Computational study of N-(2,4-Dichlorophenyl)benzamide

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ABSTRACT

The vibrational wavenumbers of N-(2,4-Dichlorophenyl)benzamide were calculated using Gaussian03 software package and the fundamental modes are assigned. The predicted infrared, Raman activities, force constants and polarization rations are reported. The first hyperpolarizability is calculated and the N-(2,4-Dichlorophenyl) benzamide is an attractive object for future studies of non linear optics. The calculated geometrical parameters are in agreement with the reported experimental values.

Key words: N-(2,4-Dichlorophenyl)benzamide, Benzamide, HF calculations, hyperpolarizability.

INTRODUCTION

Benzamide derivatives exhibit various types of biological properties such as anthelmentic, antihistaminic, antifungal, and antibacterial[1-9]. Arslan *et al.*[10] reported the molecular structure and vibrational spectra of 2-chloro-N-(diethyl carbamothioyl) benzamide by Hartree-Fock and density functional methods. Takeuchi *et al.*[11] reported the molecular structure of benzamide as studied by gas phase electron diffraction. In the past few decades, the dramatically rising prevalence of multidrug-resistant microbial infections has become a serious health care problem. In particular, the emergence of multi-drug resistant strains of Gram-positive bacterial pathogens such as methicillin-resistant *Staphylococcus aureus* and *Staphylococcus epidermis* and vancomycin-resistant *Enterococcus* is a problem of ever-increasing significance[12-16]. 6-N-(2-hydroxy-3,5-dichlorophenyl)-2-hydroxy-3,5,6-trichlorobenzamide (oxyclozanide) which has a benzamide structure,

was discovered in 1969 as an anthelmentic agent effective against *Fasciola* hepatica for the treatment of liver fluke infection[1]. 3,4-Dihydroxy-6-(N-ethylamino)benzamide is a natural product that has been found in green pepper (*Piper nigrum L.*) as an antibacterial by Pradhan *et al.*,[6]. Additionally, a benzamide derivative, BAS-118, has been found to be a novel anti-*Helicobacter pylori* agent with a potent and selective antibacterial activity, which includes clarithromycin (CAM)- and metronidazole (MNDZ)-resistant isolates[6]. Yalcin *et al.*,[5,7-9] reported some novel microbiologically active N-(2–hydroxy-5-substitutedphenyl) benzamide/phenyl acetamide/ phenoxy acetamide / thiophenoxy acetamide derivatives. The synthesis and biological evaluation of N-(2-hydroxy-4(or5) -nitro/aminophenyl) benzamides and phenyl acetamides as antimicrobial agents are reported by Ertan *et al.*,[17]. 2-hydroxy-N-phenylbenzamides have been reported as a class of compounds with a wide variety of interesting biological activities, including antimycobacterial and antifungal effects[18-22]. Gas phase structures of

fundamental amides, formamide[23] and acetamide[24] were determined by electron diffraction and their crystal structures were studied by X-ray and neutron diffraction[25-29]. The crystal structures of benzamide were determined by X-ray and neutron diffraction[30,31]. The hydrogen bonding interactions between thioacetamide and several N,N-disubstituted benzamides have been studied using near infrared absorption spectroscopy[32]. Kawski *et al.*[33] reported the X-Ray, IR investigation and quantum mechanical calculations of 2-hydroxy-benzamides. Gowda *et al.*[34] reported the crystal structure of N-(2,4-Dichlorophenyl)benzamide. In the present work, we have calculated the vibrational frequencies and geometrical parameters of the title compound theoretically using Gaussian03 software package and the geometrical parameters are compared with the results given by Gowda *et al.*[34] and other similar derivatives.

