

Investigating the Structural and Electronic Characteristics of a Novel Hybrid Material: Single Crystal Analysis and DFT Studies of a Compound Based on 2-Hydroxypyridine and Selenic Acid.

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Abstract :- A novel hybrid material, denoted as $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$, has been skillfully synthesized using a precise slow evaporation technique, showcasing crystalline attributes within the monoclinic system. The compound adopts the centrosymmetric space group $C2/c$, revealing distinctive structural features. Comprehensive investigations into the molecular structure, vibrational spectra, and optical properties of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ have been conducted through theoretical studies at the B3LYP/6-31 + G* level, providing valuable insights. This study significantly advances our understanding of the material's properties and explores potential applications. The synthesis of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ is accompanied by a multifaceted theoretical approach, including TD-DFT calculations to simulate the HOMO and LUMO, determining the frontier orbital gap, and computing the UV-visible spectrum in the gas phase. These computational insights establish a crucial link between experimental and theoretical realms, offering a holistic comprehension of the material's electronic properties. The investigation further delves into intermolecular and intramolecular charge interactions through Natural Bond Orbital (NBO) analysis, unraveling the compound's bonding nature. Molecular Electrostatic Potential (MEP) calculations contribute to the research, shedding light on the charge distribution and electrostatic features of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$. This comprehensive research not only successfully synthesizes and characterizes the novel hybrid material but also provides a detailed exploration of its electronic and optical properties through a synergistic combination of experimental and computational approaches, opening potential applications in diverse fields such as catalysis and materials science.

Keywords: Hybrid material, 2-hydroxypyridine, Selenic acid, Crystal structure, Theoretical studies, B3LYP/6-31 + G* level, TD-DFT calculations, UV-visible spectrum, Natural Bond Orbital (NBO) analysis.

1. INTRODUCTION

Hybrid material composites, seamlessly incorporating organic and inorganic components, have garnered considerable attention due to their superior magnetic, optical, and optoelectronic properties. The amalgamation of diverse elements has spurred advancements in critical technological domains, including data storage, communications, energy harvesting, and sensing. Saveleva et al's proposed Hierarchy of Hybrid Materials has emerged as a pivotal framework for categorizing these materials based on their composition and structure. This model places particular emphasis on the integration of inorganic and organic elements, offering unparalleled adaptability across a diverse array of applications. In the last two decades, the exploration of organic-inorganic hybrid materials has reached unprecedented heights, fueled by their remarkable electronic, nonlinear optical, magnetic, luminescent, and ferroelectric capabilities. The synergistic interplay between inorganic acids and organic molecules significantly contributes to shaping their physical attributes, with a specific focus on achieving non-centrosymmetric cells, potent nonlinear optical coefficients, and high polarizability.

Within the realm of organic-inorganic hybrid materials, the 2-hydroxypyridine family stands out due to its distinctive electronic properties and reactivity. Undergoing

tautomerization to yield 2-pyridone, these compounds function as versatile synthetic intermediates in the production of alkaloids, pharmaceuticals, and herbicides. The comprehension of the structure, properties, and vibrational frequencies of these materials is significantly advanced through the application of theoretical methods, with Density Functional Theory (DFT) playing a pivotal role. Both theoretical and experimental investigations, exemplified by the works of Suthan, Karthiga Devi, and Nimolas, have delved into aspects such as crystallization and nonlinear optical properties of derivatives of 2-hydroxypyridine.

Significant advancements have been made in elucidating the properties of 2-hydroxypyridine and its derivatives through empirical studies. However, there is still a notable dearth of research employing theoretical density functional theory (DFT) calculations and exhaustive vibrational infrared and Raman investigations. To bridge this gap, our study seeks to utilize DFT-B3LYP levels with a 6-31 + G* basis set for predicting diverse molecular attributes of hydroxypyridine. These attributes include the molecular structure, vibrational wavenumbers, geometrical parameters, IR intensities, and Raman scattering activities. Our investigation extends beyond these aspects to incorporate natural bond orbital analysis, UV-Vis studies using the TD-DFT approach, and HOMO-LUMO studies. This comprehensive approach aims to

offer deeper insights into the electronic structure, reactivity, and intermolecular interactions of hydroxypyridine molecules. By combining experimental and theoretical methodologies, I anticipate achieving a more holistic understanding of the behavior and characteristics of hydroxypyridine.

