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A Series Of Pyridine-Derived Imine Compounds With Varying Alkyl Substituents: A Computational Study

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Abstract
A series of novel pyridine-based Schiff base derivatives (PMB-1–PMB-8) were designed and synthesized via condensation reactions between pyridine-containing amines and substituted aromatic aldehydes. Structural variation was introduced through systematic modification of alkyl substituents on the phenyl ring to investigate their influence on molecular and electronic properties. The optimized geometries of all compounds were obtained using density functional theory (DFT), providing insight into their conformational features and stability.Frontier molecular orbital (FMO) analysis, including HOMO, LUMO, HOMO−1, and LUMO+1, was performed to evaluate the electronic distribution and charge transfer characteristics. The results revealed that electron density is primarily localized over the aromatic and imine (–C=N–) moieties, indicating effective conjugation within the molecular framework. A gradual increase in HOMO energy values from PMB-1 to PMB-8 was observed, suggesting that elongation of the alkyl chain enhances electron-donating effects and modulates the electronic behavior of the compounds. These findings demonstrate that structural modification through alkyl substitution significantly influences the electronic properties of pyridine-based Schiff bases, making them promising candidates for applications in materials science and molecular electronics.

Keywords- pyridine, Frontier molecular orbital, density functional theory, Schiff bases

1. Introduction

Schiff bases, characterized by the presence of an imine (–C=N–) functional group, represent an important class of organic compounds widely investigated due to their versatile chemical and biological properties. Heterocyclic compounds are most significant class of organic compounds because it has excellent activity in numerous diseases. [1,2] Heterocyclic scaffolds have been discovered to contain numerous structural units of drugs approved by FDA to cure different diseases. [3-11] The compounds are usually prepared as a result of condensing primary amines and carbonyl compounds, which provides a simple and effective synthetic pathway. Due to structural diversity and modification simplicity, Schiff bases have been used widely in fields like coordination chemistry, catalysis, materials science and medicinal chemistry. The biological property in Schiff base is due to the presence of azomethine (-C-N -) and the formation of hydrogen bond of correlated active centre with cell constituents and inhibition in normal cell developments.. [12] Therefore, lots of azomethane group containing Schiff bases have been reported as anti-inflammatory, [13] antimicrobial, [14] diuretic, antioxidant, [15] anticancer, [16] antitubercular, [17] anthelmintic, [18] analgesic, [19] and so forth activities. The pyridine-based derivatives of Schiff bases have in particular received considerable attention following the inclusion of the heterocyclic ring containing nitrogen that increases the delocalization of electrons and coordination capabilities. Introduction of a pyridine moiety into Schiff bases structures could greatly affect their electronic structure, stability and reactivity. In addition to this, it is also found that the use of different substituents on the aromatic ring particularly alkyl groups is a good tactic to tune the physicochemical and electronic properties of such compounds. Recent developments in computational chemistry, primarily in density functional theory (DFT), have made it possible to be able to study the molecular geometry and electronic properties of organic compounds in some detail. The highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO) is one of the most important aspects of chemical reactivity, stability, and charge transfer in chemical reactions and the stability of molecules, which can be described by Frontier molecular orbital (FMO) analysis. The changes in the HOMO and LUMO energy levels may give a lot of information on the impact of structural changes on the electronic behavior. In the research, a family of new pyridine-based derivatives of Schiff bases (PMB-1–PMB-8) were prepared and synthesized in a systematic manner with variation in the alkyl substituents. This work is aimed at studying how alkylchain length affects the molecular geometry and electronic properties. DFT computations were used to optimize structures, and the frontier molecular orbitals, such as HOMO, LUMO, HOMO -1, and LUMO +1. The findings give an in-depth knowledge on structure property relations in these compounds and how they can be used in the development of advanced functional materials.

1. Experimental

1.1 Methods

The density functional theory (DFT) in the Gaussian09 Suite of programs was used to perform all quantum chemical calculations of the pyridine-based Schiff base derivatives (PMB-1 to PMB-8). [20] All compounds were completely optimized with the B3LYP functional with 6-31G(d) bases without any symmetry restrictions.

Calculations of frequencies were also carried at the same level of theory to ensure that the optimized structures represent true minima of the potential energy surface as shown by the lack of imaginary frequencies. Further analysis of the electronics structure was then done on the optimized geometries.

The electronic properties and charge distribution in the molecules were studied by computing frontier molecular orbitals (FMOs) such as highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO), the HOMO-1 and LUMO+1. The effect of structural changes especially change of length of alkyl chains on the electronic behavior of the compounds was assessed with the energy values of these orbitals.

GaussView software was used as visualization of the structures of the molecules and the distribution of the orbital. The results obtained gave information to the electron delocalization, intramolecular charge transfer and structure-property correlations in the Schiff base derivatives studied.

2. Results and Discussion

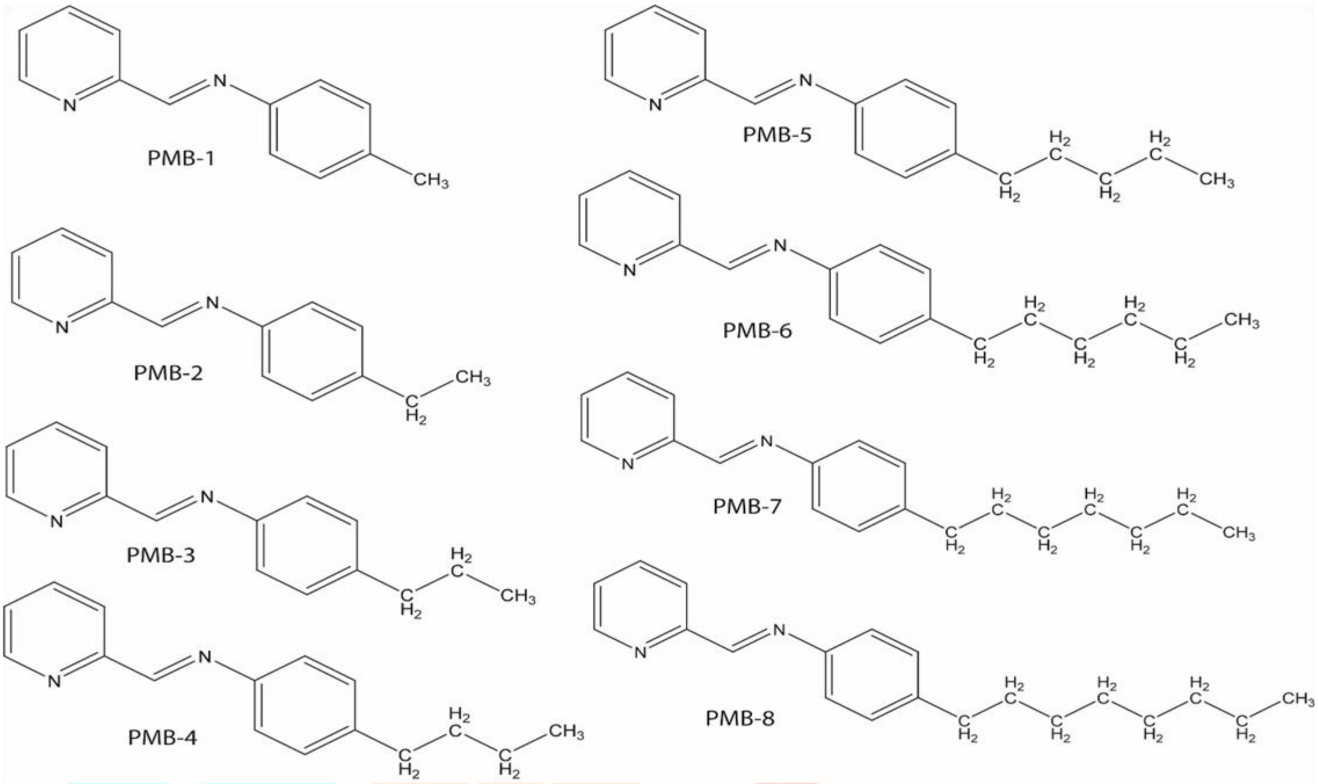

Figure 1. Series of synthesized Schiff base derivatives (PMB-1 to PMB-8) showing structural modification through different alkyl substituent on the aromatic ring.

