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Energy Spectrum and Optical Absorption Spectrum of exohedral Fullerene $C_{50}Cl_{10}$ within the Hubbard Model

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Energy spectra of fullerene C_{50} and exohedral fullerene $C_{50}Cl_{10}$ with the D_{5h} symmetry groups have been obtained within the Hubbard model and static fluctuation approximation. The energy states have been classified using the methods of group theory, and the allowed transitions in the energy spectra of molecules C_{50} and $C_{50}Cl_{10}$ have been determined. On the basis of the energy spectrum of exohedral fullerene $C_{50}Cl_{10}$ is given an interpretation of experimentally observed optical absorption bands molecule $C_{50}Cl_{10}$.

Keywords: Hubbard model, Green's functions, energy spectrum, fullerenes, nanosystems, fullerene C_{50}, exohedral fullerene $C_{50}Cl_{10}$.

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1. Introduction

After discovery of the fullerene C_{60} [1] in 1985, intense experimental studies have begun to discover other fullerenes. These studies have shown that besides the fullerenes C_n, where $n > 60$, there are also small fullerenes C_n, for which $n < 60$. Theoretical studies showed that in contrast to the fullerenes C_n, where $n \geq 60$, the small fullerenes have no isomer containing isolated pentagons. One of the small fullerenes is the fullerene C_{50}, which was discovered in 1985, simultaneously with the fullerene C_{60} when studying mass spectra of vapors of carbon clusters [1].

After the discovery of the fullerenes, studies of not only physical but chemical properties thereof have been initiated. These studies have shown that a number of the fullerenes are unstable molecules in a free state, and their chemical compounds are quite stable structures. For example, in 2004, a modified method of arc discharge [2] in a gaseous medium consisting in molecules of carbon tetrachloride CCl_4 at the partial pressure of 0.013 atm and helium atoms He at the partial pressure of 0.395 atm was applied, thereby resulting in first production of the compound $C_{50}Cl_{10}$ in an amount of about two milligrams with purity of 99.5% [3]. The studies of the molecules $C_{50}Cl_{10}$ by nuclear magnetic resonance have shown that these molecules have the D_{5h} symmetry. The carried-out studies have also shown that the $C_{50}Cl_{10}$ far more exceed the C_{60} in a static polarizability and the second hyperpolarizability. That is why the $C_{50}Cl_{10}$ is considered to be a promising material for the nonlinear optics [4]. The studies of the endohedral fullerenes He@C_{50}, Ne@C_{50} and Ar@C_{50} have shown that these molecules and the molecule $C_{50}Cl_{10}$ as well have the D_{5h} symmetry group, too [5].

As shown in the Fig. 1, the fullerene C_{50} with the D_{5h} symmetry group consists of 15 hexagons and 12 pentagons. Note that 271 isomers of the fullerene C_{50} can be built out of 50 carbon atoms [6]. It is clear from the Schlegel diagram of the Fig. 1 that the fullerene C_{50} 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 the two hexagons and one pentagon 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 the vertices of junction of the two pentagons and one hexagon 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 the two hexagons and one pentagon and, furthermore, each of these atoms has no adjacent neighbor of the same G_4 set.

The studies of the molecules $C_{50}Cl_{10}$ by the nuclear magnetic resonance have shown that chlorine atoms in these molecules are bonded to the carbon atoms, which belong to the G_2 set [3], i.e. as it is shown in Fig. 2, the chlorine atoms form a Saturn ring-like structure around the fullerene C_{50}. Quite a lot of papers [7–9] are devoted to the study of the physical and chemical properties of the fullerene C_{50}.

The Hubbard model [20] is commonly used to characterized the electron properties of the carbon fullerenes and nanotubes [10–19].

This model in the static fluctuation approximation (SFA) was used to obtain energy spectra and optical absorp-

