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Energy Spectrum and Optical Properties of Fullerene $C_{50}(D_{5h})$ within the Hubbard Model

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The energy spectra of C_{50} fullerene and molecule $C_{50}Cl_{10}$ of symmetry group D_{5h} were obtained within the Hubbard model in the mean-field approximation. Using group theory methods, the classification of energy states was carried out, and the allowed transitions in the energy spectra of C_{50} and $C_{50}Cl_{10}$ molecules of symmetry group D_{5h} were determined. On the basis of this spectrum, an interpretation of experimentally observed optical absorption bands of molecule $C_{50}Cl_{10}$ is proposed.

Keywords: Hubbard model, Green's functions, energy spectrum, nanosystems, C_{50} fullerene.

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Introduction

Today, there are many papers devoted to so called small fullerenes, i.e. C_n fullerenes with $n < 60$. These small fullerenes feature the absence of isomers, which would contain isolated pentagons. C_{50} fullerene belongs to the small fullerenes. The C_{50} fullerene was discovered in 1985, at the same time with the C_{60} and C_{70} fullerenes during the study of mass-spectra of the carbon cluster vapors [1]. Study of the carbon cluster vapor mass-spectra has shown that the C_{50} fullerene is the most stable one versus the other small fullerenes [1,2].

Along with the study of the C_{50} fullerene physical properties, its chemical properties were studied too. In 2004 as a result of application of the modified arc discharge method [3] in gaseous medium consisting of the CCl_4 (0.013 atm) and He (0.395 atm), the $C_{50}Cl_{10}$ compound was obtained for the first time, in the amount of about two milligrams with the purity of 99.5% [4]. The studies performed by using nuclear magnetic resonance have shown that the $C_{50}Cl_{10}$ molecule has the D_{5h} symmetry. Additionally, it was shown that the static polarization and the second hyperpolarization of the $C_{50}Cl_{10}$ is considerably higher than that of the C_{60}. That is why the $C_{50}Cl_{10}$ is considered to be a promising material for the nonlinear optics [5]. The studies of the endohedral fullerenes He@C_{50}, Ne@C_{50} and Ar@C_{50} have shown that these molecules have the D_{5h} symmetry group, too [6].

The C_{50} fullerene with the D_{5h} symmetry group consists of 12 pentagons and 15 hexagons, as shown in Fig. 1. Note that 271 isomers of the C_{50} fullerene can be built out of 50 carbon atoms [7]. It is clear from the Schlegel diagram of Fig. 1 that the C_{50} fullerene of the D_{5h} symmetry group contains six nonequivalent bonds and four groups of nonequivalent carbon atoms:

$G_1 = \{1, 2, 4, 5, 8, 13, 15, 20, 21, 23, 29, 31, 37, 39, 40, 42, 43, 45, 46, 48\}$,

$G_2 = \{3, 6, 7, 14, 22, 30, 38, 44, 49, 50\}$,

$G_3 = \{10, 11, 17, 18, 25, 26, 27, 33, 34, 35\}$,

$G_4 = \{9, 12, 16, 19, 24, 28, 32, 36, 41, 47\}$.

The G_1 set includes atoms, which are at vertices of junction of one pentagon and two hexagons and, furthermore, each of these atoms has one adjacent neighbor of the same G_1 set. The G_2 set includes atoms, which are at vertices of junction of one hexagon and two pentagons, and each of these atoms has one adjacent neighbor of the same G_2 set. The G_3 set includes atoms, which are at the vertices of the isolated pentagon. The G_4 set includes atoms, which are at vertices of junction of one pentagon and two hexagons and, furthermore, each of these atoms has none of adjacent neighbor of the same G_4 set. The studies performed by using the nuclear magnetic resonance have shown that chlorine atoms in the $C_{50}Cl_{10}$ molecule are bonded to the carbon atoms, which belong to the G_2 set [4], i.e. as it is shown in Fig. 2, the chlorine atoms form a Saturn ring-like structure around the C_{50} fullerene. Quite a lot of papers [8–10] are devoted to the study of the physical and chemical properties of the C_{50} fullerene.

