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Investigation of Conformational Analysis of (m-Carbamoylphenyl) Boronic Acid Molecules by Theoretical Methods

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Abstract: In this study, the structural parameters, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), hyperpolarizability (β) and vibrational frequency of (3-Carbamoylphenyl) boronic acid were calculated at Density Functional Theory (DFT) with B3LYP (Becke 3 Parameter Lee-Yang-Parr) model using the 6-311+(2d,p) basis set in gas phase. Also, using the E_{HOMO} and E_{LUMO} energy values of the molecule, the energy gap ($Eg = E_{LUMO} - E_{HOMO}$), electronegativity (χ), chemical potential (Pi), chemical hardness (η), softness (σ), ionization energy (I), electron affinity (A), electronic chemical potential (μ), global softness (S) values were calculated according to the literature. Equilibrium state (ground state) energy gap value of the molecule were calculated as 5.59 eV. The dipole moment value of the molecule was calculated as 3.41 Debye by the DFT/B3LYP/6-311+G(2d,p) method. The obtained vibrational wave numbers were scaled with appropriate scale factors and the assigning of these vibrational wavenumbers was made according to the potential energy distribution (PED) using the VEDA 4f program. The approximate geometry of the molecules in three dimensions was drawn in the Gauss View 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Keywords: (3-Carbamoylphenyl) boronic acid molecule, Vibration analysis, Hyperpolarizability, Conformational analysis.

Introduction

Heterocyclic molecules are common in nature and are used in many fields. When molecular structures, physical, theoretical, chemical and biological properties are well learned, it is possible to design molecules with desired properties (Bahçeci et al., 2016; Kardaş et al., 2016; Aktaş Yokuş et al., 2017; Bahçeci et al., 2017; Çiftçi et al., 2018; Beytur et al., 2019a; Beytur et al., 2019b; Beytur, 2020; Koç et al., 2020; Boy et al, 2021; Irak and Beytur, 2019; Kotan et al., 2020; Uğurlu, 2020; Uğurlu and Beytur, 2020; Beytur and Avinca, 2021)Boronic acids are important building blocks for organic synthesis (Miyaura et al., 1995), materials engineering, as well as supramolecular and medicinal chemistry (Soloway et al., 1998). Also, they are used as ligand in complex compounds and these ligands are utilized in organic synthesis and catalysis, as well as in biological, pharmaceutical, industrial. Boronic acid-containing compounds are very important in branch of chemistry such as organic (Quach et al., 2003; Takezawa et al., 2002), materials (Akeroy et al., 2005; Pedireddi et al., 2004), bioorganic (Jabbour et al., 2012; Zhu et al., 2006), medicinal (Baker et al., 2006; Jin et al., 2010) and chemical biology (Dickinson et al., 2008; Halo et al., 2009). Also, due to ability baryonic acid to form hydrogen bonding in the molecular complexes and coordination in metal complexes, these compounds continue to be of increasing interest and research. The several studies have been carried out experimentally and computationally on the substituted penylboronic acid derivatives (Uğurlu et al., 2020; Uğurlu; 2019; Uğurlu; 2020). In this study, (3-Carbamoylphenyl)boronic acid molecule, having the B(OH)2 and CONH2 groups is modeled theoretical and

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molecular properties such as structural and electronic properties have been investigated using Hartree-Fock (HF) and Density Functional Theory (DFT) with B3LYP (Becke 3 Parameter Lee-Yang-Parr) model using the 6-311+(2d,p) basis set in gas phase. The potential energy surface and curve of studied compound have been carried out by calculating 2D and 3D conformation analysis. Also, using HOMO-LUMO energies, energy gap values, ionization energy, electron affinity, chemical potential, electronegativity, hardness and softness indices were obtained. The molecular structure using numbering scheme of (3-Carbamoylphenyl)boronic acid is given in Figure 1.

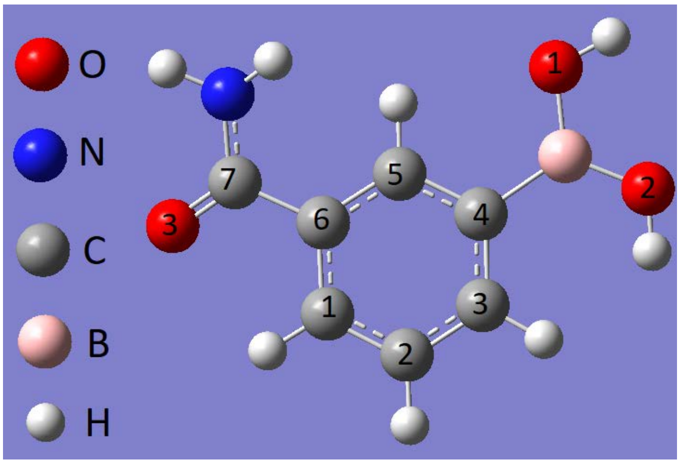

Figure 1. Molecular structure of (3-Carbamoylphenyl)boronic acid molecule numbering scheme

