A COMPLETE THEORETICAL STUDY OF INDIRUBIN-A BLUE DYE FOR DYE SENSITIZED SOLAR CELLS (DSSCs) APPLICATIONS

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ABSTRACT

The Fukui indices analysis is performed to identify the reactive regions of indirubin (IB).The most nucleophilic reactive site is identified at C16 atom. Correspondingly the most electrophilic reactive site is identified at O27 atom. The two regions are preferably used for reactions. Theoretical HOMO energy, LUMO energy and energy gaps are calculated to predict the DFT based global reactivity descriptors such as Chemical potential (μ), Chemical hardness (η), Chemical softness (s), Electro philicity index (ω), Electronegativity (χ), Maximum amount of electronic charge (ΔN_{max}). The energy gap of IB is reduced while introducing NO_2 group than CN group. This shows that the maximum charge transfer is possible in this molecule IB2. This is also well supported by ΔN_{max} of IB2. It's value is highest than other system. The chemical hardness of IB with NO_2 group is lowest than other systems such as IB and IB2. This lowest chemical hardness suggests that IB2 is a soft molecule. Out of three systems, IB2 is having more electrophilicity indexes. This is also supported well by the electronegativity of IB2 which is higher than other systems. The LHE of all the dyes fall within the range of 0.21205-0.53065 in gas phase. It can be concluded that a class of selected IB derivative dyes shows a good photo physical properties related to DSSC use but in different outstanding properties. According to LHE, IB2 in gas phase is the most efficient than that of the other derivatives studied here. From this we can assume that substitutes of acceptor and donor atoms can enrich the properties of IB derivatives dyes for the use in DSSC.

Keywords: Blue Indirubin, DFT, LHE, DSSC.

1 INTRODUCTION

Indigo is one of the oldest dyes used by mankind. The current consumption of the dye is enormous due to the popularity of blue jeans, which are dyed with indigo. The consumption of indigo and other vat dyes reaches about 33 million kg annually [1] and the reduction of indigo to leuco-indigo represents an important type of industrial process which is operated worldwide on a considerable scale [2]. Throughout history indigo was derived from various plants. Dyes's woad (Isatis tinctoria L) was cultivated in wide areas in Europe until indigofera species (indigofera tinctoria) from India started to be imported in bigger scale in the 17th century [3]. In the 19th century came the synthetic dyes and nowadays indigo is mainly synthesized from by-products of fossil fuels. Recently there has been a growing interest in natural products obtained from renewable resources instead of oil supplies, which are non-renewable [4].

1.1 INDIRUBIN- A BLUE DYE

The dark blue color indigo and the dye of the same name and color, are surely quite familiar to the reader .Intense colors in materials indicate a high degree of light absorption by their component atoms (or) molecules. That in turn implies an extensive electron resonance and delocalization in their molecular orbitals. Such a widespread electron resonance and delocalization is found in metallic solids, a topic of particular interest to me. Thus , new types of metallic compounds will be more likely derived from highly colored compounds like indigo, rather than from highly colored compounds like the saturated hydrocarbons ,for example, possible electrically –conductive indigo derivatives are examined further on in this web page.The terms indigo and indigotin are generally considered to refer to the same chemical substance. Sometimes the term indigo is applied only to the color and the natural product (which invariably contains a number of chemical compounds).while the word indigotin is reserved for the single pure compound of indigo.

Indigo is a so-called vat-dye, which means that it needs to be reduced to its water that soluble leuco–form before dying. The reduced form is absorbed into the fibers, and when oxidation back to its blue form it stays within the fiber [5]. Earlier the reduction and dyeing was done with fermentation [6,7]. Nowadays, the most of the reduction has been done chemically by sodium dithionite. It is considered environmentally unfavorable, since it produces sulphite, sulphate, thisulphate and toxic sulphides as degradation products, which then contaminate the wastes from the dyeing plants [2]. Therefore there has been interest to find new possibilities to reduce indigo.

Possible alternatives for the application of dithionite as the reducing agent are bacteria induced reduction and electro chemical reduction. A gram-positive, aerobic moderate and thermophile bacteria (clostridium isatidis) capable of reducing indigo dye was isolated

from woad vat at the University of Reading, UK [7,2]. In the electrochemical approach the possibilities are direct [9] (or) indirect [10,11] electrochemical reduction with different redox mediators. Organic reducing agents have also been investigated as possible alternatives to the sodium dithionite [12]. Glugose and other reducing sugars have recently been suggested as possible environmentally friendly alternatives as reducing agents for sulphur dyes [13] and there has also interest in using glucose to reduce indigo [14].

