Proceeding Paper

Optimization, First-Order Hyperpolarizability Studies of *o*, *m*, and *p*-Cl Benzaldehydes Using DFT Studies [†]

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Abstract: In this paper, we first optimized the structures of Cl benzaldehydes using Gaussian 09 software with the B3LYP/631-G' (d,p) basis set. The title compound's polarizability and hyperpolarizabilities values have been computed, along with an examination of its nonlinear optical characteristics. The title molecule's total initial static hyperpolarizability as determined by DFT studies may be a topic for future NLO content that is appealing.

Keywords: benzaldehydes; optimizations; NLO; MESP

1. Introduction

Due to potential future uses in photonics and optoelectronics, like optical communication, optical computing, optical data storage, optical switching, and dynamic image processing [1–4], nonlinear optical (NLO) materials have received a large amount interest in recent years [5–9]. Organic NLO materials are excellent because of their adaptability and ability to become modified for specific device applications. In comparison with inorganic NLO materials, organic NLO materials exhibit a higher nonlinear figure-of-merit for frequency conversion, a higher laser damage threshold, and a faster optical reaction time [10]. The structure of organic NLO materials is based on the bond system extended over a large length scale of the molecule. This system, known as the push–pull system, is easily manipulated by substituting electron-donating and electron-withdrawing groups to the aromatic moieties. This results in increased optical nonlinearity of the system [11]. Future optoelectronic and nonlinear optical applications hold great promise for chloro-substituted benzaldehyde derivatives with strong optical nonlinearities.

Benzaldehyde, due to its important role, and its derivatives have attracted a high degree of attention in both chemistry and biology [12–14]. Many spectroscopic investigations have been performed on benzaldehyde and its derivatives [15–42], and people have become interested in spectroscopies of halogen-derived benzaldehydes. By using matrix isolation IR spectroscopy, it has been demonstrated that trans and cis conformers of o- and m-chlorobenzaldehydes exist [43]. Although there has been a lot of research conducted on substituted benzaldehydes, a thorough analysis of chloro-benzaldehydes on electronic structure properties is still lacking. Using B3LYP/6-31G' (d,p) basic set, the molecular structure, geometric parameters, and chloro-benzaldehyde are estimated in this current work. It has been possible to determine information about charge transport inside the molecule using HOMO-LUMO research. The molecular electrostatic potential (MEP) has also been investigated.

2. Computational Details

The DFT computation of chloro-benzaldehydes was carried out using the Gaussian 09 program package at B3LYP 6-31G' (d,p) basic set. The optimized structural characteristics were assessed for use in various parameters.

3. Results and Discussion

3.1. Molecular Geometry

The titled compound's optimized geometric structure is shown in Figure 1, and a–c in Table 1 shows the optimized bond lengths, bond angles, and dihedral angles determined using the DFT-B3LYP level with 6-31G'(d,p) basic sets. All compounds have a C1 point group symmetry element.
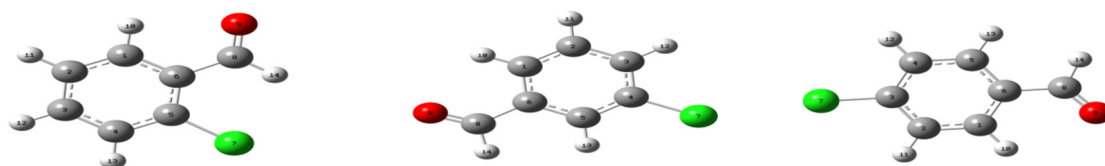

Figure 1. Molecular structure with atom numbering of *o*, *m*, and *p*-Cl benzaldehydes.

Table 1. (**a**) Optimized geometrical parameters of *o*-chlorobenzaldehyde. (**b**) Optimized geometrical parameters of *m*-chlorobenzaldehyde. (**c**) Optimized geometrical parameters of *p*-chlorobenzaldehyde.