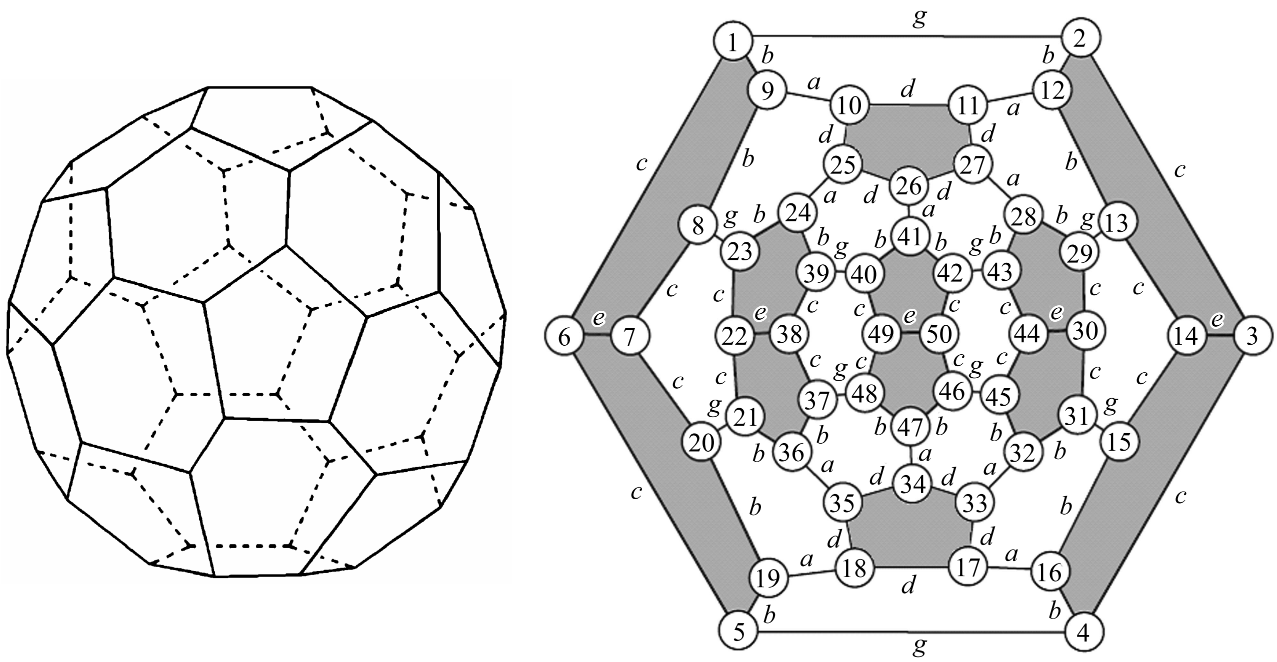

Figure 1. *a* — fullerene C_{50} with the D_{5h} symmetry group, *b* — its Schlegel diagram indicating positions of carbon atoms, bonds between carbon atoms and pentagons.

tion spectra of the fullerene C_{80} with the I_h symmetry group [10], the fullerene C_{70} [11], the fullerene C_{60} [12], the fullerene C_{36} with the D_{6h} symmetry group [13], the fullerene C_{28} with the T_d symmetry group [14], the fullerene C_{26} with the D_{3h} symmetry group [15], the fullerene C_{24} with the O_h, D_6 and D_{6d} symmetry groups [16] and the fullerene C_{20} with the I_h, D_{5d} and D_{3d} symmetry groups [17], while the paper [19] studies the electron properties of the carbon nanotubes. The results obtained in the papers [10–12] agree fairly well with experimental data.

The purpose of the present study is to study the energy spectrum of the exohedral fullerene $C_{50}Cl_{10}$ with the D_{5h} symmetry group within the Hubbard model in the static fluctuation approximation. To prepare for the study of the energy spectrum of the molecule $C_{50}Cl_{10}$, we first examine the energy spectrum of the fullerene C_{50} with the D_{5h} symmetry group.

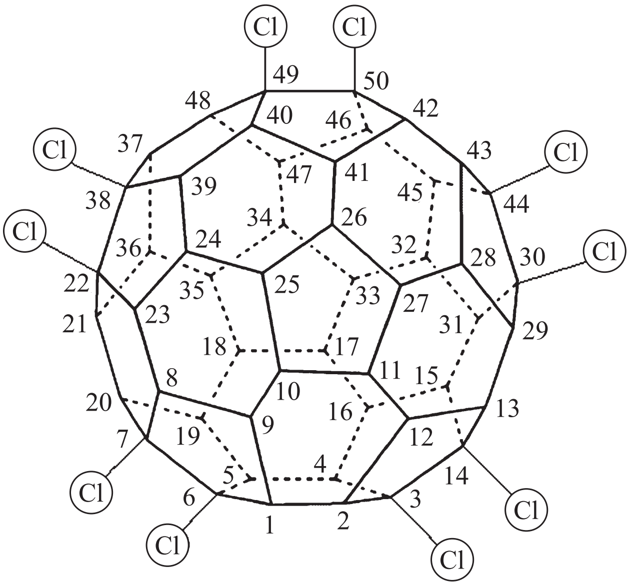

Figure 2. Molecule $C_{50}Cl_{10}$.

2. Energy spectrum of the fullerene C_{50}

To describe the π-electron system of the fullerene C_{50}, we will use the Hubbard model [20]:

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

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-m site; $\bar{\sigma} = -\sigma$.

Let us find the energy spectrum of the fullerene C_{50} in SFA. To do so, we will use the Green's functions method [21], which states that in order to find the energy spectrum of a quantum system, it is sufficient to calculate poles of the Fourier transforms of anticommutator Green's functions:

$$\langle\langle c^+_{f\sigma}|c_{f\sigma}\rangle\rangle = \langle[c^+_{f\sigma}(\tau), c_{f\sigma}(0)]\rangle, \qquad (2)$$

where $f = 1, \ldots, N$; N — a number of sites of the quantum system.

It can be shown [10,12] that the Fourier transform of the anticommutator Green's function (2) in SFA takes the following form:

$$\langle\langle c^+_{j\sigma}|c_{j\sigma}\rangle\rangle_E = \frac{i}{2\pi}\sum_{m=1}^{p}\frac{F_{j,m}}{E - E_m + ih},$$
$$E_k = \varepsilon + e_k,\ E_{k+p} = E_k + U,\ F_{j,m} = q_{m,\sigma}Q_{j,m},$$
$$Q_{j,k+6} = Q_{j,k},\ k = 1, \ldots, p, \qquad (3)$$
$$q_{m,\sigma} = \begin{cases} 1 - \dfrac{n}{2}, & m = 1, \ldots, p/2, \\ \dfrac{n}{2}, & m = p/2 + 1, \ldots, p. \end{cases}$$

where p — the number of the energy states of the quantum system, E_m — the energy of the m-th state of the quantum system, $F_{j,m}$ — the spectrum density of the m-th energy state.

