Synthesized Novel Schiff Base of 4-Hydroxybenzaldehyde with Anilines for Optoelectronic Applications

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Abstract

Optical materials organic in nature are leading materials exhibiting semiconducting properties is trend of present technology in optical and electronic applications. Active organic materials of Schiff bases are of vital importance in terms of their molecular properties, band gap, refractive index and dielectric operated at room temperature than compared to inorganic materials at elevated temperatures during synthesis. The present article focuses on the development of thin films with the synthesis of Schiff base of 4-hydroxy benzaldehydes and substituted anilines using the green synthesis method. The formation of the Schiff base compounds was confirmed with spectroscopic methods with shifts in wavenumbers in infrared spectra, transition with optical band gap with ultraviolet spectra and chemical environment with chemical shifts using proton NMR. Powdered XRD provide information of structure, composition and crystalline proximity of the synthesized Schiff base compounds. Optical properties refractive index and dielectric constant were attributed with spectroscopic ellipsometer. Computational studies were performed using the Gaussian 16 package with the B3LYP method basis set 6-311++** for all molecular compounds to confirm the molecular structures, optimized geometry, and electronic and optical properties. The insights of these properties are best visualized in terms of quantum mechanical descriptors responsible due to changes in electron density. Studies of these Schiff base compounds with nitro groups proved to exhibit optical properties and as an excellent organic semiconducting material with an energy gap of 3.08 eV; refractive index of 2.074, and dielectric constant of 4.303.

Keywords: Schiff base; Spectral studies; Computational studies; Energy gap; Refractive index.

1. Introduction

Interaction of light with materials are upcoming technologies with molecules as signatures are more accurate in identification of materials and thereafter synthesize either with inorganic material or its counterparts the organic materials. Optical materials applicable in technology require fast response, flexibility, less weight, smart towards implementation, controlling the portion of light/electromagnetic radiation that is widely implemented in glass [1-3], ceramic [4-6], polymer [7-8] and semiconductors [9-10] with the addition of dopants with changes in concentration for optoelectronic properties. Crystalline materials influenced with long-range order responsible for changes in properties such as the surface area, band gap, distribution, and compatibility. The inclusion of changes in short-range order enables the alteration of localized distortions and dipole-dipole interaction influences to a great extent with donor-acceptor group responsible for optoelectronic properties. Among these are functional materials that accommodate changes in electron density [11], the inclusion of atoms in ortho /para positions [12], bonding between host and guest molecules [13-15], and intermolecular interactions [16].

Experimental studies of Schiff base molecules [17-21] are supported by computational methods providing optimization of molecular structures with energy minima, intermolecular interactions, changes in electron density, transitions associated with energy levels, refractive index, and dielectric constant, which are responsible for the optoelectronic properties. Schiff base molecules gained importance due to interactions between the electron-donating aldehyde group and the distinct aniline of electron-deficient aldimine bonds. Optical properties refractive index and dielectric constant greatly influence the optoelectronic properties of Schiff base compounds [22-23] with changes in molecular structure. The article describes the structural importance of synthesized Schiff base compounds of 4-Hydroxybenzaldehyde with distinct anilines; HBN (4- Hydroxybenzaldehyde: *p*-nitroanilines), HBC (4- Hydroxybenzaldehyde: *p*-chloroanilines), HBA(4- Hydroxybenzaldehyde: anilines) for optoelectronic properties, as evidenced by experimental studies. These synthesized compounds are unique in their ability to determine optoelectronic properties, further extending the knowledge in scientific research.

2.Materials and Methods

The synthesis of a Schiff base molecule performed with a *p*-hydroxy-benzaldehyde and three distinct anilines. The host compound (4- hydroxybenzaldehyde- HB) and guest compounds (aniline-AN, *p*-chloroaniline-CAN, *p*-nitroaniline- NAN) were purchased from Sigma Aldrich with 98.99% purity and used without further purification. Scheme of Schiff bases synthesized is as follows.

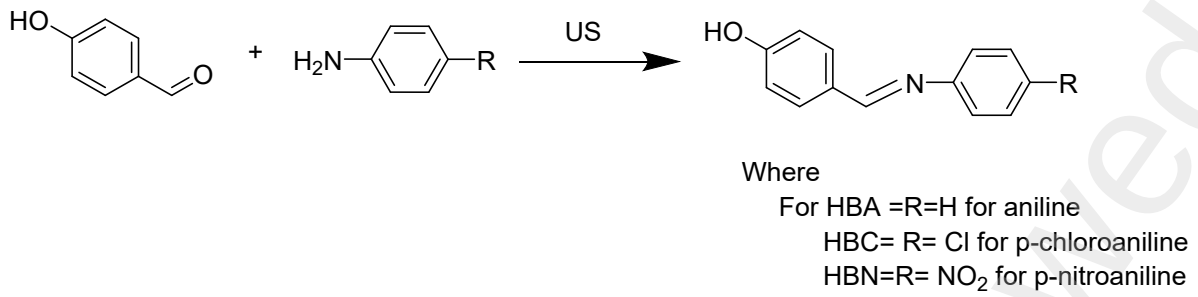
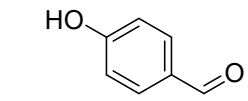
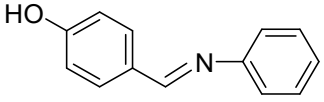


Fig.1(a): Scheme of Schiff base compounds

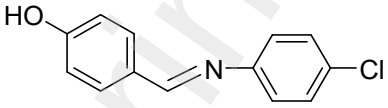
The ecofriendly ultrasonication (US) method was chosen for the synthesis of Schiff base molecules with an ultrasonic processor (250 W) operating at a fixed frequency of 50 Hz with a speed of 238 rpm for 25 mins/ 40 mins of PCI Analytics. Equimolar proportions of the host (4-hydroxybenzaldehyde-HB) and guest (substituted anillines: AN/CAN/NAN) molecules were dissolved in 10 ml of ethanol in separate beakers. Then, both solutions were mixed together in a beaker (for individual reactions) to proceed with the sonication process under the probe sonicator. The progress of the reaction was checked by TLC, and after completion, the mixture was incubated overnight. The next day, it was poured into a beaker containing ice, and the crystalline compounds were collected by filtration and dried. The structure of the fine powdered samples of Schiff base compounds with IUPAC names is shown in figure 1(b).



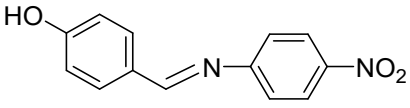
4-hydroxybenzaldehyde
HB



(*E*)-4-((phenylimino)methyl)phenol
HBA



(*E*)-4-(((4-chlorophenyl)imino)methyl)phenol
HBC



(*E*)-4-(((4-nitrophenyl)imino)methyl)phenol
HBN

Fig.1(b): IUPAC names of compounds

Formation of Schiff base compound with host and guest compounds is performed with changes in shifts in the recorded infrared spectra in functional and fingerprint regions using Bruker instrument with KBr

disc technique. The operating regions were from 400 cm^{-1} to 4000 cm^{-1} with a spectral resolution of 1cm^{-1} and 32 scans. The UV spectra of the powdered samples were obtained using the AnalytikjenaSpecord S-600 model performed with the solution method in the range of 200-500 at room temperature. Spectral observations were analysed for the optical band gap by plotting the Tauc plot and the direct band gap method. A thin film of 2 micrometer thickness was developed using a drop-casting method by dissolving the powder sample in a solvent. The film further proceeded to study the optical properties, refractive index, extinction coefficient, and real and imaginary dielectric constant values for the wavelength of the light beam at an angle of 70 °using an ellipsometer (J. A. Woollam Co. Model: Alpha-SE). Proton NMR studies were performed for the samples in DMSO-d6 with a Bruker 500 MHz instrument using TMS as the internal solvent. Powder X-ray studies with a Bruker Model D8-Advance were performed using a2.2 kW Cu anode and 40 kV/40 mA with a Linxeye detector that can measure angles from 5 °to 120 °.

The experimental studies were validated with computational studies using software Gaussian 16 consisting of the GaussView 6.1. The popular electron density method i.e. density functional theory(DFT) is employed with the hybrid correlation function 6-311++(d,p) for structural properties and optoelectronic properties of compounds. The structural properties of the compounds were attributed to optimized molecular structures and changes in electron density that were visualized in terms of frontier molecular contours, electrostatic potential contours, electrostatic potential maps, and Mulliken charges. The optoelectronic properties are elaborated in terms of electronic, optical, and nonlinear optical properties. The hybrid function consists of polarized and diffused functions to study the flexibility of orbital and intermolecular interactions.

3.Results and Discussions

Optoelectronic properties [24-26] of synthesized Schiff bases were attributed with shifts in wave numbers, optical band gap, refractive index and dielectric constant with experimental studies. Computational studies were performed and evidenced with recorded studies with changes in molecular geometry, visualizing potential maps and contours with charge transfer interactions. Optimization of the molecular geometry is attained under minimum energy conditions using local density approximation (LDA) and generalized gradient approximation (GGA) conditions. The minimum energy values of HB, HBA, HBC and HBN were given by -420.91898 Hartrees, -632.14233 Hartrees, -1091.7652 Hartrees, -836.70815 Hartrees respectively.

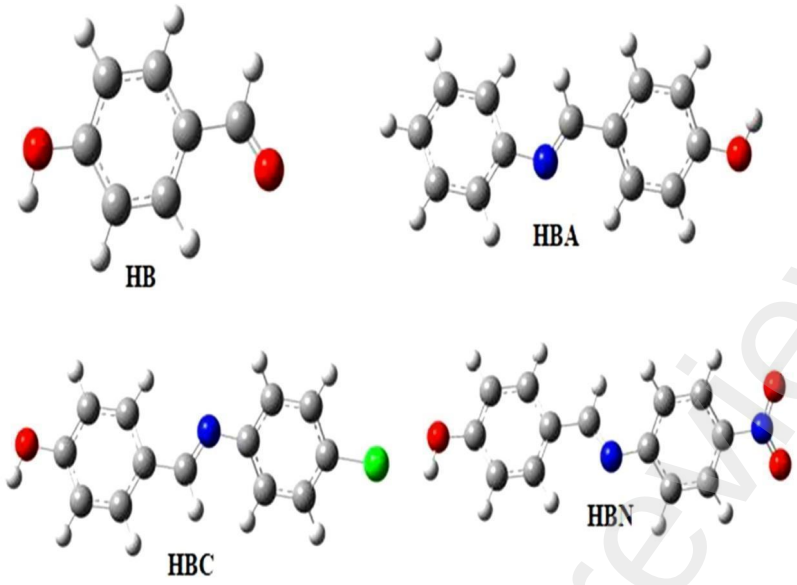


Fig 2: Optimized molecular structures of compounds

A powerful method for confirming the formation of Schiff base compounds depends on the wavenumber assignments of functional groups with the recorded infrared spectra.

The formation of Schiff base compounds could be confirmed by their IR spectrum. The major peaks appeared in the host molecule HB are 3143 cm^{-1} for aromatic CH however the doublet peak 2890 and 2785 cm^{-1} for aldehyde CH along with 1663 cm^{-1} assigned to C=O. Additionally, the guest molecule i.e. distinct anilines, two peaks observed at 3480-3460 cm^{-1} and 3360-3340 cm^{-1} could be assigned to primary amines(NH2) while 1630,1588 cm^{-1} regions could be attributed to the C-N and C=C of the aromatic ring. On the analysis of IR spectrum of target Schiff base compounds revealed that the disappearance of C=O and CH of aldehyde[HB] along with primary amine peaks of all anilines confirmed the condensation of HB with various anilines. Which is further confirmed by the aldimine bond, R-CH=NR', where R' is aniline/ chloro-aniline / nitro-aniline. In the IR spectrum of HBA [1569 cm^{-1}] and HBC [1596 cm^{-1}] these bands are appeared in little lower wave number whereas in HBN [1629 cm^{-1}] as illustrated in figure 3(a)-3(c) for Schiff base compounds. These shifts are in accordance with specified regions responsible for formation of Schiff base. Shifts in wavenumbers is consequence of allowed transitions are infrared active, no imaginary wavenumbers and change in dipole moment takes place. Wave numbers from computed infrared spectra are in agreement with recorded spectra as as illustrated in figure 4.

