Studying of Sweetening of Sour Natural Gases by Using Single-Walled Nitrogen Doped Carbon Nanotubes by DFT Method

M. Oftadeh[a], A. Rashidi[b], **M. Rezaie Sadat[a]**

[a]Chemistry Department, Payame Noor University, Tehran, I. R. of Iran
[b]Department of Developments and Nanotechnology, Tehran Oil Industry Research Laboratory, Tehran, I. R. of Iran
M_oftadeh@pnu.ac.ir

Abstract

Suitable carbon nanotubes for decreasing the process refining of sour natural gases adsorption and to reduce the high cost of amine solution is important in the petroleum technique. In this paper, investigation of physical adsorption of gases hydrogen sulfide and carbon dioxide on zigzag(5,0) carbon nanotubes doped with nitrogen by using density function theory method and B3LYP theoretical level and 6-31G average basis set on Gaussian software has been attended. The different stable and high abundance structures of carbon nanotubes doped with were considered in order to study the interaction of the mentioned gases in different situations by taking rotates of sour gas molecules in the inner and outer walls. Features such as correction of energy adsorption, energy gap, dipole moment, charge distribution, conductors and energy barrier in addition to the main parameters like as the gas adsorption energy on the nanotubes was obtained. The results suggest that the nitrogen atom in the structure of carbon nanotubes causes to increase the adsorption of hydrogen sulfide and carbon dioxide gases. Adsorption of hydrogen sulfide on the nanotubes is more effective than carbon dioxide. Also, for both gases the adsorption processes are thermodynamically favorable. These nanotubes can be economically used for separating the sour gases from natural gases and for recovering the sulfur.

References

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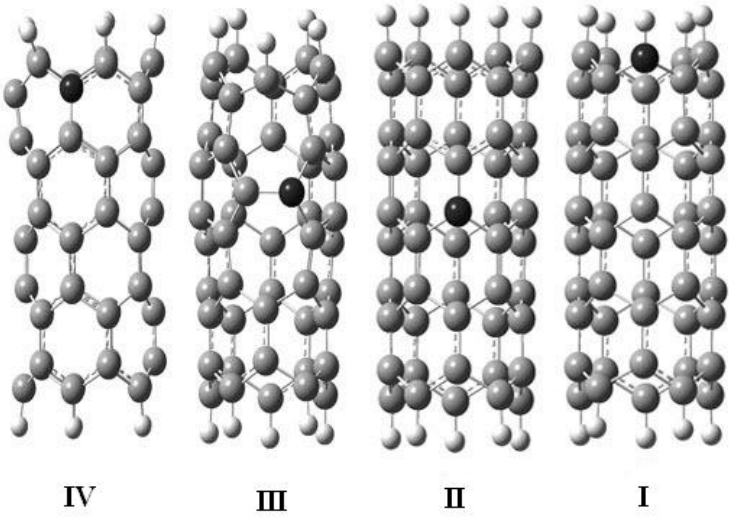

Figure 1 Four strucures of Nitrogen doped SWCNT

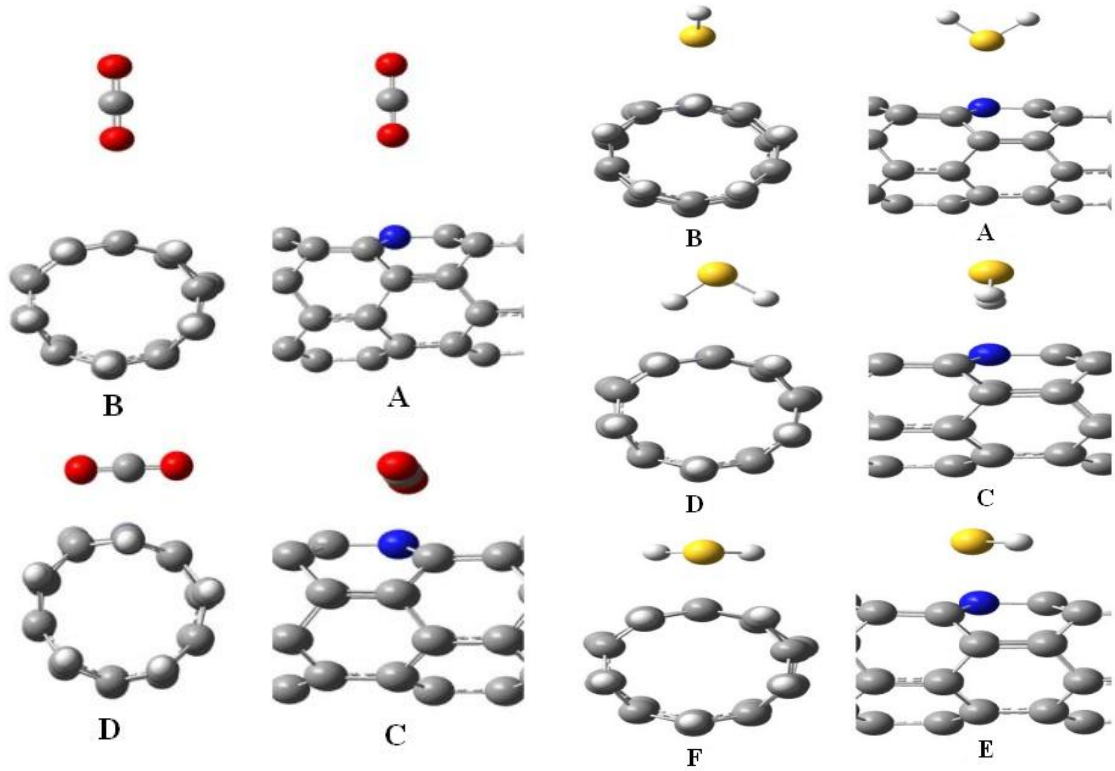

Figure 2 Right: basic positions of the H_2S interaction with the structure II of N-doped SWCN; left: basic positions of the CO_2 interaction with the structure II of N-doped SWCN