

## 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:

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

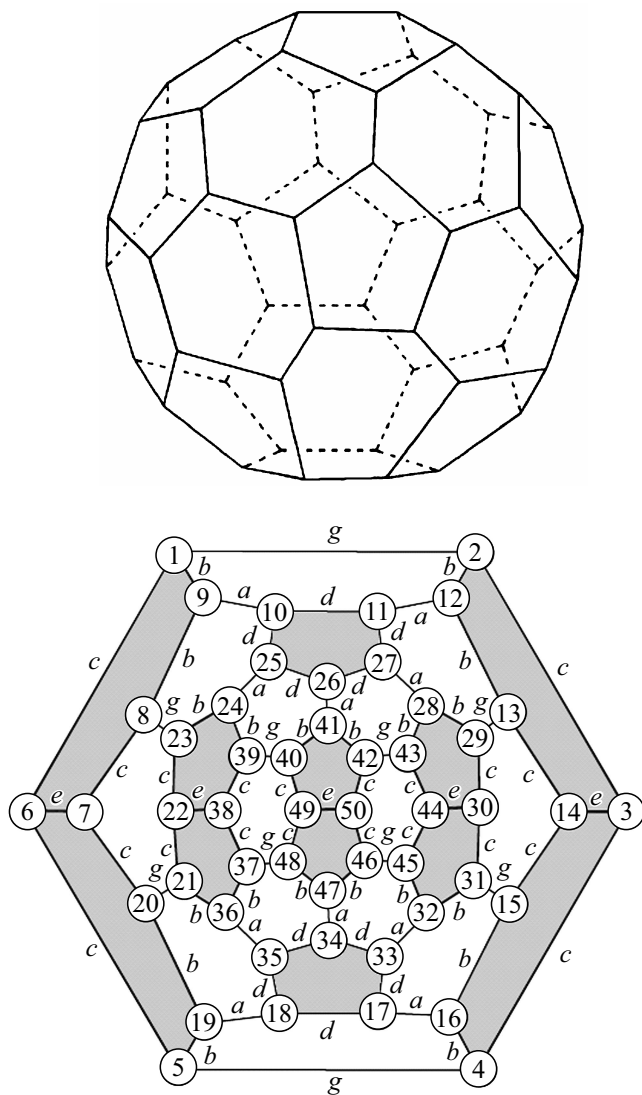
$$G_2 = \{3, 6, 7, 14, 22, 30, 38, 44, 49, 50\},$$

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

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

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<sub>50</sub> fullerene with the D<sub>5h</sub> symmetry group and its Schlegel diagram showing the position of carbon atoms, bonds between carbon atoms, and pentagons.

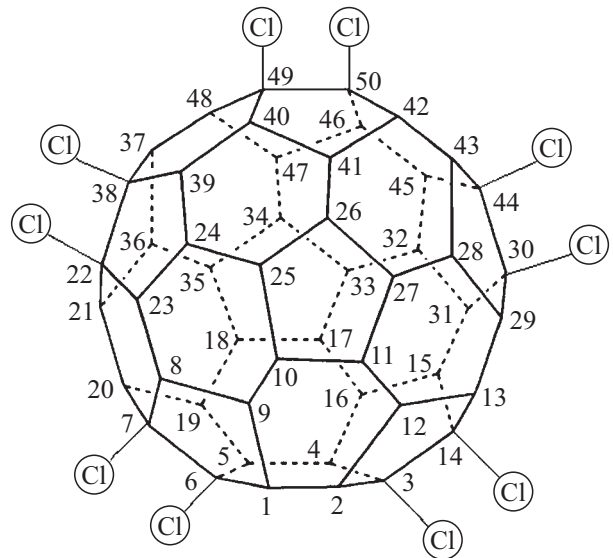
nanotubes. The results obtained in [13–15] agree fairly well with experimental data.

The objective of this paper is to investigate energy spectra of the C<sub>50</sub> fullerene and C<sub>50</sub>Cl<sub>10</sub> molecule with symmetry groups D<sub>5h</sub> under the Hubbard model in the mean-field approximation.