(a)					
Bond	**Bond Length (Å)**	**Bond Angle**	**Value (in ^{0})**	**Torsional Angle**	**Value (in ^{0})**
R(1,2)	1.3892	A(2,1,6)	121.242	D(6,1,2,3)	0.0
R(1,6)	1.4055	A(2,1,10)	121.7052	D(6,1,2,11)	180.0001
R(1,10)	1.0868	A(6,1,10)	117.0528	D(10,1,2,3)	−180.0
R(2,3)	1.3987	A(1,2,3)	119.5208	D(10,1,2,11)	0.0
R(2,11)	1.0867	A(1,2,11)	120.2455	D(2,1,6,5)	−0.0001
R(3,4)	1.3949	A(3,2,11)	120.2337	D(2,1,6,8)	−180.0001
R(3,12)	1.0873	A(2,3,4)	120.4875	D(10,1,6,5)	180.0
R(4,5)	1.3948	A(2,3,12)	120.2509	D(10,1,6,8)	0.0
R(4,13)	1.0856	A(4,3,12)	119.2615	D(1,2,3,4)	0.0
R(5,6)	1.4043	A(3,4,5)	119.3706	D(1,2,3,12)	180.0
R(5,7)	1.7638	A(3,4,13)	120.9615	D(11,2,3,4)	179.9999
R(6,8)	1.489	A(5,4,13)	119.668	D(11,2,3,12)	−0.0001
R(8,9)	1.2133	A(4,5,6)	121.2421	D(2,3,4,5)	0.0
R(8,14)	1.1071	A(4,5,7)	117.5979	D(2,3,4,13)	−180.0
		A(6,5,7)	121.16	D(12,3,4,5)	180.0
		A(1,6,5)	118.137	D(12,3,4,13)	0.0
		A(1,6,8)	118.1085	D(3,4,5,6)	0.0
		A(5,6,8)	123.7545	D(3,4,5,7)	−180.0
		A(6,8,9)	123.0545	D(13,4,5,6)	−180.0
		A(6,8,14)	115.7743	D(13,4,5,7)	0.0
		A(9,8,14)	121.1712	D(4,5,6,1)	0.0001
				D(4,5,6,8)	180.0001
				D(7,5,6,1)	180.0
				D(7,5,6,8)	0.0
				D(1,6,8,9)	0.0021
				D(1,6,8,14)	−180.0019
				D(5,6,8,9)	180.0021
				D(5,6,8,14)	−0.0019

Table 1. *Cont.*

(b)					
Bond	**Bond Length (Å)**	**Bond Angle**	**Value (in ^{0})**	**Torsional Angle**	**Value (in ^{0})**
R(1,2)	1.3911	A(2,1,6)	119.6855	D(6,1,2,3)	−0.0001
R(1,6)	1.4024	A(2,1,10)	121.7567	D(6,1,2,11)	−180.0001
R(1,10)	1.0862	A(6,1,10)	118.5579	D(10,1,2,3)	179.9999
R(2,3)	1.3993	A(1,2,3)	120.4224	D(10,1,2,11)	−0.0001
R(2,11)	1.0871	A(1,2,11)	120.2862	D(2,1,6,5)	0.0001
R(3,4)	1.3957	A(3,2,11)	119.2915	D(2,1,6,8)	180.0001
R(3,12)	1.0857	A(2,3,4)	119.3431	D(10,1,6,5)	−180.0
R(4,5)	1.3927	A(2,3,12)	120.8467	D(10,1,6,8)	0.0001
R(4,7)	1.7585	A(4,3,12)	119.8101	D(1,2,3,4)	0.0001
R(5,6)	1.4003	A(3,4,5)	121.0311	D(1,2,3,12)	180.0001
R(5,13)	1.0872	A(3,4,7)	119.4578	D(11,2,3,4)	180.0001
R(6,8)	1.4847	A(5,4,7)	119.5111	D(11,2,3,12)	0.0001
R(8,9)	1.2113	A(4,5,6)	119.1364	D(2,3,4,5)	0.0
R(8,14)	1.1145	A(4,5,13)	120.3919	D(2,3,4,7)	−180.0
		A(6,5,13)	120.4717	D(12,3,4,5)	180.0
		A(1,6,5)	120.3815	D(12,3,4,7)	0.0
		A(1,6,8)	120.2737	D(3,4,5,6)	0.0
		A(5,6,8)	119.3448	D(3,4,5,13)	−180.0001
		A(6,8,9)	124.351	D(7,4,5,6)	180.0
		A(6,8,14)	114.4592	D(7,4,5,13)	0.0
		A(9,8,14)	121.1898	D(4,5,6,1)	0.0
				D(4,5,6,8)	−180.0
				D(13,5,6,1)	−180.0
				D(13,5,6,8)	0.0
				D(1,6,8,9)	-0.0004
				D(1,6,8,14)	180.0009
				D(5,6,8,9)	−180.0004
				D(5,6,8,14)	0.0009

