
Theoretical study of the proton and methyl group transfer inside the carbon nanotubes.

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Résumé

Carbon nanotubes (CNTs) - synthesized in 1999 [1] - and other materials find applications in several fields [2–4] due to their electronic, optical and mechanical properties including their potential biocompatibility in pharmaceutical for creating versatile drug delivery systems. It is necessary to understand the biocompatibility of CNTs in either cell-based systems or animal models. This approach played an important role particularly in the targeted delivery of drugs for several diseases. We propose to study the possibility of using CNT as reaction carriers. we consider the possibility that the proton and methyl group transfer occurs inside the single-walled carbon nanotubes (SWNTs) of different diameters. This theoretical study explores the influence of the CNT confinement on the Proton and Methyl Group Transfer reactions.

Mots-Clés: Methyl Group Transfer, CNT, proton transfert, DFT, carbone nanotube

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