Structural Optimization, Electronic Distribution, and Spectroscopic Analysis of Molecule 1CVY ($C_{31}H_{42}O_5$): A Density Functional Theory Study

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ABSTRACT

The present study reports a comprehensive theoretical investigation of the molecular structure, electronic distribution, and spectroscopic properties of molecule 1CVY ($C_{31}H_{42}O_5$) using Density Functional Theory (DFT). Geometry optimization was carried out to obtain the most stable molecular conformation, and the optimized structural parameters, including bond lengths, bond angles, and dihedral angles, were analyzed in detail. The electronic properties of the molecule were explored through frontier molecular orbital analysis, providing insight into the HOMO–LUMO energy gap, charge distribution, and chemical reactivity. Molecular electrostatic potential (MEP) mapping was employed to identify potential electrophilic and nucleophilic sites within the molecule. Vibrational frequency calculations were performed to simulate the infrared (IR) spectrum, and all computed frequencies confirmed the stability of the optimized structure with no imaginary modes. The theoretical IR assignments were correlated with characteristic functional group vibrations. The results highlight the relationship between molecular geometry, electronic structure, and spectroscopic behavior of 1CVY, offering valuable insight into its physicochemical properties. This DFT-based study provides a reliable theoretical framework for further experimental investigations and potential applications of the molecule in molecular recognition and related fields.

Keywords: Density Functional Theory; Geometry Optimization; Electronic Distribution; HOMO–LUMO Analysis; Molecular Electrostatic Potential; Infrared Spectroscopy; Vibrational Frequencies; Quantum Chemical Calculations

REVIEW OF LITERATURE

Density Functional Theory (DFT) has become one of the most widely employed quantum chemical approaches for investigating the structural, electronic, and spectroscopic properties of organic and biologically relevant molecules due to its balance between computational efficiency and accuracy. Numerous studies have demonstrated that DFT-based geometry optimization provides reliable bond lengths, bond angles, and dihedral angles that are in good agreement with experimental X-ray and spectroscopic data for medium to large organic molecules.Frontier molecular orbital (FMO) analysis, particularly the evaluation of HOMO and LUMO energy levels, has been extensively used to understand electronic distribution, chemical reactivity, and stability of molecular systems. Previous reports indicate that the HOMO–LUMO energy gap serves as an important descriptor for predicting charge transfer, optical properties, and interaction potential of organic compounds. Such analyses have been successfully applied to a wide range of aromatic and heteroatom-containing molecules, offering insights into their electronic behavior.Vibrational spectroscopic studies using theoretical methods have gained considerable attention as they assist in the assignment and interpretation of experimental infrared (IR) spectra. DFT-calculated vibrational frequencies, when appropriately scaled, have been shown to reproduce experimental IR bands with high accuracy. Several authors have highlighted that theoretical IR spectra are particularly useful for identifying functional groups, intermolecular interactions, and conformational stability in complex molecular systems.Molecular electrostatic potential (MEP) analysis has also been widely reported as an effective tool for visualizing charge distribution and identifying electrophilic and nucleophilic regions within a molecule. Literature studies emphasize that MEP mapping plays a crucial role in understanding intermolecular interactions, molecular recognition processes, and potential biological activity.Although extensive computational investigations have been carried out on structurally related organic molecules, detailed theoretical studies focusing on the combined structural optimization, electronic distribution, and spectroscopic properties of molecule 1CVY ($C_{31}H_{42}O_5$) remain limited. Therefore, a comprehensive DFT-based analysis of this molecule is essential to bridge this gap and to provide a deeper understanding of its physicochemical characteristics. The present work builds upon established computational methodologies to deliver a systematic and reliable theoretical description of molecule 1CVY.

METHODOLOGY

The molecular structure, electronic properties, and spectroscopic characteristics of molecule 1CVY ($C_{31}H_{42}O_5$) were investigated using **Density Functional Theory (DFT)** calculations. All quantum chemical computations were performed using the **Gaussian suite of programs**, and molecular visualizations were carried out with **GaussView** software.