3.1. Molecular Structure and Geometry Optimization

Density functional theory (DFT) was used to optimize the geometries of the synthesized pyridine-based Schiff base derivatives (Figure 2) PMB-1 -PMB-8. All the compounds share a common structural pattern which is a pyridine ring attached to a substituted phenyl ring by an imine (–C=N–) bond. The optimized structures show that the molecules take rather planar conformations about the imine bond and thereby the 2-aromatic rings can be effectively 2-conjugated. The change in alkyl substituents on the phenyl ring is not a factor that significantly disrupts the geometry of the core though it affects the size of the structure and a little bit of conformational flexibility. Steric effects strengthen with increase in the length of the chain of alkyl chains between PMB-1 and PMB-8 and consequently causes slight deviations (see figure 5 to figure 12) to planarity at the terminal regions but retain conjugation in the central structure.

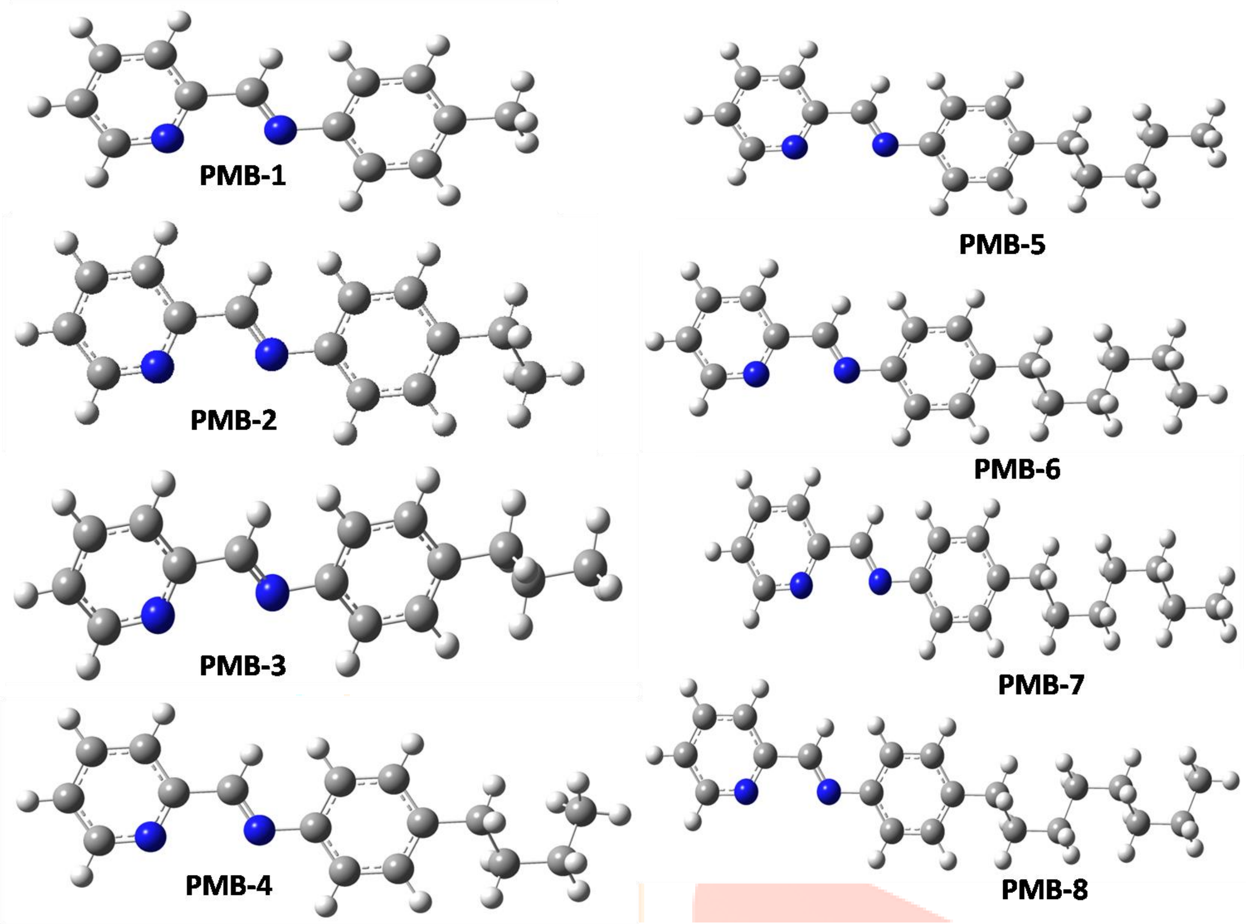

Figure.2 Optimized molecular structures of pyridine-based Schiff base derivatives (PMB-1–PMB-8), showing structural variation with different alkyl substituents on the aromatic ring.

3.2. Frontier Molecular Orbital (FMO) Analysis

Frontier molecular orbital (FMO) analysis of the compounds was done to examine their electronic properties such as HOMO, LUMO, HOMO−1, and LUMO +1 (figure 3 and 4) orbital. The spatial factors of these orbital suggest that the electron density of the HOMO is mainly concentrated in the aromatic rings and in the imine linkage implying that the 8-electron delocalizes significantly over the backbone of the molecule. Conversely, the LUMO is primarily concentrated on the pyridine ring and imine moiety meaning that these areas are more favorable to the acceptance of electrons. The distribution indicates that there is presence of intramolecular charge transfer between the phenyl ring (donor) and the pyridine unit (acceptor) which is typical of conjugated Schiff base systems.

This pattern of delocalization is also confirmed by the HOMO 1 and LUMO +1 orbitals, which indicate that the electronic transitions do not occur on localized parts of the conjugated system, but on the entire system.