Methods

Quantum chemical calculations on the (3-Carbamoylphenyl) boronic acid molecule was performed by the aid of Gaussian 09W program package and Gauss view 5.0 molecular visualization programs (Frisch et al., 2010; Dennington et al., 2009) in the gas phase. The potential energy surface (PES) have been calculated as a fuction of two dihedral angles, C4-B-O2-H and C4-B-O1-H, varied between 0 and 360° with increments of 30° at B3LYP/6-31+G(d) level of theory and potential energy curve (PEC) have been calculated as a fuction of dihedral angle C3-C4-B-O2 varied from 0 to 360° with increments of 10° both HF/6-311+G (2d,p) and B3LYP/6-311+G(2d,p)level of theory. Also, structural parameters, vibrational frequency, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α) and hyperpolarizability (β) of stuied molecule were calculated at Hartree-Fock (HF) and Density Functional Theory (DFT) with B3LYP (Becke 3 Parameter Lee-Yang-Parr) (Becke et al., 1988;Lee et al., 1988; Becke, 1993) model using the 6-31++(2d,p) basis set in gas phase. The obtained vibrational wave numbers were scaled with appropriate scale factors and the assigning of these vibrational wavenumbers was made according to the potential energy distribution (PED) using the VEDA 4f program (Jamróz., 2004). The approximate geometry of the molecules in three dimensions was drawn in the Gauss View 5.0 molecular imaging program, and all theoretical calculations were used with the Gaussian 09W package program.

Results and Discussion

Conformational Analysis and Torsional Barriers

The dihedral angles was defined as: C4-B-O2-H, C4-B-O1-H and C3-C4-B-O2. The dihedral angles are the B-O2, B-O1 and C4-B single bonds about which internal rotation forms clearly different conformations, respectively. Conformation analysis of title molecule have been carried out by calculated two (2D) and three dimensional (3D) potential energies of stuied molecule. The potential energy surface (PES) have been calculated as a fuction of two dihedral angles, C4-B-O2-H and C4-B-O1-H, varied between 0 and 360° with increments of 30° at B3LYP/6-31+G(d) level of theory and potential energy curve (PEC) have been calculated as a fuction of dihedral angle C3-C4-B-O2 varied from 0 to 360° with increments of 10° both HF/6-311+G (2d,p) and B3LYP/6-311+G(2d,p) level of theory. The potential energy surface calculated at B3LYP/6-31+G(d) level of theory is given figure 2. The potential energy curves (PEC) calculated both HF/6-311+G (2d,p) and B3LYP/6-311+G(2d,p) level of theory are given figure 3. The conformers corresponding to minimum energy on the PES have been optimized and the most stable conformer have been determined. The minimum of potential energy curves (PEC) was referred to as zero. As seen in figure 2, maxima energy conformer was seen at 0º dihedral angle at HF/6-311+G (2d,p) and B3LYP/6-311+G (2d,p) level of theory. The relative energy value at dihedral angle of 180º calculated HF/6-311+G (2d,p) is bigger than that of B3LYP/6-311+G (2d,p) and the relative energy value of orthogonal conformations are maxsima.

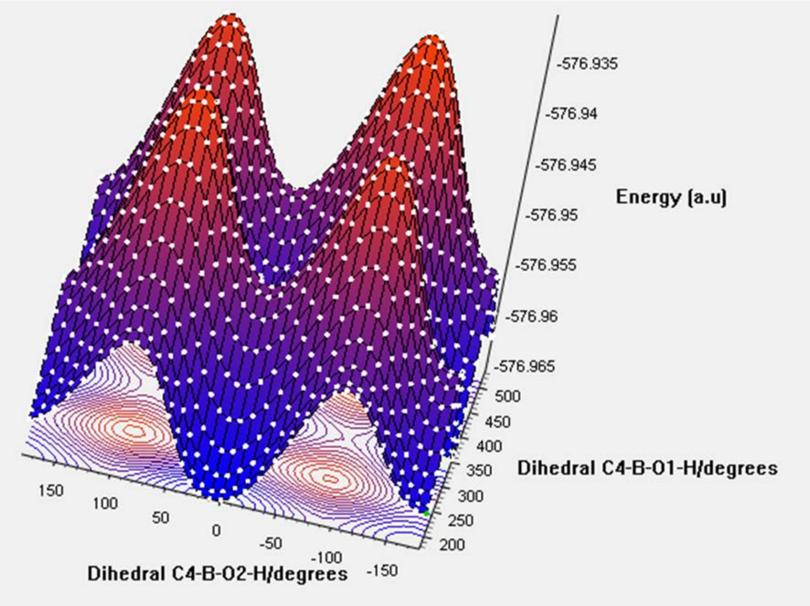

Figure 2. The potential energy surface of (3-Carbamoylphenyl) boronic acid molecule

From our previous work, conformation analysis of 4-(Methoxycarbonyl) phenylboronic acid and conformational analysis of 3-phenylthiophene and its fluoro derivatives, maximum potential energy barrier were shown at the orthogonal konformation (Uğurlu et al., 2007; Uğurlu et al., 2020).

