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An Unprecedented Hydrogen Bonded Crystal Structure Presentation of 1-(5-Chloro-2-Hydroxyphenyl)Ethanone - Complete Theoretical vs Experimental Results Survey using Reliable DFT & TD-DFT Computational Method

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ABSTRACT

1-(5-chloro-2-htdroxyphenyl)ethanone (**Compound 1**) is ortho-hydroxy aromatic ketone where crystal structure has been unambiguously confirmed by single crystal XRD at higher temperature (298 K). **Compound 1** has been characterized by different physicochemical techniques like melting point, elemental analyses (carbon, hydrogen, chlorine & oxygen), IR, UV-Vis, mass spectroscopy. Reference **Compound 1** crystallizes triclinic crystal system having space group P-1 with the values a = 7.494(4), b = 12.906(5), and c = 16.105(8) Å; α = 90.21° (2), β = 90.16° (3), and γ=90.39° (2), V=1557.7(12) Å and Z = 8. Finally crystal structure 1 was refined to R =0.1101. It is a unique crystal structure where crystal units are stabilized by intramolecular hydrogen bonding. Hydrogen bonded supramolecular network is further supported by π-π stacking interaction. The geometry of **Compound 1** optimized in the singlet ground states by DFT computation (using B3LYP functional) and proper basis sets used 6-31G (d-p). Density functional theory of optimized crystal structure having Mulliken charge distribution confirmed that both carbon and oxygen utilized sp^2 hybridization. The molecular structure, selected bond parameters and IR, UV-Vis spectral data of **Compound 1** are theoretically studied using DFT computational method. A supplementary TD-DFT calculations have been performed for optimized geometry of title **Compound 1** to get deep insight into the different spectral electronic transitions.

1. Introduction

The word of any kind of ketone was coined in 1848 by the German chemist Leopold Gmelin. Ketones are always highly reactive compound in sense that they are containing C=O double bond. Chlorine attached Ortho-hydroxy ketones reactivity always higher than that of normal ketones. Title **Compound 1** is an example of symmetrical monocyclic ketone and its conformation is best regarded as extended intramolecular hydrogen bonding. **Compound 1** is highly motivated synthetic precursor of Schiff base ligands after the discovery of Prof. Hugo Schiff during the year 1864 [1]. Schiff bases bearing additional donor groups represent an important versatile class of polydentate ligands which usually coordinate with metals in the field of coordination chemistry [2]. The special structural variety with respect to donor center flexibility makes Schiff base have significant chemical, pharmacological and biological activities [3-5]. Today the synthesized Schiff base complexes have wide applications in the treatment of cancer [5], as antibactericide agents [6-7], as antivirus agents [8-10], as fungicide agents [11-12] and finally biological properties [13-15]. They are also reported to possess good luminescence as well as pigmentation properties [16-18]. The recent research studies throw much interest to elucidate the optimized geometry of **Compound 1** with the aid of reliable DFT computational method. Hence in the current research work, we report literature survey facile synthesis of **Compound 1**, its characterization and crystal structure refinement. A thorough DFT & TD-DFT study have been performed to rationalize the spectral behavior of title **Compound 1**.

2. Experimental Methods

2.1 Materials

All chemicals were of reagent grade and used without further purification. All solvents like methanol, ethanol and other reagents used in this work were obtained from commercial sources. The synthetic reactions and work-up were done in open air.

2.2 Preparation

*2.2.1 Preparation of **Compound 1***

Compound 1 has been synthesized by following published procedure [19]. Specific details of **Compound 1** and the characterization data of product are given below. For 1 (Yield: 83%), M. Wt. (170.59), Exact Mass: 170.01, m/e: 170.00; Anal. Calc. for $C_8H_7Cl_{11}O_2$: C, 56.32; H, 4.14; O, 18.76; Cl, 20.78; Found: C, 5628; H, 4.13; O, 18.75; Cl, 20.77; IR (KBr, ν_{max}/cm^{-1}): ν(C=O) 1631. V (O-H) =3473; UV-Vis spectrum, λ_{max} (CH_3OH): 217.30 nm, 245.00 nm and 329.25 nm.

