

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

Ruchi Singh ¹, Huda Khanam ^{1,2} and Jyoti Pandey ^{1,*}

¹ Department of Chemistry, Babasaheb Bhimrao Ambedkar University, Lucknow 226025, India; ruchisingh181297@gmail.com (R.S.); kxanhuda188@gmail.com (H.K.)

² Department of Chemistry, University of Lucknow, Lucknow 226007, India

* Correspondence: drjyotibbau@gmail.com

[†] Presented at the 27th International Electronic Conference on Synthetic Organic Chemistry (ECSOC-27), 15–30 November 2023; Available online: <https://ecsoc-27.sciforum.net/>.

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.



Citation: Singh, R.; Khanam, H.; Pandey, J. Optimization, First-Order Hyperpolarizability Studies of *o*, *m*, and *p*-Cl Benzaldehydes Using DFT Studies. *Chem. Proc.* **2023**, *14*, 92. <https://doi.org/10.3390/ecsoc-27-16072>

Academic Editor: Julio A. Seijas

Published: 15 November 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

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.

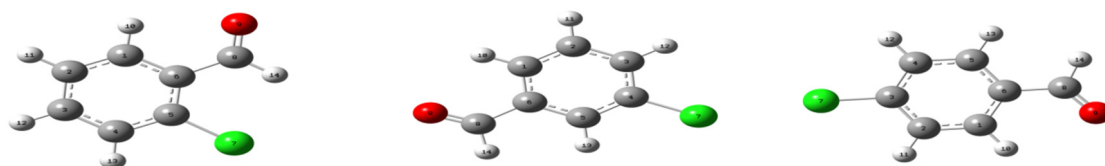


Figure 1. Molecular structure with atom numbering of *o*, *m*, and *p*-Cl benzaldehydes.

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 °)	Torsional Angle	Value (in °)
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 °)	Torsional Angle	Value (in °)
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 °)	Torsional Angle	Value (in °)
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 $155.86 \times 10^{-30} \text{ cm}^5/\text{esu}$, $240.86 \times 10^{-30} \text{ cm}^5/\text{esu}$, and $820.22 \times 10^{-30} \text{ cm}^5/\text{esu}$, 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	
μ_x	−2.7695	α_{xx}	111.140	β_{xxx}	40.2453
μ_y	−1.4438	α_{yy}	−0.255	β_{yyy}	133.6728
μ_z	0.0824	α_{zz}	103.61	β_{zzz}	−11.011
μ	3.1243	α_{xy}	−0.00066	β_{xyy}	43.186
		α_{xz}	−0.0010	β_{xxy}	0.789
		α_{yz}	32.396	β_{xxz}	−0.558
		α_0	71.49	β_{xzz}	−2.142
				β_{yzz}	−2.189
				β_{yyz}	−2.265
				β_{xyz}	−0.0012
				β_0	155.86
(b)					
Dipole Moment		Polarizability		Hyperpolarizability	
μ_x	1.4781	α_{xx}	124.426	β_{xxx}	239.0
μ_y	1.1778	α_{yy}	−0.6923	β_{yyy}	−47.06
μ_z	0.0825	α_{zz}	93.120	β_{zzz}	−95.58
μ	1.8918	α_{xy}	−0.0022	β_{xyy}	−22.57
		α_{xz}	0.0005	β_{xxy}	−1.57
		α_{yz}	32.4588	β_{xxz}	−0.927
		α_0	72.28	β_{xzz}	−0.31
				β_{yzz}	6.567
				β_{yyz}	0.346
				β_{xyz}	−0.0004
				β_0	240.81
(c)					
Dipole Moment		Polarizability		Hyperpolarizability	
μ_x	−1.1977	α_{xx}	136.97	β_{xxx}	769.984
μ_y	1.7566	α_{yy}	0.4221216	β_{yyy}	74.092
μ_z	0.0824	α_{zz}	85.6294302	β_{zzz}	−9.208
μ	2.1276	α_{xy}	0.0019948	β_{xyy}	47.957
		α_{xz}	−0.0008	β_{xxy}	−1.515
		α_{yz}	32.4628691	β_{xxz}	−1.127
		α_0	74.34	β_{xzz}	−0.737
				β_{yzz}	−2.664
				β_{yyz}	2.678
				β_{xyz}	−0.0004
				β_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).