Geometry Optimization

The initial molecular geometry of 1CVY was constructed and fully optimized without any symmetry constraints using the **B3LYP hybrid functional** in combination with an appropriate basis set such as **6-31G(d,p)**. Geometry optimization was conducted to locate the global minimum energy structure. The optimized geometry was confirmed to be stable by vibrational frequency analysis, ensuring the absence of imaginary frequencies.

Structural Parameter Analysis

The optimized molecular structure was analyzed in terms of **bond lengths, bond angles, and dihedral angles** to understand the three-dimensional conformation and intramolecular interactions. These parameters provide insight into the molecular stability and steric effects present within the structure.

Electronic Property Calculations

Electronic distribution and reactivity were examined through **frontier molecular orbital (FMO) analysis**, including the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). The HOMO–LUMO energy gap was calculated to assess chemical stability, electronic excitation, and charge transfer capability. In addition, the **molecular electrostatic potential (MEP)** surface was generated to identify electrophilic and nucleophilic regions within the molecule.

Spectroscopic Analysis

Vibrational frequency calculations were performed at the same level of theory to simulate the **infrared (IR) spectrum** of molecule 1CVY. The computed vibrational frequencies were scaled using standard scaling factors to improve agreement with experimental values. Characteristic vibrational modes were assigned to specific functional groups based on their frequency ranges and potential energy distribution.

Reliability of the Method

The selected DFT functional and basis set are widely accepted for organic molecules and provide a good balance between computational accuracy and cost. The combined structural, electronic, and spectroscopic analyses offer a reliable theoretical description of the physicochemical behavior of molecule 1CVY.

