Pamukkale Üniversitesi Mühendislik Bilimleri Dergisi
Pamukkale University Journal of Engineering Sciences

Kabul Edilmiş Araştırma Makalesi (Düzenlenmemiş Sürüm)

Accepted Research Article (Uncorrected Version)

Makale Başlığı / Title	Conformational and FTIR analyses of 2,3-dimethoxyphenylboronic acid 2,3-dimetoksifenilboronik asit molekülünün konformasyon ve FTIR analizi
Yazarlar / Authors	Duygu BİLGE1*
Referans No / Reference No	PAJES-70431
DOI	10.5505/pajes.2018.70431

Bu PDF dosyası yukarıda bilgileri verilen kabul edilmiş araştırma makalesini içermektedir. Sayfa düzeni, dizgileme ve son inceleme işlemleri henüz tamamlanmamış olduğundan, bu düzenlenmemiş sürüm bazı üretim ve dizgi hataları içerebilir.

This PDF file contains the accepted research article whose information given above. Since copyediting, typesetting and final review processes are not completed yet, this uncorrected version may include some production and typesetting errors.

Pamukkale Üniversitesi Mühendislik Bilimleri Dergisi

Pamukkale University Journal of Engineering Sciences

Ï Î Æ Ë Ï Ò Í Á Ô É Ï Î Á Ì Á Î Ä Ö Á Â É Ì Å Ô Ë Ï Ó Ù Ì Ø Ë Ø É Ã Å Ò Ö Ï Ù Ì Å

ç Ž Ö É Í Å Ô Ï Ë Ó É Æ Å Î É Ì Â Ï Ò Ï Î É Ë Á Ó É Ô Í Ï Ì Å Ë Ì Ì

$ Õ Ù Ç Õ [1*] " d , ' %

[1] 0 È Ù Ó É Ã Ó $ Å Ð Á Ò Ô Í Å Î Ô ň & Á Ã Õ Ì Ô Ù Ï Æ 3 Ã É Å Î Ã Å ň % Ç Å

duygu.bilge@ege.edu.tr

Received/ ' Å Ì É ň: 07.09.2018, Accepted/ Kabul Tarihi: 26.10.2018

doi: 10.5505/pajes.2018.70431

Research Article/ ! Ò Á ň Ô ą Ò Í Á

* Corresponding author/ 9 Á Ú ą ň ą Ì Á Î 9 Á Ú Á Ò

Abstract

The experimental and theoretical investigations of solvent effect on conformational structure and the hydroxyl stretching vibration of 2,3-dimethoxyphenylboronic acid (2,3-dmpba; C6H3(OCH3)2B(OH)2) molecule were studied by Fourier transform infrared (FTIR) spectroscopy and density functional theory (DFT). Calculations were performed by four conformational isomers of the title compound in eighteen different organic solvents by the polarizable continuum model (PCM). Scaled quantum mechanical (SQM) method was performed for the vibrational analysis. Most stable conformational isomer of the compound is independent of the solvent effect. Results of SQM method are very successful in determining the solvent effect on vibration frequency. Experimental and theoretical findings from the present search will be useful to understand structural characteristics of phenylboronic acid derivatives.

Keywords: Phenylboronic acid derivatives, FTIR, DFT, SQM, Solvent effect.

Öz

2,3-dimetoksifenil boronik asit molekülünün (2,3-dmpba; C6H3(OCH3)2B(OH)2) konformasyonel Ù Á Ð ą Ó ą Ö Å È Ç Å Ò É Ì Å Ì Å Ò É Ô É Ô Ò Å ň É Í É Ì Ú Å Ò É Î Ä Ë ą Ú ą Ì Ę Ô Å Ó É Ó Ð Å Ë Ô Ò Ï Ó É Ï Ð É Ó É ¡ & 4) 2 É Ì Å Â É Ò Ì É Ë Ô Å È Å Í Ä Å Î Ù Ó Å Ì È Å Hesaplamalar polarize sürekli É Ë Í Ï Ä Å Ì É ¡ 0 # - Ɋ Æ Á Ò Ë Ì ą Ï Ò Ç Á Î É Ë ë Ę Ú Ì Ã Ì Ä Å Ö Å Â É Ì Ú Å Ò É Î Å Ä Å Î Ì Ä Å Ì É Ì Á Î Í ą ň Ô ą Ò 8 4 É Ô Ò Å ň Í Å Ë Á Î É Ë Ì Ï Ä Å Ì É ¡ 3 1 - Ɋ Ë Õ Ì Ì Á Î ą Ì Í ą konformasyonel izi Í Å Ò É ë Ę Ú Ì Ã Ì Å Ô Ë É Ó É Î Ä Å Î Ô É Ô Ò Å ň É Í Æ Ò Å Ë Á Î Ó Ì Á Ò ą Ì Ú Å Ò É Î Ä Å Ë Â Á ň Á Ò ą Ì ą Ä ą Ò 8 " Õ ë Á Ì ą ň Í Á Ä Á Î Å Ì Ä Æ Å Î É Ì Â Ï Ò Ï Î É Ë Á Ó É Ô Ô Ì Ò Å Ö Ì Å Ò É Î Æ Á Ù Ä Á Ì ą Ï Ì Á Ã Á Ë Ô ą Ò 8

