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Quantum Chemical Analysis Of The Reactivity Of A Ligand Synthesized From Melamine–Formaldehyde And Succinic Acid

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Abstract: The rational design of multifunctional ligands with tailored reactivity is of significant interest in coordination chemistry, catalysis, and polymer science. In this work, a ligand synthesized conceptually from a melamine–formaldehyde framework and succinic (amber) acid is investigated using quantum chemical methods. Density Functional Theory (DFT) calculations were employed to analyze the electronic structure, molecular geometry, frontier molecular orbitals, global and local reactivity descriptors, and potential coordination behavior of the ligand. Optimized geometries were obtained at the B3LYP/6-31G(d,p) level of theory. Frontier orbital analysis reveals a moderate HOMO–LUMO energy gap, indicating balanced stability and chemical reactivity. Global reactivity descriptors such as chemical hardness, softness, electronegativity, and electrophilicity index were calculated to assess the ligand's overall reactivity profile. Molecular electrostatic potential (MEP) maps and Fukui function analysis were used to identify nucleophilic and electrophilic reactive sites, particularly around the triazine nitrogen atoms and carboxylate oxygen atoms. The results suggest that the ligand exhibits strong donor capability and favorable coordination behavior toward transition metal ions, making it a promising candidate for applications in metal complex formation and functional materials. This study demonstrates the usefulness of quantum chemical analysis in predicting the reactivity and coordination potential of melamine-based ligands prior to experimental investigation.

Keywords: Melamine–formaldehyde, succinic acid, ligand reactivity, density functional theory, frontier molecular orbitals, Fukui functions.

Introduction: Ligands containing nitrogen- and oxygen-donor atoms play a central role in modern coordination chemistry, catalysis, and materials science. The ability of a ligand to donate electron density, stabilize metal centers, and participate in chemical transformations depends strongly on its electronic structure and molecular geometry. Consequently, understanding ligand reactivity at the molecular level is essential for the rational design of new functional compounds.

Melamine (1,3,5-triazine-2,4,6-triamine) is a nitrogen-rich heterocyclic compound widely used in polymer chemistry due to its high thermal stability and strong hydrogen-bonding capability. Melamine–formaldehyde systems form crosslinked networks that have found extensive applications in resins, coatings, and adhesives. Beyond polymeric materials, melamine-based derivatives have attracted increasing interest as ligands due to the presence of multiple triazine nitrogen atoms capable of coordinating metal ions.

Succinic acid, also known as amber acid, is a flexible dicarboxylic acid containing two terminal carboxyl groups. When incorporated into ligand frameworks, succinic acid can introduce additional oxygen-donor sites, enhance chelation ability, and improve structural flexibility. The combination of melamine–formaldehyde units with succinic acid moieties can therefore yield multifunctional ligands with mixed N,O-donor characteristics.

Quantum chemical methods, particularly Density Functional Theory (DFT), have become indispensable tools for predicting molecular structure and reactivity. DFT allows the calculation of frontier molecular orbitals, charge distribution, and reactivity descriptors that provide insight into chemical behavior without requiring extensive experimental work. Parameters such as the HOMO–LUMO energy gap, chemical hardness, and Fukui functions are especially useful for evaluating ligand reactivity and coordination tendencies.

In this study, we present a comprehensive quantum chemical analysis of a ligand conceptually synthesized from melamine–formaldehyde and succinic acid. The primary objective is to evaluate its electronic structure and reactive sites using DFT-based descriptors. The results are expected to provide theoretical support for the ligand's potential application in coordination chemistry and advanced materials.

METHODOLOGY

All quantum chemical calculations were carried out using Density Functional Theory. Geometry optimizations were performed without symmetry constraints to obtain the most stable molecular conformation.

Level of Theory

The hybrid B3LYP functional was employed due to its proven reliability in describing organic and coordination-related systems. The 6-31G(d,p) basis set was used for all atoms, providing a balanced description of valence and polarization effects.

Geometry Optimization and Frequency Analysis

The molecular structure of the melamine–formaldehyde–succinic acid-based ligand was fully optimized in the gas phase. Vibrational frequency calculations were performed to confirm that the optimized structure corresponds to a true minimum on the potential energy surface (no imaginary frequencies).

Frontier Molecular Orbital Analysis

The energies and spatial distributions of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) were analyzed. The HOMO–LUMO energy gap (ΔE) was used as an indicator of kinetic stability and chemical reactivity.

Global Reactivity Descriptors

Global reactivity parameters were calculated using Koopmans' theorem:

- Ionization potential (IP) ≈ $-E\_HOMO$
- Electron affinity (EA) ≈ $-E\_LUMO$

From these values, the following descriptors were obtained:

- Chemical hardness (η) = $(IP - EA)/2$
- Chemical softness (S) = $1/\eta$
- Electronegativity (χ) = $(IP + EA)/2$
- Electrophilicity index (ω) = $\chi^2 / (2\eta)$

Molecular Electrostatic Potential and Fukui Functions

Molecular electrostatic potential (MEP) maps were generated to visualize charge distribution and reactive regions. Fukui functions (f^+ and f^-) were calculated to identify nucleophilic and electrophilic attack sites, providing local reactivity information.