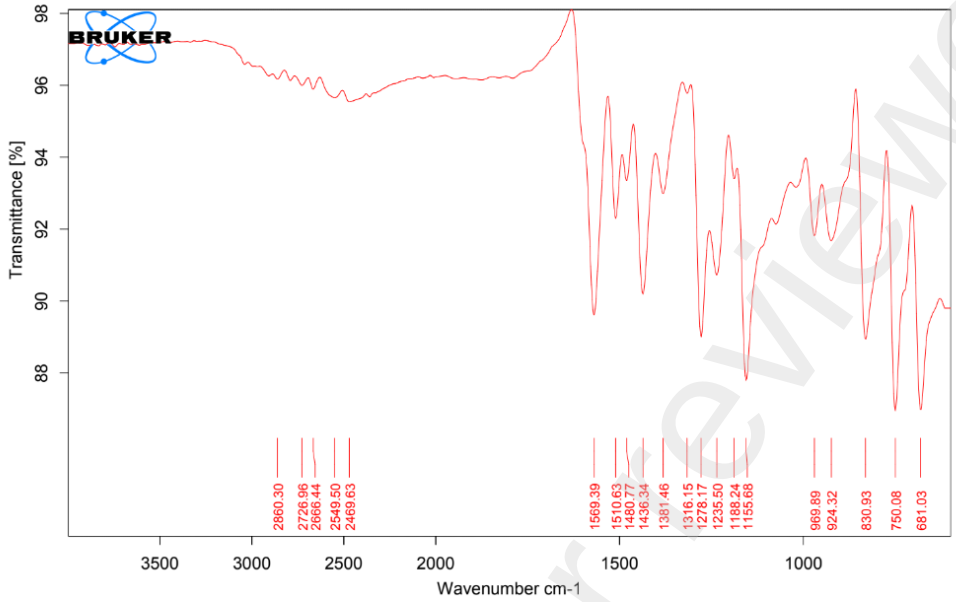


Fig.3(a). Recorded infrared spectra of HBA

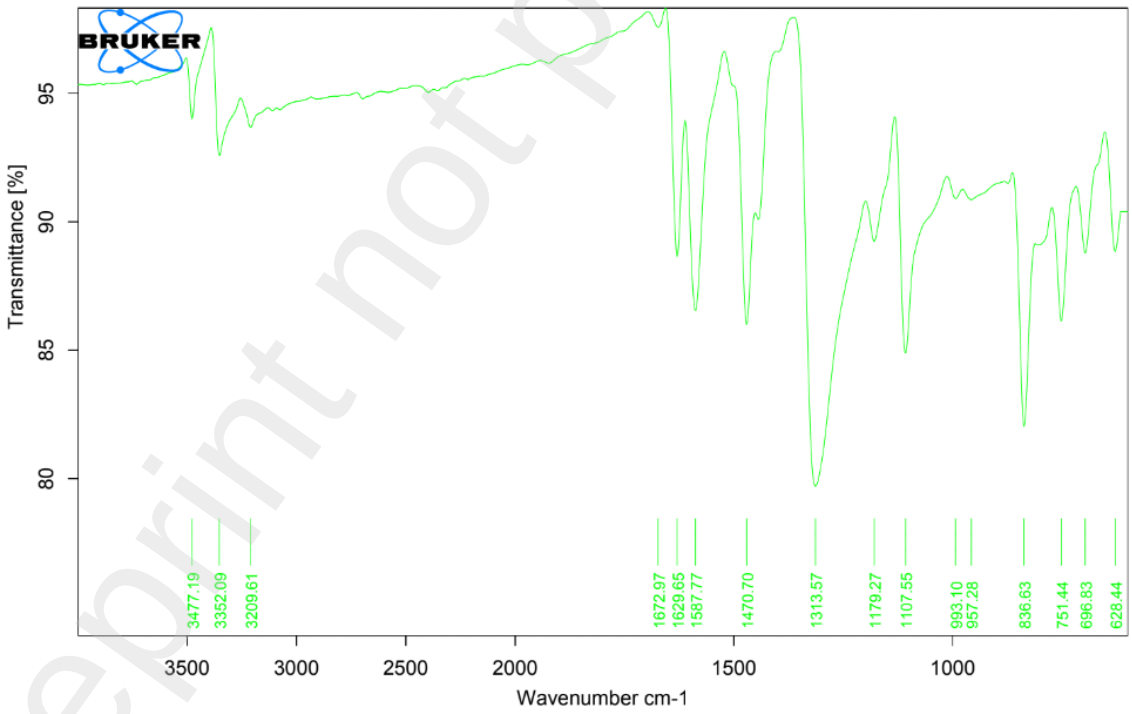


Fig.3(b). Recorded infrared spectra of HBN

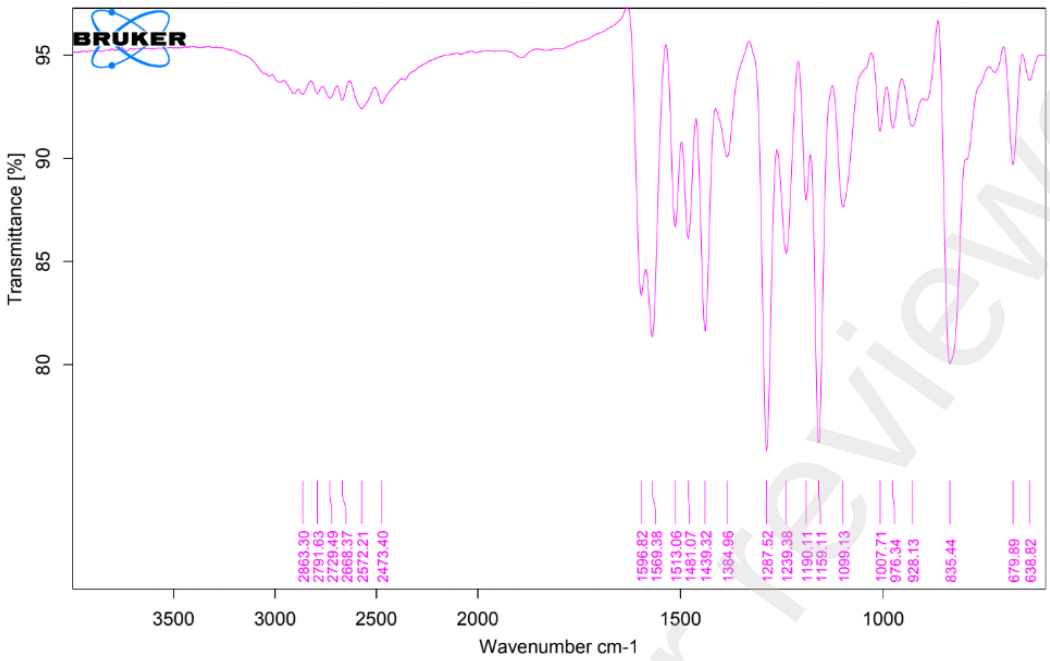


Fig.3(c). Recorded infrared spectra of HBC

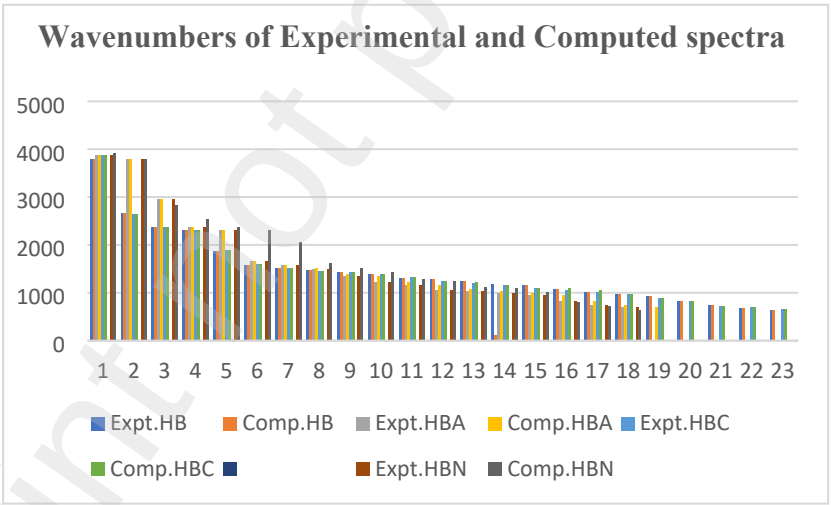


Fig.4 Recorded and Computed wavenumbers of compounds

Analysing the recorded UV spectra, only one absorption band was observed for compounds in the range 330-350 corresponding to π to π* transitions at lower energies. The optical band gap describes the solid material obtained from Gaussian curve fitting with Origin pro 8.5 with a linear correlation of the spectral data. The direct band gap of the compound was calculated using the Tauc'splot[27] method, as illustrated in figure 5(a) and figure 5(b) for the HB compound and synthesized Schiff base compound HBN (Figure 5(c) and figure 5(d)).

