

Effects of different GIAO and CSGT models and basis sets on 2-aryl-1,3,4-oxadiazole derivatives

Davut Avcı · Yusuf Atalay

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Abstract The direct molecular structure implementations of the gage-including atomic orbital (GIAO), individual gages for atoms in molecules (IGAIM) and continuous set of gage transformations (CSGT) methods for calculating nuclear magnetic shielding tensors at both the Hartree-Fock (HF) and density functional (B3LYP) levels of theory with 6-31G(d), 6-311G(d), 6-31++G(d,p), 6-311++G(d,p), and 6-311++G(df,pd) basis sets are presented. Dependence on the ^1H and ^{13}C NMR chemical shifts on the choice of method and basis set have been investigated. Also, these chemical shifts of 2-aryl-1,3,4-oxadiazoles **5a–g** have been performed related to dihedral angles (C4–C3–C2–O) of two conformers. The optimized molecular geometries and ^1H and ^{13}C chemical shift values of 2-aryl-1,3,4-oxadiazoles **5a–g** in the ground state have been obtained. The linear correlation coefficients of ^{13}C NMR chemical shifts for these molecules were given. The new nuclear magnetic shielding tensors of tetramethylsilane (TMS) were calculated. The data of 2-aryl-1,3,4-oxadiazole derivatives display significant molecular structure and NMR analysis. Also, these provide the basis for future design of efficient materials having the 1,3,4-oxadiazole core.

Keywords DFT · HF · GIAO · CSGT · ^1H · ^{13}C NMR · TMS · 2-aryl-1,3,4-oxadiazoles · Structure-correlation analysis

Introduction

1,3,4-Oxadiazoles are very interesting in medicinal chemistry. Besides, derivatives of 1,3,4-oxadiazoles have been reported to exhibit diverse biological activities. It is frequently used in pharmaceutical industry [1–6]. Various oxadiazole-containing molecular structures were synthesized [7–13]. Furthermore, the 1,3,4-oxadiazole ring which is a new NLO motifs among the heterocyclic compounds were used as a π -bridge on the ground. Its reduced aromaticity may offer better prospects for π -electron delocalization across the D–A links [13]. However, typical electron-transporting materials usually contain a π -electron deficient heterocyclic moiety, such as oxadiazoles, triazoles, triazines, etc., which can effectively improve the electron affinity [14].

Experimental measurements and theoretical calculations on NMR chemical shift become one of the key factors in the molecular structure correlations design. Theoretical determination of NMR chemical shift is quite useful both for understanding the relationship between the molecular structure and electronic properties of molecules. It also provides a guideline to experimentalists for the design and synthesis of organic materials [6].

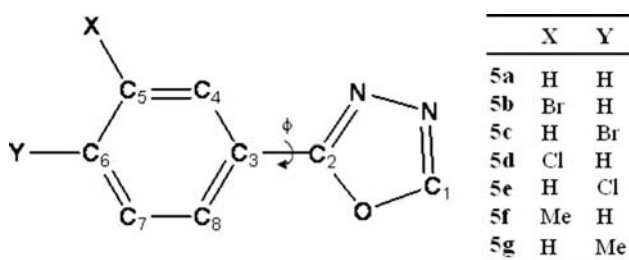
The aim of the present work is to describe and characterize the relation between the molecular structure and chemical shifts correlations of 2-aryl-1,3,4-oxadiazoles **5a–g**. A number of papers have recently appeared in the literature concerning the calculation of NMR chemical shift (c.s.) by quantum-chemistry methods [15–20]. These papers indicate that geometry optimization is a crucial factor in an accurate determination of computed NMR chemical shift. Moreover, it is known that the density functional theory (DFT) (B3LYP) method adequately takes into account electron-correlation contributions, which are

D. Avcı · Y. Atalay (✉)
Faculty of Arts and Sciences, Department of Physics,
Sakarya University, 54100 Sakarya, Turkey
e-mail: yatalay@sakarya.edu.tr

Table 1 The isotropic magnetic shielding constants (in ppm) of TMS for C and H calculated at different GIAO, IGAIM, and CSGT models with basis sets

Method/Basis set	Model/Atom					
	GIAO/C	GIAO/H	IGAIM/C	IGAIM/H	CSGT/C	CSGT/H
HF/6-31G(d)	199.9921	32.5968	196.8818	29.5524	196.882	29.5524
HF/6-311G(d)	194.5082	32.5787	187.0183	30.2072	187.0181	30.2072
HF/6-31++G(d,p)	201.8013	31.9909	202.1226	29.7036	202.1220	29.7035
HF/6-311++G(d,p)	194.8635	32.2149	192.4228	30.8871	192.4221	30.8871
HF/6-311++G(df,pd)	204.1442	30.0990	193.1035	31.0533	193.0832	31.0517
B3LYP/6-31G(d)	189.7026	32.1836	188.582	29.1962	188.5822	29.1661
B3LYP/6-311G(d)	184.2796	32.2899	177.0139	29.9581	177.0137	29.9581
B3LYP/6-31++G(d,p)	192.6804	31.6697	194.6020	29.4698	194.6015	29.4698
B3LYP/6-311++G(d,p)	184.1020	31.9713	182.3632	30.7281	182.3624	30.7281
B3LYP/6-311++G(df,pd)	193.0479	29.6572	182.7257	30.8366	182.7023	30.8348
BLYP/6-311++G(df,pd)	179.0075	31.6690	177.3744	30.6158	177.3508	30.6140

Chemical shift values are calculated using the following equation $\delta_{CSx} = \sigma_{IMSTMS} - \sigma_{IMSx}$

**Fig. 1** The schematic illustration of 2-aryl-1,3,4-oxadiazole derivatives (**5a–g**). $\phi = \text{C4–C3–C2–O}$

especially important in systems containing extensive electron conjugation and/or electron lone pairs. However, as molecular size increases, computing-time also increases. To optimize computing-time the DFT level was used. It was proposed that the single-point calculation of magnetic shielding by DFT methods was combined with a fast and reliable geometry-optimization procedure at the molecular mechanics level [19].