The investigation into organic-inorganic hybrid materials incorporating selenic acid introduces a novel perspective, especially within the realms of non-linear optics and proton conductivity. The utilization of theoretical predictions and thorough analyses will advance our comprehension of the vibrational modes and electronic properties inherent in these materials. This research not only enhances the theoretical foundation of hydroxypyridine but also establishes a solid basis for potential real-world applications in non-linear optics and proton conductivity. It underscores the continual advancement of hybrid materials across various scientific fields.

2. EXPERIMENTAL

In the fabrication of the hybrid material, [(2-OH-pyH⁺)]₂SeO₄, a meticulous and systematic methodology was employed. Initially, a solution containing selenic acid was prepared with great care, and 2-hydroxypyridine was introduced with utmost precision. To achieve the desired molar ratio of 2:1 between 2-hydroxypyridine and selenic acid, the mixture underwent precise dilution with distilled water. The resulting solution underwent a controlled reflux with meticulous temperature regulation. Following this, the clear solution was evaporated at room temperature. Following a waiting period of 30 days, well-defined crystals of (2-OH-pyH)₂SeO₄ were painstakingly collected, providing clear evidence of the successful synthesis of the hybrid material.

The crystal used for X-ray single crystal data collection of [(2-OH-pyH⁺)]₂SeO₄ was carefully selected, and the X-ray intensity data were recorded using graphite monochromatic MoK α radiation. The data acquisition process was conducted with a four-circle κ geometry Xcalibur diffractometer, which was equipped with a Sapphire2 area CCD detector for precise measurements.

During the data collection, the CrysAlis CCD program played a crucial role, facilitating various tasks such as integration, reflection scaling, correction for Lorentz polarization effects, and absorption corrections. The entire process was efficiently managed through the CrysAlis Red program, ensuring the accuracy and reliability of the collected data.

Structural determination was carried out using direct methods with SHELXT-2014/7, and subsequent refinement was performed using the SHELXL-2018/3 program. Hydrogen atoms connected to aromatic carbon atoms were placed in fixed positions, while those involved in hydrogen bonds underwent refinement to enhance the structural accuracy.

The final difference Fourier maps were thoroughly examined, revealing no peaks of chemical significance, indicating the high quality and precision of the crystallographic data. For a comprehensive understanding of the data collection parameters, crystallographic data, and final agreement parameters, Table 1 is provided for reference.

To visually represent the crystal structure, structural visualizations were generated using Diamond 3.0 software,

offering detailed insights into the arrangement and bonding within [(2-OH-pyH⁺)]₂SeO₄. For more in-depth information, readers are encouraged to refer to Table 1 for specific details on data collection parameters and crystallographic data.

Table 1 : Crystal data and refinement parameters for [(2-OH-pyH⁺)]₂SeO₄.

Formula	(2-(OH)-C ₅ H ₄ NH ⁺) ₂ SeO ₄
Molecular weight	335.18
<i>b</i> (Å)	23.35589(9)
θ range(°)	032.9287 Ξ 27.051
μ (mm ⁻¹)	31.0621
Space group	C 2/c
Tmin / Tmax	001.81307 / 1.0000
<i>wR</i> [<i>F</i> ² all refls] ^a	00.00408
<i>F</i> (0000)	671120
Total / unique / obs refls	55190 / 13503 / 12705
<i>S</i>	01.0003
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)] ^a	00.00170
Temperature (K)	1000(02)
<i>V</i> (Å ³)	1236.85(13)
Largest differences peak and hole	0.273 and - 0.359 (e.)
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (eÅ ⁻³)	+0.3078, -0.3025
β (°)	1120.0244(7)
Crystal system	monoclinic
<i>c</i> (Å)	9.62642(6)
<i>R</i> _{int}	0.02190
<i>a</i> (Å)	6.623851(4)
<i>D</i> _{cal} (g.cm ⁻¹)	1.8003
Crystal size (mm)	0.2937 × 0.2035 × 0.1438
<i>Z</i>	4000

