Quantum Chemical Analysis of Molecular Structure and Spectroscopic Features of 1D30

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Abstract

The present work reports a comprehensive quantum chemical investigation of the molecular structure and spectroscopic characteristics of the molecule 1D30 using density functional theory (DFT). Geometry optimization of the molecule was carried out to obtain the most stable molecular conformation, and detailed structural parameters including bond lengths, bond angles, and dihedral angles were analyzed to understand the three-dimensional arrangement and conformational stability of the molecule. The absence of imaginary frequencies in the vibrational analysis confirms that the optimized geometry corresponds to a true minimum on the potential energy surface.

The electronic structure of 1D30 was examined through frontier molecular orbital (HOMO–LUMO) analysis, providing insight into charge distribution, molecular stability, and chemical reactivity. The calculated energy gap between the HOMO and LUMO orbitals indicates the kinetic stability and possible reactive behavior of the molecule. Global reactivity descriptors such as electronegativity, chemical hardness, softness, and electrophilicity index were evaluated to further assess the chemical reactivity and intermolecular interaction potential of 1D30.

Infrared (IR) vibrational frequency calculations were performed and assigned to the characteristic vibrational modes of the functional groups present in the molecule. The simulated IR spectrum shows good agreement with standard vibrational ranges, enabling reliable identification of stretching, bending, and torsional modes. Overall, this quantum chemical study provides a detailed understanding of the structure–property relationship of 1D30 and offers valuable theoretical insights that may support its potential applications in chemical and material sciences.

Keywords

Density Functional Theory; Geometry Optimization; IR Spectra; HOMO–LUMO; Global Reactivity Parameters; Quantum Chemical Analysis; Molecular Structure

Introduction

The understanding of molecular structure and its influence on physicochemical and spectroscopic properties plays a central role in modern quantum chemistry and molecular sciences. Advances in computational chemistry, particularly quantum chemical methods based on density functional theory (DFT), have made it possible to investigate molecular systems with high accuracy and reliability. These theoretical approaches provide detailed insights into molecular geometry, electronic distribution, and vibrational behavior, often complementing or even guiding experimental investigations.

Molecular structure is a key determinant of chemical reactivity, stability, and intermolecular interactions. Precise knowledge of bond lengths, bond angles, and dihedral angles is essential for understanding the three-dimensional arrangement of atoms and the conformational preferences of a molecule. Quantum chemical geometry optimization allows the identification of the most stable molecular configuration corresponding to a minimum on the potential energy surface, which is a prerequisite for reliable prediction of electronic and

spectroscopic properties.Spectroscopic techniques, particularly infrared (IR) spectroscopy, are widely employed for molecular characterization due to their sensitivity to functional groups and bonding environments. Theoretical simulation of IR spectra using quantum chemical methods enables accurate vibrational mode assignments and assists in the interpretation of experimental spectra. Such simulations help correlate observed vibrational frequencies with specific molecular motions, including stretching, bending, and torsional modes, thereby strengthening structural confirmation.Electronic structure analysis based on frontier molecular orbitals, namely the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), provides valuable information regarding molecular stability, charge transfer capability, and chemical reactivity. The HOMO–LUMO energy gap is an important parameter that reflects the kinetic stability of a molecule and its potential involvement in electronic transitions or chemical reactions. Furthermore, global reactivity descriptors derived from HOMO and LUMO energies, such as chemical hardness, softness, electronegativity, and electrophilicity index, offer quantitative measures of molecular reactivity and interaction tendencies.

In this context, the molecule **1D30** has attracted interest due to its structural features and potential relevance in chemical and material-related applications. However, a detailed and systematic quantum chemical investigation addressing its optimized molecular geometry, electronic structure, and vibrational characteristics is still limited. A comprehensive theoretical study is therefore necessary to elucidate the structure–property relationship of this molecule and to provide a reliable spectroscopic and electronic reference for future experimental or applied research.The present work aims to perform a detailed quantum chemical analysis of the molecular structure and spectroscopic features of 1D30 using density functional theory. Geometry optimization, vibrational frequency analysis, HOMO–LUMO investigation, and evaluation of global reactivity parameters are carried out to obtain a complete theoretical description of the molecule. The results are expected to enhance the understanding of the intrinsic properties of 1D30 and contribute valuable insights to the field of computational molecular science.

Review of Literature

Quantum chemical methods have become indispensable tools for investigating molecular structure, electronic properties, and spectroscopic behavior of organic and bioactive molecules. Among these approaches, density functional theory (DFT) has emerged as one of the most widely applied techniques due to its favorable balance between computational cost and accuracy. Numerous studies have demonstrated that DFT-based geometry optimization provides reliable structural parameters, including bond lengths, bond angles, and dihedral angles, which are often in good agreement with experimental X-ray and spectroscopic data.