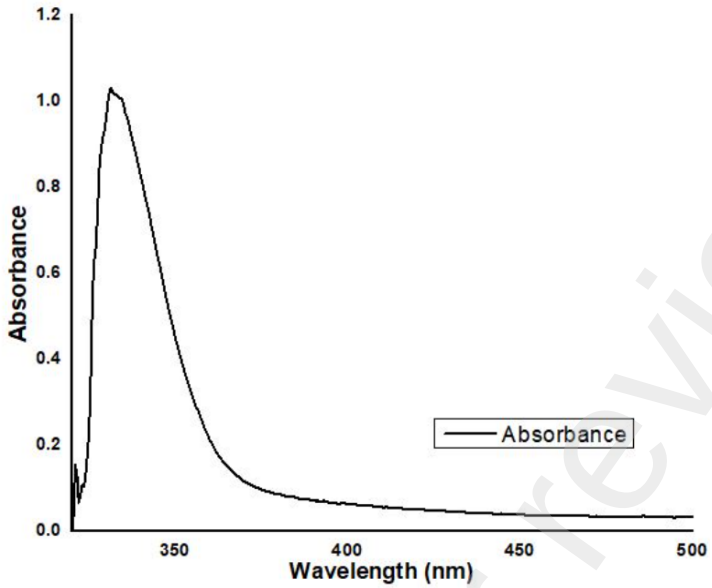


Fig.5(a)UV Spectra of HB

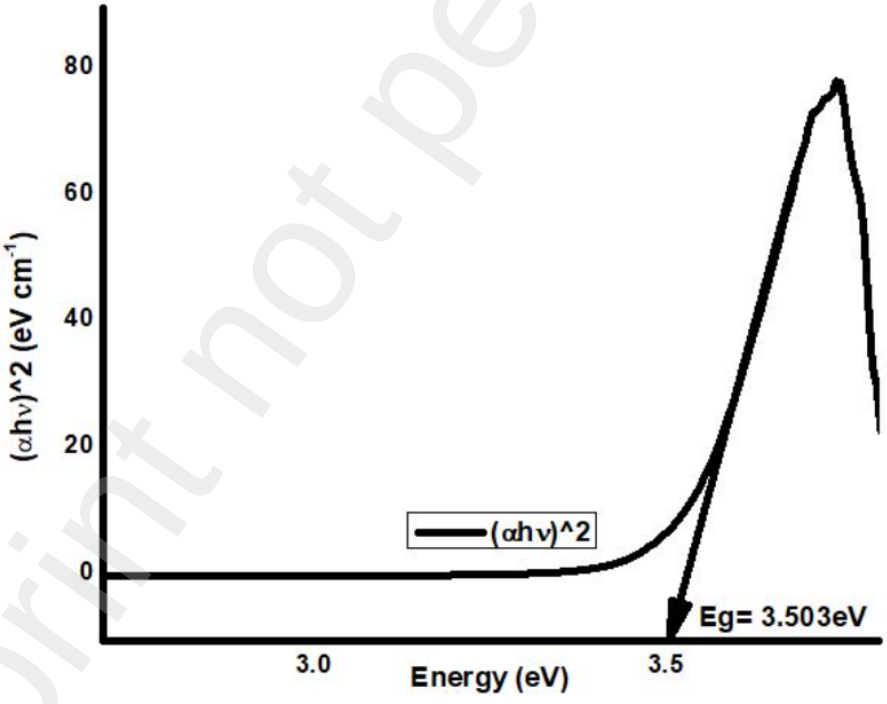


Fig.5(b) UV Spectra of HB with energy

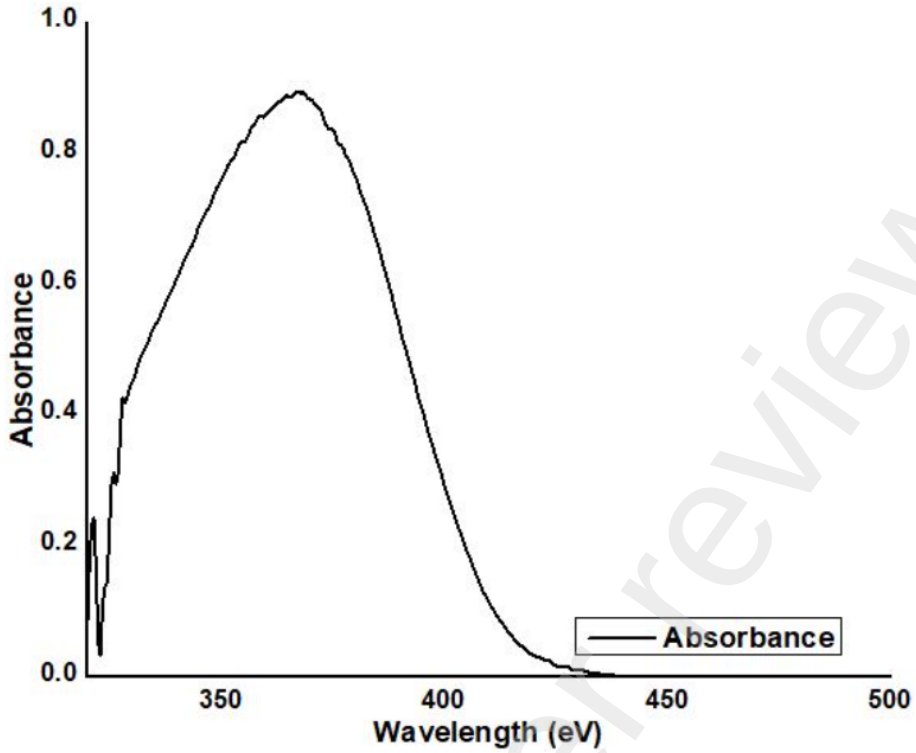


Fig.5(c) UV Spectra of HBN

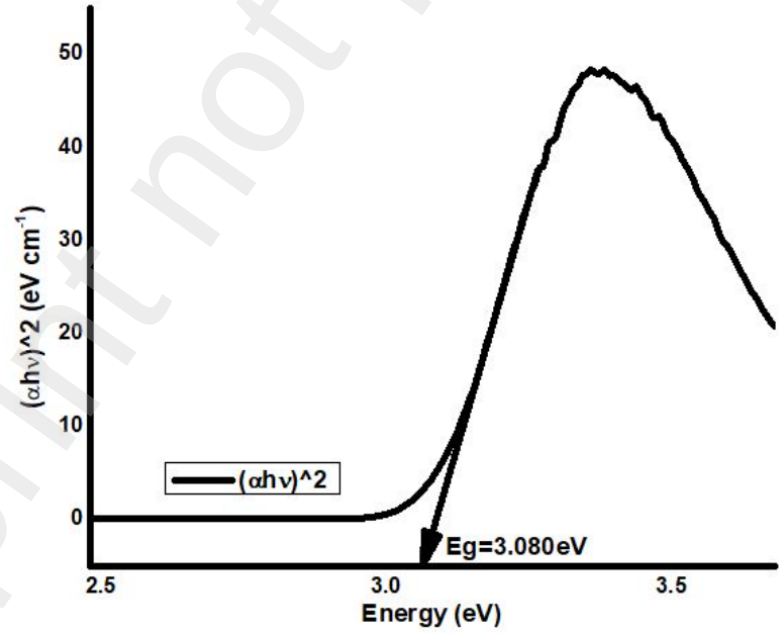
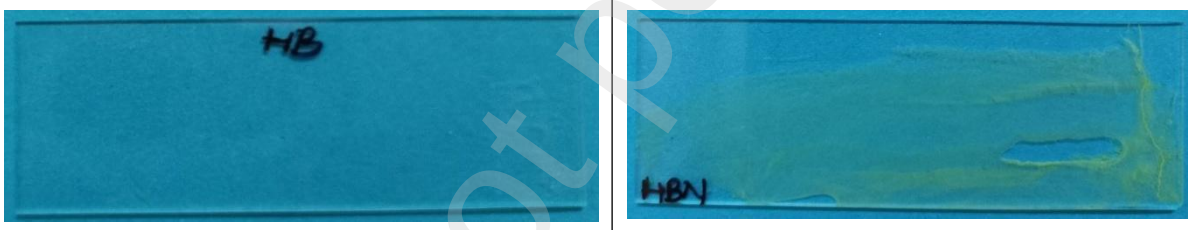


Fig.5(d) UV Spectra of HBN with energy

Optoelectronic studies attribute the capacity of light absorbed by molecules, that determines the mass extinction coefficient per unit mass density, and is expressed in terms of molar mass and molar extinction coefficient [27-28]. Calculated optical band gap 3.503 eV for HB and 3.50 eV(HBA) 3.46 eV(HBC) and 3.08 eV for HBN corresponds to optical transition helps to determine refractive index HB(2.282);HBA(2.282);HBC(2.288) and HBN(2.357) of compounds [29-31]. Studies on synthesized Schiff base compounds with nitro groups are convinced with a refractive index as a semiconducting material [32] suitable for technological applications.

Ellipsometer studies provide optical properties like refractive index (n), extinction coefficient (k) and dielectric behavior (ε) of materials. The powder samples were diluted to a suitable solution and coated on a glass slide (Figure 6) using a drop-casting method to form a thin film with a uniform thickness of ~2µm.



HB	HBN

Fig.6: Films of compounds

Polarized light was incident on the glass film to study the optical properties refractive index, extinction coefficient and dielectric constant of compounds. A graphical representation is obtained from a database of spectroscopic ellipsometers using the B-spline method. B represents the basis set for the polynomial splines. The real (ε1) and imaginary (ε2) dielectric values with respect to wavelength are shown in Figure 7a, and figure 7b shows the graph for n and k for the typical compound HBA. The calculated refractive indices of the compounds were 1.419(HB), 2.028(HBA), 1.831(HBC), and 1.634(HBN), confirming that the synthesized compounds are in agreement with studies performed using UV spectroscopy.

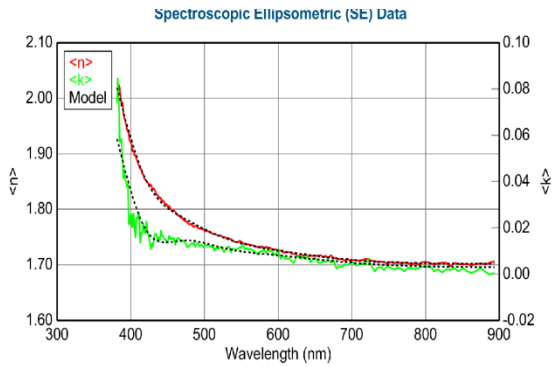


Fig. 7a: Refractive index and extinction coefficient of HBA

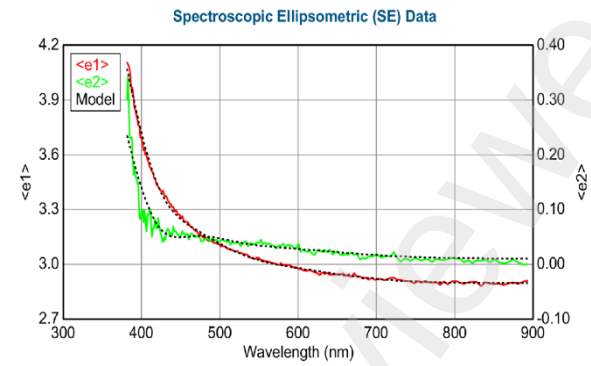


Fig.7b: Real and Imaginary part of optical dielectric constant of HBA molecule

Studies of powdered X-ray diffraction of the host compound and synthesized Schiff base compound are illustrated in figure 8(a) and 8(b) with intensity on the ordinate and diffraction angle on the abscissa.