Computational Details

Calculations of the title compound were carried out with Gaussian03 program[35] using the HF/6-31G* level of theory to predict the molecular structure and wavenumbers. Molecular geometry was fully optimized by Berny's optimization algorithm using redundant internal coordinates. Harmonic vibrational wavenumbers were calculated using the analytic second derivatives to confirm the convergence to minimum on the potential surface. The wavenumber values computed theoretically contain known systematic errors due to the negligence of electron correlation[36]. We therefore, have used the scaling factor value of 0.8929 for HF/6-31G* basis set. The absence of imaginary wavenumber on the calculated vibrational spectrum confirms that the structure deduced corresponds to minimum energy. The geometrical parameters corresponding to the optimized geometry is given in table 1 together with reported values.
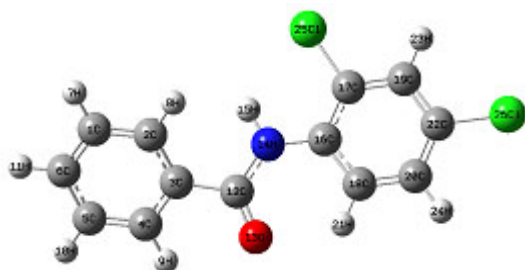

Fig. 1: Optimized geometry

RESULTS AND DISCUSSION

The calculated (scaled) wavenumbers and their assignments are given in Table 2. The carbonyl stretching C=O vibrations[37,38] are expected in the region 1715-1680 cm^{-1} and in the present study the calculated value corresponding to this mode appears at 1749 cm. El-Shahawy *et al.*[39] reported a value 1640 cm^{-1} in the IR spectrum as νC=O for paracetamol. The deviation of the calculated value for this mode can be attributed to the under estimation of the large degree of π-electron delocalization due to conjugation in the molecule[40]. The NH stretching vibration[37] appears as a strong and broad band in the region 3390 ± 60 cm^{-1}. For the title compound, the calculated value for this mode is 3489 cm^{-1}. The CNH vibration, in which the N and H atoms move in opposite direction of the carbon atom in the amide moiety appears at 1528 cm^{-1} and the CNH vibration, in which the N and H atoms move in the same direction of the carbon atom in the amide group appears at 1253 cm^{-1}. The calculated value of NH rocking is 1097 cm^{-1}. The band at 828 cm^{-1} is assigned as out-of-plane wagging mode of NH.

For simple organic molecules, CCl stretching vibrations are expected in the region 750-700 cm^{-1}. Sundaraganesan *et al.*[41] reported δCCl at 704 (IR), 705 (Raman) and at 715 cm^{-1} theoretically. In the following discussion, the mono and tri-substituted phenyl rings are designated as PhI and PhII, respectively. The benzene ring possesses six ring stretching vibrations of which the four with the highest wavenumbers occurring near 1600, 1580, 1490 and 1440 cm^{-1} are good group vibrations[37]. With heavy substituents, the bands tend to shift to somewhat lower wavenumbers, and the greater the number of substituents on the ring, the broader the absorption region[37]. In the case of C=O substitution, the band near 1490 cm^{-1} can be very weak[37]. The fifth ring stretching vibration is active near 1315 ± 65 cm^{-1}, a region that overlaps strongly with that of the CH in-plane deformation[37]. The sixth ring stretching vibration, the ring breathing mode, appears as a weak band near 1000 cm^{-1} in mono, 1,3-di and 1,3,5-trisubstituted benzenes. In the otherwise substituted benzenes, however, this vibration is substituent sensitive and difficult to distinguish from other modes.