The energy spectrum is importantly characterized by a degeneration degree, which can be found by knowing the spectrum density of their states [10,12]:

$$g_i = \sum_{j=1}^{N} Q_{j,i}, \qquad (4)$$

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

As the fullerene C_{50} has four groups of nonequivalent sites, then in order to find the energy spectrum of the fullerene C_{50} , it is necessary to compute the anticommutator Green's functions for any four nonequivalent sites of this fullerene. In order to find the Green's functions, first of all, we determine a time dependence of birth operators. To do so, using the Hamiltonian (1) and the Schlegel diagram of the Fig. 1, as it is in the papers [10–17], we write motion equations in SFA for the $c^+_{1\sigma}(\tau)$, $c^+_{1\sigma}n_{1\bar\sigma}(\tau), \ldots, c^+_{50\sigma}(\tau)$, $c^+_{50\sigma}n_{50\bar\sigma}(\tau)$ operators, specified in the Heisenberg representation:

$$\begin{cases} \dfrac{dc^+_{1\sigma}}{d\tau} = \varepsilon c^+_{1\sigma} + t_g c^+_{2\sigma} + t_c c^+_{6\sigma} + t_b c^+_{9\sigma} \\ \dfrac{d(c^+_{1\sigma}n_{1\bar\sigma})}{d\tau} = (\varepsilon + U)c^+_{1\sigma}n_{1\bar\sigma} + t_g c^+_{2\sigma}n_{2\bar\sigma} \\ \qquad + t_c c^+_{6\sigma}n_{6\bar\sigma} + t_b c^+_{9\sigma}n_{9\bar\sigma} \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \dfrac{dc^+_{50\sigma}}{d\tau} = \varepsilon \cdot c^+_{50\sigma} + t_c(c^+_{42\sigma} + c^+_{46\sigma}) + t_e c^+_{49\sigma} \\ \dfrac{d(c^+_{50\sigma}n_{50\bar\sigma})}{d\tau} = (\varepsilon + U)c^+_{50\sigma}n_{50\bar\sigma} + t_c(c^+_{42\sigma}n_{42\bar\sigma} \\ \qquad + c^+_{46\sigma}n_{46\bar\sigma}) + t_e c^+_{49\sigma}n_{49\bar\sigma} \end{cases}, \qquad (5)$$

where $\tau = it$, t — time.

The system of equations (5) is a closed system of differential equations. Before solving this system, we find numerical values for the transfer integrals, which correspond to the fullerene C_{50}. For this we will use the following relationship [10,11]:

$$t_s = -8.17065\exp(-1.69521x_s). \qquad (6)$$

The studies of the fullerene C_{50} [4] have shown that distances between carbon atoms in this fullerene are as follows:

$$x_a = 1.399\,\text{Å},\quad x_b = 1.449\,\text{Å},\quad x_c = 1.444\,\text{Å},$$
$$x_d = 1.450\,\text{Å},\quad x_e = 1.400\,\text{Å},\quad x_g = 1.387\,\text{Å}. \qquad (7)$$

Now, substituting (7) into the relationship (6), we obtain the numerical values for the transfer integrals for the fullerene C_{50} with the D_{5h} symmetry group:

$$t_a = -0.76258\,\text{eV},\quad t_b = -0.70061\,\text{eV},$$
$$t_c = -0.70657\,\text{eV},\quad t_d = -0.69942\,\text{eV},$$
$$t_e = -0.76129\,\text{eV},\quad t_g = -0.77825\,\text{eV}. \qquad (8)$$

As it follows from (3), in order to find the energy spectrum of the fullerene C_{50}, it is necessary to know numerical values of the ε and U parameters. The required values ($\varepsilon = -7.824$ eV, $U = 5.662$ eV) were determined in the paper [12] based on the experimentally measured optical absorption spectrum of the fullerene C_{60} within the Hubbard model in SFA. Note that the numerical value of the parameter $U = 5.662$ eV agrees with the results presented in the paper [22], where $U \sim 5$ eV was obtained.

Substituting the numerical values of the transfer integrals (8), as well as the numerical values of the parameters $\varepsilon = -7.824$ eV and $U = 5.662$ eV into the system of differential equations (5) and solving this system, we obtain expressions for the birth operators $c^+_{1\sigma}(\tau), \ldots, c^+_{50\sigma}(\tau)$. Using the solution of the system of equations (5), as well as relationships (2), (3) and (4), we obtain the numerical values for E_k, $\bar{e}_k$ and g_k, see Table 1, where $\bar{e}_k$ — the energy value of the k-th level in relation to $\varepsilon + U/2$, which, as it is clear from the relationship (3), is correlated to the magnitude E_k as follows:

$$E_k = \varepsilon + \frac{U}{2} + \bar{e}_k, \qquad (9)$$

where

$$\bar{e}_k = \begin{cases} e_k - \dfrac{U}{2}, & k = 1, \ldots, p/2, \\ e_k + \dfrac{U}{2}, & k = p/2 + 1, \ldots, p. \end{cases} \qquad (10)$$

As it follows from the relationships (9) and (10), the energy states of the fullerene C_{50} form two Hubbard subbands, wherein the lower Hubbard subband is formed by the energy states focused near the energy ε, while the upper Hubbard subband is formed by the energy states focused near the energy $\varepsilon + U$. The energy states forming the energy spectrum of the fullerene C_{50} with the D_{5h} symmetry group can be classified by irreducible representations of the D_{5h} group, see Table 1. The energy spectrum of the fullerene C_{50} is shown in the Fig. 3.

