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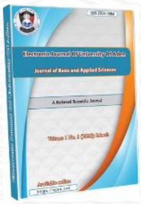

RESEARCH ARTICLE

INVESTIGATION OF BASICITY AND PROTONATED SITES OF SOME COUMARIN DERIVATIVES
A DFT STUDY

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Abstract

Hymecromone and umbelliferone are hydroxycoumarin compounds, which are highly significant because of their wide applications in organic chemistry, medicine, and industry. They show photochemical, antagonist, anticoagulants, anticancer, antioxidant, antiviral, and antimicrobial properties. The ground-state equilibrium geometries of two molecules and their protonated forms were optimized at the density functional theory (DFT)/6-311++G(d) level of theory. Proton affinities on two protonated sites of the studied compounds were calculated at the DFT/ B3LYP / 6-311++G(d). The results indicated that heterogeneous oxygen atom in lactonic ring was strongly favored over hydroxy oxygen atom as sites of protonation for the series studied. A comprehensive investigation of the effect of solvent on the process of protonation of the studied compounds was performed using CPCM method at the B3LYP/6-311++G(d) level of theory. The results showed that the solvent increased the dipole moments of the bare molecules compared with the gas phase and the solvation was enhanced in a protic polar solvent such as water and ethanol.

Keywords: CPCM; DFT (B3LYP / 6-311++G(d); Hymecromone; Proton affinity (PA); Umbelliferone.

Introduction

Basicity is the measure of a substance's ability to accept protons. This includes proton-transfer reactions where lone pair of electrons on the basic atom N, O, or S is protonated. Knowledge of the protonation process and acidity constants of weakly basic substances are of central importance to study the reaction mechanisms specially at acidic media. They also play an important role in the biochemical interactions. For example, many weakly basic anticancer drugs are accumulated in the acidic medium that surrounding cancer cells which improve the selectivity uptake of drugs by tumor cells, and increase of ionic interactions with negatively charged in target proteins binding sites [1-3]. Antifungal agents such as polyenes, and echinocandins have basic characteristics that causing damage of fungal cell walls and membranes and inhibiting fungal growth [4-7]. Furthermore, the basicity of the molecules enhances their binding affinity to the bacterial wall, and this can lead to the disruption of bacterial cell walls [8-12].

Coumarin and its derivatives were studied extensively for their spasmolytic, anticancer, antibacterial, antiviral, anti-inflammatory, anticonvulsant, anticoagulant, antidiabetic, anti-hyperpigmentation effects, and fluorescent activities [13-18]. Hymecromone is a 4-methyl-7-hydroxy coumarin and it is a choleretic (increasing bile flow), and antispasmodic drug [19,20]. Moreover, it is used as standard for the fluorometric determination of enzyme activity and as an optical brightening agent due to its fluorescent [21,22]. Another synthetic coumarin derivative is umbelliferone (7-Hydroxy coumarin). Umbelliferone and its derivatives are known as antimicrobials and antifungal activities [23-25].

Experimental investigation of the sites of protonation and the proton transfer reactions are not easy, and a density functional theory (DFT) approaches is another quantum candidate method for reliable calculation of theses parameters.

Proton affinity (PA) is the energy released when a base accepts a proton, and it is calculated thermodynamically as the negative enthalpy of the protonation reaction: $H^+ + B \rightarrow BH^+$, in the gas phase [26-28]: $PA = -\Delta H$

Most of the available experimental data on basicity and acidity have been obtained in solutions, and the enthalpy of solvation is defined as the heat released or absorbed when one mole of a solute dissolves in a solvent, typically at constant pressure, and representing the net energy from breaking intermolecular forces within the solute [29,30].

In the present study we used a density functional theory (DFT) calculation to investigate the sites of protonation of hymecromone and umbelliferone as coumarin derivatives. The theoretical proton affinities enthalpies of the studied compounds are computed. Since most protonation process occurs in solution, it is necessary to understand how the solvation processes influence on the protonation process. Therefore, the investigation of solvent effect are computed using solvation model CPCM. The total energies of the studied compounds are performed by using a DFT method at the B3LYP/6-311++G(d).

2. Computational methods:

The molecular geometry optimization, and energy calculations were carried out for the studied compounds using Gaussian 03W software package. [31] Full geometry optimizations were performed on each species without any symmetry constraint. Each optimized structure was characterized by positive eigen-value of the second derivative Hessian matrix that implies a minimum on the potential energy surface.