The Hubbard model [11] is widely used to describe the electronic properties of carbon nanosystems. This model in the mean-field approximation was used to obtain the energy spectra and optical absorption spectra of the C_{80} fullerene with the I_h symmetry group [12], the C_{70} fullerene [13], the C_{60} fullerene [14], the C_{36} fullerene with the D_{6h} symmetry group [15], the C_{28} fullerene with the T_d symmetry group [16], the C_{26} fullerene with the D_{3h} symmetry group [17], the C_{24} fullerene with the O_h, D_6 and D_{6d} symmetry groups [18] and the C_{20} fullerene with the I_h, D_{5d} and D_{3d} symmetry groups [19]. The authors of [20] used it to determine the electronic properties of carbon

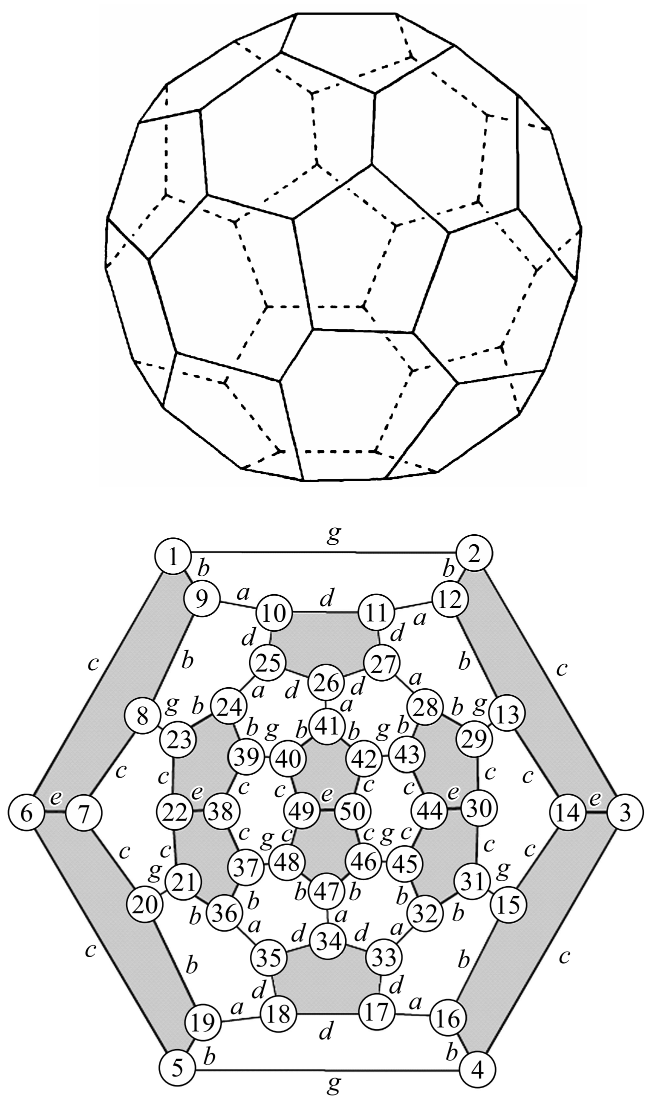

Figure 1. The C_{50} fullerene with the D_{5h} symmetry group and its Schlegel diagram showing the position of carbon atoms, bonds between carbon atoms, and pentagons.

nanotubes. The results obtained in [13–15] agree fairly well with experimental data.

The objective of this paper is to investigate energy spectra of the C_{50} fullerene and $C_{50}Cl_{10}$ molecule with symmetry groups D_{5h} under the Hubbard model in the mean-field approximation.

Energy spectrum of the C_{50} fullerene

As known, the electronic properties of carbon fullerenes and nanotubes generally depend on the behavior of π-electrons in these molecules. We use the Hubbard model [11] to characterize the π-electron system of the C_{50} fullerene:

$$H = \sum_{\sigma,i} \varepsilon_i n_{i\sigma} + \sum_{\sigma,i\neq j} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{\sigma,i} U_i n_{i\sigma} n_{i\bar{\sigma}}, \qquad (1)$$

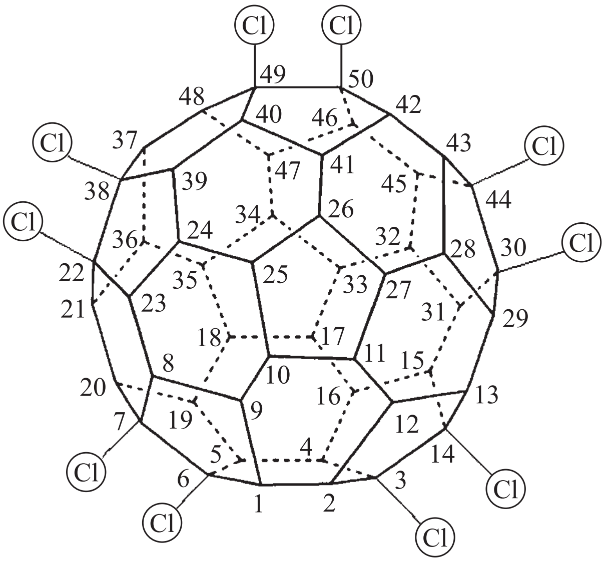

Figure 2. The $C_{50}Cl_{10}$ molecule.