2.2.2 Physical Measurements

Elemental analyses (carbon, hydrogen, oxygen and chlorine) of **Compound 1** were performed on a Perkin-Elmer-240 C elemental analyzer. IR spectra in KBr (4000-400 cm^{-1}) were recorded using a Perkin-Elmer model 883 infrared spectrophotometer. Electronic UV-Vis spectra in methanol were recorded using UV-spectrometer. Mass spectra were done with a JEOLJMS-AX 500 spectrophotometer. Melting Point of title **Compound 1** has been determined on a Melting Point B-545 apparatus and is uncorrected.

2.2.3 X-Ray Crystallographic Structure Determination

Compound 1, the data collections were made using a CCD area detector equipped with a graphite monochromated MO-K_α (K = 0.71073 Å) source in the ω scan mode at 293 K. The program SMART was used for collecting different frames of data, determination of lattice parameters and finally indexing reflections. The molecular structure of 1 has been solved by direct methods and refinement by full-matrix least squares on F^2 using the SHELXS-97 package [20]. Non-hydrogen's atoms were refined with anisotropic thermal parameters. Hydrogen atoms were fixed at calculated positions, and their positions were refined by a riding model. Multi-scan

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empirical absorption corrected were applied to the collected data using the program SADABS [21]. Hence during crystal structure refinement different programs used are SHELXS-97, ORTEP, DIAMOND and MERCURY. The crystallographic figures were generated using Diamond 3.1 e software.

2.2.4 Theory and Computational Methods

All computations for **Compound 1** were performed using the Gaussian 09 (G09) software package [25] by using the Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr non-local correlation functional (B3LYP). In the calculation the 6-31G (d-p) basis set was assigned to all elements. The geometric structure of **Compound 1** in the ground state (singlet) was fully optimized at the B3LYP level. During calculation the Los Alamos effective core potentials plus the Double Zeta (LanL.2DZ) basis set were employed [26]. The vibration frequency calculations were performed to ensure that the optimized geometries represent local minima associated with positive Eigen values only. Vertical electronic excitations based on B3LYP were obtained with the time-dependent density functional theory (TD-DFT) formalism in methanol using the conductor-like polarizable continuum model (CPCM). Gauss Sum was used to calculate the fractional contributions of various groups to each molecular orbital.

3. Result and Discussion

3.1 Synthesis

Compound 1 synthesis has been successfully fulfilled in our laboratory by published procedure [19]. X-ray diffraction quality white crystal obtained upon slow evaporation of the methanolic reaction mixture & subsequent recrystallization at room temperature. **Compound 1** has been characterized by different physicochemical techniques like melting point, IR, UV-Vis and mass spectroscopy (m/e).

*3.2 IR and Other Characterization of **Compound 1***

The infrared spectra data of **Compound 1** are consistent with the structural data given in this paper. An intense strong IR band in the region 1630-1631 cm^{-1} for **Compound 1** indicates the presence of $\nu_{C=O}$ group. **Compound 1** significant IR peak in the region 3200-3500 cm^{-1} reveals that there will be free ν_{O-H} group positively present. The obtained UV-Vis spectra in methanol solvent of **Compound 1** are 217.30 nm, 245.00 nm and 329.25 nm confirmed $\pi \rightarrow \pi^*$ transition takes place in the O-hydroxy ketone. On the basis of elemental analysis the molecular formula of **Compound 1** must be $C_8H_7Cl_{11}O_2$. A strong mass highest base peak 170.00 conclusively confirmed the molecular formula of **Compound 1**.

*3.3 Crystal Structure Description of **Compound 1***

In order to confirm the chemical structure, single crystal X-ray analysis was used to determine the structure of **Compound 1**. A summary of perspective view of important crystal metrical refinement parameters of **1** shown in Table 1, and selected bond parameters are listed in Tables 2 and 3. An ORTEP view of **Compound 1** with atom numbering scheme shown in Fig. 1. For **Compound 1**, X-ray analysis confirmed that it is totally triclinic crystal system having one phenyl ring linked by one C=O and –OH group. The most promising and striking features in this crystal structure belongs that several bond angles are nearly equal to 120° supporting carbon and oxygen utilized purely sp^2 hybridization. From Table 1a, different C-C and C-O experimental bond distances in the crystal structure support that bonding nature are purely σ covalent & π. A strong intramolecular hydrogen bonding (Fig. 2) is extended over the crystal system and this leads to supramolecular network supported by π-π stacking interactions (Fig. 3). To the best of our knowledge this is the first example where intramolecular hydrogen bond developed supramolecular network and is further supported by π-π stacking.