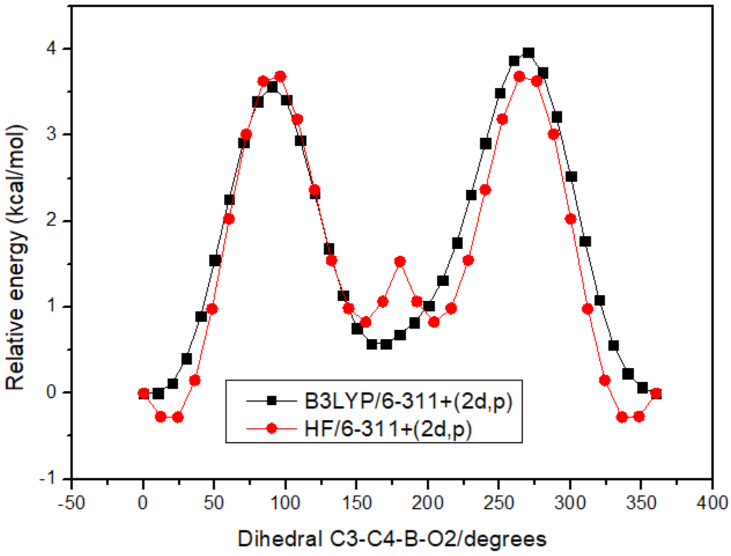

Figure 3. The potential energy curves of (3-Carbamoylphenyl)boronic acid molecule

Molecular Structure

Since the (3-Carbamoylphenyl)boronic acid was modeled theoretically for the first time, there are no molecular and crystal structures in the literature. After the conformational analysis, geometric optimization of the title molecule was performed by both methods mentioned above. Afterward, values of the electronic, dipole moment, polarizability, hyperpolarizability, HOMO, LUMO energy and energy gap (Eg) at the ground-state equilibrium geometry of studied molecules are calculated and listed in Table 1. The calculated parameter of studied molecule of both at the B3LYP/6-311+G (2d, p) and the HF/6-311+ G (2d,p) methods in the ground state are tabulated in the Table 2. The dipole moment value of the molecule was calculated as 3.41 Debye by the B3LYP/6-311+G(2d,p) method and as 3.41 Debye by the HF/6-311+G(2d,p) method, respectively and energy gap of the molecule was calculated as 5.59 eV by the B3LYP/6-311+G(2d,p) method and as 10.69 e energy gap by the HF/6-311+G(2d,p) method, respectively.

Table 1. The electronic, HOMO, LUMO energy, dipole moment, polarizability, hyperpolarizability, and energy gap (Eg) of (3-Carbamoylphenyl)boronic acid

B3LYP/6-311+G(2d. p)						
Electronic Energy (a.u)	μ (D)	α (a.u)	β(a.u)	E_{HOMO} (a.u)	E_{LUMO} (a.u)	Eg
-577.170457207	3.41	115,11	88,28	-0,264757	-0,059189	5,59
HF/6-311+G(2d. p)						
Electronic Energy (a.u)	μ (D)	α (a.u)	β(a.u)	E_{HOMO} (a.u)	E_{LUMO} (a.u)	ΔE
-577.170457207	3.41	103,25	64,81	-0,351156	0,0416	10,69