Based on above applications Indirubin (IB) is selected for the theoretical investigations to analyse the light harvesting efficiency (LHE) and the electronic properties such as Fukui indices, hardness (η), chemical potential (μ), softness (s), electronegativity(χ) and electrophilicity index (ω) and charge transfer(ΔN_{max}).

1.2. THEORETICAL BACKROUND OF FUKUI FUNCTION

Fukui function f(r), as proposed by parr and yang ,is defined as the Partial derivative of the electron density $\rho(r)$ with respect to the total number of electrons N of the system at the constant external potential v(r):

$$f(r) = (\partial \rho(r)/\partial N)_{v(r)} \qquad \ldots\ldots\ldots(1)$$

Applying finite difference approximation ,f(r) can be written as a difference between the electron densities of the molecular system. For reaction with the electrophiles

$$f^{-}(r) \cong \rho_N(r) - \rho_{N-1}(r) \qquad \ldots\ldots\ldots(2a)$$

For reaction with the nucleophiles

$$f^{+}(r) \cong \rho_{N+1}(r) - \rho_N(r) \qquad \ldots\ldots\ldots(2b)$$

where $\rho_N(r)$, $\rho_{N+1}(r)$ and $\rho_{N-1}(r)$ are the electron densities of the system with N, N+1 and N-1 electrons , respectively .

condensed Fukui function calculations are based on the finite difference approximation and partitioning of the electron density $\rho(r)$ between atoms in a molecular system yang and Mortier proposed f_c calculations from atomic charges using equations. For reactions with the electrophiles

$$f_c^{-} = q_N - q_{N-1} \qquad \ldots\ldots\ldots(3a)$$
$$f_c^{+} = q_{N+1} - q_N \qquad \ldots\ldots\ldots(3b)$$

where q_N , q_{N+1} , q_{N-1} are the atomic charges of the system with N , N+1 , N-1 electrons ,respectively .condensed Fukui function is local reactivity descriptor and could be used only for comparing reactive atomic centres within the same molecule .

1.3 GLOBAL REACTIVITY DESCRIPTORS

The prediction of the reactivity of chemical species is one of the main purposes of theoretical chemistry and a lot of work has been done on this line. Density functional theory

has been successful in providing theoretical background of popular qualitative chemical concepts. In this context, several reactivity descriptors have been proposed and used to analyze chemical reactivity and site selectivity .Hardness, global softness, electro negativity and polarizability are the global reactivity descriptors widely used to understand the global nature of molecules in terms of their stability and it is possible to gain knowledge about the Reactivity of molecules.

From the Koopman's theorem , the ionization potential (IP) and electron affinity (EA) are the Eigen value of the HOMO and LUMO with change of sign

$$IP \approx -E_{HOMO} \quad \text{and} \quad E_A \approx -E_{LUMO} \tag{1}$$

Several global chemical reactivity descriptors of molecules such as hardness (η),chemical potential (μ),softness (s),electronegativity(χ) and elctrophilicity index (ω) were calculated based on the density functional theory (DFT) .The global hardness (η),and chemical potential (μ) is defined as the second and first derivatives of the Energy (E) with Respect to the number of electrons (N),at constant external potential ,$V\overrightarrow{(r)}$ captures the resistance of a chemical species to changing its electronic number

$$\eta = 1/2 \ (\partial^2 E/\partial N^2)_V \overrightarrow{(r)} \quad \text{and} \quad \mu = (\partial E/\partial N)_V \overrightarrow{(r)} \tag{2}$$

In equation (2), E and $V\overrightarrow{(r)}$, are electronic energy system potential of an N- electron system respectively .softness is a property of molecules that measures the extent of chemical reactivity. It is the reciprocal of hardness and electronegativity has been defined as the negativity of the electronic chemical potential in muliken sense.

$$S= 1/2\eta \quad \text{and} \quad \chi = -\mu = (\partial E/\partial N)_V \ \overrightarrow{(r)} \tag{3}$$

