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(4-Carbamoylphenyl)Boronic Acid: A DFT Study On The Structural And Spectral Properties

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Makalenin Alanı: Kimya

Makale Bilgileri	**Öz**
Geliş Tarihi 16.07.2021 **Kabul Tarihi** 28.12.2021 **Anahtar Kelimeler** DFT Boronik asit türevleri Moleküler yapı Tautomerik formlar	Başlangıç bileşiği; CAPBA, B3LYP düzeyinde ve 6.31G* temel setinde DFT yöntemi kullanılarak hesaplama yöntemleriyle analiz edilmiştir. Hesaplamalı analiz için SPARTAN-14 yazılımı kullanıldı. Hesaplanan sonuçlar literatürdeki deneysel değerlerle karşılaştırıldı. Bağ uzunlukları, bağ açıları, dihedral açılar ve elektronik özellikler spektroskopik bilgilere göre araştırılmış ve açıklanmıştır. Hesaplanan değerler ve deneysel sonuçların %0,1 ile %3 arasında bir hata payı ile mükemmel bir uyum içinde olduğu gözlemlenmiştir.

Article Info	**Abstract**
Received 16.07.2021 **Accepted** 28.12.2021 **Keywords** DFT Boronic acid derivatives, Molecular structure, Tautomeric forms	Title compound; CAPBA was analyzed via computational methods using the DFT method in the B3LYP level and 6.31G* basis set. The SPARTAN-14 software was used for computational analysis. The calculated results were compared to experimental values from the literature. Bond lengths, bond angles, dihedral angles and electronic properties were investigated and explicated according to spectroscopic knowledge. The calculated values and experimental results were observed to be in perfect agreement in an error margin between 0,1% and 3%.

INTRODUCTION

Boronic acid and its derivatives (BAs) are well known for their wide use in, especially medicinal chemistry. Their chemical and biological activities depend upon their additional substituents (Hall, 2006, pp. 1-99). BAs exhibit Lewis acid properties due to the lack of e^- in

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the valence shell of the Boron atom. Boron atom attracts a OH^- anion from water in aqueous solutions to fill its valence shell (Zepeda-Valesquez, 2015, pp.6-7)

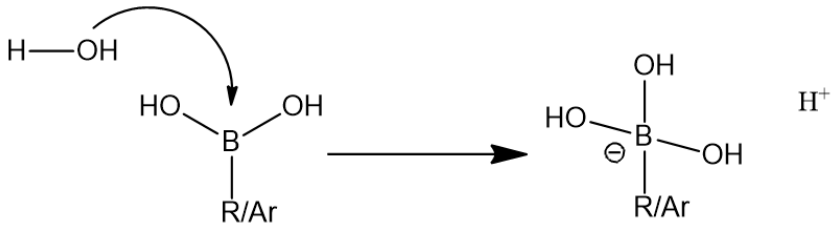

Figure 1. Acidic behavior of boronic acid in aqueous solution.

Previously, all boron-containing compounds were assumed to be poisonous, and their use was limited except for some ant poisoning chemicals. But recently, this prejudice has been broken and boron compounds have been acquitted in this regard, so their use in pharmaceutical chemistry has been paved (Baker et al., 2009). Because of their importance in chemical and medicinal studies such as Boron Neutron Capture Therapy (BNCT) (Tjarks et al.,1992) preparing medicines (Kar, 2003, pp.143-146), etc. a huge number of studies has been undergone about spectroscopic and structural properties of the organoboron compounds particularly on boronic acids and their esters. These studies generally survey the molecular structures as a dimer or monomer-dimer equilibrium Lu et al., Zheng et al., Rani et al., Karabacak et al., 2012, Zheng et al., 2011, Sachan et al., 2014, Erdoğdu et al., 2009).

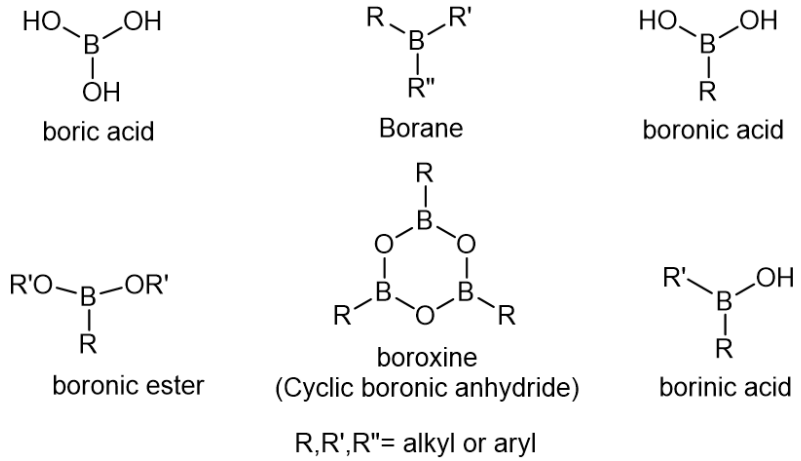

Figure 2. Oxygen-containing organoboron compounds (Hall 2006)

In some recent studies, researchers have handled their effect on the formation of biofilm, production of virulence factors (elastase and pyocyanin) and swarming motility in Pseudomonas aeruginosa (Akalın&Ulusoy, 2018).

CAPBA is a white to Brown solid with a melting point of 229-234°C (URL1). Apostolova et al. experimentally found the molecular properties of the title compound 4-Carbamoylphenylboronic acid (AKA 4-Aminocarbonylphenylboronic acid / CAPBA) in a crystallographic study (Apostolova et al., 2010). But unfortunately, there is no other experimental spectral data for this compound so far.

