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Complexation Energies and Electronic-Structural Properties of Adamantane Derivatives: A DFT Study

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Abstract

This article is an investigation related to the complexation energies, binding abilities, frontier molecular orbital's energy gaps and dipole moments on dimeric forms of 1-adamantanol, 1-adamantanemethylamine and 1-adamantanecarboxylic acid as the adamantane derivatives. All the optimizations, counterpoise corrections and complexation energy computations have been achieved by density functional theory with B3LYP and WB97XD functionals. In all counterpoise calculations have been used the empirical dispersion method with B3LYP and WB97XD for non-covalent interactions. The more favorable complexation energies have been obtained by B3LYP with the addition of dispersion correction. In addition, the images mapped with total density and electrostatic potential have been obtained in this study.

Keywords: Adamantane derivatives, Complexation energy, Density functional theory

Adamantan Türevlerinin Kompleksleşme Enerjileri ve Elektronik-Yapısal Özellikleri: Bir DFT Çalışması

Öz

Bu makale, adamantan türevleri olarak 1-adamantanol, 1-adamantanmetilamin ve 1-adamantan karboksilik asit yapılarının dimerik formlarında kompleksleşme enerjileri, bağlanma yetenekleri, sınır moleküler orbital enerji boşlukları ve dipol momentleri ile

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ilgilidir. Tüm optimizasyonlar, counterpoise düzeltmeleri ve kompleksleşme enerji hesaplamaları, B3LYP ve WB97XD ile yoğunluk fonksiyonel teorisi yardımıyla elde edilmiştir. Tüm counterpoise hesaplamalarında kovalent olmayan etkileşimler için B3LYP ve WB97XD ile ampirik dispersiyon metodu kullanılmıştır. B3LYP yaklaşımında dispersiyon düzeltmesinin eklenmesiyle daha uygun kompleksleşme enerjileri elde edilmiştir. Ek olarak, bu çalışmada toplam yoğunluk ve elektrostatik potansiyel ile haritalanan görüntüler elde edilmiştir.

Anahtar Kelimeler: Adamantan türevleri, Kompleksleşme enerjisi, Yoğunluk fonksiyon teorisi

1. Introduction

Adamantane is a crystalline, colorless compound highly soluble in hydrocarbons and it has four cyclohexane rings. Adamantane derivatives are organic compounds that are effective in medical practice, extensively [1-3]. The first adamantane-derived drug is amantadine developed for the treatment of Parkinson's and influenza diseases [4-8]. Other biological characteristics of adamantane-like compounds such as anticancer, antihypertensive, central nervous and antimicrobial activities are reported in literature [9-13]. Also, the chemical and physical characteristics of adamantane derivatives such as low surface energy, thermal stabilities and oxidative stabilities have been the focus of several scientific studies [14, 15].

Adamantane derivatives have been recently analyzed by computational approaches as potential hole transport materials for perovskite solar cells [16], porous materials for energy conversion, gas storage [17] and optical materials [18]. The crystal structure and data, electronic structure calculations, spectral analysis, molecular orbitals (MO) analysis, natural bond analysis (NBO), non-linear optical (NLO) properties, molecular docking studies and electrostatic potential analysis on the several adamantane derivatives have been the main topics of the previous studies [19–26].

Structural properties of Adamantane derivatives have been studied due to the use as technological materials in the industrial areas and the synthesis and spectroscopic analysis of very novel compounds in recent years. Hydrogen bond geometries between the hydroxyl, methylamine and carboxylic components have attracted our attention in

these dimers. The main objective is to examine the interactions that are caused by the effective hydrogen bonds in the selected dimer structures. In this research article; the dimeric forms of 1-adamantanol (AD1), 1-adamantanemethylamine (AD2) and 1-adamantane carboxylic acid (AD3) as the adamantane derivatives are optimized by computational quantum chemistry methods. AD1 and AD2 compounds are also called as 1-hydroxyadamantane and 1- (amino methyl) adamantane in literature, respectively. In addition, we aimed to obtain corrected complexation energies by using Grimme's dispersion correction in B3LYP and compare without dispersion contribution. The corrected complexation energies, dipole moments and non-covalent interactions of the adamantane derivatives are evaluated in this study.