Using koopman's theorem for closed –shell molecules η , μ and χ can be redefined

as;

$$\eta \approx 1/2 \ (IP\text{-}EA) \approx 1/2 \ (\varepsilon_{HOMO} - \varepsilon_{LUMO}) \tag{4}$$

$$\mu \approx -1/2 \ (IP\text{+}EA) \approx 1/2 \ (\varepsilon_{HOMO} + \varepsilon_{LUMO}) \tag{5}$$

$$\chi = IP\text{+}EA/2 \tag{6}$$

The concept of electrophilicity viewed as a reactivity index was introduced by parr et al. It is based on a second order expansion of the electronic energy with respect to the charge transfer Δ N at fixed geometry .This index, which measures the stabilization in energy when the system acquires an additional electronic charge Δ N from the environment ,is defined by the following simple and more familiar from in terms of the electronic chemical potential (μ)

and the chemical hardness (η).Electrophilicity is a useful in structural depictor of reactivity and is frequently used in the analysis of the chemical Reactivity of molecules.

$$\omega = \mu^2 / 2\eta \tag{7}$$

Maximum amount of electronic charge that an electrophile system may accept is given by,

$$\Delta N_{max} = -\mu/\eta \tag{8}$$

The maximum charge transfer ΔN_{max} towards the electrophile was evaluated using equation (8). Thus, while the quantity defined by equation (8) describes the propensity of the system to acquire additional, electronic charge from the environment the quantity defined in equation (7) describes the charge capacity of the molecule.

Very recently, Ayers and co-workers have proposed two new reactivity indices to quantify nucleophilic and electrophilic capabilities of leaving group, nucleofugality (ΔE_n) and electrofugality (ΔE_e), defined as follows

$$\Delta E_n = EA + \omega = (\mu+\eta)^2 / 2\eta \tag{9}$$

$$\Delta E_e = IP + \omega = (\mu-\eta)^2 / 2\eta \tag{10}$$

1.4 COMPUTATIONAL DETAILS

GAUSSVIEW software was used to generate the molecular structures, and calculations were performed using GAUSSIAN 09W [34]. Density functional theory (DFT) was implemented for the energy optimizations. For all the study 6-311G basis set and the Becke 3- parameter –Lee-Yang-Parr (B3LYP) functional were employed. The optimized structure is shown in Fig 1.

1.5 RESULTS AND DISCUSSION

1.5.1 ANALYSIS OF FUKUI INDICES

Fukui indices of all atoms of Blue Indirubin are calculated to identify the most reactive sites. Fukui indices of Blue Indirubin are presented in Table 1. The most nucleophilic reactive site is identified at C16 atom. Correspondingly the most electrophilic reactive site is identified at O27 atom. The two regions are preferably used for reactions.

1.5.2 CALCULATION OF THE HOMO, LUMO AND BAND GAPS ENERGIES

Energies of HOMO and LUMO are popular quantum mechanical descriptors. The highest occupied molecular orbital (HOMO), it represents the distribution and energy of the least tightly held electrons in the molecule and the lowest unoccupied molecular orbital (LUMO) because it describes the easiest route to the addition of more electrons to the systems. In fact, the energy of the HOMO is a good approximation to the lowest ionization potential of the molecule but the energy of the LUMO generally is poor approximation to the molecule's electron affinity. A molecule whose HOMO is not doubly occupied or that does not have a large HOMO-LUMO energy gap is chemically reactive. High value of HOMO

energy is likely to indicate a tendency of the molecule to donate electrons to appropriate acceptor molecule of low empty molecular orbital energy. The lower values of LUMO energy show more probability to accept electrons. The concept of hard and soft nucleophiles and electrophiles has been also directly related to the relative energies of the HOMO and LUMO orbital's. Hard nucleophiles have a low energy HOMO, soft nucleophiles have a high energy HOMO, hard electrophiles have a high energy LUMO and soft electrophiles have a low energy LUMO. HOMO-LUMO gap is an important stability index. Fig.2 shows the HOMO-LUMO pictorial representations of indirubin and its derivatives. The calculated HOMO energy, LUMO energy and the energy gaps of IB and its derivatives are presented in Table 2. As seen from this table, the energy gap of BI is reduced while introducing NO_2 group than CN group. This shows that the maximum charge transfer is possible in this molecule IB2. This is also well supported by ΔN_{max} of IB2. It's value is highest than other system as seen in Table 2.

1.5.3 CHEMICAL HARDNESS (η)

Chemical hardness is a useful concept for understanding the behaviour of chemical systems .It is measures the resistance to change in the electron distribution in a collection of nuclei and electrons. Chemical hardness was calculated by using of equation (4) and is presented in Table 2. The chemical hardness of IB with NO_2 group is lowest than other systems such as IB and IB2. This lowest chemical hardness suggests that IB2 is a soft molecule.

