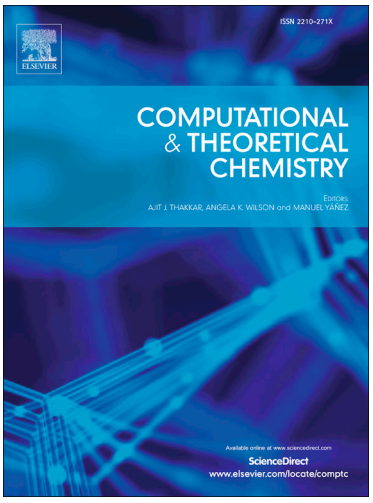

The nature of the noncovalent interactions between fullerene C_{60} and aromatic hydrocarbons

Yu Zhang, Weizhou Wang, Yi-Bo Wang

PII: S2210-271X(17)30474-7
DOI: https://doi.org/10.1016/j.comptc.2017.11.004
Reference: COMPTC 2661

To appear in: *Computational & Theoretical Chemistry*

Received Date: 19 October 2017
Revised Date: 2 November 2017
Accepted Date: 3 November 2017

Please cite this article as: Y. Zhang, W. Wang, Y-B. Wang, The nature of the noncovalent interactions between fullerene C_{60} and aromatic hydrocarbons, *Computational & Theoretical Chemistry* (2017), doi: https://doi.org/10.1016/j.comptc.2017.11.004

The nature of the noncovalent interactions between fullerene C_{60} and aromatic hydrocarbons

Yu Zhang [a], Weizhou Wang [a,*], Yi-Bo Wang [b,*]

[a] *College of Chemistry and Chemical Engineering, and Henan Key Laboratory of Function-Oriented Porous Materials, Luoyang Normal University, Luoyang 471934, China*

[b] *Department of Chemistry, and Key Laboratory of Guizhou High Performance Computational Chemistry, Guizhou University, Guiyang 550025, China*

ABSTRACT

To better understand the solubility of fullerenes in common aromatic organic solvents such as benzene, toluene, tetralin, 1,2,4-trimethylbenzene and 1-methylnaphthalene, the structures, energies and electronic properties of the complexes formed by fullerene C_{60} with benzene, toluene, tetralin, 1,2,4-trimethylbenzene and 1-methylnaphthalene, respectively, have been investigated by the density functional theory with long-range dispersion correction. It was found that the solubility of C_{60} in these solvents is generally proportional to the intermolecular force between solute molecule and solvent molecule. In order to further understand the nature of the noncovalent interactions between C_{60} and these aromatic hydrocarbons, interaction energy decomposition analyses were performed with the symmetry adapted perturbation theory. The results clearly show that the noncovalent interactions between C_{60} and the aromatic hydrocarbons are mainly dependent on both electrostatic and dispersion components, with dispersion playing the dominant role. The other important finding is