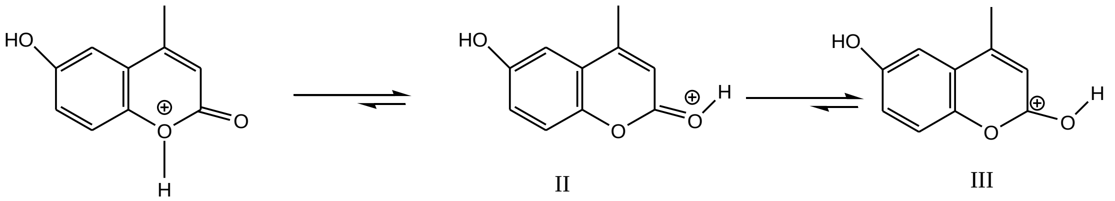
All the calculations have been performed using the Becke's three-parameter exchange functional with the correlation functional of Lee, Yang, and Parr (B3LYP) combined with the standard 6-311++G(d) basis set [32-36]. The solvation model CPCM [36-37] have been used in the present work to study the effect of the solvent on the protonation process.

3. Results and discussion:

3.1 Proton affinity:

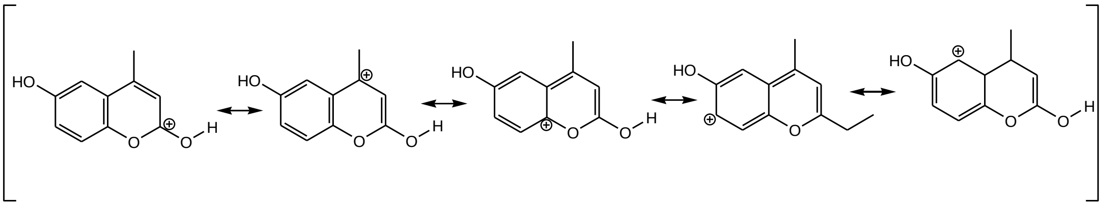
The proton affinity (PA) is defined as the negative of the enthalpy change associated with protonation reaction B $+ H^+ = HB^+$ in the gas phase. The heterogeneous oxygen atom of lactonic ring site (prot1), the hydroxy oxygen atom site (prot2), as well as both oxygenated sites (diprot)) in the hymecromone and umbelliferone (neutral compounds) were investigated for protonation using density function theory (DFT). The geometries of the neutrals and their protonated species (prot1, prot2, diprot) obtained after energy minimization at the B3LYP/6-311++G(d) level of the theory.

The results were displayed in figures 1,2, and tabulated in table1. The data in figures reflected the most significant change in geometrics associated with the proton sites as significant bond lengths. Figures 1 and 2 displayed a deformation in the prot1 and diprot forms, where the lactonic rings were opened. This may be occurred to reduce the strain inside the rings after protonation process. On the other hand, we observed that the length of C_7-O bond increased in the prot2 forms compared with neutral forms. We noted the C_7-O bond length became 1.50648 A° instead of 1.36166 A° in neutral hymecromone, and it became 1.5054866 A° compared with 1.3634652 A° in the neutral umbelliferone. This indicated that the charge density took place in this region. Table 1 represented the DFT/B3LYP energies for the hymecromone and umbelliferone and their protonated species in the gas phase. The results indicated clearly that the heterogeneous oxygen atom (prot1) was more energetically favored for accepting proton compared with the hydroxy oxygen atom (prot2). The prot1 of hymecromone was more stable than prot2 form by 82.88 kJ/mol. Also, the prot1 of umbelliferone was more stable than the prot2 form by 94.20 kJ/mol. This would suggest that protonation took place preferably on the heterogeneous oxygen atom in both hymecromone and umbelliferone. The stabilization energies values in table 1 indicated that the deformation in lactonic ring was overcome. This can be interpreted by equilibrium between prot1 and an intermediate III through the structure II as shown in scheme1. The intermediate III is more stable. It has five resonance structures as illustrated in scheme2.