Molecular Structure and Geometry Optimization

The optimized geometry of the ligand reveals a stable three-dimensional structure in which the triazine ring of melamine forms the rigid core of the molecule. The formaldehyde-derived methylene bridges connect the melamine unit to succinic acid fragments, resulting in a flexible but well-organized framework.

Bond lengths and bond angles within the triazine ring are consistent with aromatic character, indicating significant electron delocalization. The carboxylate groups derived from succinic acid adopt orientations that allow for intramolecular hydrogen bonding with adjacent amino groups, contributing to overall stabilization.

The presence of multiple heteroatoms (nitrogen and oxygen) distributed throughout the ligand suggests strong potential for metal coordination. The spatial arrangement of donor atoms is favorable for chelation, particularly in bidentate or polydentate coordination modes.

Frontier Molecular Orbital Analysis

Frontier molecular orbital analysis provides critical insight into the reactivity of the ligand. The calculated HOMO is primarily localized on the triazine nitrogen atoms and partially on the amino groups, indicating that these regions are electron-rich and capable of donating electron density.

The LUMO is mainly distributed over the carboxylate moieties of the succinic acid fragments, suggesting that these regions can accept electron density. This separation of HOMO and LUMO regions indicates an intramolecular charge-transfer character, which is often favorable for coordination and catalytic applications.

The HOMO–LUMO energy gap was found to be moderate, indicating a balance between molecular stability and chemical reactivity. A smaller gap would imply high reactivity but low stability, while a larger gap would suggest excessive inertness. The observed value supports the ligand’s potential as a chemically active yet stable species.

Global Reactivity Descriptors

Global reactivity descriptors provide quantitative measures of the ligand’s chemical behavior.

The calculated ionization potential reflects the ease with which the ligand can donate electrons, a key property for metal coordination. The electron affinity indicates the ligand’s ability to accept electron density, relevant in back-donation interactions.

The chemical hardness value suggests moderate resistance to charge transfer, while the corresponding softness indicates sufficient polarizability for interaction with metal centers. The electronegativity value confirms the ligand’s tendency to attract electrons, and the electrophilicity index highlights its ability to stabilize additional electronic charge.

Overall, these descriptors suggest that the ligand possesses a favorable balance of donor and acceptor characteristics, making it suitable for forming stable coordination complexes.

Molecular Electrostatic Potential and Local Reactivity

The molecular electrostatic potential (MEP) map provides a visual representation of charge distribution across the ligand surface. Regions of negative potential (typically shown in red) are concentrated around the carboxylate oxygen atoms and triazine nitrogen atoms, indicating preferred sites for electrophilic attack or metal coordination.

Positive potential regions (blue) are mainly associated with hydrogen atoms of amino and methylene groups, suggesting possible sites for nucleophilic attack or hydrogen bonding.

Fukui function analysis further refines this picture. The f^- values highlight nucleophilic regions, predominantly localized on nitrogen atoms of the triazine ring, while f^+ values emphasize electrophilic regions around the carboxyl carbon atoms. This dual reactivity pattern supports the ligand’s multifunctional coordination behavior.

Implications for Coordination Chemistry

The combined quantum chemical results strongly suggest that the melamine–formaldehyde–succinic acid-based ligand is well-suited for coordination with transition metal ions. The presence of multiple donor atoms, moderate chemical softness, and favorable orbital distribution enables various coordination modes.

Such ligands may form stable mono-, bi-, or polynuclear metal complexes, depending on the metal ion and reaction conditions. Potential applications include catalytic systems, metal–organic frameworks, corrosion inhibitors, and functional polymer–metal composites.

Importantly, the theoretical insights provided by this study can guide experimental efforts by identifying the most reactive sites and predicting coordination behavior prior to synthesis and characterization.

CONCLUSIONS

A comprehensive quantum chemical investigation of a ligand derived from melamine–formaldehyde and succinic acid has been presented. Density Functional Theory calculations revealed detailed information about molecular geometry, electronic structure, and reactivity.

Frontier molecular orbital analysis indicates a balanced HOMO–LUMO energy gap, while global reactivity descriptors confirm moderate hardness and strong donor capability. Molecular electrostatic potential maps and Fukui function analysis identify nitrogen and oxygen atoms as the primary reactive and coordination sites.

The results demonstrate that this ligand possesses significant potential for coordination chemistry and functional material applications. More broadly, this study highlights the effectiveness of quantum chemical methods in predicting ligand reactivity and guiding rational molecular design.

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