where $c^{+}_{i\sigma}$, $c_{i\sigma}$ — the operators of creation and annihilation of electrons with the σ spin at the i site; $n_{i\sigma}$ — the operator of the number of particles with the σ spin at the i site; ε_i — the energy of the one-electron atomic state at the i site; t_{ij} — the transfer integral characterizing electron hops from the i site to the j site; U_i — the energy of the Coulomb repulsion of two electrons at the i site; $\bar{\sigma} = -\sigma$.

In order to find the energy spectrum of the C_{50} molecule in the mean-field approximation, one should perform the following substitution in Hamiltonian (1):

$$n_{i\sigma} n_{i\bar{\sigma}} \rightarrow n_{i\sigma}\langle n_{i\bar{\sigma}}\rangle + n_{i\bar{\sigma}}\langle n_{i\sigma}\rangle, \qquad (2)$$

where $\langle n_{i\sigma}\rangle$ — average number of electrons with spin σ in the i site.

Substituting expression (2) to expression (1), we will get Hamiltonian of the Hubbard model in the mean-field approximation:

$$H = \sum_{\sigma,i} \varepsilon'_{i\sigma} n_{i\sigma} + \sum_{\sigma,i\neq j} t_{ij} c^{+}_{i\sigma} c_{j\sigma}, \qquad (3)$$

where

$$\varepsilon'_{i\sigma} = \varepsilon_i + U\langle n_{i\bar{\sigma}}\rangle \qquad (4)$$

The performed studies of the C_{50} fullerene with the D_{5h} symmetry group [21] have shown that the distances between carbon atoms are as follows:

$$x_a = 1.399\,\text{Å},\ x_b = 1.449\,\text{Å},\ x_c = 1.444\,\text{Å},$$

$$x_d = 1.450\,\text{Å},\ x_e = 1.400\,\text{Å},\ x_g = 1.387\,\text{Å}. \qquad (5)$$

We use the following relation to determine the numerical values of the transfer integrals corresponding to the C_{50} molecule [13,14]:

$$t_s = -8957.33 \exp(-6.0207 x_s). \qquad (6)$$

Substituting (5) into formula (6), we obtain the numerical values for the transport integrals for the C_{50} fullerene with the symmetry group D_{5h}:

$$t_a = -1.96856\,\text{eV}, t_b = -1.45684\,\text{eV}, t_c = -1.50136\,\text{eV},$$

$$t_d = -1.44809\,\text{eV}, t_e = -1.95675\,\text{eV}, t_g = -2.511605\,\text{eV}. \tag{7}$$

In order to find the spectrum of energy of the C_{50} fullerene, finding the anticommutator Green functions [22] for all non-equivalent points of that fullerene is enough:

$$G_{f\sigma}(\tau) = \langle\langle c^{+}_{f\sigma}|c_{f\sigma}\rangle\rangle = \langle[c^{+}_{f\sigma}(\tau), c_{f\sigma}(0)]_{+}\rangle, \tag{8}$$

where $\tau = it$, t — time, i — imaginary unit.

Since the C_{50} fullerene has a total of four non-equivalent points, then to find the spectrum of energy of that fullerene, finding the Green functions, for example, for the points 1, 3, 9, and 10, is enough.

As known, the spectrum of energy of the quantum system is determined by Fourier transforms of anticommutator Green functions, which, in the mean-field approximation, refer to the following [13,14]:

$$\langle\langle c^{+}_{j\sigma}|c_{j\sigma}\rangle\rangle = \frac{i}{2\pi}\sum_{m=1}^{p}\frac{Q_{j,m}}{E - E_m + ih},$$

$$E_m = \varepsilon' + e_m, \tag{9}$$

where p — the number of the energy state of the quantum system, E_m — the energy of the m-th state of the quantum system, e_m — the energy of the m-th state of the quantum system versus ε', $Q_{j,m}$ — the spectrum density of the m-th energy state.

Note that with the known spectrum density of the energy state, one can find the degeneration degree of each energy level [13,14]:

$$g_i = \sum_{j=1}^{N} Q_{j,i}, \tag{10}$$

where g_i — the degeneration degree of the i-th energy level, N — the number of the sites of the nanosystem.