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

The experimental studies show that the fullerene C_{50} is an unstable molecule, which can be stabilized by forming chemical compounds of this fullerene with other molecules. The paper [3] states that the stable exohedral fullerene $C_{50}Cl_{10}$ was produced in macroscopic quantities.

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

№	e_j	E_j, eV	g_j	Γ_j	№	e_j	E_j, eV	g_j	Γ_j
1	−5.005	−9.998	1	$E_1(a'_1)$	31	.657	−4.336	1	$E_{31}(a'_1)$
2	−4.805	−9.798	2	$E_2(e'_1)$	32	.857	−4.136	2	$E_{32}(e'_1)$
3	−4.766	−9.759	1	$E_3(a''_2)$	33	.896	−4.097	1	$E_{33}(a''_2)$
4	−4.445	−9.437	2	$E_4(e'_2)$	34	1.217	−3.776	2	$E_{34}(e'_2)$
5	−4.390	−9.383	1	$E_5(a'_1)$	35	1.272	−3.721	1	$E_{35}(a'_1)$
6	−4.362	−9.355	2	$E_6(e''_1)$	36	1.300	−3.693	2	$E_{36}(e''_1)$
7	−3.931	−8.924	1	$E_7(a''_2)$	37	1.731	−3.262	1	$E_{37}(a''_2)$
8	−3.918	8.911	2	$E_8(e'_2)$	38	1.744	−3.249	2	$E_{38}(e'_2)$
9	−3.899	−8.892	2	$E_9(e''_2)$	39	1.763	−3.230	2	$E_{39}(e''_2)$
10	−3.780	−8.773	2	$E_{10}(e'_1)$	40	1.882	−3.111	2	$E_{40}(e'_1)$
11	−3.419	−8.412	2	$E_{11}(e''_1)$	41	2.243	−2.750	2	$E_{41}(e''_1)$
12	−3.417	−8.410	2	$E_{12}(e'_1)$	42	2.245	−2.748	2	$E_{42}(e'_1)$
13	3.396	−8.389	2	$E_{13}(e''_2)$	43	2.266	−2.727	2	$E_{43}(e''_2)$
14	−3.356	−8.349	2	$E_{14}(e'_2)$	44	2.306	2.687	2	$E_{44}(e'_2)$
15	−3.064	−8.056	1	$E_{15}(a'_1)$	45	2.598	−2.395	1	$E_{45}(a'_1)$
16	−3.061	−8.054	1	$E_{16}(a'_2)$	46	2.601	−2.392	1	$E_{46}(a'_2)$
17	−2.695	−7.688	2	$E_{17}(e'_1)$	47	2.967	−2.026	2	$E_{47}(e'_1)$
18	−2.442	−7.435	2	$E_{18}(e''_1)$	48	3.220	−1.773	2	$E_{48}(e''_1)$
19	−2.053	−7.046	1	$E_{19}(a''_1)$	49	3.609	−1.384	1	$E_{49}(a''_1)$
20	−1.973	−6.966	1	$E_{20}(a''_2)$	50	3.689	−1.304	1	$E_{50}(a''_2)$
21	−1.859	−6.852	2	$E_{21}(e''_2)$	51	3.803	−1.190	2	$E_{51}(e''_2)$
22	−1.804	−6.797	1	$E_{22}(a'_1)$	52	3.858	−1.135	1	$E_{52}(a'_1)$
23	−1.745	−6.738	1	$E_{23}(e'_2)$	53	3.917	−1.076	1	$E_{53}(e'_2)$
24	−1.669	−6.662	2	$E_{24}(e'_1)$	54	3.993	−1.000	2	$E_{54}(e'_1)$
25	−1.533	−6.526	2	$E_{25}(e''_1)$	55	4.129	−.864	2	$E_{55}(e''_1)$
26	−1.493	−6.486	2	$E_{26}(e'_2)$	56	4.169	−.824	2	$E_{56}(e'_2)$
27	−1.062	−6.054	1	$E_{27}(a'_2)$	57	4.600	−.393	1	$E_{57}(a'_2)$
28	−1.051	−6.044	2	$E_{28}(e'_1)$	58	4.611	−.382	2	$E_{58}(e'_1)$
29	1.039	−6.032	2	$E_{29}(e''_2)$	59	4.623	−.370	2	$E_{59}(e''_2)$
30	−.897	−5.890	2	$E_{30}(e'_2)$	60	4.765	−.228	2	$E_{60}(e'_2)$