EXPERIMENTAL

Computational Details

In all calculations, the SPARTAN 14 computational chemistry suite (Hehre, 2014) was used. Calculations were undergone according to the DFT method in the B3LYP level and 6.31G* basis set (Becke, 1993, Hehre, 2014, Jensen, 2017, Onishi, 2018, Peter et al., 2011, Silverstein et al., 2005). The calculated and experimental results were tabulated in relational tables for comparisons. Recently, DFT method has gained a rising popularity among the researchers. Most researchers especially the ones investigating d-block metal complexes prefer to use this method with or instead of HF. (Beytur&Yuksek, 2018). Some small molecules such as boronic acid derivatives or benzoic acid derivatives are investigated using both DFT and HF and mostly In many studies, it was seen that the results of the DFT method were more compatible with the experimental results than the HF method (Kotan&Yüksek, 2019).

The DFT method has also been successfully used in the study of other small groups of molecules such as pyrazoles and their derivatives (Turhan İrak&Beytur 2019).

Molecular Structure CAPBA has a dimeric structure like other boronic acid derivatives which has been investigated in depth so far. But in these studies, CAPBA never was handled for its tautomeric forms. Due to the lack of a survey on its tautomers, in the following study, it has been handled considering its tautomeric forms and conformational isomers on the same hand. The dimeric structure was omitted for clarity (Figure 3 a and b). The group of $–B(OH)_2$ has four conformers which will be abbreviated as “CC”, “CT”, “TC” and “TT” in the following pages (C= Cis, T=Trans).

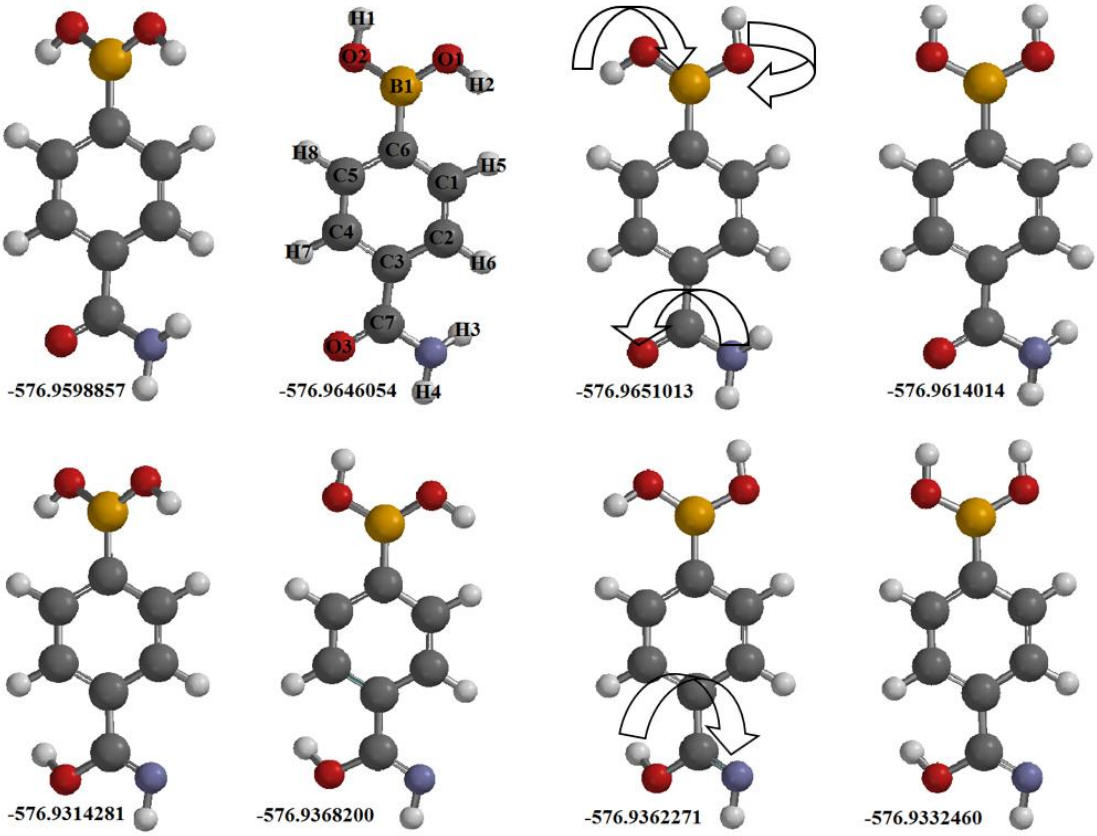

Figure 3. The isomeric forms and tautomeric transformation of the compound CAPBA (energies in Hartree)

Molecular Structure

As mentioned before, CAPBA had been investigated for its crystallographical structure via single-crystal X-ray spectroscopy (Apostolova et al., 2010). Both the experimental and the calculated bond lengths and bond angles have been tabulated in Table 1 and Table 2 respectively. Besides calculated dihedral angles have been given in Table 3 for gaining an idea about the torsion of some parts in the molecule. Unfortunately, experimental dihedral angles are not available in the literature.

As seen in Table 1, the calculated bond lengths are very close to the experimentally measured ones. Since the least energetic form of the compound is TC the error% values were calculated between the experimental values and the ones that belong to TC.

