DFT STUDY OF PHYSISORPTION EFFECT OF CO AND CO_2ON FURANOCOUMARINS FOR AIR PURIFICATION

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First For the first time in the present work, the adsorption properties of the Furanocoumarins derivatives at the non-bonded interaction withCO and CO_2 were investigated by density functional theory (DFT/B3LYP/6-311+G* level of theory) in the solvent water.

*Keywords:*Physisorption, DFT method, Furanocoumarins, Air Purification.

The non-bonded interaction of the title compounds with CO and CO_2 on the electronic properties such as E_{HOMO}, E_{LUMO}, the energy gap between LUMO and HOMO, global hardness was determined. The Furthermore, chemical shift tensors and, natural charge of the Furanocoumarins derivatives and the related complexes were determined and discussed. We have also investigated the charge distribution for the related complexes by molecular electrostatic potential (MEP) calculations using the B3LYP/6-311+G* level of theory. The electronic spectra of the Furanocoumarins derivatives and the related complexes were calculated bytime dependent DFT (TD-DFT) for investigation of the maximum wavelength value of the Furanocoumarins derivatives before and after the non-bonded interaction with the CO and CO_2. Furanocoumarins can be used as strong absorber absorbers for air purification in contaminated territories and cities.According to the results of the chemical shift tensors, non-bonded interaction of the title compounds with CO and CO_2 changes CS^I and CS^A have been described consequently. The calculated results have shownnon-bonded interaction between the Furanocoumarins derivatives and CO and CO_2. Therefore, Furanocoumarins may be used for solving to solve the ecological problems of CO and CO_2 in worldwide may be used across the whole world.

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