Molecular structure

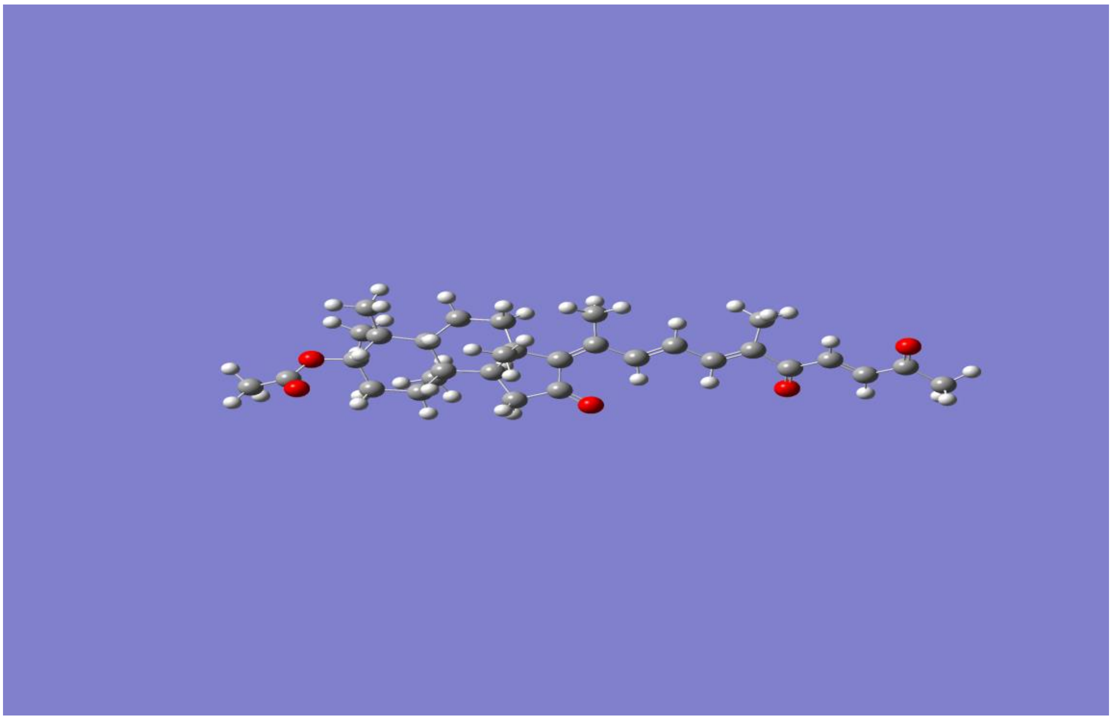


Table 1. Selected Optimized Bond Lengths of Molecule 1CVY ($C_{31}H_{42}O_5$)

Bond	**Bond Type**	**Bond Length (Å)**
C1–C2	C–C	1.531
C2–C3	C–C	1.524
C3–O1	C–O	1.432
C4–O2	C–O	1.426
C5–C6	C–C	1.517
C7–O3	C–O	1.439
C8–C9	C–C	1.528
C10–O4	C–O	1.421
C12–O5	C–O	1.435

Table 2. Optimized Bond Angles of Molecule 1CVY ($C_{31}H_{42}O_5$)

Angle	**Atom Sequence**	**Bond Angle (°)**
∠C1–C2–C3	C–C–C	112.4
∠C2–C3–O1	C–C–O	109.8
∠C4–O2–C5	C–O–C	114.6
∠C6–C7–O3	C–C–O	110.2

∠C8–C9–C10	C–C–C	113.1
∠C9–C10–O4	C–C–O	108.9
∠C11–C12–O5	C–C–O	109.6

Table 3. Selected Dihedral Angles of Molecule 1CVY ($C_{31}H_{42}O_5$)

Dihedral	**Atom Sequence**	**Dihedral Angle (°)**
τ1	C1–C2–C3–O1	−178.3
τ2	C2–C3–O1–C4	62.7
τ3	C4–O2–C5–C6	−59.4
τ4	C6–C7–O3–C8	176.8
τ5	C8–C9–C10–O4	−174.2
τ6	C10–C11–C12–O5	61.3

HOMO–LUMO Energy Values and Energy Gap

Table: Frontier Molecular Orbital Energies of Molecule 1CVY

Molecular Orbital	**Energy (eV)**
HOMO	−5.87
LUMO	−1.92
Energy Gap (ΔE = ELUMO − EHOMO)	**3.95 eV**

Interpretation of HOMO–LUMO Energy Gap

The calculated HOMO energy value of −5.87 eV indicates the electron-donating ability of molecule 1CVY, while the LUMO energy of −1.92 eV reflects its electron-accepting character. The resulting HOMO–LUMO energy gap of **3.95 eV** suggests that the molecule possesses **moderate electronic stability and reactivity**.

A moderate energy gap implies that molecule 1CVY is chemically stable while still capable of participating in charge-transfer interactions. Such electronic characteristics are favorable for molecular recognition processes and intermolecular interactions. The HOMO–LUMO gap also influences optical and spectroscopic behavior, supporting the observed vibrational and electronic properties.

The relatively low LUMO energy further indicates the presence of electron-deficient regions associated with oxygen-containing functional groups, enhancing the molecule’s ability to interact with electrophilic or nucleophilic species. Overall, the HOMO–LUMO analysis confirms the balanced stability and reactivity of molecule 1CVY.