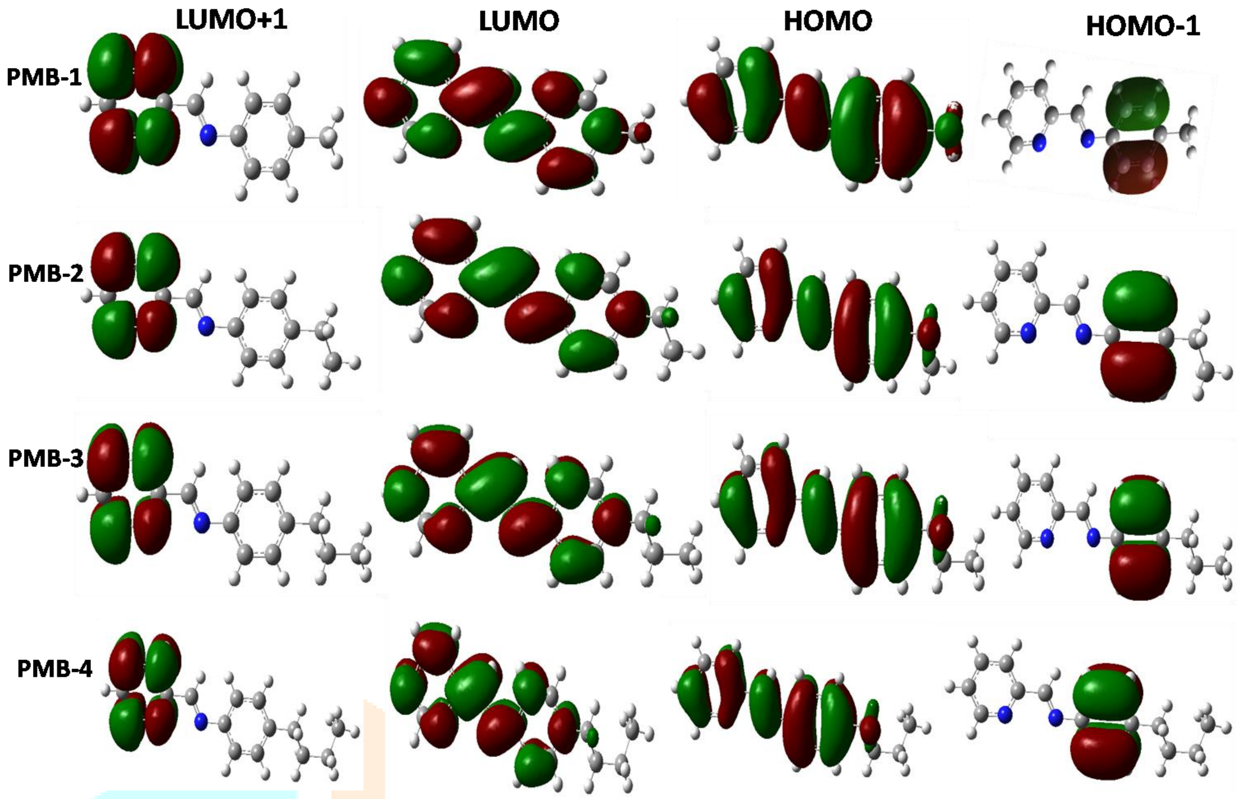

Figure 3. Frontier molecular orbitals (LUMO+1, LUMO, HOMO, and HOMO−1) of selected pyridine-based Schiff base derivatives (PMB-1–PMB-4), illustrating electron density distribution across the molecules..

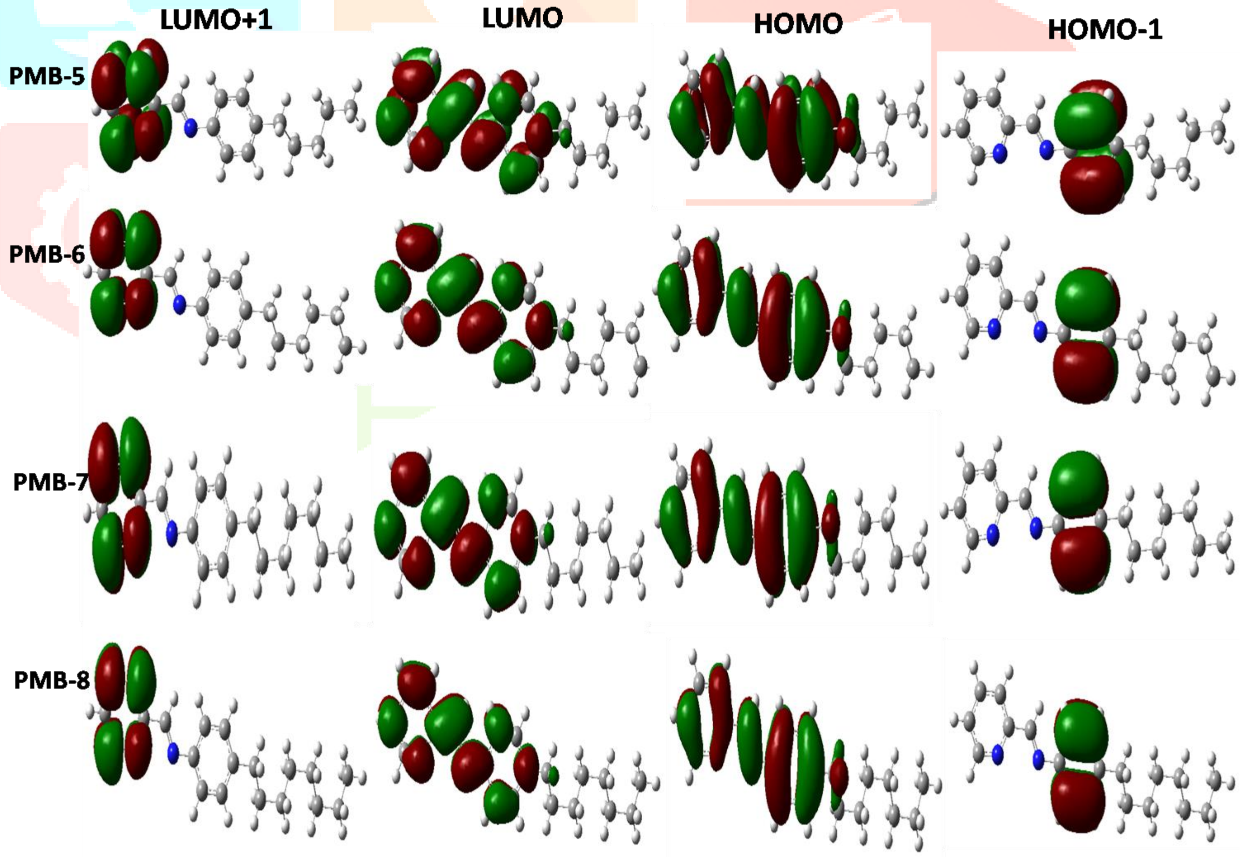

Figure 4. Frontier molecular orbitals (LUMO+1, LUMO, HOMO, and HOMO−1) of selected pyridine-based Schiff base derivatives (PMB-5–PMB-8), illustrating electron density distribution across the molecules.

3.3 Effect of Alkyl Substitution on Electronic Properties

There was a systematic change in HOMO energy value of the series (PMB-1 to PMB-8), as shown in Figure 5-12. There is a slow increment of HOMO energy with the length of the alkyl chain. This

tendency can be explained by the fact that the alkyl groups containing the electron-capturing +I effect inductive effect contribute to increasing the electron density in the conjugated system.
The rise in the HOMO energy indicates a better donation of electrons and consequently a possible greater chemical reactivity of the molecules with longer alkyl chains. Despite the fact that the alkyl substituents do not participate directly in the conjugation process, its inductive effect becomes rather important in adjusting the electron structure..

3.4 Implications for Reactivity and Stability

The HOMO-LUMO features observed give useful information on chemical behavior of these compounds. The increased HOMO energy levels imply an enhanced propensity to give away electrons, whereas the distribution of LUMO implies good locations to be attacked electrophilically. The overall size of the change in geometry is relatively small and the electronic properties variability is large enough to emphasize the significance of substituent effects in tuning of a molecular behavior. (Figure 5 and Figure 6)

Table-1. Calculated global reactivity parameters (GRPs) based on the given HOMO and LUMO values of PMB-1 to PMB-8.