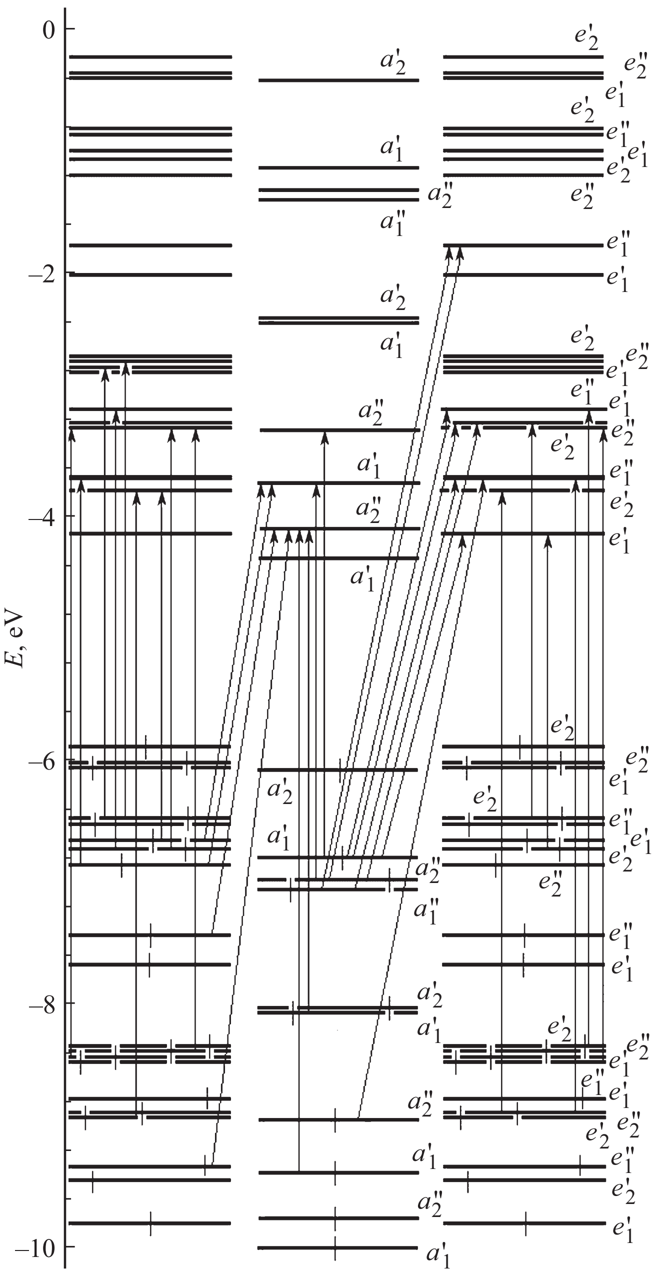

Figure 3. Energy spectrum of the fullerene C_{50}.

Let us consider the energy spectrum of the exohedral fullerene $C_{50}Cl_{10}$, which has the D_{5h} symmetry group as per studies [4]. The studies of the exohedral fullerene $C_{50}Cl_{10}$ [4] have also shown that distances between carbon atoms in this molecule are as follows:

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

$$x_d = 1.430\,\text{Å},\ x_e = 1.598\,\text{Å},\ x_g = 1.373\,\text{Å}. \qquad (11)$$

It follows from the relationships (6) and (11) that for the molecule $C_{50}Cl_{10}$ the transfer integrals have the following numerical values:

$$t_a = -0.75743\,\text{eV}, \quad t_b = -0.73094\,\text{eV},$$

$$t_c = -0.62645\,\text{eV}, \quad t_d = -0.72354\,\text{eV},$$

$$t_e = -0.54422\,\text{eV}, \quad t_g = -0.79694\,\text{eV}. \qquad (12)$$

Knowing numerical values for the transfer integrals (12), as well as the numerical values for the parameters $\varepsilon = -7.824\,\text{eV}$ and $U = 5.662\,\text{eV}$, and using the relationships (5) and (2)−(4), we will obtain the numerical values for the magnitudes E_k, $\bar{e}_k$ and g_k for the $C_{50}Cl_{10}$ molecule, see Table 2. The Fig. 4 shows the energy spectrum of the exohedral fullerene $C_{50}Cl_{10}$. It is clear from the Figures 3 and 4 that the fullerene C_{50} has the lower Hubbard subband fully occupied, while the exohedral fullerene $C_{50}Cl_{10}$ has ten energy states in the lower Hubbard subband unoccupied. It is due to the fact that when the molecule $C_{50}Cl_{10}$ is formed, the ten valence electrons of the fullerene C_{50} are spent to form strong chemical bonds with the chlorine atoms.

