

# Molecular Structure, NBO Analysis NLO of Iodo -4-Oxo-4H Chromene-3 Carbaldehyde Using Density Functional Theory

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**Abstract**— The first objective of this computational work is to determine the optimized geometry of Iodo -4-Oxo-4H Chromene-3 Carbaldehyde C<sub>10</sub>H<sub>5</sub>IO<sub>3</sub>. The optimized structural parameters such as the lengths and angles of the bonds were determined by the B3LYP density functional model with Lan L2DZ basis set by Gaussian program 09. The optimized structural parameters calculated by density functional theory (DFT) were compared with the results of X-ray diffraction in the literature. The second objective is natural bond orbital (NBO) analysis which provides an efficient method to study the stability of the molecule. The dipole moment ( $\mu$ ), molecular electrostatic potential (MEP), frontier orbital energy gap was illustrated. Nonlinear Optical Effects (NLO) properties related to polarizability and hyperpolarizability was also discussed.

**Keywords**— Density Functional Theory; NBO; electrostatic potential, NLO.

## I. INTRODUCTION

7-iodo-4-oxo-4H-chromene-3-carbaldehyde is an organic compound of formula C<sub>10</sub>H<sub>5</sub>IO<sub>3</sub> geometrical structure is shown in Fig.1. The synthesis and crystallization of the title compound was described by Yoshinobu Ishikawa [1]. 3-Formylchromone and its derivatives show versatile biological activities such as anti-inflammatory activity [2], and the inhibition of protein tyrosine phosphatase 1B [3], thymidine phosphorylase [4], carbonic anhydrase [5], and metallo-lactamase [6]. Ishikawa & Motohashi, [1] concluded that, the position of halogen atoms on the chromone ring should be associated with the urease inhibitory activity.

## II. COMPUTATIONAL DETAILS

Geometry optimization is an important part of most quantum chemical calculations; it is a key component of most

, “This work was supported in part by the 1st National Conference on Synthesis and Catalysis, Tiaret (CNSCT, 2021)

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computational chemistry studies that are concerned with the structure and/or reactivity of molecules.

Many of physical and chemical properties are determined from the geometry of molecule. The optimization of the geometry for the molecule was achieved by energy minimization; using DFT at the B3LYP level, employing the basis set LanL2DZ Figure 1 and Table 1 below represent the diagram of the optimized molecule, these bond lengths and its angle measurements. All calculations was made with the Gaussian 09 program [7]

## A. Abbreviations and Acronyms

B3LYP is the nonlocal correlation functional of Lee, Yang, and Parr, HOMO is highest occupied molecular orbital and LUMO lowest unoccupied molecular orbital,  $F_{i,j}$  is the corresponding Fock matrix element,  $q_i$  is the donor orbital occupancy and  $\epsilon_j, \epsilon_i$  are the orbital energy. Finally, in order to select optimal,  $E^2$  is the stabilization energy, ED is electron density, NBO is natural bond orbital, NLO is, Nonlinear Optical Effects,  $\mu$  is dipole moment, MEP is molecular electrostatic potential,  $\alpha_0$  is polarizability,  $\alpha$  is anisotropy of the polarizability,  $\beta$  first order hyperpolarizability, au is atomic units.

## III. GEOMETRY OPTIMISATION

The formulae of studied compounds are depicted in Fig. 1. Initially the optimized geometrical data of title compound has been determined by using B3LYP function with Lan L2DZ basis set. Title compound has been chosen for this step because its structure was analyzed by x-ray diffraction method.[1]

The optimized geometrical parameters and X-ray crystallographic data [1] were collected in Table 1. In general, the bond length between two atoms is approximately the sum of the covalent radii of the two atoms. For covalent bonds, bond energies and bond lengths depend on many factors like electron affinities, sizes, electro-affinity of atoms involved in the bond, differences in their electronegativity, and the overall structure of the molecule [8]. As can be seen from the Table I the computed values are in good harmony with experimental values (Fig.2).

#### IV. III HOMO-LUMO ANALYSIS AND MULLIKEN ATOMIC CHARGES

Both the highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) play a role in the chemical stability of compounds. For instance, the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) show the ability of donating and accepting an electron in any molecule, respectively. [9].