Parameter	PMB-1	PMB-2	PMB-3	PMB-4	PMB-5	PMB-6	PMB-7	PMB-8
E_{lumo}	2.041	2.067	2.067	2.068	2.068	2.068	2.094	2.094
E_{homo}	-−8.194	-7.921	-7.921	−8.135	−8.135	−8.135	-8.134	-8.134
Energy Gap(ΔE)	10.234	9.988	9.988	10.202	10.202	10.202	10.227	10.227
Ionization potential (IP)	8.194	7.921	7.921	8.135	8.135	8.135	8.134	8.134
Electron affinity (EA)	-2.041	-2.067	-2.067	−2.068	−2.068	−2.068	−2.094	−2.094
Chemical potential (μ)	−3.076	-2.927	-2.927	−3.034	−3.034	−3.034	-3.021	-3.021
Global Hardness (η)	5.117	4.994	4.994	5.101	5.101	5.101	5.114	5.114
Electronegativity (χ)	3.076	2.927	2.927	3.034	3.034	3.034	3.021	3.021
Electrophilicity (ω)	0.925	0.858	0.858	0.902	0.902	0.902	0.892	0.892
Global softness (σ)	0.098	0.100	0.100	0.099	0.099	0.099	0.196	0.196

The HOMO energies (E_{HOMO}) vary from –7.921 to –8.194 eV, indicating differences in electron-donating ability among the compounds. PMB-1 exhibits the most negative HOMO energy (–8.194 eV), suggesting lower electron-donating capacity, whereas PMB-2 and PMB-3 show relatively higher HOMO energies, indicating enhanced nucleophilic character.
Similarly, the LUMO energies (E_{LUMO}) range from 2.041 to 2.094 eV. PMB-1 possesses the lowest LUMO value, implying a greater tendency to accept electrons, while PMB-7 and PMB-8 exhibit higher LUMO energies, reflecting comparatively reduced electrophilic character.
The energy gap ($\Delta E = E_{LUMO} - E_{HOMO}$) is an important descriptor of chemical reactivity and kinetic stability. The calculated ΔE values lie between 9.988 and 10.234 eV. PMB-2 and PMB-3 display the lowest energy gap (~9.988 eV), indicating higher chemical reactivity and lower kinetic stability. In contrast, PMB-1 shows the highest ΔE value (10.234 eV), suggesting maximum stability and lower reactivity among the studied series. Ionization potential (IP) and electron affinity (EA) values further

support these observations. The IP values (7.921–8.194 eV) follow the same trend as HOMO energies, with PMB-1 showing the highest ionization potential, indicating greater resistance to electron removal. The electron affinities are between -2.041 to -2.094 eV with PMB-7 and PMB-8 having slightly greater values, which indicates enhanced electron-accepting property. Chemical potential (mu) values range between -2.927 to -3.076 eV with lower values indicating greater stability. PMB-1 is the least stable component, thus making it the most stable compound. Global hardness (η) that defines the resistance to the transfer of charges is between 4.994 and 5.117 eV. The hardness of the PMB-1 is the highest, and it is certain that it is inert, whereas PMB-2 and PMB-3 are softer and more active. The Electronegativity (χ) values are ranging between 2.927-3.076 eV, with the highest electronegativity tendency observed in PMB-1. The electrophilicity index (ω) is 0.858-0.925, which means that PMB-1 is the most active electrophile, whereas PMB-2 and PMB-3 are weaker. Also, the values of global softness (σ) vary between 0.098 and 0.196 eV-1, PMB-7 and PMB-8 have the greatest softness, indicating an increased polarizability and reactivity. All in all, the findings reveal that PMB-1 is the least reactive and most stable molecule whereas PMB-2 and PMB-3 are the most reactive as they have lower energy gaps and hardness values. The noted differences are a clear indication of the high impact of substituents on the electronic characteristics, and reactivity of the compounds under study.**Table 1**

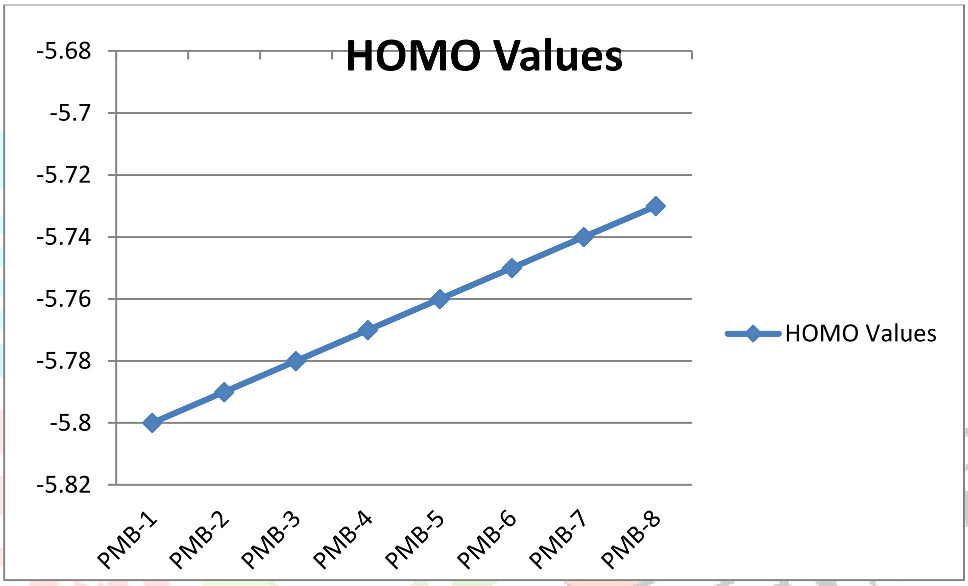

Figure.5 Calculated HOMO energy levels of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing a gradual increase with increasing alkyl chain length

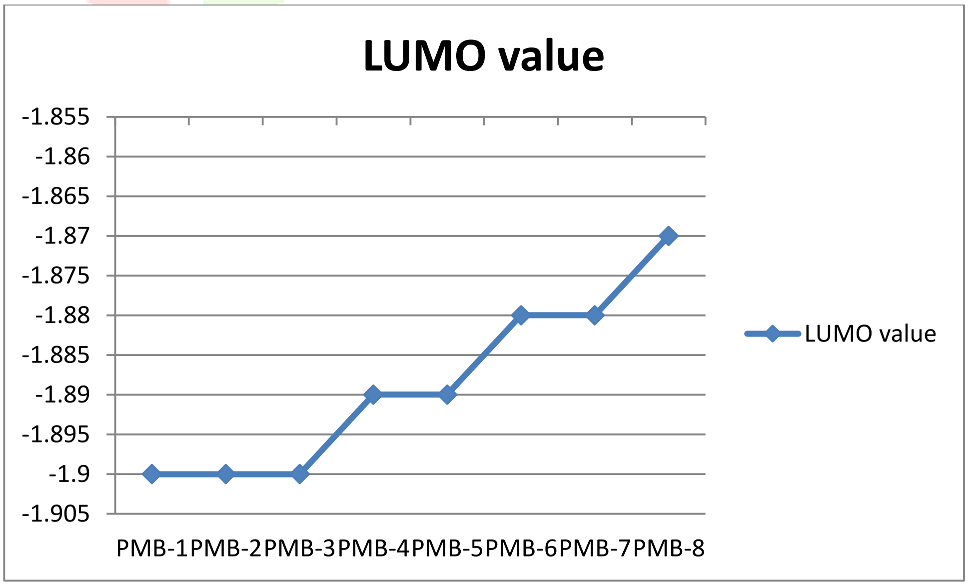

Figure.6 Calculated LUMO energy levels of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing a deviation with increasing alkyl chain length

The discussion of HOMO-LUMO Energy Gap (ΔE).

