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Quant-Chemical Modeling Solvatofobic Effect Bei Sorption and Partition Organic Compounds Nanocomposit Sorbent

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ABSTRACT

Solvation plays a key role in the regulation of many chemical sorption processes. The solvent can be used not only as a environment, but also as an effective means to study the nature of the chemical interaction and reactivity of substances. Therefore, understanding and a priori assessment of the effects of the environment remains one of the important practical tasks of modern chemistry. We present some results of experimental studies of heterogeneous catalytic reactions occurring through several elementary stages on the surface of the nanocomposit. Nanostructures in a polymer composite are defined as regular micro heterogeneities (i.e. areas of a polymer material with an interfacial surface) of nanometer dimensions, which largely determine the unique properties (catalytic, magnetic, semiconductor, nonlinear optical, etc.) of Nanocomposites. As nanostructure, polymer systems, providing the formation of nanoparticles in solutions, the most promising are block copolymer micelles and dendrimers, which can be adsorbed on the surface to form monolayers. Most special properties of nanostructures are the result of two main effects: a. the share of surface atoms in the total number of atoms is a significant share, which leads to the dominant role of the surface (surface-dominated effects); b. the electrons in the nanostructure are in a bounded region of space, which leads to quantum dimensional effects and reduced-dimensional effects.

With the use of the density functional theory (DFT) is investigated solvatofobic effect in the organic compound separation in Nanocomposites sorbent gas chromatographic method. On the basis of electrostatic pseudo phase model of micellar catalysis the coefficients of activity of transfer of organic molecules from solvent to micellar pseudo phase are calculated. According to the principles of the theory hard and soft acid and alkali (HSAF) calculated energy non-valent interactions, contributing to the processes of self-assembly. Hypothesis that the formation of bifurcate halogen bonds during salvation can contribute to the formation of molecular bridge between the associated molecules.

***Keywords:** Solvatofobic effect, density functional theory (DFT), non-valent interaction, molecular bridge, halogen bond, hydrogen bond, bifurcatnaja galogen bond, mechanism division*

INTRODUCTION

Gas chromatography is one of the universal methods of qualitative and quantitative analysis of complex mixtures of organic compounds. The main element of this method is a chromatographic column, in as a sorbent are used nanocomposit. Nanomaterials are of interest to researchers for their unique chemical, catalytic, electrochemical, magnetic, optical photochemical adsorption properties, due to which their application in catalysis/electro catalysis, photonics, sensor biology, medicine and other fields is expanding [1].

Prospects for the use of nanocomposite materials are associated with studies of a large number of complex liquids, which are characterized by strong micro- heterogeneity and diverse supramolecular architecture arising on mesoscopic scales [2, 3].

The main purpose of most molecular solvation models is to study conformational, tautomeric and other transformations of solvates, as well as to determine the conditions for the formation of their dimers, tees and other complexes [4]. Sorbate particles not only compete with each other for sorption centers, but also change the sorption ability of the centers in relation to competitors. Solvation of molecules can be accompanied by various specific solvation effects. For the formation of solvation models and study of solvation effects using numerical experiments, including quantum chemical methods, based on the calculation in which the expected schrödinger equation. Supramolecular formation formed in the process of self-assembly is characterized by the spatial arrangement of their components, their architecture, "suprastructure", as well as types of intermolecular interactions that hold the components together. In general, non-covalent interactions are weaker than covalent bonds, so that supramolecular associates are less stable thermodynamically, more labile kinetically, and more flexible dynamically than molecules [5].

MATERIAL AND METHOD

This work is devoted to study solvational effect and continues research started in [6]. The calculations of intermolecular interactions in the process of self-assembly, as well as the energy of non-covalent interactions are presented here. Researches carry out bu a method gas chromatograph with application of a column 1 m, with an internal diameter of 3 mm and a sorbent of 10% 3-nitrilpropanamin on color chrome (fr.0.14/0.25 mm). In quality adsorbate investigated aceton, acetilaceton, butilacetat.

RESULT AND DISCUSSION

The study of the electronic structure of crystals, interfaces, supramolecular associates was carried out using the density functional theory (DFT) [7]. To calculate the ground state of the system of interacting electrons, the Hohenberg-Kohn theorems were used, from which it follows that all the properties of the system are completely determined by the density distribution (ρ) of the particles entering it. If the calculated potential surface of the main electronic state of the supramolecular system (the selected ensemble of atoms) has a minimum, it is possible to assume the existence of a stable supramolecule. The calculations used the potential of the ground state of the interacting electron system:

$$V_{KS}^{\sigma}(r) = V_{ext}(r) + V_{H}(r) + V_{XC}^{\sigma}(r) \tag{1}$$

where $V_H(r)$ - the Hartree potential; $V_{ext}(r)$ - the external potential does not depend on the spin of electrons (for example, an external electrostatic field or hydrostatic pressure); $V_{KS}^{\sigma}(\rho)$ - the potential of the ground state of the interacting electron system; $V_{XC}^{\sigma}(r)$ - exchange- correlation potential.