Anahtar kelimeler: Fenilboronik asit türevleri, FTIR, DFT, SQM, Çözücü etkisi.

1 Introduction

Boronic acid is a compound related to boric acid in which one of the three hydroxyl groups is replaced by an alkyl or aryl group. Boron and boronic acid-based include large number of potentials of related application in medicine, biology, material science and supramolecular or analytical chemistry [1-2]. A variety of typical properties of boronic acids enable them to be well suitable for practices in biomedicine [2]. Polymers including boronic acid have a wide range of uses in various biomedical applications such as management of HIV, obesity, diabetes, and cancer [3].

Phenylboronic acid (PBA) containing a phenyl substituent is an example of boronic acid. PBA and its derivatives have also attracted much attention as modifier of layer by layer films or microcapsules [4]. Molecular characteristics of PBA and its some derivatives have been studied for years. Crystal and molecular structures or some spectroscopic properties of PBA [5] and its dimer [6], diphenyl phenylboronate [7], 3-fluorophenylboronic acid [8], 4-chloro- or -bromo-phenylboronic acid [9], 2- and 4-iodo-phenylboronic acid [9], 2,4-difluorophenylboronic acid [10], 3-formylphenylboronic acid [11], 3-aminophenylboronic acid [12] were investigated.

There are many theoretical and experimental structural investigations on boronic acid derivatives such as 4-pyridineboronic acid [13], methylboronic acid [14], acenaphthene-5-boronic acid [15] and 2-thienylboronic acid [16]. Furthermore, conformational, vibrational or electronic properties of phenylboronic acid derivatives such as 4-chloro- or -bromo-phenylboronic acid [17], 3,4-dichlorophenylboronic acid [18], 2,4- or 2,6-dimethoxy phenylboronic acids [19, 20], 2,3-difluorophenylboronic [21], 3-bromophenylboronic acid [22], 3,5-difluorophenylboronic acid [23], 3-fluorophenylboronic acid [24], 4-mercaptophenylboronic acid [25], 4-carboxy phenylboronic acid [26], 3-(acrylamido)phenylboronic acid [27], 5-bromo-2-ethoxyphenylboronic acid [28] and pentafluorophenylboronic acid [29] were reported by combining both experimental and theoretical works. This research is a continuation of these previous studies [17-29] and according to the detailed literature survey there is no any theoretical or experimental studies on the structural and vibrational properties of 2,3-dmpba. The detailed analysis was performed to examine the solvent effect on conformational isomerism of 2,3-dmpba. Further, the frequencies of hydroxyl stretch vibrations of the compound were reported by FTIR and DFT studies.

2 Experimental

2,3-dmpba was commercially obtained from Sigma Aldrich and chloroform, methanol, ethanol and dichloromethane solvents were procured from Merck. FTIR spectrum of free and solid 2,3-dmpba were optimi reported via Potassium Bromide (KBr) pellet technique by Perkin Elmer Frontier FTIR spectrophotometer at a resolution of 2 cm^{-1}. Infrared spectra of 2,3-dmpba in solutions were recorded by a deuterated triglycine sulfate detector. Concentrations of 2,3-dmpba in the pure solvents ranged from 0.28 to 0.31 mol/l. Solvents of 25 µl were placed between CaF_2 windows whose cell thickness was 12 µm.

3 Calculational details

Many possible conformational isomers could be proposed for 2,3-dmpba molecule. However, the discussion in this research

is limited to cis ↔cis (*CC*), cis ↔trans (*CT*), trans ↔cis (*TC*) and trans ↔trans (*TT*) forms (Figure 1). Gaussian 09 was used for all calculations [30]. The optimized molecular structures were viewed with the GaussView program [31]. Calculations were performed by DFT method at B3LYP/6-31++G** in the gas phase and solutions. PCM model was employed to assess the solvent effect [32]. After, optimization processes were repeated with no geometric constraints until imaginary frequencies were not seen, calculations were performed for vibrational frequency under the same theory. Harmonic vibrational frequencies were scaled according to 0.955 [33] and SQM [34, 35]. Mole fractions for the isomers were calculated as given before [36, 37].