The optical absorption spectrum is an essential physical characteristic of any molecule. Using the above energy spectrum of the exohedral fullerene $C_{50}Cl_{10}$ with the D_{5h} symmetry group, it is possible to find the transitions which form the optical spectrum of this molecule. The group theory [23] may be used to demonstrate that a molecule with the D_{5h} symmetry group has the following allowed transitions in its energy spectrum:

$$a'_1 \leftrightarrow e'_1,\ a'_1 \leftrightarrow a''_2,\ a'_2 \leftrightarrow e'_1,\ e'_1 \leftrightarrow e'_2,$$

$$e'_1 \leftrightarrow e''_1,\ e'_2 \leftrightarrow e'_2,\ e''_2 \leftrightarrow e''_2,\ a''_1 \leftrightarrow e''_1,$$

$$e'_2 \leftrightarrow e''_2,\ a'_2 \leftrightarrow a''_1,\ a''_2 \leftrightarrow e''_1,\ e''_2 \leftrightarrow e''_1. \qquad (13)$$

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

Table 2. The energy spectrum of the fullerene $C_{50}Cl_{10}$: level energy values, multiplicity of their degeneration and irreducible representations of the D_{5h} group, to which they belong

№	e_j	E_j, eV	g_j	Γ_j	№	e_j	E_j, eV	g_j	Γ_j
1	−4.957	−9.950	1	$E_1(a'_1)$	31	0.705	−4.288	1	$E_{31}(a'_1)$
2	−4.811	−9.804	1	$E_3(a''_2)$	32	0.851	−4.142	1	$E_{33}(a''_2)$
3	−4.709	−9.702	2	$E_2(e'_1)$	33	0.953	−4.040	2	$E_{32}(e'_1)$
4	−4.402	−9.395	2	$E_6(e''_1)$	34	1.260	−3.733	2	$E_{36}(e''_1)$
5	−4.332	−9.325	1	$E_5(a'_1)$	35	1.330	−3.663	1	$E_{35}(a'_1)$
6	−4.324	−9.317	2	$E_4(e'_2)$	36	1.338	−3.655	2	$E_{34}(e'_2)$
7	−3.978	−8.971	1	$E_7(a''_2)$	37	1.684	−3.309	1	$E_{37}(a''_2)$
8	−3.931	−8.924	2	$E_9(e''_2)$	38	1.731	−3.262	2	$E_{39}(e''_2)$
9	−3.836	−8.829	2	$E_8(e'_2)$	39	1.826	−3.167	2	$E_{38}(e'_2)$
10	−3.720	−8.713	2	$E_{10}(e'_1)$	40	1.942	−3.051	2	$E_{40}(e'_1)$
11	−3.428	−8.421	2	$E_{11}(e''_1)$	41	2.234	−2.759	2	$E_{41}(e''_1)$
12	−3.406	−8.399	2	$E_{13}(e''_2)$	42	2.256	−2.737	2	$E_{43}(e''_2)$
13	−3.346	−8.339	2	$E_{12}(e'_1)$	43	2.316	−2.677	2	$E_{42}(e'_1)$
14	−3.288	−8.281	2	$E_{14}(e'_2)$	44	2.374	−2.619	2	$E_{44}(e'_2)$
15	−3.055	−8.048	1	$E_{16}(a'_2)$	45	2.607	−2.386	1	$E_{46}(a'_2)$
16	3.025	−8.018	1	$E_{15}(a'_1)$	46	2.637	−2.356	1	$E_{45}(a'_1)$
17	−2.718	−7.711	2	$E_{17}(e'_1)$	47	2.944	−2.049	2	$E_{47}(e'_1)$
18	−2.446	−7.439	2	$E_{18}(e''_1)$	48	3.216	−1.777	2	$E_{48}(e''_1)$
19	−2.034	−7.027	1	$E_{19}(a''_1)$	49	3.628	−1.365	1	$E_{49}(a''_1)$
20	−1.948	−6.941	1	$E_{20}(a''_2)$	50	3.714	−1.279	1	$E_{50}(a''_2)$
21	−1.892	−6.885	2	$E_{23}(e'_2)$	51	3.770	−1.223	2	$E_{53}(e'_2)$
22	−1.821	−6.814	2	$E_{21}(e''_2)$	52	3.841	−1.152	2	$E_{51}(e''_2)$
23	−1.798	−6.791	1	$E_{22}(a'_1)$	53	3.864	−1.129	1	$E_{52}(a'_1)$
24	−1.777	−6.770	2	$E_{24}(e'_1)$	54	3.885	−1.108	2	$E_{54}(e'_1)$
25	−1.595	−6.588	2	$E_{26}(e'_2)$	55	4.067	−0.926	2	$E_{56}(e'_2)$
26	−1.496	−6.489	2	$E_{25}(e''_1)$	56	4.166	−0.827	2	$E_{55}(e''_1)$
27	−1.266	−6.259	1	$E_{27}(a'_2)$	57	4.396	−0.597	1	$E_{57}(a'_2)$
28	−1.163	−6.156	2	$E_{28}(e'_1)$	58	4.498	−0.494	2	$E_{58}(e'_1)$
29	−0.996	−5.989	2	$E_{29}(e''_2)$	59	4.666	−0.327	2	$E_{59}(e''_2)$
30	−0.882	−5.875	2	$E_{30}(e'_2)$	60	4.780	−0.213	2	$E_{60}(e'_2)$