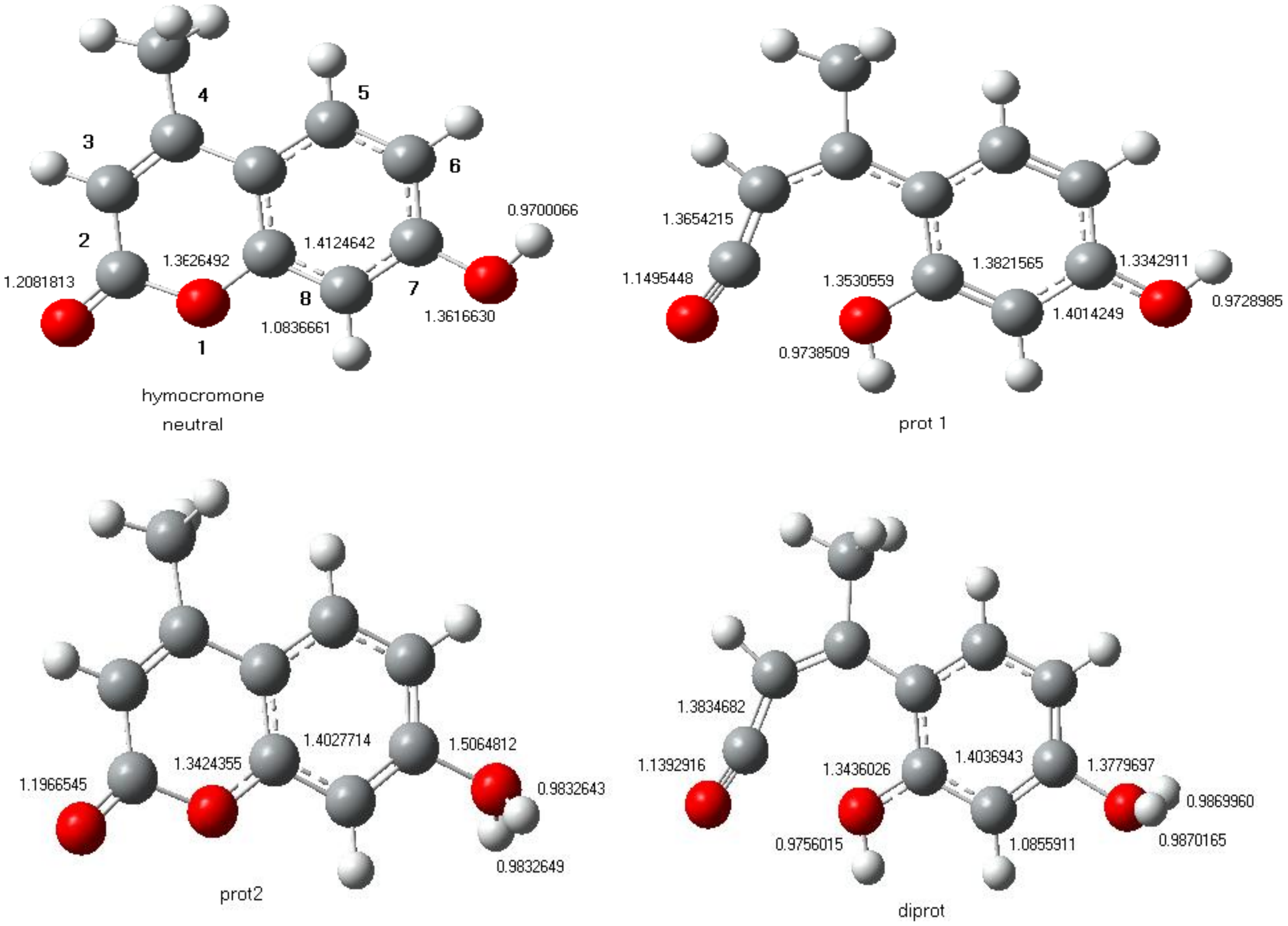


I (Prot1)
II
III

Scheme1: The equilibrium of Prot1 with structure III through structure II



Scheme2: Five resonance structures of intermediate III



hymocromone
neutral

prot 1

prot2

diprot

Fig. 1: The optimized structures (bond lengths in angstrom) of the neutral and the corresponding protonated forms of hymecromone at B3LYP / 6-311++G(d) level of the theory