1.5.4 ELECTROPHILICITY INDEX (ω)

The electrophilicity index has been used as structural depictor for the analysis of the chemical reactivity of molecules. It measures the propensity of a species them to accept electron. A good, more reactive nucleophile is characterized by a lower value of (ω),in opposite a good electrophile is characterized by a high value of (ω).The electrophilicity index values were calculated by equation (6). All the calculated the electrophilicity indexes are tabulated in Table 2. Out of three systems, IB2 is having more electrophilicity indexes. This is also supported well by the electronegativity of IB2 which is higher than other systems.

1.5.5 CHEMICAL POTENTIAL (μ)

Physically, chemical potential (μ) describes the escaping tendency of electrons from an equilibrium system. The values of μ were calculated by equation (5) and for all compounds are presented in Table 2. The greater the electronic chemical potential, the less stable or more reactive is the compound. The chemical potential of BI is -0.16275 a.u .It is the highest value than other systems. Hence IB is less stable and more reactive.

1.6 LIGHT HARVESTING EFFICIENCY (LHE) AND OSCILLATOR STRENGTH

In the present section, we propose structural modifications improving the electron injection efficiency of the BI based DSSCs. Of course, all modifications are theoretically possible and a large panel of new structure can be tested. We focus on two properties that can be the light harvesting efficiency (LHE) of the dye has to be as high as possible to maximize the photocurrent response. More precisely, LHE is expressed as,

$$LHE = 1 - 10^{-A} = 1 - 10^{-f}$$

where A(f) is the absorption (oscillator strength) of the dye associated to the λ_{max}. The light harvesting efficiency (LHE) is the efficiency of dye in responding to light .It is another factor which indicates the efficiency of DSSC.

The light harvesting efficiency (LHE) of the dye should be as high as possible to maximize the photocurrent response. The value of LHE of the dyes has to b33333e as high as possible to maximize the photocurrent response. The LHE of all the dyes are calculated and listed in Table 3 The LHE of all the dyes fall within the range of 0.21205-0.53065 in gas phase. It can be concluded that a class of selected BI derivative dyes shows a good photo physical properties related to DSSC use but in different outstanding properties. According to LHE, IB2 in gas phase is the most efficient than that of the other derivatives studied here. From this we can assume that substitutes of acceptor and donor atoms can enrich the properties of BI derivatives dyes for the use in DSSC.

CONCLUSION

The Fukui indices analysis is performed to identify the reactive regions. The most nucleophilic reactive site is identified at C16 atom. Correspondingly the most electrophilic reactive site is identified at O27 atom. The two regions are preferably used for reactions. Theoretical HOMO energy, LUMO energy and energy gaps are calculated to predict the DFT based global reactivity descriptors such as Chemical potential (μ), Chemical hardness (η), Chemical softness (s), Electro philicity index (ω), Electronegativity (χ), Maximum amount of electronic charge (ΔN_{max}). The energy gap of BI is reduced while introducing NO_2 group than CN group. This shows that the maximum charge transfer is possible in this molecule IB2. This is also well supported by ΔN_{max} of IB2. It's value is highest than other system. The chemical hardness of IB with NO_2 group is lowest than other systems such as BI and IB2. This lowest chemical hardness suggests that BI2 is a soft molecule. Out of three systems, BI2 is having more electrophilicity indexes. This is also supported well by the electronegativity of IB2 which is higher than other systems. The LHE of all the dyes fall within the range of 0.21205-0.53065 in gas phase. It can be concluded that a class of selected BI derivative dyes shows a good photo physical properties related to DSSC use but in different outstanding properties. According to LHE, IB2 in gas phase is the most

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Table **1 Fukui indices of Blue Indirubin using DFT/B3LYP method.**