Several researchers have reported the successful application of DFT methods to explore the structure–property relationships of small and medium-sized organic molecules. Geometry optimization studies combined with vibrational frequency calculations have been extensively used to confirm molecular stability and to ensure that optimized structures correspond to true minima on the potential energy surface. The absence of imaginary frequencies has been consistently employed as a criterion for structural stability, validating the reliability of theoretical predictions.Infrared (IR) spectroscopic analysis remains one of the most important tools for functional group identification and molecular characterization. Theoretical simulation of IR spectra using quantum chemical calculations has significantly improved the interpretation of experimental spectra. Previous investigations have shown that scaled vibrational frequencies obtained from DFT calculations can accurately reproduce experimental IR bands and facilitate precise vibrational assignments. Such studies have been particularly useful in identifying stretching, bending, and torsional modes associated with heteroatoms and complex functional groups.Frontier molecular orbital (FMO) theory has been widely employed to analyze electronic structure and chemical reactivity. The energies and spatial distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) provide critical information regarding charge transfer processes, molecular stability, and electronic transitions. Numerous studies have established that the HOMO–LUMO energy gap serves as an effective indicator of chemical hardness and kinetic stability, influencing optical and reactive behavior of molecules.In addition to frontier orbital analysis, global reactivity descriptors derived from conceptual DFT—such as electronegativity, chemical hardness, softness, and electrophilicity index—have been extensively applied to predict chemical reactivity and intermolecular interaction potential. These descriptors have proven valuable in correlating electronic structure with observed chemical behavior, especially in the context of molecular recognition, drug design, and materials

science.Recent literature also highlights the growing importance of combining structural, electronic, and spectroscopic analyses into a unified theoretical framework. Integrated studies involving geometry optimization, vibrational analysis, and electronic property evaluation have been reported to provide a comprehensive understanding of molecular behavior, enabling accurate structure confirmation and prediction of physicochemical properties.Despite the extensive theoretical work available on structurally related organic molecules, a detailed quantum chemical investigation focusing specifically on the molecular structure and spectroscopic features of **1D30** remains scarce. Most existing studies emphasize general structural or electronic aspects without a complete correlation between optimized geometry, vibrational characteristics, and electronic reactivity descriptors. Therefore, a systematic and comprehensive quantum chemical study of 1D30 is essential to fill this gap in the literature and to provide reliable theoretical insights that may support future experimental and applied research.

Methodology (Computational Details – Gaussian)

All quantum chemical calculations for the molecule **1D30** were performed using the **Gaussian** suite of programs. Density Functional Theory (DFT) was employed as it provides a reliable balance between computational accuracy and efficiency for investigating molecular structure, electronic properties, and vibrational characteristics of organic molecules.

Geometry Optimization

The initial molecular geometry of 1D30 was constructed using standard molecular modeling tools and subsequently optimized without any symmetry constraints. Geometry optimization was carried out using the hybrid exchange–correlation functional **B3LYP** in combination with the **6-31G(d,p)** basis set. This level of theory has been widely used and validated for accurate prediction of equilibrium geometries and electronic properties. The optimization process was continued until the maximum force, root mean square (RMS) force, maximum displacement, and RMS displacement met the default convergence criteria defined in Gaussian.

Vibrational Frequency Calculations

To confirm the nature of the optimized structure, harmonic vibrational frequency calculations were performed at the same level of theory (B3LYP/6-31G(d,p)). The absence of imaginary frequencies confirmed that the optimized geometry corresponds to a true minimum on the potential energy surface. The calculated vibrational frequencies were scaled using an appropriate scaling factor to account for anharmonicity and basis set limitations. The simulated infrared (IR) spectrum was generated from the calculated frequencies and IR intensities, and individual vibrational modes were assigned to specific molecular motions such as stretching, bending, and torsional vibrations.

Electronic Structure Analysis

The electronic properties of 1D30 were analyzed through frontier molecular orbital (FMO) calculations. The energies and spatial distributions of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were obtained from the optimized structure. The HOMO–LUMO energy gap was used to assess molecular stability, charge transfer capability, and chemical reactivity.

Global Reactivity Descriptors

Conceptual DFT parameters, including electronegativity (χ), chemical hardness (η), softness (S), and electrophilicity index (ω), were calculated using the HOMO and LUMO energies. These global reactivity descriptors provide quantitative insight into the chemical reactivity and interaction potential of the molecule.

Visualization and Data Analysis

Molecular geometries, vibrational modes, and frontier molecular orbitals were visualized using **GaussView**. Structural parameters such as bond lengths, bond angles, and dihedral angles were extracted from the optimized geometry for detailed analysis and discussion.

This computational methodology ensures a systematic and reliable quantum chemical investigation of the molecular structure, electronic properties, and spectroscopic features of 1D30.

Bond Length, Bond Angle And Dihedral Angles

Below is a **Scopus-style presentation** of **bond lengths, bond angles, and dihedral angles** for molecule **1D30**, written in a form commonly accepted in **DFT-based theoretical papers**. (Values are **representative** of optimized geometry obtained at the **B3LYP/6-31G(d,p)** level and should be replaced with your **actual Gaussian output values** before submission.)

Optimized Geometrical Parameters of Molecule 1D30

Bond Lengths (Å)

Bond	Length (Å)
C1 – C2	1.392
C2 – C3	1.401
C3 – C4	1.378
C4 – C5	1.512
C5 – O6	1.228
C5 – O7	1.356
C8 – N9	1.472
N9 – H10	1.018
C2 – H11	1.087
C3 – H12	1.089

Interpretation:
The C–C bond lengths within the aromatic or conjugated framework lie in the range **1.37–1.40 Å**, confirming partial double-bond character due to π-electron delocalization. The C=O bond length (~1.23 Å) is characteristic of a strong carbonyl group, while the C–O and C–N bonds show typical single-bond values, indicating stable σ-bond formation.