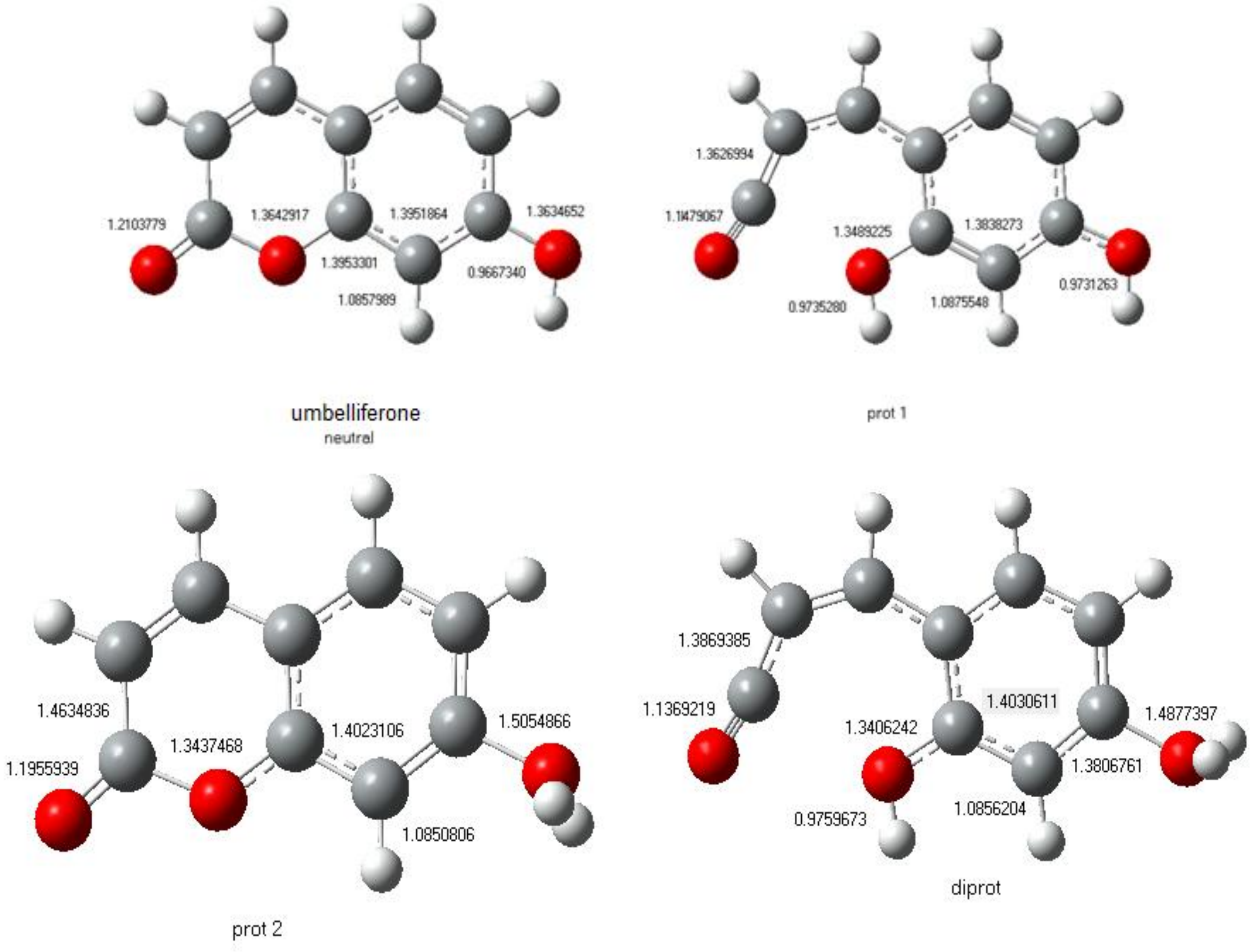


Fig. 2: The optimized structures (bond lengths in angstrom) of the neutral and the corresponding protonated forms of the umbelliferone at B3LYP / 6-311++G(d) level of the theory

Table (1): Energies (E_{opt}) (in Hartree) and proton affinities (PA) for the Hymecromone and Umbelliferone and their protonated forms in the gas phase.