Table 2. Selected structural parameters of 3-Carbamoylphenyl boronic acid

	Bond length (Å)		
Atoms	Exp[a]	B3LYP/6-311+G(2d,p)	HF/6-311+G(2d,p)
C1-C2	1.397(8)	1,3873	1,3781
C1-C6	1.388(8)	1,3967	1,3877
C2-C3	1.384(8)	1,3910	1,3833
C3-C4	1.391(8)	1,3998	1,3889
C4-C5	1.391(8)	1,4012	1,3929
C4-B	1.546(6)	1,5674	1,5745
C5-C6	1.384(8)	1,3940	1,3831
C7-N	1.298(7)	1,3680	1,3587
C7-O3	1.246(7)	1,2202	1,1946
B-O1	1.351(8)	1,3663	1,3525
B-O2	1.393(8)	1,3705	1,3568
	Bond angle (°)		
C2-C1-C6	117.8(5)	120.19	120.14
C1-C2-C3	121.1((5)	119.91	119.79
C2-C3-C4	120.8(5)	121.39	121.50
C3-C4-C5	118.2(5)	117.61	117.59
C3-C4-B	119.5(8)	122.70	122.90
C5-C4-B	122.2(8)	119.69	119.50
C4-C5-C6	120.8(5)	121.72	121.63
C1-C6-C5	121.2(6)	119.17	119.34
C5-C7-N	--	116.80	117.02
C5-C7-O3	--	121.66	121.36
N-C7-O3	120.8(16)	121.54	121.61
C4-B-O1	119.4(13)	118.29	118.29
C4-B-O2	121.6(12)	124.41	124.26
O1-B-O2	118.9(15)	117.31	117.45
	Dihedral angle (°)		
C2-C3-C4-B	--	-179.29	-179.36
H3-C3-C4-B	--	0.79	0.79
B-C4-C5-C6	--	179.61	179.49
B-C4-C5-H4	--	1.39	1.13
C3-C4-B-O1	--	-175.21	-173.72
C3-C4-B-O2	--	4.74	6.28
C5-C4-B-O1	--	4.90	6.32
C5-C4-B-O2	--	-175.15	-173.68
H4-C5-C6-C7	--	-1.52	-1.06
C5-C6-C7-N	--	-15.54	-18.30
C5-C6-C7-O3	--	163.49	160.67
C4-B-O1-H7	--	-179.18	-178.98
C4-B-O2-H8	--	1.71	2.53

(a) taken from (Apostolova et al. 2010)

Since there are no the structural parameter (bond length, bond and dihedral angle) of studied molecule, the table 2 compares with those obtained experimental data of similar molecule (Apostolova et al., 2010)

The C4-B bond length have been calculated as 1.5674 Å (B3LYP/6-311+G(2d,p), 1,5745 Å (HF/6-311+G(2d,p). This value determined as 1.546(6) Å. The $B(OH)_2$ and $CONH_2$ functional groups are twisted out of the plane of the benzene ring by 4.90° and -15.54° (B3LYP) and 6.32° and -18.30°, respectively. These values determined experimenally as 23.9° (5) and 24.6° (6), respectively. The studied molecule olmost is planar. The electron affinity (A), global hardness (η)/softness (S), electronegativity (χ), chemical potential (μ), ionization potential (I), chemical potential (Pi) calculated by using HOMO-LUMO energies calculated the B3LYP/6-311+G (2d, p) for the compound were given in Table 3.

Table 3. Electronic properties of 3-Carbamoylphenyl)boronic acid molecule

		Hatree	**eV**	**kcal/mol**	**KJ/mol**
	LUMO	-0,059189	-1,61057	-37,1413	-155,401
	HOMO	-0,264757	-7,20422	-166,136	-695,12
A	elektron ilgisi	0,059189	1,61057	37,1413	155,401
I	İyonlaşma potansiyeli	0,264757	7,20422	166,136	695,12
ΔE	energy gap	0,205568	5,59365	128,995	539,719
χ	electronegativity	0,161973	4,4074	101,639	425,26
Pi	chemical potential	-0,161973	-4,4074	-101,639	-425,26
ω	electrophilic index	0,001348282	0,03669	0,84605	3,53991
IP	Nucleophilic index	-0,01664823	-0,45301	-10,4468	-43,7099
S	molecular softness	0,0514	1,39841	32,2486	134,93
η	molecular hardness	0,102784	2,79682	64,4973	269,859

The HOMO, LUMO and the MEP plots of 3-Carbamoylphenyl)boronic acid molecule are shown in Figure 4. As seen in the figure.4, the frontier molecular orbital HOMO of all the studied molecule have exhibited similar behavior at the both methods.