Table 1. Bond distances (Å) for the compound CAPBA

Distance (Å)	CC1	CC2	CT1	CT2	TC1	TC2	TT1	TT2	EXP*	Error%
H3,O3	3.149	0.971	3.145	0.971	3.149	0.971	3.145	0.971	xx	X
H4,O3	2.460	2.354	2.457	2.351	2.459	2.353	2.456	2.349	xx	X
O1,H2	0.966	0.966	0.966	0.966	0.970	0.970	0.967	0.967	0.820	18.29
O2,H1	0.966	0.966	0.970	0.970	0.967	0.966	0.967	0.967	0.820	17.93
H4,N1	1.012	1.024	1.012	1.024	1.012	1.024	1.012	1.024	0.860	17.67
H3,N1	1.010	3.084	1.010	3.085	1.010	3.083	1.010	3.084	0.860	17.44
N1,C7	1.376	1.271	1.378	1.272	1.376	1.271	1.378	1.272	1.298	6.01
O3,C7	1.224	1.371	1.224	1.371	1.225	1.372	1.225	1.372	1.246	-1.69
C7,C3	1.504	1.490	1.503	1.489	1.503	1.489	1.503	1.489	1.505	-0.13
C2,C1	1.394	1.390	1.393	1.390	1.393	1.390	1.393	1.390	1.384	0.65
C3,C2	1.401	1.403	1.402	1.402	1.402	1.403	1.402	1.403	1.397	0.36
C4,C3	1.401	1.402	1.401	1.403	1.400	1.402	1.401	1.403	1.388	0.86
C5,C4	1.391	1.394	1.391	1.393	1.391	1.394	1.391	1.394	1.384	0.51
C6,C5	1.407	1.404	1.407	1.405	1.406	1.404	1.407	1.404	1.391	1.08
C1,C6	1.406	1.408	1.405	1.407	1.406	1.409	1.406	1.408	1.391	1.08
B1,O1	1.368	1.367	1.374	1.374	1.367	1.366	1.375	1.374	1.351	1.18
B1,O2	1.367	1.368	1.366	1.367	1.374	1.374	1.374	1.374	1.393	-1.36
C6,B1	1.580	1.580	1.571	1.571	1.571	1.571	1.564	1.564	1.546	1.62
H6,C2	1.087	1.085	1.087	1.085	1.087	1.085	1.087	1.085	0.930	16.88
H5,C1	1.089	1.089	1.090	1.089	1.086	1.086	1.086	1.086	0.930	16.77
H7,C4	1.085	1.088	1.085	1.088	1.085	1.088	1.085	1.088	0.930	16.67
H8,C5	1.089	1.089	1.086	1.086	1.090	1.089	1.086	1.086	0.930	17.20

*Received from Ref. (Erdoğdu et al., 2009) xx=no data for this value in lit. X= not calculated.

As seen in the table, the bonds between C and C or C and Heteroatom were calculated with small deviations which are between 0.36% and 6%, from the experimental values. But the bonds between H and C or H and heteroatoms were calculated with deviations between 16% to 18%. Also, another point to notice, most values are very close to each other despite the tautomeric activity except for the H3-O3 bond which changes dramatically from one form to another due to H3 immigration between N1 to O3. As the last word for bond distances, between two tautomers for every isomer, the bond distances change slightly between 0 to 2 Å on the phenyl and $–B(OH)_2$ parts. But the differences increase to 100 Å's when the turn comes to bonds between N1, C7 and O3.

The bond angles for the compound have been tabulated in table 2. According to these values, the most mobile parts of the molecule are again the group of $-B(OH)_2$ and carbamoyl part.