The gage-including atomic orbital (GIAO) [21–24], individual gages for atoms in molecules (IGAIM) [25] and continuous set of gage transformations (CSGT) [25–28] methods are three of the most common approaches for calculating nuclear magnetic shielding tensors. GIAO has been shown to provide results that are often more accurate than those calculated with other approaches, at the same basis set size [29]. In most cases, in order to take into account correlation effects, post-Hartree-Fock calculations of organic molecules have been performed using (i) Møller-Plesset perturbation methods, which are very time consuming and hence applicable only to small molecular systems, and (ii) density functional theory (DFT) methods, which usually provide significant results at a relatively low computational cost [30]. In this regard, DFT methods in

which the electron-correlation contributions are not negligible have been preferred in the study of large organic molecules [31], metal complexes [32], organometallic compounds [33]. For these cases GIAO ^{13}C c.s. calculations [29] were used.

2-Aryl-1,3,4-oxadiazoles **5a–g** were synthesized and characterized by ^1H NMR, ^{13}C NMR, IR, and elemental analysis [6]. And also, theoretical analysis of vibrational spectra and scaling-factor of these molecules were studied in our previous work [34]. To the best of our knowledge, the theoretical calculations of chemical shifts and the effects on chemical shifts of different NMR methods and basis sets for 2-aryl-1,3,4-oxadiazoles **5a–g** have not been investigated yet. In this study, GIAO, IGAIM, and CSGT ^1H and ^{13}C NMR chemical shifts of the title compounds in the ground state have been calculated by using the Hartree-Fock (HF) and DFT (B3LYP) methods with 6-31G(d), 6-311G(d), 6-31++G(d,p), 6-311++G(d,p), and 6-311++G(df,pd) basis sets. These results were compared with the experimental ^1H and ^{13}C NMR chemical shifts (CDCl_3). A comparison of the experimental and theoretical spectra can be very useful in making correct assignments and understanding the basic chemical shift-molecular structure relationship. And so, these calculations are valuable for providing insight into molecular structure analysis.

Computational details

The molecular structures of the title compounds (**5a–g**) in the ground state (in vacuo) are optimized HF and B3LYP methods with 6-31G(d), 6-311G(d), 6-31++G(d,p), 6-311++G(d,p), and 6-311++G(df,pd) basis sets. The geometry of tetramethylsilane (TMS) is fully optimized. ^1H

and ^{13}C NMR chemical shifts for TMS and the title compounds (**5a–g**) are calculated with GIAO, IGAIM, and CSGT approaches [21–28]. First, these approaches were applied to the B3LYP and HF methods [29, 35] with 6-31G(d), 6-311G(d), 6-31++G(d,p), 6-311++G(d,p), and 6-311++G(df,pd) [36–38] basis sets for dihedral angles at 180.0 (C4–C3–C2–O) and 0.0 (C4–C3–C2–N) degrees. Second, conformational analysis formation was performed by B3LYP/6-31G(d) level; it was carried out by changing the torsional angle (dihedral angle, ϕ , C–C–C–O). For each conformer, the torsional angle was held fixed while all other geometric parameters were optimized. And so, two conformers were obtained at dihedral angles: -135 and -90° . These conformers for the chemical shift calculations of the title compounds (**5a–g**) were used. Besides, the calculations of ^1H and ^{13}C NMR chemical shifts using GIAO and CSGT approaches with the BLYP/6-311++G(df,pd) level for **5a–e** were done. The theoretical NMR ^1H and ^{13}C chemical shift values were obtained by subtracting isotropic magnetic shielding (IMS) values which are calculated with GIAO, IGAIM, and CSGT from the IMS values of TMS [29, 35, 39]. For instance, the average ^{13}C IMS of TMS are taken into account for the calculation of ^{13}C c.s. of any X carbon atom, and so c.s. can be calculated using the following equation $\delta_{\text{CSx}} = \sigma_{\text{IMS-TMS}} - \sigma_{\text{IMSx}}$. The ^1H and ^{13}C IMS values of TMS were given in Table 1. And these values were used for the calculation of c.s. All the calculations are performed by using Gauss-View molecular visualization program [40] and Gaussian 98 program package [41].

Results and discussion

The atomic numbering with the geometric structure of the title compounds (**5a–g**) are shown in Fig. 1.

The dihedral angles between the five-membered 1,3,4-oxadiazole ring and the aryl ring are 0.0 or 180.0°. Therefore, the molecular structures of **5a–e** molecules are planar (C_s -symmetry) and are displayed in Fig. 1. The other molecular structures of **5f,g** which are non-planar (adopted C_1 -symmetry) are demonstrated in Fig. 1. Since these molecular structures of **5f,g** include methyl group bounded to the aryl ring. The different meta and para substituents (–Br, –Cl, and –Methyl) dependent on the aromatic ring are defined by molecular structure and chemical shifts correlations. Also, the orientation of the substituents with respect to the aryl ring is determined by the torsion angles C–C–C–Br [180.0°] and C–C–C–Cl [180.0°] and C–C–C–CH₃ [different from 180.0°] [34]. Besides, two conformers with C_1 -symmetry of **5a–g** which have dihedral angles ($\phi = \text{C4–C3–C2–O}$) have been obtained to be -135.0 and -90.0° using B3LYP/6-31G(d) level.