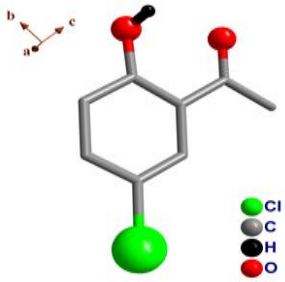


Fig. 1 ORTEP of **Compound 1**

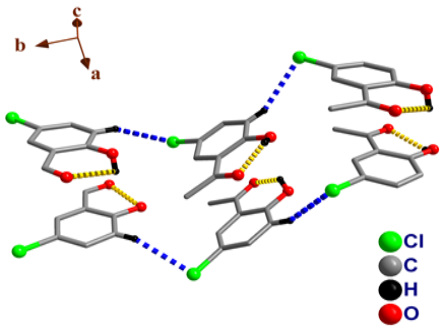


Fig. 2 H-bonding of **Compound 1**

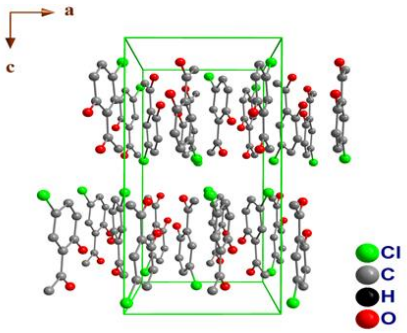


Fig. 3 π-π molecular stacking

Table 1 Crystal data and refinement details for **Compound 1**

Empirical formula	$C_8H_7Cl_{11}O_2$
Formula weight	170.59
Temperature (K)	294(2) K
Wavelength (Å)	0.71073
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	
a (Å)	7.494(4)
b (Å)	12.906(5)
c (Å)	16.105(8)
α (°)	90.4(2)
β (°)	90.16(3)
γ (°)	90.39(2)
Volume (A^3)	1557.7(12)
z	8
$Density_{cal}$ (Mgm^{-3})	1.455
Absorption coefficient (mm^{-1})	0.431
F (000)	704
θ Range (°) for data collection	25.50
Index ranges	-9≤h≤9
	-15≤k≤15
	-19≤l≤16
Goodness-of-fit on F^2	1.408
Completeness to theta	25.50
Independent reflections [R_{int}]	0.0438
Refinement method	Full-matrix least squares on F^2
Reflections collected	5725
Final R indices [I>2σ (I)]	R_1=0.1101, ωR_2=0.2685.
Largest difference peak and hole((eA^{-3})	1.455

Table 2 Selected some bond distances (Å) and angles (°) for **Compound 1**

Selected some Bond distances	Bond distances value (Å)
C1-C7	1.4640
C1-C2	1.4018
C7-O2	1.2341
C7-C8	1.4769
C8-O2	2.3433
C8-H8B	0.9598
C8-H8A	0.9598
C8-H8C	0.9603
O2-H1	1.9299
C9-O4	2.3279
C9-O3	2.430
C1-C6	1.4127

Table 3 Selected some bond distances (Å) and angles (°) for **Compound 1**

Selected some Bond angles	Bond angles value (°)
C1-C2-C6	118.627
C1-C2-C7	121.341
C1-C2-O2	148.679
C1-C2-C3	29.573
C1-C2-O1	146.747
C1-C6-O2	92.693
C1-C6-O1	28.127
C1-C7-O2	27.341
C1-C7-O1	91.906
C1-O2-C3	177.979
C1-O2-C5	122.183
C1-O2-O1	64.573
C1-O3-O1	17.191
C1-C5-O1	57.638
C2-C3-C1	120.012
C2-C3-C4	29.926
C2-C3-C6	89.204
C2-C3-C7	150.027
C3-C2-Cl1	120.059
C3-C4-Cl1	119.079
C3-C4Cl1	119.079
C3-Cl1-C5	149.084
C3-Cl1-C1	150.471
C3-Cl1-H2	96.308
C3-Cl1-H4	95.821
C3-Cl1-C5	149.084
C3-Cl1-C1	150.471
C6-O1-C5	117.943
C6-O1-C1	122.117
H1-O1-C6	45.020
H1-O1-O2	130.056
H1-O1-C1	77.695
H1-O1-C7	108.358