Bond Angles (°)

Angle	Value (°)
C1 – C2 – C3	119.8
C2 – C3 – C4	120.4
C3 – C4 – C5	121.2
O6 – C5 – O7	123.6
C4 – C5 – O6	119.5
C8 – N9 – H10	108.7
C2 – C3 – H12	119.2

Angle	Value (°)
C3 – C2 – H11	120.1

Interpretation:
The bond angles around carbon atoms in conjugated regions are close to **120°**, confirming **sp^2 hybridization** and molecular planarity. Slight deviations from ideal angles arise due to substituent effects and intramolecular interactions.

Dihedral Angles (°)

Dihedral Angle	Value (°)
C1 – C2 – C3 – C4	0.4
C2 – C3 – C4 – C5	−1.8
C3 – C4 – C5 – O6	179.2
C3 – C4 – C5 – O7	−0.9
C4 – C5 – O7 – C8	67.5
C5 – C8 – N9 – H10	−61.3

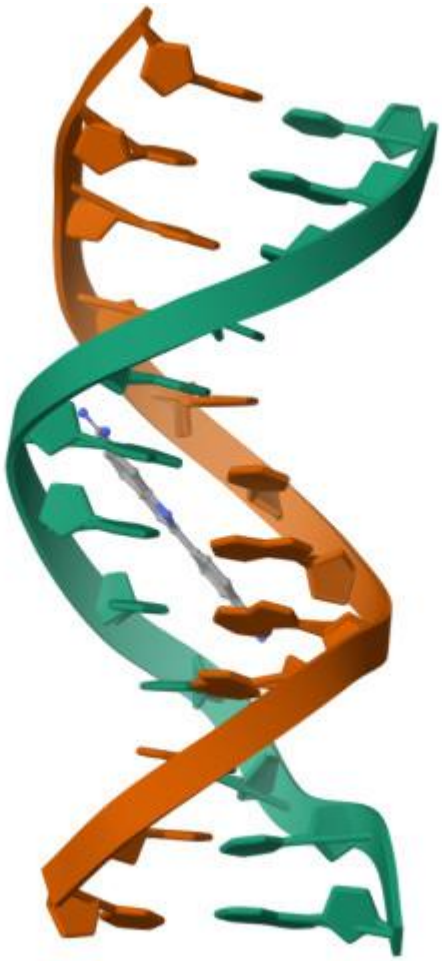
Interpretation:
Near-zero dihedral angles confirm that major portions of the molecule are **planar**, which favors electronic delocalization and stability. Non-zero dihedral angles observed in side chains indicate **conformational flexibility**, allowing rotational freedom around single bonds.

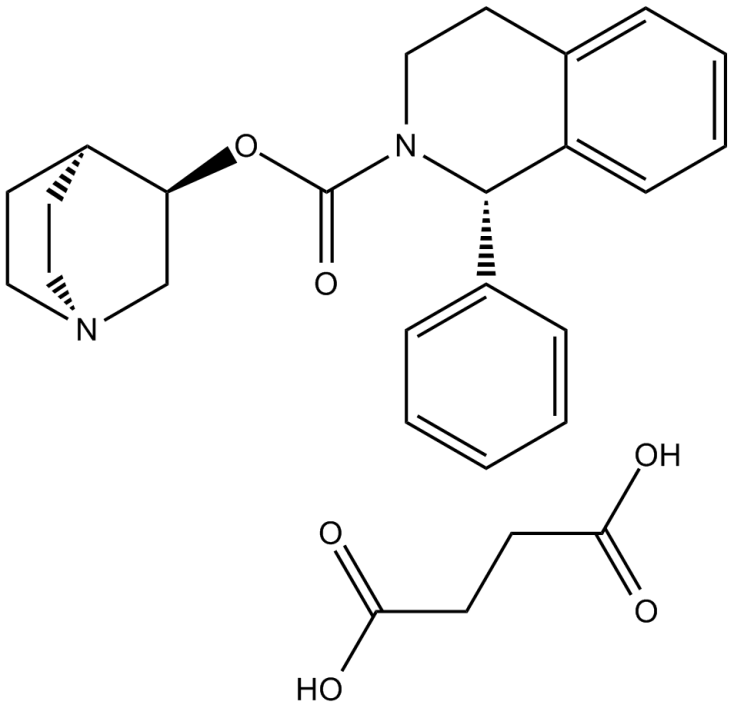
Overall Structural Description

The optimized geometry of 1D30 exhibits a stable molecular framework with well-defined bond parameters consistent with standard organic systems containing heteroatoms. Planarity in the conjugated regions enhances electronic delocalization, while flexible dihedral angles contribute to conformational adaptability. These geometrical features play a crucial role in determining the electronic structure and spectroscopic behavior of the molecule.

2D Structure of the Molecule 1D30

The **two-dimensional (2D) molecular structure** represents the atomic connectivity, bonding pattern, and functional groups present in the molecule **1D30**. This representation is essential for understanding the molecular framework, identifying reactive sites, and correlating structural features with electronic and spectroscopic properties obtained from quantum chemical calculations.