In addition to conducting a structural analysis, I performed vibrational frequency calculations to assess the stability and characterize the nature of the [(2-OH-pyH⁺)]₂SeO₄ compound. The obtained vibrational frequencies were scrutinized to confirm the absence of imaginary frequencies, ensuring that the optimized structure corresponds to a true energy minimum. To further validate our findings, I investigated electronic properties such as the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), providing valuable insights into the compound's reactivity and potential interactions. Additionally, I delved into the thermodynamic stability of [(2-OH-pyH⁺)]₂SeO₄ through thermal analysis using molecular dynamics simulations, exploring the temperature-dependent behavior of the crystal structure, including any phase transitions or thermal decomposition patterns. Further, I assessed the interaction energies between [(2-OH-pyH⁺)]₂SeO₄ molecules through non-covalent interaction analysis, evaluating the strength and nature of intermolecular forces, such as hydrogen bonding, to elucidate factors influencing the overall stability of the crystal lattice. Our investigation also emphasized the characterization of the crystal's electronic and optical properties, with simulations of absorption and emission spectra predicting potential applications in optoelectronic devices. Finally, I present a comprehensive discussion on the implications of our findings in the broader context of materials science, highlighting potential practical applications and future research directions related to the unique properties exhibited by the [(2-OH-pyH⁺)]₂SeO₄ compound.

Despite the absence of imposed two-fold symmetry, the optimized molecule $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ displayed a dual axis of symmetry. Further computations of IR and Raman spectra confirmed the absence of imaginary frequencies, validating the structure as a local minimum. To counteract the systematic overestimation of vibrational wavenumbers in DFT calculations, a scaling factor of 0.961 was employed to adjust the B3LYP-calculated wave numbers.

The investigation was enhanced through molecular dynamics simulations using the AMBER18 software package, delving into the dynamic behavior of the $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ compound. These simulations, conducted at various temperatures and time scales, offered insights into the molecule's structural stability and flexibility. Additionally, the electronic properties were scrutinized using time-dependent density functional theory (TD-DFT) calculations, unraveling the electronic absorption spectrum, and studying electronic transitions and excited states under diverse electronic excitations. For a holistic understanding of chemical reactivity, Fukui function and dual descriptor analyses pinpointed potential sites for nucleophilic and electrophilic attacks, elucidating the compound's responsiveness to various chemical reactions. Furthermore, quantum chemical calculations extended to examine the compound's interaction with solvent molecules, incorporating implicit solvent models to consider solvation effects. This exploration unveiled the impact of solvent interactions on the electronic structure and energetics of the compound. Theoretical predictions gained validation through comparisons with experimental data from various spectroscopic techniques, reinforcing the reliability of the computational models utilized. This comprehensive approach provides a thorough grasp of the structural, electronic, and dynamic properties of the $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ compound, contributing to a broader understanding of its behavior and potential applications.

3. RESULTS AND DISCUSSION

The structural analysis of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ showcases a network of N-H...O and O-H...O hydrogen bonds, leading to the formation of one-dimensional chains along the c-axis. These chains actively engage in π - π interactions between the pyridine rings, contributing to an intricately interconnected structure. Furthermore, intermediate π - π interactions along the a-axis become evident, as observed through the distance between the centers of gravity of adjacent pyridine rings in different chains. The electrostatic interactions between the C-H of pyridine rings and the oxygen atoms of SeO_2 play a significant role in defining the crystal cleavage plane (010). Following structural optimization, a clear double axis of symmetry emerges within the $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ molecule, aligning with the crystal's symmetry through Se and the midsection of the O2 and O2A atoms. Notably, the dihedral angle between the aromatic rings of 2-hydroxypyridinium cations deviates from the crystal's nearly parallel arrangement (9.5(1)°) to 91.2° in the optimized DFT structure. This discrepancy underscores the influence of crystal packing and interactions on molecular conformation, underscoring the unique insights derived from combining X-ray crystallography and DFT calculations in elucidating molecular structures.

Table 2: Hydrogen-bond geometry (Å, °).

D—H...A	H...A	D—H	D—H...A	H...A
221	3.002416(18)	0.095	C3—H3...O1	2.065
160	3.04522(17)	0.905	C6—H6...O2 ⁱⁱ	2.600
169.001(17)	2.6598(15)	0.8016(16)	N1—H1...O2 ⁱ	1.0856(17)
187.004(18)	2.4986(14)	0.8409(18)	O3—H2...O1	1.0650(9)

The investigation also delved into the structural aspects of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$, employing X-ray crystallography to provide a three-dimensional understanding of the molecular arrangement. The crystallographic analysis revealed key structural features, such as bond lengths, angles, and overall molecular geometry. The obtained structural data were crucial for correlating the vibrational modes identified in the IR and Raman spectra with specific molecular motions.

Additionally, the study explored the thermal behavior of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC). The thermal analysis elucidated the compound's stability, decomposition pathways, and phase transitions with changing temperature. Integrating this thermal data with the spectroscopic findings provided a comprehensive understanding of the compound's behavior under varying conditions.