In previous work, nuclear magnetic shielding values of TMS were calculated with GIAO and CSGT approach applying B3LYP/6-311+G(2d,p) and HF/6-31G(d) levels [29]. For ^{13}C and ^1H chemical shift values, the values of TMS display significant. The convergence of the GIAO and CSGT methods with HF/6-31G(d) and B3LYP/6-311+G(2d,p) levels for absolute shielding constants were demonstrated [29]. The shielding constant of GIAO and CSGT with HF/6-31G(d) and B3LYP/6-311+G(2d,p) levels for C were calculated to be 195.1 and 188.5, and 190.8 and 188.6 ppm, respectively [29]. Besides, nuclear magnetic shielding values of TMS were obtained from GIAO model applying B3LYP method with 6-31G(d), 6-31+G(d), 6-31+G(d,p), 6-31++G(d,p) basis sets and HF method with 6-31G+(d) basis set [42, 43]. These calculations are not sufficient in our study. Since obtained nuclear magnetic shielding values of TMS using the different NMR models and basis sets are different from each other. So, the calculation of new TMS values for C and H are beneficial to compare with experimental chemical shifts. The nuclear magnetic shielding values of TMS are calculated using GIAO, IGAIM, and CSGT approaches applying B3LYP and HF methods with 6-31G(d), 6-311G(d), 6-31++G(d,p), and 6-311++G(d,p) basis sets. These TMS values are depicted in Table 1, and these are used in calculations of chemical shifts. Initially, nuclear magnetic shielding calculations have been based on optimized molecular structures which are dihedral angles at 180.0 (C4–C3–C2–O) and 0.0 (C4–C3–C2–N) degrees by using B3LYP method with 6-31G(d), 6-311G(d), 6-31++G(d), and 6-311++G(d,p). Then, GIAO, IGAIM, and CSGT ^{13}C and ^1H c.s. calculations of the title compounds (**5a–g**) have been carried out using B3LYP and HF method with these basis sets. The ^{13}C and ^1H chemical shift values (with respect to TMS) were compared to the experimental ^{13}C and ^1H chemical shift values [6]. These results are shown in Tables 2–8. The IGAIM ^{13}C and ^1H c.s. calculations of the title compounds (**5a–g**) are identical to the CSGT ones. Therefore, the results of IGAIM were not given. According to performed calculations for **5a–g**, we have found ~ 176.0 to ~ 20.0 ppm and ~ 9.0 to ~ 1.0 ppm for ^{13}C and ^1H the chemical shift values (with respect to TMS). The experimental results were observed to be ~ 165.0 to ~ 21.0 ppm and ~ 8.50 to ~ 2.0 ppm [6], and so the accuracy ensures reliable interpretation of spectroscopic parameters. As can be seen from Fig. 1, molecular structure of the title compounds (**5a–g**) includes Br, Cl, and methyl bounded to aromatic rings. The electronegative properties of Br, Cl, etc. atoms are well known, and the resonance at 8.11–7.48 ppm was assigned to the aromatic ring-H atom [6] for **5a**. This c.s. calculated at ~ 9.0 to ~ 4.8 ppm for all calculations. Besides, in 1,3,4-oxadiazole ring C bounded H chemical shift were observed

Table 4 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts (with respect to TMS, all values in ppm) for 2-(4-Bromophenyl)-1,3,4-oxadiazole (**5c**)

Atom	NMR [6] (CDCl ₃)	HF/6-31G(d)		HF/6-311G(d)		HF/6-31++G(d,p)		HF/6-311++G(df,pd)			
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT		
C2	164.11	165.8484	171.6464	172.8871	160.5888	167.5561	175.4465	170.4278	184.1686	171.1105	
C1	152.74	153.6723	160.9877	159.898	149.784	154.9726	162.7729	158.2354	171.4794	158.5366	
C7	131.83	130.3843	131.4156	137.1852	128.1603	132.0166	135.3803	134.2764	147.9657	135.9557	
C5	131.83	131.1044	132.141	137.9345	128.8679	132.7274	136.3107	135.0547	148.7838	136.789	
C4	128.51	130.7734	132.3527	137.4435	129.0393	132.2007	136.0141	135.3412	148.4388	136.6553	
C8	128.51	128.5663	130.0729	134.7574	127.2172	129.8739	133.9556	133.1124	145.9468	134.4068	
C3	126.82	122.6102	123.51	129.2575	119.8409	125.7948	129.459	126.8052	139.3198	128.5305	
C6	122.35	141.6999	141.9425	148.4832	141.3557	143.6581	146.4906	147.3707	159.2082	148.49	
H(C1)	8.47 (s)	8.3584	4.2569	8.1098	5.2715	8.5151	5.8166	7.0073	6.3514	7.0863	
H(C8)	7.98–7.87 (m)	8.2169	4.8496	8.2531	5.4138	8.4182	6.158	6.9139	6.2922	6.9991	
H(C4)	7.98–7.87 (m)	8.9763	5.482	8.9544	6.0496	9.1872	6.8131	7.5839	7.0184	7.6784	
H(C7)	7.70–7.50 (m)	7.6781	4.1285	7.7411	4.6472	8.0075	5.4645	6.3214	5.7666	6.4231	
H(C5)	7.70–7.50 (m)	7.7564	4.2114	7.8066	4.7233	8.0708	5.5502	6.3902	5.8277	6.5045	
Atom	NMR [6] (CDCl ₃)	B3LYP/6-31G(d)		B3LYP/6-31++G(d,p)		B3LYP/6-311++G(d,p)		B3LYP/6-311++G(df,pd)		BLYP/6-311++G(df,pd)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
C2	164.11	157.7144	163.4049	170.0228	157.6896	161.1096	168.1992	167.8084	180.8307	173.1167	169.1711
C1	152.74	144.2677	151.5806	155.1865	145.8896	147.6441	154.0265	153.7755	165.9618	156.5939	153.3882
C7	131.83	125.6509	126.5753	137.0526	128.3688	128.4008	132.0606	134.3938	147.1362	136.8397	134.1611
C5	131.83	126.2301	127.2153	137.7161	129.0001	128.4635	132.8532	135.0762	147.9161	137.4941	134.7449
C4	128.51	122.851	124.4105	133.822	125.7001	126.0981	129.6799	131.9292	143.8283	133.1958	131.0471
C8	128.51	120.872	122.3286	131.3327	123.998	123.6569	127.748	129.7566	141.3182	130.6514	128.8966
C3	126.82	117.5598	118.8369	129.0798	119.1797	121.8972	126.3905	126.4622	138.2575	128.1911	126.5044
C6	122.35	139.2677	139.7682	151.6241	144.3194	141.5253	146.148	150.6907	161.08	154.1147	153.7256
H(C1)	8.47 (s)	7.7749	4.1243	7.8006	5.2302	8.2274	5.7287	6.94	6.0579	8.2932	7.0318
H(C8)	7.98–7.87 (m)	7.6439	4.5497	7.8491	5.2274	7.9792	5.8811	6.699	5.8032	7.8483	6.6345
H(C4)	7.98–7.87 (m)	8.3688	5.1684	8.5138	5.8629	8.7219	6.5141	7.3527	6.5579	7.4611	7.2787
H(C7)	7.70–7.50 (m)	7.2436	3.9402	7.4795	4.5842	7.7627	5.3364	6.2453	5.4428	7.5311	6.2269
H(C5)	7.70–7.50 (m)	7.295	4.0102	7.5204	4.6524	7.77	5.4087	6.3031	5.4734	7.5523	6.2879