(c)					
Bond	**Bond Length (Å)**	**Bond Angle**	**Value (in ^{0})**	**Torsional Angle**	**Value (in ^{0})**
R(1,2)	1.3896	A(2,1,6)	120.3956	D(6,1,2,3)	−0.0001
R(1,6)	1.4034	A(2,1,10)	121.0573	D(6,1,2,11)	−180.0001
R(1,10)	1.0867	A(6,1,10)	118.5472	D(10,1,2,3)	180.0
R(2,3)	1.3997	A(1,2,3)	118.9399	D(10,1,2,11)	−0.0001
R(2,11)	1.0856	A(1,2,11)	121.1629	D(2,1,6,5)	0.0
R(3,4)	1.3963	A(3,2,11)	119.8973	D(2,1,6,8)	180.0001
R(3,7)	1.7547	A(2,3,4)	121.6657	D(10,1,6,5)	−180.0
R(4,5)	1.3933	A(2,3,7)	119.1476	D(10,1,6,8)	0.0
R(4,12)	1.0854	A(4,3,7)	119.1867	D(1,2,3,4)	0.0001
R(5,6)	1.4005	A(3,4,5)	118.6961	D(1,2,3,7)	−179.9999
R(5,13)	1.0887	A(3,4,12)	120.0761	D(11,2,3,4)	180.0001
R(6,8)	1.4813	A(5,4,12)	121.2278	D(11,2,3,7)	0.0001
R(8,9)	1.2123	A(4,5,6)	120.6123	D(2,3,4,5)	0.0
R(8,14)	1.1148	A(4,5,13)	119.7285	D(2,3,4,12)	−180.0
		A(6,5,13)	119.6591	D(7,3,4,5)	180.0
		A(1,6,5)	119.6904	D(7,3,4,12)	0.0
		A(1,6,8)	120.1889	D(3,4,5,6)	0.0
		A(5,6,8)	120.1207	D(3,4,5,13)	−180.0
		A(6,8,9)	124.4964	D(12,4,5,6)	180.0
		A(6,8,14)	114.3928	D(12,4,5,13)	0.0
		A(9,8,14)	121.1107	D(4,5,6,1)	0.0
				D(4,5,6,8)	−180.0
				D(13,5,6,1)	−180.0
				D(13,5,6,8)	0.0
				D(1,6,8,9)	−0.0005
				D(1,6,8,14)	180.0009
				D(5,6,8,9)	−180.0004
				D(5,6,8,14)	0.0009

3.2. NLO

First-order hyperpolarizability (β_{tot}) and its components, as well as the total molecule polarizability (α_{tot}) and its components, were calculated using the DFT/B3LYP/6-31G′

level of theory. Nonlinear optical (NLO) effects can be measured using first-order hyperpolarizability. A common molecule employed in the NLO characteristics of molecular systems is urea. As a result, it is widely utilized as a comparison threshold value. According to DFT calculations as shown in Table 2, the titled compound's dipole moment and first-order hyperpolarizability are calculated to be 3.1243, 1.8918, and 2.1276 Debye, respectively, and 155.86×10^{-30} cm^5/esu, 240.86×10^{-30} cm^5/esu, and 820.22×10^{-30} cm^5/esu, respectively.

Table 2. (**a**) Dipole moment (μ_{tot}), polarizability (α_{tot}), and hyperpolarizability (β_{tot}) of *o*-Cl benzaldehyde. (**b**) Dipole moment (μ_{tot}), polarizability (α_{tot}), and hyperpolarizability (β_{tot}) of *m*-Cl benzaldehyde. (**c**) Dipole moment (μ_{tot}), polarizability (α_{tot}), and hyperpolarizability (β_{tot}) of *p*-Cl benzaldehyde.