In order to find Green functions (8), first of all let us find the creation operators $c^{+}_{f\sigma}(\tau)$. To do this, we write the equations of motion for all creation operators $c^{+}_{f\sigma}(\tau)$ in the Heisenberg representation:

$$\frac{dc^{+}_{f\sigma}(\tau)}{d\tau} = [H, c^{+}_{f\sigma}(\tau)]. \tag{11}$$

By substituting Hamiltonian (3) into the equation of motion (11), we obtain a close system of differential equations:

$$\begin{cases} \dfrac{dc^{+}_{1\sigma}}{d\tau} = \varepsilon'_{\sigma}c^{+}_{1\sigma} + t_g c^{+}_{2\sigma} + t_c c^{+}_{6\sigma} + t_b c^{+}_{9\sigma} \\ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots . \\ \dfrac{dc^{+}_{50\sigma}}{d\tau} = \varepsilon'_{\sigma}c^{+}_{50\sigma} + t_c(c^{+}_{42\sigma} + c^{+}_{46\sigma}) + t_e c^{+}_{49\sigma} \end{cases} \tag{12}$$

By substituting the numerical values for transfer integrals (7) into the system of equations (12) and by solving the obtained system of differential equations, we obtain expressions for the creation operators $c^{+}_{f\sigma}(\tau)$. By using this solution and ratios (8), (9), we obtain for the C_{50} fullerene numerical values of energy states e_k versus the energy ε' and their degradation degree. The numerical values e_k and g_k are given in Table 1.

The energy states of the C_{50} fullerene with the D_{5h} symmetry group can be classified in accordance with the irreducible representations of this group, which has the following irreducible representations: a'_1, a'_2, a''_1, a''_2, e'_1, e'_2, e''_1, e''_2 [23]. Table 1 shows, which irreducible representations of the D_{5h} group the C_{50} fullerene energy states relate with.

Therefore, the results of these calculations have shown that the energy spectrum of the C_{50} fullerene with the D_{5h} symmetry group consists of 30 energy states, ten out of which are non-degenerated, and twenty two ones are generated.

As it follows from (9), the energy spectrum of the C_{50} fullerene is described by the following formula:

$$E_k = \varepsilon' + e_k, \tag{13}$$

where $\varepsilon' = -4.979\,\text{eV}$ [13].

Now, by substituting numerical values for e_k from Table 1, and numerical value for ε' in ratio (13) we get the energy spectrum of the C_{50} fullerene with the D_{5h} symmetry group. The calculation results are given in Table 1, as well as in Fig. 3. As seen from ratio (13) and Fig. 3, energy levels of fullerene C_{50} are concentrated near energy

$$\varepsilon' = \varepsilon + U\langle n_{\bar{\sigma}}\rangle. \tag{14}$$

where $U = 5.662\,\text{eV}$ [24].

Energy spectrum of the $C_{50}Cl_{10}$ molecule

According to experimental studies, the C_{50} molecule is a non-stable one. The C_{50} fullerene can be stabilized, e.g., by making chemical bonds of that fullerene with other molecules. The paper [4] deals with a stable $C_{50}Cl_{10}$ compound in a macroscopic quantity. The process of that molecule formation can be described as follows. When the $C_{50}Cl_{10}$ molecule is formed, ten valent electrons of the C_{50} fullerene and one valent electron out of each of ten chlorine atoms are coupled and form strong bonds between the chlorine and carbon atoms.

The studies described in the paper [21] have shown that the $C_{50}Cl_{10}$ molecule has the D_{5h} symmetry group, besides, these studies revealed that the distances between carbon atoms in this molecule are as follows:

$$x_a = 1.403\,\text{Å},\ x_b = 1.424\,\text{Å},\ x_c = 1.515\,\text{Å},$$

$$x_d = 1.430\,\text{Å},\ x_e = 1.598\,\text{Å},\ x_g = 1.373\,\text{Å}. \tag{15}$$

Substituting (15) into ratio (6), we obtain the numerical values for the transfer integrals in the molecule $C_{50}Cl_{10}$:

$$t_a = -1.92172\,\text{eV}, t_b = -1.69348\,\text{eV}, t_c = -1.979125\,\text{eV},$$

Table 1. Energy spectrum of the C_{50} fullerene with the D_{5h} symmetry group: values of levels energy, multiplicity of their degeneration and irreducible representations of the D_{5h} group, to which they belong