2. Material and Method

Geometry optimizations of the adamantane derivatives were provided by density functional theory (DFT) [27] with Becke's three-parameter exchange function [28] along with Lee-Yang-Parr correlation exchange functional (LYP) [29] and wB97XD in combination with 6-31G (*d, p*) basis set. WB97XD is in the group of long range corrected functionals and includes empirical dispersion [30]. The description of atomic coordinates, initially, for all the geometry optimizations and molecular orbitals were formed by Gauss View software database [31]. All the optimizations, counterpoise (CP) corrections [32], basis set superposition error (BSSE) corrections and complexation energy computations were performed by using Gaussian 09W program package [33]. Monomer components (monomers A and B) as Gaussian fragments 1 and 2 were selected in Gauss View software. Corrected complexation energy is a value calculated by the CP approach. Raw (uncorrected) complexation energy does not contain CP correction. CP correction is a method for removing BSSE [34]. Gap between corrected and raw complexation energy is equal to BSSE energy. In all CP calculations empirical dispersion method, D2 version of Grimme's dispersion correction [35], was applied with B3LYP and WB97XD by defining the values of the functional-specific global parameters for non-covalent interactions [36, 37].

3. Results and Discussion

The modeling images of the dimeric structures are given in Fig. 1. The energies of the monomeric and dimeric structures, complexation energies and hydrogen bond geometries ($\text{H}\cdots\text{X}'$ distances) for AD1, AD2 and AD3 are shown in Table 1. The stronger binding abilities between the monomer components with the hydrogen bond are computed as 1.86 ($\text{H3}\cdots\text{O2}'$), 2.11 ($\text{H3}\cdots\text{N2}'$), and 1.62 Å ($\text{H3}\cdots\text{O4}'$) by WB97XD methodology for AD1, AD2 and AD3, respectively. It is noteworthy that the binding abilities with $\text{O2-H3}\cdots\text{O4}'$ hydrogen bond geometry and corrected complexation energies results are more effective in AD3 dimer.

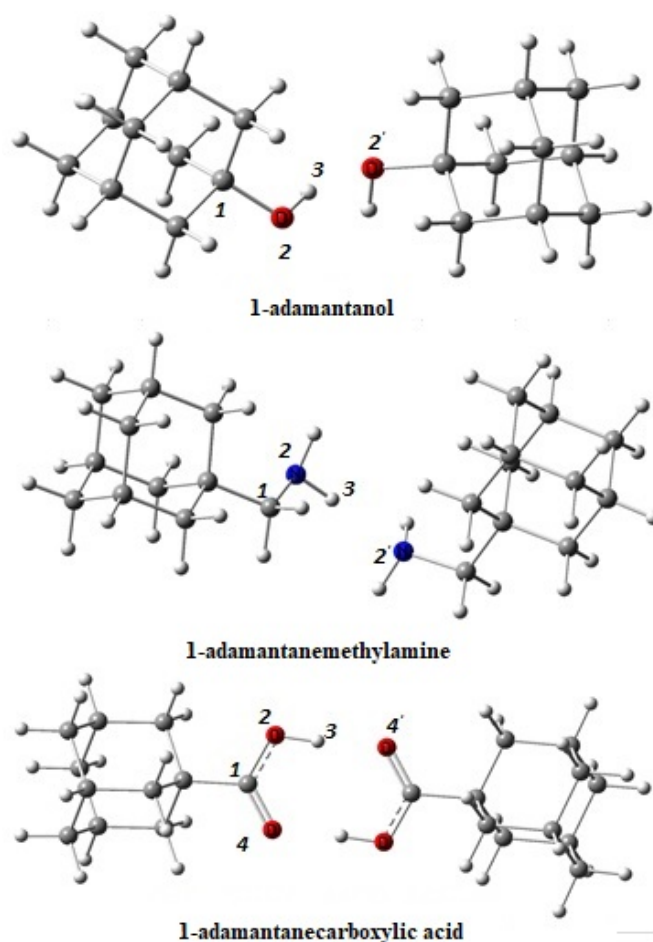


Figure 1. Dimeric forms of the adamantane derivatives

Corrected complexation energies are -4.26 (AD1), -2.60 (AD2) and -20.35 (AD3) kcal/mole without dispersion contribution in B3LYP. As shown in Table 1, corrected

complexation energies are computed as -8.61 (AD1), -6.04 (AD2) and -23.75 (AD3) kcal/mole by using Grimme's dispersion correction in B3LYP. Adding dispersion correction in WB97XD approach did not affect the complexation energies in CP calculations (Table 1). This indicates that the WB97XD function already contains dispersion correction. There are strong intermolecular hydrogen bonds in dimers. Non-covalent interactions (van der Waals and steric interactions) are weak physical interactions and lower than hydrogen bonds.