Table 1: Geometrical Parameters

Bond lengths(Å)			Bond angles (º)			Dihedral angles (º)		
	HF	XRD[a]		HF	XRD[a]		HF	XRD[a]
C_1-C_2	1.3851	1.3874	A(2,1,6)	120.0	120.1	D(6,1,2,3)	-0.3	-0.2
C_1-C_6	1.3847	1.3665	A(2,1,7)	119.8	119.9	D(2,1,6,5)	0.7	0.5
C_1-H_7	1.0748	0.9300	A(6,1,7)	120.2	119.9	D(1,2,3,4)	-0.8	-0.8
C_2-C_3	1.3905	1.3753	A(1,2,3)	120.2	119.7	D(1,2,3,12)	-179.1	179.4
C_2-H_8	1.0752	0.9300	A(1,2,8)	118.9	120.2	D(2,3,4,5)	1.4	1.6
C_3-C_4	1.3906	1.3713	A(3,2,8)	120.8	120.2	D(12,3,4,5)	179.8	179.8
C_3-C_{12}	1.5011	1.4883	A(2,3,4)	119.5	119.3	D(2,3,12,13)	152.0	146.7
C_4-C_5	1.3826	1.3874	A(2,3,12)	123.3	122.3	D(2,3,12,14)	-28.9	-33.6
C_4-H_9	1.0731	0.9300	A(4,3,12)	117.3	118.4	D(4,3,12,13)	-26.4	-31.9
C_5-C_6	1.3868	1.3564	A(3,4,5)	120.3	120.9	D(4,3,12,14)	152.7	147.8
C_5-H_{10}	1.0749	0.9300	A(3,4,9)	119.0	119.6	D(3,4,5,6)	-0.9	-1.3
C_6-H_{11}	1.0752	0.9300	A(5,4,9)	120.8	119.6	D(4,5,6,1)	-0.1	0.2
C_{12}-O_{13}	1.1985	1.2212	A(4,5,6)	120.0	119.2	D(3,12,14,16)	178.4	176.4
C_{12}-N_{14}	1.3681	1.3483	A(4,5,10)	119.9	120.4	D(13,12,14,16)	-2.6	-3.9
N_{14}-H_{15}	0.9926	0.8052	A(6,5,10)	120.1	120.4	D(12,14,16,17)	175.6	145.5
C_{16}-N_{14}	1.3990	1.4083	A(1,6,5)	120.0	120.8	D(12,14,16,18)	-5.2	35.3
C_{16}-C_{17}	1.3951	1.3803	A(1,6,11)	120.0	119.6	D(14,16,17,19)	179.4	179.8
C_{16}-C_{18}	1.3948	1.3883	A(5,6,11)	120.0	119.6	D(14,16,17,25)	-0.6	1.0
C_{17}-C_{19}	1.3814	1.3743	A(3,12,13)	121.3	121.6	D(18,16,17,19)	0.1	-1.0
C_{17}-Cl_{25}	1.7500	1.7352	A(3,12,14)	114.9	115.9	D(18,16,17,25)	-179.8	-179.7
C_{18}-C_{20}	1.3814	1.3743	A(13,12,14)	123.9	122.5	D(14,16,18,20)	-179.3	-179.2
C_{18}-H_{21}	1.0676	0.9300	A(12,14,15)	116.1	119.5	D(17,16,18,20)	-0.1	1.6
C_{19}-C_{22}	1.3785	1.3743	A(12,14,16)	128.4	126.5	D(16,17,19,22)	-0.1	-0.6
C_{19}-H_{23}	1.0719	0.9300	A(15,14,16)	115.2	114.0	D(25,17,19,22)	179.8	178.1
C_{20}-C_{22}	1.3811	1.3663	A(14,16,17)	119.1	120.1	D(16,18,20,22)	-0.0	-0.5
C_{20}-H_{24}	1.0732	0.9300	A(14,16,18)	123.6	122.2	D(17,19,22,20)	-0.0	1.7
C_{22}-Cl_{26}	1.7408	1.7432	A(17,16,18)	117.4	117.8	D(17,19,22,26)	180.0	-177.5
			A(16,17,19)	122.1	122.2	D(18,20,22,19)	0.1	-1.2
			A(16,17,25)	120.6	119.2	D(18,20,22,26)	-179.9	178.1
			A(19,17,25)	117.4	118.6			
			A(16,18,20)	120.9	120.9			
			A(16,18,21)	119.3	119.5			
			A(20,18,21)	119.9	119.5			
			A(17,19,22)	119.2	118.1			
			A(17,19,23)	119.9	120.9			
			A(22,19,23)	120.9	120.9			
			A(18,20,22)	120.3	119.4			
			A(18,20,24)	119.6	120.3			
			A(22,20,24)	120.1	120.3			
			A(19,22,20)	120.2	121.6			
			A(19,22,26)	119.6	119.1			
			A(20,22,26)	120.2	119.3			