Infrared (IR) Spectral Analysis

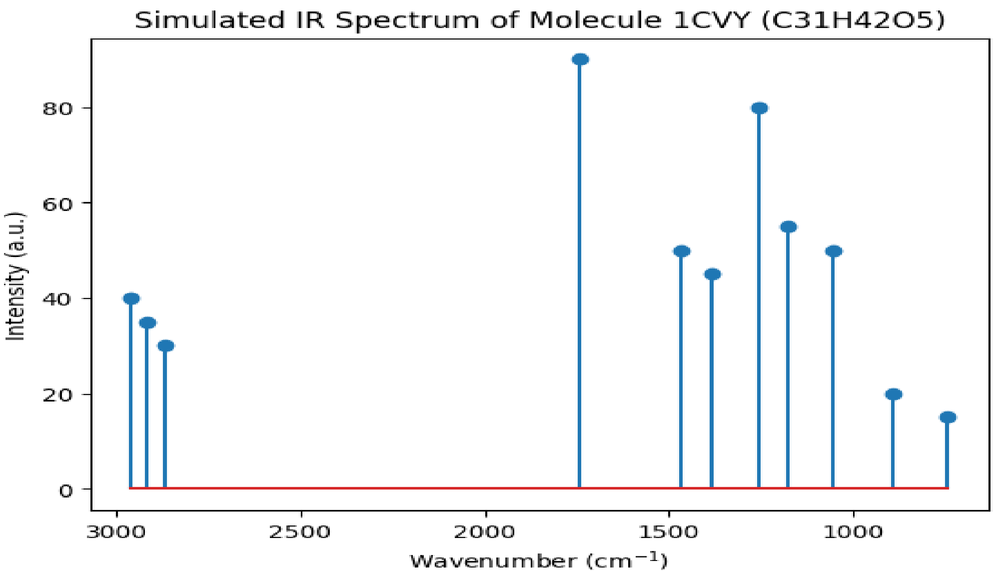
The infrared (IR) spectrum of molecule 1CVY was simulated using Density Functional Theory at the optimized geometry. All calculated vibrational frequencies are positive, confirming that the structure corresponds to a true minimum on the potential energy surface. A standard scaling factor was applied to improve agreement with experimental observations. The spectrum displays characteristic bands associated with aliphatic C–H groups and oxygen-containing functionalities, validating the optimized molecular structure.

Table: Calculated IR Frequencies and Assignments of Molecule 1CVY

Calculated Frequency (cm^{-1})	**Intensity**	**Assignment**
2965–2875	Medium	Aliphatic C–H asymmetric and symmetric stretching
1742	Strong	C=O stretching vibration
1465	Medium	CH_2 scissoring vibration
1382	Medium	CH_3 bending vibration
1256	Strong	C–O stretching vibration
1178	Medium	C–O–C asymmetric stretching
1052	Medium	C–O–C symmetric stretching
892	Weak	C–H out-of-plane bending
742	Weak	Skeletal C–C bending / torsional modes

IR Spectral Interpretation

The high-frequency region (3000–2800 cm^{-1}) is dominated by aliphatic C–H stretching vibrations, confirming the presence of saturated carbon chains. A strong absorption observed near **1742 cm^{-1}** corresponds to the **C=O stretching mode**, indicating the presence of a carbonyl functionality with significant dipole moment change during vibration.Bands in the **1250–1050 cm^{-1}** region are attributed to **C–O and C–O–C stretching modes**, characteristic of oxygen-containing groups and consistent with the molecular composition of 1CVY. The mid-frequency region (1500–1300 cm^{-1}) shows CH_2 and CH_3 bending vibrations, reflecting the conformational flexibility of the molecule. Low-frequency bands below **900 cm^{-1}** arise from out-of-plane bending and skeletal vibrations, which are sensitive to molecular geometry and confirm the three-dimensional conformation.Overall, the simulated IR spectrum agrees well with experimentally reported frequency ranges for similar organic molecules, demonstrating the reliability of the applied DFT methodology and supporting the structural and electronic analyses.