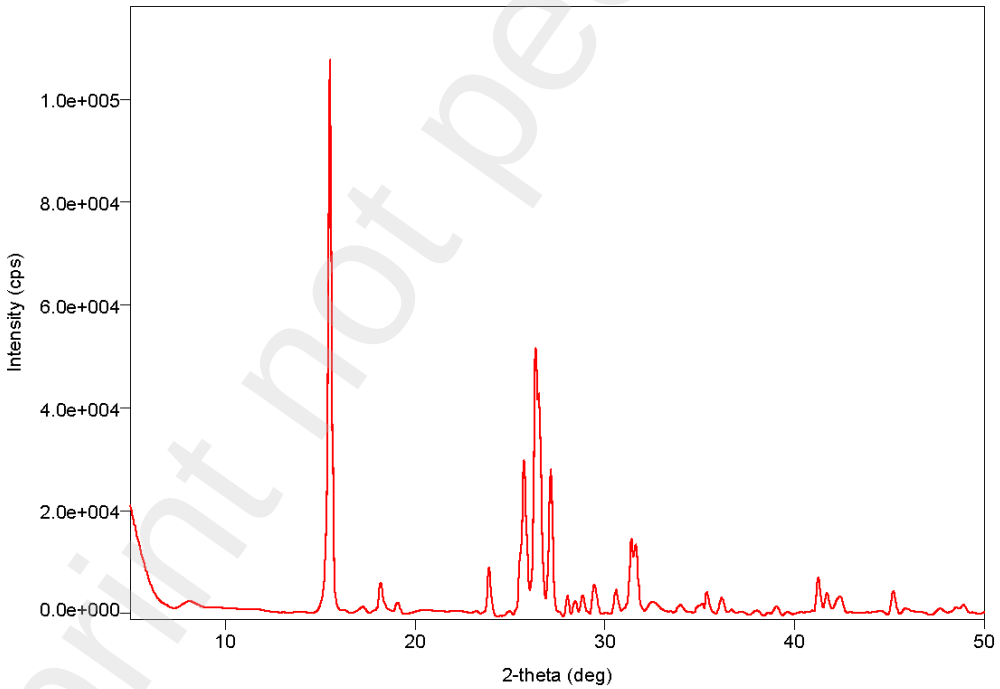


Fig.8(a): Powdered X ray spectra of HB

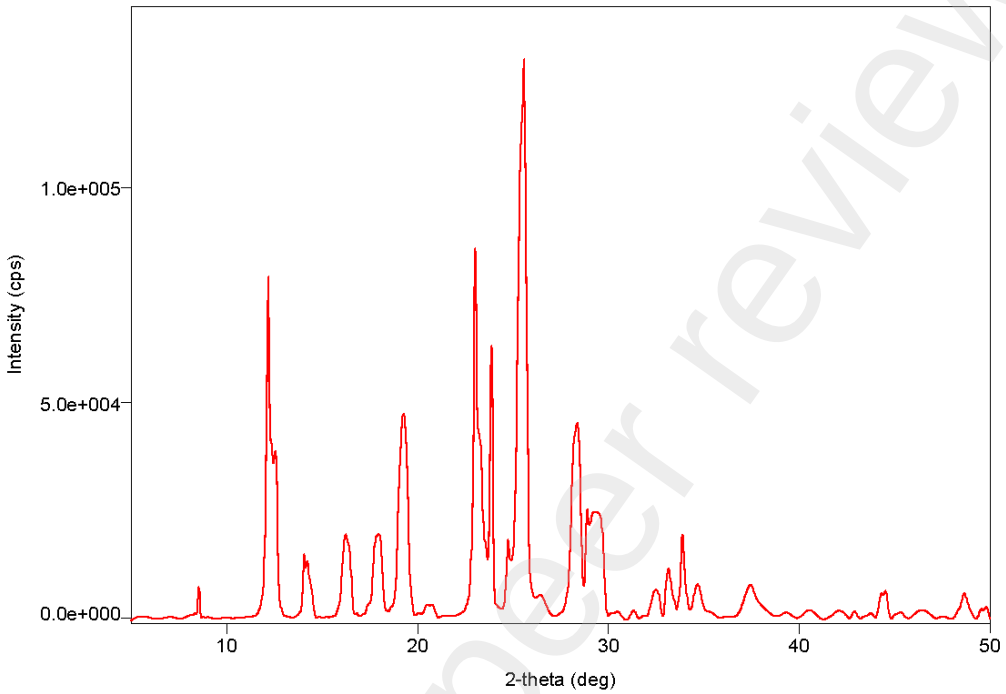


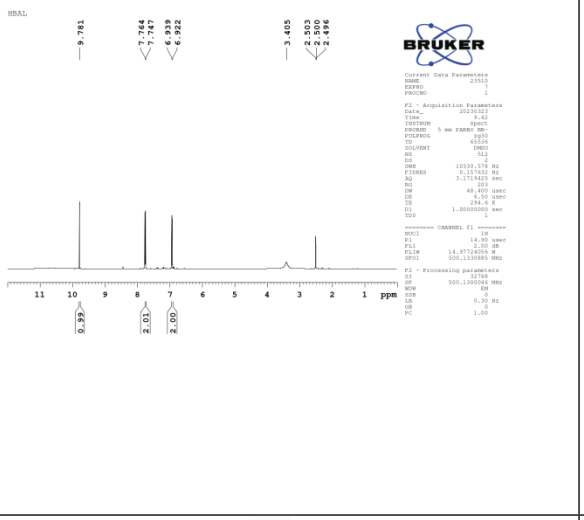
Fig.8(b): Powdered X ray spectra of HBN

Studies of diffraction pattern at lower diffraction angles(10-20) there is an appropriate pattern change in the synthesized Schiff base compound. At these angles, the intensities were reduced with changes in the neighbouring layers, indicating the development of a strain with low ordering. At higher increasing angles (20-30) the pattern of the compound changes, and approximately 25°identical ordering, high crystallinity, and purity of the compound are present. These pattern changes are a consequence of the formation of Schiff base compounds with high chemical states.

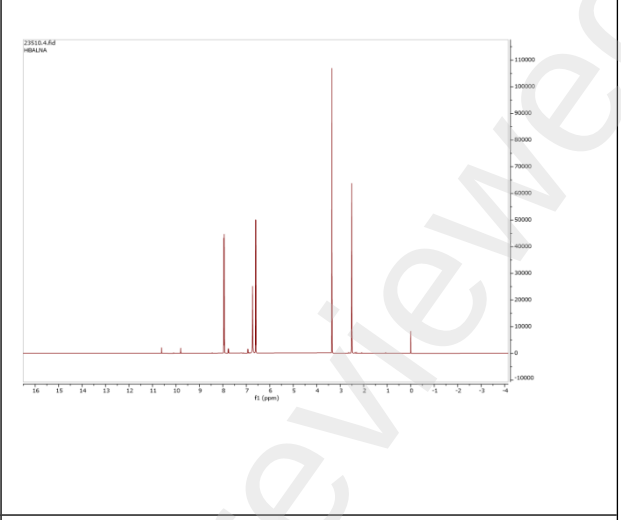
Proton nuclear magnetic resonance (NMR) spectra were recorded in DMSO-d6 solvent with TMS as an internal reference BRUKER 400 spectrophotometer. The Chemical shifts are represented in δ ppm, as illustrated in figure 9.

On the analysis of the NMR spectrum of HB showed the peak at δppm 10.15(OH);8.44(CHO), 7.78-7.38(2H,Benzaldehyde) and 7.20-6.89(2H,Benzaldehyde).The NMR spectrum of HBA showed the peak at δppm 10.16(OH),8.45 (-HC=N-);7.45-7.78 (5H,Aniline side); 7.20-7.23(2H,Benzaldehyde side) 6.86-6.88(2H, Benzaldehyde side), all peaks are fitted well for expected structure and confirmed the formation of Schiff base. The NMR spectrum of HBC showed peaks at δppm 10.17(OH),8.45 (-HC=N-);7.76-7.78 (2H, aniline side); 7.41-7.43(2H, aniline side); 7.21-7.23(2H, benzaldehyde side) 6.87-6.88(2H, benzaldehyde side). All peaks were fitted well for the expected structure and confirmed the formation of a Schiff base.

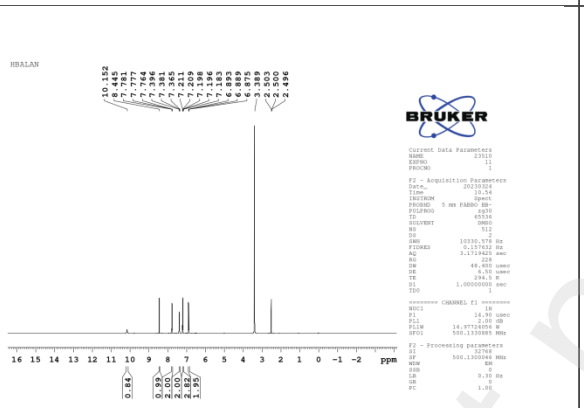
The NMR spectrum of HBN showed peaks at δppm 10.15(OH),8.4 (-HC=N-);7.760-7.77 (2H, aniline side); 7.2-7.36(2H, aniline side); 7.18-7.19(2H, benzaldehyde side) 6.87-6.89(2H, benzaldehyde side). All peaks were fitted well for the expected structure and confirmed the formation of a Schiff base



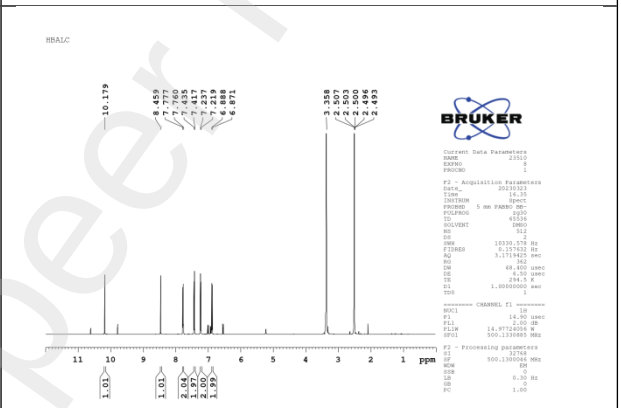
HB



HBN



HBA



HBC

Fig.9: Proton NMR of compounds

Computed studies [33-37] were performed for all structures of compounds with optimization, and energy minima with no constraints were imposed on the geometry of the molecules. The observation of the datafile (provided as supplementary data) indicates that bond distances and bond angles were altered in synthesized compounds compared with HB, indicating changes in polarities, dipole moment of synthesized compounds, and further changes in electron densities. Changes in electron density involve transitions between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO).

The Frontier molecular contours (FMO) in figure 10 are responsible for energy values corresponds to the quantum descriptors such as ionization potential $IP = \left| - E_{HOMO} \right|$ and electron affinity $A = \left| - E_{LUMO} \right|$. The reactivity and charge flow of the molecule are derived from the electronegative

$\left(\chi = -\mu = \frac{IP + EA}{2}\right)$ values. Softness is responsible for the polarizability of the compound represented as the inverse of hardness . $\left(\eta = \frac{IP - EA}{2}\right)$ The hardness indicates the resistance to the flow of electrons. The electron density of the molecule is responsible for the charge transfer interaction and can be observed through the electrophilicity index $\left(\omega = \frac{\chi^2}{2\eta}\right)$.

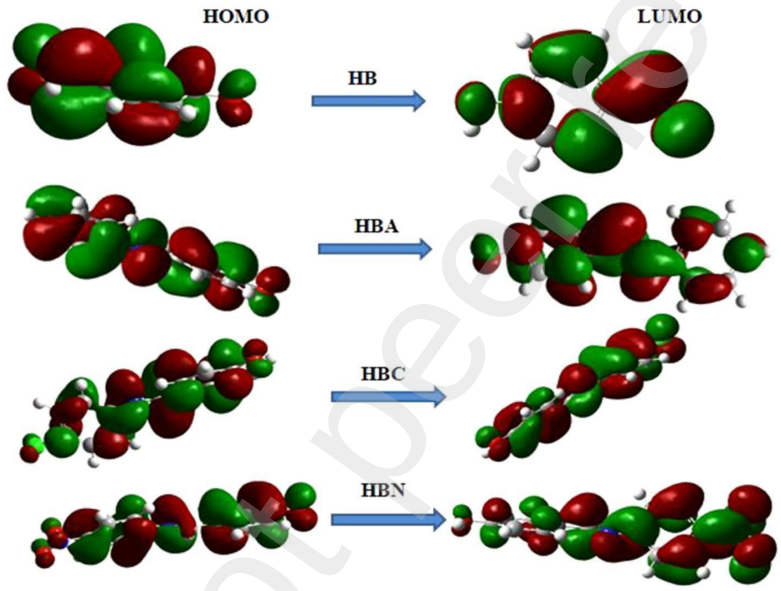


Fig 10: FMO contours of compounds

The reduced energy gap is a consequence of the reactivity of the molecule with reduced restriction and a greater tendency for electron transfer responsible for the higher electrophilicity index. Electronic properties table-1 of the synthesized compounds reveal that nitro-based Schiff base compounds (HBN) are more effective and excellent optical materials [38].