[a]XRD data from reference 34

Table 2: Calculated scaled wavenumbers and assignments

υ (cm⁻¹)	IR intensity	Raman activity	Force constants	Depolarization ratio (P)	Depolarization ratio (U)	Assignments
3489	45.05	55.02	9.70	0.16	0.27	υNH
3103	7.70	58.43	7.78	0.20	0.33	υCH II
3053	0.10	65.64	7.54	0.28	0.44	υCH II
3046	4.32	99.15	7.51	0.15	0.27	υCH I
3039	2.76	89.49	7.46	0.33	0.49	υCH II
3029	21.84	222.36	7.45	0.12	0.21	υCH I
3020	31.14	58.03	7.37	0.73	0.84	υCH I
3010	7.84	106.49	7.30	0.70	0.82	υCH I
3002	1.89	37.74	7.24	0.72	0.84	υCH I
1749	262.03	94.22	20.04	0.23	0.37	υCO
1616	33.51	86.35	9.77	0.51	0.67	υPh I
1606	84.77	173.67	10.05	0.44	0.61	υPh II
1597	172.20	14.31	6.45	0.71	0.83	υPh II
1591	25.87	2.57	9.05	0.48	0.65	υPh I
1528	615.55	11.62	4.55	0.55	0.71	δNH
1491	49.37	0.17	3.61	0.60	0.75	υPh I
1467	46.85	15.69	3.68	0.33	0.50	υPh II
1440	7.44	4.48	3.25	0.40	0.57	υPh I
1379	105.49	12.33	4.52	0.30	0.46	υPh II
1317	0.63	0.84	1.71	0.68	0.81	υPh I
1282	411.29	72.68	2.50	0.22	0.37	υPh II, δCH I
1253	146.13	14.33	2.26	0.20	0.33	δNH, δCH II
1225	0.49	5.69	2.85	0.34	0.50	υCN
1200	8.65	1.75	1.82	0.38	0.55	υPh I
1166	10.87	3.28	1.167	0.39	0.56	δCH I
1149	4.43	9.20	1.53	0.18	0.31	δCH I
1102	1.29	8.96	2.04	0.48	0.65	δCH II
1097	11.69	13.94	2.44	0.26	0.42	δCH II
1085	67.44	13.18	3.59	0.58	0.73	υPh II
1079	26.31	7.15	3.01	0.25	0.41	ρNH
1061	6.51	0.57	1.46	0.54	0.70	δCH I
1031	17.87	2.23	2.91	0.38	0.55	δCH I
1015	0.09	1.47	1.04	0.21	0.34	γCH I
1007	6.09	15.33	1.86	0.12	0.21	υPh I
993	0.73	0.06	1.00	0.55	0.71	γCH I
993	2.46	0.95	0.97	0.75	0.85	γCH II
974	1.65	36.74	4.21	0.12	0.21	Ring breath I
951	1.00	1.597	0.95	0.70	0.82	γCH I
906	12.91	1.67	0.85	0.75	0.86	γCH I
877	30.22	10.40	3.71	0.11	0.19	δCO, υNH
860	0.07	3.43	0.69	0.41	0.58	γCH II
854	48.06	1.06	0.76	0.71	0.83	γCH I
828	31.73	8.59	2.89	0.17	0.29	Ring breath II
797	1.72	0.52	1.37	0.67	0.80	γCH II

Table 2 Cont..