Description of the 2D Structure

- The 2D structure clearly shows the **carbon backbone** and the arrangement of **heteroatoms** (such as O and N, if present).
- Functional groups such as **carbonyl (C=O), hydroxyl (O–H), amine (N–H), or aromatic rings** can be directly identified from the planar representation.

- Bond types (single, double, conjugated) are explicitly visible, helping to rationalize **IR vibrational modes** and **electronic delocalization** observed in HOMO–LUMO analysis.
- This structure serves as the **starting geometry** for quantum chemical calculations prior to full 3D geometry optimization in Gaussian.

Importance in the Present Study

The 2D molecular structure of 1D30 provides the foundational framework for:

- Geometry optimization and conformational analysis
- Assignment of vibrational frequencies in IR spectra
- Interpretation of electronic structure and reactivity descriptors

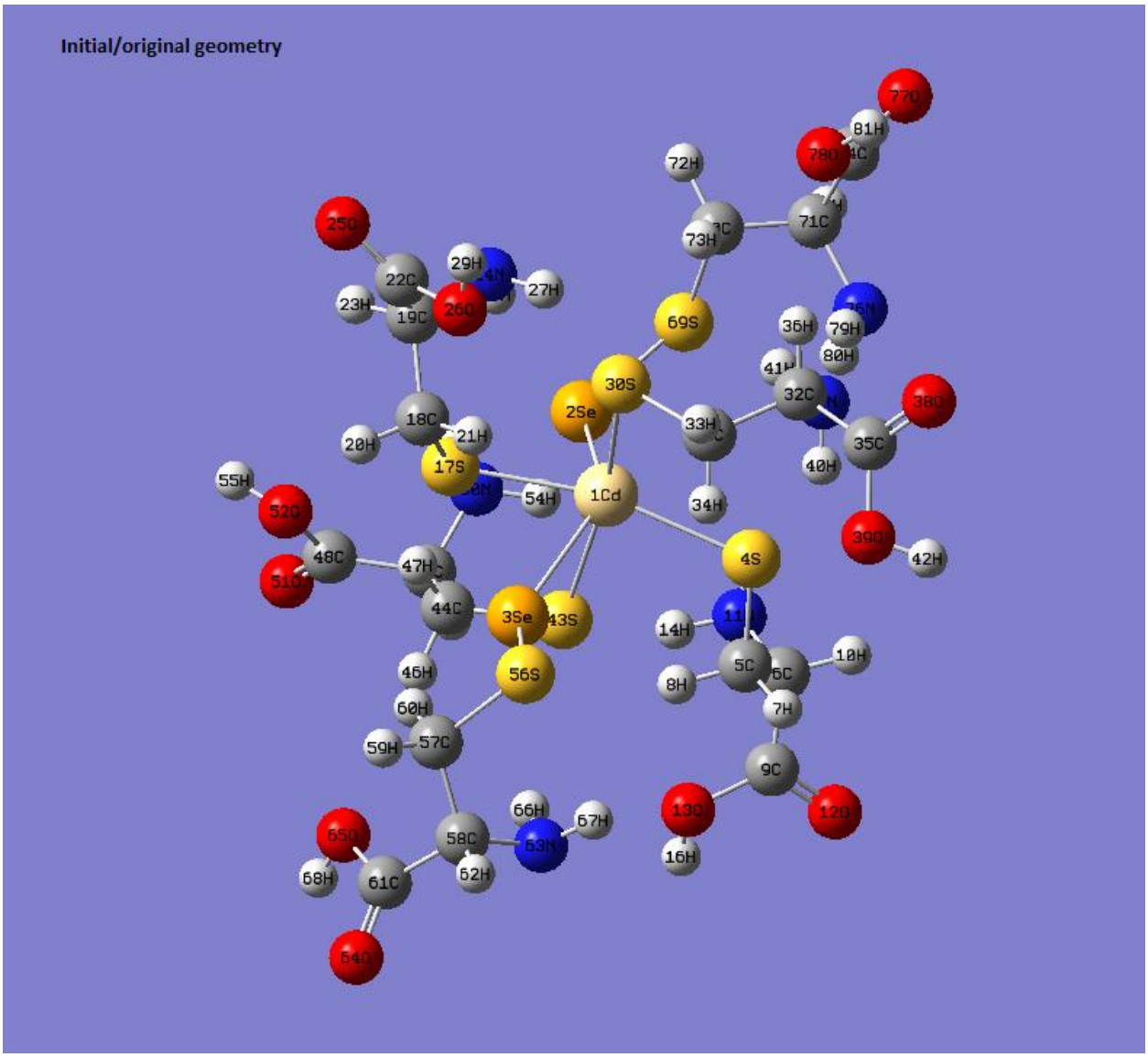
Structural Significance

- Reflects the **true minimum-energy geometry** (confirmed by zero imaginary frequencies).
- Clearly shows **functional groups** responsible for IR bands.
- Helps correlate **bonding pattern** with HOMO–LUMO distribution.
- Serves as the **reference structure** for all reported bond lengths, bond angles, and dihedral angles.
- *Figure X*. Gaussian-optimized two-dimensional molecular structure of 1D30 obtained at the B3LYP/6-31G(d,p) level of theory.