Table-1: Electronic properties

Name of the compound	IP	EA	ΔE	χ	η	ω
HB	6.922	1.941	4.981	4.431	2.490	3.943
HBA	6.057	1.779	4.278	3.918	2.139	3.588
HBC	6.135	1.954	4.181	4.044	2.091	3.912
HBN	6.641	2.826	3.815	4.733	1.908	5.873

Extending the molecular interpretation with changes in electron densities favours the determination of dipole moment ρ , polarizability α and first order hyperpolarizability β which contribute to the nonlinear optical properties responsible for the electronic behaviour of the molecules. Optical materials are very accurate and precise for technological advancements that require the absorption and emission of energies during transition. These transitions are characterized by the HOMO(donor) and LUMO(acceptor) levels, which contribute to the change in electron densities. Factors such as molecular radius (R), volume of the material (R^3), polarization. Optical materials are very accurate and precise towards advancements in technological purposes require absorption and emission of energies during transition. These transitions are characterized with HOMO(donor) level and LUMO(acceptor) level that contribute to change in electron densities. The factors like molecular radius (R), volume of the material (R^3), polarization density $\left(P=\frac{\mu}{V}\right)$ and electric field generated during iterations $\left(E=\frac{\mu}{\alpha}\right)$, electric susceptibility $\left(\chi_e=\frac{P}{\varepsilon_o E}\right)$, refractive index $n=\sqrt{\chi_e+1}$, and dielectric constant $\left(\varepsilon_r=\chi_e+1\right)$ are responsible for optical behaviour. Studies of Schiff base compounds nitro compound contributed with enhancement in optoelectronic properties than compared to other compounds. Increased refractive index and dielectric constant are confirmed with experimental methods performed.

Table-2: Optoelectronic properties

Name of the compound	R_O	R_o^3	P	E	χ_e	ε_r	n	ρ	α	β
HB	4.09	68.418	0.168	7.677	2.473	3.473	1.864	3.455	13.477	7.157
HBA	4.90	117.649	0.086	3.265	2.976	3.976	1.994	3.023	27.726	11.297
HBC	5.08	131.096	0.112	4.334	2.920	3.920	1.979	4.407	30.452	5.023
HBN	5.11	133.433	0.196	7.309	3.030	4.303	2.074	7.856	32.188	57.047

An enhancement in molecular properties dipole moment, polarizability and hyperpolarizability [34] is consequence of reactivity of during the formation of Schiff base compounds at reduced electric field. First order hyperpolarizability is proportional to dipole moment and inversely proportional to energy gap a consequence of applicative phenomenon the change of state [24]. These are best visualized using electrostatic potential (ESP) contours with red-coloured delocalized contours that are highly reactive and responsible for bonding. In HB, the aldehyde bond is more reactive than the hydroxyl group. The aldimine bonds for all the synthesized molecules were also reactive, but in HBN, the nitro group also showed reactive delocalized contours, as shown in Figure 11. Electron transition is best visualized during formation of Schiff base compound corresponding to π to π* transitions at lower energies is confirmed with UV spectral studies [38].

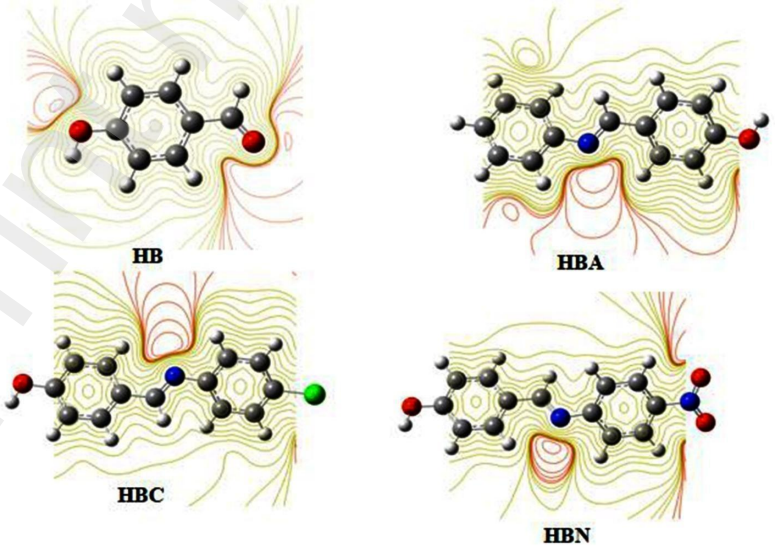


Fig. 11: ESP Contours of compounds

The electrostatic potential (ESP) maps are responsible for the compounds that were visualized using a gradient of colours in figure 12. The electrophilic sites are observed in the aldehyde and aldimine bonding regions with yellow colour for the host and formerly synthesized molecules with negative potential. However, around the nitro bond, the electrophilic nature is dominant in HBN because of its dominance over other bonded regions. The positive potential with nucleophilicity remains the same for the hydroxyl group in the blue region.

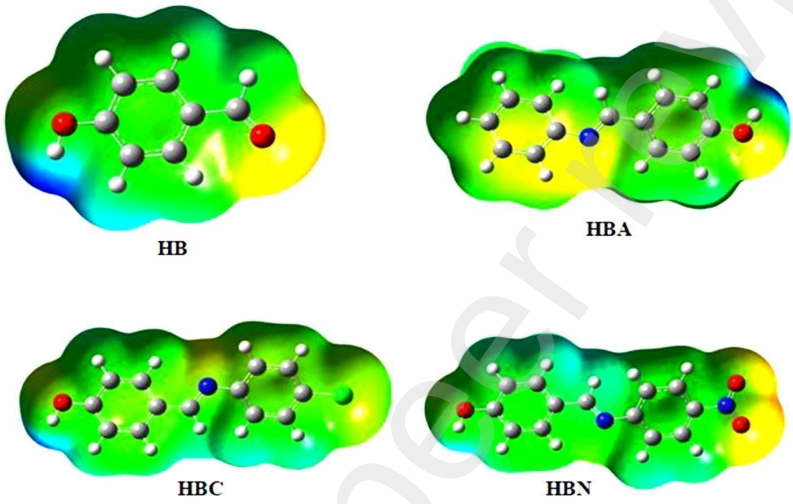


Fig 12: ESP maps of compounds

Charge transfer [39] properties provide the distribution of atoms responsible for changes in donor and acceptor behaviour of atoms in the molecule. An illustration of density of atomic charges for the molecules is shown in figure 13 with atoms of molecule. The higher values of electron accepting power ω_{+} and electron donating power ω_{-} confirms the electrophilic nature of the molecule. Table 3 shows that among the synthesized molecules HBN shows the least nucleophilic nature N^{I} with maximum charge transfer capacity ΔN.

Table-3: Charge transfer properties

Name of the compound	ω_+	ω_-	ΔN	N
HB	4.809	0.378	1.779	2.079
HBA	4.288	0.369	0.428	2.332
HBC	4.501	0.457	1.934	2.222
HBN	5.780	1.047	2.481	1.730

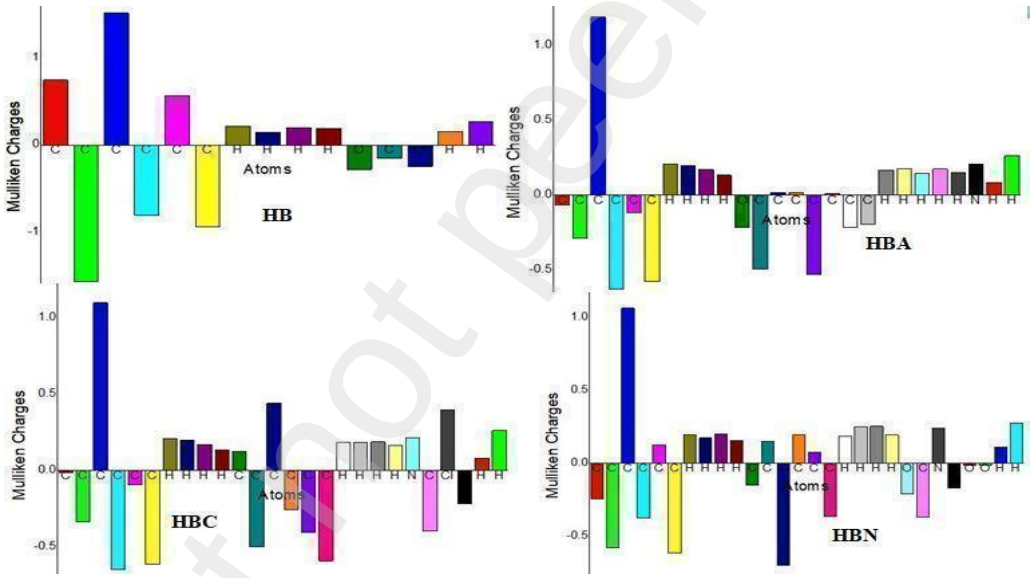


Fig 13: Mulliken Charge distribution

4.Conclusion

Schiff base compounds were synthesized using an eco-friendly green synthesis mechanism, that is, sonication. Structural and performance parameters with experimental methods reveal (i) formation of Schiff base compound with secondary aldemine, (ii) electronic transitions at a unique wavelength, (iii) the optical properties determined with two experimental are approximately the same; (iv) chemical environment convinced with chemical shifts refractive index; (v) changes in diffraction pattern to ordered nature at high angles of diffraction and intensities confirm that the Schiff base compound with

a nitro group is the most suitable semiconducting material with an energy gap of (3.08 eV HBN). Experimental studies are validated with computational methods that optimize molecular structures, reduce the energy gap, electrophilicity index, visualization of changes in electron density with reduced restriction, and contribution of nitrogroups in electrostatic potential contours and maps. Studies have concluded that Schiff base compounds with nitro groups exhibit good optical properties and behave as excellent organic semiconducting materials.

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Conflict of Interest

The authors declare no conflict of interest

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Figure Captions

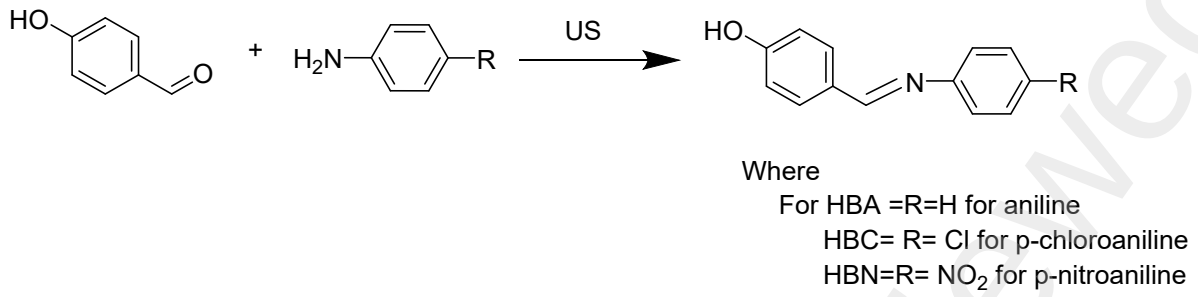


Fig.1(a): Scheme of Schiff base compounds

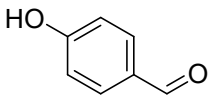
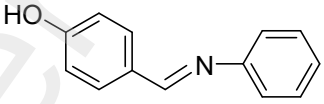
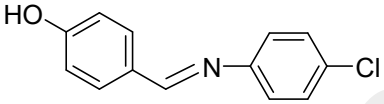
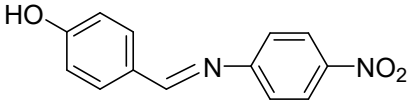
 4-hydroxybenzaldehyde **HB**	 (*E*)-4-((phenylimino)methyl)phenol **HBA**
 (*E*)-4-(((4-chlorophenyl)imino)methyl)phenol **HBC**	 (*E*)-4-(((4-nitrophenyl)imino)methyl)phenol **HBN**