№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$	№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$
1	−4.975	−9.954	1	$E_1(a_1')$	16	−0.883	−5.068	1	$E_{16}(a_2')$
2	−4.531	−9.511	2	$E_2(e_1')$	17	0.534	−4.445	2	$E_{17}(e_1')$
3	−4.410	−9.390	1	$E_3(a_2'')$	18	1.171	−3.809	2	$E_{18}(e_1'')$
4	−3.668	−8.647	2	$E_4(e_2')$	19	1.876	−3.104	1	$E_{19}(a_2'')$
5	−3.586	−8.566	2	$E_5(e_1'')$	20	2.116	−2.863	1	$E_{20}(a_1'')$
6	−3.509	−8.489	1	$E_6(a_1')$	21	2.125	−2.854	1	$E_{21}(a_1')$
7	−2.550	−7.529	2	$E_7(e_2')$	22	2.225	−2.754	2	$E_{22}(e_2'')$
8	−2.494	−7.473	2	$E_8(e_2')$	23	2.408	−2.572	2	$E_{23}(e_2')$
9	−2.478	−7.457	1	$E_9(a_2'')$	24	2.561	−2.418	2	$E_{24}(e_1')$
10	−2.338	−7.318	2	$E_{10}(e_1')$	25	3.060	−1.920	2	$E_{25}(e_2')$
11	−1.542	−6.522	2	$E_{11}(e_1'')$	26	3.063	−1.916	2	$E_{26}(e_1'')$
12	−1.466	−6.445	2	$E_{12}(e_2'')$	27	4.133	−0.846	2	$E_{27}(e_2'')$
13	−1.391	−6.371	2	$E_{13}(e_2')$	28	4.150	−0.829	2	$E_{28}(e_1')$
14	−1.271	−6.251	2	$E_{14}(e_1')$	29	4.161	−0.818	1	$E_{29}(a_2')$
15	−0.610	−5.589	1	$E_{15}(a_1')$	30	4.428	−0.551	2	$E_{30}(e_2')$

Table 2. Energy spectrum of the $C_{50}Cl_{10}$ molecule with the D_{5h} symmetry group: values of levels energy, multiplicity of their degeneration and irreducible representations of the D_{5h} group, to which they belong

№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$	№	e_j, eV	E_j, eV	g_j	$E(\Gamma_j)$
1	−4.907	−11.018	1	$E_1(a_1')$	16	−0.179	−6.290	1	$E_{16}(a_2')$
2	−4.773	−10.884	1	$E_3(a_2'')$	17	0.262	−5.849	2	$E_{17}(e_1')$
3	−4.196	−10.307	2	$E_2(e_1')$	18	1.130	−4.981	2	$E_{18}(e_1'')$
4	−3.916	−10.027	2	$E_5(e_1'')$	19	1.137	−4.974	2	$E_{23}(e_2')$
5	−3.221	−9.332	2	$E_4(e_2')$	20	1.807	−4.304	2	$E_{24}(e_1')$
6	−3.176	−9.287	1	$E_6(a_1')$	21	2.024	−4.087	1	$E_{19}(a_2'')$
7	−2.820	−8.931	1	$E_9(a_2'')$	22	2.187	−3.924	1	$E_{21}(a_1')$
8	−2.799	−8.910	2	$E_7(e_2'')$	23	2.302	−3.809	1	$E_{20}(a_1'')$
9	−1.939	−8.050	2	$E_8(e_2')$	24	2.494	−3.617	2	$E_{22}(e_2'')$
10	−1.931	−8.042	2	$E_{10}(e_1')$	25	2.749	3.362	2	$E_{25}(e_2')$
11	−1.590	−7.701	2	$E_{11}(e_1'')$	26	3.075	−3.036	1	$E_{29}(a_2')$
12	−1.530	−7.641	2	$E_{12}(e_2'')$	27	3.367	−2.744	2	$E_{26}(e_1'')$
13	−0.703	−6.814	2	$E_{13}(e_2')$	28	3.708	−2.403	2	$E_{28}(e_1')$
14	−0.659	−6.770	2	$E_{14}(e_1')$	29	4.478	−1.633	2	$E_{27}(e_2'')$
15	−.2670	−6.378	1	$E_{15}(a_1')$	30	4.620	1.491	2	$E_{30}(e_2')$

$$t_d = -1.63340\,\text{eV},\, t_e = -1.59404\,\text{eV},\, t_g = -2.30214\,\text{eV}. \tag{16}$$

Using relations (16), (12), (8) and (9), we will obtain for the $C_{50}Cl_{10}$ molecule the numerical values for the values e_k, which are given in Table 2.