The HOMO is delocalized on ring of oxygen atoms while LUMO is localized on atoms of oxygen and on second ring also of the title compound Fig.3. The distribution pattern revealed the intra-molecular charge transfer from HOMO to LUMO. The energy gap of the title compound is 4,409936 eV at B3LYP by Lan L2DZ level of theory has been tabulated in Table 2. It is noteworthy that the C9 atom of the title compound exhibited more positive charge, whereas the O11, O12 O13 atoms exhibited the most negative charges (Fig.1).

#### V. MOLECULAR ELECTROSTATIC POTENTIAL SURFACE

The electrostatic potential of a molecule is a good guide in assessing the molecules reactivity towards positively or negatively charged reactants [10]. The negative attractive potential appears in red and yellow coloured regions of MEP surface (Fig.4) were related to electrophilic reactivity, while the positive repulsive potential appear in blue regions to nucleophilic reactivity.

Negative electrostatic potential corresponds to an attraction of the proton by the concentrated electron density in the molecules (from lone pairs, pi-bonds, etc.). Positive electrostatic potential corresponds to repulsion of the proton by the atomic nuclei in regions where low electron density exists and the nuclear charge is incompletely shielded. In the title molecule the negative potentials are located over the formyl O atom. While the positive potentials are located near the hydrogens

#### VI. NATURAL BOND ORBITAL ANALYSIS (NBO)

NBO analysis provides an efficient method for studying intra and intermolecular bonding and interaction among bonds, and also provides a convenient basis for investigation of charge transfer or conjugative interactions in molecular system [11]. The second Fock matrix was carried out to evaluate donor-acceptor interactions in the NBO analysis [12].

The interaction results in a loss of occupancy from the localized NBO of the idealized Lewis structure into an empty non-Lewis orbital. For each donor (*i*) and acceptor (*j*), the stabilization energy,  $E^2$ , associated with the delocalization,  $i \rightarrow j$ , is estimated as:

$$E^{(2)} = q_i \frac{(F_{ij})^2}{\epsilon_j - \epsilon_i} \quad (1)$$

where  $q_i$  is the orbital occupancy,  $\epsilon_i$ ,  $\epsilon_j$  are diagonal elements and  $F_{ij}$  is the off-diagonal NBO Fock matrix element. In the perturbation energies of donor acceptor interactions are presented.. In the title molecule 7-iodo-4-oxo-4H-chromen-3-

carbaldehyde.  $\pi(C1-C2) \rightarrow \pi^*(C3-O12)$  was

25.10 kcal/mol,  $\pi(C4-C5) \rightarrow \pi^*(C6-C7)$  was 23,11 kcal/mol therefore they give a stronger stabilization to the structure, it is noted that the maximum occupancies 1,98452 ; 1,98838 , 1,99072 ; 1,98227 are obtained  $\sigma(C1-C2)$ ,  $\sigma(C1-O11)$ ,  $\sigma(C3-O12)$ , et  $\sigma(C5-C6)$  respectively. Therefore, the results suggest that  $\sigma(C1-C2)$ ,  $\sigma(C1-O11)$ ,  $\sigma(C3-O12)$   $\sigma(C5-C6)$  are mainly controlled by the p character of hybrid orbitals Table II.

The same kind of interaction is calculated in the same kind of interaction energy, related to the resonance in the molecule, is electron donating (Table III) LP(2) O13 to  $\sigma^*(C10-H16)$  shows less stabilization of 16.40kJ/mol and further LP(2)O11 and  $\pi^*(C1-C2)$ , leads to strong stabilization energy of 31,47kJ/mol and LP(2) O11 to  $\pi^*(C8-C9)$  resulting in an enormous stabilization of 22,81 kJ/mol. The strong intra-molecular hyper conjugation hyper conjugation interaction of the  $\sigma$  and the  $\pi$  electrons of C-C to the anti C-C bond in the ring leads to stabilization of some part of the ring as evident from

#### VII. NON-LINEAR OPTICAL EFFECTS (NLO)

When a beam of light propagates through a material, the interaction of the optical field with organic molecules in the material induces charge variation and displacement of associated atoms [13].

