the patch there are h^2 carbon atoms which are symmetrically distributed from upward to downward about the symmetry plane σ_d in the manner of the following distribution function:

$$D\left(h^2\right) = (0, 1) + (1, 2) + \cdots + (h - 1, h) \tag{8}$$

as illustrated in Fig. 2. When all the elements of the tetrahedral group T operate on the polyhedron $\mathrm{C}_n(T_d, n = 12h^2)$ separately, the representative patch will move over all 12 equivalent patches, and they cover the whole surface of the polyhedron $\mathrm{C}_n(T_d, n = 12h^2)$.

2.2 $\mathrm{C}_n(T_d, n = 4h^2; h = 1, 2, \ldots)$

The representative patch of $\mathrm{C}_n(T_d, n = 4h^2)$ is characterized by the presence of three threefold axes ($\mathrm{OP}'_3, \mathrm{OP}_3$, and OP'''_3) and one twofold axis (OP_2) on its boundaries. Furthermore, there is a symmetry plane σ'_d determined by OP'_3 and OP_2 across the patch, as shown in Fig. 3.

Inside the patch, there are $h^2/3$ carbon atoms which are symmetrically distributed about the plane σ'_d. For those carbon atoms on both the boundaries determined by OP'_3 and OP_3, and the other one by OP'_3 and OP'''_3, we can only take the carbon atoms on one boundary to be in the patch. The distribution of carbon atoms about the symmetry plane σ'_d is according to the following three distribution functions in three cases, so we need to consider the three cases separately.

$$D\left(h^2/3\right) = (1, 2) + (4, 5) + \cdots + (3m - 2, 3m - 1)$$
$$(h = 3m, m = 1, 2, \ldots) \tag{9}$$

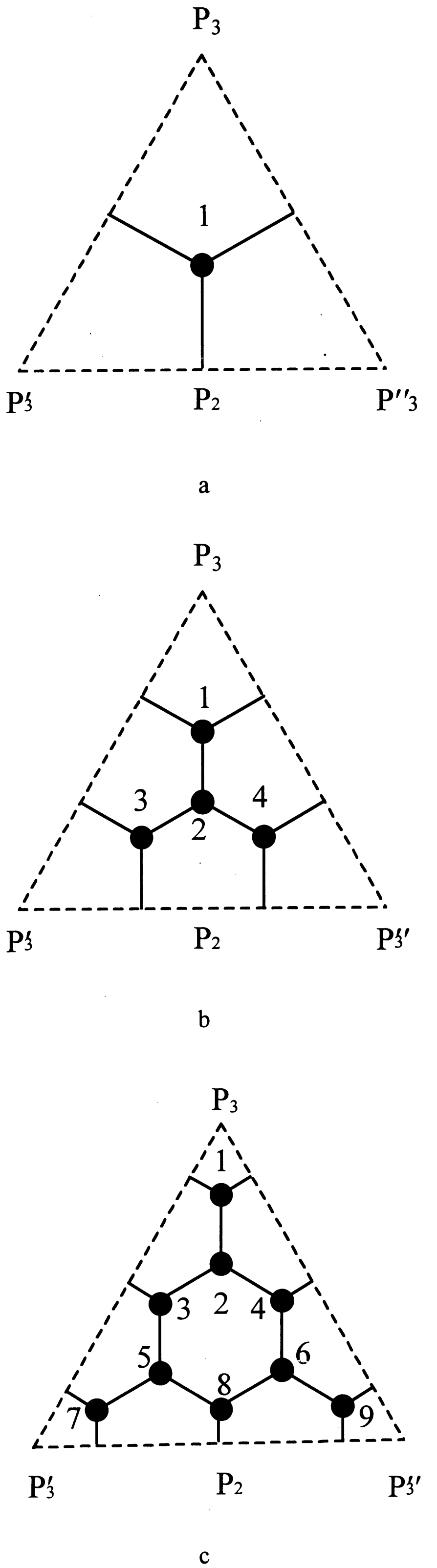

Fig. 2a–c. Patches of fullerenes $C_n(T_d,\ n=12h^2)$: **a** $C_{12}(h=1)$; **b** $C_{48}(h=2)$; **c** $C_{108}(h=3)$