According to ratio (14), when the $C_n^q X_k^{(-q)}$ molecule is formed, the energy ε' is changed:

$$\varepsilon' = \begin{cases} \varepsilon'_{C_n}, & \text{for } C_n, \\ \varepsilon'_{C_n} - qU/n, & \text{for } C_n^{+q} X_k^{(-q)}, \end{cases} \tag{17}$$

where ε'_{C_n} corresponds to the C_n fullerene; q — number of electrons passing from the C_n fullerene to k atoms of X.

From ratio (17) it follows that:

$$\varepsilon'_{C_{50}Cl_{10}} = \varepsilon'_{C_{50}} - \frac{qU}{n} = -4.979 - \frac{10 \cdot 5.662}{50} = 6.111\,\text{eV}, \tag{18}$$

where $U = 5.662\,\text{eV}$ [24], $\varepsilon' = -4.979\,\text{eV}$ [13].

Now, by substituting the numerical values for e_k from Table 2, as well as numerical value for $\varepsilon' = \varepsilon'_{C_{50}Cl_{10}}$ to ratio (13), we obtain the energy spectrum of the $C_{50}Cl_{10}$ molecule with the D_{5h} symmetry group. The calculation results are given in Table 2, as well as in Fig. 4.

From Figs. 3 and 4, Tables 1 and 2 we can see that the energy spectra of the C_{50} and $C_{50}Cl_{10}$ molecules differ from each other by the relative position of their energy state $E_2(a_1')$, $E_3(a_2'')$, $E_4(e_2')$, $E_5(e_1'')$, $E_9(a_2'')$, $E_{20}(a_1'')$, $E_{21}(a_1')$, $E_{23}(e_2')$, $E_{24}(e_1')$, $E_{27}(e_2'')$, $E_{28}(e_1')$, $E_{29}(a_2')$.

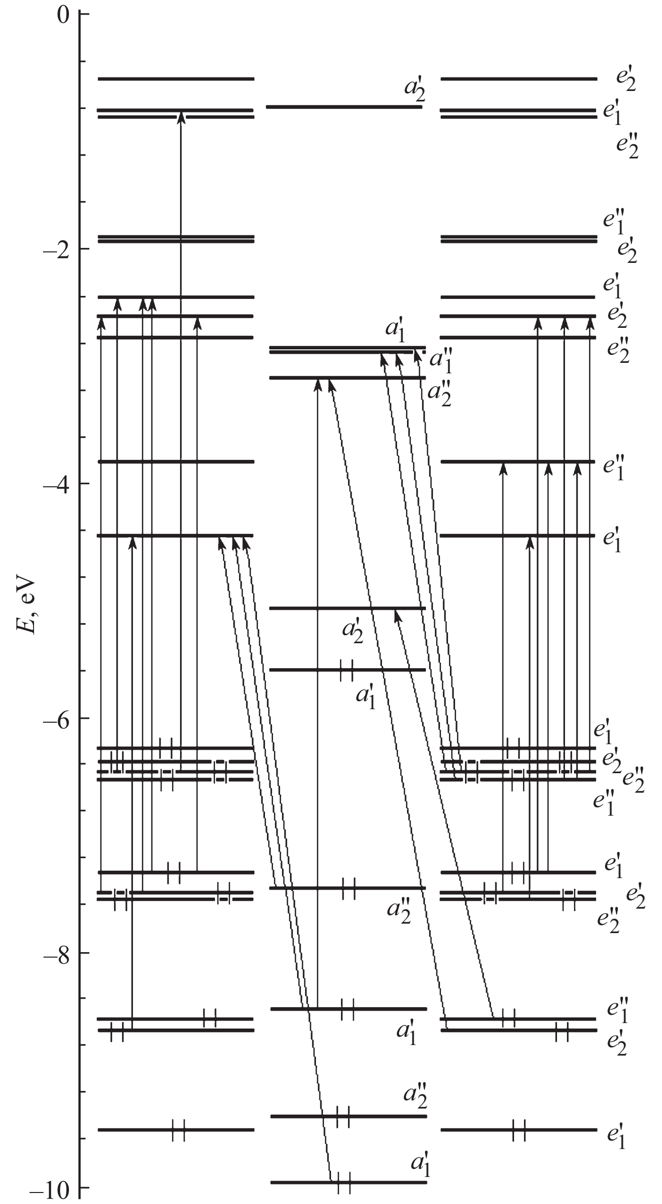

Figure 3. Energy spectrum of the C_{50} fullerene with the D_{5h} symmetry group.