Table 2. Some bond angles (°) for the compound CAPBA

Angle (°)	CC1	CC2	CT1	CT2	TC1	TC2	TT1	TT2	EXP*	err%
H3,O3,C7	22.92	109.71	23.06	109.65	22.94	109.55	23.08	109.45	xx	x
O3,C7,N1	121.86	121.85	121.78	121.75	121.77	121.80	121.61	121.67	120.80	0.80
C7,N1,H4	115.13	110.00	114.90	109.92	115.12	109.94	114.94	109.84	120.00	4.07
H3,N1,C7	120.23	19.13	119.88	19.06	120.23	19.15	119.93	19.03	120.00	0.19
H4,N1,H3	116.32	91.25	116.11	91.20	116.36	91.18	116.23	91.14	120.00	3.03
N1,C7,C3	116.24	121.26	116.16	121.34	116.26	121.40	116.19	121.56	118.80	2.14
O3,C7,C3	121.88	116.89	122.05	116.90	121.96	116.79	122.18	116.76	120.40	1.30
C7,C3,C2	123.52	119.29	123.28	119.21	123.58	119.40	123.33	119.37	122.20	1.13
C3,C2,C1	120.17	120.17	120.03	120.03	120.30	120.29	120.19	120.21	121.10	0.66
C4,C3,C2	119.06	118.91	119.11	118.91	119.08	118.93	119.15	118.96	117.80	1.09
C5,C4,C3	120.25	120.34	120.36	120.49	120.12	120.22	120.30	120.41	121.20	0.89
C6,C5,C4	121.59	121.54	121.36	121.30	121.68	121.60	121.24	121.20	120.80	0.73
C1,C6,C5	117.35	117.25	117.49	117.37	117.46	117.37	117.85	117.74	118.20	0.63
C2,C1,C6	121.57	121.78	121.63	121.88	121.35	121.58	121.26	121.47	120.80	0.46
B1,O1,H2	111.96	112.14	113.16	113.29	110.65	110.76	114.84	114.96	xx	x
B1,O2,H1	112.05	112.04	110.73	110.69	113.22	113.27	114.92	114.87	xx	x
C6,B1,O2	122.22	122.17	118.41	118.38	123.83	123.92	118.01	117.94	121.60	1.83
C6,B1,O1	122.15	122.21	123.87	123.85	118.43	118.34	117.98	117.97	119.40	0.81
C1,C6,B1	121.25	121.44	122.20	122.40	120.21	120.32	120.98	121.23	119.50	0.59
C5,C6,B1	121.40	121.30	120.31	120.23	122.32	122.31	121.16	121.03	122.20	0.10
H6,C2,C1	119.39	121.38	119.55	121.44	119.32	121.27	119.43	121.32	119.50	0.15
H5,C1,C6	119.67	119.57	120.21	120.08	119.00	118.91	119.22	119.11	119.60	0.50
C2,C1,H5	118.74	118.63	118.15	118.02	119.64	119.51	119.52	119.42	119.60	0.03
H7,C4,C5	121.45	119.15	121.32	119.02	121.52	119.20	121.39	119.09	119.40	1.78
C3,C2,H6	120.39	118.45	120.39	118.53	120.34	118.44	120.33	118.46	119.50	0.70
H8,C5,C4	118.79	118.69	119.66	119.60	118.16	118.07	119.57	119.48	xx	x
O1,B1,O2	115.63	115.62	117.73	117.77	117.73	117.74	124.02	124.09	118.90	0.98
C2,C3,C7	123.52	119.29	123.28	119.21	123.58	119.40	123.33	119.37	xx	x
C7,C3,C4	117.41	121.80	117.60	121.88	117.34	121.67	117.52	121.67	120.00	2.22
H7,C4,C3	118.30	120.46	118.32	120.44	118.37	120.53	118.31	120.45	119.40	0.86
C6,C5,H8	119.62	119.75	118.97	119.09	120.15	120.32	119.18	119.31	119.60	0.46

As seen from Table 2 the error margin is between 0.03% and 4%. An important point to be noticed from the table, there is a 5-6° difference between the tautomeric forms when it comes to carbamoyl groups such as N1, C7, C3 and O3, C7, C3 angles. But in the phenyl part and $-B(OH)_2$ group, the values only change slightly. For example for C6, B1, O2 the values are 123.83° and 123.92°, for O1, B1, O2 angle 117.73° and 117.74° between two tautomers for TC isomer.

In the literature, there is no data for the torsional properties of CAPBA, for this reason, Table 3 has no experimental values column. Since the values in Table1 and Table 2 are close to the experimental results enough, it can be considered that Table 3 is also reliable.

As seen in Table 3 torsion angles in the CAPBA molecule differs according to the sections. In the phenyl part, as expected, for example, dihedral angles are about 1-2 degrees. For instant H6, C2, C1, H5 –1.93 / 0.64° for TC isomer and C1, C2, C3, C4 has 0.78 / -0.93°. But O3, C7, C3, C2 and N1, C7, C3, C4 has 160.83° / 157.24° and –162.87° / –155.72° respectively.

Table 3. Dihedral angles for CAPBA and conformers.

Dihedral	CC1	CC2	CT1	CT2	TC1	TC2	TT1	TT2
H3,O3,N1,H4	135.70	-155.87	-134.05	-157.00	135.86	-155.61	-134.62	-157.49
H3,O3,C7,C3	-165.14	16.94	164.54	16.02	-165.26	17.05	164.79	15.61
H4,N1,C7,O3	-9.66	2.41	10.09	2.33	-9.83	2.47	10.23	2.30
H3,N1,C7,O3	-156.81	14.32	155.79	13.65	-157.05	14.49	156.36	13.42
H4,N1,C7,C3	171.67	-178.70	-171.31	-178.65	171.45	-178.57	-171.02	-178.58
H3,N1,C7,C3	24.53	-166.79	-25.61	-167.33	24.22	-166.55	-24.89	-167.46
H3,O3,C7,N1	16.27	-164.12	-16.95	-164.92	16.09	-163.94	-16.53	-165.23
H1,O2,O1,H2	-20.84	-21.27	170.00	171.95	172.16	-170.16	-0.08	0.12
H1,O2,B1,O1	173.43	173.23	-1.88	-1.49	175.90	-174.84	-0.24	-0.13
H2,O1,B1,O2	173.36	173.30	174.76	175.78	-1.46	1.82	0.15	0.26
C5,C6,B1,O1	147.07	146.74	163.07	164.96	166.06	-164.50	179.26	-179.71
C5,C6,B1,O2	-32.94	-33.22	-16.70	-14.68	-14.26	15.73	-0.82	0.24
C1,C6,B1,O1	-33.42	-32.85	-16.47	-14.50	-14.55	15.82	-0.36	0.61
C3,C2,C1,C6	-0.39	-0.06	-0.45	0.18	-0.26	0.85	-0.17	0.42
C3,C4,C5,C6	0.23	-0.43	-1.21	-0.38	0.48	0.32	-0.73	0.04
H7,C4,C5,H8	1.25	-1.37	-0.90	-2.30	1.33	-2.79	-0.57	-2.11
B1,C6,C1,C2	-179.91	-179.85	-179.96	179.62	-179.56	179.51	-179.68	-179.92
B1,C6,C1,H5	-1.62	-1.11	-0.64	-1.58	-0.05	-0.55	0.75	-0.07
B1,C6,C5,H8	-1.02	-1.67	0.57	-0.09	-1.51	0.49	0.03	-0.82
B1,C6,C5,C4	179.99	-179.91	-179.22	-179.53	179.44	179.91	-179.86	179.69
H6,C2,C1,H5	-1.08	1.04	2.33	1.11	-1.93	0.64	1.66	0.34
C1,C6,B1,O2	146.56	147.19	163.75	165.86	165.12	-163.96	179.56	-179.44
N1,C7,C3,C4	-162.43	-156.40	161.28	-157.32	-162.87	-155.72	162.34	-156.67
N1,C7,C3,C2	18.66	22.73	-19.56	22.10	17.90	23.75	-18.43	22.76
C1,C2,C3,C4	1.08	-0.68	-0.42	-0.61	0.78	-0.93	-0.80	-1.00
H1,O2,B1,C6	-6.56	-6.80	177.91	178.18	-3.78	4.94	179.85	179.92
H2,O1,B1,C6	-6.65	-6.67	-5.02	-3.86	178.23	-177.97	-179.94	-179.80
O3,C7,C3,C2	-160.00	-158.33	159.03	-158.84	-160.83	-157.24	160.31	-158.08
O3,C7,C3,C4	18.90	22.54	-20.13	21.74	18.41	23.29	-18.92	22.49