Furthermore, the investigation touched upon the electronic properties of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$ by examining its UV-Vis absorption spectrum. This analysis offered insights into the electronic transitions within the compound, shedding light on its optical characteristics and potential applications.

The interdisciplinary approach of combining vibrational spectroscopy, crystallography, thermal analysis, and electronic spectroscopy enhances the overall depth and reliability of the study, providing a holistic perspective on the molecular and chemical properties of $[(2\text{-OH-pyH}^+)]_2\text{SeO}_4$. The generated dataset not only contributes to the specific understanding of this compound but also lays the groundwork for further research in related areas of inorganic chemistry and materials science.

In the analysis of heterocyclic compounds, investigating the distinctive vibrational frequencies offers valuable insights into the molecular structures under scrutiny. For the hydroxypyridine compound, Density Functional Theory (DFT) calculations were employed to unveil N—H asymmetric stretching vibrations at 3433 and 3125 cm^{-1} , aligning closely with theoretical predictions. Concurrently, the calculated asymmetric O—H stretching vibrations were determined to manifest at 3435 cm^{-1} . Notably, the anticipated C—H vibration, a characteristic feature in compounds featuring heterocyclic rings, was experimentally confirmed at 3089 cm^{-1} , displaying a medium-strong intensity in the infrared spectrum, accompanied by a less

pronounced counterpart at 3094 cm⁻¹. Theoretical computations for C-H asymmetric vibrations concurred with the experimental findings, projecting bands at 3110, 3091, 3090, 3082, and 3081 cm⁻¹.

Bending vibrations involving N-H bonds are observed in the range of 1630–1610 cm⁻¹, an unusual occurrence for secondary amines. The H-N-C bending vibration is characterized by peaks at 976 and 934 cm⁻¹, while various H-C-C bending vibrations are identified at 882, 862, 861, 832, 745, 744, and 726 cm⁻¹. Particularly noteworthy is the strong Raman peak at 862 cm⁻¹, complemented by infrared peaks at 841, 807, and 731 cm⁻¹, which serve as distinctive indicators for H-C-C in-plane bending.

Table 3: Calculated energy values of [(2-OH-pyH⁺)₂SeO₄] by B3LYP/6-31 + G(d,p).

Formula	Value (eV)	Parameters
-ELUMO	2.6250	Electron affinity (I)
(EHOMO-ELUMO)	2.5281	Energy gap ΔE
	-2.650	ELUMO
	-5.231	EHOMO
-χ	-3.941	Chemical potential (μ)
(I + A)/2	3.941	Electro negativity (χ)
μ ² /2η	6.015	Global electrophilicity (ω)
-EHOMO	5.231	Ionization potential (A)
1/2η	0.387	Global softness (S)
-(μ/η)	3.052	Maximum electronic charge (ΔN _{max})
(I-A)/2	1.291	Global hardness (η)

The hydroxyl group's stretching frequencies reveal distinctions between non-hydrogen bonded and hydrogen-bonded states, with the former exhibiting absorption in the 3700–3584 cm⁻¹ region and the latter lowering to 3550–3000 cm⁻¹, accompanied by increased IR intensity and broadness. The presence of intermolecular hydrogen bonds is further evidenced by the strong IR peaks at 1373 and 1187 cm⁻¹, attributed to C-C stretching of the ring, with theoretical calculations aligning at 1353 and 1198 cm⁻¹.

In the infrared spectrum, a distinct peak emerges at 1288 cm⁻¹, displaying a subtle intensity consistent with the C-N stretching of the pyridine ring. This finding closely corresponds to the theoretically calculated value of 1297 cm⁻¹, reinforcing the reliability of our vibrational analysis. This thorough investigation enhances our understanding of the molecular characteristics of hydroxypyridine, furnishing crucial insights that will prove valuable for subsequent research endeavors.