Table 7 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts (with respect to TMS, all values in ppm) for 2-m-Tolyl-1,3,4-oxadiazole (**5f**)

Atom	NMR [6] (CDCl ₃)	HF/6-31G(d)		HF/6-31++G(d,p)		HF/6-311++G(d,p)		HF/6-311++G(df,pd)			
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT		
C2	164.90	166.7313	172.5826	173.806	161.5795	168.3503	176.3362	175.9842	171.4805	185.1328	172.1106
C1	152.56	153.3709	160.8417	159.6352	149.7048	154.5951	162.5753	162.4188	158.0774	171.2499	158.412
C5	139.02	136.4856	136.0029	144.7598	137.166	140.6002	143.2834	147.0071	144.391	155.8247	145.7766
C4	132.80	130.1284	132.942	136.2178	127.9841	131.1359	135.7521	138.0296	133.6329	146.9241	135.0114
C6	129.01	132.8819	134.8365	139.8945	132.9857	134.1313	138.4319	141.6221	138.2234	150.5145	139.528
C7	127.61	126.7472	128.629	133.3906	126.706	128.4957	132.5911	135.6035	132.241	144.5053	133.4346
C8	124.21	125.4044	127.5088	131.3011	124.3148	126.2244	130.643	133.1096	129.4309	141.8692	130.6913
C3	123.33	123.0224	123.8538	130.0016	120.8333	126.5487	130.3172	131.7433	128.0717	140.3999	129.8355
C(CH ₃)	21.32	20.4593	20.7972	20.7706	18.8608	20.8317	22.9103	21.39	20.32	30.5338	20.858
H(C1)	8.46 (s)	8.3231	4.318	8.0847	5.338	8.4768	5.8413	8.3061	7.0337	6.3137	7.113
H(C8)	7.90–7.80 (m)	8.0896	5.038	8.1568	5.5714	8.2401	6.2131	8.2334	6.9284	6.1441	6.9878
H(C4)	7.90–7.80 (m)	8.7895	5.909	8.8131	6.2513	8.9989	6.8456	8.9566	7.6449	6.8994	7.7245
H(C6)	7.43–7.31 (m)	7.7122	5.0362	7.7836	5.6219	7.8932	6.0583	7.8173	6.8114	5.7434	6.8874
H(C7)	7.43–7.31 (m)	7.6161	4.9575	7.685	5.4223	7.737	5.9002	7.6977	6.6551	5.6245	6.7265
H(CH ₃)	2.43 (s)	2.5949	1.5338	2.7054	1.6336	2.6892	1.8774	2.6792	2.0225	0.5852	2.1235
H(CH ₃)	2.43 (s)	2.2317	1.087	2.3663	1.167	2.342	1.4745	2.3419	1.6353	0.2905	1.7445
H(CH ₃)	2.43 (s)	2.5951	1.534	2.7056	1.634	2.6886	1.8768	2.6844	2.0283	0.5904	2.1287
Atom	NMR [6] (CDCl ₃)	B3LYP/6-31G(d)		B3LYP/6-31++G(d,p)		B3LYP/6-311++G(d,p)		B3LYP/6-311++G(df,pd)			
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT		
C2	164.90	158.4449	164.2114	170.886	158.5763	162.2139	169.0146	172.7564	168.8144	181.6494	169.2073
C1	152.56	144.0504	151.4557	154.9344	145.8282	147.4378	153.862	157.1912	153.6151	165.7627	153.779
C5	139.02	132.7046	132.118	145.3663	137.968	139.0878	140.8098	147.1893	145.2775	155.4699	146.3067
C4	132.80	122.7873	125.713	133.0516	125.3167	125.5632	130.2512	134.7991	131.0825	142.6466	132.1424
C6	129.01	125.2323	127.4881	136.9733	130.6078	127.461	132.8076	138.5411	135.7543	147.0448	136.7821
C7	127.61	121.8472	123.2134	132.822	126.314	124.6095	128.8692	134.5705	131.8273	143.1084	132.7735
C8	124.21	117.7821	119.8718	127.9143	121.2585	120.6653	124.7219	129.169	126.3036	137.6366	127.2924
C3	123.33	118.6679	119.5689	130.1557	120.5885	123.3671	127.6156	131.1658	128.1591	139.5272	129.6658
C(CH ₃)	21.32	21.8537	22.2735	23.1511	21.3595	23.5903	24.8664	23.5292	22.7764	32.4294	23.1602
H(C1)	8.46 (s)	7.7472	4.1877	7.7824	5.302	8.2099	5.7585	8.1233	6.9768	6.0273	7.0682
H(C8)	7.90–7.80 (m)	7.5767	4.7822	7.8151	5.4407	7.8526	5.9888	7.9655	6.7719	5.7451	6.8563
H(C4)	7.90–7.80 (m)	8.2634	5.3412	8.4483	6.1526	8.058	6.5892	8.6904	7.4858	6.4555	7.5765
H(C6)	7.43–7.31 (m)	7.2291	4.7066	7.4491	5.4376	7.677	5.7729	7.56	6.6024	5.3443	6.6966
H(C7)	7.43–7.31 (m)	7.2678	4.7452	7.4713	5.3675	7.5646	5.7625	7.5536	6.5741	5.3174	6.6657

Table 8 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts (with respect to TMS, all values in ppm) for 2-p-Tolyl-1,3,4-oxadiazole (**5g**)