732	39.21	1.03	2.93	0.72	0.84	δPh(X)I, υCCl
718	89.58	3.78	0.80	0.72	0.84	γCH I, υCCl
710	14.52	0.67	1.11	0.69	0.82	γCH I
681	4.59	1.14	1.06	0.24	0.38	γPh I
664	16.21	11.03	2.20	0.15	0.26	δPh I, II
632	2.40	3.09	2.06	0.42	0.59	δPh I, II
605	0.91	6.74	1.68	0.74	0.85	δPh I
562	0.12	0.12	0.83	0.75	0.86	γPh II
541	91.45	91.5	0.26	0.74	0.85	γPh(X) II
502	7.55	7.55	0.95	0.55	0.71	γPh(X) I
459	5.70	2.14	1.02	0.35	0.52	δPh(X) I
445	5.51	0.45	0.51	0.73	0.84	δPh(X) II
421	17.63	1.78	0.68	0.75	0.85	δPh(X) II
407	0.12	0.14	0.36	0.71	0.83	γPh I
396	2.14	6.53	1.02	0.22	0.36	δPh(X) I
378	3.98	4.03	0.96	0.23	0.38	δCX(X) I
351	0.89	1.08	0.57	0.75	0.86	δCX'(X) II
300	11.42	0.97	0.57	0.57	0.72	γCX(X) II
231	0.13	3.61	0.36	0.27	0.42	δCX'(X) I
209	2.16	3.18	0.23	0.74	0.85	δCX'(X) II
181	0.92	2.21	0.25	0.72	0.84	δCX'(X) II
171	0.05	1.66	0.13	0.75	0.86	δCX(X) I
152	2.02	3.46	0.14	0.68	0.81	γCX'(X) II
123	0.78	1.74	0.06	0.74	0.85	γPh(X) I,II
74	2.41	1.45	0.03	0.72	0.83	γPh(X) I
51	2.48	3.48	0.01	0.74	0.85	γPh(X) I
29	0.04	0.91	0.01	0.75	0.86	γPh(X) II
16	2.89	3.65	0.01	0.75	0.86	γPh(X) I

υ-stretching; δ- in-plane deformation; γ- out-of-plane deformation; ρ -rocking; ω-waging; PhI- mono substituted phenyl ring; PhII-trisubstituted phenyl ring; X-substituent sensitive

In asymmetric trisubstituted benzenes, when all the three substituents and light, the wavenumber interval of the breathing mode[42] is between 500 and 600 cm^{-1}. When all the three substituents are heavy, the wavenumber appears above 1100 cm^{-1}. In the case of mixed substituents[42], the wavenumber is expected to appear between 600 and 750 cm^{-1}. The in-plane and out-of-plane CH deformations[37] of the phenyl ring are expected above 1000 cm and below 1000 cm^{-1} and these modes are assigned (Table 2).

At C_3 position, the angle C_4-C_3-C_{12} is reduced by 2.7^0 and C_2-C_3-C_{12} is increased by 3.3^0 from 120^0, and this asymmetry of exocyclic angles reveals the interaction between O_{13} and the phenyl ring I. The C-C bond lengths in the phenyl ring lie between 1.3564 to 1.3874Å whereas for the phenyl ring II, the range is 1.3663 to 1.3883Å. The CH bond lengths lie between 1.0731 and 1.0752Å for ring I and between 1.0676 and 1.0732Å for ring II. According to Noveron *el al.*[43] for complexes of N-(4-pyridyl)benzamide, the bond lengths for C_{16}-N_{14}, C_{12}-O_{13}, C_{12}-N_{14}, C_{12}-C_3, C_3-C_2, C_3-C_4 and N_{14}-H_{15} are 1.3953, 1.2253, 1.3703, 1.4943, 1.3923, 1.3933 and 0.773Å, respectively and for the title compound the corresponding bond values are 1.399, 1.1985, 1.3681, 1.5011, 1.3905, 1.3906 and 0.9926Å, respectively. For N-(2-pyridyl)benzamide complexe[44], the bond lengths for C_{12}-O_{13}, N_{14}-C_{12}, N_{14}-C_{16} and C_{12}-C_3 are 1.2445, 1.3646, 1.4156 and 1.4810Å, respectively and in the present case, the