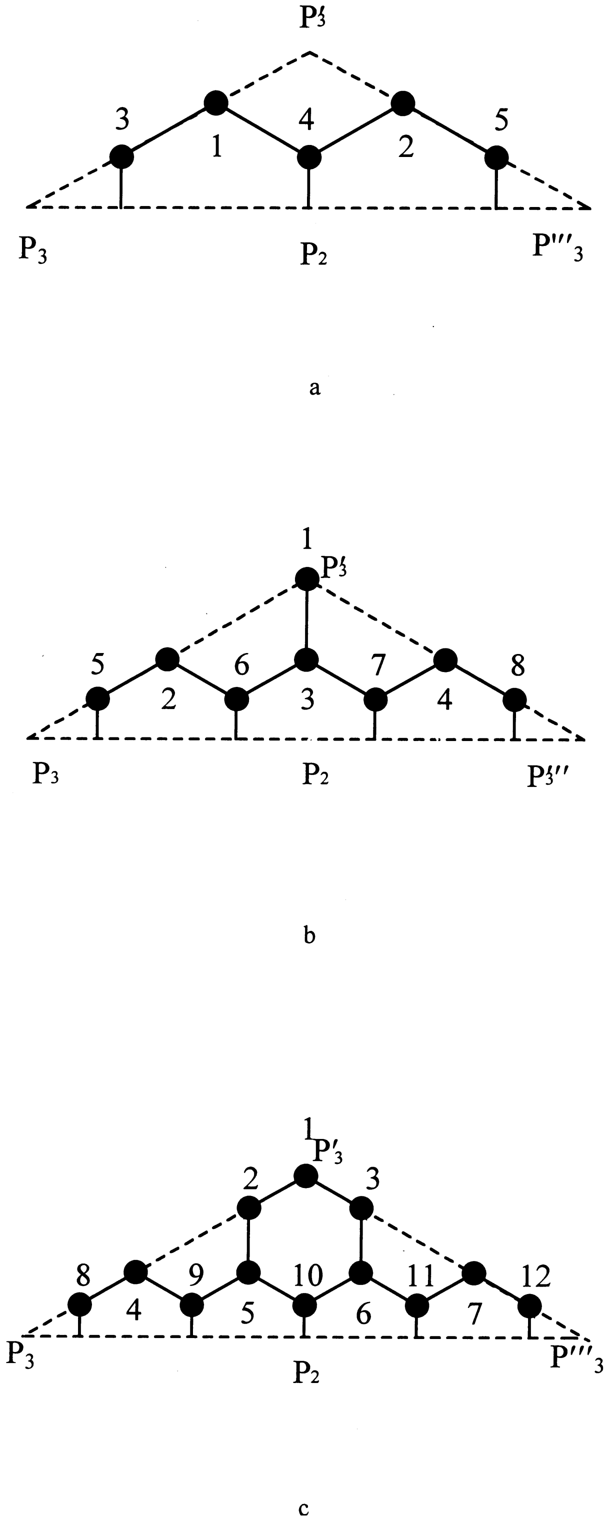

Fig. 3a–c. Patches of fullerenes $C_n(T_d, n=4h^2)$: **a** $C_{36}(h=3m;\ m=1)$; **b** $C_{64}(h=3m+1; m=1)$; **c** $C_{100}(h=3m+2;\ m=1)$

$$D(h^2/3) = \tfrac{1}{3} + (2,3) + \cdots + (3m-1, 3m) \quad (h = 3m+1, m = 0, 1, \ldots) \tag{10}$$

$$D(h^2/3) = \tfrac{1}{3} + 1 + (3,4) + \cdots (3m, 3m+1) \quad (h = 3m+2, m = 0, 1, \ldots) \tag{11}$$

where $\frac{1}{3}$ means the presence of one carbon atom lying on the threefold axis OP_3'.