Fig.1(b): IUPAC names of compounds

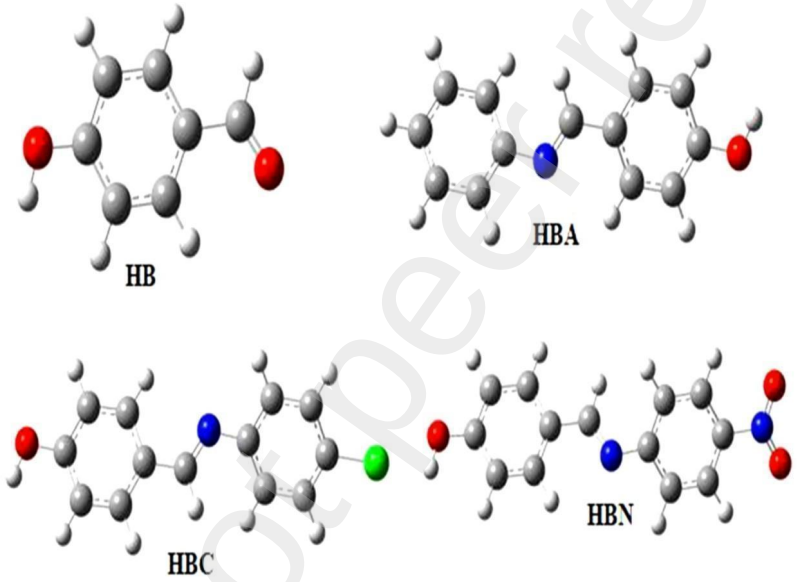


Fig 2: Optimized molecular structures of compounds

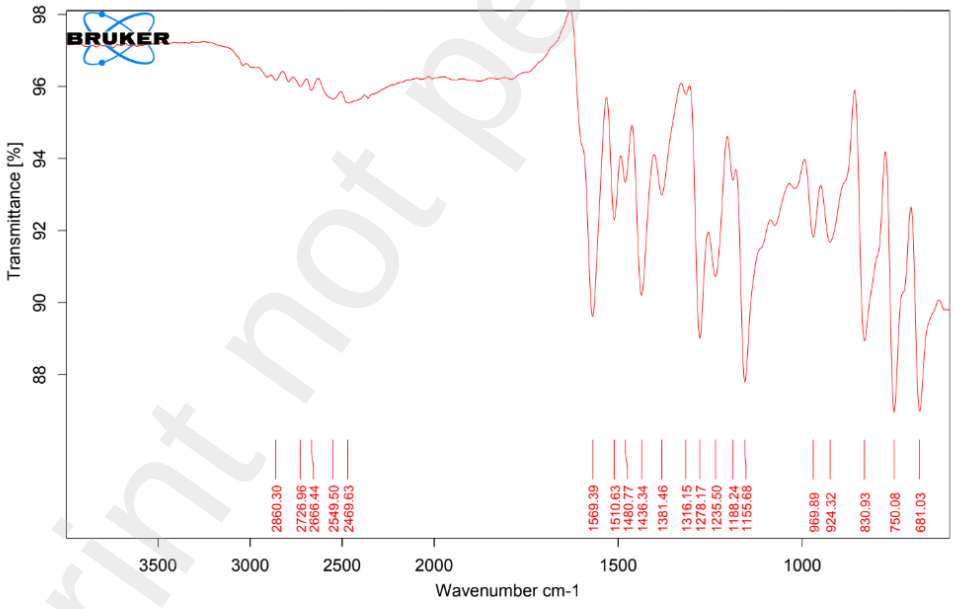


Fig.3(a): Recorded infrared spectra of HBA

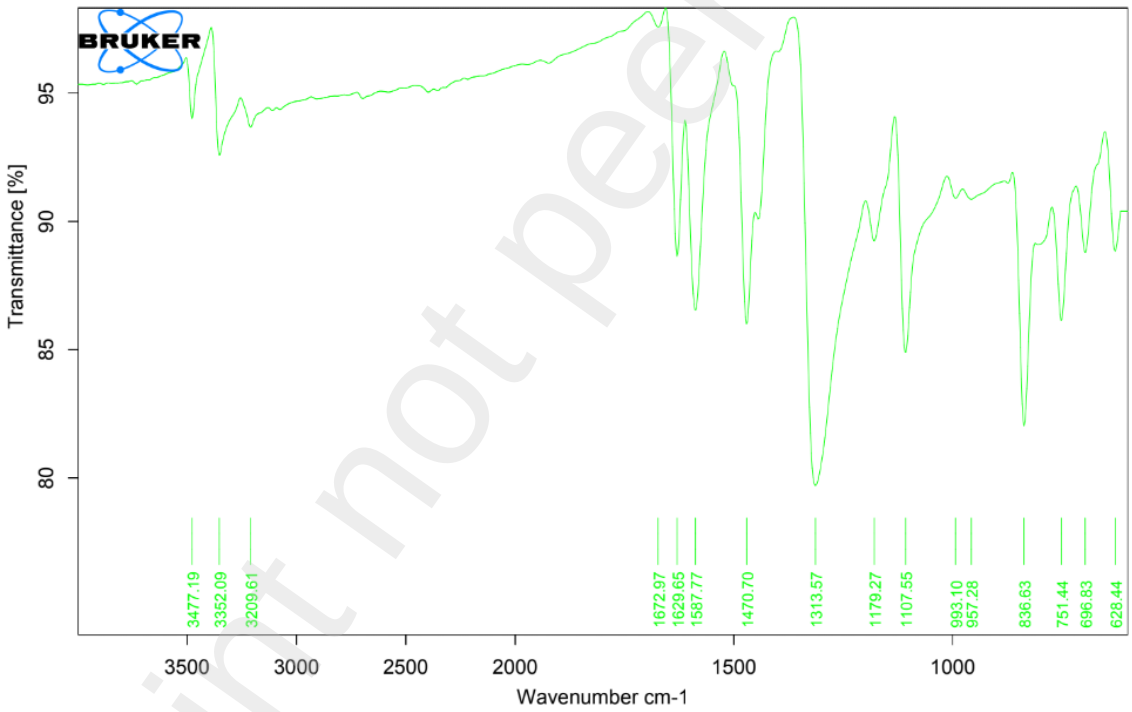


Fig.3(b): Recorded infrared spectra of HBN

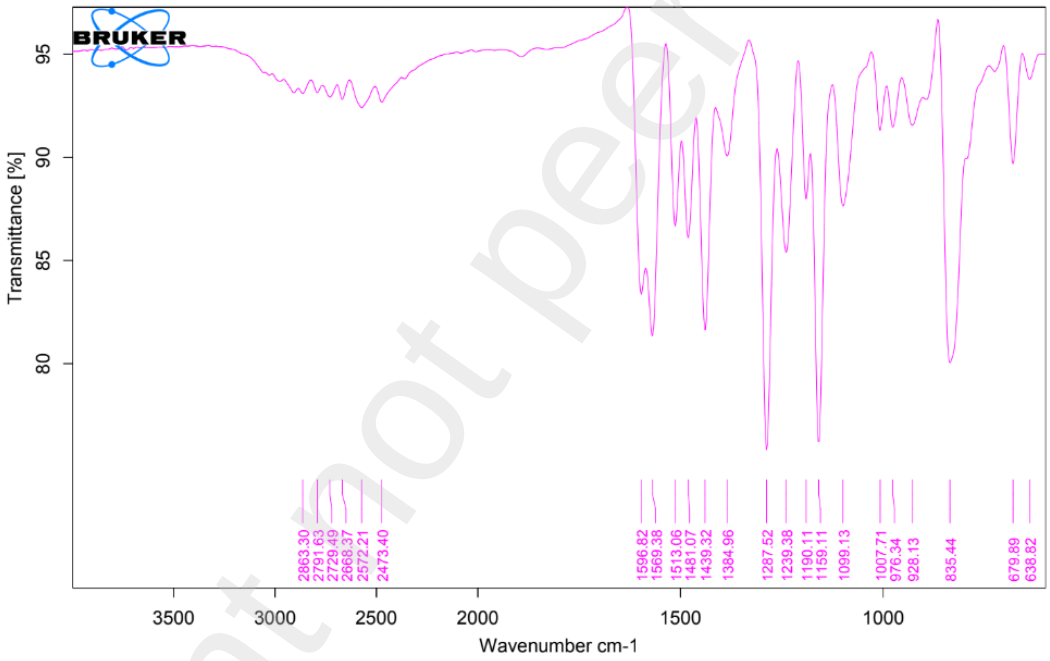


Fig.3(c): Recorded infrared spectra of HBC

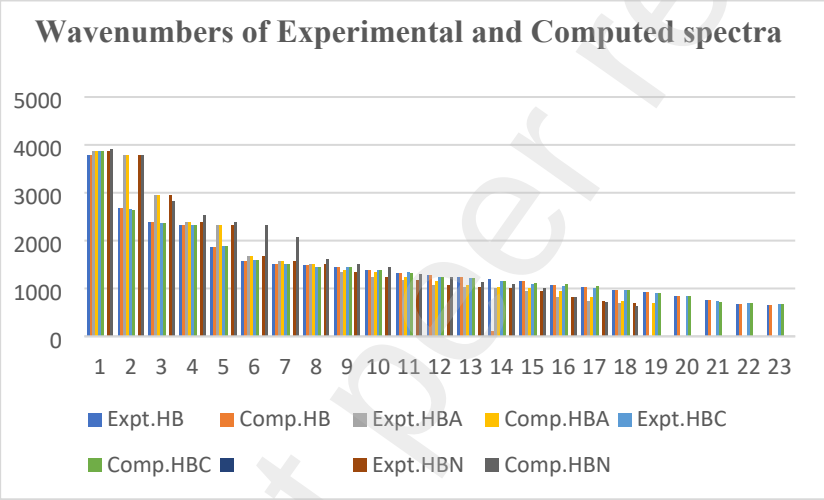


Fig.4 Recorded and Computed wavenumbers of compounds

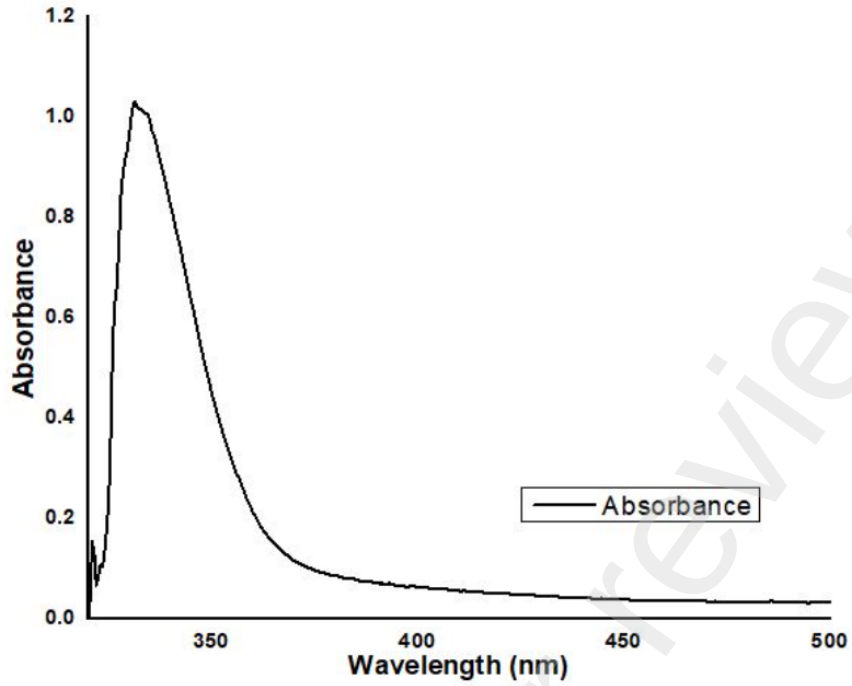


Fig.5(a): UV Spectra of HB

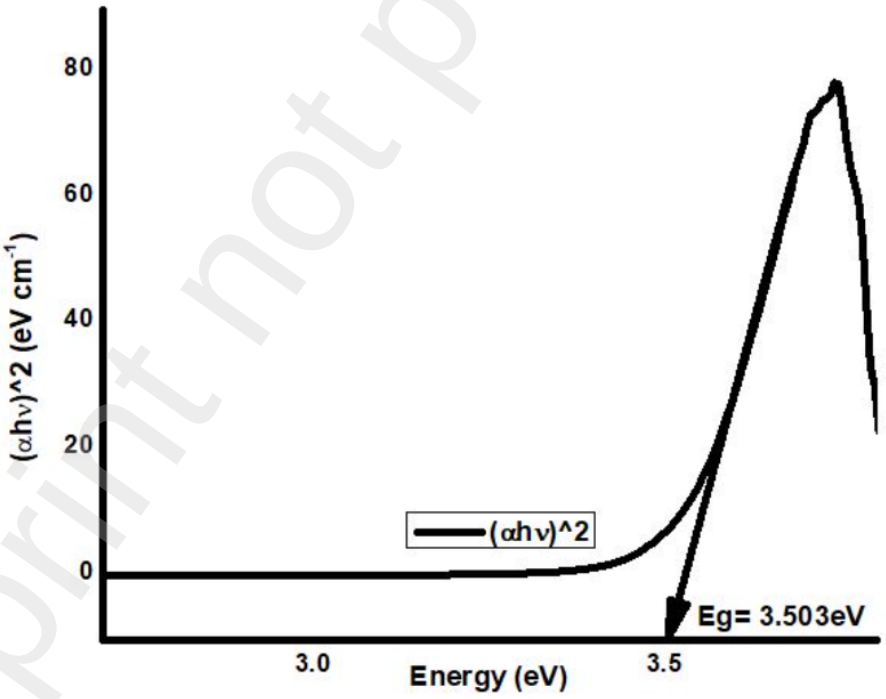


Fig.5(b): UV Spectral of HB with energy

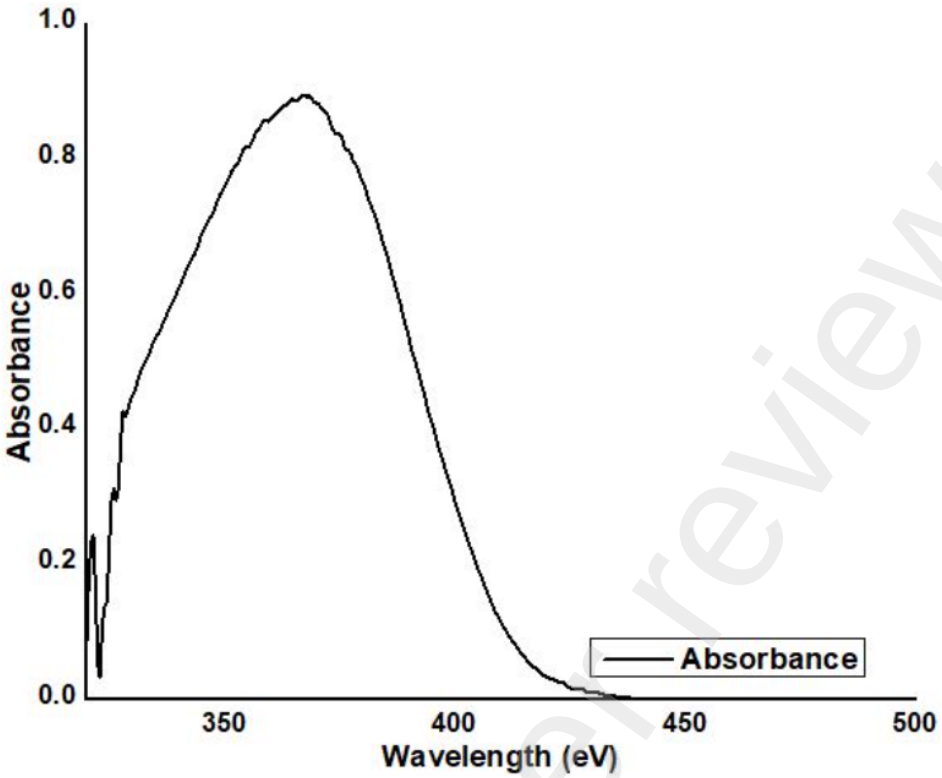


Fig.5(c): UV Spectra of HBN

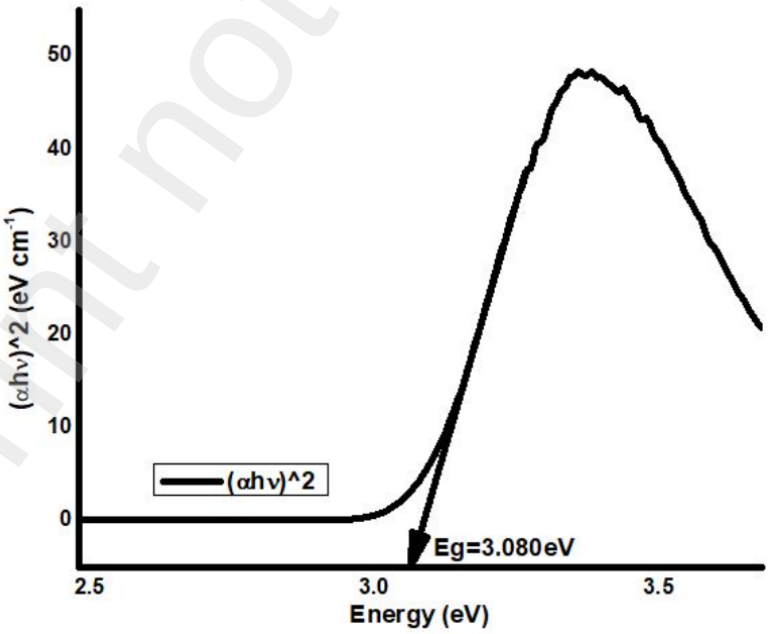


Fig.5(d): UV Spectra of HBN with energy

	
HB	HBN
Fig.6: Films of compounds	

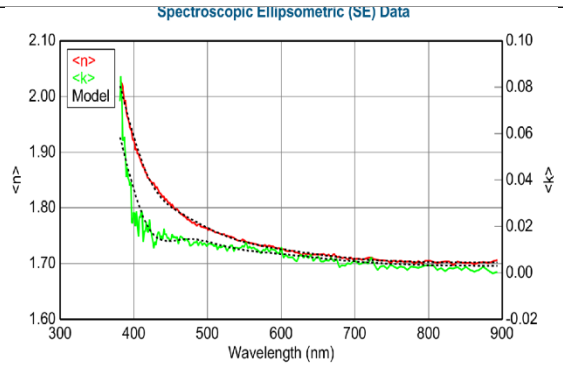