In order to study the relationships between photocurrent generation, molecular structures and NLO, polarizabilities and hyperpolarizabilities were calculated using various methods and different bases, depending on the finite field approach. First order hyperpolarizability is a third rank tensor that can be described using 3x3x3 matrices. The 27 components of the 3D matrix can be reduced to 10 components according to Kleinman symmetry [14]. The components of  $\beta$  are defined as the coefficients of a Taylor series expansion of the energy in an external electric field. When the external electric field is weak and homogeneous, the expansion becomes:

$$E = E^0 - \mu_\alpha F_\alpha + \frac{1}{2} \alpha_{\alpha\beta} F_\alpha F_\beta - \frac{1}{6} \beta_{\alpha\beta\gamma} F_\alpha F_\beta F_\gamma + \dots \quad (3)$$

where  $E^0$  is the energy of the unperturbed molecules,  $F_\alpha$  the field at the origin and  $\mu_\alpha$ ,  $\alpha_{\alpha\beta}$  and  $\beta_{\alpha\beta\gamma}$  are the components of dipole moment, polarizability and the first hyperpolarizabilities, respectively.

The total static dipole moment ( $\mu$ ), mean polarizability ( $\alpha_0$ ) anisotropy of the polarizability ( $\alpha$ ) and mean first order hyperpolarizability ( $\beta$ ), using the *x*, *y* and *z* components, are defined as follows:

$$\alpha_0 = \frac{1}{3} \sum_i \alpha_{ii} \quad (4)$$

$$\alpha = 2((\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6\alpha_{xx}^2)^{0.5} \quad (5)$$

$$\begin{cases} \beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz} \\ \beta_y = \beta_{yyy} + \beta_{xxy} + \beta_{yzz} \\ \beta_z = \beta_{zzz} + \beta_{xxz} + \beta_{yyz} \end{cases} \quad (6)$$

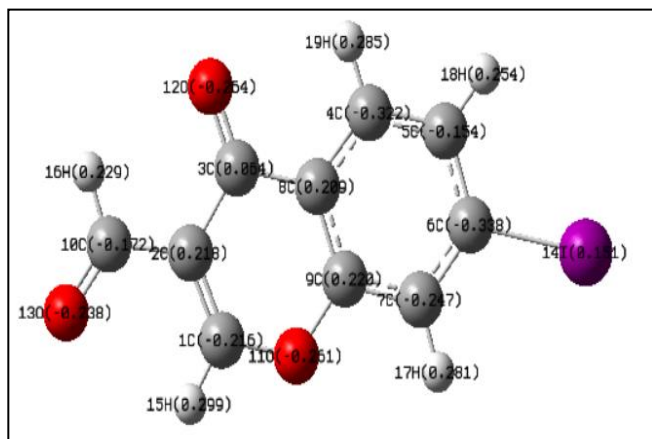


Fig. 1. Optimized structure and Mulliken atomic charges obtained by B3LYP/ Lan L2DZ for *C10H5IO3*