ATO	$q_k(N)$	$q_k(N+1)$	$q_k(N-1)$	F_K^+	F_K^-	F_K^0
C1	0.369373	0.329014	0.351243	-0.040359	0.01813	-
C2	-0.302860	-0.247724	-0.296640	0.055136	-0.00622	0.024458
C3	-0.025830	0.003525	-0.078201	0.029355	0.052371	0.040863
C4	-0.169854	-0.144453	-0.177670	0.025401	0.007816	0.0166085
C5	-0.138329	-0.129141	-0.168350	0.009188	0.030021	0.0196045
C6	-0.057151	-0.017269	-0.067883	0.039882	0.010732	0.025307
C7	0.246287	0.287473	0.228668	0.041186	0.017619	0.0294025
C8	0.297037	0.275690	0.246600	-0.021347	0.050437	0.014545
H9	0.182489	0.219050	0.140808	0.036561	0.041681	0.039121
H10	0.159103	0.201851	0.110603	0.042748	0.0485	0.045024
H11	0.155779	0.197994	0.107730	0.042215	0.048049	0.045132
H12	0.169473	0.207438	0.128690	0.037965	0.040783	0.039374
H13	0.341154	0.379056	0.321995	0.037902	0.019159	0.0285305
C14	0.280325	0.290483	0.281660	0.010158	-	0.0044115
C15	-0.124574	-0.083357	-0.168810	0.041217	0.044236	0.0427265
C16	-0.055776	0.003857	-0.102692	0.059633	0.046916	0.0532745
C17	-0.182770	-0.165807	-0.187686	0.016963	0.004916	0.021879
C18	-0.135203	-0.107386	-0.165120	0.027817	0.029917	0.028867
C19	-0.052725	-0.014029	-0.077188	0.038696	0.024463	0.0315795
C20	0.524870	0.545231	0.459746	0.020361	0.065124	0.0427425
C21	-0.096367	-0.110126	-0.093047	-0.013759	-0.00332	-
H22	0.154035	0.185378	0.139579	0.031343	0.014456	0.0228995
H23	0.148285	0.198224	0.103714	0.049939	0.044571	0.047255
H24	0.152730	0.204481	0.103813	0.051751	0.048917	0.050335
H25	0.168544	0.218153	0.122418	0.049609	0.046126	0.0478675
H26	0.345144	0.389796	0.301976	0.044652	0.043168	0.04391
O27	-0.282146	-0.227351	-0.412112	0.054795	0.129966	0.0923805
O28	-0.333179	-0.249521	-0.421609	-0.083658	0.088443	0.086044
N29	-0.889605	-0.827117	-0.880221	-0.062488	-	0.026552
N30	-0.848259	-0.813414	-0.852015	0.034845	-	0.0193005

Table **2: Calculated global reactivity descriptors of Blue Indirubin using DFT/B3LYP/ method.**

PARAMETERS	BI	BI1	BI2
HOMO ENERGY (E_H)	-0.21493	-0.22607	-0.23117
LUMO ENERGY (E_L)	-0.11057	-0.12642	-0.13538
ENERGY GAP(E_G)	0.10436	0.09965	0.09579
CHEMICAL POTENTIAL	-0.16275	-0.17624	-0.18327
CHEMICAL HARDNESS	0.05218	0.049825	0.047895
CHEMICAL SOFTNESS(S)	9.58221	10.03512	10.43950
ELECTRO PHILICITY	0.25380	0.311713	0.350652
ELECTRONEGATIVITY	0.16275	0.176245	0.183275
CHARGE TRANSFER	3.119011	3.4611138	3.826599
NUCLEOFUGALITY (ΔE_n)	0.1171425	0.160368	0.191332
ELECTROFUGALITY(ΔE_e)	0.442640	0.512844	0.557881

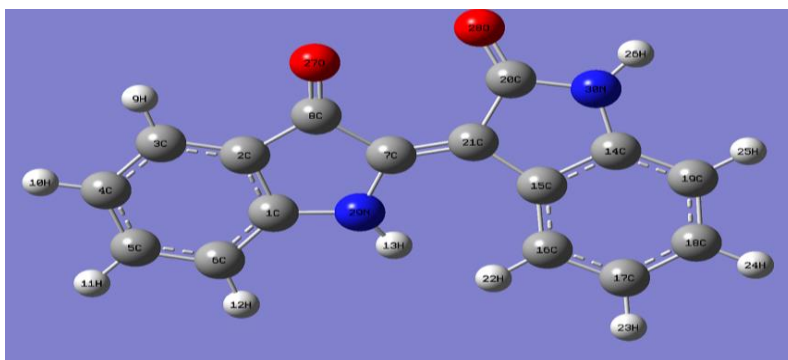BI - BLUE INDIRUBIN; BI1- Donor - Benzene; Acceptor - CN

Table 3 Theoretically calculated values of the light harvesting efficiency of Blue indirubin and its derivatives.