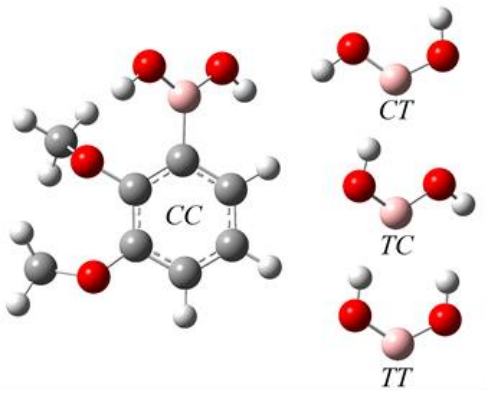

Figure 1: Conformational isomers of 2,3-dmpba.

4 Results and discussion

Optimization energies of four isomers of the compound in eighteen different solvents are given in Table 1. Optimization energy vs. solvent dielectric constant plot of 2,3-dmpba in *CT* form are also depicted in Figure 2.

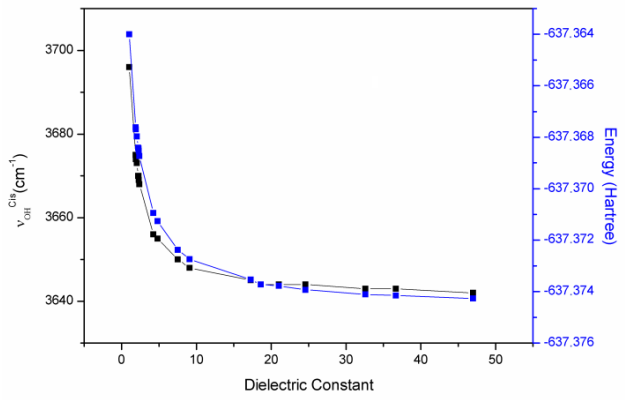

Figure 2: Plot of optimized energy and OH stretching frequency vs. dielectric constant.

Solvation is the process of interaction between solvent and solute molecules and is in part due to the attraction of a charge for a dipole. If the solute has polarity, solvent molecules will be thus drawn to the solute molecules. The greater the polarity of the solvent, the more the attraction is and therefore the more close attraction of the solvent molecules to the solute molecules is. Thus more electrostatic work is performed and so is more energy lost by the system, which inevitably turns more stable [38]. As seen from Table 1 and Figure 2, since dielectric constant of the solvent increases for the all forms, the molecule becomes more stable.

According to direction of various substituents in the gas phase, 3,4-dichloro [18], 2,4-dimethoxy [19], 2,3-difluoro [21] and 3,5-difluoro phenylboronic acid [23] prefer to *CT* form whereas the *CC* conformer is the most stable for 2,6-dimethoxy phenylboronic acid [20]. Optimized relative energies and mole fractions for all forms of 2,3-dmpba in different medium are listed in Table 2. Computed optimize energies indicate that the *CT* form is more stable than *CC*, *TC* and *TT* forms by 7.77 ↔9.57 kcal/mol, 9.11-10.63 kcal/mol and 10.10 ↔13.97 kcal/mol correspondingly. According to results of mole fraction computations of isomers, the title molecule prefers to *CT* conformational isomer with the probability of 100% for all medium (Table 2).

Table 3 presents the calculated lengths of hydroxyl bond and dipole moments of 2,3-dmpba, from which the OH bond lengths in *CT* form are seen to exhibit a linear correlations with the hydroxyl stretching frequencies of the compound as (R^2 = 0.99484 (C) and 0.99554 (T). Dipole moment of the compound increases gradually by solvent polarity. It is in agreement with the literature. However, it is inversely proportional with the hydroxyl stretching frequencies. As seen from Figure 3, there is good and linear correlation between OH stretching frequencies and dipole moments (R^2 = 0.99466).