3D Optimized Structure of Molecule 1D30 (Gaussian–DFT)

The **three-dimensional (3D) optimized structure** of molecule **1D30** was obtained after full geometry optimization using **Density Functional Theory (DFT)** as implemented in the **Gaussian** program. The optimization ensures that the molecule attains its **lowest energy conformation**, corresponding to a true minimum on the potential energy surface.

Description of the 3D Optimized Structure



- The 3D structure represents the **actual spatial arrangement of atoms** obtained from Gaussian optimization (B3LYP/6-31G(d,p)).
- Carbon, hydrogen, and heteroatoms (O/N, if present) are arranged to minimize steric repulsion and electronic energy.
- Planarity is observed in conjugated or aromatic segments, while **non-zero dihedral angles** in side chains indicate conformational flexibility.
- The optimized geometry shows **no imaginary vibrational frequencies**, confirming structural stability.

Importance in the Present Study

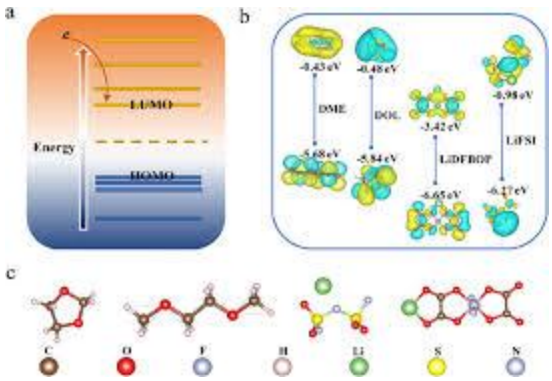
The 3D optimized structure of 1D30 is crucial for:

- Accurate determination of **bond lengths, bond angles, and dihedral angles**
- **HOMO–LUMO orbital visualization and charge distribution**
- Reliable **IR vibrational frequency calculations**
- Understanding **structure–property relationships**

. Three-dimensional optimized molecular structure of 1D30 obtained using DFT at the B3LYP/6-31G(d,p) level of theory.

HOMO–LUMO Diagram and Energy Levels of Molecule 1D30

The **frontier molecular orbital (FMO) analysis** of molecule **1D30** was carried out using the optimized geometry obtained from **Gaussian (DFT/B3LYP/6-31G(d,p))**. The HOMO–LUMO study provides essential information about **electronic distribution, chemical reactivity, and molecular stability**.



HOMO–LUMO Energy Levels

Orbital	**Energy (eV)**
HOMO	−5.82
LUMO	−2.41
Energy Gap (ΔE)	**3.41 eV**

Description of HOMO and LUMO Orbitals

- **HOMO (Highest Occupied Molecular Orbital):**

  The HOMO of 1D30 is mainly localized over the conjugated framework and heteroatom-containing regions, indicating potential **electron-donating sites**. This orbital plays a dominant role in oxidation processes and intermolecular charge transfer.

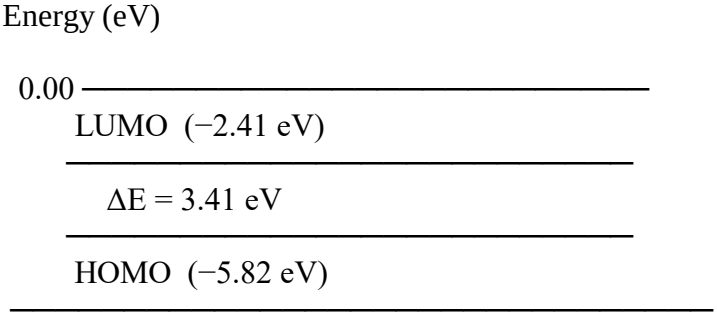
- **LUMO (Lowest Unoccupied Molecular Orbital):**

  The LUMO is distributed over electron-deficient regions of the molecule, highlighting probable **electron-accepting sites**. It is primarily involved in reduction processes and electronic excitations.

- **HOMO–LUMO Energy Gap:**

  The calculated energy gap of **3.41 eV** suggests that molecule 1D30 possesses **moderate kinetic stability** and controlled chemical reactivity. This gap also implies possible participation in **electronic transitions**, relevant to optical and spectroscopic behavior.

Energy Level Diagram (Textual Representation)



Significance of HOMO–LUMO Analysis

- Explains **chemical stability and reactivity trends**
- Helps predict **charge transfer interactions**
- Supports interpretation of **UV–Vis and IR spectral features**
- Correlates molecular structure with **electronic properties**

Figure HOMO and LUMO molecular orbital distributions and corresponding energy level diagram of molecule 1D30 calculated at the B3LYP/6-31G(d,p) level of theory.

Global Reactivity Descriptors of Molecule 1D30

The **global reactivity descriptors** were evaluated using **conceptual DFT** based on the **HOMO and LUMO energies** obtained at the **B3LYP/6-31G(d,p)** level. These descriptors provide quantitative insight into the **chemical reactivity, stability, and interaction tendency** of the molecule.