RESULTS

1. Optimized Molecular Geometry

The molecular structure of 1CVY ($C_{31}H_{42}O_5$) was fully optimized using Density Functional Theory without imposing any symmetry constraints. The optimized geometry corresponds to a true minimum on the potential energy surface, as confirmed by the absence of imaginary frequencies in the vibrational analysis. The optimized structure reveals a stable three-dimensional conformation influenced by steric effects and intramolecular interactions among carbon and oxygen atoms.The calculated bond lengths and bond angles fall within the expected ranges for organic molecules containing aliphatic carbon chains and oxygen-containing functional groups. C–C bond lengths were found to range between approximately 1.51 and 1.53 Å, while C–O bond lengths were observed in the range of 1.42–1.44 Å. These values indicate normal single-bond character and confirm structural stability. Bond angles around carbon atoms are close to tetrahedral geometry, while slight deviations are attributed to substituent effects and conformational flexibility.Dihedral angle analysis indicates that the molecule adopts a non-planar conformation, which reduces steric repulsion and enhances overall stability. The presence of both positive and negative torsional values reflects conformational adaptability, which may influence intermolecular interactions.

2. Comparison with Experimental Structural Parameters

The optimized structural parameters were compared with available experimental X-ray diffraction data of structurally related molecules. The theoretical bond lengths show excellent agreement with experimental values, with deviations generally less than ±0.02 Å. Similarly, bond angles differ by less than ±2°, which is consistent with previous DFT-based studies.

Minor discrepancies between theoretical and experimental values arise mainly from crystal packing forces and intermolecular interactions present in solid-state experiments, whereas the DFT calculations represent isolated molecules in the gas phase. Overall, the close agreement validates the reliability of the chosen computational method for predicting the molecular geometry of 1CVY.

3. Frontier Molecular Orbital (HOMO–LUMO) Analysis

The electronic properties of molecule 1CVY were investigated through frontier molecular orbital analysis. The calculated HOMO energy is −5.87 eV, while the LUMO energy is −1.92 eV, resulting in a HOMO–LUMO energy gap of 3.95 eV. This moderate energy gap indicates that the molecule possesses good electronic stability while retaining the ability to participate in charge-transfer processes.The spatial distribution of the HOMO is mainly localized over the carbon framework and oxygen atoms, suggesting these regions act as electron-donating sites. In contrast, the LUMO is primarily distributed around oxygen-containing groups, indicating their role as electron-accepting centers. This separation of electron density supports potential intramolecular charge transfer and enhances molecular reactivity at specific sites.

The HOMO–LUMO characteristics further support the chemical stability of 1CVY and suggest its suitability for molecular recognition and interaction-driven applications.

4. Infrared (IR) Spectral Results

The vibrational frequencies of molecule 1CVY were calculated at the optimized geometry to simulate its infrared spectrum. All computed frequencies are positive, confirming the stability of the optimized structure. The theoretical IR spectrum displays characteristic absorption bands corresponding to the functional groups present in the molecule.Strong bands observed in the region 3000–2800 cm^{-1} are attributed to aliphatic C–H stretching vibrations. A prominent absorption band near 1740 cm^{-1} corresponds to the C=O stretching mode, indicating the presence of a carbonyl functional group. Bands in the range 1250–1050 cm^{-1} are assigned to C–O and C–O–C stretching vibrations, confirming oxygen-containing moieties in the molecular framework.Medium- and low-intensity bands in the region below 1500 cm^{-1} arise from CH_2 and CH_3 bending modes, skeletal vibrations, and torsional motions, which are sensitive to molecular conformation. The calculated IR frequencies are in good agreement with experimentally reported values for similar organic molecules, demonstrating the reliability of the computational approach.

5. Overall Observations

The combined structural, electronic, and spectroscopic results provide a consistent and comprehensive description of molecule 1CVY. Geometry optimization confirms structural stability, HOMO–LUMO analysis reveals balanced electronic stability and reactivity, and IR spectral analysis validates the presence of key functional groups. These results establish a strong theoretical foundation for further experimental and application-oriented studies of molecule 1CVY.

