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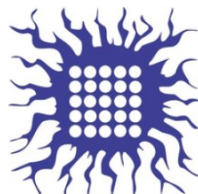
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**2<sup>nd</sup> International Conference on Chemo and Bioinformatics**

**ICCBIKG\_2023**



# BOOK OF PROCEEDINGS





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## Interaction energy and decomposition of interaction energy of halo-substituted phthalimide with carbon nanotube

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**Abstract:** Interaction energy of phthalimide (ph) with carbon nanotube (CNT) calculated at SAPT0 level with a mixed basis set (6-31G\* for CNT and 6-311G\* for ph) is -19.51 kcal/mol. Halo-substitution of the phthalimide generally strengthens its interaction with the CNT and interaction energies are in the range from -21.02 kcal/mol to -22.62 kcal/mol going from ph-Cl to ph-I. However, interaction energy for phthalimide substituted with F atom (ph-F) is weaker (-18.81 kcal/mol) than for non-substituted phthalimide. For ph-Cl, ph-Br, ph-I, the total interaction energy increases with the higher halogen atomic number, because of the significant dispersion term and, less pronounced, electrostatic term increase. The smallest dispersion is calculated for ph-F/CNT (-28.72 kcal/mol), while the remaining systems range from -31.51 kcal/mol for ph/CNT to -35.78 kcal/mol for ph-I/CNT. Apart from dispersion, the system with fluorine has a less pronounced electrostatic term than other substituted phthalimides and does not follow trends observed for other systems.

**Keywords:** phthalimide, SAPT, quantum chemistry, carbon nanotube, halogen

### 1. Introduction

It has been proposed that aromatic interactions consist of van der Waals and electrostatic forces, as well as hydrophobic effects [1]. The relative ratio of these components is complicated to define due to the fact that aromatic groups interact in one of several geometries, depending on the nature of the rings involved. The solvent studies on aromatic interactions addressed the importance of electrostatic and solvophobic components in aromatic interactions. The influence of substituents on both edge-face and stacking interactions was analyzed. It was found that the position of fluorine on a phenyl ring has a significant influence on its interaction with a flavin ring in chloroform. This system provides a good example of polar interactions influencing the magnitude of aromatic interactions [2].

In this work, we studied the influence of halo-substitution of the phthalimide (ph) on stacking interactions with carbon nanotube (CNT). We performed Symmetry Adapted Perturbation Theory (SAPT) calculations on stacking interaction geometries and energies for ph/CNT, ph-F/CNT, ph-Cl/CNT, ph-Br/CNT, and ph-I/CNT systems.

## 2. Results

Geometry optimization of phthalimide (ph) and its halo-substituted structures (ph-F, ph-Cl, ph-Br, and ph-I) (**Figure 1**) was performed at  $\omega$ B97XD/6-311G\* level using Gaussian 09 program package. CNT was built using the VMD Nanotube builder plugin by choosing 30.1 nm diameter armchair (222,222) type CNT, cutting out an 82-carbon curved square sheet and saturating it with 24 hydrogen atoms.

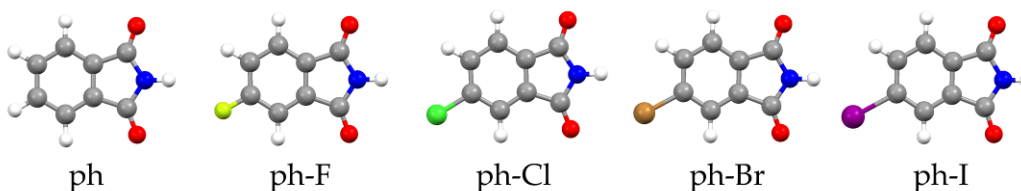


Figure 4. Optimized structures of phthalimide (ph) and phthalimide substituted with fluorine (ph-F), chlorine (ph-Cl), bromine (ph-Br) and iodine (ph-I).

Using phthalimides and CNT sheet prepared as explained above, each system was built by placing a phthalimide or a substituted phthalimide above a CNT sheet, parallel to it and performing geometry optimizations starting from this geometry. Geometry optimizations at  $\omega$ B97XD/6-311G\* level were done with frozen CNT coordinates to preserve the CNT curvature and the resulting coordinates are presented in **Figure 2**.

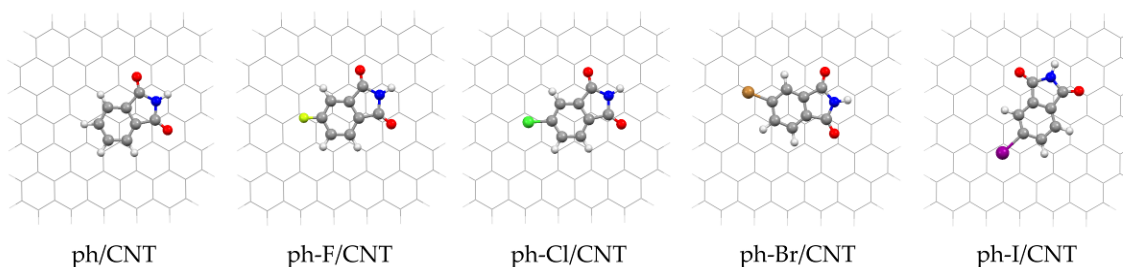


Figure 2. Optimized geometries of ph/CNT, ph-F/CNT, ph-Cl/CNT, ph-Br/CNT and ph-I/CNT systems.