Atom	NMR [6] (CDCl ₃)	HF/6-31G(d)		HF/6-31G(d)		HF/6-31++G(d,p)		HF/6-31++G(d,p)		HF/6-31++G(df,pd)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
C2	164.89	167.7388	172.6217	173.7655	161.5722	168.344	176.3157	175.9671	171.4542	185.0242	179.4136
C1	152.37	153.1484	160.618	159.3399	149.4232	154.4116	162.2933	162.0847	157.7898	170.944	163.9182
C6	142.58	142.8827	142.2571	151.5107	144.0344	146.798	149.4027	153.7342	151.098	162.5252	159.8194
C7	129.81	126.276	128.9439	132.3442	125.426	127.3941	131.9856	134.1704	130.5785	142.9919	143.4381
C5	129.81	127.0218	129.2471	133.7594	126.7559	128.3636	132.7275	135.6128	132.1521	144.4745	144.3038
C8	127.03	128.9409	130.5594	135.3356	128.0563	130.3908	134.5849	137.6211	133.7927	146.5421	140.7169
C4	127.03	130.9853	132.8961	137.6091	129.7231	132.4518	136.5806	139.6565	135.6813	148.6435	142.6631
C3	120.70	119.8372	121.0732	126.4476	117.376	122.8435	126.864	127.798	124.0875	136.3804	137.287
C(CH ₃)	21.65	20.7742	21.1239	21.0654	19.1512	21.224	23.1946	21.5726	20.5828	30.71	33.7705
H(C1)	8.44 (s)	8.3032	4.3027	8.0593	5.316	8.4448	5.8192	8.284	7.0091	6.2832	7.2615
H(C8)	7.99–7.83 (m)	8.2172	5.1455	8.2818	5.7095	8.3908	6.3399	8.3782	7.0677	6.291	7.1666
H(C4)	7.99–7.83 (m)	8.9913	5.815	9.0118	6.3906	9.1631	7.0245	9.0897	7.7929	7.026	7.8774
H(C7)	7.34–7.18 (m)	7.4042	4.7396	7.452	5.2987	7.5614	5.7063	7.5212	6.4697	5.4492	6.7463
H(C5)	7.34–7.18 (m)	7.5825	4.9226	7.6746	5.5044	7.7233	5.9086	7.707	6.7106	5.6407	6.95
H(CH ₃)	2.43 (s)	2.173	1.0656	2.2234	1.0635	2.2688	1.4313	2.1916	1.5217	0.13	1.7648
H(CH ₃)	2.43 (s)	2.6098	1.5642	2.7181	1.6618	2.7591	1.9489	2.6952	2.0575	0.6027	2.3818
H(CH ₃)	2.43 (s)	2.4969	1.4201	2.7181	1.6618	2.5712	1.7512	2.6952	2.0575	0.6028	2.3818
Atom	NMR [6] (CDCl ₃)	B3LYP/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31++G(d,p)		B3LYP/6-31++G(d,p)		B3LYP/6-31++G(df,pd)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
C2	164.89	158.4073	164.1975	170.7631	158.5042	161.8923	168.8934	172.8236	168.6583	181.6562	169.0358
C1	152.37	143.8376	151.2986	154.7102	145.6035	147.1679	153.6551	156.8856	153.399	165.4279	153.5404
C6	142.58	135.0803	134.9962	148.6627	141.4154	139.8971	143.4523	150.1434	148.4242	158.3793	149.4416
C7	129.81	122.8984	125.071	133.6248	126.61	125.923	129.9879	135.0615	132.0237	143.4704	133.0603
C5	129.81	123.1618	124.9954	134.3449	127.4142	125.8606	130.3128	135.7701	132.969	144.1635	133.926
C8	127.03	120.2869	121.8231	130.7941	123.7758	123.1371	127.413	132.4877	129.3277	140.9704	130.3391
C4	127.03	122.1104	124.0386	132.9702	125.4798	124.9673	129.2915	134.5115	131.2842	143.1544	132.2853
C3	120.70	116.4335	117.8821	127.9397	118.3456	121.1844	125.3725	128.7615	125.4523	136.9997	126.9092
C(CH ₃)	21.65	22.2662	22.5993	23.3899	21.6764	22.6029	25.159	23.597	23.0048	32.243	23.3927
H(C1)	8.44 (s)	7.7445	4.1791	7.7693	5.2876	8.2216	5.7439	8.1406	6.958	6.0092	7.0448
H(C8)	7.99–7.83 (m)	7.6681	4.8532	7.8936	5.5316	8.0633	6.0729	8.0814	6.8624	5.872	6.9499
H(C4)	7.99–7.83 (m)	8.4113	5.5137	8.5893	6.2187	8.7719	6.7351	8.7558	7.5729	6.5729	7.6607
H(C7)	7.34–7.18 (m)	7.0983	4.5621	7.2778	5.2881	7.3697	5.588	7.4121	6.439	5.2433	6.5296
H(C5)	7.34–7.18 (m)	7.2384	4.7143	7.4727	5.4498	7.4743	5.768	7.5544	6.6432	5.5591	6.7333

Table 9 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts in different dihedral angles (with respect to TMS, all values in ppm) for 2-Phenyl-1,3,4-oxadiazole (**5a**)

Atom	NMR [6] (CDCl_3)	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
		5a ($\phi = -135.0^\circ$)		5a ($\phi = -90.0^\circ$)		5a ($\phi = -135.0^\circ$)		5a ($\phi = -90.0^\circ$)	
C2	164.79	168.0781	173.6794	167.593	172.4389	160.0464	165.6756	159.4408	164.5983
C1	152.67	154.895	162.4672	154.8819	162.4165	145.6814	153.2451	145.2829	152.8187
C8	132.03	129.4981	131.3621	131.1238	133.0152	121.9493	123.9295	124.2337	126.3107
C4	132.03	132.3101	134.2165	131.1464	133.0375	124.5159	126.686	124.2558	126.3315
C7	129.13	126.3508	127.9423	126.4359	128.0063	121.5626	122.8231	121.1595	122.4463
C5	129.13	126.864	128.4579	126.4338	128.0034	122.0099	123.3351	121.1554	122.4418
C6	127.10	131.9155	133.1761	131.1569	132.6042	124.0359	125.4353	123.6781	125.2554
C3	123.43	124.5414	125.0521	125.9082	125.9565	120.2314	121.0837	121.2899	121.9892
H(C1)	8.42 (s)	8.3937	4.4289	8.3902	4.4537	7.8547	4.3261	7.848	4.3382
H(C8)	8.11–8.05 (m)	7.9814	4.9697	7.6834	4.7494	7.4878	4.7116	7.2303	4.524
H(C4)	8.11–8.05 (m)	8.3116	5.2143	7.6831	4.7497	7.7763	4.9445	7.2301	4.5242
H(C7)	7.59–7.48 (m)	7.6926	4.9845	7.6874	5.0099	7.3605	4.7924	7.3599	4.811
H(C5)	7.59–7.48 (m)	7.7164	5.0276	7.6873	5.0096	7.3873	4.8302	7.3596	4.8107
H(C6)	7.59–7.48 (m)	7.8628	5.1406	7.8704	5.1714	7.42	4.8473	7.4586	4.9071