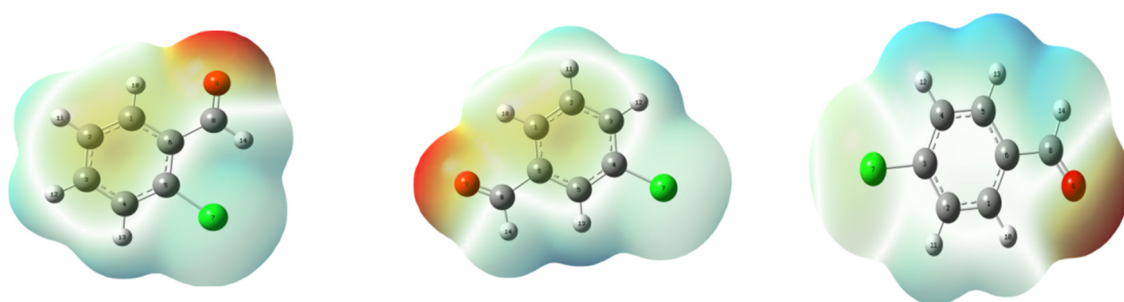


Figure 2. Molecular electrostatic potential (MEP) map of title compounds calculated at B3LYP/6-31G' (d,p) level.

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.

Author Contributions: R.S. and H.K.: Investigation, methodology, data correction, original draft, editing, communication. J.P.: Supervision, review and editing. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no external funding.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Datta, A.; Pati, S.K. Effects of dipole orientations on nonlinear optical properties of oxo-bridged dinitroaniline systems. *J. Phys. Chem. A* **2004**, *108*, 320. [[CrossRef](#)]
2. Petrosyan, A.M. Salts of l-histidine as nonlinear optical materials: A review. *J. Cryst. Phys. Chem.* **2010**, *1*, 33–56.
3. Karakas, A.; Elmalı, A.; Unver, H.; Svoboda, I. Nonlinear optical properties of some derivatives of salicylaldehyde-based ligands. *J. Mol. Struct.* **2004**, *702*, 103. [[CrossRef](#)]