### Energy spectrum of the C<sub>50</sub> 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<sub>50</sub> fullerene:

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



**Figure 2.** The C<sub>50</sub>Cl<sub>10</sub> molecule.

where  $c_{i\sigma}^+$ ,  $c_{i\sigma}$  — the operators of creation and annihilation of electrons with the  $\sigma$  spin at the  $i$  site;  $n_{i\sigma}$  — the operator of the number of particles with the  $\sigma$  spin at the  $i$  site;  $\varepsilon_i$  — 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<sub>50</sub> molecule in the mean-field approximation, one should perform the following substitution in Hamiltonian (1):

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

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

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

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

where

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

The performed studies of the C<sub>50</sub> fullerene with the D<sub>5h</sub> symmetry group [21] have shown that the distances between carbon atoms are as follows:

$$\begin{aligned} x_a &= 1.399 \text{ \AA}, \quad x_b = 1.449 \text{ \AA}, \quad x_c = 1.444 \text{ \AA}, \\ x_d &= 1.450 \text{ \AA}, \quad x_e = 1.400 \text{ \AA}, \quad x_g = 1.387 \text{ \AA}. \end{aligned} \quad (5)$$

We use the following relation to determine the numerical values of the transfer integrals corresponding to the C<sub>50</sub> molecule [13,14]:

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



**Table 1.** Energy spectrum of the C<sub>50</sub> fullerene with the D<sub>5h</sub> symmetry group: values of levels energy, multiplicity of their degeneration and irreducible representations of the D<sub>5h</sub> group, to which they belong

| N <sup>o</sup> | e <sub>j</sub> , eV | E <sub>j</sub> , eV | g <sub>j</sub> | E(Γ <sub>j</sub> )                  | N <sup>o</sup> | e <sub>j</sub> , eV | E <sub>j</sub> , eV | g <sub>j</sub> | E(Γ <sub>j</sub> )                  |
|----------------|---------------------|---------------------|----------------|-------------------------------------|----------------|---------------------|---------------------|----------------|-------------------------------------|
| 1              | -4.975              | -9.954              | 1              | E <sub>1</sub> (a' <sub>1</sub> )   | 16             | -0.883              | -5.068              | 1              | E <sub>16</sub> (a' <sub>2</sub> )  |
| 2              | -4.531              | -9.511              | 2              | E <sub>2</sub> (e' <sub>1</sub> )   | 17             | 0.534               | -4.445              | 2              | E <sub>17</sub> (e' <sub>1</sub> )  |
| 3              | -4.410              | -9.390              | 1              | E <sub>3</sub> (a'' <sub>2</sub> )  | 18             | 1.171               | -3.809              | 2              | E <sub>18</sub> (e'' <sub>1</sub> ) |
| 4              | -3.668              | -8.647              | 2              | E <sub>4</sub> (e' <sub>2</sub> )   | 19             | 1.876               | -3.104              | 1              | E <sub>19</sub> (a' <sub>2</sub> )  |
| 5              | -3.586              | -8.566              | 2              | E <sub>5</sub> (e'' <sub>1</sub> )  | 20             | 2.116               | -2.863              | 1              | E <sub>20</sub> (a'' <sub>1</sub> ) |
| 6              | -3.509              | -8.489              | 1              | E <sub>6</sub> (a' <sub>1</sub> )   | 21             | 2.125               | -2.854              | 1              | E <sub>21</sub> (a' <sub>1</sub> )  |
| 7              | -2.550              | -7.529              | 2              | E <sub>7</sub> (e' <sub>2</sub> )   | 22             | 2.225               | -2.754              | 2              | E <sub>22</sub> (e'' <sub>2</sub> ) |
| 8              | -2.494              | -7.473              | 2              | E <sub>8</sub> (e' <sub>2</sub> )   | 23             | 2.408               | -2.572              | 2              | E <sub>23</sub> (e' <sub>2</sub> )  |
| 9              | -2.478              | -7.457              | 1              | E <sub>9</sub> (a'' <sub>2</sub> )  | 24             | 2.561               | -2.418              | 2              | E <sub>24</sub> (e' <sub>1</sub> )  |
| 10             | -2.338              | -7.318              | 2              | E <sub>10</sub> (e' <sub>1</sub> )  | 25             | 3.060               | -1.920              | 2              | E <sub>25</sub> (e' <sub>2</sub> )  |
| 11             | -1.542              | -6.522              | 2              | E <sub>11</sub> (e'' <sub>1</sub> ) | 26             | 3.063               | -1.916              | 2              | E <sub>26</sub> (e'' <sub>1</sub> ) |
| 12             | -1.466              | -6.445              | 2              | E <sub>12</sub> (e'' <sub>2</sub> ) | 27             | 4.133               | -0.846              | 2              | E <sub>27</sub> (e'' <sub>2</sub> ) |
| 13             | -1.391              | -6.371              | 2              | E <sub>13</sub> (e' <sub>2</sub> )  | 28             | 4.150               | -0.829              | 2              | E <sub>28</sub> (e' <sub>1</sub> )  |
| 14             | -1.271              | -6.251              | 2              | E <sub>14</sub> (e' <sub>1</sub> )  | 29             | 4.161               | -0.818              | 1              | E <sub>29</sub> (a' <sub>2</sub> )  |
| 15             | -0.610              | -5.589              | 1              | E <sub>15</sub> (a' <sub>1</sub> )  | 30             | 4.428               | -0.551              | 2              | E <sub>30</sub> (e' <sub>2</sub> )  |