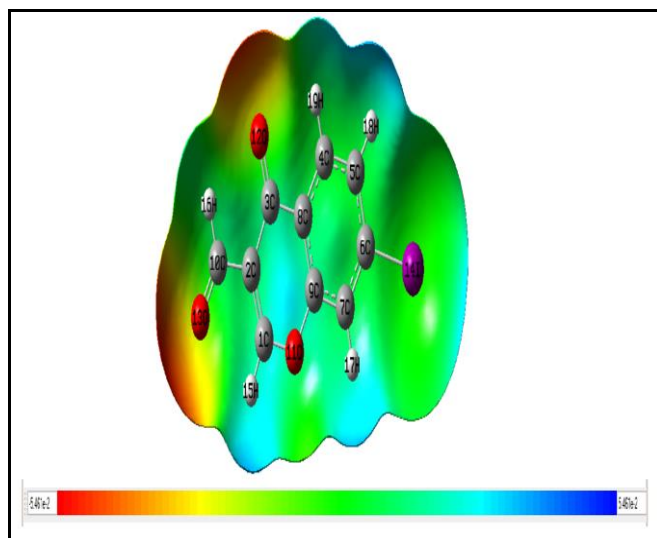


Fig 4 : Molecular electrostatic potential surface map

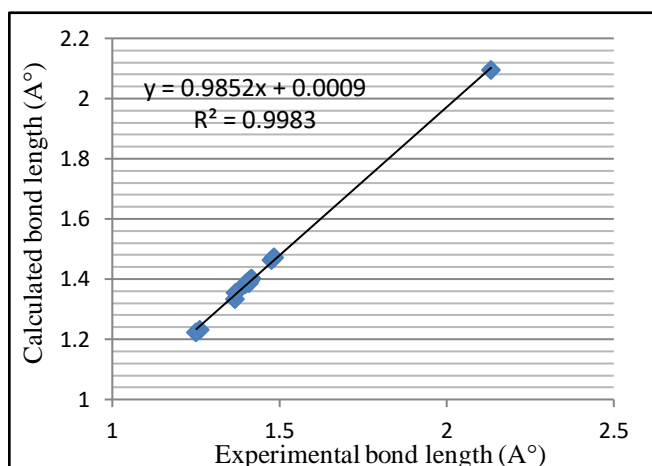


Fig. 2. Calculated bond lengths in comparison with experimental data.

TABLE I

SELECTED OPTIMIZED PARAMERS OF *C10H5IO3*

bond length (Å°)	Calculated values	Experimental values [1]
I14—C6	2.13258	2.094
O11—C1	1.36838	1.334
O11—C9	1.40884	1.386
O12—C3	1.26140	1.230
O3—C10	1.25142	1.222
C1—C2	1.36991	1.355
C2—C3	1.47719	1.462
C2—C10	1.48401	1.462
C3—C8	1.4853	1.471
C4—C5	1.39867	1.471
C4—C8	1.41308	1.400
C5—C6	1.41680	1.401
C6—C7	1.40135	1.387
C7—C9	1.40340	1.389
C8—C9	1.41092	1.392
C1—H15	1.08440	0.9500
C4—H19	1.08599	0.9500
C5—H18	1.08455	0.9500
C7—H17	1.08413	0.9500
C10—H16	1.10089	0.9500

