

Investigation of carbon nanotube activity to heavy organic molecules

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The high specific surface area of carbon nanotubes, which in several times exceeds the surface area of the best contemporary sorbents [1, 2], opens up the possibility of their using in filters and other equipment of chemical technology. Nanotubes can adsorb impurities on the outer and the inner surface. This allows to produce the selective adsorption. The effectiveness of nanotubes with respect to organic molecules is in ten times greater than the activity of graphite adsorbents, which are most popular means of treatment in this time. So proposed to use carbon nanotubes for purification of liquids, such as alcohol-based liquids, from the side (and / or toxic) products. These products include heavy organic alcohols.

In this work have been made the quantum-chemical researches of the adsorption interaction of carbon nanotubes with heavy organic molecules (in particular the isopropyl alcohol: n-propanol and i-propanol) using methods of MNDO, MNDO/PM3, DFT and program packages of MNDO92, HyperChem, Gamess. Energy curves of interaction processes are built and main geometric parameters of adsorption complexes and energy characteristics of the process are defined. It has been theoretically proved the carbon nanotube activity to heavy organic molecules.

Cleaning of the alcohol-based liquids by the extra small quantity of carbon nanomaterials was made. To prove the purification of water-alcohol solutions from the heavy organic alcohols have been used methods such as IR-spectroscopy, titrimetry, chromatography. We have proved, that the cleaning the water-ethanol mixtures of nanotubes contributes to a decrease in their content of heavy alcohols and other impurity substances.

This research was supported by Russian Federal Target Program "Scientists and pedagogical workers of innovation's Russia", 2009-2013 (Grant No. P328).

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