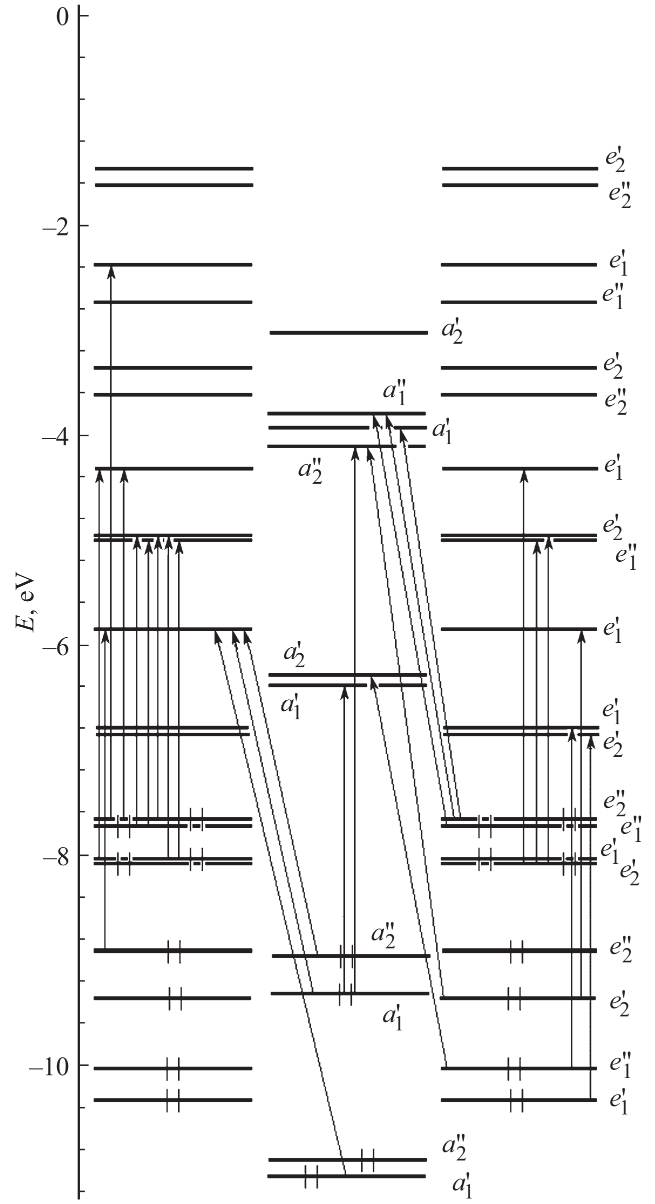

Figure 4. Energy spectrum of the $C_{50}Cl_{10}$ molecule with the D_{5h} symmetry group.

The optical absorption spectrum is an essential characteristic of any molecule. Using the above energy spectra of the C_{50} and $C_{50}Cl_{10}$ molecules with the D_{5h} symmetry group, by means of the group theory one may determine the transitions that shape the optical spectra of these molecules. It can be shown, that the following transitions are allowed in the energy spectrum of a molecule with the D_{5h} symmetry group [23]:

$$\begin{gathered} a'_1 \leftrightarrow e'_1,\ a'_1 \leftrightarrow a''_2,\ a'_2 \leftrightarrow e'_1,\ e'_1 \leftrightarrow e'_2, \\ e'_1 \leftrightarrow e''_1,\ e'_2 \leftrightarrow e'_2,\ e''_2 \leftrightarrow e''_2,\ a''_1 \leftrightarrow e''_1, \\ e'_2 \leftrightarrow e''_2,\ a'_2 \leftrightarrow a''_1,\ a''_2 \leftrightarrow e''_1,\ e''_2 \leftrightarrow e''_1. \end{gathered} \tag{19}$$

From energy spectra of the $_{50}$ and $C_{50}Cl_{10}$ molecules with the D_{5h} symmetry group and ratios (19) it follows that the C_{50} fullerene has 94 allowed transitions, and the $C_{50}Cl_{10}$ molecule has 90 allowed transitions. It can be seen in Figs. 3 and 4 that when the $C_{50}Cl_{10}$ molecule is generated, 20 allowed transitions disappear from the C_{50} fullerene and 16 allowed transitions appear simultaneously.

The paper [4] performed experimental studies dealing with study of the optical absorption spectrum of the $C_{50}Cl_{10}$ molecule in cyclohexane. The studies have shown that eight distinct absorption bands can be picked up in the $C_{50}Cl_{10}$ molecule optical spectrum: a, b, c, d, e, f, g, h, which are given in Table 3.