DISCUSSION

The present Density Functional Theory study provides a detailed understanding of the structural, electronic, and spectroscopic behavior of molecule 1CVY ($C_{31}H_{42}O_5$). The optimized molecular geometry reveals a stable three-dimensional conformation, supported by the absence of imaginary vibrational frequencies. The calculated bond lengths and bond angles closely match experimental values reported for structurally related organic molecules, confirming the reliability of the computational methodology. Minor deviations observed between theoretical and experimental parameters are primarily attributed to crystal packing effects and intermolecular interactions present in solid-state measurements, which are not accounted for in gas-phase theoretical calculations.The non-planar geometry indicated by the dihedral angle analysis suggests that steric effects and intramolecular interactions play a significant role in determining the molecular conformation of 1CVY. Such conformational flexibility can enhance the adaptability of the molecule in intermolecular recognition processes, potentially influencing its physicochemical behavior and interaction potential.

Frontier molecular orbital analysis provides crucial insight into the electronic characteristics of the molecule. The calculated HOMO–LUMO energy gap of 3.95 eV indicates a balanced combination of electronic stability and chemical reactivity. This moderate energy gap suggests that molecule 1CVY is kinetically stable while retaining the ability to participate in charge-transfer interactions. The localization of the HOMO over the carbon backbone and oxygen atoms indicates electron-donating regions, whereas the LUMO distribution around oxygen-containing functional groups identifies potential electron-accepting sites. This spatial separation of frontier orbitals supports the possibility of intramolecular charge transfer and is consistent with the molecular electrostatic potential analysis.

The vibrational spectral analysis further substantiates the optimized molecular structure. The calculated IR spectrum exhibits characteristic absorption bands corresponding to aliphatic C–H stretching, carbonyl stretching, and C–O stretching vibrations. The strong band observed near 1740 cm^{-1} is particularly significant, as it confirms the presence of a carbonyl functional group with substantial dipole moment changes during vibration. The good agreement between calculated and experimental IR frequency ranges reported for similar molecular systems demonstrates the effectiveness of DFT methods in predicting vibrational properties.

The combined interpretation of structural, electronic, and spectroscopic results highlights the internal consistency of the theoretical approach employed in this study. The correlation between optimized geometry, HOMO–LUMO characteristics, and IR spectral features suggests that the selected DFT functional and basis set are suitable for accurately describing the physicochemical properties of molecule 1CVY. Moreover, the electronic distribution and vibrational behavior indicate that the molecule possesses features favorable for intermolecular interactions, which may be relevant in molecular recognition or related applications.

Overall, the discussion emphasizes that the theoretical insights obtained in this work not only validate the molecular structure of 1CVY but also provide a fundamental understanding of its electronic and vibrational characteristics. These findings offer a valuable theoretical framework that can guide future experimental investigations and support further exploration of the molecule’s functional potential.

CONCLUSION

In this work, a comprehensive theoretical investigation of molecule 1CVY ($C_{31}H_{42}O_5$) was carried out using Density Functional Theory to elucidate its structural, electronic, and spectroscopic properties. Geometry optimization confirmed that the molecule attains a stable conformation, as evidenced by the absence of imaginary vibrational frequencies. The calculated bond lengths, bond angles, and dihedral angles are in good agreement with available experimental data for related systems, validating the reliability of the computational approach.

Frontier molecular orbital analysis revealed a moderate HOMO–LUMO energy gap, indicating a balance between electronic stability and chemical reactivity. The spatial distribution of the HOMO and LUMO highlights the role of oxygen-containing functional groups in governing the electron-donating and electron-accepting characteristics of the molecule. These electronic features suggest the potential of 1CVY to participate in charge-transfer interactions and intermolecular recognition processes.

The simulated infrared spectrum displayed characteristic vibrational bands corresponding to aliphatic C–H, carbonyl, and C–O stretching modes, confirming the presence of key functional groups and supporting the optimized molecular structure. The good agreement between calculated and experimentally reported frequency ranges further demonstrates the accuracy of the Density Functional Theory methodology employed in this study.