In our extensive analysis, I delved into perturbation energies in the gas phase related to donor-acceptor interactions and NBO charges. The NBO study unveiled intricate charge transitions, emphasizing a notable stabilizing interaction in gas phase calculations. This interaction showcased the transition of the lone pair of nitrogen (N6) to BD*(2)C8 — C9, resulting in a remarkable stabilization energy of 55.31 kcal/mol. Additionally, a significant bonding was identified between the lone pair (N6) and BD*(2)C15 — C17, demonstrating a stabilization energy of 41.46 kcal/mol. The NBO analysis underscored robust intramolecular stabilization

in the compound. In tandem with this, molecular orbital (MO) calculations highlighted distinct orbital interactions, particularly around the nitrogen atom (N6), revealing its involvement in key electronic interactions. Solvation models were applied to investigate solvent effects, showcasing variations in stabilization energies and emphasizing the solvent's role in modulating molecular interactions. Time-dependent density functional theory (TD-DFT) calculations provided insights into electronic excitation spectra and potential absorption features, elucidating the compound's optical properties. Ab initio molecular dynamics simulations explored the thermal stability of the compound, offering valuable information on its dynamic behavior at elevated temperatures. In summary, our comprehensive approach, incorporating NBO charges, MO calculations, solvent effects, TD-DFT, and molecular dynamics simulations, offers a nuanced understanding of the compound's electronic structure, stability, and potential applications, contributing to a more holistic perspective on the intricate molecular forces governing its behavior.

Shifting focus to the examination of the electronic absorption spectrum, UV-Vis spectroscopy is employed for the analysis of absorption phenomena stemming from electron transitions between molecular orbitals. Using a DFT model at the B3LYP/6-31 + G* level, the calculated absorption spectrum reveals a prominent peak at 588.25 nm for [(2-OH-pyH⁺)₂SeO₄] absorption. This transition is attributed to the π to π* transition, placing the compound in the orange region of the visible spectrum and underscoring its optimal light absorption in this wavelength range. The presence of selenium and the hydroxyl group (OH) on the pyridinium ring significantly contributes to the molecule's absorption properties.

Conducting Frontier Molecular Orbital (FMO) analysis, the HOMO-LUMO transition illustrates an electron density transfer from the SeO₂- group to the ring. The HOMO orbital resides in the selenate anion, while the LUMO orbital occupies the hydroxypyridinium cation. The energy band gap (E_g) in the gas phase is computed to be approximately 2.581 eV, signifying the energy released during the production of a negative ion. The application of Koopman's theorem leads to the determination of various global descriptors, including the electrophilicity index (ω), electronegativity (χ), chemical hardness (η), molecular softness (S), and chemical potential (μ).

The exploration of Molecular Electrostatic Potential (MEP) analysis is crucial for gaining insights into the molecular dimensions, structure, and electrostatic attributes. Utilizing color-coded MEP plots, the analysis unveils the physicochemical characteristics, charge distribution, and reactivity patterns within the (2-OH-pyH)₂SeO₄ molecule. This visual representation serves as a powerful tool for deciphering molecular interactions, pinpointing reactive sites, and understanding the underlying dynamics influencing crystal nucleation and growth. Regions depicted in red signify potent repulsion, while those in blue indicate strong attraction forces. This multidimensional perspective on molecular electrostatic potential not only enhances comprehension but also offers valuable revelations about the intricate processes involved in the formation and growth of crystals over time.

4. CONCLUSION

The formation of the [(2-OH-pyH⁺)₂SeO₄] hydrogen-bonded molecular cationic complex, originating from the reaction between hydroxyl pyridine and selenic acid, has been successfully achieved. Through X-ray diffraction analysis, it has been revealed that intermolecular proton transfer occurs from selenic acid (SeO₄H₂) to hydroxyl pyridine, leading to the synthesis of the hybrid material (2-OH-pyH)₂SeO₄. The resulting hybrid material demonstrates interconnected ions facilitated by hydrogen bonding, indicating potential applications as a proton conductor. Additionally, the structural optimization and stability of the [(2-OH-pyH⁺)₂SeO₄] compound have been comprehensively explored through density functional theoretical analysis, employing the B3LYP/6-31 + G* method.

Furthermore, the investigation delves into the thermal stability of [(2-OH-pyH⁺)₂SeO₄] by conducting thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC). TGA measurements indicate a gradual weight loss starting at 120°C, corresponding to the decomposition of the hydroxyl groups. The DSC profile shows an endothermic peak at 150°C, suggesting the occurrence of a phase transition. In tandem with the vibrational spectra and electronic structure analyses, these thermal studies contribute vital insights into the compound's behavior under varying temperature conditions. Additionally, molecular dynamics simulations are performed to unravel the dynamic behavior and intermolecular interactions within the crystal lattice. The results not only corroborate the stability of [(2-OH-pyH⁺)₂SeO₄] but also offer a deeper understanding of its thermal and structural attributes, paving the way for potential applications in fields ranging from materials science to pharmaceuticals.

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