**Table 2.** Energy spectrum of the C<sub>50</sub>Cl<sub>10</sub> molecule with the D<sub>5h</sub> symmetry group: values of levels energy, multiplicity of their degeneration and irreducible representations of the D<sub>5h</sub> group, to which they belong

| N <sup>o</sup> | e <sub>j</sub> , eV | E <sub>j</sub> , eV | g <sub>j</sub> | E(Γ <sub>j</sub> )                  | N <sup>o</sup> | e <sub>j</sub> , eV | E <sub>j</sub> , eV | g <sub>j</sub> | E(Γ <sub>j</sub> )                  |
|----------------|---------------------|---------------------|----------------|-------------------------------------|----------------|---------------------|---------------------|----------------|-------------------------------------|
| 1              | -4.907              | -11.018             | 1              | E <sub>1</sub> (a' <sub>1</sub> )   | 16             | -0.179              | -6.290              | 1              | E <sub>16</sub> (a' <sub>2</sub> )  |
| 2              | -4.773              | -10.884             | 1              | E <sub>3</sub> (a'' <sub>2</sub> )  | 17             | 0.262               | -5.849              | 2              | E <sub>17</sub> (e' <sub>1</sub> )  |
| 3              | -4.196              | -10.307             | 2              | E <sub>2</sub> (e' <sub>1</sub> )   | 18             | 1.130               | -4.981              | 2              | E <sub>18</sub> (e'' <sub>1</sub> ) |
| 4              | -3.916              | -10.027             | 2              | E <sub>5</sub> (e'' <sub>1</sub> )  | 19             | 1.137               | -4.974              | 2              | E <sub>23</sub> (e' <sub>2</sub> )  |
| 5              | -3.221              | -9.332              | 2              | E <sub>4</sub> (e' <sub>2</sub> )   | 20             | 1.807               | -4.304              | 2              | E <sub>24</sub> (e' <sub>1</sub> )  |
| 6              | -3.176              | -9.287              | 1              | E <sub>6</sub> (a' <sub>1</sub> )   | 21             | 2.024               | -4.087              | 1              | E <sub>19</sub> (a' <sub>2</sub> )  |
| 7              | -2.820              | -8.931              | 1              | E <sub>9</sub> (a'' <sub>2</sub> )  | 22             | 2.187               | -3.924              | 1              | E <sub>21</sub> (a' <sub>1</sub> )  |
| 8              | -2.799              | -8.910              | 2              | E <sub>7</sub> (e'' <sub>2</sub> )  | 23             | 2.302               | -3.809              | 1              | E <sub>20</sub> (a'' <sub>1</sub> ) |
| 9              | -1.939              | -8.050              | 2              | E <sub>8</sub> (e' <sub>2</sub> )   | 24             | 2.494               | -3.617              | 2              | E <sub>22</sub> (e'' <sub>2</sub> ) |
| 10             | -1.931              | -8.042              | 2              | E <sub>10</sub> (e' <sub>1</sub> )  | 25             | 2.749               | 3.362               | 2              | E <sub>25</sub> (e' <sub>2</sub> )  |
| 11             | -1.590              | -7.701              | 2              | E <sub>11</sub> (e'' <sub>1</sub> ) | 26             | 3.075               | -3.036              | 1              | E <sub>29</sub> (a' <sub>2</sub> )  |
| 12             | -1.530              | -7.641              | 2              | E <sub>12</sub> (e'' <sub>2</sub> ) | 27             | 3.367               | -2.744              | 2              | E <sub>26</sub> (e'' <sub>1</sub> ) |
| 13             | -0.703              | -6.814              | 2              | E <sub>13</sub> (e' <sub>2</sub> )  | 28             | 3.708               | -2.403              | 2              | E <sub>28</sub> (e' <sub>1</sub> )  |
| 14             | -0.659              | -6.770              | 2              | E <sub>14</sub> (e' <sub>1</sub> )  | 29             | 4.478               | -1.633              | 2              | E <sub>27</sub> (e'' <sub>2</sub> ) |
| 15             | -2.670              | -6.378              | 1              | E <sub>15</sub> (a' <sub>1</sub> )  | 30             | 4.620               | 1.491               | 2              | E <sub>30</sub> (e' <sub>2</sub> )  |