corresponding values are 1.1985, 1.3681, 1.399 and 1.5011Å. The C=O and C-N bond lengths[11] in benzamide, acetamide and formamide are, respectively, 1.2253, 1.2203, 1.2123 and 1.3801, 1.3904, 1.3683Å. According to literature[25,27,31,45] the changes in bond lengths in C=O and C-N are consistent with the following interpretation: that is hydrogen bond decreases the double bond character of C=O bond and increases the double bond character of C-N bond. The values of the angles C_4-C_3-C_{12} (117.3º) and C_3-C_{12}-O_{13} (121.3º) are smaller than those of benzaldehyde[46], 121.0º and 123.6º. These differences are due to the steric repulsion between H_8 and H_{15} atoms.

The dihedral angles C_2-C_3-C_{12}-O_{13} was determined to be 152.0º by the HF method. On the contrary, the equilibrium structure of benzaldehyde[46] is planar. The steric repulsion in the present case is also considered to cause the nonplanar skeleton. The C_3-C_{12} bond length (1.5011) is larger than the corresponding length of benzaldehyde[46] (1.4794) by 0.0217. Saeed *et al.*[47] reported C_{12}-O_{13}, N_{14}-C_{12} and N_{14}-C_{16} bond lengths as 1.2132, 1.3612 and 1.4042 for benzamide derivatives. For the title compound, the bond lengths obtained are 1.1985, 1.3681 and 1.399. For the benzamide moiety of the title compound, the calculated values of the bond angles C_{12}-N_{14}-C_{16}, C_{18}-C_{16}-N_{14}, O_{13}-C_{12}-N_{14}, O_{13}-C_{12}-C_3, N_{14}-C_{12}-C_3, C_4-C_3-C_{12} and C_2-C_3-C_{12} are 128.4, 123.6, 123.9, 121.3, 114.9, 117.3 and 123.3º, respectively. Sun *et al.*[48] reported the corresponding angles as 124.7, 116.6, 123.1, 118.7, 118.3, 115.6 and 124.3º, respectively. Also, the HF calculations give the torsional angles C_{19}-C_{17}-C_{16}-N_{14}, N_{14}-C_{16}-C_{19}-C_{20}, O_{13}-C_{12}-C_3-C_2, N_{14}-C_{12}-C_3-C_2, O_{13}-C_{12}-C_3-C_4 and N_{14}-C_{13}-C_3-C_4 as 177.4, -179.3, 152.0, -28.9, -26.4 and 152.7º around the benzamide group, which are in agreement with the reported values[43] 178.5, -178.9, -16.8, 163.8, 161.6 and -17.8º. The C_{12}-N_{14} bond is twisted from the phenyl ring I and II as is evident from the torsion angles C_{18}-C_{16}-N_{14}-C_{12} = -5.2º, C_{17}-C_{16}-N_{14}-C_{12} = 175.6º and N_{14}-C_{12}-C_3-C_4 = 152.7º, N_{14}-C_{12}-C_3-C_2 = -28.9º.

Analysis of organic molecules having conjugated π-electron systems and large hyperpolarizability using infrared and Raman spectroscopy has evolved as a subject of research[49]. The potential application of the title compound in the field of non linear optics demands the investigation of its structural and bonding features contributing to the hyperpolarizability enhancement, by analyzing the vibrational modes using the IR and Raman spectrum. The first hyperpolarizability (β_0) of this novel molecular system is calculated using HF method, based on the finite field approach. In the presence of an applied electric field, the energy of a system is a function of the electric field. First hyperpolarizability is a third rank tensor that can be described by a 3×3×3 matrix. The 27 components of the 3D matrix can be reduced to 10 components due to the Kleinman symmetry[50]. The calculated first hyperpolarizability of the title compound is 1.610^{-30} esu, which is comparable with the reported values of similar derivatives[51] and experimental evaluation of this data is not readily available. We conclude that the title compound is an attractive object for future studies of non linear optical properties.

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