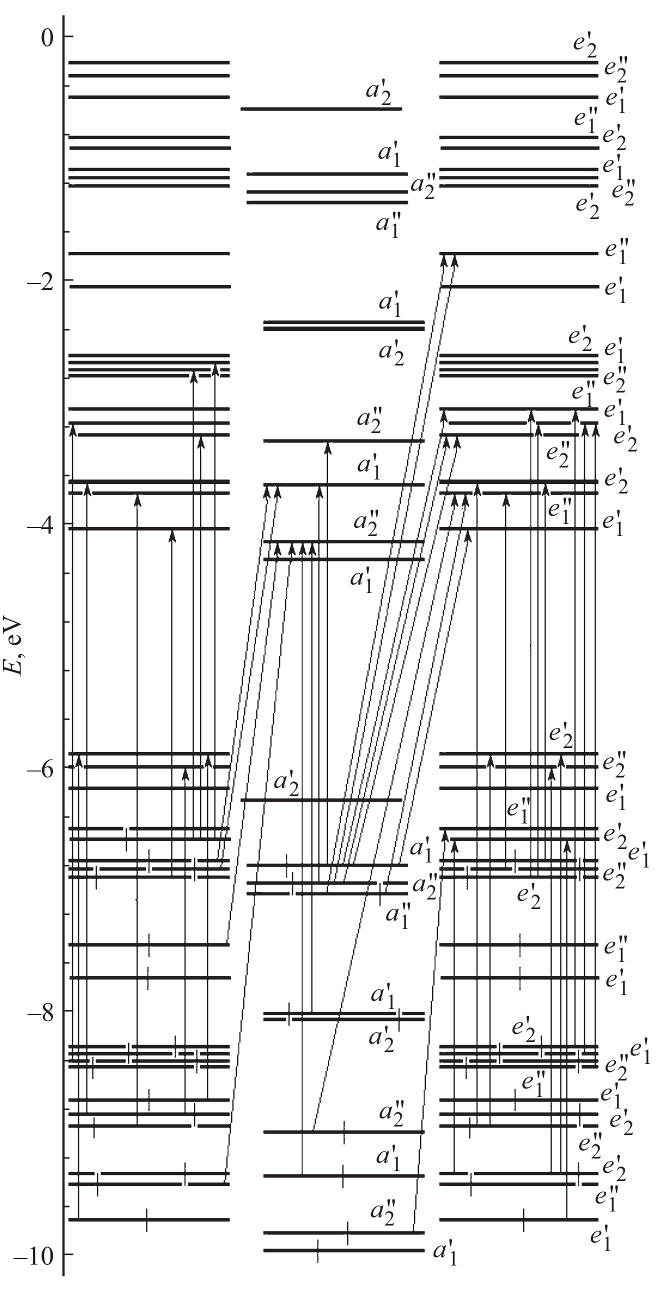

Figure 4. Energy spectrum of the molecule $C_{50}Cl_{10}$.

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

Bands of absorption	[3], λ, nm	[3] E, eV	Theoret. E, eV
a	454.6	2.73	2.7294
b	433.8	2.86	2.8448
c	400.8	3.10	3.1076
d	376.6	3.30	3.2971
e	356.6	3.48	3.4822
f	334.0	3.72	3.7177
g	322.0	3.86	3.8510
h	238.5	5.21	5.2295

Table 4. Transitions forming the absorption bands $a, b, c, d, e, f, g, h, y$ of the molecule $C_{50}Cl_{10}$