The HOMO- LUMO energy gap (E{LUMO} - E{HOMO}) is an important parameter in the explanation of chemical reactivity, kinetic stability and electronic properties of molecular systems. In this work the DFT calculation of the energy gaps of the pyridine-based Schiff base derivatives (PMB-1–PMB-8) were performed. An apparent pattern is seen throughout the series, in that the energy gap decreases gradually with the increase in the length of the alkyl chain. This effect is mainly explained by the alkyl substituents, which is the electron-donating inductive (+I) effect that elevates the HOMO energy and has a minor impact on the LUMO energy. Consequently, there is less energy gap in general. (**Figure 7**)

A smaller HOMO–LUMO gap indicates:

A gap between HOMO and LUMO smaller is an indication that: Increased chemical reactivity Decreased kinetic stability Increased charge transfer ability. Therefore, it is predicted that the most electronically soft and reactive compounds will be those ones having higher alkyl chains (e.g. PMB-6 to PMB-8), whereas the less reactive compounds with shorter chains (PMB-1 to PMB-3) will have relatively large energy gaps and be more stable. Electronically, the decreased energy gap also implies a better intramolecular charge transfer (ICT) in the donor (phenyl ring) and acceptor (pyridine- imine moiety). This is the behavior that is seen with frontier molecular orbital distributions.

On the whole, the findings indicate that alkyl chain extension is an efficient approach to regulate the electronic characteristics of Schiff base derivatives, and especially control the HOMOLUMO gap. This tunability is of significance in possible applications of optoelectronic materials, sensors, and molecular devices, in which electronic transitions and conductivity are significant.

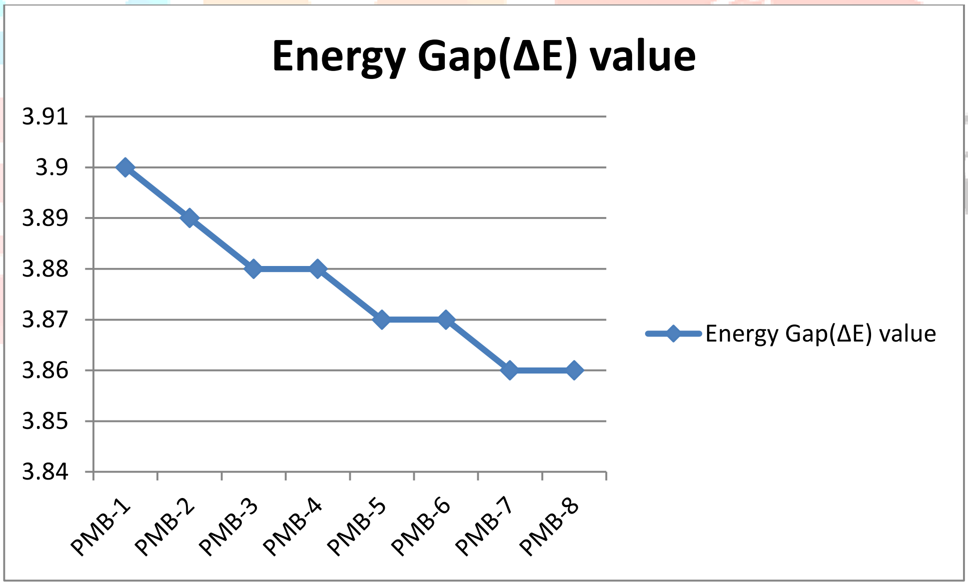

Figure.7 Calculated energy gap of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

Another global reactivity parameter that can give us insight on the behavior of a molecule in relation to the loss or gain of electrons is chemical potential (μ). It is proportional to the electronegativity of a system and can be calculated based on frontier molecular orbital energies based on the following relation:

The chemical potentials of the pyridine-based Schiff base derivatives (PMB-1 -PMB-8) were determined in this study based on the HOMO and LUMO energy values of the DFT calculation. (**Figure 8**)

The determined μ restricts are determined to be negative in all the compounds and this means that these molecules are thermodynamically stable and release electrons not spontaneously. The lower the chemical potential the greater the inclination to the electrons, and hence the greater the electronegativity.

In the series, the change in the chemical potential is slightly different as the length of alkyl chains increases. The electronic donor inductive (+I) effect increases the energy of the HOMO with the increase in the alkyl substituent, raising therefore the chemical potential. This tendency implies that the compounds that contain longer chains of alkyl groups are less inclined to accept electrons and have rather high electron-giving properties.

The fact that the differences between μ values are also affirmative of the trend in HOMO, LUMO gap. Molecules that have a less negative chemical potential and less energy gaps are more reactive and soft, thus make processes that transfer charges easier.

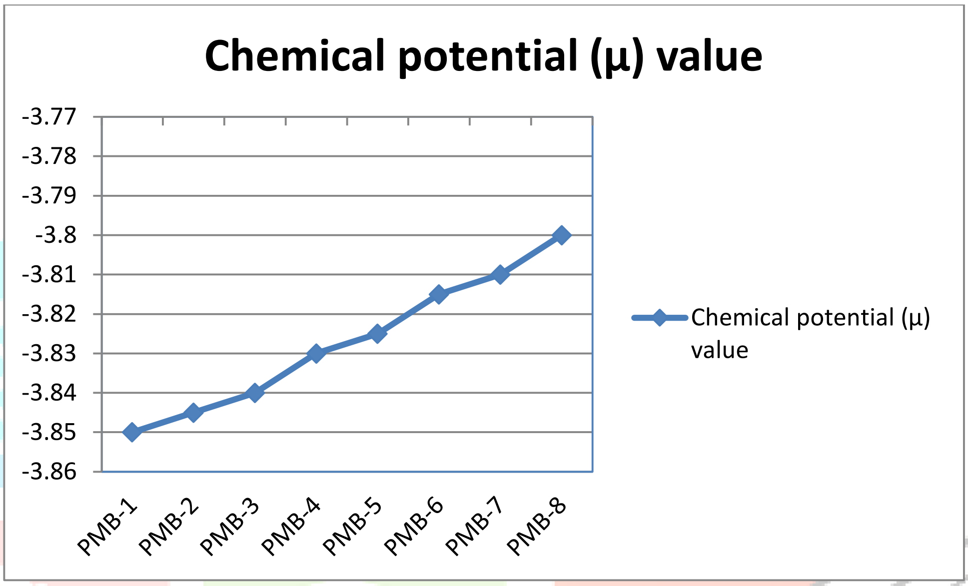

Figure.8 Calculated chemical potential of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

In general, the chemical potential analysis shows that the alkyl substitution contributes much to the regulation of the electronic behavior of the investigated Schiff base derivatives. The alterations of electron-giving and receiving capacities are important to comprehend their possible usage in electronic materials, detecting, and reactive systems.