2.3 $\mathrm{C}_n(T, n = 4(h^2 + hk + k^2); h > k; h, k = 1, 2, \ldots)$

As the T group has no symmetry planes, the fullerenes C_n with T group symmetry can be divided into three cases:

1. $h - k = 3m, \quad n = 12(k^2 + 3km + 3m^2)$ (12)
2. $h - k = 3m+1, \quad n = 12(k^2 + 3km + 3m^2 + 2m + k) + 4$ (13)
3. $h - k = 3m+2, \quad n = 12(k^2 + 3km + 3m^2 + 4m + 2k + 1) + 4$ (14)

Obviously, there are four carbon atoms on the threefold axes in the latter two cases, which are different from the first case.

3 Vibration spectra of tetrahedral fullerenes

Once the point group of a fullerene is known, its vibrations can be analyzed and the Infrared (IR)-active, Raman-active, polarized Raman, and IR/Raman coincident modes can be counted, fully characterizing the spectrum. A fullerene C_n has $3n - 6$ vibrations and their symmetries can be obtained by subtracting the translational and rotational symmetries from the representation of the $3n$ Cartesian atomic displacement coordinates.

A mode can in general be IR active, Raman active, or neither, or both. A fundamental transition is IR active if the normal mode involved belongs to the same representation of the point group as one or more components of the dipole moment, and is Raman active if the mode shares a representation with one or more components of the polarizability tensor.

Now let us discuss the decomposition of fullerene nuclear motions into irreducible representations. The n vectors of the small nuclear displacements of C_n can be used as the bases of a representation of a corresponding point group, and their characters are equal to $n(\hat{g})\chi(\hat{g})$ ($\hat{g}$ are the elements of the point group), where $n(\hat{g})$ and $\chi(\hat{g})$ are the number of unmoved carbon atoms and the trace of the vector displacement matrix with respect to the operation $\hat{g}$, respectively. Then, by use of characters of the point group and the orthogonality relationship, we obtain the decomposition of nuclear motions into any non-equivalent irreducible representations of the point group as follows:

$$n_\alpha = \frac{1}{q} \sum_{\hat{R}} n(\hat{g}) \chi(\hat{g}) \chi^{(\alpha)}(\hat{g}) \tag{15}$$

where q is the order of the point group and n_α is the number of irreducible representation α involved in the nuclear motions.

3.1 Vibration spectra of $\mathrm{C}_n(T_d,\ n = 12h^2,\ h = 1,\ 2,\ \ldots)$

In the T_d group the 24 group elements are divided into five classes: $\hat{e}$, $8(\hat{C}_3, \hat{C}_3^{-1})$, $3\hat{C}_2$, $6\hat{S}_4$, $6\hat{\sigma}_d$. The T_d group has five non-equivalent irreducible representations denoted by A_1, A_2, E, T_1, and T_2. Their characters are listed in Table 1.

From the patch shown in Fig. 2 and distribution function (8), we could know that only $12h$ carbon atoms in $\mathrm{C}_n(T_d, n = 12h^2)$ are lying on the symmetry planes σ_d. All the remaining $12h(h-1)$ carbon atoms are not lying on any symmetry element. Therefore we have:

$$n_\alpha = \tfrac{3}{2} h^2 \chi^{(\alpha)}(\hat{e}) + \tfrac{1}{2} h \chi^{(\alpha)}(\hat{\sigma}_d) \tag{16}$$

where $\alpha = A_1$, A_2, E, T_1, and T_2, respectively.