Table 10 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts in different dihedral angles (with respect to TMS, all values in ppm) 2-(3-Bromophenyl)-1,3,4-oxadiazole (**5b**) and 2-(4-Bromophenyl)-1,3,4-oxadiazole (**5c**)

Atom	NMR [6] (CDCl_3)	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
		5b ($\phi = -135.0^\circ$)		5b ($\phi = -90.0^\circ$)		5b ($\phi = -135.0^\circ$)		5b ($\phi = -90.0^\circ$)	
C2	163.53	166.905	172.4448	166.3916	171.1682	158.9724	164.5948	158.1827	163.404
C1	152.87	155.2024	162.6348	155.111	162.5191	145.9395	153.3637	145.4644	152.8896
C4	135.01	135.7245	137.1175	134.9738	136.2962	127.6199	129.5858	127.6791	129.5893
C6	130.73	135.7663	136.5983	135.176	136.1858	127.654	129.0017	127.425	128.9736
C7	129.96	127.199	128.6633	127.2404	128.7106	122.602	123.7139	122.2164	123.3743
C8	125.63	128.7991	130.7754	130.6227	132.617	120.3247	122.566	122.7262	125.1231
C3	125.25	125.8654	126.1089	127.273	127.0451	121.7272	122.573	123.0196	123.3943
C5	123.14	135.2474	135.7194	134.7153	135.2097	136.4025	136.32	135.4251	135.4865
H(C1)	8.50 (s)	8.4181	4.3676	8.4134	4.3899	7.8676	4.2614	7.8544	4.2702
H(C4)	8.24–8.23 (m)	8.3115	4.4357	7.6961	3.9695	7.6924	4.1876	7.1492	3.7637
H(C8)	8.04–8.01 (m)	7.8893	4.698	7.6036	4.4856	7.3016	4.3685	7.0565	4.1882
H(C7)	7.72–7.67 (m)	7.6416	4.69	7.6359	4.714	7.2465	4.4562	7.2418	4.4746
H(C4)	7.44–7.34 (m)	7.8777	4.3398	7.894	4.3752	7.3261	4.0621	7.3754	4.1266

Atom	NMR [6] (CDCl_3)	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO	CSGT	GIAO	CSGT	GIAO	CSGT	GIAO	CSGT
		5c ($\phi = -135.0^\circ$)		5c ($\phi = -90.0^\circ$)		5c ($\phi = -135.0^\circ$)		5c ($\phi = -90.0^\circ$)	
C2	164.11	167.1837	172.7431	166.5659	171.3644	159.1812	164.7814	158.4852	163.5701
C1	152.74	155.1391	162.5811	155.1387	162.5704	145.8579	153.2975	145.5489	153.0011
C7	131.83	130.5708	131.6601	130.6117	131.7139	125.376	126.5911	125.0116	126.2488
C5	131.83	131.0753	132.1853	130.6091	131.711	125.8411	127.1124	125.0068	126.2445
C4	128.51	132.8688	134.64	131.9246	133.6539	125.3771	127.3983	125.3089	127.2192
C8	128.51	130.0166	131.725	131.9041	133.6335	122.7311	124.562	125.2895	127.201
C3	126.82	124.3396	124.8304	125.6976	125.7253	119.0119	120.0282	120.0543	120.9216

Table 10 continued

Atom	NMR [6] (CDCl ₃) 5c	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO 5c ($\phi = -135.0^\circ$)	CSGT	GIAO 5c ($\phi = -90.0^\circ$)	CSGT	GIAO 5c ($\phi = -135.0^\circ$)	CSGT	GIAO 5c ($\phi = -90.0^\circ$)	CSGT
C6	122.35	141.2563	141.4676	140.4186	140.7798	139.2775	139.5634	138.8066	139.2039
H(C1)	8.47 (s)	8.4133	4.365	8.4123	4.3936	7.855	4.2569	7.8568	4.2788
H(C8)	7.98–7.87 (m)	7.9121	4.651	7.6216	4.4374	7.3633	4.3563	7.1054	4.1727
H(C4)	7.98–7.87 (m)	8.2465	4.8987	7.6213	4.4378	7.6577	4.5937	7.1053	4.173
H(C7)	7.70–7.50 (m)	7.7219	4.1982	7.7144	4.2191	7.2816	4.0121	7.2764	4.0296
H(C5)	7.70–7.50 (m)	7.7444	4.2407	7.7143	4.2189	7.3033	4.0498	7.2762	4.0293

Table 11 Theoretical and experimental ¹³C and ¹H isotropic chemical shifts in different dihedral angles (with respect to TMS, all values in ppm) for for 2-(3-Chlorophenyl)-1,3,4-oxadiazole (**5d**) and 2-(4-Chlorophenyl)-1,3,4-oxadiazole (**5e**)

Atom	NMR [6] (CDCl ₃) 5d	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO 5d ($\phi = -135.0^\circ$)	CSGT	GIAO 5d ($\phi = -90.0^\circ$)	CSGT	GIAO 5d ($\phi = -135.0^\circ$)	CSGT	GIAO 5d ($\phi = -90.0^\circ$)	CSGT
C2	163.17	166.9283	172.47	166.3689	171.1414	159.0143	164.593	158.2089	163.3466
C1	152.84	155.1987	162.6505	155.0954	162.5138	145.938	153.3866	145.4749	152.8971
C5	135.28	137.4049	134.9999	136.8948	134.5377	137.5515	134.8615	136.6283	134.0073
C4	132.09	132.7896	134.4994	131.9999	133.6279	124.9547	127.1235	124.9682	127.0855
C6	130.52	132.6327	133.7872	132.0526	133.3773	124.8039	126.3654	124.5857	126.3366
C7	127.11	127.3274	128.9603	127.3665	129.0032	122.5611	123.8706	122.1491	123.516
C8	125.20	128.0545	130.1214	129.9074	131.9885	119.8467	122.1545	122.2879	124.7386
C3	125.07	125.9634	126.3185	127.3403	127.2408	121.694	122.4223	122.9526	123.4415
H(C1)	8.50 (s)	8.4119	4.3728	8.4076	4.3945	7.8641	4.268	7.8514	4.2766
H(C4)	8.05–7.95 (m)	8.2184	4.4084	7.5968	3.9354	7.61	4.1149	7.0564	3.6824
H(C8)	7.86–7.78 (m)	7.8463	4.7086	7.5596	4.497	7.2764	4.3979	7.0302	4.2192
H(C5)	7.58–7.44 (m)	7.771	4.3042	7.7886	4.3416	7.2455	3.9809	7.2923	4.048
H(C7)	7.58–7.44 (m)	7.6474	4.7254	7.6416	4.7504	7.2702	4.5015	7.2647	4.5205