	Eopt(au)	PA(KJ/mol)
Hymecromone	-611.6019170	0.00
Prot1	-611.8985801	-778.877233799
Prot2	-611.8670117	-695.995609825
Diprot	-612.0585780	-1198.94529407
Umbelliferone	-572.2551496	0.00
Prot1	-572.5630686	-808.4414476
Prot2	-572.5271897	-714.2412
Diprot	-572.7231155	-1228.644493

3.2 Solvation:

More precise calculations were undertaken using the CPCM model at the B3LYP/6-311++G(d) level of theory to investigate the effect of a solvent on the studied protonation. Tables (2) and (3) presented the DFT/B3LYP 6-31G++(d) energies hymecromone and umbelliferone and their protonated forms in the gas phase and in solution. The results in table 2 showed that the neutral hymecromone had a positive value of enthalpy change of solution in carbon tetrachloride, which indicated that the solvation not occurred in this solvent. The data in table 3 indicated that the solvent increased the dipole moments of the bare molecules compared with the gas phase. For example, the computed solvation energy for prot2 of hymecromone in water was -611.9931 kJ/mol ((dipole moment =18.173 Debye)), larger than the -611.8670 kJ/mol ((dipole moment = 13.4685 Debye)) which computed in the gas phase.

Table (2): the DFT/B3LYP 6-311++G(d) energies (E, in Hartree) of Hymecromen and Umbelliferone with their protonated forms in the gas phase, and in the liquid phases by CPCM method

	Enthalpy change of solution (Hartree)			
	ΔE_{Water}	$\Delta E_{Ethanol}$	$\Delta E_{Chloroform}$	$\Delta E_{Carbontetrachloride}$
Hymocromone	-0.0122183	-0.01076316	-0.00509256	0.00236172
Prot1	-0.0960730	-0.09243765	-0.07605617	-0.05213315
Prot2	-0.1261666	-0.12174317	-0.09915017	-0.06701373
Diprot	-0.3054985	-0.29570049	-0.24424705	-0.170102717
Umbelliferone	-0.05287894	-0.05102913	-0.04359609	-0.03558493
Prot1	-0.14289068	-0.14015946	-0.13147397	-0.11971654
Prot2	-0.19822755	-0.19405591	-0.17481276	-0.10632104
Diprot	-0.40987653	-0.40477565	-0.38336585	-0.36031777

Table (3): the DFT/B3LYP 6-311++G(d) energies(E, in Hartree) ,and dipole moments (μ)(Debye) of Hymecromen and Umbelliferone and their protonated forms in the gas phase, and in the liquid phases by CPCM method

	E_{gas}	μ in gas	E_{water}	μ in H_2O	$E_{ethanol}$	μ in EtOH	E_{CHCl3}	μ in $CHCl_3$	E_{CCl4}	μ in CCl_4
HYMECROMONE	-611.6019	7.1474	-611.6141	10.812	-611.6126	10.6079	-611.60700	9.7801	-611.5995	8.7768
Prot1	-611.8985	2.0024	-611.9946	2.107	-611.9910	2.0122	-611.97463	2.0113	-611.9507	2.0089
Prot2	-611.8670	13.4685	-611.9931	18.173	-611.9887	17.9740	-611.96616	16.9809	-611.9340	15.7065
diprot	-612.0585	9.1499	-612.3640	11.928	-612.3542	11.8186	-612.30282	11.2325	-612.2286	10.4769
Umbelliferone	-572.2551	3.9432	-572.3080	6.791	-572.3061	6.6319	-572.29874	5.9738	-572.2907	5.2606
Prot1	-572.5630	1.1978	-572.7059	6.984	-572.7032	6.8433	-572.69454	5.4668	-572.6827	4.8649
Prot2	-572.5271	12.8581	-572.7254	23.417	-572.7212	23.0193	-572.70200	21.1363	-572.6335	16.5884
diprot	-572.7231	8.1386	-573.1329	22.0065	-573.1278	21.5462	-573.10648	19.4244	-573.0834	16.9359

The water predicted very high solvation energies and the order of stabilization of the protonated structures in the four used solvents was:

Water > Ethanol >> Chloroform > Carbon tetrachloride

In conclusion, the computational calculations indicated that heterogeneous oxygen atom in hemecromone and umbelliferone compounds was more preferred to accept proton over the hydroxy oxygen atom, and the solvation increased the stability of the protonated species, especially in the polar protic solvent. It can be concluded that the studied compounds have basic nature and can be acted as weak bases in the acidic environment in which they accept proton and converted to protonated forms. So, they behave as weak bases, which are similar to the some coumarin derivatives [38-42].

