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THE SEMI-EMPIRICAL RESEARCH OF THE ADSORPTION OF BIOLOGICALLY ACTIVE MOLECULES ON THE OUTER SURFACE OF CARBON NANOTUBES

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The object of this work is to research the interaction of carbon nanotubes with organic molecules containing the diphenyloxide fragment in order to identify new properties for the obtained compounds.

Keywords: Carbon nanotube, Adsorption, The semi-empirical research, MNDO, Diketones.

1. Introduction

Closed surface structure of carbon (fullerenes and nanotubes) shows a number of specific properties suitable for use it as a sort of materials and treat it as objects of interesting physical and chemical systems [1]. At the present time, nanotubes (or tubulenes) have changed from exotic objects to become the subject of large-scale physical and chemical research. Their unusual properties have become the basis of many challenging technical solutions. Now, nanotubes are the materials with a wide array of practical applications, the subject of commercial production, marketing and research. The outstanding feature of carbon nanotubes is their unique adsorption characteristics. The greatly curved surface of nanotubes (compared with a flat layer of graphite) can adsorb sufficiently large and heavy molecules including naturally-occurring organic molecules on its surface. Modern medicine development advances a need for new materials, one of which may be carbon tubulenes. Nanotubes with the drug substances deposited on their surface may be used to deliver drugs into infected human organs, followed by excretion of the tube from the human body. This should increase the effectiveness of existing drugs [2].

2. The conduct of the calculations

In this study, we will discuss the model of adsorption for organic molecules on the surface of carbon nanotubes. Many biologically active substances have heterocycles present in their structure. In these studies, a pair of model compounds were selected as biomolecule mimetics 1-(3-phenoxyphenyl)butane-1,3-dione and 2-(3-phenoxybenzoyl)cyclohexanone – both diketones containing the diphenylether fragment, which are new structures, characterized by high levels of similarity to known drugs, the absence of toxic properties in the model compounds , and a wide range of pharmacological properties which should be of practical and research interest to those in the medical field [3]. Software package Gaussian was used to build the model and calculations were performed using the MNDO scheme. Selection of this scheme was made for the following reasons: the method has worked well for calculations of molecules and solids; the error of the method is small compared to all previously known semi-empirical

schemes; low cost of computer computation time; the method is most effective for today's personal computers. Particular spatial configuration of molecules and their basic geometric characteristics were identified as a result of this research. The calculations were performed using the molecular cluster. To do this, the model of a single-walled zigzag type nanotube (0,5) diameter $r = 4.5$ Åwas used. The molecular tubulene clusters contained 96 carbon atoms; the dangling bonds at the boundaries were closed by pseudoatoms (these were selected as hydrogen atoms). Several connection options have been considered for adsorbed biologically active molecules:

- for the 2-(3-phenoxybenzoyl)cyclohexanone molecule, a single-center connection to the CNT surface was considered (Fig. 1);
- for the 1-(3-phenoxyphenyl)butane-1,3-dione molecule, a multicenter interconnection of two centers was considered (Fig. 2).

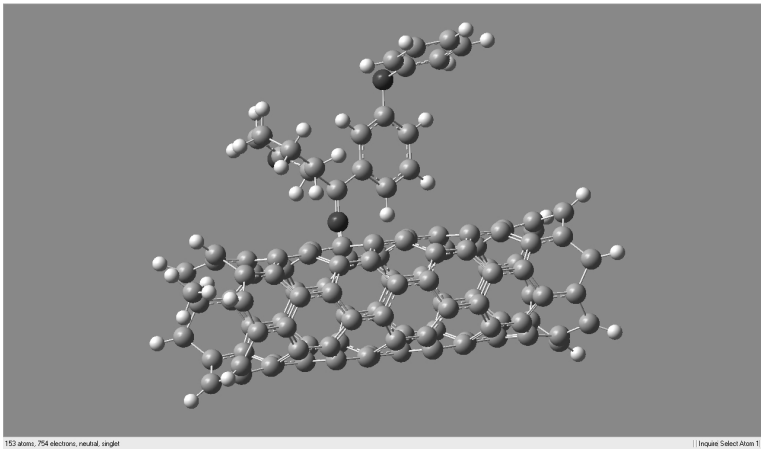

FIG. 1. The interaction of the molecule 2-(3-phenoxybenzene)-cyclohexanone with a carbon nanotube

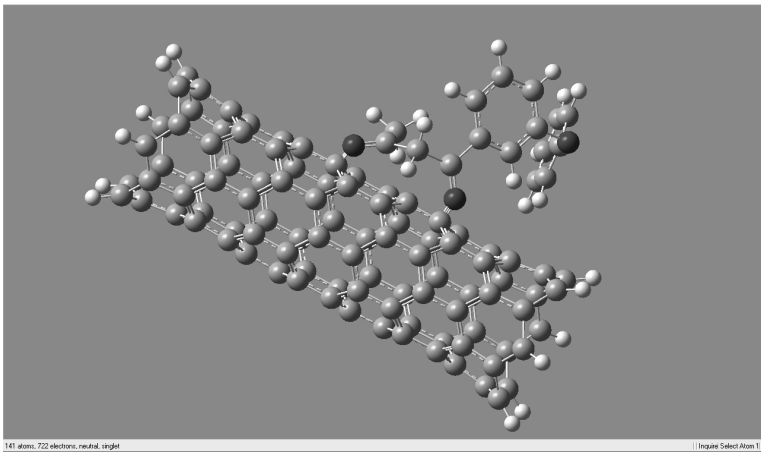

FIG. 2. The interaction of the molecule of 1-(3-phenoxyphenyl)-butan-1.3-dione with a carbon nanotube