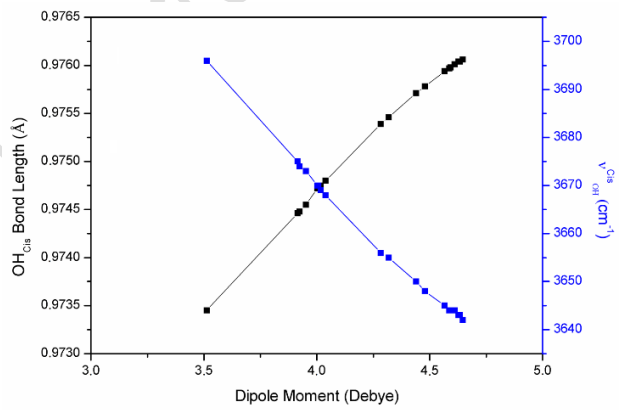

Figure 3: Plot of OH bond length and stretching frequency vs. dipole moment.

Length of OH bond increases as the polarity of the solvent does. Hydroxyl stretching frequency should therefore decrease. It follows from Table 3 that this requirement is significantly fulfilled for the compound and OH frequencies decreases by increases in the bond lengths (R^2 = 0.99956). Hydroxyl stretching frequencies are inversely proportional to the polarity of the sdvent (Figure 2).

OH stretching vibrations of the investigated molecule needs to special attention. Once these bands of some PBA derivatives are investigated, they are comprehensible and this suggests that the intramolecular hydrogen bondings occur in different environments of boronic acids [25]. The hydroxyl stretching bands in the infrared spectra of free 3,4-dichlorophenylboronic acid [18], 2,4- and 2,6-dimethoxyphenylboronic acid [19, 20], 2,3-difluorophenylboronic acid [21] and 5-bromo-2-ethoxyphenylboronic acid [28] were observed at 3465 / 3425, 3480/3339, 3335 and 3400/3332 and 3371 cm^{-1} correspondingly. However, there is no any peak for 3,5-difluorophenylboronic acid [14]. OH stretching band of free 2,3-dmpba is shown at 3368 cm^{-1} for the solid phase This observation is consistent with previously reported paper [18, 21, 28]. As seen from Table 4, they are observed at 3468 cm^{-1}, 3351 cm^{-1}, 3350 cm^{-1} and 3351 cm^{-1} in chloroform,

dichloromethane, ethanol and methanol, respectively, as one strong and broad band. These experimental OH stretching frequencies also decrease by increasing of the dielectric constant of the solvent.

In Table 4, theoretical OH stretching vibrations scaled by literature coefficient and SQM are also given together with their experimental values. Correlation values between the experimental and computed vibrational frequencies are found to be 0.76684 for scaling factor and 0.99872 for SQM. The biggest difference between the experimental and theoretical frequencies is 133 cm^{-1} for scaling factor in literature and 29 cm^{-1} for SQM. Hence, there is a poor agreement between the theoretically scaled frequencies by scaling factor of the B3LYP/6-31++G** and those obtained experimentally. However, the predicted values by SQM show a good correlation with experimental data and this method constitutes a reliable complement the understanding of vibrational bands of the investigated compound.

Table 1: Optimization energy (Hartree) of 2,3-dmpba in various medium.

Medium	2,3-dmpba			
	CC	*TT*	*CT*	*TC*
Gas phase	-637.34875320	-637.34173799	-637.36400100	-637.34706046
n-hexane	-637.35319394	-637.34696008	-637.36762019	-637.35111167
n-heptane	-637.35329185	-637.34707820	-637.36769830	-637.35120243
Cyclohexane	-637.35362546	-637.34748170	-637.36796394	-637.35151230
1,4-dioxane	-637.35417813	-637.34815308	-637.36840238	-637.35202775
Tetrachloromethane	-637.35422626	-637.34821172	-637.36844044	-637.35207277
Benzene	-637.35433731	-637.34834717	-637.36852819	-637.35217673
Toluene	-637.35459477	-637.34866174	-637.36873128	-637.35241822
Diethylether	-637.35743615	-637.35235039	-637.37094067	-637.35514797
Chloroform	-637.35785270	-637.35288547	-637.37125964	-637.35556333
Tetrahydrofuran	-637.35933333	-637.35480220	-637.37238275	-637.35706528
Dichloromethane	-637.35980249	-637.35541587	-637.37273492	-637.35754950
2-butanol	-637.36088794	-637.35684683	-637.37354195	-637.35868563
2-propanol	-637.36113953	-637.35718054	-637.37372740	-637.35895230
Acetone	-637.36121295	-637.35727806	-637.37378141	-637.35903041
Ethanol	-637.36141711	-637.35754951	-637.37393128	-637.35924822
Methanol	-637.36164963	-637.35785914	-637.37410146	-637.35949737
Acetonitrile	-637.36171457	-637.35794572	-637.37414888	-637.35956717
Dimethylsulfoxide	-637.36187993	-637.35816643	-637.37426945	-637.35974535

Table 2: Relative energy and mole fraction for 2,3-dmpba in various medium.