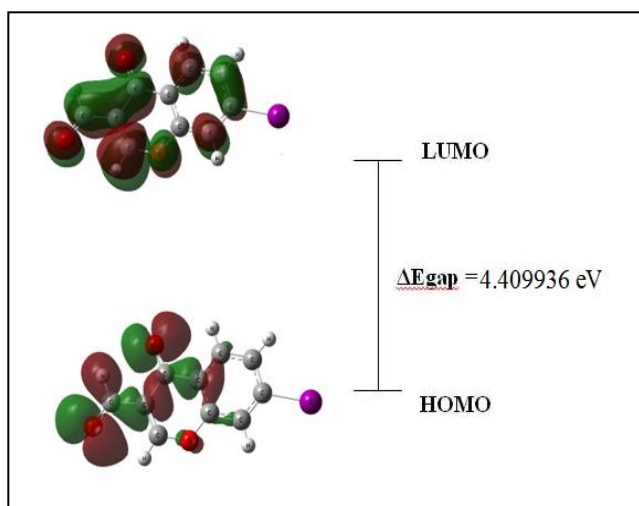


Fig. 3. Frontier molecular orbital surfaces and energy gap for *C10H5IO3*

bond angles (°)	Calculated values	Experimental values [1]
C1—O11—C9	118.93093	118.2
O11—C1—C2	124.19949	125.1
O11—C1—H15	112.61513	117.4
C1—C2—C3	123.18539	120.5
C1—C2—C10	120.63342	119.4
C3—C2—C10	119.85735	120.1
O12—C3—C2	122.95470	123.2
O12—C3—C8	122.48349	122.8
C2—C3—C8	114.56182	113.9
C5—C4—C8	120.86113	120.8
C5—C4—H19	121.10559	119.6
C8—C4—H13	118.03329	119.6
C4—C5—C6	119.62427	120.5
C4—C5—C6	119.62427	120.5
C4—C5—H18	120.12946	120.5
C7—C6—C5	120.97712	121.6
C7—C6—H14	119.54788	118.6
C5—C6—H14	119.47500	119.8
C6—C7—C9	118.01454	117.7
C6—C7—H17	122.61125	121.2
C9—C7—H17	119.37421	121.2
C9—C8—C4	117.84021	118.2
C9—C8—C3	120.65476	120.2
C4—C8—C3	121.50502	121.5
O11—C9—C7	116.29769	115.5
O11—C9—C8	121.01958	122.0
C7—C9—C8	122.68273	122.5
O13—C10—C2	123.57290	123.9
O13—C10—H16	121.76497	118.0
C2—C10—H16	114.66213	118.0
C7—C6—C5	120.97712	121.6
C6—C5—H18	120.24627	
Torsion angle(°)	Calculated values	Experimental values [1]
C9-O11-C1-C2	0.00000	0.1
O1-C1-C2-C3	0.00034	1.1
O11-C1-C2-C10	-180.00000	-178.8
C1-C2-C3-O12	-179.99897	178.6
C10-C2-C3-O12	0.00119	-1.5
C1-C2-C3-C8	-0.00074	-2.3
C10-C2-C3-C8	-0.00074	177.6
C8-C4-C5-C6	0.00000	1.6
C4-C5-C6-C7	0.00000	-1.5
C4-C5-C6-H14	180.00000	177.9
C5-C6-C7-C9	0.00000	0.3
H14-C6-C7-C9	180.00000	-179.1

C5-C4-C8-C9	0.00000	-0.6
C5-C4-C8-C3	-180.00000	179.7
O12-C3-C8-C9	179.99894	-178.5
C2-C3-C8-C9	0.00070	2.4
O12-C3-C8-C4	-0.00120	1.2
C2-C3-C8-C4	-179.99944	-177.9
C1-O11-C9-C7	180.00000	179.6
C1-O11-C9-C8	0.00000	0.0
C6-C7-C9-O11	-180.00000	-178.8
C6-C7-C9-C8	0.00000	0.7
C4-C8-C9-O11	180.00000	179.0
C3-C8-C9-O11	-0.00026	-1.4
C4-C8-C9-C7	0.00000	-0.6
C3-C8-C9-C7	180.00000	179.1
C1-C2-C10-O13	0.00115	4.9
C3-C2-C10-O13	-179.99901	-175.0

TABLE II  
HYBRIDS OF 7-IODO-4-OXO-4H-CHROMENE-3-CARBALDEHYDE  
CALCULATED BY B3LYP/ Lan L2DZ basis set. FOR C, H, I, O atoms.

Donor Lewis-type NBOs	Hybrid	AO [%]
C1 - C2	S p <sup>1.39</sup>	s( 41.85%)p ( 58.15%)
C1 - C2	Sp	s( 0.00%)p (100.00%)
C1 - O11	S p <sup>2.98</sup>	s( 25.15%) p( 74.85%)
C1 - H15	S p <sup>2.03</sup>	s( 33.01%)p ( 66.99%)
C2 - C 3	S p <sup>2.01</sup>	s( 33.25%)p ( 66.75%)
C2 - C10	S p <sup>2.12</sup>	s( 32.01%)p ( 67.99%)
C3 - C8	S p <sup>1.91</sup>	s( 34.40%)p ( 65.60%)
C3 - O12	S p <sup>2.20</sup>	s( 31.29%)p ( 68.71%)
C4 - C5	S p <sup>1.80</sup>	s( 35.77%)p (64.23%)
C4 - C5	S p <sup>2.20</sup>	s( 0.00%)p (100.00%)
C4 - C8	S p <sup>1.88</sup>	s( 34.72%)p ( 65.28%)
C4 - H19	S p <sup>2.39</sup>	s( 29.49%)p ( 70.51%)
C5 - C6	S p <sup>1.86</sup>	s( 34.95%)p( 65.05%)
C5 - H18	S p <sup>2.43</sup>	s( 29.19%)p ( 70.81%)
C6 - C7	S p <sup>1.54</sup>	s( 39.35%)p ( 60.65%)
C6 - C7	Sp	s( 0.00%)p(100.00%)
C6 - H14	S p <sup>3.67</sup>	s( 21.42%)p ( 78.58%)
C7 - C9	S p <sup>1.91</sup>	s( 34.42%)p ( 65.58%)
C7 -H17	S p <sup>2.39</sup>	s( 29.48%)p ( 70.52%)
C8 - C9	S p <sup>2.02</sup>	s( 33.14%)p( 66.86%)
C9 - O11	S p <sup>3.34</sup>	s( 23.06%)p ( 76.94%)
C10 - O13	Sp	s( 0.00%)p(100.00%)
C10 - H16	S p <sup>2.05</sup>	s( 32.76%)p ( 67.24%)