Knowing the energy spectrum of the $C_{50}Cl_{10}$ molecule, its experimentally observed spectrum of optical absorption can be interpreted as follows. The optical absorption spectrum bands of the molecule, which correspond to the

Table 3. Experimental and theoretical values of the wavelengths and energies, which correspond to the absorption bands within the optical spectrum of the $C_{50}Cl_{10}$ molecule

Absorption Theory	[4] λ, nm	[4] E, eV	bands E, eV
a	454.6	2.73	2.67
b	433.8	2.86	2.91
c	400.8	3.10	3.07
d	376.6	3.30	3.36
e	356.6	3.48	3.48
f	334.0	3.72	3.75
g	322.0	3.86	3.89
h	238.5	5.21	5.20

Table 4. Transitions forming the absorption bands *a*, *b*, *c*, *d*, *e*, *f*, *g*, *h*

ΔE	ΔE, eV	δ	ΔE	ΔE, eV	δ	ΔE	ΔE, eV	δ
a			*d*			*g*		
$E_{18}-E_{12}$	2.66	$-$	$E_{22}-E_{10}$	3.21	$-$	$E_{20}-E_{12}$	3.83	$-$
$E_{23}-E_{12}$	2.67	$+$	$E_{14}-E_{5}$	3.26	$+$	$E_{20}-E_{11}$	3.89	$+$
$E_{18}-E_{11}$	2.72	$-$	$E_{24}-E_{12}$	3.34	$-$	$E_{15}-E_{2}$	3.93	$-$
$E_{23}-E_{11}$	2.73	$-$	*e*			$E_{18}-E_{7}$	3.93	$-$
b			$E_{17}-E_{6}$	3.44	$+$	*h*		
$E_{15}-E_{6}$	2.91	$-$	$E_{17}-E_{4}$	3.48	$+$	$E_{17}-E_{1}$	5.17	$+$
$E_{15}-E_{4}$	2.95	$-$	$E_{13}-E_{2}$	3.49	$+$	$E_{19}-E_{6}$	5.20	$+$
c			*f*			$E_{28}-E_{12}$	5.24	$-$
$E_{17}-E_{7}$	3.06	$-$	$E_{21}-E_{12}$	3.72	$-$	$E_{19}-E_{4}$	5.24	$-$
$E_{18}-E_{10}$	3.06	$+$	$E_{24}-E_{10}$	3.74	$-$			
$E_{18}-E_{8}$	3.07	$-$	$E_{16}-E_{5}$	3.74	$-$			
$E_{23}-E_{10}$	3.07	$+$	$E_{24}-E_{8}$	3.75	$+$			
$E_{17}-E_{9}$	3.08	$-$	$E_{21}-E_{11}$	3.78	$-$			
$E_{23}-E_{8}$	3.08	$+$						

experimentally observed energies E_a, E_b, E_c, E_d, E_e, E_f, E_g, E_h, as given in Table 3, can be interpreted as bands, which are formed by transitions as given in Table 4. It is clear from Table 4 that energies of these transitions are close to the experimental values [4]. The δ symbol in Table 4 shows the transitions as allowed and not allowed in terms of symmetry. If $\delta = +$, then such a transition is allowed in terms of symmetry, if $\delta = -$, then such a transition is not allowed. It should be noted that the atoms in the $C_{50}Cl_{10}$ molecule make small oscillations around an equilibrium. This leads to the asymmetry of the $C_{50}Cl_{10}$ molecule. As a result, optical transitions not allowed in terms of the system symmetry become allowed. As a result of the asymmetry, some of the unallowed transitions may form a clearly observed band of optical absorption. In case of the $C_{50}Cl_{10}$ molecule, such an absorption band is the absorption band with the energy of E_b.

Conclusion

Conducted research also demonstrated that optical absorption spectrum of the $C_{50}Cl_{10}$ molecule, which is observed experimentally [4], is rather well agreed with the optical absorption spectrum obtained within the Hubbard model in the mean-field approximation.

We also note that studies of the optical properties of the C_{60} and C_{70} fullerenes, as well as the $Y_3N@C_{80}$ endofullerene, carried out within the Hubbard model in the mean-field approximation in papers [14,13,12], have shown good agreement between the experimental data and theoretical results. This allows one to state that the Hubbard model in the mean-field approximation characterizes fairly well the electron properties of carbon nanosystems.

Conflict of interest

The author declares that he has no conflict of interest.

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