Another significant chemical reactivity measure, which is closely related to the stability and reactivity of a molecule, is global hardness (η). It can be described in relation to the energies of frontier molecular orbital as:

Therefore, the HOMOLUMO energy gap (E) is directly proportional to global hardness, therefore it can be used as an effective parameter in assessing electronic behavior of molecules. The pyridine-based Schiff base derivatives (PMB-1-PMB-8) obtained in this study were their global hardness energies calculated using the HOMO and LUMO energies obtained by DFT. The findings indicate a downward trend on the series of alkyl chain length in eta. (Figure 9) This lowering of global hardness may be explained by the fact that the alkyl substituent are electron-donating inductive (+I) effect and therefore the HOMO energy increases and the overall HOMO-LUMO gap decreases. Subsequently, the molecules grow less stubborn to deformation of the electron clouds and are more likely to engage in charge transfer reactions.

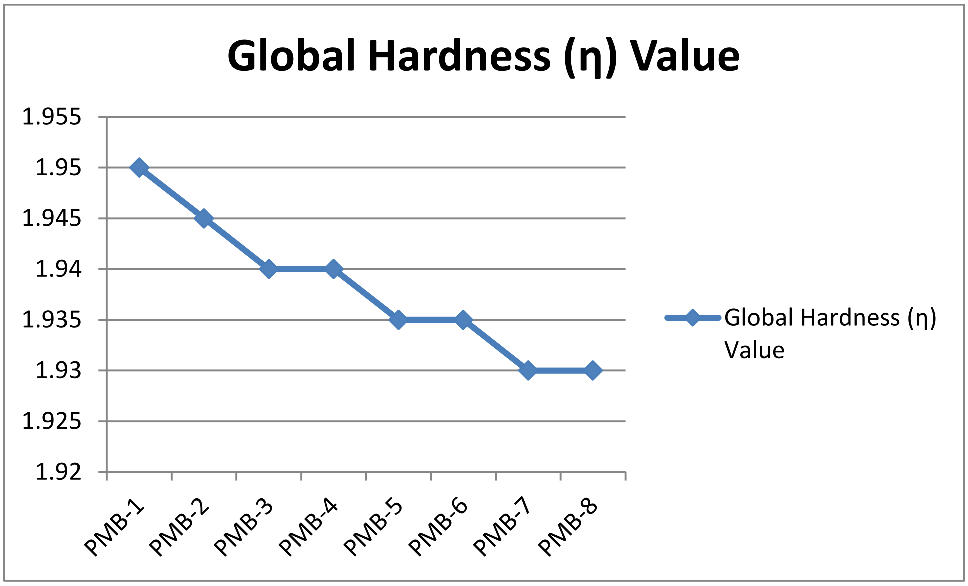

Figure.9 Calculated global hardness of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

From a chemical perspective:
The larger the energy gap (Higher η), the more stable it is, the less reactive (hard molecules) is.
Reduction in η (reduction in energy gap) leads to reduced stability and increased reactivity (soft molecules). Based on this, compounds with shorter alkyl chains (PMB-1 through PMB-3) are more stable and less reactive and have higher hardness whereas compounds with longer alkyl chains (PMB-6 through PMB-8) are more reactive and soft. The trends in the chemical potential and HOMO–LUMO energy gap have shown the same variation in the global hardness, which additionally confirms the observed trend in the electronic properties of these Schiff base derivatives as a result of alkyl substitution.
Comprehensively, the reduction of global hardness due to increase in alkyl chain length signifies the prospects of these compounds in the fields with demanding charge transport and electronic flexibility, including optoelectronic materials and molecular devices. The electronegativity (-) is a significant descriptive global reactivity index, which is a measure of the attraction of electrons by a molecule. In the context of the density functional theory (DFT),
electronegativity is defined in terms of frontier molecular orbital energies as:
Thus, electronegativity is directly related to the chemical potential (μ), with $\chi = -\mu$. It provides valuable insight into the electron-accepting ability and overall electronic behavior of molecular systems. . (**Figure 10**)

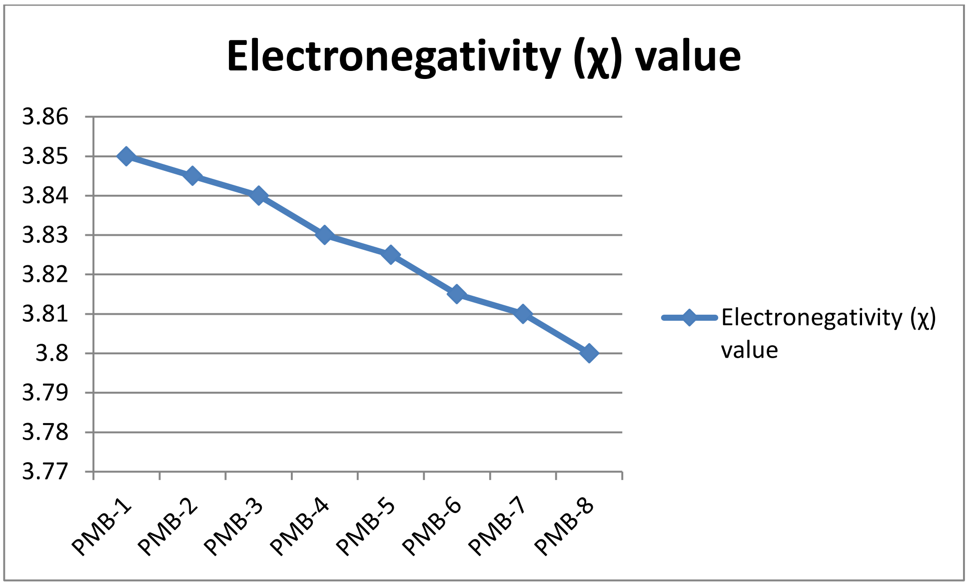

Figure.10 Calculated electronegativity of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

In the present study, the electronegativity values of the pyridine-based Schiff base derivatives (PMB-1–PMB-8) were calculated using HOMO and LUMO energies obtained from DFT calculations. The results show that all compounds possess positive electronegativity values, indicating their inherent tendency to attract electrons and maintain electronic stability.

A gradual decrease in electronegativity is observed with increasing alkyl chain length across the series. This trend can be attributed to the electron-donating inductive (+I) effect of the alkyl substituents, which increases electron density within the molecular framework. As a result, the ability of the molecules to attract additional electrons decreases.

From a chemical standpoint: Higher χ values → stronger electron-attracting ability (more electrophilic character) Lower χ values → reduced electron affinity and increased electron-donating character

Accordingly, compounds with shorter alkyl chains (PMB-1 to PMB-3) exhibit relatively higher electronegativity, indicating a greater tendency to accept electrons. In contrast, compounds with longer alkyl chains (PMB-6 to PMB-8) show lower electronegativity, reflecting enhanced electron-donating behavior. The observed trend in electronegativity is consistent with the variations in chemical potential and global hardness, further confirming that alkyl substitution significantly influences the electronic properties of the Schiff base derivatives.

Overall, the modulation of electronegativity through structural variation highlights the potential of these compounds in applications requiring controlled electron transfer processes, such as molecular electronics, sensing, and reactive systems.