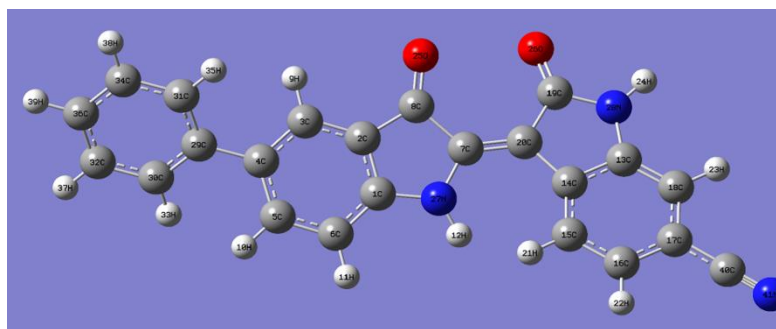| SYSTEM	E(eV)	λ(nm)	F	LHE
BI	2.6050	475.95	0.1035	0.21205
BI1	2.2942	540.43	0.1789	0.33764
BI2	2.2786	544.13	0.3285	0.53065

BI - BLUE INDIRUBIN; BI1- Donor - Benzene; Acceptor - CN
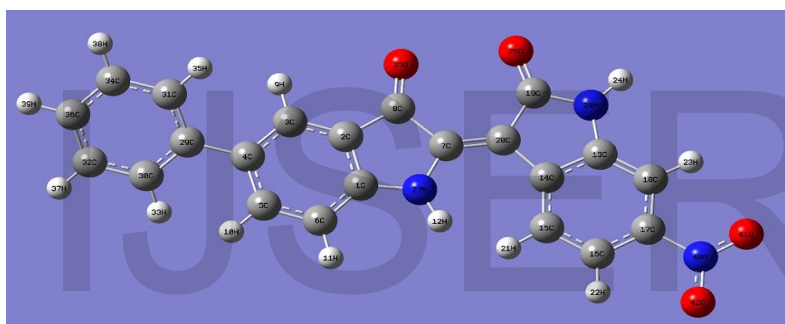
BI2- Donor - Benzene; Acceptor - NO$_2$

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(a) IB- Indirubin

(b) IB1-Donor (Benzene) ;Acceptor (CN)

(c) IB2- Donor (Benzene); Acceptor (NO₂)

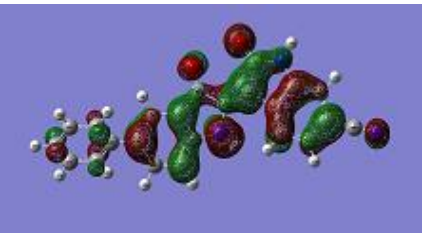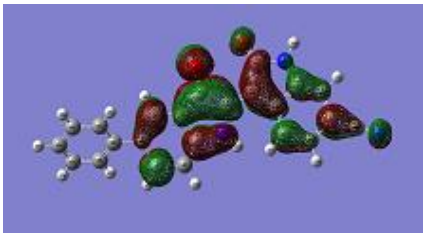**Figure 1 Optimized structures of indirubin(IB) and its derivatives**
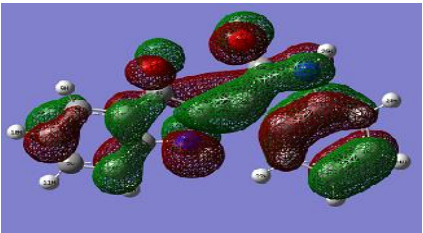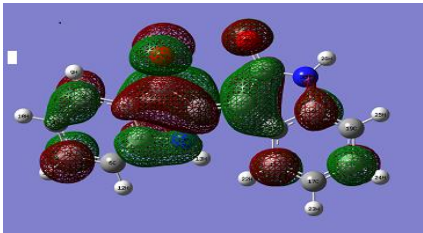
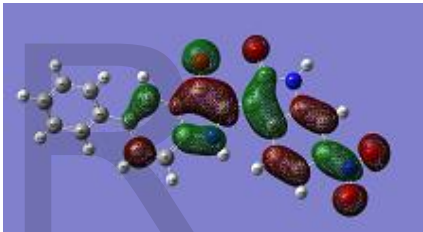| SYSTEMS	HOMO	LUMO
IB		
IB1		
IB2		

Figure 2 HOMO AND LUMO pictorial representations of indirubin and its

Derivatives

IB - INDIRUBIN; IB1- Donor - Benzene; Acceptor - CN

IB2- Donor - Benzene; Acceptor - NO$_2$