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## Volatile Organic Molecules Sorption onto Carbon Nanotubes: Experiment and Molecular Modeling.

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### Abstract

Two organic compounds (naphthalene and formaldehyde) were investigated for their sorption properties on to multiwall carbon nanotubes in original state and purified using acid treatment. Nice enhancement of sorptive ability was observed after nanotube purification. Smaller organic molecule was adsorbed in higher weight percentage (reaching 30 wt.%) than naphthalene (approx.13 wt.%). Molecular modeling confirmed adsorption centers of organics on carbon nanotubes being located on the outside area or close to center of nanotube, then having the lowest energy of adsorption.

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### 1. Introduction

A carbon nanotube (CNT) consists of one or more graphene sheets rolled into a hollow cylinder. Typical lengths and internal diameters range from 1 to 100  $\mu\text{m}$  and from 1 to 25 nm, respectively. The unique combination of physical and chemical properties attributed to CNTs has made them one of the most widely utilized classes of

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engineered nanomaterials. CNTs are developed as sensors, imaging agents in gene therapy, vehicles for targeted drug delivery, nanocomposite reinforcement, hydrogen storage devices, and catalyst supports (Rümmeli 2011, Bachmatiuk 2010, Martynkova 2014, Martynkova 2007, Martynkova 2011, Matějka 2014). Multiwalled and single-walled carbon nanotubes (MWCNTs and SWCNTs) are also effective sorbents for low-molecular weight organics due to their high surface areas and hydrophobic graphene properties. Several recent studies have shown CNTs to be effective sorbents for vapor-phase toxins. CNT sorption properties in water have also begun to attract research interest with respect to the uptake of hydrophobic organic chemicals (HOCs) (Matlochová 2013). Indeed, Li 2004 reported that MWCNTs are better sorbents than carbon black for the sorption of volatile HOCs from water, and Peng 2003 and Lu 2005 observed that CNTs can effectively remove 1,2-dichlorobenzene and trihalomethanes, respectively, from water.

Two possible types of adsorption sites were proposed for carbonaceous sorbents: (i) adsorption on external surfaces, and (ii) adsorption in nanopores.

The aim of our study was to analyze adsorbed amount of organics onto MWCNT using thermal analysis. Molecular modeling was employed for prediction of adsorption centers of CNTs.

### 1.1. Experiment and samples

Multiwall carbon nanotubes (Nanocyl<sup>TM</sup> NC 7000) were used in both form: as received and purified by acid treatment.

Purification process removes impurity and partly oxidizes the nanotube to help sorption process. At first intensive humidification in oven (heat at 5 °C/min from ambient to 250 °C and hold for 12 h) was performed. This was followed with acid treatment (2 mol. dm<sup>-3</sup> HCl, stirring for 2 h), washing using distilled water till pH 7 and then centrifuged at 4000 rpm; next similarly (3 mol. dm<sup>-3</sup> HNO<sub>3</sub> for 0.5 hour), washing using distilled water till neutral pH and then centrifuged at 4000 rpm. Last step was treatment with 20% H<sub>2</sub>O<sub>2</sub> and maintained in suspension by stirring for 1 hour.

Purification morphology, observing appearance of the sample for amorphous matter, was examined using SEM. The images of original (Fig.1a) and purified samples (Fig.1b) are proving successful process of cleaning, because purified sample exposed truly fibrous character of the sample while original sample looks covered with fine amorphous particles.

Purified carbon nanotubes were exposed volatile organics for 48h in closed container at room temperature (Plachá 2008).

Two organic compounds sorption were compared: naphthalene and formaldehyde.

### 1.2. Analytical methods

Thermal gravimetric analysis (multi-modular thermal analyser SETSYS 1200 by SETARAM with two measurement heads (TG-ATD 1600°C rod for the simultaneous measurement of TG and DTA curves and the head TMA – Quartz for the simultaneous measurement of thermal dilatation) was performed under 400°C in Ar inert atmosphere.

The X-ray powder diffraction (XRD) patterns were measured on X-ray diffractometer Rigaku Ultima IV (reflection mode, Bragg-Brentano arrangement, CuK $\alpha$ 1 radiation) in ambient atmosphere under constant conditions (40 kV, 40 mA).

The micrographs of samples were performed by scanning electron microscopy (SEM) on PHILIPS XL-30.

### 1.3. Molecular modeling system

The computational study was made using Forcite and Adsorption locator in Biovia Materials Studio software environment. The studied structure is MWCNT containing 2 concentric nanotubes (6,6) with inner tube diameter 0.81nm and length 0.74nm, nanotubes separation is 0.3347nm. We performed a series of total energy calculations

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