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

Using relations (16), (12), (8) and (9), we will obtain for the C<sub>50</sub>Cl<sub>10</sub> molecule the numerical values for the values e<sub>k</sub>, which are given in Table 2.

According to ratio (14), when the C<sub>n</sub>X<sub>k</sub><sup>(-q)</sup> molecule is formed, the energy ε' is changed:

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

where ε'<sub>C<sub>n</sub></sub> corresponds to the C<sub>n</sub> fullerene; q — number of electrons passing from the C<sub>n</sub> fullerene to k atoms of X.

From ratio (17) it follows that:

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

where U = 5.662 eV [24], ε' = -4.979 eV [13].

Now, by substituting the numerical values for e<sub>k</sub> from Table 2, as well as numerical value for ε' = ε'<sub>C<sub>50</sub>Cl<sub>10</sub></sub> to ratio (13), we obtain the energy spectrum of the C<sub>50</sub>Cl<sub>10</sub> molecule with the D<sub>5h</sub> 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<sub>50</sub> and C<sub>50</sub>Cl<sub>10</sub> molecules differ from each other by the relative position of their energy state E<sub>2</sub>(a'<sub>1</sub>), E<sub>3</sub>(a''<sub>2</sub>), E<sub>4</sub>(e'<sub>2</sub>), E<sub>5</sub>(e''<sub>1</sub>), E<sub>9</sub>(a''<sub>2</sub>), E<sub>20</sub>(a''<sub>1</sub>), E<sub>21</sub>(a'<sub>1</sub>), E<sub>23</sub>(e'<sub>2</sub>), E<sub>24</sub>(e'<sub>1</sub>), E<sub>27</sub>(e''<sub>2</sub>), E<sub>28</sub>(e'<sub>1</sub>), E<sub>29</sub>(a'<sub>2</sub>).



**Table 3.** Experimental and theoretical values of the wavelengths and energies, which correspond to the absorption bands within the optical spectrum of the C<sub>50</sub>Cl<sub>10</sub> molecule