Atom	NMR [6] (CDCl ₃) 5e	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO 5e ($\phi = -135.0^\circ$)	CSGT	GIAO 5e ($\phi = -90.0^\circ$)	CSGT	GIAO 5e ($\phi = -135.0^\circ$)	CSGT	GIAO 5e ($\phi = -90.0^\circ$)	CSGT
C2	164.01	167.1601	172.7231	166.5732	171.3802	159.1383	164.7432	158.4731	163.5814
C1	152.73	155.1045	162.5646	155.1393	162.5788	145.8413	153.2958	145.5567	153.0086
C6	138.36	142.8277	140.2041	142.0707	139.5954	140.0208	137.649	139.6284	137.3629
C7	129.55	127.498	128.8868	127.5323	128.9327	122.5777	123.975	122.2096	123.6227
C5	129.55	127.9849	129.3869	127.5299	128.9297	123.0335	124.4746	122.2046	123.618
C8	128.38	130.2683	132.1465	132.1333	134.0367	122.7821	124.7664	125.3269	127.4041
C4	128.38	133.1432	135.0841	132.1519	134.0553	125.4453	127.6251	125.3446	127.4205
C3	121.92	123.577	124.1624	124.9083	125.0324	118.5959	119.6284	119.6178	120.4994
H(C1)	8.49 (s)	8.4034	4.3659	8.4047	4.3967	7.8514	4.2597	7.8546	4.283
H(C8)	8.03 (d)	7.9255	4.6969	7.633	4.4819	7.3865	4.4103	7.1289	4.2257
H(C4)	8.03 (d)	8.2604	4.9444	7.6326	4.4822	7.6819	4.6471	7.1286	4.226
H(C7)	7.50 (d)	7.6134	4.1624	7.6073	4.1843	7.1862	3.9333	7.181	3.951
H(C5)	7.50 (d)	7.6361	4.2058	7.6073	4.1842	7.2087	3.9724	7.1808	3.9509

Table 12 Theoretical and experimental ^{13}C and ^1H isotropic chemical shifts in different dihedral angles (with respect to TMS, all values in ppm) for for 2-m-Tolyl-1,3,4-oxadiazole (**5f**) and 2-p-Tolyl-1,3,4-oxadiazole (**5g**)

Atom	NMR [6] (CDCl_3) 5f	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO 5f ($\phi = -135.0^\circ$)	CSGT	GIAO 5f ($\phi = -90.0^\circ$)	CSGT	GIAO 5f ($\phi = -135.0^\circ$)	CSGT	GIAO 5f ($\phi = -90.0^\circ$)	CSGT
C2	164.90	168.2079	173.8119	167.7256	172.5908	160.1884	165.786	159.5498	164.7563
C1	152.56	154.7995	162.3972	154.7977	162.3501	145.5566	153.1354	145.1872	152.7408
C5	139.02	136.584	136.2119	136.0825	135.6928	132.44	132.1003	131.4615	131.0764
C4	132.80	132.2024	135.1457	131.1538	134.0879	125.2627	128.5048	125.0313	128.2805
C6	129.01	132.2248	134.2496	131.4103	133.6007	125.0032	127.2036	124.5286	126.9056
C7	127.61	127.0125	128.831	127.0885	128.9094	121.6396	123.118	121.2317	122.7443
C8	124.21	126.5798	128.9164	128.1699	130.5566	119.4852	121.9705	121.7211	124.3428
C3	123.33	124.9078	125.4131	126.3729	126.4061	120.114	120.9033	121.2881	121.829
C(CH ₃)	21.32	20.4733	20.8739	20.4502	20.8351	21.932	22.3843	21.9072	22.3184
H(C1)	8.46 (s)	8.377	4.4275	8.3757	4.4527	7.8333	4.3215	7.8312	4.3356
H(C8)	7.90–7.80 (m)	7.7737	4.8402	7.4747	4.6174	7.2891	4.5939	7.033	4.4028
H(C4)	7.90–7.80 (m)	8.0782	5.0433	7.4339	4.5642	7.5607	4.7934	6.9938	4.3554
H(C6)	7.43–7.31 (m)	7.7299	5.0765	7.7399	5.1068	7.2894	4.7748	7.322	4.8321
H(C7)	7.43–7.31 (m)	7.6538	5.0181	7.6479	5.0414	7.3032	4.8024	7.2913	4.818
H(CH ₃)	2.43 (s)	2.6556	1.6137	2.6474	1.6089	2.5632	1.5523	2.5653	1.5541
H(CH ₃)	2.43 (s)	2.2429	1.1309	2.1323	1.0445	2.0411	1.0325	1.9393	0.9431
H(CH ₃)	2.43 (s)	2.4605	1.4049	2.4961	1.4458	2.3247	1.3218	2.3651	1.6694
Atom	NMR [6] (CDCl_3) 5g	HF/6-31G(d)		HF/6-31G(d)		B3LYP/6-31G(d)		B3LYP/6-31G(d)	
		GIAO 5g ($\phi = -135.0^\circ$)	CSGT	GIAO 5g ($\phi = -90.0^\circ$)	CSGT	GIAO 5g ($\phi = -135.0^\circ$)	CSGT	GIAO 5g ($\phi = -90.0^\circ$)	CSGT
C2	164.89	168.1493	173.8016	167.7001	172.6022	160.0208	165.7281	159.5632	164.7821
C1	152.37	154.7149	162.3126	154.8974	162.4618	145.4918	153.0768	145.3007	152.8725
C6	142.58	142.2831	141.6081	141.3248	140.8711	134.8776	134.6207	134.3461	134.2977
C7	129.81	126.5825	129.287	126.6008	129.0864	122.6679	125.0829	122.042	124.3121
C5	129.81	127.0158	129.316	126.5915	129.0614	122.8041	124.8966	122.042	124.2791
C8	127.03	132.1846	132.0185	131.7633	133.7245	122.0041	123.9539	124.295	126.4169
C4	127.03	132.9203	135.0308	131.7401	133.7107	124.5609	126.9252	124.2746	126.4046
C3	120.70	121.493	122.3305	122.682	123.0731	117.7835	118.9689	118.6046	119.6567
C(CH ₃)	21.65	20.7109	21.0669	20.7418	21.1417	22.1729	22.5135	22.2212	22.6147
H(C1)	8.44 (s)	8.3671	4.4206	8.3782	4.4619	7.8283	4.3195	7.8385	4.3507
H(C8)	7.99–7.83 (m)	7.9034	4.9411	7.6211	4.7416	7.3807	4.6571	7.1406	4.4909
H(C4)	7.99–7.83 (m)	8.2652	5.2323	7.6223	4.7436	7.7098	4.942	7.1422	4.4932
H(C7)	7.34–7.18 (m)	7.454	4.8156	7.4913	4.8851	7.1415	4.6351	7.172	4.6896
H(C5)	7.34–7.18 (m)	7.5695	4.9501	7.4947	4.8885	7.2358	4.7487	7.1746	4.6923
H(CH ₃)	2.43 (s)	2.1904	1.1015	2.3677	1.2963	1.9786	0.9936	2.189	1.2041
H(CH ₃)	2.43 (s)	2.6254	1.5932	2.6202	1.6069	2.5316	1.5286	2.5335	1.5548
H(CH ₃)	2.43 (s)	2.5392	1.4792	2.3794	1.3088	2.3977	1.3942	2.2034	1.2174