Among the irreducible representations obtained by the above equations, one T_2 belongs to the translation, one T_1 to the rotation, and all the others belong to the vibration modes. The number of IR, Raman, and polarized Raman active modes are respectively

$(9h^2/2) + (h/2) - 1$	for IR and Raman active (T_2)
$3h^2$	for depolarized Raman active (E)
$(3h^2/2) + (h/2)$	for polarized Raman active (A_1)

3.2 Vibration spectra of $\mathrm{C}_n(T_d,\ n = 4h^2,\ h = 1, 2, \ldots)$

For this type of fullerene, as there are carbon atoms on both boundaries $\mathrm{P}_3'\mathrm{P}_3$ and $\mathrm{P}_3'\mathrm{P}_3'''$ in the patches shown in Fig. 2, we can only take the carbon atoms on one boundary to be in the patch. Since the three planes

Table 1. Characters for the point groups T and T_d, where $\varepsilon = \exp(i2\pi/3)$

T	$\hat{E}$	$4\hat{C}_3$	$4\hat{C}_3^2$	$3\hat{C}_2$	Basis functions
A	1	1	1	1	$x^2 + y^2 + z^2$
E	1	ε^*	ε	1	$(2z^2 - x^2 - y^2,$
	1	ε	ε^*	1	$x^2 - y^2)$
T	3	0	-1	1	(x, y, z) (R_x, R_y, R_z) $(xy,\ yz,\ xz)$

T_d	$\hat{E}$	$8\hat{C}_3$	$3\hat{C}_2$	$6\hat{\sigma}_d$	$6\hat{S}_4$	Basis functions
A_1	1	1	1	1	1	$x^2 + y^2 + z^2$
A_2	1	1	1	-1	-1	
E	2	-1	2	0	0	$(2z^2 - x^2 - y^2,\ x^2 - y^2)$
T_1	3	0	-1	-1	1	$(R_x,\ R_y,\ R_z)$
T_2	3	0	-1	1	-1	$(x,\ y,\ z)\ (xy,\ yz,\ xz)$

determined respectively by OP'_3 and OP_3, OP'_3 and OP_2, and OP'_3 and OP'''_3 are equivalent with respect to the threefold axis, according to distribution functions (9), (10), and (11), there are $3m$, $3m+1$, and $3m+2$ carbon atoms respectively on the symmetry planes σ_d in the patch for the three cases $h = 3m$, $h = 3m+1$, and $h = 3m+2$. By using Eq. (15) and taking $\chi(\hat{C}_3) = 0$ into consideration, we obtain the formula for the decomposition of nuclear motions into the irreducible representations in $C_n(T_d,\ n = 4h^2)$ as follows:

$$n_\alpha = \tfrac{1}{2}h^2\chi^{(\alpha)}(\hat{e}) + \tfrac{1}{2}h\chi^{(\alpha)}(\hat{\sigma}_d) \tag{17}$$

where $\alpha = A_1$, A_2, E, T_1, and T_2, respectively.

Among the irreducible representations obtained by the above equations, one T_2 belongs to the translation, one T_1 to rotation, and all the others belong to the vibration modes. Thus we obtain the number of IR and Raman active modes of $C_n(T_d,\ n = 4h^2)$ to be respectively

$(3h^2/2) + (h/2) - 1$	for IR and Raman active (T_2)
h^2	for depolarized Raman active (E)
$(h^2/2) + (h/2)$	for polarized Raman active (A_1)

3.3 Vibration spectra of $C_n(T, n = 4(h^2 + hk + k^2);\ h > k;\ h, k = 1,\ 2, \ldots)$

As the T group has no symmetry planes, it has 12 elements, four classes, and four non-equivalent irreducible representations denoted by A, E (a pair of conjugate representations), and T as shown in Table 1.

According to Eqs. (12), (13), and (14), the tetrahedral fullerenes should be divided into three cases to discuss the vibration spectra. The presence of four carbon atoms on the threefold axes in the latter two cases could introduce different properties from those of the first case, but it does not affect the decomposition formula of nuclear motions owing to the fact $\chi(\hat{C}_3) = 0$.