Briefly, it can be said, the molecule is almost planar in the phenyl section and twisted about 15° and 35° in the substituted parts (Figure 4).

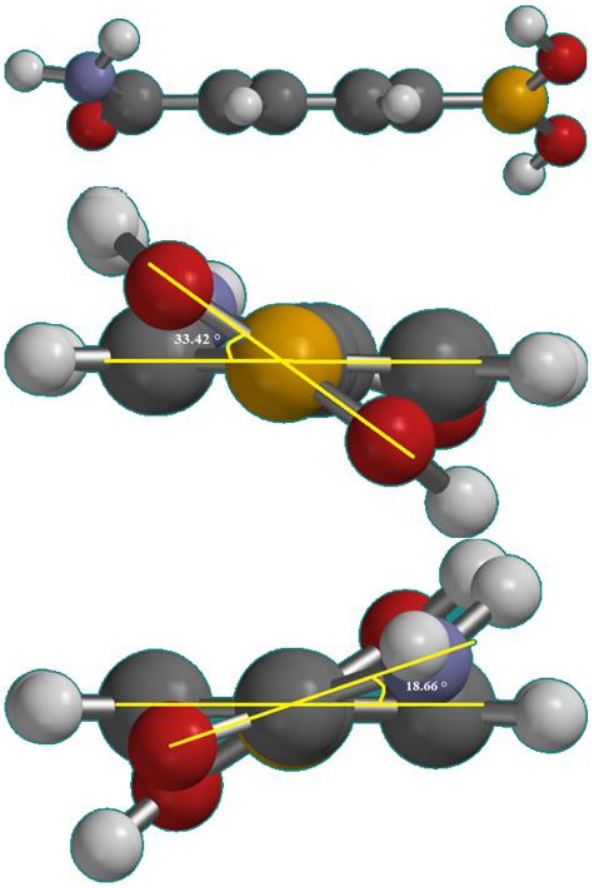

Figure 4. Deviation from planarity in parts of CAPBA

Mulliken Charges Analysis

Like every molecule, CAPBA's atoms have different electronegativities. For this reason, the electronic distribution on the molecule is not homogenous. The more an atom is electronegative, the more electrons it gathers up. This heterogeneity causes different partial charges on atoms of the same molecule. If a certain section of a molecule is electronically rich, it is a partially negative site and so on. Electron-rich parts of the molecules are more suitable for electrophilic attacks and electron-poor sites are open for nucleophilic attacks. Mulliken charge distribution is important for predicting the potential reaction mechanisms that the molecule is involved (Jensen, 2016). ESPMap surface determines the distance that a certain positive charge can interact with the molecule enough to form an attraction or repulsion so

that they can have a bonding possibility for complexation reaction. Molecular ESP (Vr) is calculated via Eq. 2 (Peter et al., 2011).

$$Vr = \sum_{A} \frac{Z_A}{R_A - r} - \int \frac{\rho(r')}{(r'-r)} dr' \qquad \text{Eq.2}$$

Figure 5 and Table 4 exhibit the Mulliken charges of CAPBA which are also depicted in figure 2 as colors. At a glance the most remarkable points are briefly:

1- C atoms of the molecule are divided into two parts; C1,2,4 and 5 are negatively charged and C3, 6 and 7 are charged positively. C7 has the highest positive charge and its charge dramatically changes between tautomeric forms.

2- All H atoms have positive charges and the most striking differences are seen on H4 and H8 according to tautomeric changes.

3- All O atoms have negative charges and according to tautomeric activity only the charge of O3 changes.

4- N atom has a considerable negative charge and as expected it changes between tautomeric forms.

5- B1, O1, O2, H1, H2 and H3 are not affected by tautomeric transformations.