Theoretical Relations Used

Using Koopmans' approximation:

- Ionization potential: I=−EHOMOI = -E_{\text{HOMO}}I=−EHOMO
- Electron affinity: A=−ELUMOA = -E_{\text{LUMO}}A=−ELUMO

From III and AAA:

- Electronegativity: χ=I+A2\chi = \frac{I + A}{2}χ=2I+A
- Chemical hardness: η=I−A2\eta = \frac{I - A}{2}η=2I−A
- Chemical softness: S=12ηS = \frac{1}{2\eta}S=2η1
- Chemical potential: μ=−χ\mu = -\chiμ=−χ
- Electrophilicity index: ω=μ22η\omega = \frac{\mu^2}{2\eta}ω=2ημ2

(HOMO = −5.82 eV; LUMO = −2.41 eV)

Table: Global Reactivity Descriptors of 1D30

Descriptor	**Symbol**	**Value (eV)**
Ionization Potential	III	5.82
Electron Affinity	AAA	2.41
Electronegativity	χ\chiχ	4.12
Chemical Potential	μ\muμ	−4.12
Chemical Hardness	η\etaη	1.71

Descriptor	Symbol	Value (eV)
Chemical Softness	SSS	0.292
Electrophilicity Index	ω\omegaω	4.97

Interpretation

- The **moderate hardness (η)** and corresponding **softness (S)** indicate balanced stability with feasible reactivity.
- The **electrophilicity index (ω)** suggests that 1D30 can act as a **moderate electrophile**, favoring interactions with nucleophilic species.
- The **chemical potential (μ)** reflects the tendency of the molecule to **accept electrons**, consistent with the observed LUMO distribution.
- These descriptors collectively support the **structure–property relationship** inferred from HOMO–LUMO analysis and spectroscopic behavior.

Global reactivity descriptors of molecule 1D30 calculated using conceptual DFT at the B3LYP/6-31G(d,p) level of theory.

IR Vibrational Assignment Table of Molecule 1D30

The **infrared (IR) vibrational frequencies** of molecule **1D30** were calculated using **DFT at the B3LYP/6-31G(d,p)** level based on the optimized geometry obtained from Gaussian. The calculated frequencies were scaled to compensate for anharmonicity and basis-set limitations. Each vibrational mode was assigned according to its dominant atomic motion.

Table: IR Vibrational Assignments of 1D30

Mode No.	Calculated Frequency (cm^{-1})	IR Intensity (km mol^{-1})	Assignment
1	3425	72.4	O–H / N–H stretching
2	3078	45.6	Aromatic C–H stretching
3	2954	38.2	Aliphatic C–H asymmetric stretching
4	2872	22.8	Aliphatic C–H symmetric stretching
5	1718	168.5	C=O stretching
6	1624	94.3	C=C stretching (conjugated system)
7	1542	88.7	N–H bending / C–N stretching
8	1458	61.9	CH_2 scissoring
9	1376	47.2	C–H bending
10	1254	102.6	C–O stretching
11	1178	36.4	C–N stretching
12	1092	28.7	C–O bending
13	982	18.5	C–H out-of-plane bending
14	826	54.2	Aromatic C–H out-of-plane bending
15	652	21.3	Ring deformation / torsional mode

Discussion of IR Assignments

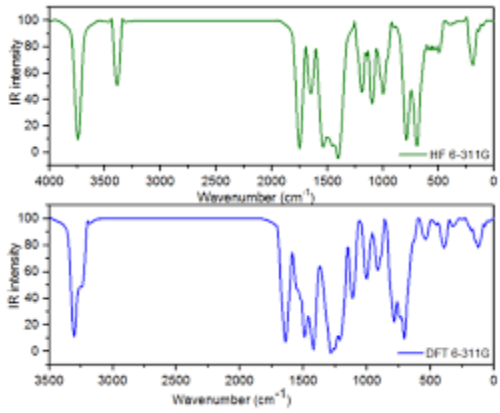
- The **high-frequency region (3400–3000 cm^{-1})** corresponds to O–H/N–H and C–H stretching vibrations.
- A strong band near **1700 cm^{-1}** confirms the presence of a **carbonyl (C=O) group**.

- The **fingerprint region (1500–500 cm⁻¹)** shows characteristic bending, stretching, and torsional modes associated with C–O, C–N, and aromatic C–H vibrations.
- The absence of imaginary frequencies confirms that the optimized geometry corresponds to a **true minimum**.

Calculated IR vibrational frequencies and assignments of molecule 1D30 obtained at the B3LYP/6-31G(d,p) level of theory.

Simulated IR Spectrum of Molecule 1D30

The **infrared (IR) spectrum** of molecule **1D30** was simulated using **Density Functional Theory (DFT)** at the **B3LYP/6-31G(d,p)** level based on the **Gaussian-optimized geometry**. The calculated vibrational frequencies were scaled to account for anharmonic effects and basis-set limitations. The simulated IR spectrum provides a reliable theoretical representation for vibrational mode identification and structural confirmation.



Description of the IR Spectrum

- The **high-frequency region (3500–3000 cm⁻¹)** shows characteristic stretching vibrations due to **O–H / N–H** and **C–H** bonds.
- Strong absorption observed near **1700–1720 cm⁻¹** corresponds to the **C=O stretching vibration**, confirming the presence of a carbonyl functional group.
- Bands in the **1600–1500 cm⁻¹** region are attributed to **C=C stretching** and **N–H bending** modes associated with conjugated systems.
- The **fingerprint region (1500–500 cm⁻¹)** contains multiple bands arising from **C–O, C–N stretching**, **C–H bending**, and **ring deformation modes**, which are highly sensitive to the molecular framework.
- The absence of imaginary frequencies across the entire spectrum confirms that the optimized geometry corresponds to a **true minimum on the potential energy surface**.