Medium	Relative energy (kcal/mol)				Mole fraction (%)			
	CC	*TT*	*CT*	*TC*	*CC*	*TT*	*CT*	*TC*
Gas phase	9.57	13.97	-	10.63	0	0	100	0
n-hexane	9.05	12.96	-	10.36	0	0	100	0
n-heptane	9.04	12.94	-	10.35	0	0	100	0
Cyclohexane	9.00	12.85	-	10.32	0	0	100	0
1,4-dioxane	8.93	12.71	-	10.28	0	0	100	0
Tetrachloromethane	8.92	12.70	-	10.27	0	0	100	0
Benzene	8.90	12.66	-	10.26	0	0	100	0
Toluene	8.87	12.59	-	10.24	0	0	100	0
Diethylether	8.47	11.67	-	9.91	0	0	100	0
Chloroform	8.41	11.53	-	9.85	0	0	100	0
Tetrahydrofuran	8.19	11.03	-	9.61	0	0	100	0
Dichloromethane	8.12	10.87	-	9.53	0	0	100	0
2-butanol	7.94	10.48	-	9.32	0	0	100	0
2-propanol	7.90	10.38	-	9.27	0	0	100	0
Acetone	7.89	10.36	-	9.26	0	0	100	0
Ethanol	7.85	10.28	-	9.21	0	0	100	0
Methanol	7.81	10.19	-	9.16	0	0	100	0
Acetonitrile	7.80	10.17	-	9.15	0	0	100	0
Dimethylsulfoxide	7.77	10.10	-	9.11	0	0	100	0

Table 3: Dipole moment, OH stretching and bond length of 2,3-dmpba (*CT*).

Medium	μ (Debye)	O-H: *C* (Å)	n_{OH}: *C* (cm^{-1})	O-H: *T* (Å)	n_{OH}: *T* (cm^{-1})
Gas phase	3.513	0.97345	3696	0.96613	3846
n-hexane	3.915	0.97446	3675	0.96653	3841
n-heptane	3.924	0.97448	3674	0.96653	3840
Cyclohexane	3.953	0.97455	3673	0.96656	3840
1-4-dioxane	4.003	0.97472	3670	0.96669	3838
Tetrachlorometha	4.007	0.97473	3670	0.96670	3838
Benzene	4.017	0.97475	3669	0.96671	3838
Toluene	4.039	0.97480	3668	0.96673	3838
Diethylether	4.283	0.97539	3656	0.96704	3833
Chloroform	4.318	0.97546	3655	0.96709	3833
Tetrahydrofuran	4.440	0.97571	3650	0.96723	3831
Dichloromethane	4.479	0.97578	3648	0.96727	3830
2-butanol	4.567	0.97594	3645	0.96737	3829
2-propanol	4.587	0.97597	3644	0.96739	3828
Acetone	4.593	0.97598	3644	0.96739	3828
Ethanol	4.610	0.97601	3644	0.96741	3828
Methanol	4.628	0.97604	3643	0.96743	3828
Acetonitrile	4.634	0.97604	3643	0.96744	3828
Dimethylsulfoxide	4.647	0.97606	3642	0.96745	3827

Table 4. Comparison of OH stretching frequencies (cm^{-1}).

Medium	Exp. n_{OH}	n_{OH}^{1} (*C*)	n_{OH}^{2} (*C*)
Chloroform	3468	3491	3440
Dichloromethane	3351	3484	3380
Ethanol	3350	3480	3379
Methanol	3351	3479	3375

n_{OH}^{1} (C) and n_{OH}^{2} (C) are scaled frequencies by 0.955 [33] and SQM [34, 35].

5 Conclusions

Theoretical and experimental works have been performed by using DFT and FTIR to investigate solvent effect on the structure and hydroxyl stretching vibration of 2,3-dmpba as phenylboronic acid derivatives. There is no solvent effect on conformational isomers of the compound. Solvent-induced OH frequencies are inversely proportional with the dipole moment, bond length and dielectric constant. Unscaled and scaled frequencies by B3LYP/6-31++G** have poor correlations with experimental data whereas SQM results are in excellent agreement and it is very successful in revealing the dielectric-induced solvent effect on the vibrational frequency.

6 Acknowledgements

This work was supported by Research Fund of the Ege University (Project number: 2016-FEN-032).

7 References

[1] Hall DG. Boronic Acids: Preparation and Applications in Organic Synthesis and Medicine. Alberta/Canada, Wiley-VCH, Weinheim, 2005.