The results of the study indicate a solvatofobic effect (data $V_{ext}(r)$), as a result of which the organic molecules enter the micellar pseudo phase or are pushed into the interphase space. The equation of the pseudo phase model of micellar catalysis can be applied to the experimental data: the electrostatic model of solubilization of organic substances in micelles is based on the expression for the free transfer energy from the solvated phase to the charged micellar surface:

$$\Delta G = RT \ln \gamma_i + \psi F \tag{2}$$

where ψ - the electrical potential in the localization of bound ions or molecules (in the case of not too hydrophobic reagents ψ corresponds to the Stern lauer); γ_i - the activity coefficient of the transfer of associates from the solvent to the micellar pseudo phase. According to experimental data γ_i =0,5 (for acetone); γ_i=0,84 (for ether); γ_i =0,093 (for acetilacetone).

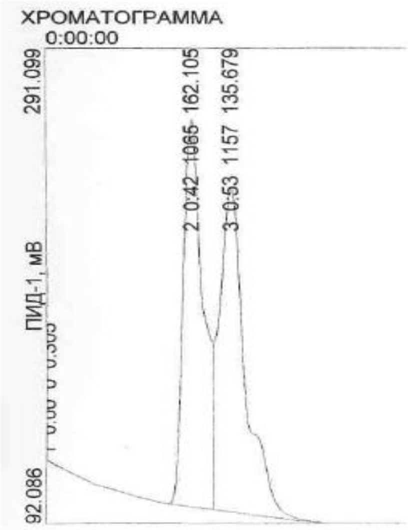

Fig1. *Chromatogramma partition tautomer aceton*

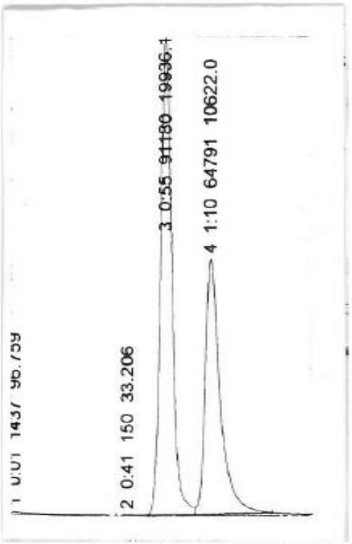

Fig2. *Chromatogramma Partition butilacetata*

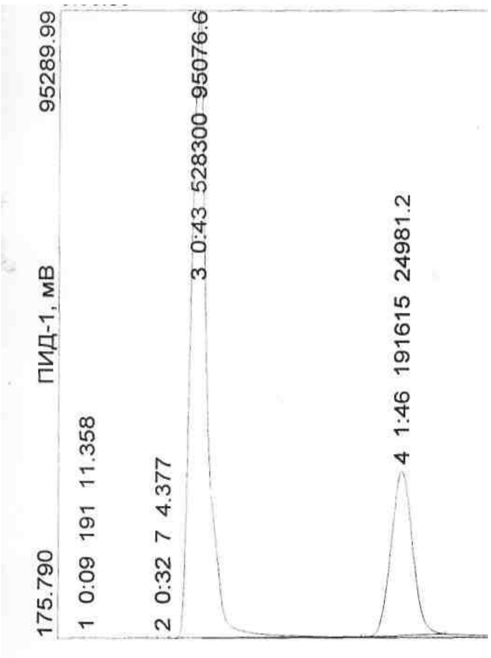

Fig3. *Chromatogramma Partition acetilaceton*

The calculation of the energies of non-valent interactions [8] is based on the equation J. L. Gaskesa and the principle JMKO, proving that the interaction between particles with approximately the same softness energetically favorable, in contrast to the interaction between the molecular systems, differing greatly in softness:

$$E_{(\rho)} = N_e \cdot \mu - 0{,}5N_e^2 \cdot \eta + \varepsilon_{core}(\rho) \qquad (3)$$

where N_e - is the effective number of valence electrons; μ- chemical potential; η- hard; - contribution skeleton in absolute energy.

Table. *Summary table of studies of the halogen bond coexisting with hydrogen bond bei partition organic compound*

Adsorbat	**$T_{кол.}$ K**	**Mechanism partition**	**k_p**	**α**	**E J/mol *Galogen bond***	**E J/mol *Hydrogen bond***	***E^** *J/mol***	***Commentary* [9]**
aceton	343	solvatofobic interaction with micells	1,4	1	$-4{,}23 \cdot 10^3$	$-308{,}05 \cdot 10^3$	31,2	*Systems in which display the weakening effect. Two halogen bonds are formed by one electron acceptor*
Acetilaceton *(bifurcatnaja galogen bond)*	355	Isoelectric point	0,64	0,001	$-10{,}14 \cdot 10^3$	-43,03	1,23	*Synergistic effect for cases where the system transfers charge from anion over connected to the halogen bond*
butilacetat	423	motive bond	3	1	-45,25	$-984{,}4 \cdot 10^3$	25,2	*The cooperative effect of the mutual influence of two closely disposed donor centers.Intensification of halogen bonds, if the binding carry out between O and CL*

E^*- barrier transfer proton to aceptor..

k_p (partition constant) calculate according to equation [10]:

$$k_p = \frac{\Delta l}{\mu_{0,5}^1 + \mu_{0,5}^2} \qquad (4)$$

where Δl – distance between maximum partition peak; $\mu_{0,5}$ - semi width chromatograph peak 1 and 2-go component on half height.

CONCLUSION

Thus, the separation of organic molecules on the gas chromatograph "Crystal - 2000M" was carried out by capillary electrophoresis. The various separation mechanisms manifested in the method are listed. The energies of non-valent interactions during self-assembly are calculated. According to the Brensted-Polyani ratio, the coefficient α of catalytic processes is given.

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