TABLE II  
NLO PROPERTIES OF -IODO-4-OXO-4H-CHROMENE-3-CARBALDEHYDE CALCULATED BY B3LYP/ Lan L2DZ

Parameters	Lan L2DZ/ B3LYP	Parameters	Lan L2DZ/ B3LYP
$\mu_x$	1.63179		
$\mu_y$	-0.26353		
$\mu_z$	0.00009	$\beta_{xxx}$	-1816.8592
$\mu(D)$	1,65293	$\beta_{xxy}$	158.70592
$\alpha_{xx}$	240.8779	$\beta_{xyy}$	148.65988
$\alpha_{xy}$	-5.5228	$\beta_{yyy}$	50.31617
$\alpha_{yy}$	125.9107	$\beta_{xxz}$	0.03187
$\alpha_{xz}$	-0,0009	$\beta_{xyz}$	-0.00495
$\alpha_{yz}$	-0,0007	$\beta_{yyz}$	0.004
$\alpha_{zz}$	45.5701	$\beta_{xzz}$	-38.64089
$\alpha_0(u.a)$	135.612	$\beta(u.a)$	1720.0037
$\alpha \times 10^{23}(esu)$	2.007	$\beta \times 10^{-30}(esu)$	14.8596

TABLE III  
SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS IN C10H5IO3 CALCULATED BY B3LYP/Lan L2DZ