[2] Yang W, Gao X, Wang B. Biological and medicinal applications of boronic acids. Hall DG. Preparation and Applications in Organic Synthesis and Medicine. 481-512, Alberta/Canada, Weinheim: Wiley-VCH, 2005.

[3] #ÁÍÂÒÅ *.ȟ 3ÕÍÅÒÌÉÎ "38 Ȱ"ÉÏ ÂÏÒÏÎÉÃ ÁÃÉÄ ÐÏÌÙÍÅ 4043, 2011. 0ÏÌÙÍ

[4] 7ÁÎÇ "ȟ 9ÏÓÈÉÄÁ +ȟ 3ÁÔÏ -+ȟ !Î Functionalized Layer-by-Layer Assemblies for Biomedical !ÐÐÌÉÃÁÔÉÏÎÓȱȢ 0ÏÌÙÍÅÒÓȟ ωȟ ς

[5] 2ÅÔÔÉÇ 3*ȟ 4ÒÏÔÔÅÒ *Ȣ Ȱ#ÒÙÓÔ ÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄȟ #φ(υ"ɉ/(Ɋ Chemistry,. 55, 3071-3075, 1977.

[6] Cyran´ski MK, Jezierska A, Klimentowska P, Panek JJ, 3ÐÏÒÚÙÎÓǇËÉ !!Ȣ Ȱ)ÍÐÁÃÔ ÏÆ ÉÎ on structural properties of phenylboronic acid: quantum ÃÈÅÍÉÃÁÌ ÁÎÄ 8ǕÒÁÙ ÓÔÕÄÉÅÓȱȢ * Chemistry, 21, 472-482, 2008.

[7] &ÁÎÉÒÁÎ *.ȟ 3ÈÕÒÖÅÌÌ (&Ȣ Ȱ phenylboronic acid (normal and deuterated) and diphenyl ÐÈÅÎÙÌÂÏÒÏÎÁÔÅȱȢ #ÁÎÁÄÉÁÎ *Ï 2089-2095, 1968.

[8] 7Õ 9-ȟ $ÏÎÇ ##ȟ ,ÉÕ 3-ȟ :ÈÕ Fluorophe ÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄȱȢ !ÃÔÁ Section E, 62 (10), 4236-4237, 2006.

[9] Shimpi MR, SeethaLekshmi N, Pedireddi VR. Ȱ3ÕÐÒÁÍÏÌÅÃÕÌÁÒ ÁÒÃÈÉÔÅÃÔÕÒÅ ÈÁÌÏÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄÓȱȢ #ÒÙÓ 1958-1963, 2007.

[10] Rodriguez-Cuamatzi P, 4ÌÁÈÕÅØÔ (ȟ -(ĘÐÆÌ $ÉÆÌÕÏÒÏÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄȱȢ Section E, 65, 44-45, 2009.

[11] Zarychta B, Zaleski J, Sporzynski A, Dabrowski M, Crystallographica Section C, C 60, 344-345, 2004.