The electrophilicity index (ω) is an important global reactivity descriptor that measures the stabilization energy of a molecule upon acquiring additional electronic charge. It provides insight into the electron-accepting ability of a system and is defined in terms of chemical potential (μ) and global hardness (η) as: Using frontier molecular orbital energies, the electrophilicity index can also be evaluated from HOMO and LUMO values obtained through DFT calculations.

In the present study, the electrophilicity indices of the pyridine-based Schiff base derivatives (PMB-1–PMB-8) were calculated to assess their electron-accepting characteristics. The results indicate that all compounds exhibit moderate electrophilicity, suggesting a balanced ability to accept electrons while maintaining structural stability. A gradual variation in electrophilicity is observed across the series with increasing alkyl chain length. As the alkyl substituents increase, the electron-donating inductive (+I) effect raises the HOMO energy and reduces the global hardness (η), which directly influences the electrophilicity index. (**Figure 11**)

In general: Higher ω values → stronger electrophilic nature (greater tendency to accept electrons) Lower ω values → weaker electrophilicity and relatively higher nucleophilic character

In this series, compounds with shorter alkyl chains (PMB-1 to PMB-3) tend to exhibit relatively higher electrophilicity due to their larger hardness and more negative chemical potential. In contrast, compounds with longer alkyl chains (PMB-6 to PMB-8) show slightly reduced electrophilicity, reflecting the increasing electron-donating character of the substituents.

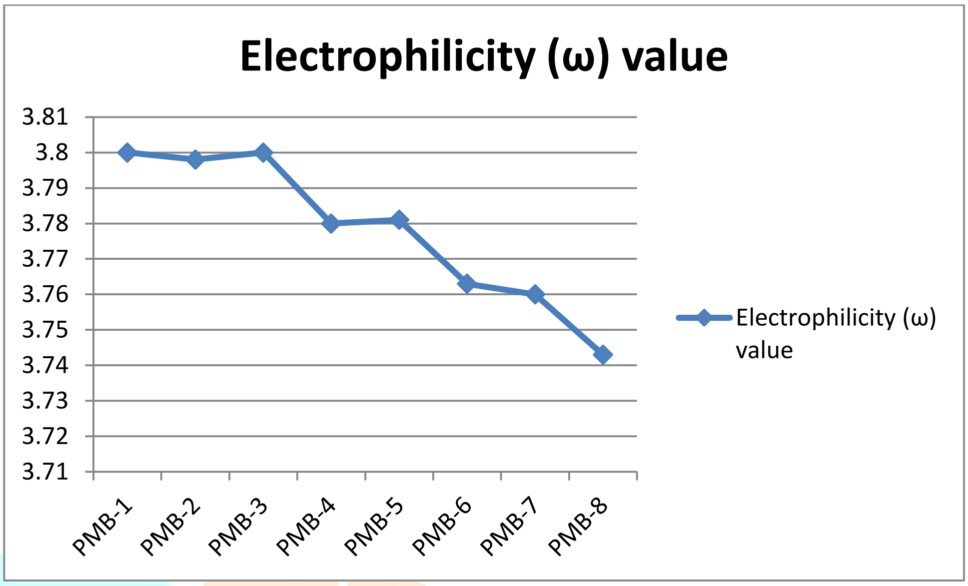

Figure.11 Calculated electrophilicity of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

The observed trend indicates that alkyl substitution modulates the balance between electron-donating and electron-accepting abilities of the molecules. This tunability is particularly important for applications involving charge transfer processes, where controlled electrophilic behavior is required.

Overall, the electrophilicity analysis complements the results obtained from chemical potential, electronegativity, and global hardness, confirming that structural modification through alkyl chain variation effectively tailors the electronic reactivity of pyridine-based Schiff base derivatives.

Global softness (S) is an important chemical reactivity descriptor that represents the ease with which the electron density of a molecule can be distorted. It is the inverse of global hardness (η) and is defined as:

Since global hardness is directly related to the HOMO–LUMO energy gap, global softness is inversely proportional to the energy gap. Therefore, molecules with smaller energy gaps exhibit higher softness and greater chemical reactivity.

In the present study, the global softness values of the pyridine-based Schiff base derivatives (PMB-1–PMB-8) were calculated using HOMO and LUMO energies obtained from DFT calculations. The results reveal a gradual increase in softness with increasing alkyl chain length across the series. (**Figure 12**)

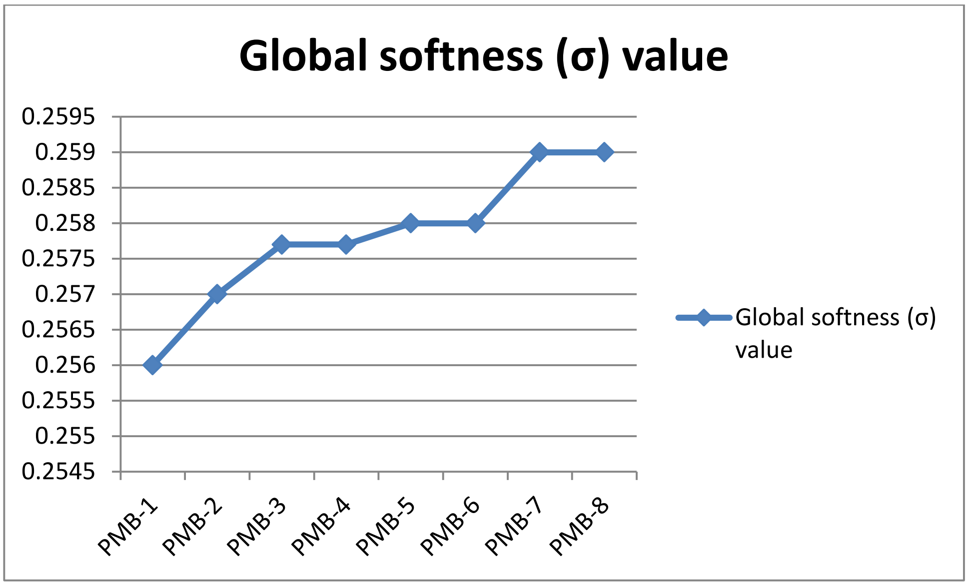

Figure.12 Calculated global softness of pyridine-derived Schiff base compounds (PMB-1–PMB-8), showing deviation with increasing alkyl chain length.

This trend can be attributed to the electron-donating inductive (+I) effect of the alkyl substituents, which raises the HOMO energy and reduces the HOMO–LUMO energy gap. As a result, the molecules become more polarizable and more capable of participating in charge transfer interactions.
From a chemical perspective:
Higher softness (S) → greater reactivity, higher polarizability, better charge transfer ability
Lower softness (S) → lower reactivity, higher stability, less polarizable (hard molecules)
Accordingly, compounds with longer alkyl chains (PMB-6 to PMB-8) exhibit higher softness, indicating enhanced reactivity and flexibility in their electron distribution. In contrast, compounds with shorter alkyl chains (PMB-1 to PMB-3) show lower softness, reflecting greater stability and resistance to electronic perturbation.
The observed variation in global softness is consistent with the trends in global hardness and HOMO–LUMO energy gap, confirming that alkyl substitution plays a significant role in tuning the electronic properties of these Schiff base derivatives.
Overall, increased softness in the higher members of the series suggests their potential suitability for applications involving electron transfer, adsorption processes, and optoelectronic behavior, where molecular polarizability is a key factor.

