Hydrogen bonds between phthalimide chloride and carboxylic acids: A theoretical study

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Introduction

It is well known that cyclic imides can be compounds potential biological activities[1,2]. For example, the phthalimide is a potent hypolipidemic agent when administered at relatively low doses. It was observed that, in mice, the serum cholesterol level decreases to 43% of its initial value after a few days[1,2]. The existence of two carbonyl groups in cyclic imides allows the formation of hydrogen bonded complexes[3].

In this work, we study the molecular and vibrational properties of the complexes between phthalimide chloride (PHT, Figure 1) and carboxylic acids: HOOCH and HOOCCF$_3$. In order to obtain these properties, we employed the PBE1PBE functional with the 6-31++G(d,p) basis set. All calculations were performed with the Gaussian 2009 software.

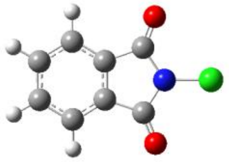

Figure 1. Molecular structure of the phthalimide chloride (PHT).

Results and Discussion

We calculated the fully optimized geometries of the isolated molecules and the hydrogen bonded complexes. No imaginary frequencies were found. This indicates that all structures correspond to minimum points on their potential energy surfaces. Figure 2 shows the PBE1PBE/6-31++G(d,p) fully optimized molecular structures of the complexes between phthalimide chloride and RCOOH in 1:1 stoichiometric ratios. We verified that the length of the hydrogen bonds were 1.845Å for the complex PHT···HOOCH and 1.748Å for complex PHT···HOOCCF$_3$.

Table 1 shows the uncorrected binding energies (ΔE), the binding energies after ZPE corrections (ΔE^{ZPE}), and the binding Gibbs energies (ΔG) obtained. We observed that the ΔE^{ZPE} value of the hydrogen bond in complex PHT···HOOCH (-23.1 kJ mol^{-1}) is less negative than the corresponding value in the PHT···HOOCCF$_3$ (-33.5 kJ mol^{-1}).

However, the spontaneity of the binding reaction is greater for the complex PHT···HOOCH (-10.3 kJ mol^{-1}) when compared with the corresponding value in the PHT···HOOCCF$_3$ complex (-5.0 kJ mol^{-1}).

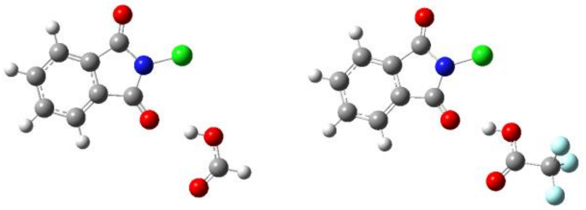

Figure 2. DFT PBE1PBE/6-31++G(d,p) optimized molecular structures of the complexes between phthalimide chloride and RCOOH in 1:1 stoichiometric ratio.

Table 1. Uncorrected binding energies (ΔE), binding energies after ZPE corrections (ΔE^{ZPE}), and binding Gibbs energies (ΔG) obtained from PBE1PBE/6-31++G(d,p) calculations.

Complex	ΔE (kJ mol^{-1})	ΔE^{ZPE} (kJ mol^{-1})	ΔG (kJ mol^{-1})
PHT···HOOCH	-26.5	-23.1	-10.3
PHT···HOOCCF$_3$	-36.1	-33.5	-5.0

Conclusions

We calculated the molecular properties of the hydrogen bonded complexes between phthalimide chloride and RCOOH. We verified that the spontaneity of the binding reaction is greater for the PHT···HOOCH complex when compared with the corresponding value in the PHT···HOOCCF$_3$ complex.

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CNPq, PRONEX/FACEPE and PROAES/UFPE.

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