[12] 6ÅÇÁ !ň :ÁÒÁÔÅ .ň 4ÌÁ-ÈÕÅ ÁÍÉÎÏÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄ Crystallographica Section E, 66, o1260, 2010.
[13] +ÕÒÔ -ň 3ÅÒÔÂÁËÁÎ 4 2ň vÚÄÕÒÁÎ Theoretical Study of Molecular Structure and Vibrational Spectra of 3- and 4-Pyridineboronic Acid Molecules by $ÅÎÓÉÔÙ &ÕÎÃÔÉÏÎÁÌ 4ÈÅÏÒÙ #ÁÌÃÕÌÁÔÉÏÎÓ Acta Part A: Molecular and Biomolecular Spectroscopy, 70, 664-673, 2008.
[14] 2ÁÎÉ 5ň +ÁÒÁÂÁÃÁË -ň 4ÁÎÒą 3ÕÎÄÁÒÁÇÁÎÅÓÁÎ .8 Ŏ4-Raman, FT-IR, 1H, 13C NMR and UV), first-order hyperpolarizability and HOMO-,5-/ ÁÎÁÌÙÓÉÓ ÏÆ ÍÅÔÈÙÌÂÏÒÏÎÉÃ Acta Part A: Molecular and Biomolecular Spectroscopy, 92, 67-77, 2012.
[15] +ÁÒÁÂÁÃÁË -ň 3ÉÎÈÁ ,ň 0ÒÁÓÁÄ experimental and theoretical investigation of Acenaphthene-5-boronic acid: conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-2ÁÍÁÎň .-2 ÁÎÄ 56 ÓÐÅÃÔÒÁ ō8 3ÐÅÃÔÒÏÃÈÉÍÉÃÁ Molecular and Biomolecular Spectroscopy, 115, 753-766, 2013.
[16] Sachan AK, Pathak SK, Sinha L, Prasad O, Karabacak M, !ÓÉÒÉ !-8 Ŏ! ÃÏÍÂÉÎÅÄ ÅØÐÅÒÉÍÅÎÔÁÌ investigation of 2-Thienylboronic acid: Conformational search, molecular structure, NBO, NLO and FT-IR, FT-2ÁÍÁÎň .-2 ÁÎÄ 56 ÓÐÅÃÔÒÁÌ Journal of Molecular Structure, 1076, 639-650, 2014.
[17] +ÕÒÔ -8 Ŏ$&4 ÓÉÍÕÌÁÔÉÏÎÓ ÁÎÄ chloro and 4-ÂÒÏÍÏÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄÓ Journal of Raman Spectroscopy, 40, 67-75, 2009.
[18] +ÕÒÔ -ň 3ÅÒÔÂÁËÁÎ 4 2ň vÚÄÕÒÁÎ and Raman spectrum, molecular structure and theoretical calculation of 3,4-ÄÉÃÈÌÏÒÏÐÈÅÎÙÌÂÏÒÏÎÉÃ Molecular Structure, 92, 178-187, 2009.
[19] !ÌÖÅÒ v 8 Ŏ& 4-IR, Raman, 13C solution and solid state NMR studies of 2,4-dimethoxyphenylboronic acid ō8 Comptes Rendus Chimie, 14, 446-455, 2011.
[20] !ÌÖÅÒ vň 0ÁÒÌÁË #8 Ŏ& 4-IR, Raman, liquid and solid state NMR studies of 2,6-ÄÉÍÅÔÈÏØÙÐÈÅÎÙÌÂÏÒÏÎÉÃ Vibrational Spectroscopy, 54, 1-9, 2010.
[21] Karabacak M, Kose E, Atac A, Cipiloglu MA, Kurt M. Ŏ-lecular structure investigation and spectroscopic studies on 2,3-difluorophenylboronic acid: A combined ÅØÐÅÒÉÍÅÎÔÁÌ ÁÎÄ ÔÈÅÏÒÅÔÉÃÁÌ Acta Part A: Molecular and Biomolecular Spectroscopy, 97, 892-908, 2012.
[22] Karabacak M, Kose E, Atac A, Sas EB, Asiri AM, Kurt M. Ŏ%ØÐÅÒÉÍÅÎÔÁÌ (FT-IR, FT-Raman, UV-Vis, 1H and 13C NMR) and computational (density functional theory) studies on 3-ÂÒÏÍÏÐÈÅÎÙÌÂÏÒÏÎÉÃ ÁÃÉÄ Molecular Structure, 1076, 358-372, 2014.
[23] Karabacak M, Kose E, Atac A, Asiri AM, Kurt M. Ŏ-ÏÎÏÍÅÒÉÃ and dimeric structures analysis and spectroscopic characterization of 3,5-difluorophenylboronic acid with experimental (FT-IR, FT-Raman, 1H and 13C NMR, UV) ÔÅÃÈÎÉÑÕÅÓ ÁÎÄ ÑÕÁÎÔÕÍ ÃÈÅÍÉÃÁÌ Molecular Structure, 1058, 79-96, 2014.
[24] Karabacak M, Kose E, Sas EB, Kurt M, Asiri AM, Atac A. Ŏ$&4 ÃÁÌÃÕÌÁÔÉÏÎÓ, FT-IR, FT-Raman, 1H, 13C NMR, UV-Vis spectral studies of 3-fluorophenylboronic ÁÃÉÄ ō8 3ÐÅÃÔÒÏÃÈÉÍÉÃÁ !ÃÔÁ 0ÁÒÔ !ą -ÏÌÅÃÕÌÁÒ ÁÎÄ Biomolecular Spectroscopy, 136, 306-320, 2015.
