



Original Research Article

## Adsorption of Tetryl on the Surface of Carbon Nanocone: A Theoretical Investigation

Azar Mohasseb\*

*Department of Pharmacology, Isfahan Medical University, Isfahan, Iran.*

\*Corresponding author phone number: Tel.: +98 9395951692

\*E-mail: dr.azarmohasseb@yahoo.com

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### ABSTRACT

In this paper, the performance of carbon nanocone as an ideal adsorbent and sensing material for tetryl was investigated by density functional theory. For this aim, the structures of tetryl, carbon nanocone and their complexes were optimized geometrically. Afterwards, IR and FMO computations were done on them. The obtained thermodynamic parameters showed the interaction of carbon nanocone with tetryl is spontaneous, exothermic and experimentally possible. The Molecular orbital parameters like band gap, maximum transferred charge, electrophilicity, chemical potential and chemical hardness was also inspected and the results indicated that carbon nanocone can be used as an excellent sensing material for electrochemical detection of tetryl. The specific heat capacity values have also proved the heat sensitivity has abated after tetryl adsorption on carbon nanocone surface.

**Keywords:** Tetryl, Carbon Nanocone, Adsorption, Density Functional Theory, Explosives

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