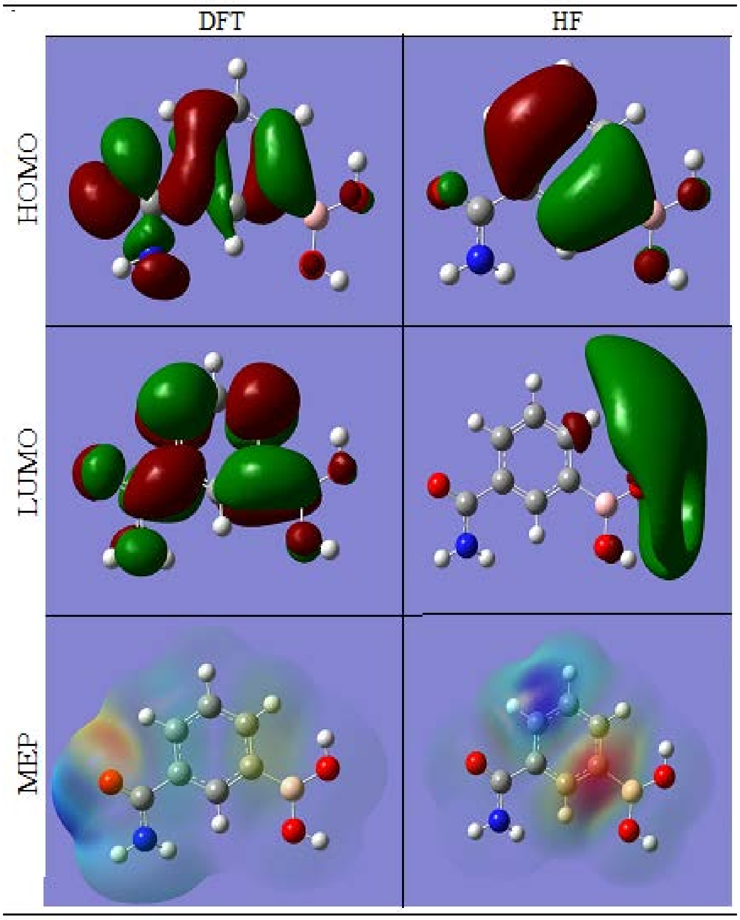

Figure 4. MEP and HOMO-LUMO surface of (3-Carbamoylphenyl) boronic acid

Table 4. Theoretical wavenumbers of (3-Carbamoylphenyl) boronic acid

B3LYP		HF		
Unsc.	Sc.	Unsc.	Sc.	Assignments with PED (≥10 %)
3880	3717	4222	3800	νO1H7(52) νO2H8(48)
3840	3679	4172	3755	νO1H7(48) νO2H8(52)
3711	3556	3939	3545	νNHb(99)
3586	3436	3813	3431	νNHa(99)
3201	3066	3369	3032	νC1H1(35) νC2H2(10) νC3H3(12) νC5H4(42)
3181	3047	3356	3020	νC1H1(21) νC2H2(13) νC3H3(34) νC5H4(32)
3176	3043	3337	3003	νC1H1(10) νC2H2(62) νC3H3(17) νC5H4(11)
3134	3003	3301	2971	νC1H1(33) νC2H2(14) νC3H3(37) νC5H4(15)
1733	1661	1917	1725	νO3C7(76)
1637	1568	1788	1609	νC3C2(39) γH3C3C4(16) γC5C6C1(11)
1619	1551	1773	1595	γHaNHb(70)
1618	1550	1762	1586	νC1C6(24)νC2C1(10)νC4C3(23)γH1C1C2(10)γH2C2C3(10)
1521	1457	1644	1480	νC3C2(18) γH1C1C2(20) γH2C2C3(20) γH4C5C6(13)
1446	1385	1556	1401	νO1B(12) γH1C1C2(17) γC5C6C1(21)
1397	1338	1489	1340	νO1B(34) νO2B(13) νC4B(12)
1377	1319	1473	1325	νC2C1(11) νO1B(27)
1356	1299	1457	1311	νC2C1(10) γH4C5C6(65)
1343	1286	1440	1296	νNC7(17) νO2B(10) γH2C2C3(11)
1303	1248	1317	1185	νC2C1(30) νC4C3(27) γH4C5C6(10)
1204	1153	1251	1126	νC3C2(10) γH3C3C4(62)
1159	1110	1242	1118	νC5C6(12) γC4C3C2(14)
1136	1088	1197	1077	γHbNC7(13) γH2C2C3(28) γC5C6C1(15)
1107	1060	1188	1069	νC1C6(38) γH1C1C2(24)
1082	1036	1171	1054	νNC7(29) γHbNC7(44)
1026	983	1115	1004	νO2B(14) γH8O2B(69)
1019	977	1106	995	νC5C6(43) γC4C3C2(50)
1005	963	1086	978	βH2C2C1C6(57) βH3C3C4C5(22)
990	949	1066	960	νO2B(24) γH7O1B(45) γH8O2B(21)
953	913	1056	950	βH2C2C1C6(26) βH3C3C4C5(40)
940	901	1050	945	βH4C5C6C7(71) βC5C6C1C2(12)
837	802	892	803	νO2B(10) νC7C6(17) νC4B(11) γC3C2C1(22)
831	797	771	694	βH1C1C6C5(25) βH3C3C4C5(19) βC5C6C1C2(14) βO3NC6C7(13) βC7C5C1C6(10)
766	734	754	679	βO3NC6C7(53)
713	683	722	650	βH1C1C6C5(43) βC5C6C1C2(20)
706	677	680	612	γC2C1C6(25) γC4C3C2(13)
668	640	603	543	βC5C6C1C2(21) βO2C4O1B(51)
629	603	576	518	γO3C7N(46) γC3C2C1(14)
577	553	573	516	βH7O1BC4(59) βHaNC7C6(12)
547	524	554	498	βH7O1BC4(11) βHaNC7C6(61)
537	514	491	442	γC2C1C6(20) γO2BO1(38)
515	493	461	415	γNC7C6(26) γC7C6C1(10)
479	459	456	410	βH7O1BC4(12) βH8O2BC4(80)
430	412	444	399	γO1BC4(26) γBC4C5(10)
419	402	401	361	γNC7C6(13) γO1BC4(10) βC4C3C2C1(26)
409	392	394	355	γNC7C6(10) βC3C2C1C6(53)
370	355	331	298	νC7C6(21) γO3C7N(14) γC3C2C1(18)
321	308	253	227	βHbNC7C6(83)
310	297	183	164	νC4B(22) γC2C1C6(14) γO1BO1(32)
234	225	139	125	NC7C6(16) O1BC4(20) C7C6C1(34) BC4C5(13)
166	159	126	114	βC4C3C2C1(31) βBC3C5C4(19) βC7C5C1C6(23)
128	123	69	62	βBC3C5C4(37) βC7C5C1C6(17)