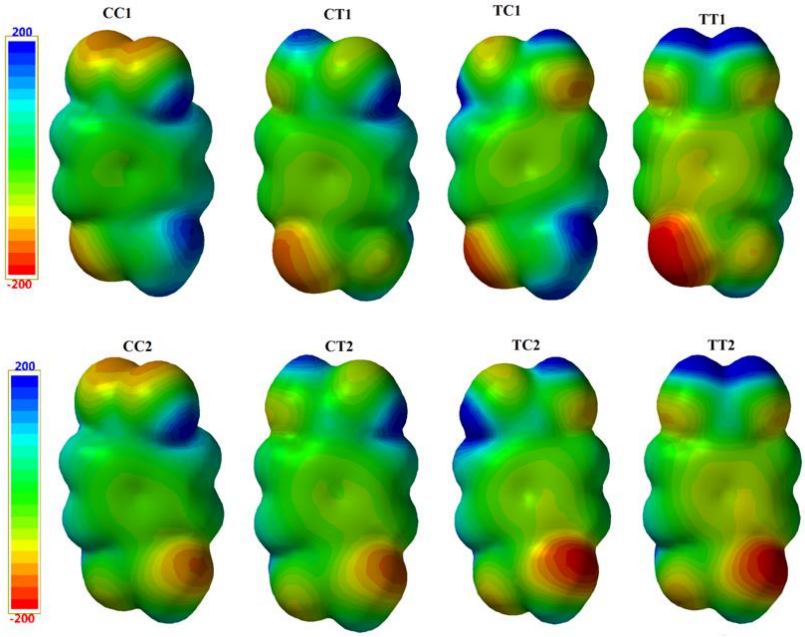

Figure 5. Mulliken Charge distribution of CAPBA according to isomeric and tautomeric forms

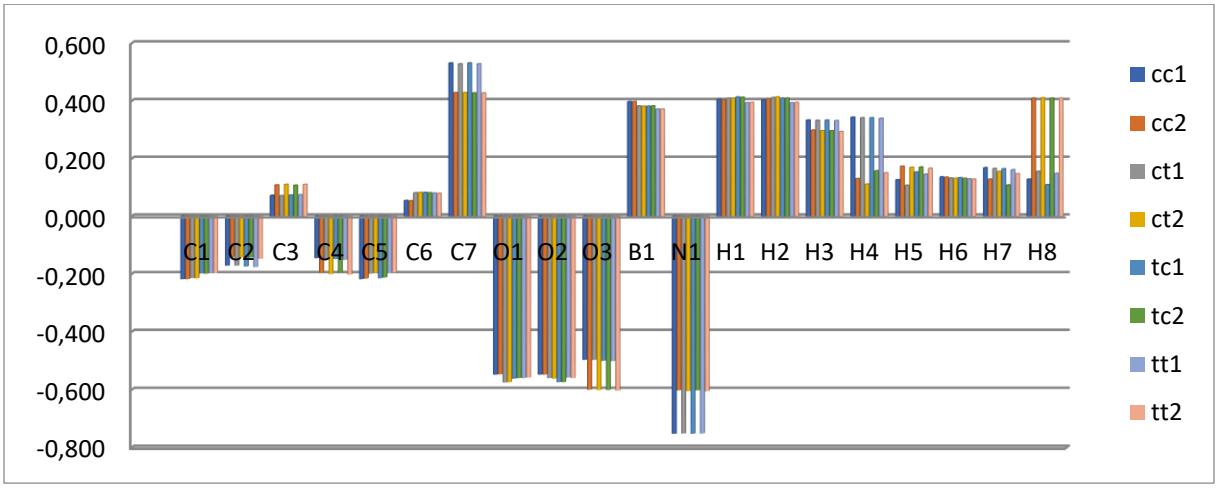

Figure 6. Mulliken Charge distribution of CAPBA

Table 4. Mulliken Charge distribution of CAPBA

Charges	CC1	CC2	CT1	CT2	TC1	TC2	TT1	TT2
C1	-0.218	-0.218	-0.214	-0.215	-0.198	-0.199	-0.196	-0.197
C2	-0.171	-0.141	-0.171	-0.143	-0.174	-0.143	-0.176	-0.147
C3	0.072	0.108	0.071	0.110	0.073	0.107	0.074	0.110
C4	-0.145	-0.196	-0.148	-0.200	-0.148	-0.196	-0.151	-0.202
C5	-0.218	-0.216	-0.199	-0.196	-0.215	-0.212	-0.197	-0.194
C6	0.054	0.053	0.081	0.082	0.082	0.081	0.080	0.079
C7	0.531	0.428	0.528	0.428	0.531	0.427	0.528	0.427
O1	-0.548	-0.547	-0.575	-0.574	-0.562	-0.560	-0.560	-0.558
O2	-0.548	-0.548	-0.560	-0.562	-0.574	-0.574	-0.558	-0.560
O3	-0.497	-0.600	-0.497	-0.601	-0.500	-0.601	-0.501	-0.603
B1	0.397	0.397	0.382	0.381	0.381	0.382	0.371	0.371
N1	-0.752	-0.602	-0.751	-0.605	-0.752	-0.602	-0.751	-0.605
H1	0.405	0.403	0.409	0.409	0.413	0.412	0.393	0.394
H2	0.403	0.406	0.411	0.413	0.409	0.409	0.393	0.394
H3	0.333	0.298	0.332	0.296	0.333	0.296	0.331	0.293
H4	0.343	0.130	0.341	0.111	0.341	0.157	0.339	0.150
H5	0.126	0.173	0.107	0.169	0.153	0.170	0.145	0.166
H6	0.136	0.135	0.132	0.131	0.133	0.131	0.129	0.128
H7	0.168	0.128	0.165	0.155	0.164	0.108	0.161	0.147
H8	0.128	0.409	0.155	0.410	0.109	0.409	0.148	0.409

Molecular Orbitals analysis (HOMO-LUMO) and UV-Vis spectra

HOMO (Highest Occupied Molecular Orbital) represents the highest energy level that at least one electron exists around the molecule. As just opposite LUMO (Lowest Unoccupied Molecular Orbital) represents the lowest energy level around the molecule in which there is no electron. The HOMO-LUMO gap is very important for charge transfers which affect the biological and chemical reactivities of the molecules. The molecules with small energy gaps

are expected to be chemically reactive and called soft molecules. HOMO LUMO levels also determine the acidity or basicity of the molecules.