Fig. 7(a): Refractive index and extinction coefficient of HBA

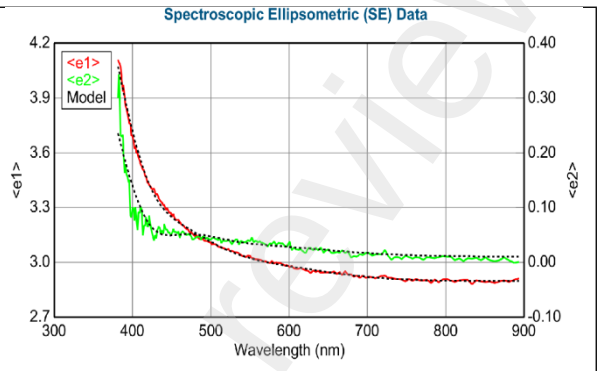


Fig.7(b): Real and Imaginary part of optical dielectric constant of HBA

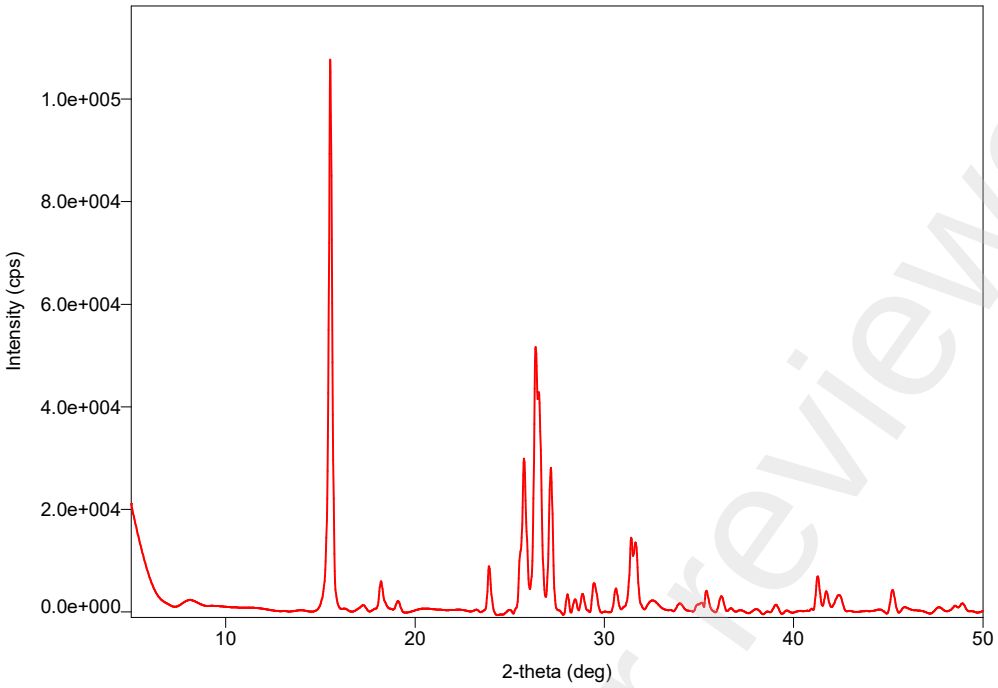


Fig.8(a): Powdered X ray spectra of HB

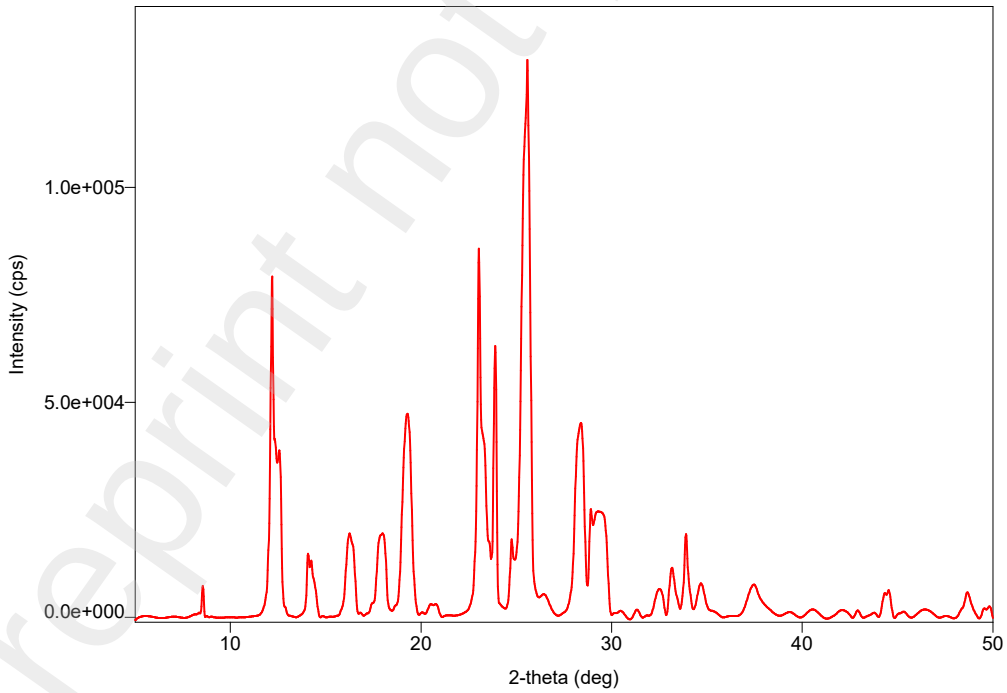
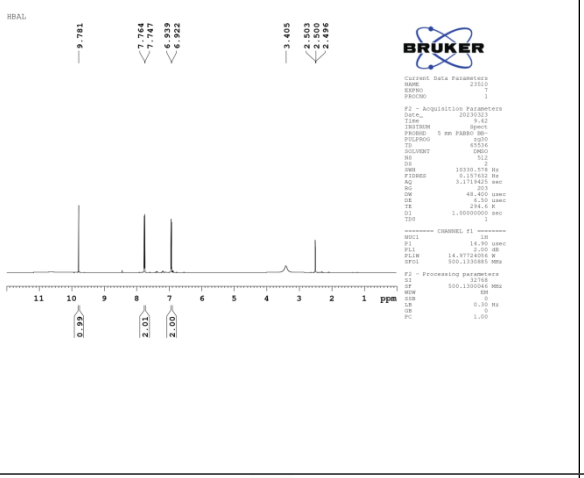
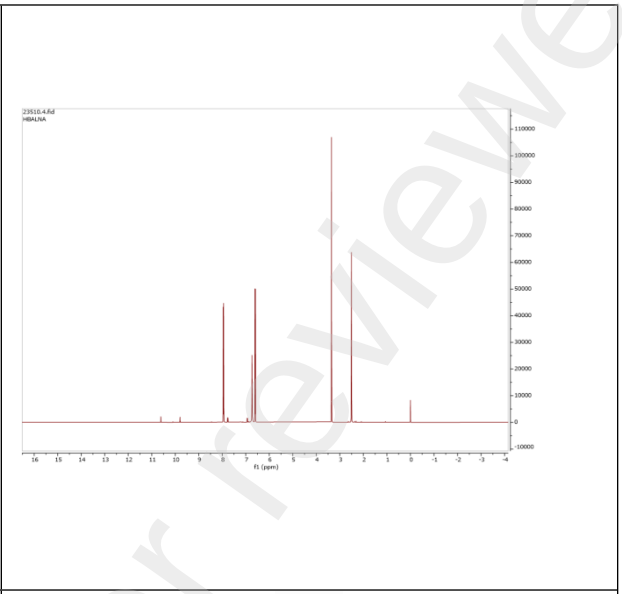


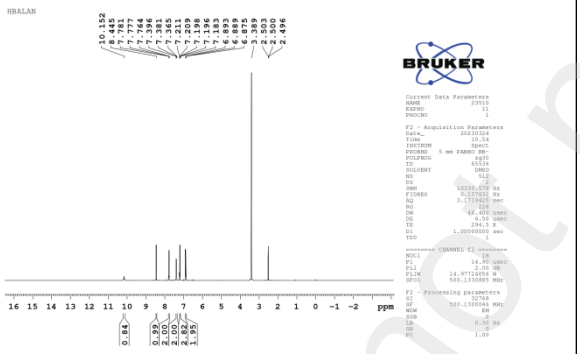
Fig.8(b): Powdered X ray spectra of HBN



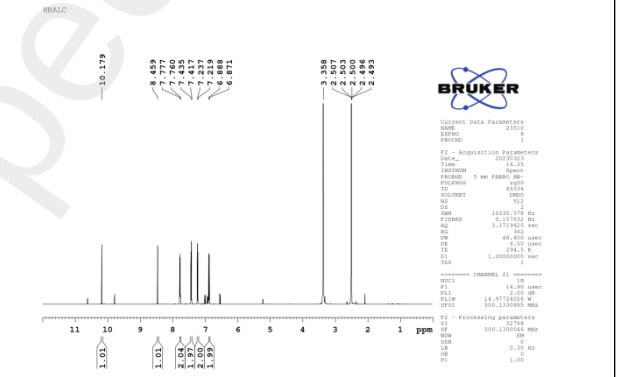
HB



HBN



HBA



HBC

Fig.9: Proton NMR of compounds

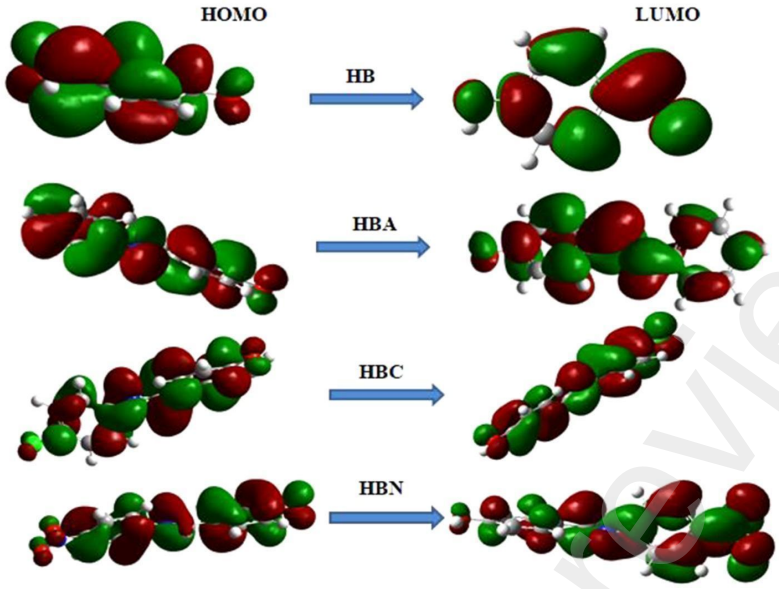


Fig 10: FMO contours of compounds

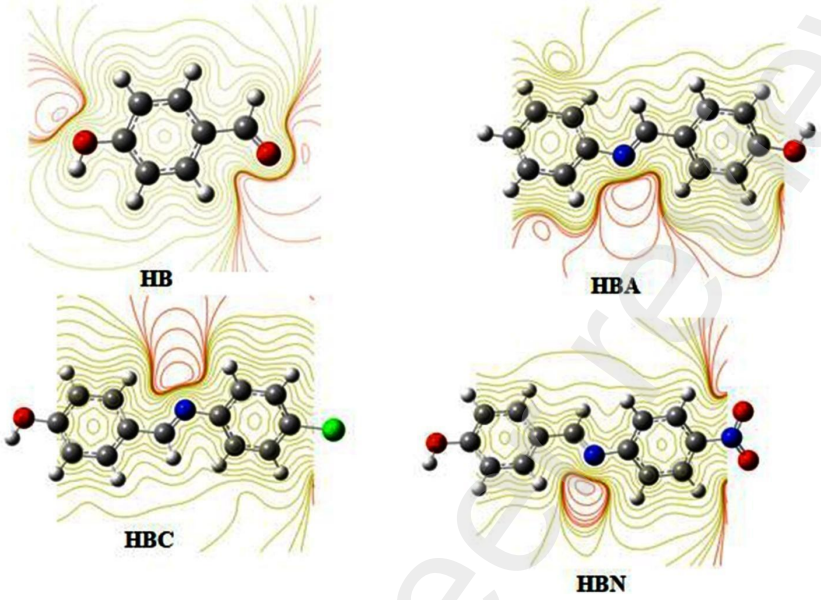


Fig. 11: ESP Contours of compounds

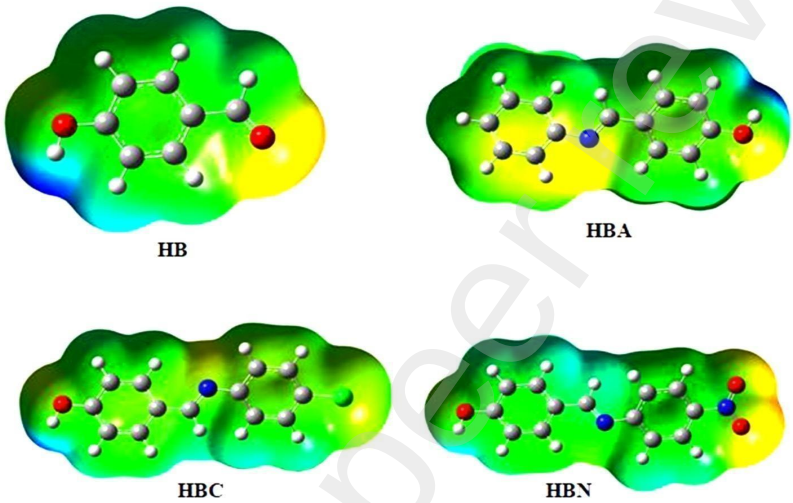


Fig 12: ESP maps of compounds

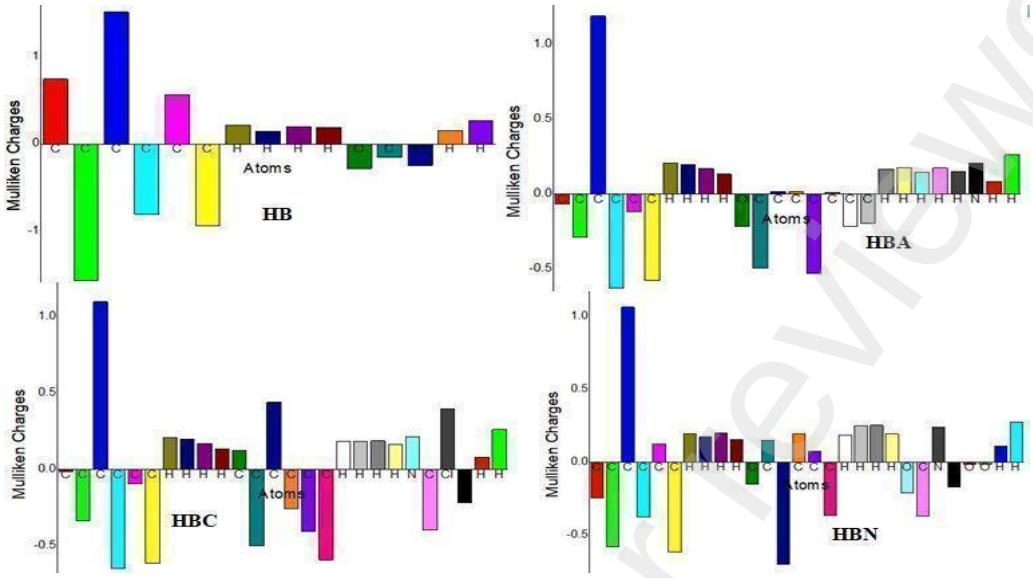


Fig 13: Mulliken Charge distribution