Psi4 program was used to perform Symmetry Adapted Perturbation Theory (SAPT) energy decomposition on optimized systems into electrostatic ( $\Delta E_{el}$ ), exchange ( $\Delta E_{ex}$ ), induction ( $\Delta E_{ind}$ ), and dispersion ( $\Delta E_{disp}$ ) interactions at the SAPT0 ( $\Delta E_{SAPT0}$ ) level. Basis set 6-311G\* was proven to be too demanding for such large systems, so a mixed basis set was used: 6-31G\* on CNT atoms and 6-311G\* on the atoms belonging to ph or

substituted phthalimides. **Table 1** represents normal distances ( $d$ ) between phthalimides and a CNT sheet and the results of SAPT energy decomposition analysis. Normal distances represent the distance from the center of phthalimide C6 ring to the CNT plane.

In all systems, phthalimides stayed parallel to the CNT sheet after geometry optimization. In ph-I/CNT system, iodine is slightly bent away from the CNT sheet because of its large diameter. Normal distances ( $d$ ) are rising uniformly from hydrogen to iodine in the range from 3.33 to 3.39 Å with an exception for ph-F/CNT system which has a longer  $d$  distance (3.37 Å) than ph-Cl/CNT system (3.35 Å) (**Table 1**).

**Table 1.** Normal distances  $d$  (Å) and decomposition of interaction energy  $\Delta E_{\text{SAPT0}}$ , at SAPT0 level with 6-31G\* basis on CNT atoms and 6-311G\* on the remaining atoms, into electrostatic  $\Delta E_{\text{el}}$ , exchange  $\Delta E_{\text{ex}}$ , induction  $\Delta E_{\text{ind}}$ , and dispersion  $\Delta E_{\text{disp}}$  terms of optimized systems. All energies are expressed in kcal/mol.

	$d$	$\Delta E_{\text{el}}$	$\Delta E_{\text{ex}}$	$\Delta E_{\text{ind}}$	$\Delta E_{\text{disp}}$	$\Delta E_{\text{SAPT0}}$
ph/CNT	3.33	-10.96	+25.80	-2.84	-31.51	-19.51
ph-F/CNT	3.37	-8.61	+20.68	-2.16	-28.72	-18.81
ph-Cl/CNT	3.35	-11.32	+26.84	-2.89	-33.65	-21.02
ph-Br/CNT	3.38	-11.43	+27.39	-2.86	-34.63	-21.54
ph-I/CNT	3.39	-11.81	+27.97	-3.00	-35.78	-22.62

The total SAPT0 interaction is becoming stronger with an increased atomic number of the halogen substituent. However, ph-F/CNT system does not follow the trend and its total SAPT0 interaction energy is the weakest (-18.8 kcal/mol) (**Table 1**). The SAPT0 energies of ph, ph-Cl, ph-Br and ph-I with the CNT sheet are -19.51, -21.02, -21.54, and -22.62 kcal/mol, respectively (**Table 1**).

Dispersion interaction has the strongest attractive contribution to the total SAPT0 energy with values having the same trend as  $\Delta E_{\text{SAPT0}}$ . The smallest dispersion is calculated for ph-F/CNT (-28.72 kcal/mol), while the remaining systems range from -31.51 kcal/mol for ph/CNT to -35.78 kcal/mol for ph-I/CNT (**Table 1**). Dispersion interaction is rising because of the larger surface area between a phthalimide molecule and a CNT sheet, even though the distances are also slightly rising. Such a drastic difference between ph-F/CNT and ph/CNT  $\Delta E_{\text{disp}}$  values compared to the other neighboring values could also be caused by a large distance of ph-F from the CNT sheet. The same trend observed in total and dispersion interactions can be noticed for electrostatic terms which is also the second largest attractive contribution. The system with fluorine has a significantly weaker electrostatic interaction (-8.61 kcal/mol) than the ph/CNT system (-10.96 kcal/mol) which could probably be explained in the same manner as for dispersion interactions. Electrostatic terms for ph-Cl/CNT, ph-Br/CNT and ph-I/CNT are -11.32, -11.43 and -11.81 kcal/mol (**Table 1**). Induction terms are very small and have similar values with again fluorine system having the considerably smaller value (-2.16 kcal/mol) than the remaining systems (from -2.84 to -3.00 kcal/mol) (**Table 1**).

Exchange interaction is the only repulsive interaction at the SAPT0 level, and its values also follow the same trend as mentioned above with the fluorine system having the smallest exchange (+20.68 kcal/mol), while the other systems have values from +25.80 for ph/CNT to +27.97 kcal/mol for ph-I/CNT.

#### 4. Conclusions

Halo-substitution of phthalimide generally strengthens its interaction with the CNT with ph-F/CNT being the exception. For other systems, the total interaction increases with the higher halogen atomic number, because of the significant dispersion and less pronounced electrostatic term increase. The system with fluorine does not follow trends observed for other systems and its interaction with CNT is weaker than for ph/CNT system.

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