In the molecule, CAPBA HOMO-LUMO gap is 5.4 eV which means this molecule can be supposed to be a “soft” molecule and of course the opposite is also true (figure 6.). The larger HOMO–LUMO gap always refers to higher kinetic stability and lower chemical reactivity. Molecule's hardness can be calculated via Eq. 3a and softness (*S*) can be calculated via Eq 3b.

$\eta = (\varepsilon_{LUMO} - \varepsilon_{HOMO})$ Eq. 3a

$S = 1/\eta$ Eq. 3b

While hard molecules which have a large gap between HOMO&LUMO do not change their electron density easily, the soft molecules with a small gap of HOMO&LUMO change their electron density relatively easily (Sahin et al., 2015, Pearson, 2005).

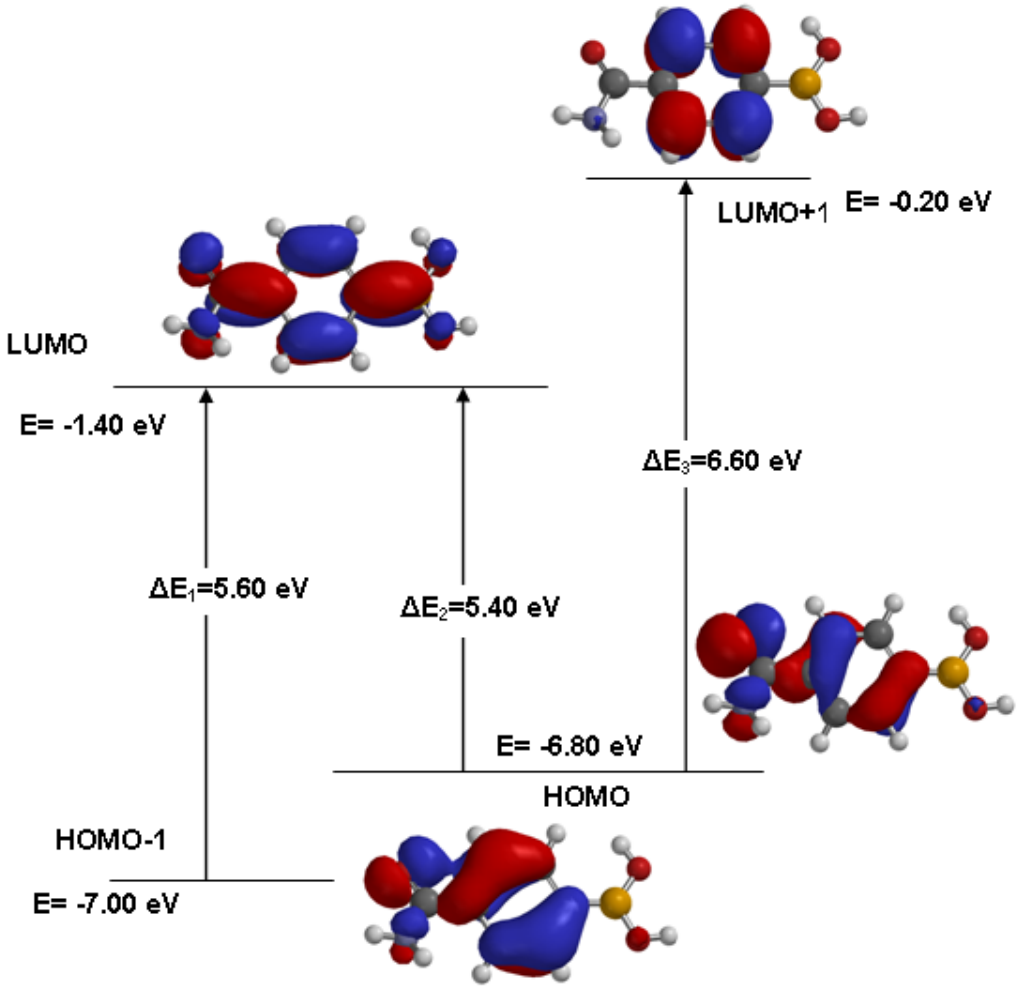

Figure 7. Electron transfers and corresponding E values and HOMO-LUMO gap (ΔE_2) for TC form of CAPBA

Table 5. The energy equivalencies for the transitions between conformers for the compound CAPBA

Conformers	Energy (Hartree)	Energy Diff. (Hartree)	Energy Diff. (kcalmol^{-1})	Energy Diff. (eV)	Eq. Freq. (cm^{-1})	Dip. Moment (Debye)
CC	-	0.0052150	3.272463	0.141907	1144.56	3.57
CT	-	0.0004960	0.311245	0.013497	108.86	4.09
TC	-	0.0000000	0.00	0.00	0.00	2.29
TT	-	0.0037000	2.321786	0.100682	812.06	5.24

Table 6. MO energies and differences with λ_{max} values (simplified) for conformers of the compound CAPBA