The calculations were conducted in the medium of toluene as a solvent. The process was modeled as follows: a molecule was brought nearer to the outer surface of the carbon nanotubes in a stepwise fashion (0, 5) along a perpendicular drawn to the surface of the carbon

atom of the selected molecular cluster selected handset (in increments of 0.1 Å). The maximum convergence was chosen on the distance of 0.85 Å.

3. Inference

The calculations allowed us to construct profiles for the potential energy surface adsorption processes for the case of a single-site interaction mentioned above. The graph (Fig. 3) shows that there is an energy minimum on the distance between atomic systems at 2.3 Å, which corresponds to the Van-der-Waals force between tubulenes and the molecule, i.e. the so-called physical adsorption. The adsorption energy is $E = -10.42$ eV in this case. However, it is clear that being in this state, the molecule can also move into a more stable position, having overcome the potential barrier equal to 0.79 eV, i.e. a molecule of 2-(3-phenoxybenzoyl)cyclohexanone ceases to interact with the surface of the carbon nanotube.

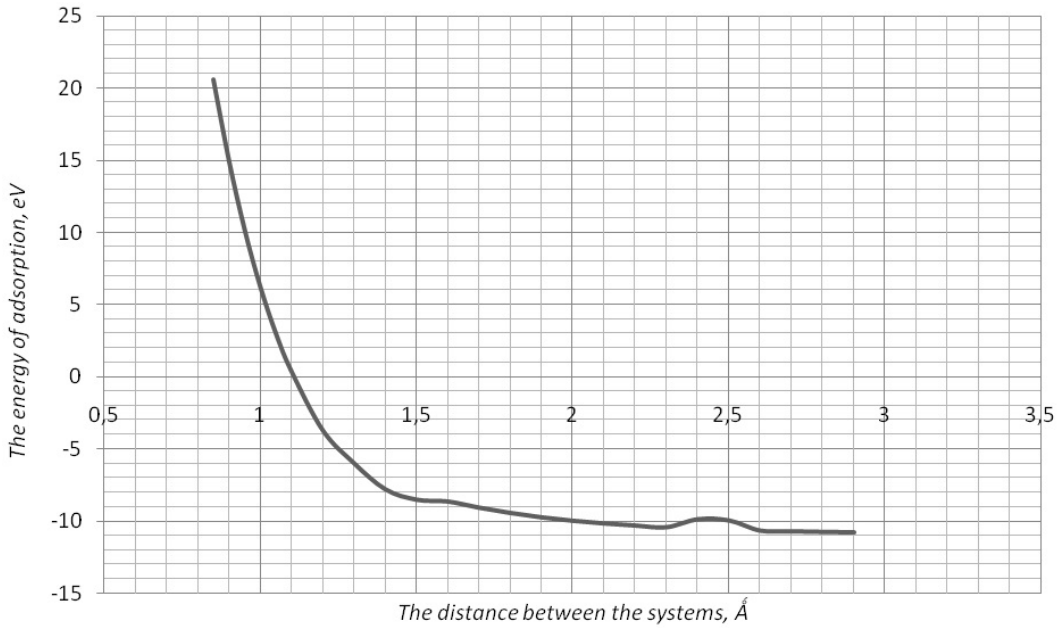

FIG. 3. The surface profile of the potential energy of interaction between molecules of 2-(3-fenoksibenzoil)-cyclohexanone with the surface of the carbon nanotube 'zig-zag' (0.5)

Theoretical calculations show that under these conditions (chosen sorption center, design scheme, etc.) the physical adsorption of a biologically active molecule on the surface of the tube was considered. It will be necessary to carry out future calculations with varying conditions and to conduct experiments to determine the means by which the chemical adsorption of organic molecules containing diphenylether fragment occurs on the external surface of the carbon nanotubes.

References

[1] Sidorov L.N., Yurovskaya M.A., et al. *Fullerenes*. Publishing house 'Exam', Moscow, 2005, 688p. (In Russian).

[2] Piotrowski L.B., Kiselev O.I. In: *Fullerenes in biology*. Publishing house 'Sprout', Saint Petersburg, 2006, p. 246–251.

[3] Popov U.V., Korchagina T.K., Kalmykova G.V., Shinkarenko E.A. Synthesis of 2-(3-fenoksibenzoil)cyclohexanone. *Russian J. General Chem.*, **82** (7), P. 1220–1221 (2012).