

Theoretical study on noncovalent interactions in the carbon nanotube-formic acid dimer system.

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Streszczenie

The noncovalent interaction of the formic acid dimer (FAD) with pyrene and single-walled carbon nanotubes (SWCNTs) is studied using both density functional theory with an empirical dispersion correction as well spin-component-scaled and F12 variants of second-order Møller–Plesset perturbation theory. For the FAD–pyrene model system, it is shown that the dispersion-corrected DFT methods provide similar accurate results for the noncovalent interaction of carboxylic acid dimers with large conjugated π -systems such as MP2 and SCS-MP2. The binding energy of FAD in SWCNTs is found to be sensitive to the radius of the nanotube. It amounts to ca. 22 kcal/mol in the armchair (6,6) SWCNT and decreases with increasing tube radius. In the armchair (8,8) SWCNT, the binding energy is already 25% smaller. To facilitate an experimental identification of FAD inside SWCNTs, we report results for the shifts of the vibrational frequency, where we could identify intense C–O, C=O and O–H stretch modes as promising infrared signatures for an experimental detection of such complexes.

Adres publiczny

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Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>