Table 1. Energies and hydrogen-bond geometry of the adamantane derivatives by B3LYP and WB97XD type calculations

	Derivatives					
	AD1		AD2		AD3	
	B3LYP	WB97XD	B3LYP	WB97XD	B3LYP	WB97XD
Monomer (a.u.)	-465.96654	-465.84689	-485.40854	-485.28688	-579.31875	-579.16709
Dimer/CP corrected (a.u.)	-932.04213	-931.70840	-970.94357	-970.58679	-1158.77246	-1158.36309
Raw Complexation Energy (kcal.mole ⁻¹)	-12.23	-12.41	-8.14	-8.52	-27.84	-25.93
Corrected Complexation Energy (kcal.mole ⁻¹)	-8.61	-8.75	-6.04	-6.43	-23.75	-22.52
d(H...X)* (Å)	1.93	1.86	2.19	2.11	1.63	1.62

The relationship between the binding ability and interaction energy has been highlighted in earlier study [38]. The interaction energy was -19.815 kcal/mole as a lower level by the M06-2X of density functional than the B3LYP functional for a dimer linked with strong C-H...O interaction and N-H...O hydrogen bonds in this study [38]. In a similar study on the intermolecular interactions in aromatic amino acid residues, the binding energies have been computed at -5.8 and -6.6 kcal/mole by second-order Møller-Plesset perturbation (MP2) theory and the molecular mechanics modeling for para-cresol dimer, respectively [39].

Hydrogens interact symmetrically with atoms with higher electronegativity in AD3 dimeric form. So, it has minimum complexation energy values and stronger binding abilities with H3...O4' hydrogen bond geometry. Along with that, C1-O2-H3, C1-N2-H3 and C1-O2-H3 bond angles as (shown in Fig. 1) are respectively calculated by B3LYP as 107.37° , 110.98° and 105.71° in AD1, AD2 and AD3 monomeric forms. These angles are respectively 108.85° , 109.39° and 110.44° in AD1, AD2 and AD3 dimers as a result of intermolecular interactions. The analysis of the interaction energy and the decrease in

bridging angles are reviewed in a previous study involving the interactions of polyaniline emeraldine salt with NH₃, CO₂, and CO [40].

Table 2 includes the energy gaps between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) and dipole moments for the monomeric and dimeric forms by B3LYP approach. As shown in the table, the minimal dipole moment is resulted in AD3 dimeric forms. The charge distribution and geometry of a molecule determines the polarity of this molecule. Polar or apolar properties of a molecule relate to electronegativity and molecular geometry. The dipole moment near zero indicates that the bond moments are of equal magnitude and opposite direction in AD3 dimeric forms.

Table 2. HOMO-LUMO energy gaps and dipole moments of the adamantane derivatives by RB3LYP /6-31G(d, p) type calculations

	HOMO-LUMO gap -monomer- (eV)	HOMO-LUMO gap -dimer- (eV)	Dipole moment -monomer - (Debye)	Dipole moment -dimer- (Debye)
AD1	8.63	8.04	1.54	2.16
AD2	8.11	7.71	1.46	2.91
AD3	7.46	7.24	1.71	0.22

HOMO-LUMO plots, molecular orbital energy levels for the AD1 dimeric form are displayed in Fig. 2. The frontier molecular orbital energy gaps (HOMO-LUMO gaps) of the AD1, AD2 and AD3 dimeric forms are calculated as 8.04, 7.71 and 7.27 eV, respectively (Table 2). The frontier molecular orbital energy gaps of the dimers are lower than those of monomers. The visuals mapped with electrostatic potential (ESP) onto AD1, AD2 and AD3 dimers are given in Fig. 3. Red, green, and blue tones represent negative, neutral and positive potential values, respectively. ESP is effectively observed onto dimer interaction regions. It is used to explore the electron richness or poorness of the molecular regions and to discuss the suitability of the electrophilic and nucleophilic attack. That is, it presents the distribution of positive and negative potentials on the molecule. The negative ESP generally refers to the lone pair of an electronegative atom [41]. In monomers, the hydroxyl, methylamine and carboxylic regions act as electrophilic attack. The regions with the positive electrostatic potential tone act as a nucleophilic attack. The surface map values are approximately -0.017 (around the oxygen), -0.013 (around the nitrogen) and -0.012 (around the symmetric atom group) for AD1, AD2 and AD3 dimeric forms, respectively.