*3.4 DFT Calculations and TD-DFT Analysis of **Compound 1***

The geometry of **Compound 1** as derived from X-ray crystallographic data, were optimized without any symmetry restrictions by means of density functional theory (DFT) calculations using the hybrid DFT (B3LYP) method with the proper basis set 6-31G(d-p) and the GAUSSIAN 09 software package after revision. For the geometry optimized DFT models of **Compound 1** (Fig. 4), the input structures were acquired from the CIF data. The experimental results like bond parameters, IR and UV-Vis spectral data's were compared with the theoretical values in (Table 4).

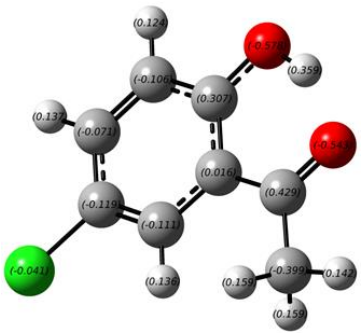


Fig. 4 Optimized structure of **Compound 1** with Mulliken charge distribution

Table 4 Comparative Survey of IR & UV-Vis spectral data of **compound 1**

Experimental Data			Theoretical DFT Computation		
IR (cm^{-1})	UV-Vis	Transition	IR	UV-Vis (nm)	Transition
1630-1631	217.30, 245.00, 329.25	$\pi\rightarrow\pi^*$ in the aromatic ring	1631	215.44, 242.13, 327.32	$\pi\rightarrow\pi^*$ in the aromatic ring
3473	NA	NA	3500	NA	NA

According to this table, the best agreement between the most of the common geometrical parameters calculated at the different DFT levels with 6-31G (d-p) basis set used attained maximum satisfactory results. Hence DFT model as well as proper basis set used 6-31G (d-p) should also be capable of producing a maximum reliable geometry of **Compound 1**. The slight discrepancies with respect bond parameters could be attributed to the fact that crystallographic X-ray measurement has been purely carried out in solid state but the computed DFT model refers to the isolated gaseous phase [Theoretical target optimization curve, IR & UV-Vis spectral curves are depicted from Figs. 5-7. DFT and TD-DFT computations of optimized structure of **Compound 1** was performed in order to establish its electronics structure and different spectral transitions. The geometric structures of the isolated **Compound 1** was fully optimized at the Becke's three parameter hybrid exchange functional and the Lee-Yang-Parr non-local correlation functional (B3LYP) level in the ground state. The optimized structure with Mulliken charge distribution is depicted in Fig. 4, TD-DFT calculations in methanol using CPCM model was performed and theoretically possible spin allowed (singlet-singlet) electronic transitions with their assignment is listed in Table 5. HOMO→LUMO+9 and HOMO→LUMO are the possible highest and lowest energy electronic transitions respectively. The theoretical electronic spectral band at 215.44, 242.13 and 327.32 nm in methanol may be assigned as HOMO →LUMO+1, HOMO-2 →LUMO and HOMO→LUMO respectively. The experimental spectral bands like 217. 30 nm, 245.00 nm and 329.25 nm also confirmed the reference type transitions. All the bands correspond to $\pi\rightarrow\pi^*$ transitions (Table 5). The orbital surface diagram, energies and contributions from the different part of compounds are given in Fig. 8 and Table 6. The energies of highest occupied molecular orbital and lowest unoccupied molecular orbital are -6.31 and -1.97 eV respectively. Contribution of aromatic ring, keto group, hydroxyl group and chlorine atom to HOMO and LUMO are 67%, 3%, 18%, 12% and 50%, 48%, 2%, 0% respectively. Finally for **Compound 1** both the MOs mostly characterized by aromatic ring (Table 7).