Conf.	HOMO-1	HOMO	LUMO	LUMO+1	ΔE (eV)			λ_{max}		
					ΔE_1	ΔE_2	ΔE_3	Calc. (Vac)		
CC	-7.3	-6.9	-1.5	-0.6	5.8	5.4	6.3	213.77	229.60	196.80
CT	-7	-6.8	-1.4	-0.3	5.6	5.4	6.5	221.40	229.60	190.74
TC	-7	-6.8	-1.4	-0.2	5.6	5.4	6.6	221.40	229.60	187.85
TT	-6.8	-6.6	-1.2	0	5.6	5.4	6.6	221.40	229.60	187.85

Table 7 Calculated Allowed electron transitions and corresponding λmax values for CAPBA

	nm	Strength	MO Comp.%			nm	Strength	MO Comp.%	
	203.46	0.0046	HOMO-4 -> LUMO	66		193.13	0.0039	HOMO-5 -> LUMO	7
			HOMO-5 -> LUMO	23				HOMO-3 -> LUMO+1	16
	203.92	0.0794	HOMO -> LUMO+1	34		214.71	0.0616	HOMO -> LUMO+1	58
			HOMO-3 -> LUMO+1	22				HOMO-1 -> LUMO+1	28
			HOMO-2 -> LUMO+1	20		220.24	0.1069	HOMO-3 -> LUMO	55
			HOMO-1 -> LUMO	14				HOMO -> LUMO+1	13
CC	206.77	0.037	HOMO-3 -> LUMO	76	**TC**			HOMO -> LUMO	12
	228.57	0.2988	HOMO -> LUMO	66		222.74	0.2627	HOMO-2 -> LUMO	41
			HOMO-2 -> LUMO	16				HOMO-3 -> LUMO	32
	239.69	0.0361	HOMO-2 -> LUMO	79				HOMO-1 -> LUMO	12
	249.07	0.0103	HOMO-1 -> LUMO	55		250.42	0.0175	HOMO-1 -> LUMO	45
			HOMO -> LUMO+1	33				HOMO-2 -> LUMO	22
								HOMO-2 -> LUMO+1	15
						284.98	0.0035	HOMO -> LUMO	70
								HOMO-1 -> LUMO	19
	192.87	0.0024	HOMO-5 -> LUMO	88		211.18	0.0292	HOMO -> LUMO+1	61
	200.45	0.081	HOMO -> LUMO+1	42				HOMO-2 -> LUMO+1	26
			HOMO-3 -> LUMO+1	24		219.6	0.0438	HOMO-3 -> LUMO	80
			HOMO-2 -> LUMO+1	15		223.93	0.4045	HOMO-2 -> LUMO	61
			HOMO-1 -> LUMO	13		252.89	0.019	HOMO-1 -> LUMO	65
	208.03	0.0564	HOMO-3 -> LUMO	82				HOMO-2 -> LUMO+1	14
CT	230.32	0.3379	HOMO -> LUMO	62	**TT**	284.51	0.0036	HOMO -> LUMO	64
			HOMO-2 -> LUMO	17				HOMO-2 -> LUMO	23
	240.37	0.0442	HOMO-2 -> LUMO	78					
	251.23	0.0214	HOMO-1 -> LUMO	55					
			HOMO -> LUMO+1	26					
			HOMO -> LUMO	13					

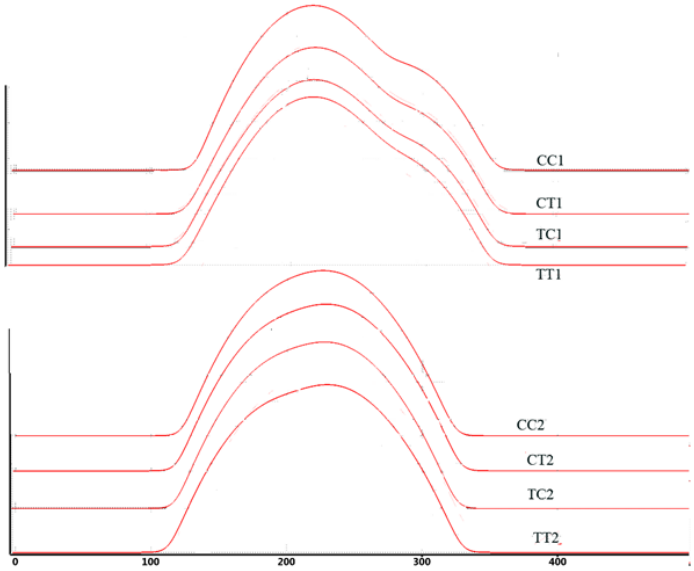

Figure 8. Calculated UV-Vis spectra for the compound CAPBA

CONCLUSIONS

In this study, the compound CAPBA was investigated for mainly its molecular structure using computational methods. Imported experimental values such as bond lengths and bond angles were compared to corresponding calculated ones (and were found to agree). Also, the molecule was surveyed for its UV-Vis spectra and HOMO&LUMO analysis beside Mulliken charge distribution. The HOMO&LUMO energy gap and UV-Vis spectra and also the hardness of the molecule were discussed. The obtained results were tabulated in corresponding sections and some results were depicted in graphs and figures. In calculations, the 6.31G* basis set was used under DFT's B3LYP level. The SPARTAN 14 quantum chemical calculation software was used in this study. The experimental and calculated results were compared in tables and verified each other.

The author declares that there is no Conflict of Interest with any person and/or institution.

Supplementary material

All requests from the readers who would like to obtain extra information such as pictures, tables, etc. will be responded with pleasure by the corresponding author.

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