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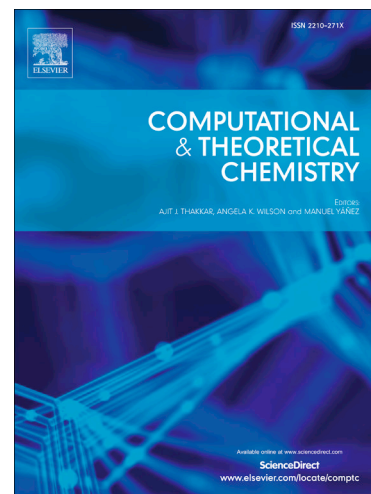
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# The nature of the noncovalent interactions between fullerene C<sub>60</sub> and aromatic hydrocarbons

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## 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<sub>60</sub> 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<sub>60</sub> 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<sub>60</sub> 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<sub>60</sub> and the aromatic hydrocarbons are mainly dependent on both electrostatic and dispersion components, with dispersion playing the dominant role. The other important finding is

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