Table Captions

Table-1: Electronic properties

Table-2: Optoelectronic properties

Table-3: Charge transfer properties

Table-1: Electronic properties

Name of the compound	IP	EA	ΔE	χ	η	ω
HB	6.922	1.941	4.981	4.431	2.490	3.943
HBA	6.057	1.779	4.278	3.918	2.139	3.588
HBC	6.135	1.954	4.181	4.044	2.091	3.912
HBN	6.641	2.826	3.815	4.733	1.908	5.873

Table-2: Optoelectronic properties

Name of the compound	R_O	R_o^3	P	E	χ_e	ε_r	n	ρ	α	β
HB	4.09	68.418	0.168	7.677	2.473	3.473	1.864	3.455	13.477	7.157
HBA	4.90	117.649	0.086	3.265	2.976	3.976	1.994	3.023	27.726	11.297
HBC	5.08	131.096	0.112	4.334	2.920	3.920	1.979	4.407	30.452	5.023
HBN	5.11	133.433	0.196	7.309	3.030	4.303	2.074	7.856	32.188	57.047

Table-3: Charge transfer properties

Name of the compound	ω_+	ω_-	ΔN	N^I
HB	4.809	0.378	1.779	2.079
HBA	4.288	0.369	0.428	2.332
HBC	4.501	0.457	1.934	2.222
HBN	5.780	1.047	2.481	1.730