Table 5 Selected list of excitation energies of compound 1 in Methanol using CPCM model

Excitation	Wavelength λ (nm)	Oscillatory strength (*f*)	Major Contribution	Assignment
1	327.32	0.0975	HOMO→LUMO (97%)	$\pi\rightarrow\pi^*$
2	307.25	0.0001	HOMO-1 →LUMO (97%)	$n\rightarrow\pi^*$, $\pi\rightarrow\pi^*$
3	242.13	0.1516	HOMO-2 →LUMO (85%)	$\pi\rightarrow\pi^*$
4	215.44	0.3284	HOMO →LUMO+1 (69%)	$\pi\rightarrow\pi^*$
5	213.71	0.0006	HOMO → LUMO+2 (99%)	$\pi\rightarrow\pi^*$
6	206.42	0.0284	HOMO-3 →LUMO (71%)	$n\rightarrow\pi^*$

Table 6 Selected MOs along with their energies and compositions of compound 1

MOs	Energy (eV)	% of Composition			
		Ring	keto	hydroxyl	Cl
LUMO+15	7.9	51	10	1	37
LUMO+14	6.82	63	27	0	10
LUMO+13	6.31	62	28	5	5
LUMO+12	5.74	32	59	7	2
LUMO+11	4.92	45	27	26	2
LUMO+10	4.84	18	81	0	0
LUMO+9	4.71	90	8	1	1
LUMO+8	4.3	46	39	14	1
LUMO+7	4.13	75	23	2	1
LUMO+6	3.99	38	51	11	1
LUMO+5	3.18	68	17	13	2
LUMO+4	2.92	33	65	0	2
LUMO+3	0.64	60	39	0	1
LUMO+2	0.58	55	1	0	43
LUMO+1	-0.27	91	2	5	2
LUMO	-1.97	50	48	2	0
HOMO	-6.31	67	3	18	12
HOMO -1	-7.45	14	76	10	1
HOMO -2	-7.55	92	8	0	0
HOMO -3	-8.71	31	2	18	49
HOMO -4	-8.77	9	1	0	90
HOMO -5	-9.92	61	10	25	3
HOMO -6	-10.09	6	82	10	1
HOMO -7	-10.46	43	9	16	32
HOMO -8	-10.7	32	55	6	6
HOMO -9	-11.01	52	36	3	8
HOMO -10	-11.11	44	8	33	15
HOMO -11	-11.47	47	27	23	3
HOMO -12	-11.94	11	81	7	1
HOMO -13	-12.34	88	8	4	1
HOMO -14	-12.45	20	75	5	0
HOMO -15	-12.59	52	25	7	16

Table 7 Energy and others physical properties of **Compound 1**

Charge	0
Spin	Singlet
Energy (eV)	-25027.465375226
Dipole moment (D)	1.9666
Point group	C1