4. Mendes, P.J.; Ramalho, J.P.P.; Candeias, A.J.E.; Robalo, M.P.; Garcia, M.H. Density functional theory calculations on η^5 -monocyclopentadienyltrilecobalt complexes concerning their second-order nonlinear optical properties. *J. Mol. Struct. (Theochem.)* **2005**, *729*, 109.
5. Ahmed, A.B.; Elleuch, N.; Feki, H.; Abid, Y.; Minot, C. Vibrational spectra and non-linear optical proprieties of l-histidine oxalate: DFT studies. *Spectrochim. Acta A* **2011**, *79*, 554–561. [[CrossRef](#)] [[PubMed](#)]
6. Ravikumar, C.; Joe, I.H. Electronic absorption and vibrational spectra and nonlinear optical properties of 4-methoxy-2-nitroaniline. *Phys. Chem. Chem. Phys.* **2010**, *12*, 9452–9460.
7. Borbone, F.; Carella, A.; Roviello, A.; Casalboni, M.; De Matteis, F.; Stracci, G.; della Rovere, F.; Evangelisti, A.; Dispenza, M. Outstanding poling stability of a new cross-linked nonlinear optical (NLO) material from a low molecular weight chromophore. *J. Phys. Chem. B* **2011**, *115*, 11993–12000. [[CrossRef](#)] [[PubMed](#)]
8. Ivanova, B.B.; Spiteller, M. Physical optical properties and crystal structures of organic 5-sulfosalicylates—Theoretical and experimental study. *J. Mol. Struct.* **2011**, *1003*, 1–9. [[CrossRef](#)]
9. Linet, J.M.; Das, S.J. Optical, mechanical and transport properties of unidirectional grown l-tartaric acid bulk single crystal for non-linear optical application. *Mater. Chem. Phys.* **2011**, *126*, 886–890.
10. Sajan, D.; Ravindra, H.J.; Misra, N.; Joe, I.H. Intramolecular charge transfer and hydrogen bonding interactions of nonlinear optical material N-benzoyl glycine: Vibrational spectral study. *Vib. Spectrosc.* **2010**, *54*, 72–80. [[CrossRef](#)]
11. Chis, V.; Oltean, M.; Pirnau, A.; Miclaus, V.; Filip, S. Spectral and theoretical studies of 2-naphthalenol: An organic nonlinear optical crystalline material. *J. Optoelectron. Adv. Mater.* **2006**, *8*, 1143–1147.
12. Atkins, P.; Jones, L. *Chemistry: Molecules Matter and Change*; W.H. Freeman and Co.: New York, NY, USA, 1997.
13. Available online: <http://www.intermesh.net/Benzald.htm> (accessed on 1 November 2023).
14. Available online: <https://en.wikipedia.org/wiki/Benzaldehyde> (accessed on 1 November 2023).
15. Bednarek, P.; Bally, T.; Gebicki, J. Characterization of Rotameric Mixtures in *o*- and *m*-Substituted Benzaldehydes by Matrix Isolation IR Spectroscopy. *J. Org. Chem.* **2002**, *67*, 1319. [[PubMed](#)]
16. Ribeiro-Claro, P.J.A.; de Carvalho, L.A.E.B.; Amado, A.M. Evidence of dimerization through C—H...O interactions in liquid 4-methoxybenzaldehyde from Raman spectra and ab initio calculations. *J. Raman Spectrosc.* **1997**, *28*, 867. [[CrossRef](#)]
17. Karger, N.; da Costa, A.M.A.; Ribeiro-Claro, P.J.A. C—H...O bonded dimers in liquid 4-methoxybenzaldehyde: A study by NMR, vibrational spectroscopy, and ab initio calculations. *J. Phys. Chem. A* **1999**, *103*, 8672. [[CrossRef](#)]
18. Ribeiro-Claro, P.J.A.; Drew, M.G.B.; Felix, V. C—H...O bonded dimers in 2-methoxy-benzaldehyde studied by X-ray crystallography, vibrational spectroscopy, and ab initio calculations. *Chem. Phys. Lett.* **2002**, *356*, 318. [[CrossRef](#)]
19. Marques, M.P.M.; da Costa, A.M.A.; Ribeiro-Claro, P.J.A. Evidence of C—H...O Hydrogen Bonds in Liquid 4-Ethoxybenzaldehyde by NMR and Vibrational Spectroscopies. *J. Phys. Chem. A* **2001**, *105*, 5292. [[CrossRef](#)]
20. Schaeffer, T.; Cox, K.J.; Sebastian, R. Experimental and theoretical conformer distributions of 3-methylbenzaldehyde. *Can. J. Chem.* **1991**, *69*, 908. [[CrossRef](#)]
21. Anjaneyulu, A.; Rao, G.R. Vibrational analysis of substituted benzaldehydes: Part I. Vibrational spectra, normal co-ordinate analysis and transferability of force constants of monohalogenated. *Spectrochim. Acta A* **1999**, *55*, 749.
22. Ahmad, S.; Verma, P.K. Laser Raman and infrared and far infrared spectra of 3, 4, 5-trimethoxybenzaldehyde. *Ind. J. Phys.* **1990**, *64B*, 50.
23. Aralakkanavar, M.K.; Katti, N.R.; Jeeragal, P.R.; Kalakoti, G.B.; Rao, R.; Shashidhar, M.A. $\pi^* \leftarrow \pi$ systems in the electronic absorption spectra of some trisubstituted benzenes. *Spectrochim. Acta* **1992**, *48A*, 983.
24. Yadav, R.A.; Singh, I.S. Vibrational studies, barrier height and thermodynamic functions for biomolecules: 5-Trifluoromethyl uraci. *Ind. J. Phys.* **1994**, *58B*, 556.
25. Singh, D.N.; Singh, I.D.; Yadav, R.A. Vibrational Spectra and Force Fields for 2, 3-; 2, 4-; 2, 5-and 3, 4-Dihydroxybenzaldehydes. *Ind. J. Phys.* **2002**, *76B*, 35.
26. Hinchliffe, A.; Munn, R.W. Molecular Electromagnetism. In *Molecular Electromagnetism*; John Wiley and Sons Ltd.: Chichester, UK, 1985.
27. Lampert, H.; Mikenda, W.; Karpfen, A. Molecular geometries and vibrational spectra of phenol, benzaldehyde, and salicylaldehyde: Experimental versus quantum chemical data. *J. Phys. Chem. A* **1997**, *101*, 2254.
28. Mollendal, H.; Gundersen, S.; Tafipolsky, M.A.; Volden, H.V. The molecular structure of benzene derivatives, part 2: 4-chloro-benzaldehyde by joint analysis of gas electron diffraction, microwave spectroscopy and ab initio molecular orbital calculations. *J. Mol. Struct.* **1998**, *444*, 47. [[CrossRef](#)]
29. Bhattacharjee, D.; Ghosh, A.; Mishra, T.N. Solvent-Induced Vibrational Relaxation in Benzaldehyde. *Bull. Chem. Soc. Jpn.* **1995**, *68*, 1269.
30. Das, K.; Kumar, J. Solvent-dependent study of anisotropy shift in the C=O stretching mode of benzaldehyde. *Raman Spectrosc.* **1999**, *30*, 563.
31. Speakman, L.D.; Papas, B.N.; Woodcock, H.L.; Schaefer, H.F. The microwave and infrared spectroscopy of benzaldehyde: Conflict between theory and experimental deductions. *J. Chem. Phys.* **2004**, *120*, 4247. [[CrossRef](#)] [[PubMed](#)]
32. Kushto, G.P.; Jagodzinski, P.W. Vibrational spectra and normal coordinate analysis of 4-(dimethylamino) benzaldehyde and selected isotopic derivatives. *Spectrochim. Acta* **1998**, *54A*, 799. [[CrossRef](#)]