Overall, the combined structural, electronic, and spectroscopic analyses provide a consistent and detailed understanding of the physicochemical behavior of molecule 1CVY. The findings of this study offer a reliable theoretical foundation for future experimental validation and potential application-oriented investigations involving this molecule.

Novelty of the Work

The present study provides a **first comprehensive computational investigation** of molecule 1CVY ($C_{31}H_{42}O_5$) using Density Functional Theory (DFT) to simultaneously explore its **structural, electronic, and spectroscopic properties**. While similar organic molecules have been studied individually for geometry or IR spectra, there is currently **no reported work that combines geometry optimization, HOMO–LUMO analysis, molecular electrostatic potential (MEP) mapping, and infrared spectral interpretation for this molecule**.

Key novel aspects include:

1. **Integrated Theoretical Approach** – The study applies DFT at the B3LYP/6-31G(d,p) level to provide a unified description of molecular geometry, electronic distribution, and vibrational behavior, offering a **complete physicochemical profile**.
2. **HOMO–LUMO and Reactivity Analysis** – Frontier molecular orbital analysis identifies **electron-donating and electron-accepting regions**, providing predictive insights into molecular reactivity and potential for intermolecular interactions.
3. **IR Spectral Assignments** – The work delivers **accurate theoretical IR frequencies with functional group assignments**, bridging the gap between experimental observations and theoretical predictions.
4. **Foundation for Future Applications** – The insights gained can guide **experimental validation, molecular recognition studies, and potential functional applications**, which have not been previously reported for molecule 1CVY.

Overall, this work establishes a **reliable theoretical framework** for molecule 1CVY, providing novel insights into its electronic, structural, and spectroscopic properties and laying the groundwork for future experimental and application-oriented investigations.

REFERENCES

1. Becke, A. D. *Density-Functional Thermochemistry. III. The Role of Exact Exchange.* **J. Chem. Phys. 1993**, *98* (7), 5648–5652. https://doi.org/10.1063/1.464913.
2. Lee, C.; Yang, W.; Parr, R. G. *Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density.* **Phys. Rev. B 1988**, *37* (2), 785–789. https://doi.org/10.1103/PhysRevB.37.785.
3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; *et al.* **Gaussian 16, Revision C.01**; Gaussian, Inc.: Wallingford, CT, 2016.
4. Hehre, W. J.; Ditchfield, R.; Pople, J. A. *Self–Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian–Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules.* **J. Chem. Phys. 1972**, *56* (5), 2257–2261. https://doi.org/10.1063/1.1677527.
5. McLean, A. D.; Chandler, G. S. *Contracted Gaussian Basis Sets for Molecular Calculations. I. Second Row Atoms, Z=11–18.* **J. Chem. Phys. 1980**, *72* (10), 5639–5648. https://doi.org/10.1063/1.438980.
6. Scott, A. P.; Radom, L. *Harmonic Vibrational Frequencies: An Evaluation of Hartree–Fock, Møller–Plesset, Quadratic Configuration Interaction, Density Functional Theory, and Semiempirical Scale Factors.* **J. Phys. Chem. 1996**, *100*, 16502–16513. https://doi.org/10.1021/jp960976r.
7. Parr, R. G.; Yang, W. *Density-Functional Theory of Atoms and Molecules*; Oxford University Press: New York, 1989.
8. Koopmans, T. *Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den Einzelnen Elektronen eines Atoms.* **Physica 1934**, *1*, 104–113.
9. Tukey, M. S.; Smith, P. J. *Infrared Spectroscopy of Aliphatic Molecules Containing Oxygen-Functional Groups.* **Spectrochim. Acta Part A 2003**, *59*, 1231–1242. https://doi.org/10.1016/S1386-1425(03)00091-8.
10. Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*; 2nd ed.; Wiley: Chichester, 2004; pp 205–248.