116	112	53	48	βO1BC4(12) γC7C6C1(23) γBC4C5(41)
45	43	30	27	βNC7C6C5(89)
27	26	0	0	βO1BC4C3(92)
				ν; stretching, τ; in plane bending, β; out of plane bending,

Vibrational Frequencies

The (3-Carbamoylphenyl) boronic acidm olecule consist of 20 atoms having 54 normal modes of vibrations. The calculated vibrational wavenumbers, FT-IR and FT-Raman intensity of the title compounds are given in Table 4. The obtained vibrational wave numbers were scaled with appropriate scale factors.

Conclusions

In this work, the structural parameters, the electronic energy, the dipole moment (μ), the highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy, the polarizability (α), hyperpolarizability (β) and vibrational frequency of (3-Carbamoylphenyl) boronic acid were calculated at DFT/ B3LYP/v an HF6-311+(2d,p) level of theory in gas phase. The dipole moment value of the molecule was calculated as 3.41 Debye by the B3LYP/6-311++G(2d,p) method and as 3.41 Debye by the HF/6-311++G(2d,p) method, respectively and energy gap of the molecule was calculated as 5.59 eV by the B3LYP/6-311++G(2d,2p) method and as 10.69 e energy gap by the HF/6-311++G(2d,2p) method, respectively. C4-B bond length have been calculated as 1.5674 Å (B3LYP/6-311+G(2d,p), 1,5745 Å (HF/6-311+G(2d,p). This value determined as 1.546(6) Å. The $B(OH)_2$ and $CONH_2$ functional groups are twisted out of the plane of the benzene ring by 4.90° and -15.54° (B3LYP) and 6.32° and -18.30°, respectively. These values determined as 23.9° (5) and 24.6° (6), respectively. It was seen that there was a good agreement between the calculated values of the structural parameters and the experimental values.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM journal belongs to the authors.

Acknowledgements or Notes

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References

Akeroy, C.B. & Salmon, D.J. (2005). Building co-crystals with molecular sense and supramolecular sensibility. *CrystEngComm journal*, *7,* 439-448.

Aktaş-Yokuş, Ö., Yüksek, H. Manap, S. Aytemiz, F. Alkan, M. Beytur, M. & Gürsoy-Kol, Ö. (2017). In-vitro biological activity of some new 1, 2, 4-triazole derivatives with their potentiometric titrations, *Bulgarian Chemical Communications*, *49,* 98-106.

Apostolova, M. D., Nikolovab, R. P. & Shivachevb, B. L. (2010). (4-Carbamoylphenyl)boronic acid. *Acta Crystallographica Section A, 66,* 1273.

Bahçeci, Ş., Yıldırım, N., Gürsoy-Kol, Ö. Manap, S. Beytur, M. & Yüksek, H. (2016). Synthesis, characterization and antioxidant properties of new 3-alkyl (aryl)-4-(3-hydroxy-4-methoxybenzylidenamino)-4,5-dihydro-1h-1,2,4-triazol-5-ones. *Rasayan Journal of Chemistry*. *9,* 494-501.

Bahçeci, Ş. Yıldırım, N. Alkan, M. Gürsoy-Kol Ö., Manap, S., Beytur, M. & Yüksek, H. (2017). Investigation of antioxidant, biological and acidic properties of new 3-alkyl(aryl)-4-(3-acetoxy-4-methoxybenzylidenamino)-4,5-dihydro-1h-1,2,4-triazol-5-ones, *The Pharmaceutical and Chemical Journal*. *4* (4), 91-101.

Baker, S.J., Akama, T., Zhang, Y.K., Sauro, V., Pandit, C., Singh, R., Kully, M., Khan, J., Plattner, J.J., Benkovic, S.J., Lee, V. & Maples, K.R. (2006). Identification of a novel boron-containing antibacterial agent (AN0128) with anti-inflammatory activity, for the potential treatment of cutaneous diseases. *Bioorganic & Medicinal Chemistry Letters, 16*, 5963-5967.