explicitly displayed. The comparison of the GIAO and CSGT methods shows that the latter are more sensitive to the quality of the basis set employed. In other words, convergence of calculated chemical shifts is faster with the CSGT method. In particular, calculations by HF method with 6-31G(d), 6-31++G(d,p), and 6-311++G(df,pd)

basis sets provide quite good results for **5a–d** and **5f**. While the linear correlation coefficients of GIAO and CSGT models for the molecules (**5b–d**) which aromatic ring is bounded at meta or para positions of different electronegative atoms (Cl and Br) are different, the molecules (**5a**, **5e–g**) are roughly similar. Although the B3LYP level of

Table 13 Linear correlation coefficients (R^2) of linear regression analysis of theoretical and experimental ^{13}C isotropic chemical shifts for 2-aryl-1,3,4-oxadiazole derivatives (**5a–g**)

Molecules	Basis sets	HF		B3LYP	
		GIAO ^{13}C	CSGT ^{13}C	GIAO ^{13}C	CSGT ^{13}C
5a	6-31G(d)	0.95407	0.9553	0.95404	0.95875
	6-311G(d)	0.95154	0.93501	0.94585	0.9333
	6-31++G(d,p)	0.95851	0.96343	0.95366	0.9578
	6-311++G(d,p)	0.95199	0.94816	0.94413	0.94249
	6-311++G(df,pd)	0.88217	0.87642	0.90183	0.89361
5b	6-31G(d)	0.8131	0.83943	0.69455	0.76742
	6-311G(d)	0.81299	0.76539	0.68441	0.62318
	6-31++G(d,p)	0.82782	0.8519	0.71672	0.74789
	6-311++G(d,p)	0.80753	0.80456	0.68087	0.66638
	6-311++G(df,pd)	0.89429	0.8791	0.70145	0.6965
5c	6-31G(d)	0.77289	0.82153	0.67231	0.7463
	6-311G(d)	0.77058	0.70485	0.65104	0.58198
	6-31++G(d,p)	0.77232	0.8167	0.69691	0.71685
	6-311++G(d,p)	0.76514	0.74555	0.65701	0.62773
	6-311++G(df,pd)	0.77387	0.74585	0.67177	0.61972
5d	6-31G(d)	0.84235	0.90353	0.66914	0.79589
	6-311G(d)	0.82452	0.77423	0.64858	0.5869
	6-31++G(d,p)	0.8125	0.8697	0.60203	0.72361
	6-311++G(d,p)	0.81282	0.79775	0.6609	0.61413
	6-311++G(df,pd)	0.98889	0.97774	0.93126	0.88292
5e	6-31G(d)	0.9802	0.98749	0.95483	0.99186
	6-311G(d)	0.97543	0.942	0.94044	0.90085
	6-31++G(d,p)	0.96913	0.98642	0.95094	0.97213
	6-311++G(d,p)	0.97274	0.95831	0.94735	0.92314
	6-311++G(df,pd)	0.97401	0.95593	0.9477	0.91557
5f	6-31G(d)	0.96852	0.96987	0.9636	0.96749
	6-311G(d)	0.96606	0.95978	0.96044	0.95298
	6-31++G(d,p)	0.96598	0.9688	0.95802	0.96476
	6-311++G(d,p)	0.96581	0.9617	0.95998	0.95516
	6-311++G(df,pd)	0.99793	0.99727	0.99659	0.99534
5g	6-31G(d)	0.99669	0.99413	0.99925	0.99636
	6-311G(d)	0.99685	0.99609	0.99853	0.99829
	6-31++G(d,p)	0.99645	0.99619	0.99863	0.99833
	6-311++G(d,p)	0.99666	0.99646	0.99892	0.99869
	6-311++G(df,pd)	0.99653	0.99813	0.99897	0.99813

theory includes the effects of electron correlation, the B3LYP is not quite as accurate as HF for ^{13}C chemical shifts. In these state, geometric parameters and chemical shifts for diverse molecular structure analysis change with respect to the different theoretical approaches. However, the NMR spectrum is used in chemical analysis to determine the structures of complicated organic molecules.

The ^{13}C chemical shifts calculations of the title compounds (**5a–g**) are directly related to linear correlation coefficients (R^2) of GIAO and CSGT calculations. Linear

correlation coefficients (R^2) of the larger molecules **5f** and **5g** have been obtained as better than the others (**5a–e**). Further variation in meta and para positions of the aromatic-substituent groups and the π -conjugation network containing the oxadiazole ring in the core structure is necessary for reaching a concrete inference.

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