33. Kushto, G.P.; Jagodzinski, P.W. Formation of a ground state twisted-internal-charge-transfer conformer of 4-(dimethylamino) benzaldehyde. *J. Mol. Struct.* **2000**, *516*, 215.
34. Ribeiro-Claro, P.J.A.; Marques, M.P.M.; Amado, A.M. Experimental and Theoretical Evidence of C—H···O Hydrogen Bonding in Liquid 4-Fluorobenzaldehyde. *ChemPhysChem* **2002**, *3*, 599.
35. Qayyum, M.; Reddy, B.V.; Rao, G.R. Vibrational analysis of mononitro substituted benzamides, benzaldehydes and toluenes: Part I. Vibrational spectra, normal coordinate analysis and transferability of force constants of nitrobenzamides, nitrobenzaldehydes and nitrotoluenes. *Spectrochim. Acta A* **2004**, *60*, 279. [[CrossRef](#)] [[PubMed](#)]
36. Akai, N.; Kudoh, S.; Takayanagi, M.; Nakata, M. Photoinduced rotational isomerization mechanism of 2-chlorobenzaldehyde in low-temperature rare-gas matrices by vibrational and electronic spectroscopies. *J. Photochem. Photobiol. A* **2002**, *150*, 93.
37. Jeeragal, P.R.; Kalakoti, G.B.; Navati, M.S.; Aralakkanavar, M.K.; Shashidhar, M.A. FT-Raman and infrared spectra and vibrational assignments for 3-chloro-4-methoxybenzaldehyde, as supported by ab initio, hybrid density functional theory and normal coordinate calculations. *Ind. J. Pure Appl. Phys.* **1994**, *32*, 521.
38. Shashidhar, M.A.; Shanabhag, P.V.; Ayachit, N.H.; Rao, K.S. infrared and electronic absorption-spectra of 3-cyanobenzaldehydes and 4-cyanobenzaldehydes. *Ind. J. Pure Appl. Phys.* **1984**, *22*, 433.
39. Abdulridha, A.A.; Allah, M.A.A.H.; Makki, S.Q.; Sert, Y.; Salman, H.E.; Balakit, A.A. Corrosion Inhibition of Carbon Steel in 1 M H₂SO₄ Using New Azo Schiff Compound: Electrochemical, Gravimetric, Adsorption, Surface and DFT Studies. *J. Mol. Liq.* **2020**, *315*, 113690. [[CrossRef](#)]
40. Green, J.H.S.; Harrison, D.J. Vibrational spectra of benzene derivatives—XVI. Benzaldehyde and mono-substituted benzaldehydes. *Spectrochim. Acta A* **1976**, *32*, 1265.
41. Pinchas, S. Infrared absorption of aldehydic CH group. *Anal. Chem.* **1957**, *29*, 334.
42. Abraham, R.J.; Mobli, M. Prediction of ¹H NMR Coupling Constants with Associative Neural Networks Trained for Chemical Shifts 2004. Available online: <http://www.spectroscopyeurope.com> (accessed on 1 November 2023).
43. Alkorta, I.; Perez, J.J. Molecular polarization potential maps of the nucleic acid bases *Int. J. Quantum Chem.* **1996**, *57*, 123–135. [[CrossRef](#)]
44. Scrocco, E.; Tomasi, J. Advances in quantum chemistry. In *Advances in Quantum Chemistry*; Lowdin, P., Ed.; Academic Press: New York, NY, USA, 1978; Volume 2.
45. Luque, F.J.; Orozco, M.; Bhadane, P.K.; Gadre, S.R. SCRF calculation of the effect of water on the topology of the molecular electrostatic potential. *J. Phys. Chem.* **1993**, *97*, 9380–9384. [[CrossRef](#)]
46. Sponer, J.; Hobza, P. DNA base amino groups and their role in molecular interactions: Ab initio and preliminary density functional theory calculations. *Int. J. Quantum Chem.* **1996**, *57*, 959–970. [[CrossRef](#)]
47. Murray, J.S.; Sen, K. Molecular electrostatic potentials: Concepts and applications. In *Molecular Electrostatic Potentials, Concepts and Applications*; Elsevier: Amsterdam, The Netherlands, 1996.
48. Politzer, P.; Truhlar, D.G. (Eds.) Chemical applications of atomic and molecular electrostatic potentials: Reactivity, structure, scattering, and energetics of organic, inorganic, and biological. In *Chemical Application of Atomic and Molecular Electrostatic Potentials*; Plenum: New York, NY, USA, 1981.

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.