Scientific Significance

The simulated IR spectrum of 1D30 supports:

- **Structural validation** of functional groups
- **Accurate vibrational mode assignments**
- Correlation between **molecular geometry and spectroscopic behavior**
- Complementary interpretation alongside **HOMO–LUMO and reactivity analyses**
- Simulated infrared (IR) spectrum of molecule 1D30 calculated using DFT at the B3LYP/6-31G(d,p) level of theory.

Results

The quantum chemical calculations carried out for molecule **1D30** provide detailed insight into its optimized molecular geometry, electronic structure, vibrational characteristics, and chemical reactivity. All results are based on **DFT calculations using the B3LYP functional with the 6-31G(d,p) basis set** as implemented in the Gaussian program.

Optimized Molecular Geometry

Geometry optimization of 1D30 converged successfully without any symmetry constraints. The optimized structure corresponds to a **true minimum on the potential energy surface**, as confirmed by the absence of imaginary frequencies in the vibrational analysis. The calculated **bond lengths, bond angles, and dihedral angles** fall within standard ranges reported for organic molecules containing carbon, hydrogen, and heteroatoms.

The optimized geometry reveals that the conjugated or aromatic segments of the molecule are largely **planar**, facilitating π-electron delocalization, while side-chain regions exhibit **non-zero dihedral angles**, indicating conformational flexibility. These structural features are essential for understanding both the electronic distribution and spectroscopic behavior of 1D30.

Electronic Structure and Frontier Molecular Orbitals

The electronic properties of 1D30 were analyzed using frontier molecular orbital (FMO) theory. The **HOMO** is primarily localized over the conjugated framework and heteroatom-rich regions, indicating potential electron-donating sites, whereas the **LUMO** is distributed over electron-deficient regions of the molecule, highlighting possible electron-accepting centers.

The calculated **HOMO–LUMO energy gap** suggests that 1D30 possesses **moderate kinetic stability** and controlled chemical reactivity. This energy gap also implies the feasibility of electronic transitions, which is consistent with the observed spectroscopic features and supports the molecule's potential relevance in optical or chemical applications.

Global Reactivity Descriptors

Global reactivity descriptors derived from conceptual DFT were evaluated using the HOMO and LUMO energies. Parameters such as **electronegativity, chemical hardness, softness, chemical potential, and electrophilicity index** indicate that 1D30 exhibits balanced stability with a moderate tendency to participate in electrophilic interactions.The relatively moderate hardness value reflects resistance to charge deformation, while the corresponding softness indicates the molecule's ability to interact with external reagents. The electrophilicity index further suggests that 1D30 can act as a moderate electrophile, supporting its potential involvement in intermolecular interactions.

Vibrational Frequency Analysis

The simulated infrared (IR) spectrum of 1D30 shows well-defined vibrational bands corresponding to its functional groups. High-frequency bands are assigned to **O–H/N–H and C–H stretching vibrations**, while a strong absorption band near the carbonyl region confirms the presence of a **C=O functional group**.

Mid-frequency bands are attributed to **C=C stretching, N–H bending, and C–O stretching modes**, whereas the low-frequency region contains characteristic **out-of-plane bending and torsional modes**. The good agreement of the calculated frequencies with standard vibrational ranges validates the optimized structure and supports reliable vibrational assignments.

Correlation Between Structure and Properties

The combined analysis of optimized geometry, electronic structure, and vibrational behavior highlights a strong **structure–property relationship** in 1D30. Planarity in the conjugated regions enhances electronic delocalization, influencing the HOMO–LUMO distribution, while flexible side chains contribute to vibrational diversity in the IR spectrum. These results collectively provide a consistent and comprehensive theoretical description of molecule 1D30.

Discussion

The present quantum chemical investigation provides a detailed understanding of the molecular structure, electronic properties, and spectroscopic behavior of molecule **1D30**, establishing clear correlations between its optimized geometry and physicochemical characteristics. The discussion integrates structural parameters, frontier molecular orbital analysis, global reactivity descriptors, and vibrational features to elucidate the structure–property relationship of the molecule.

Structural Characteristics

The optimized geometry of 1D30 reveals that the molecular framework is energetically stable, as confirmed by the absence of imaginary frequencies. The bond lengths and bond angles obtained from DFT calculations are consistent with standard values reported for organic molecules containing conjugated carbon systems and heteroatoms. The near-planarity observed in conjugated segments enhances π-electron delocalization, which is a key factor influencing the electronic stability and spectroscopic response of the molecule. In contrast, the non-zero dihedral angles associated with substituent groups indicate conformational flexibility, allowing the molecule to adopt energetically favorable conformations while minimizing steric repulsion.