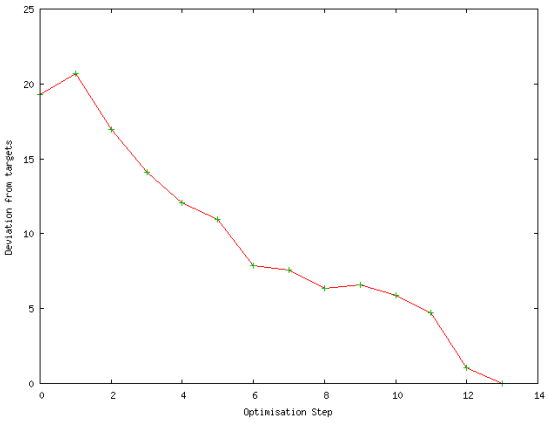


Fig. 5 Optimization step vs deviation from target curve

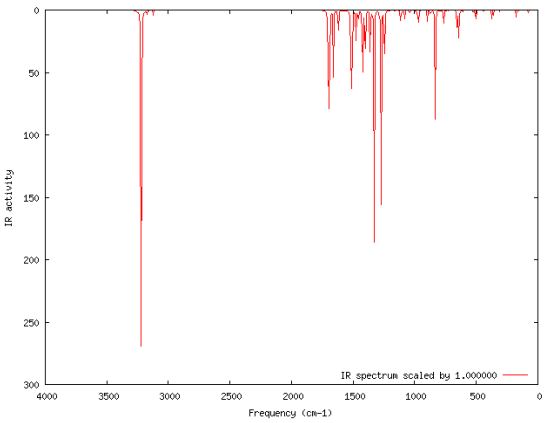


Fig. 6 Theoretical IR spectrum of **compound 1**

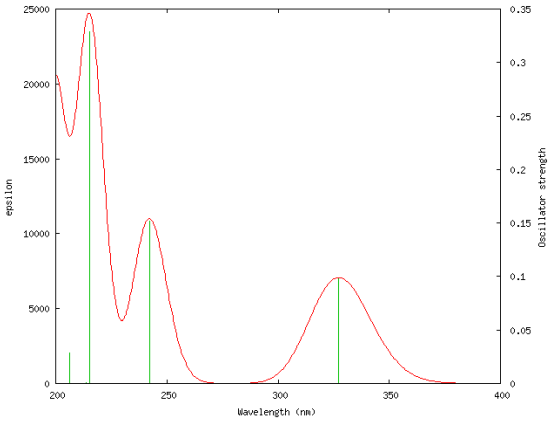
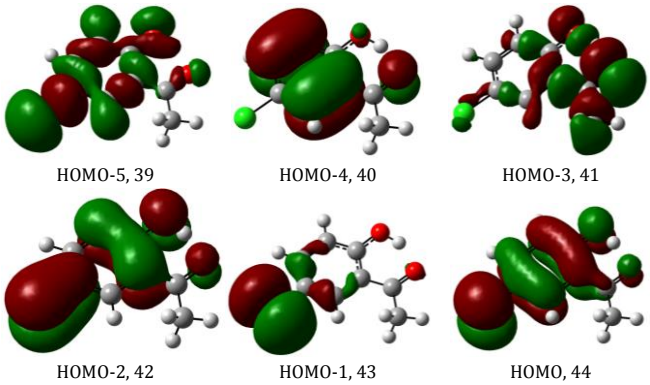


Fig. 8 Theoretical UV-Vis spectra of **compound 1**



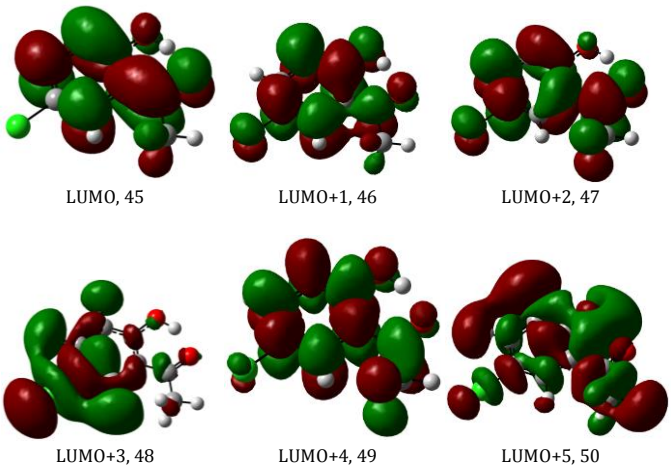


Fig. 8 Surface plot of the frontier orbital of **compound 1**

4. Conclusion

Compound 1 successfully synthesized in our laboratory by published procedure. X-ray single crystal analysis confirmed **compound 1** belongs to triclinic crystal system and characterized by melting point, FT-IR, UV-Vis and mass spectroscopic study. The geometry of **compound 1** optimized with the DFT-B3LYP level computation method using LanL.2DZ basis sets. The best agreement between most of the common bond parameters theoretical and experimental results were obtained by using B3LYP level with 6-31G(d-p) basis set. Thus we can conclude that beside single XRD analysis for crystal structure refinement, today in the same field DFT & TD-DFT are another reliable methods to the same extent.

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