Donor(i)	Type	ED(e)	Acceptor(j)	Type	ED(e)	$E^{(2)a}$ [Kcal/mol]	$E(j)-E(i)^b$ [a.u.]	$F_{ij}^c$ [a.u.]
C 1 - C2	$\sigma$	1.98452	C1- H 15	$\sigma^*$	1.9732	1.01	1.25	0.032
	$\sigma$		C2 - C3	$\sigma^*$	1.9732	1.66	1.20	0.040
	$\sigma$		C 2 - C 10	$\sigma^*$	1.9745	1.32	1.18	0.036
	$\sigma$		C 3 - O 12	$\sigma^*$	1.9902	2.67	1.25	0.052
	$\sigma$		C 9 - O 11	$\sigma^*$	1.9876	0.66	1.01	0.023
	$\sigma$		C 10 - H 16	$\sigma^*$	1.9856	1.44	1.22	0.038
C 1 - C2	$\pi$	1.77434	C1 - C2	$\pi^*$	1.7744	4.99	0.30	0.035
	$\pi$		C3 - O12	$\pi^*$	1.9628	25.10	0.29	0.077
	$\pi$		C10 - O13	$\pi^*$	1.9764	19.89	0.29	0.070
C 1-O11	$\sigma$	1.98838	C2 - C10	$\sigma^*$	1.9745	2.56	1.35	0.053
	$\sigma$		C7 - C9	$\sigma^*$	1.9652	2.24	1.45	0.051
C 3-O12	$\sigma$	1.99072	C 1- C2	$\sigma^*$	1.98452	1.84	1.56	0.048
	$\sigma$		C 2- C3	$\sigma^*$	1.97392	1.11	1.44	0.036
	$\sigma$		C 3- C8	$\sigma^*$	1.97116	1.20	1.43	0.037
	$\sigma$		C 8- C9	$\sigma^*$	1.97615	2.22	1.52	0.052
C 3-O12	$\pi$	1.96218	C 1- C2	$\pi^*$	1.77434	6.72	0.36	0.046
	$\pi$		C 8- C9	$\pi^*$	1.63290	6.20	0.36	0.047
C 4- C5	$\pi$	1.66002	C 6- C7	$\pi^*$	1.69435	23.11	0.27	0.070
	$\pi$		C 8- C9	$\pi^*$	1.63290	20.55	0.27	0.068
C 5- C6	$\sigma$	1.98227	C 4- C5	$\sigma^*$	1.97002	1.60	1.27	0.040
	$\sigma$		C 4- H19	$\sigma^*$	1.97262	2.87	1.24	0.053
	$\sigma$		C 5- H18	$\sigma^*$	1.97541	1.27	1.23	0.035
	$\sigma$		C 6- C7	$\sigma^*$	1.97799	1.87	1.24	0.043
	$\sigma$		C 7- H17	$\sigma^*$	1.97183	3.18	1.21	0.055
C 6- C7	$\pi$	1.69435	C 4- C5	$\pi^*$	1.66002	17.24	0.31	0.066
	$\pi$		C 8- C9	$\pi^*$	1.63290	20.84	0.27	0.071
C 8- C9	$\pi$	1.63290	C 3- O12	$\pi^*$	1.96218	22.25	0.31	0.071
	$\pi$		C 4- C5	$\pi^*$	1.66002	18.55	0.29	0.069
	$\pi$		C 6- C7	$\pi^*$	1.69435	20.31	0.29	0.068
	$\pi$		C 8- C9	$\pi^*$	1.63290	1.21	0.29	0.017
C 9-O11	$\sigma$	1.98706	C 1- H15	$\sigma^*$	1.97312	1.36	1.40	0.039
	$\sigma$		C 4- C8	$\sigma^*$	1.96904	2.31	1.43	0.051
	$\sigma$		C 6- C7	$\sigma^*$	1.97799	2.28	1.42	0.051
C10-O13	$\sigma$	1.99336	C2 - C3	$\sigma^*$	1.97392	2.23	1.44	0.051
	$\sigma$		C2 - C10	$\sigma^*$	1.97465	0.51	1.43	0.024
C10-O13	$\pi$	1.97654	C1- C2	$\pi^*$	1.77434	6.01	0.37	0.044
C10-H16	$\sigma$	1.98556	C1- C2	$\sigma^*$	1.98452	5.29	1.08	0.068
O11	LP(2)		C1- C2	$\pi^*$	1.77434	31.47	0.36	0.097
	LP(2)		C8- C9	$\pi^*$	1.63290	22.81	0.36	0.085
O12	LP(2)		C2- C3	$\sigma^*$	1.97392	16.71	0.69	0.097
	LP(2)		C3- C8	$\sigma^*$	1.97116	17.17	0.68	0.097
O13	LP(2)		C2- C10	$\sigma^*$	1.97465	16.87	0.68	0.097
	LP(2)		C10- H16	$\sigma^*$	1.98556	16.40	0.72	0.098

a  $E^{(2)}$  means energy of hyper conjugative interaction (stabilization energy).

b  $E(j)-E(i)^b$  Energy difference between donor and acceptor i and j NBO orbitals.

c  $F(i; j)$  is the Fock matrix element between i and j NBO orbitals.

## VIII. VCONCLUSION

The calculated parameters (bond lengths and bond angles) show a good agreement with the corresponding experimental data [1] showing the strength of density functional calculations.

The HOMO, LUMO orbital localization confirm the intramolecular charge transfer, also HOMO-LUMO energy gap reflected the chemical activity of C10H5IO3.

The MEP shows that the negative potential sites are on electronegative atoms as well as the positive potential

The NBO analysis has provided the detailed in-sight into the the nature of bonding in C10H5IO3. The  $\sigma$  bond (C6 - I14) is formed from the hybrid S p<sup>3.67</sup> on an iodine atom and the bond  $\sigma$ (C1 - O11) is formed from a hybrid S p<sup>2.98</sup> on oxygen and the  $\pi$  bond (C3 -O12) is formed from a hybrid Sp<sup>2.20</sup> on oxygen. The strongest electron donation occurs from a single LP (2) O11 pair to the anti-binding acceptor  $\pi^*$  (C1-C2), leading to a strong stabilizing energy of 31.47kJ / mol..

The predicted first order hyperpolarizability shows that the molecule might have a reasonably good NLO behavior.