[25] Parlak C, Ramasami P, Tursun M, Rhyman L, Kaya MF, Atar N, et al. 4-Mercaptophenylboronic acid: Conformation, FT-IR, Raman, OH stretching and theoretical studies. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 144, 131-138, 2015.
[26] !ÌÖÅÒ v8 3ÐÅÃÔÒÏÓÃÏÐÉÃ ÁÎÁÌÙÓÉÓ solvent dependent behavior and XRD structural properties of 4-carboxy phenylboronic acid: A DFT study. Journal of Molecular Structure, 1099, 208-215, 2015.
[27] Alver Ö, Kaya MF, Dikmen G. Ŏ3ÔÒÕÃÔÕÒÅ ÁÎÄ Solvent effects on nuclear magnetic shielding tensors, experimental and theoretical DFT studies on the vibrational and NMR spectra of 3-(methoxycarbonyl)phenylboronic acid. Journal of Molecular Structure, 1102, 285-294, 2015.
[28] 3ÁÓ %"ň +ÏÓÅ %ň +ÕÒÔ -ň +ÁÒÁÂÁÃÁË -8 FT-IR, FT-Raman, NMR and UV-Vis spectra and DFT calculations of 5-bromo-2-ethoxyphenylboronic acid (monomer and dimer structures). Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 137, 1315-1333, 2015.
[29] +ÕÒÔ -ň Ŏ!Î ÅØÐÅÒÉÍÅÎÔÁÌ ÁÎÄ ÔÈÅÏÒÅÔÉÃÁÌ molecular structure and vibrational spectra of pentafluorophenylboronic acid molecule by density functional theory and ab initio Hartree Fock calculations. Journal of Molecular Structure, 874, 159-169, 2008.
[30] Frisch MJ, Trucks, GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Mennucci B, Petersson GA, Nakatsuji H, Caricato M, Li X, Hratchian HP, Izmaylov AF, Bloino J, Zheng G, Sonnenb DJ., Gaussian 09, Revision A.1, Gaussian Inc., 340 Quinnipiac St., Bldg. 40, Wallingford, CT 06492, USA, 2008.
[31] Dennington RD, Keith TA, Millam JM. GaussViev 5.0.8, Gaussian Inc., 340 Quinnipiac St., Bldg. 40, Wallingford, CT 06492, USA, 2008.
[32] Miertus S, Scrocco E, Tomasi J. Ŏ%ÌÅÃÔÒÏÓÔÁÔÉÃ ÉÎÔÅÒÁÃÔÉÏÎ of a solute with a continuum. A direct utilizaion of AB initio ÍÏÌÅÃÕÌÁÒ ÐÏÔÅÎÔÉÁÌÓ ÆÏÒ ÔÈÅ ÐÒÅÖÉÓÉÏÎ ÏÆ ÓÏÌÖÅÎÔ Chemical Physics, 55, 117-129, 1981.
[33] "ÁÌÃą +ň !ËÙÌÚ 38 Ŏ! ÖÉÂÒÁÔÉÏÎÁÌ investigation on benzoylacetone molecules. Spectroscopy, 48, 215-218, 2008.
[34] "ÁËÅÒ *ň *ÁÒÚÅÃËÉ !!ň 0ÕÌÁÙ 0ň Ŏ! 3ÃÁÌÅÄ 1ÕÁÎÔÕÍ -ÅÃÈÁÎÉÃÁÌ &ÏÒÃÅ &ÉÅÌÄ Physical Chemistry A, 102, 1412-1424, 1998.
[35] 2ÁÕÈÕÔ 'ň 0ÕÌÁÙ 08 Ŏ4ÒÁÎÓÆÅÒÁÂÉÌÉÔÙ ÏÆ $ÅÎÓÉÔÙ &ÕÎÃÔÉÏÎÁÌ $ÅÒÉÖÅÄ 6ÉÂÒÁÔÉÏÎÁÌ Journal of Physical Chemistry, 99, 3093-3100, 1995.
[36] 0ÁÒÌÁË #ň Ŏ4ÈÅÏÒÅÔÉÃÁÌ ÁÎÄ spectroscopic study of 4-(1-0ÙÒÒÏÌÉÄÉÎÙÌ)ÐÉÐÅÒÉÄÉÎÅ Journal of Molecular Structure, 966, 1-7, 2010.
[37] 4ÕÒÓÕÎ -ň 0ÁÒÌÁË #8 Ŏ#ÏÎÆÏÒÍÁÔÉÏÎÁÌ ÁÎÁÌÙÓÉÓ solvent effects on CO stretching of 4-chloro-3-ÈÁÌÏÇÅÎÏÂÅÎÚÁÌÄÅÈÙÄÅÓō8 3ÐÅÃÔÒÏÃÈÉÍÉÃÁ Molecular and Biomolecular Spectroscopy, 141, 1-53, ÏÆ 2015.
[38] Sharma RK. Stereochemistry. New Delhi/India, Discovery Publishing House, p 270, 2007.