

HF and DFT Analysis of 3,5-Dimethyl-2-pyridylselenium Compounds: A Combined Experimental and Theoretical Analysis

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The chemistry of pyridylselenium compounds has seen a lot activity in recent years due to some unique properties of these compounds.¹ A combined theoretical and experimental approach plays an important role in determining molecular properties and solving problems encountered in experimental techniques. This is especially beneficial in cases where molecules (such as organoseleniums) are either unstable or difficult to synthesize. Advances in computer technology and emergence of chemistry related software programs have led to the utilization of quantum chemistry as a practical investigating tool.² Although experimental aspect of pyridylselenium chemistry has been extensively reported, however to the best of our knowledge, there is no study on the theoretical aspect of pyridylselenium chemistry in combination with experimental results. Therefore, there is a need to develop and explore a quantum chemical model to determine and understand molecular properties of these compounds. The present study, for the first time, attempts to theoretically explore molecular geometry, HOMO-LUMO energy gap, thermodynamic parameters such as entropy, enthalpy, specific heat capacity, etc., and spectroscopic properties such as FT-IR, ¹H and ¹³C NMR spectra of pyridylselenium compounds. The results have been computed and validated with the experimental data. For this, three compounds namely; bis(3,5-dimethyl-2-pyridyl)diselenide (1), 3,5-dimethyl-2,6-bis(methyl selenenyl)pyridine (2) and 3,5-dimethyl-2-(methylselenenyl)pyridine (3) were synthesized in the laboratory and quantum computations were carried out by HF and DFT methods. The molecular structure of 1 has a characteristic Se-Se bridge, the molecule 2 has two methylselenenyl units at two different positions on the pyridine ring, whereas 3 encompasses a single methylselenenyl unit on the pyridine ring. The objective was to investigate the impact of these structural variations on molecular properties of the pyridylselenium compounds.

References

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Ligand-controlled Regioselective Deprotonation: Au-catalyzed Acyloxy Dienes Synthesis from Propargylic Esters

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By functionalizing biphenyl-2-ylphosphine ligand with a basic amino group on the remote benzene ring, the derived gold(I) complexes enable a facile synthesis of acyloxy dienes from easily accessible propargylic esters under exceptionally mild conditions. Regio- and stereoselectivity of the acyloxy diene products is well controlled by further rationally tuning the location and bulkiness of the amino group on the ligands as well as the size of acyl groups on the propargylic esters.