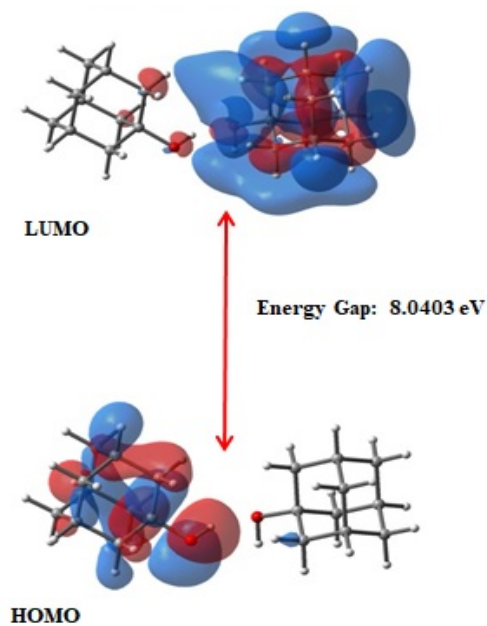


Figure 2. The frontier molecular orbitals and energy levels of 1-Adamantanol dimeric form

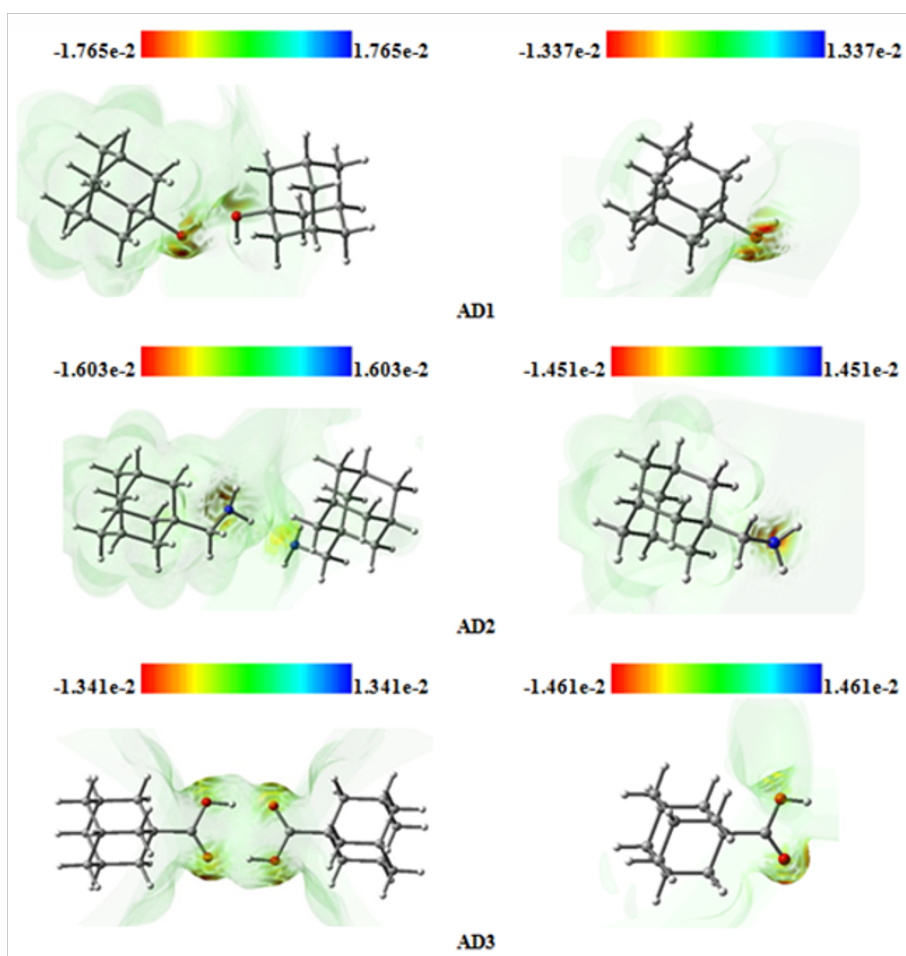


Figure 3. The visuals mapped with ESP of the dimer and monomer structures

4. Conclusions

In this study, the monomer and dimer optimizations of the adamantane derivatives have been performed via density functional theory. The binding abilities with the hydrogen bond geometries and complexation energies have been evaluated in dimer structures. Complexation energies and binding abilities with the hydrogen bond geometry are much more effective in AD3 dimer with atoms with higher electronegativity. D2 version of Grimme's dispersion correction has been tested with density functional theory for non-covalent interactions. In B3LYP the more favorable complexation energies have been obtained with dispersion correction. In all dimers the binding abilities computed by WB97XD functional are stronger for containing empirical dispersion. The energy gaps and dipole moment values for the monomeric and dimeric forms of the adamantane derivatives have been calculated. The relations of polarity and apolarity properties to electronegativity and molecular geometry have been commented. The surface map values have been calculated by ESP analysis observed onto dimer interaction regions and monomers. The hydroxyl, methylamine and carboxylic regions in dimers and monomers act as electrophilic attack.

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