ΔE	ΔE, eV	δ	ΔE	ΔE, eV	δ	ΔE	ΔE, eV	δ
a			$E_{27}-E_6$	3.1361	$-$	$E_{40}-E_{22}$	3.7398	$+$
$E_{27}-E_7$	2.7120	$-$	$E_{31}-E_{18}$	3.1505	$-$	$E_{31}-E_{16}$	3.7598	$-$
$E_{29}-E_{10}$	2.7236	$-$	$E_{35}-E_{21}$	3.1509	$+$	$E_{40}-E_{21}$	3.7627	$-$
$E_{26}-E_4$	2.7294	$+$	$E_{36}-E_{23}$	3.1519	$-$	$E_{39}-E_{19}$	3.7655	$-$
$E_{32}-E_{24}$	2.7307	$-$	**d**			$E_{38}-E_{20}$	3.7747	$-$
$E_{26}-E_5$	2.7373	$-$	$E_{35}-E_{20}$	3.2786	$+$	$E_{35}-E_{18}$	3.7762	$-$
$E_{31}-E_{19}$	2.7386	$-$	$E_{37}-E_{26}$	3.2789	$-$	**g**		
$E_{33}-E_{23}$	2.7426	$-$	$E_{34}-E_{20}$	3.2865	$-$	$E_{29}-E_3$	3.8145	$-$
$E_{32}-E_{22}$	2.7511	$+$	$E_{36}-E_{19}$	3.2945	$+$	$E_{30}-E_2$	3.8267	$+$
$E_{28}-E_9$	2.7675	$-$	$E_{33}-E_{18}$	3.2971	$+$	$E_{41}-E_{26}$	3.8286	$-$
$E_{32}-E_{21}$	2.7740	$-$	$E_{25}-E_3$	3.3153	$+$	$E_{40}-E_{23}$	3.8335	$+$
b			$E_{39}-E_{26}$	3.3260	$+$	$E_{43}-E_{26}$	3.8510	$+$
$E_{26}-E_6$	2.8070	$-$	$E_{29}-E_4$	3.3275	$+$	$E_{38}-E_{19}$	3.8603	$-$
$E_{28}-E_7$	2.8145	$-$	$E_{29}-E_5$	3.3354	$-$	$E_{33}-E_{15}$	3.8762	$+$
$E_{25}-E_4$	2.8284	$-$	**e**			$E_{40}-E_{20}$	3.8904	$-$
$E_{25}-E_5$	2.8363	$-$	$E_{30}-E_4$	3.4420	$+$	$E_{33}-E_{16}$	3.9064	$-$
$E_{30}-E_{10}$	2.8381	$+$	$E_{27}-E_2$	3.4432	$+$	$E_{42}-E_{26}$	3.9102	$+$
$E_{29}-E_8$	2.8393	$+$	$E_{30}-E_5$	3.4499	$-$	**h**		
$E_{32}-E_{23}$	2.8448	$+$	$E_{37}-E_{24}$	3.4618	$-$	$E_{48}-E_{20}$	5.1645	$+$
$E_{36}-E_{26}$	2.8550	$-$	$E_{25}-E_1$	3.4619	$-$	$E_{35}-E_8$	5.1659	$-$
$E_{33}-E_{19}$	2.8851	$-$	$E_{37}-E_{22}$	3.4822	$+$	$E_{38}-E_{12}$	5.1725	$+$
$E_{32}-E_{20}$	2.9018	$-$	$E_{37}-E_{21}$	3.5051	$-$	$E_{34}-E_8$	5.1739	$+$
$E_{25}-E_6$	2.9060	$-$	$E_{39}-E_{24}$	3.5089	$-$	$E_{33}-E_4$	5.1750	$-$
c			$E_{30}-E_6$	3.5196	$-$	$E_{33}-E_5$	5.1829	$+$
$E_{30}-E_9$	3.0486	$+$	$E_{39}-E_{22}$	3.5293	$+$	$E_{36}-E_9$	5.1909	$+$
$E_{36}-E_{22}$	3.0582	$-$	**f**			$E_{49}-E_{26}$	5.2225	$-$
$E_{27}-E_4$	3.0584	$-$	$E_{32}-E_{17}$	3.6710	$-$	$E_{40}-E_{14}$	5.2295	$+$
$E_{27}-E_5$	3.0663	$-$	$E_{39}-E_{20}$	3.6800	$+$	$E_{38}-E_{13}$	5.2318	$+$
$E_{36}-E_{21}$	3.0811	$+$	$E_{27}-E_1$	3.6919	$-$	$E_{36}-E_7$	5.2380	$+$
$E_{30}-E_7$	3.0956	$-$	$E_{36}-E_{18}$	3.7064	$-$	$E_{48}-E_{19}$	5.2500	$+$
$E_{35}-E_{24}$	3.1076	$+$	$E_{29}-E_2$	3.7122	$-$	$E_{33}-E_6$	5.2527	$+$
$E_{26}-E_2$	3.1141	$+$	$E_{38}-E_{23}$	3.7177	$+$	$E_{38}-E_{11}$	5.2542	$+$
$E_{34}-E_{24}$	3.1155	$+$	$E_{37}-E_{19}$	3.7184	$-$	$E_{41}-E_{15}$	5.2591	$-$
$E_{35}-E_{22}$	3.1280	$-$	$E_{40}-E_{24}$	3.7194	$-$	$E_{35}-E_9$	5.2607	$-$
$E_{34}-E_{22}$	3.1359	$-$	$E_{31}-E_{15}$	3.7296	$-$	$E_{34}-E_9$	5.2686	$+$

Knowing the energy spectrum of the exohedral fullerene $C_{50}Cl_{10}$, its experimentally observed spectrum of optical absorption can be interpreted as follows. The optical absorption spectrum bands of the molecule $C_{50}Cl_{10}$, which correspond to the 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 the Table 4 that energies of these transitions are close to the experimental values [3]. The δ symbol of the Table 4 shows the transitions as allowed and unallowed in terms of the symmetry. If $\delta = +$, then such a transition is allowed in terms of the symmetry, if $\delta = -$, then such a transition is unallowed. Note that in the molecule $C_{50}Cl_{10}$ the atoms make small oscillations around an equilibrium. This lead to asymmetry of the molecule $C_{50}Cl_{10}$. As a result, optical transitions unallowed 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.

4. Conclusion

Thus, the optical absorption of the exohedral fullerene $C_{50}Cl_{10}$, which is observed experimentally, agrees fairly well with the optical absorption spectrum of this molecule, which is obtained from the energy spectrum of the molecule $C_{50}Cl_{10}$ within the Hubbard model in the static fluctuation approximation.

Note that the energy spectra of the fullerenes C_{60}, C_{70} and the endohedral fullerenes $Lu_3N@C_{80}$ and $Y_3N@C_{80}$ were also studied in the papers [12,11,10], as determined within the Hubbard model in the static fluctuation approximation. These studies showed that the optical absorption spectra of these molecules, which were observed experimentally, also agree fairly well with the optical absorption spectra of the molecules C_{60}, C_{70}, $Y_3N@C_{80}$ and $Y_3N@C_{80}$, which have been obtained within the Hubbard model in the static fluctuation approximation. This allows one to state that the Hubbard model in the static fluctuation 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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