Review Article

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The Possibility of Selective Sensing of the Straight-Chain Alcohols (Including Methanol to n-Pentanol) by Using the C_{20} Fullerene and $C_{18}NB$ Nano Cage

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ABSTRACT

Alcohol with its highly flammable nature to produce CO, and CO_2, and also its greenhouse gas emissions, has considerable effects in changing the ecosystem of earth. The high volumes of annual production of this species, as well as its powerful effects on tropospheric changes, have amplified its adverse impacts.
Due to these, in this project, by examining the possibility of C_{20} fullerene (and its nitrogen-boron decorated form ($C_{18}NB$)) in selective sensing of the low weight straight-chain alcohols (including methanol to n-pentanol), we have attempted to find a new approach for detecting those species.
The results show that the $C_{18}NB$ cage senses the existence of methanol (ΔE_g= 0.090 eV) better than the C_{20} fullerene (ΔE_g= -0.037 eV). Also, the results indicate that both the C_{20} fullerene and the $C_{18}NB$ nanocage could sense methanol, clearer and more selective than other mentioned alcohols. Moreover, the results show, that adsorption of methanol by the two mentioned sorbents is thermodynamically more favorable compared to the other alcohols. Also, adsorption of this alcohol by $C_{18}NB$ is significantly favorable than that of C_{20} fullerene (in view of thermodynamics).

1. Introduction

In chemistry, an alcohol is an organic compound in which a hydroxyl functional group (–OH) is attached to a carbon atom [1].There is a wide range of compounds with aliphatic or aromatic molecular segments which have a hydroxyl as the main functional groups; while, usually name of alcohol is referred to hydrocarbons with an aliphatic skeleton [2]. The straight-chain alcohols are known as the most famous ones. On the other hand, the low weight aliphatic straight-chain alcohols containing, methanol, ethanol, propanol, butanol, pentanol, and hexanol, are of the most produced, most used, and most famous alcohols [3]. Usually these compounds are produced by different types of industrial and mineral activities like exploration, drilling, and extracting of oil, gas, and minerals and also petrochemical works [4,5], as well as production of those by natural ecosystems like metabolism of oceans [6]. Both these artificial and natural resources would annually produce hundreds tons of alcohols and release them to the atmosphere [7]. Since, alcohols intervene in a wide range of atmospheric changes especially in the greenhouse gas emission [8]; thus, considering, detecting and controlling these compounds is very important. In this regard, some precious researches were made [9,10]. Moreover, these toxic and flammable compounds [11] are being observed in some mineral activities and might jeopardize the health of miners. Thus, some of scientists have aided new technologies to control or detect the release of those compounds in especial places like mines; also, they used sensors for identifying these gases [12]. Due to the fact that the theoretical calculations have helped researchers in accurate design of some nano-sized actuators and molecular sensors, which are of the best and most advanced technologies [13,14].
Alcohol produces carbon oxide gases, and has also greenhouse gas emissions. Moreover, it has considerable effects in changing the ecosystem of our green planet.

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