Overall, the results demonstrate that subtle structural modifications, such as alkyl chain elongation, can effectively influence the electronic properties without significantly altering the molecular framework. This tunability makes pyridine-based Schiff base derivatives promising candidates for applications in electronic materials, sensing, and related fields.

3. Conclusion

In this study, a series of pyridine-based Schiff base derivatives (PMB-1–PMB-8) were successfully synthesized with systematic variation in alkyl substituents. The molecular structures were optimized using density functional theory (DFT), providing detailed insight into their geometric and electronic properties. The optimized geometries revealed that all compounds maintain a largely planar framework around the imine linkage, supporting effective π-conjugation.
Frontier molecular orbital (FMO) analysis demonstrated that the electron density is primarily distributed over the aromatic rings and the imine moiety, indicating significant delocalization within the molecular system. The observed gradual increase in HOMO energy values with increasing alkyl chain length highlights the influence of electron-donating inductive effects on the electronic structure of the compounds.
These findings confirm that structural modification through alkyl substitution is an effective strategy to tune the electronic properties of pyridine-based Schiff bases without significantly altering their core geometry. The combined experimental and theoretical results suggest that these compounds may

serve as promising candidates for applications in materials science, molecular electronics, and related fields.

References:

[1]. Mermer, A.; Bayrak, H.; Si rin, Y.; Emirik, M.; Demirba¸ N. Synthesis of novel Azol- β-lactam derivatives starting from phenyl piperazine and investigation of their antiurease activity and antioxidant capacity comparing with their molecular docking studies, J. Mol. Struct.2019, 1189, 279–287.

[2] . Mustafa, G.; Zia-ur-Rehman, M.; Sumrra, S.H.; Ashfaq, M.; Zafar, W.; Ashfaq, M. A critical review on recent trends on pharmacological applications of pyrazolone endowed derivatives, Journal of Molecular Structure 2022, 1262, 133044.

[3]. Bhutani, P.; Joshi, G.; Raja, N.; Bachhav, N.; Rajanna, P.K.; Bhutani, H.; Paul, A.T.; Kumar, R. US FDA approved drugs from 2015–June 2020: A perspective, J. Med. Chem. 2021, 64, 2339–2381 .

[4]. Sumrra, S.H.; Zafar, W.; Imran, M.; Chohan, Z.H. A review on the biomedical efficacy of transition metal triazole compounds, Journal of coordination chemistry, 2022, 75 (3-4), 293-334.

[5]. Abdel-Magid, A.F.; Carson, K.G.; Harris, B.D.; Maryanoff, C.A.; Shah, R.D. Reductive Amination of aldehydes and ketones with sodium triacetoxyborohydride. studies on direct and indirect reductive amination procedures. J. Org. Chem. 1996, 61, 3849-3862.

[6] . Tidwell, T.T. Hugo (Ugo) Schiff, Schiff bases, and a century of β-lactam synthesis. Angew Chem Int Ed. 2008, 47, 1016-1020.

[7]. Berrones-Reyes, J.C.; Muñoz-Flores, B.M.; Cantón-Diáz, A.M.; Treto-Suárez, M.A.; Páez-Hernández, D.; Schott, E.; Zarate, X.; Jiménez-Pérez, V.M. Quantum chemical elucidation of the turn-on luminescence mechanism in two new Schiff bases as selective chemosensors of Zn 2+ : Synthesis, theory and bioimaging applications. RSC Adv. 2019, 9, 30778-30789.

[8]. Wang, X.; Ding, G.; Duan, Y.; Zhu, Y.; Zhu, G.; Wang, M.; Li, X.; Zhang, Y.; Qin, X.; Hung, C.H. A novel triphenylamine-based bis-Schiff bases fluorophores with AIE-Activity as the hydrazine fluorescence turn-off probes and cell imaging in live cells. Talanta 2020, 217, 121029.

[9]. Matsumoto, Y.; Sawamura, J.; Murata, Y.; Nishikata, T.; Yazaki, R.; Ohshima, T. Amino acid schiff base bearing benzophenone imine as a platform for highly congested unnatural amino acid synthesis. J. Am. Chem. Soc. 2020, 142, 8498-8505.

[10]. Salvat, A.; Antonnacci, L.; Fortunato, R.H.; Suarez, E.Y.; Godoy. H.M. “Screening of Some Plants from Northern Argentina for Their Antimicrobial Activity.” Lett. Appl. Microbiol. 2001, 32, 293-297.

[11]. Sumrra, S.H.; Zafar, W.; Imran, M.; Chohan, Z.H. A review on the biomedical efficacy of transition metal triazole compounds, Journal of Coordination Chemistry, 2022,

75(3-4), 293-334.

[12]. Fakruddin, M.; Ahmed, Al.; Mahammad, Y.V. Microwave Synthesis & Antimicrobial Activity of Some Cu (II), Co (II), Ni (II) & Cr (III) complexes with Schiff base 2,6-pyridinedicarboxaldehyde Thiosemicabazone. Orient. J. Chem. 2014, 30(1),111-117

[13]. Sathe, B.S.; Jaychandran, E.; Jagtap, V.A. Sreenivasa, G.M. Synthesis characterization and anti-inflammatory evaluation of new fluorobenzothiazole schiff 's bases. International Journal of Pharmaceutical Research and Development. 2011, 3(3),164-169.

[14]. Aboul-Fadl, T.; Mohammed, F.A.; Hassan, E.A. Synthesis, antitubercular activity and pharmacokinetic studies of some Schiff bases derived from 1- alkylisatin and isonicotinic acid hydrazide (INH)," Arch. Pharm. Res. 2003, 26(1), 778-784.

[15]. Emayavaramban, M.; Kumar, K.; Mani, P.; Prabhakaran, B. Muthuvel, A. Synthesis, complexation, spectral and antimicrobial study of some novel 5 bromofluorobenzaldehydeoxime and semicarbazone under ultrasonic irradiation. Int. J. Adv. Chem. 2014, 2(1), 20-23.

[16]. H. Schiff. Ann. Chem. Pharm., Eine neue Reihe organischer Basen. 1864, 131, 118-119.

17. Wei, D.; Li, N.; Lu, G.; Yao, K. Synthesis, catalytic and biological activity of novel dinuclear copper complexwith Schiff base. Science in China B. 2006, 49(3), 225-229.

[18]. Khan, S.A.; Asiri, A.M.; Al-Amry, K.; Malik, M.A. Synthesis, Characterization, Electrochemical Studies, and In vitro Antibacterial Activity of Novel Thiosemicarbazone and Its Cu (II), Ni (II), and Co (II) Complexes. Hindawi Publishing Corporation Scientific World Journal, 2014, Article ID 592375:9

[19]. Mounika, K.; Anupama, B.; Pragathi, J.; Gyanakumari, C. Synthesis, characterization and biological activity of a Schiff base derived from 3-ethoxy salicylaldehyde and 2-amino benzoic acid and its transition metal complexes. J. Sci. Res. 2010, 2(3), 513-524.

[20]. Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, J. A. Jr, Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C., Iyengar, S. S., Tomasi, J., Cossi, M., Rega, N., Millam, J. M., Klene, M., Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, Ö., Foresman, J. B., Ortiz, J. V., Cioslowski, J. & Fox, D. J. (2009). *GAUSSIAN 09*. Gaussian Inc., Wallingford, CT, USA.