## REFERENCES

- [1] Yoshinobu Ishikawa. (2016, Oct.). Acta Cryst. Section E Structure.[Online]. (72), pp. 1724–1727. Available:
- [2] Khan, K. M., Ambreen, N., Mughal, U. R., Jalil, S., Perveen, S. & Choudhary, "3-Formylchromones: Potential antiinflammatory agents," *Eur. J. Med. Chem.*, vol. 45, pp. 4058–4064, Jun., 2010.
- [3] Shim, Y. S., Kim, K. C., Lee, K. A., Shrestha, S., Lee, K. H., Kim, C. K. & Cho, H., "Formylchromone derivatives as irreversible and selective inhibitors of human protein tyrosine phosphatase 1B. Kinetic and modeling studies," *Bioorg. Med. Chem* vol. 13, pp. 1325–1332, 2005.
- [4] Khan, K. M., Ambreen, N., Hussain, S., Perveen, S. & Choudhary, M. I, "Schiff bases of 3-formylchromone as thymidine phosphorylase inhibitors," *Bioorg. Med. Chem.*, vol. 17, pp. 2983–2988, Mar. 2009.
- [5] Ekinci, D., Al-Rashida, M., Abbas,, "Chromone containing sulfonamides as potent carbonic anhydrase inhibitors," *J. Enzyme Inhib. Med. Chem.* vol. 27, pp. 744–747, 2012.
- [6] Christopheit, T., Albert, A. & Leiros, H. K. "Discovery of a novel covalent non- $\beta$ -lactam inhibitor of the metallo- $\beta$ -lactamase NDM-1," *Bioorg. Med. Chem.*, vol. 24, pp. 2947–2953, Jul. 2016.
- [7] M.J. Frisch, G.W. Trucks, H.B. Schlegel.(2009,June). GAUSSIAN 09.[Online]. Revision B.03, Gaussian, Inc., Pittsburgh PA.
- [8] A. Kumer, Md. Sarker, S. Paul, "The theoretical investigation of HOMO, LUMO, thermophysical properties and QSAR study of some aromatic carboxylic acids using HyperChem programming," *Int. J. Chem. Technol.*, vol. 3, pp26-37, Jun., 2019.
- [9] S. Gunasekaran, R.A. Balaji, S. Kumaresan, G. Anand, S. Srinivasan, "Experimental and theoretical investigations of spectroscopic properties of N-acetyl-5-methoxytryptamine," *Can. J. Anal. Sci. Spectrosc.*, vol. 53, pp. 149-162, Jan. 2008.
- [10] Yiwei Wang, Yu Zhang, "Experimental and DFT studies on the vibrational and electronic spectra of 9-ptolyl-9H-carbazole-3-carbaldehyde Spectrochimica Acta Part A: *Molec. and Biomolec. Spectrosc.*, vol. 135, pp. 296–306 2015.
- [11] Rubarani P. Gangadharana and S. Sampath Krishnanb, "Natural Bond Orbital (NBO) Population Analysis of 1-Azanaphthalene-8-ol," *Acta Physica Polonica A.*, vol. 125, pp. 18–22. 2014.
- [12] Raj R.K., Gunasekaran S., Gnanasambandan T., Seshadri S. "Structural, Spectroscopic (FT-IR, FT-Raman & UV-Vis) and theoretical studies of 4,6-dichloro-3-formyl coumarin, *Int. J. Curr. Res. Aca.* vol., 3, pp. 130–149 ,2015.
- [13] Zeynep Demircioglu<sup>a,\*</sup>, Cigdem Albayrak Kastan<sup>b</sup>, Orhan Buyukgungor<sup>a</sup>, "Theoretical analysis (NBO, NPA, Mulliken Population Method) and molecular orbital studies (hardness, chemical potential, electrophilicity and Fukui function analysis) of (E)-2-((4-hydroxy- 2-methylphenylimino)methyl)-3-methoxyphenol," *J. of Molec. Struc.*, vol. 1091, pp. 183–195, Mar. 2015.
- [14] Maha S. Almutairi, S. Muthu, Johanan C. Prasana, B. Chandralekha, Alwah R. Al-Ghamdi, Mohamed I. Attia\*, "Comprehensive spectroscopic (FT-IR, FT-Raman, 1H and 13C NMR) identification and computational studies on 1-acetyl-1H-indole-2,3-dione," *Open Chem.*, vol. 15, pp. 225–237, Sep., 2017.