The three cases of tetrahedral fullerenes with T symmetry have the same form of decomposition formula:

$$n_\alpha = \left(h^2 + hk + k^2\right)\chi^{(\alpha)}(\hat{e}) \tag{18}$$

where α is A, E, and T, respectively.

Among the irreducible representations obtained by the above equations, one T belongs to the translation, one T to the rotation, and all the others belong to the vibration modes. The number of IR and Raman active modes are respectively

$3(h^2 + hk + k^2) - 2$	for IR and Raman active (T)
$(h^2 + hk + k^2)$	for depolarized Raman active (E)
$(h^2 + hk + k^2)$	for polarized Raman active (A)

As examples, the number of IR, Raman, and polarized Raman active modes for some tetrahedral (T_d and T) fullerenes are listed in Tables 2 and 3, respectively.

4 NMR spectra of tetrahedral fullerenes

In natural abundance, only one in every 100 carbon nuclei is a ^{13}C nucleus, and in ideal circumstances the ^{13}C NMR spectrum of a tetrahedral fullerene will be very simple. It will consist of a number of peaks, one for each equivalent set of atomic sites, with intensities proportional to the number of sites in each set. A symmetry analysis by means of the patch and its distribution function can therefore predict the number of peaks and their relative intensities in the hypothetical ^{13}C NMR spectrum of a tetrahedral fullerene. Here symmetry places a very useful limitation on the ^{13}C NMR spectrum. There are only three kinds of equivalent sets of atomic sites in a fullerene. Therefore, the idealized stick spectrum of a fullerene may contain three different peak heights at most.

4.1 NMR spectra of $C_n(T_d, n = 12h^2)$

Inside the patch shown in Fig. 1 there are h^2 carbon atoms, which are symmetrically distributed about the symmetry plane σ_d in the manner according to the distribution function (8).

Obviously, there are h carbon atoms on the symmetry plane σ_d and $h(h-1)$ carbon atoms located symmetrically on the two sides of the plane in the patch. In totality, there are h different sets with 12 carbon atoms in each set lying on the symmetry planes, and $h(h-1)/2$ different sets with 24 carbon atoms in each set not lying

Table 2. Infrared (IR) and Raman active modes of $C_n(T_d)$

Fullerenes	$n = 12h^2$				$n = 4h^2$			
	C_{12}	C_{48}	C_{108}	...	C_{36}	C_{64}	C_{100}	...
IR and Raman active (T_2)	4	18	41		14	25	39	
Depolarized Raman active (E)	3	12	27		9	16	25	
Polarized Raman active (A_1)	2	7	15		6	10	15	

Table 3. IR and Raman active modes of $C_n(T, n = 4(h^2 + hk + k^2))$

Fullerenes	C_{28} ($h = 2, k = 1$)	C_{52} ($h = 3, k = 1$)	C_{84} ($h = 4, k = 1$)
IR and Raman active (T)	19	37	61
Depolarized Raman active (E)	7	13	21
Polarized Raman active (A)	7	13	21

on any symmetry element of the T_d group. Therefore, the total number of NMR spectrum lines, N_{NMR}, for the tetrahedral fullerenes $\mathrm{C}_n(T_d,\ n = 12h^2)$ is

$$N_{\mathrm{NMR}} = h + h(h-1)/2$$

4.2 NMR spectra of $\mathrm{C}_n(T_d,\ n = 4h^2)$

According to patch of $\mathrm{C}_n(T_d,\ n = 4h^2)$ shown in Fig. 3 and its distribution functions (9), (10), and (11), we need to consider the three cases separately.