(a)					
Dipole Moment		**Polarizability**		**Hyperpolarizability**	
μx	−2.7695	αxx	111.140	βxxx	40.2453
μy	−1.4438	αyy	−0.255	βyyy	133.6728
μz	0.0824	αzz	103.61	βzzz	−11.011
μ	3.1243	αxy	−0.00066	βxyy	43.186
		αxz	−0.0010	βxxy	0.789
		αyz	32.396	βxxz	−0.558
		$\alpha 0$	71.49	βxzz	−2.142
				βyzz	−2.189
				βyyz	−2.265
				βxyz	−0.0012
				$\beta 0$	155.86
(b)					
Dipole Moment		**Polarizability**		**Hyperpolarizability**	
μx	1.4781	αxx	124.426	βxxx	239.0
μy	1.1778	αyy	−0.6923	βyyy	−47.06
μz	0.0825	αzz	93.120	βzzz	−95.58
μ	1.8918	αxy	−0.0022	βxyy	−22.57
		αxz	0.0005	βxxy	−1.57
		αyz	32.4588	βxxz	−0.927
		$\alpha 0$	72.28	βxzz	−0.31
				βyzz	6.567
				βyyz	0.346
				βxyz	−0.0004
				$\beta 0$	240.81
(c)					
Dipole Moment		**Polarizability**		**Hyperpolarizability**	
μx	−1.1977	αxx	136.97	βxxx	769.984
μy	1.7566	αyy	0.4221216	βyyy	74.092
μz	0.0824	αzz	85.6294302	βzzz	−9.208
μ	2.1276	αxy	0.0019948	βxyy	47.957
		αxz	−0.0008	βxxy	−1.515
		αyz	32.4628691	βxxz	−1.127
		$\alpha 0$	74.34	βxzz	−0.737
				βyzz	−2.664
				βyyz	2.678
				βxyz	−0.0004
				$\beta 0$	820.22

As a result, we observe that the (α_{tot}) and (β_{tot}) values for titled compounds are higher than the equivalent threshold values for urea. The extent of the first-order hyperpolarizabil-

ity leads to the conclusion that titled compounds may be considered potential applicants in the development of NLO material.

3.3. Molecular Electrostatic Potential Analysis

For analyzing and predicting molecular behavior, we used the molecular electrostatic potential (MEP), which is produced by the nuclei and electrons and is viewed as static distributions of charge reacting in a particular manner; this investigation benefits greatly by studies of molecular electrostatic mapping (MEP) in regard to the molecular structure connecting with its physiochemical properties [44–47]. This has been especially helpful as an indication of active areas or places on a molecule shown with specific colors. Initially, electrophile attracts, and it has also been successfully used in the investigation of interactions involving a certain optimal reactants' relative orientation [48]. MEP usually reflects its values onto the molecular electron to create a visual density.

The MEP plot of the titled compounds material as shown in Figure 2 demonstrates that the oxygen atoms of carbonyl have the greatest negative potential and are the main active nucleophilic centers, respectively, whereas chlorine atoms have a negative potential (blue color).
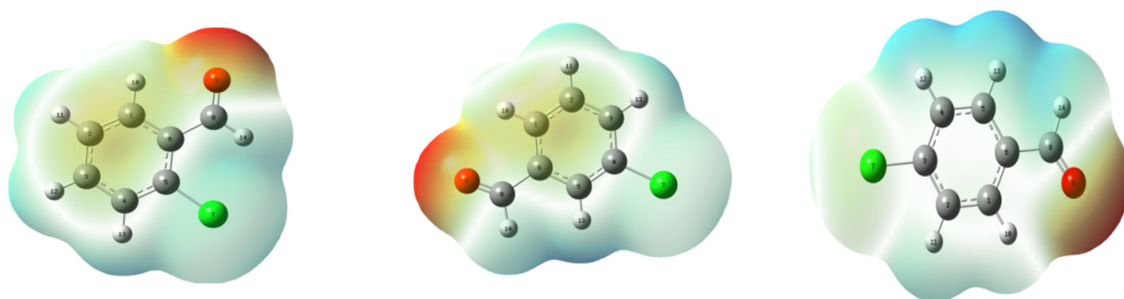
Figure 2. Molecular electrostatic potential (MEP) map of title compounds calculated at B3LYP/6-31G' (d,p) level.

4. Conclusions

The structural characteristics of titled compounds have been explained theoretically using B3LYP/6-31G' (d,p) techniques. The NBO outcome displays the transmission of charges inside the molecules. According to MEP, the hydrogen and chlorine atoms were on the positive potential site, whereas the oxygen atoms in the aldehyde group were on the negative potential site.

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