Becke, A. D. (1988). Density-functional exchange-energy approximation with correct asymptotic behavior. *Physical Review A, 38*(6), 3098–3100.

Becke, A. D. (1993). Density-functional thermochemistry .3. The role of exact exchange. *The Journal of Chemical Physics, 98*(7), 5648-5652.

Beytur, M. (2020). Fabrication of platinum nanoparticle/boron nitride quantum dots/6-methyl-2-(3-hydroxy-4-methoxybenzylidenamino)-benzothiazole (Ils) nanocomposite for electrocatalytic oxidation of methanol. *Journal of the Chilean Chemical Society, 65*, 4929-4933.

Beytur, M. & Avinca, I. (2021). Molecular, electronic, nonlinear optical and spectroscopic analysis of heterocyclic 3-substituted-4-(3-methyl-2-thienylmethyleneamino)-4,5-dihydro-1h-1, 2, 4-triazol-5-ones: experiment and DFT calculations. *Heterocyclic Communications, 27*, 1-16.

Beytur, M., Manap, S., Özdemir, G., Gürsoy-Kol, Ö., Aytemiz, F., Alkan, M. & Yüksek, H. (2019). Preparation of some new bis-[4-(3-alkyl/aryl-4, 5-dihydro-1h-1, 2, 4-triazol-5-on-4-yl)-azomethinphenyl] phtalate derivatives with their antioxidant and antimicrobial activities. *Research Journal of Pharmaceutical Biological and Chemical Sciences, 10*(1), 426-436.

Beytur, M. Irak Z. T., Manap, S. & H. Yüksek, (2019). Synthesis, characterization and theoretical determination of corrosion inhibitor activities of some new 4,5-dihydro-1*H*-1,2,4-Triazol-5-one derivatives. *Heliyon*, 5, e01809.

Boy, S., Aras, A., Türkan, F., Akyıldırım, O., Beytur, M., Sedef Karaman, H., Manap, S., & Yüksek, H. (2021). Synthesis, spectroscopic analysis, and in vitro/in silico biological studies of novel piperidine derivatives heterocyclic schiff-mannich base compounds. *Chemistry & Biodiversity, 18*(12), e2100433.

Çiftçi, E., Beytur, M. Calapoğlu, M., Gürsoy-Kol, Ö., Alkan, M. Toğay, V. A., Manap, S. & Yüksek. (2017). Synthesis, characterization, antioxidant and antimicrobial activities and DNA damage of some novel 2-[3-alkyl (aryl)-4,5-dihydro-1h-1,2,4-triazol-5-one-4-yl]-phenoxyacetic acids in human lymphocytes. *Research Journal of Pharmaceutical, Biological and Chemical Sciences, 9* (5), 1760-1771.

Dennington, R., Keith T., Millam, J. (2009). *Semichem Inc., GaussView*, Version 5, Shawnee Mission KS.

Dickinson, B.C. & Chang, C.J. (2008). A targetable fluorescent probe for ımaging hydrogen peroxide in the mitochondria of living cells. *Journal of the American Chemical Society, 130*, 9638-9639.

Gürsoy-Kol, Ö., Manap, S., Ozdemir, G., Beytur, M., Agdaş, E., Azap, F., Yuca, S., Alkan, M. & Yüksek, H. (2020). Synthesis, antioxidant and antimicrobial activities of novel 4-(2-cinnamoyloxybenzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives, *Heterocyclic Letters, 10*(4), 575-587.

Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Robb M A, Cheeseman J R, Scalmani G, Barone V, Mennucci B, Petersson G A, Nakatsuji H, Caricato M, Li X, Hratchian H P, Izmaylov A F, Bloino J, Zheng G, Sonnenberg J L, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida,M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Montgomery J A, Vreven T J, Peralta J E, Ogliaro F, Bearpark M, Heyd J. J, Brothers E, Kudin N, Staroverov V N, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant J C, Iyengar S S, Tomasi J, Cossi M, Rega N, Millam J M, Klene,M, Knox J E, Cross J B, Bakken V, Adamo C, Jaramillo J, Gomperts R, Stratmann R E, Yazyev O, Austin A J, Cammi R, Pomelli C J, Ochterski W, Martin L R, Morokuma K, Zakrzewski V G, Voth G A, Salvador P, Dannenberg J J, Dapprich S, Daniels A D, Farkas O, Foresman J B, Ortiz J V, Cioslowski J, Fox D J. (2009). *Gaussian Inc.*, (Wallingford, CT).

Halo, T.L., Appelbaum, J. ,Hobert, E.M., Balkin, D.M. & Schepartz, A. (2009). Selective recognition of protein tetraserine motifs with a cell-permeable, pro-fluorescent bis-boronic acid. *J. Am. Chem. Soc. 131*, 438-439.