4. Conclusion:

1- In this work, density functional theory was used to investigate of the electronic structure and basic properties of the two biologically important coumarin derivatives. Proton affinities of heterogeneous oxygen atom (in lactonic ring) and hydroxy oxygen atom sites in hemecromone and umbelliferone compounds were calculated at B3LYP / 6-311++G(d) theoretical level in the gas phase and in solution. The results suggested that the protonation at heterogeneous oxygen atom was more stable and favored over hydroxy oxygen atom site.

2- Although protonation at heterogeneous oxygen atom introduced geometry deformations, but the values of stabilization energies indicated that a deformation may be overcome by equilibrium and resonance which illustrated in schemes 1 and 2, respectively.

3- CPCM as solvation model at the B3LYP/6-311++G(d) level of theory was used to study the effect of solvent on protonation process. The obtained results exhibited that the solvent increased the dipole moments of the bare molecules compared with the gas phase and the order of the stability was: Water > Ethanol >> Chloroform > Carbon tetrachloride.

4- In conclusion, the results showed that the studied compounds have basic nature, and they can behave as the weak bases in acidic media in which they accept proton and converted to protonated structures which play a central role in acid catalyzed reactions. This behavior of studied compounds is similar to the some coumarin derivatives [38-42].

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مقالة بحثية

التحقق من قاعدية ومواقع دخول البروتونات في بعض مشتقات الكومارين دراسة باستخدام نظرية الكثافة الوظيفية (DFT)

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المُلخّص

يُعدّ كلٌّ من الهايميكرومون والأومبليفيرون من مركبات الهيدروكسي كومارين، وهما مركبان بالغا الأهمية نظراً لتطبيقاتهما الواسعة في الكيمياء العضوية والطب والصناعة. يظهر المركبان خصائص كيميائية ضوئية، وصفات مناهضة (antagonist)، كما ان لهما نشاط بيولوجي مثل الخصائص المضادة لكل من التخثر، السرطان، الأكسدة، الفيروسات، والميكروبات. في هذا البحث تم دراسة قابلية موقعين في هذين المركبين لاكتساب البروتون باستخدام نظرية الكثافة الوظيفية (DFT) وهي طريقة تستخدم في الكيمياء الحاسوبية وتعتمد على علم ميكانيكا الكم حيث تُستخدم لدراسة البنية الإلكترونية أو البنية النووية وخاصة في الحالة الأرضية للذرات والجزيئات والأطوار المكثفة وبها يمكن دراسة حاسوبيا خصائص نظام متعدد الإلكترونات باستخدام الدوال الوظيفية. تم دراسة الالفة البروتونية على موقعين في مركبي الهايميكرومون والأومبليفيرون على مستوى نظرية الكثافة الالكترونية باستخدام هجين B3LYP للتبادل والارتباط، مع مجموعة أساس 6-311++G(d) وأشارت النتائج إلى أن دخول البروتون (البرتنة) على ذرة الأكسجين غير المتجانسة في حلقة اللاكتون في المركبات المدروسة هو مفضل جدا من حيث الطاقة مقارنة بدخوله على ذرة الأكسجين في مجموعة الهيدروكسيل في تلك المركبات. ولان معظم عمليات البرتنة تحدث في المحاليل تم أيضا دراسة تأثير المذيب على عملية البرتنة باستخدام نموذج الوسط المتصل القابل للاستقطاب الشبيه بالموصل (CPCM) عند مستوى نظرية B3LYP/6-311++G(d). حيث أظهرت النتائج أن احاطة الهايميكرومون والأومبليفيرون وأشكالها المبرتنة بجزئيات المذيب (solvation) يزيد من عزم ثنائي القطب لها (dipole moments) كما يزيد من استقرارها ايضا خاصة في المذيبات القطبية البروتونية مثل الماء والإيثانول.

الكلمات المفتاحية: CPCM نموذج الوسط المتصل القابل للاستقطاب الشبيه بالموصل؛ نظرية الكثافة الالكترونية (DFT B3LYP/ 6-311++G(d))؛ هايميكرومون؛ الالفة البروتونية؛ أومبليفيرون.

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