| Absorption Theory | [4]<br>λ, nm | [4]<br>E, eV | bands<br>E, eV |
|-------------------|--------------|--------------|----------------|
| <i>a</i>          | 454.6        | 2.73         | 2.67           |
| <i>b</i>          | 433.8        | 2.86         | 2.91           |
| <i>c</i>          | 400.8        | 3.10         | 3.07           |
| <i>d</i>          | 376.6        | 3.30         | 3.36           |
| <i>e</i>          | 356.6        | 3.48         | 3.48           |
| <i>f</i>          | 334.0        | 3.72         | 3.75           |
| <i>g</i>          | 322.0        | 3.86         | 3.89           |
| <i>h</i>          | 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 |
|---|--------|---|---|--------|---|---|--------|---|
| <i>a</i>  |        |   | <i>d</i>  |        |   | <i>g</i>  |        |   |
| <i>E</i> <sub>18</sub> – <i>E</i> <sub>12</sub> | 2.66   | – | <i>E</i> <sub>22</sub> – <i>E</i> <sub>10</sub> | 3.21   | – | <i>E</i> <sub>20</sub> – <i>E</i> <sub>12</sub> | 3.83   | – |
| <i>E</i> <sub>23</sub> – <i>E</i> <sub>12</sub> | 2.67   | + | <i>E</i> <sub>14</sub> – <i>E</i> <sub>5</sub>  | 3.26   | + | <i>E</i> <sub>20</sub> – <i>E</i> <sub>11</sub> | 3.89   | + |
| <i>E</i> <sub>18</sub> – <i>E</i> <sub>11</sub> | 2.72   | – | <i>E</i> <sub>24</sub> – <i>E</i> <sub>12</sub> | 3.34   | – | <i>E</i> <sub>15</sub> – <i>E</i> <sub>2</sub>  | 3.93   | – |
| <i>E</i> <sub>23</sub> – <i>E</i> <sub>11</sub> | 2.73   | – | <i>e</i>  |        |   | <i>E</i> <sub>18</sub> – <i>E</i> <sub>7</sub>  | 3.93   | – |
| <i>b</i>  |        |   | <i>E</i> <sub>17</sub> – <i>E</i> <sub>6</sub>  | 3.44   | + | <i>h</i>  |        |   |
| <i>E</i> <sub>15</sub> – <i>E</i> <sub>6</sub>  | 2.91   | – | <i>E</i> <sub>17</sub> – <i>E</i> <sub>4</sub>  | 3.48   | + | <i>E</i> <sub>17</sub> – <i>E</i> <sub>1</sub>  | 5.17   | + |
| <i>E</i> <sub>15</sub> – <i>E</i> <sub>4</sub>  | 2.95   | – | <i>E</i> <sub>13</sub> – <i>E</i> <sub>2</sub>  | 3.49   | + | <i>E</i> <sub>19</sub> – <i>E</i> <sub>6</sub>  | 5.20   | + |
| <i>c</i>  |        |   | <i>f</i>  |        |   | <i>E</i> <sub>28</sub> – <i>E</i> <sub>12</sub> | 5.24   | – |
| <i>E</i> <sub>17</sub> – <i>E</i> <sub>7</sub>  | 3.06   | – | <i>E</i> <sub>21</sub> – <i>E</i> <sub>12</sub> | 3.72   | – | <i>E</i> <sub>19</sub> – <i>E</i> <sub>4</sub>  | 5.24   | – |
| <i>E</i> <sub>18</sub> – <i>E</i> <sub>10</sub> | 3.06   | + | <i>E</i> <sub>24</sub> – <i>E</i> <sub>10</sub> | 3.74   | – |   |        |   |
| <i>E</i> <sub>18</sub> – <i>E</i> <sub>8</sub>  | 3.07   | – | <i>E</i> <sub>16</sub> – <i>E</i> <sub>5</sub>  | 3.74   | – |   |        |   |
| <i>E</i> <sub>23</sub> – <i>E</i> <sub>10</sub> | 3.07   | + | <i>E</i> <sub>24</sub> – <i>E</i> <sub>8</sub>  | 3.75   | + |   |        |   |
| <i>E</i> <sub>17</sub> – <i>E</i> <sub>9</sub>  | 3.08   | – | <i>E</i> <sub>21</sub> – <i>E</i> <sub>11</sub> | 3.78   | – |   |        |   |
| <i>E</i> <sub>23</sub> – <i>E</i> <sub>8</sub>  | 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  $\delta$  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<sub>50</sub>Cl<sub>10</sub> molecule make small oscillations around an equilibrium. This leads to the asymmetry of the C<sub>50</sub>Cl<sub>10</sub> 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<sub>50</sub>Cl<sub>10</sub> 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<sub>50</sub>Cl<sub>10</sub> 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<sub>60</sub> and C<sub>70</sub> fullerenes, as well as the Y<sub>3</sub>N@C<sub>80</sub> 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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