4.2.1 $h = 3m,\ m = 1, 2, \ldots$

In the patch shown in Fig. 3a the plane defined by OP'_3 and OP_3 is also a symmetry plane since it is equivalent to the plane σ'_d with respect to the threefold axis OP'_3. According to distribution function (9), therefore, there are $3m$ carbon atoms lying on the symmetry planes, and $3m(m-1)$ carbon atoms located symmetrically on the two sides of the symmetry plane σ'_d. In totality, of the 12 equivalent patches, there are $3m$ different sets with 12 carbon atoms in each set lying on the symmetry planes, and $3m(m-1)/2$ different sets with 24 carbon atoms in each set not lying on any symmetry element of the T_d group. Therefore, for the fullerenes $\mathrm{C}_n(T_d,\ n = 4h^2,\ h = 3m)$ the number of NMR spectrum lines, N_{NMR}, is determined by

$$N_{\mathrm{NMR}} = 3m + 3m(m-1)/2$$

4.2.2 $h = 3m + 1,\ m = 0, 1, 2, \ldots$

In this case there are $(3m+1)^2/3$ carbon atoms in the patch shown in Fig. 3b, and they are symmetrically located about the plane σ'_d in the manner according to the distribution function (10). Therefore, 1/3 carbon atom located on the threefold axis OP'_3, $3m$ carbon atoms lying on the symmetry planes and $m(3m-1)$ carbon atoms located symmetrically on the two sides of the plane σ'_d in the patch. Taking the 12 equivalent patches as a whole, we have one set of four carbon atoms on the threefold axes, $3m$ different sets with 12 carbon atoms in each set lying on the symmetry planes, and $m(3m-1)/2$ different sets with 24 carbon atoms not lying on any symmetry element of the T_d group. Therefore, for the fullerenes $\mathrm{C}_n(T_d,\ n = 4h^2,\ h = 3m+1)$ the number of NMR spectrum lines, N_{NMR}, is

$$N_{\mathrm{NMR}} = 3m + m(3m-1)/2 + 1$$

4.2.3 $h = 3m + 2,\ m = 0, 1, 2, \ldots$

In this case the $(3m+2)^2/3$ carbon atoms in the patch as shown in Fig. 3c are symmetrically located about the plane σ'_d in the manner according to the distribution function (11).

In the patch, there is 1/3 carbon atom located on the threefold axis OP'_3, $(3m+1)$ carbon atoms lying on the symmetry planes, and $m(3m+1)$ carbon atoms located symmetrically on the two sides of the plane σ'_d. Taking the 12 equivalent patches as a whole, we have one set of four carbon atoms located on the threefold axes, $(3m+1)$ different sets with 12 carbon atoms in each set lying on the symmetry planes, and $m(3m+1)/2$ different sets with 24 carbon atoms in each set not lying on any symmetry element of the T_d group. Therefore, for the fullerenes $\mathrm{C}_n(T_d,\ n = 4h^2, h = 3m+2)$ the number of NMR spectrum lines, N_{NMR}, is

$$N_{\mathrm{NMR}} = (3m+1) + m(3m+1)/2 + 1$$

4.3 NMR spectra of $\mathrm{C}_n(T,\ n = 4(h^2 + hk + k^2), h > k)$

The fullerenes with T symmetry have been divided into three cases, according to Eqs. (12), (13), and (14).

For case 1, there are $k^2 + 3mk + 3m^2$ different sets with 12 carbon atoms in each set, so the number of NMR spectrum lines, N_{NMR}, is

$$N_{\mathrm{NMR}} = k^2 + 3mk + 3m^2$$

For case 2 there are $k^2 + (3m+1)k + 3m^2 + 2m$ different sets with 12 carbon atoms in each set. Furthermore, there is one set of four carbon atoms lying on the threefold axes. Therefore, the number of NMR spectrum lines, N_{NMR}, is

$$N_{\mathrm{NMR}} = \left[k^2 + (3m+1)k + 3m^2 + 2m\right] + 1$$

For case 3, similar to case 2, the number of NMR spectrum lines, N_{NMR}, is

$$N_{\mathrm{NMR}} = \left[k^2 + (3m+2)k + 3m^2 + 4m + 1\right] + 1$$

in which the last number 1 is due to the presence of four carbon atoms located on the threefold axes.

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