Jabbour, A., Steinberg, D. ,Dembitsky, V.M., Moussaieff, A., Zaks, B. & Srebnik, M. (2004). Synthesis and evaluation of oxazaborolidines for antibacterial activity against streptococcus mutans. *Journal of Medicinal Chemistry, 47*, 2409-2410.

Jamróz, M. H. (2004). *Vibrational energy distribution analysis: VEDA 4 program*, Warsaw.

Jin, S., Cheng, Y.F. Reid, S.; Li, M.Y. & Wang, B.H. (2010). Carbohydrate recognition by boronolectins, small molecules, and lectins. *Medicinal Research Reviews, 30*, 171-257.

Kardas, F., Manap, S., Gürsoy-Kol, Ö., Beytur, M., & Yüksek, H. (2016). Synthesis and antioxidant properties of some 3-alkyl(aryl)-4-[3-ethoxy-2-(4-toluenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-ones. *Der Pharma Chemica. 8*, 274–281.

Koç, E. Yüksek, H. Beytur, M. Akyıldırım, O. Akçay, M. & Beytur, C. (2020). Heterosiklik 4, 5-dihidro-1H-1, 2, 4-triazol-5-on türevinin antioksidan özelliğinin erkek ratlarda (wistar albino) in vivo olarak belirlenmesi. *Bitlis Eren Üniversitesi Fen Bilimleri Dergisi, 9*, 542-548.

Kotan, G., Gökce, H., Akyıldırım, O., Yüksek, H., Beytur, M., Manap, S., & Medetalibeyoğlu, H. (2020). Synthesis, spectroscopic and computational analysis of 2-[(2-Sulfanyl-1H-benzo[d]imidazol-5-yl)iminomethyl]phenyl Naphthalene-2-sulfonate. *Russian Journal of Organic Chemistry*, *56*(11), 1982–1994.

Lee, C. T., Yang, W. T. & Parr, R. G. (1988). Development of the colle-salvetti correlation-energy formula into a functional of the electron density, *Physical Review B*, *37*, 785-789.

Miyaure, N. & Suzuki, A. (1995). Palladium-catalyzed cross-coupling reactions of organoboron compounds. *Chemical Reviews*, *95*, 7, 2457-2483.

Pedireddi, V.R. & Seethalekshmi, N. (2004). Boronic acids in the design and synthesis of supramolecular assemblies. *Tetrahedron Letters*, *45*, 1903-1906.

Quach, T.D. & Batey, R.A. (2003). Ligand- and base-free copper(ıı)-catalyzed c-n bond formation: cross-coupling reactions of organoboron compounds with aliphatic amines and anilines. *Organic Letters*, *5*, 4397-4400.

Soloway, A. H., Tjarks, W., Barnum, B. A., Rong, F.G., Barth, R. F., Codogni, I. M. & Wilson J. G. (1998). The chemistry of neutron capture therapy. *Chemical Reviews*, *98*(4), 1515-1562.

Takezawa, A., Yamaguchi, K., Ohmura, T., Yamamoto, Y. & Miyaura, N. (2002). Inter- and intramolecular additions of 1-alkenylboronic acids or esters to aldehydes and ketones catalyzed by rhodium(ı) complexes in basic, aqueous solutions. *Synlett*, *18*, 1733-1735.

Turhan Irak Z., & Beytur, M. (2019). 4-benzilidenamino-4, 5-dihidro-1h-1, 2, 4-triazol-5-on türevlerinin antioksidan aktivitelerinin teorik olarak incelenmesi. *Journal of the Institute of Science and Technology*, *9*(1), 512-521.

Uğurlu G., & Beytur, M. (2020). Theoretical studies on the structural, vibrational, conformational analysis and nonlinear optic (NLO) property of 4-(methoxycarbonyl) phenylboronic acid. *Indian Journal of Chemistry-Section A*, *59*(10), 1504-1512.

Ugurlu, G., Kasap, E., Kantarci, Z. & Bahat M. (2007). A theoretical study of the linear, nonlinear optical properties and conformational analysis of 3-phenylthiophene and its fluoro derivatives with torsional dependence. *Journal of Molecular Structure*, 834–836 508–515.

Uğurlu, G. (2019). theoretical studies of the molecular structure, conformational and nonlinear optical properties of (2-benzyloxy-pyrimidin-5-yl) boronic acid. *The Eurasia Proceedings of Science, Technology, Engineering & Mathematics*, *6*, 101-105.

Uğurlu, G. (2020). Theoretical examination of the conformational effect on the molecular structure and electronic properties of the orthorhombic metaboric acid molecule, *Boron* *5*(2), 91-99.

Zhu, L., Zhong, Z. & Anslyn, E.V. (2005). Guidelines in implementing enantioselective indicator displacement assays for α-hydroxycarboxylates and diols. *Journal of the American Chemical Society*, *127*, 4260-4269.

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