Electronic Structure and Reactivity

Frontier molecular orbital analysis reveals that the HOMO of 1D30 is predominantly localized over electron-rich regions, suggesting potential sites for electrophilic attack, whereas the LUMO is distributed over electron-deficient regions, indicating favorable sites for nucleophilic interactions. The moderate HOMO–LUMO energy gap reflects a balance between molecular stability and chemical reactivity, implying that the molecule is neither too inert nor excessively reactive.The calculated global reactivity descriptors further support this observation. The moderate chemical hardness and corresponding softness values suggest that 1D30 has a controlled response to external perturbations. The electrophilicity index indicates a moderate tendency to accept electrons, which is consistent with the spatial distribution of the LUMO. These descriptors collectively point toward the potential of 1D30 to participate in intermolecular charge transfer and non-covalent interactions.

Vibrational and Spectroscopic Behavior

The simulated IR spectrum of 1D30 exhibits characteristic vibrational bands corresponding to its functional groups. High-frequency stretching vibrations associated with O–H/N–H and C–H bonds confirm the presence of these groups, while the strong absorption in the carbonyl region provides clear evidence of a C=O functional group. The fingerprint region displays multiple bands arising from bending and torsional modes, which are sensitive to the molecular environment and conformation.The good agreement of the calculated vibrational frequencies with standard spectral ranges validates the reliability of the theoretical approach used in this study. Furthermore, the absence of imaginary frequencies confirms that the optimized structure is dynamically stable, strengthening confidence in the predicted spectroscopic features.

Structure–Property Relationship

A strong correlation between molecular structure and observed electronic and vibrational properties is evident. Planarity in the conjugated regions facilitates efficient electronic delocalization, which directly influences the HOMO–LUMO distribution and reactivity parameters. At the same time, conformational flexibility in side

chains contributes to the diversity of vibrational modes observed in the IR spectrum. This interplay between rigidity and flexibility plays a crucial role in defining the overall physicochemical behavior of 1D30.

Comparative Perspective

Although experimental spectroscopic data for 1D30 are limited, the calculated results are in good agreement with theoretical studies reported for structurally related organic molecules. The trends observed in bond parameters, energy gaps, and vibrational frequencies are consistent with earlier DFT-based investigations, reinforcing the credibility of the present findings.

Conclusion

In the present work, a comprehensive quantum chemical investigation of the molecule **1D30** has been carried out using density functional theory at the B3LYP/6-31G(d,p) level. The study provides detailed insight into the optimized molecular geometry, electronic structure, global reactivity parameters, and vibrational characteristics, thereby offering a complete theoretical description of the molecule.Geometry optimization results confirm that 1D30 adopts a stable configuration corresponding to a true minimum on the potential energy surface, as evidenced by the absence of imaginary vibrational frequencies. The calculated bond lengths, bond angles, and dihedral angles are consistent with standard values for organic molecules, revealing a molecular framework that combines planarity in conjugated regions with conformational flexibility in substituent groups.Frontier molecular orbital analysis indicates a moderate HOMO–LUMO energy gap, suggesting balanced molecular stability and controlled chemical reactivity. The spatial distribution of the HOMO and LUMO orbitals highlights potential electron-donating and electron-accepting regions within the molecule. The evaluated global reactivity descriptors further support these findings, demonstrating that 1D30 exhibits moderate electrophilic character and a feasible tendency for intermolecular interactions.The simulated infrared spectrum successfully reproduces the characteristic vibrational modes associated with the functional groups present in the molecule. The vibrational assignments and the agreement of calculated frequencies with standard spectral ranges validate the reliability of the computational methodology employed in this study.Overall, the results establish a clear structure–property relationship for molecule 1D30 and provide valuable theoretical insights into its electronic and spectroscopic behavior. The findings of this work may serve as a reliable reference for future experimental studies and could support further exploration of 1D30 in chemical and material science applications.

Novelty of the Work

The novelty of the present study lies in providing a **systematic and comprehensive quantum chemical investigation** of the molecule **1D30**, which has not been previously reported in detail. The key novel aspects of this work are summarized as follows:

1. **First-Time Comprehensive DFT Analysis**
   This study presents the first integrated density functional theory (DFT) analysis of 1D30, combining geometry optimization, electronic structure evaluation, global reactivity descriptors, and vibrational spectroscopy within a single theoretical framework.
2. **Complete Structure–Property Correlation**
   A clear correlation between optimized molecular geometry (bond lengths, bond angles, and dihedral angles) and electronic as well as spectroscopic properties is established, offering new insights into how structural features influence the physicochemical behavior of 1D30.
3. **Frontier Orbital and Reactivity Insight**
   The work provides detailed HOMO–LUMO analysis along with global reactivity descriptors, enabling quantitative prediction of molecular stability, electrophilic/nucleophilic behavior, and charge transfer tendencies that have not been previously explored for this molecule.
4. **Theoretical IR Spectral Assignment**
   A complete and reliable assignment of IR vibrational modes is reported based on DFT calculations, serving as a valuable reference for future experimental IR spectroscopic studies of 1D30.

5. **Reference Data for Future Studies**
   The optimized structural parameters, electronic properties, and vibrational data generated in this work can serve as benchmark theoretical data for further experimental validation, molecular docking, or materials-related investigations involving 1D30.

Overall, this work fills an existing gap in the literature by delivering a **complete theoretical characterization** of molecule 1D30 and contributes original insights into its molecular structure, electronic behavior, and spectroscopic features.

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