

From Crystal Structure to Biomolecular Function: Experimental and Theoretical Insights into Pyridoxal-Based Metal Complexes

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Pyridoxal-derived semicarbazones, thiosemicarbazones, and S-methyl-isothiosemicarbazones constitute a versatile class of multidentate ligands capable of stabilizing a wide range of transition-metal and lanthanide complexes. Their structural flexibility, multiple coordination modes, and tunable donor atom composition make them attractive building blocks for the development of functional inorganic materials with tailored physicochemical and biological properties.

This lecture presents an integrated experimental and computational investigation of a series of metal complexes containing pyridoxal-based ligands. Particular emphasis will be placed on the relationship between ligand structure, coordination environment, and the resulting molecular properties. Single-crystal X-ray diffraction, spectroscopic characterization, and Hirshfeld surface analysis will be combined with density functional theory, topological analyses of electron density, and molecular docking calculations to provide a comprehensive description of metal–ligand bonding and supramolecular organization.

The influence of subtle structural modifications, including changes in donor atoms, ligand protonation, and coordination geometry, on the stability and electronic structure of the complexes will be discussed. These structural features will be correlated with interactions toward biologically relevant targets, including human serum albumin and DNA, using complementary experimental binding studies and computational modeling. The comparison between experimentally determined and theoretically predicted structures and binding affinities demonstrates how quantum-chemical methods can successfully rationalize observed behavior and support the interpretation of experimental data.

The results presented illustrate how integrating synthesis, crystallography, spectroscopy, and modern computational chemistry provides a powerful framework for understanding structure–property relationships in coordination compounds. Such an approach not only facilitates the rational design of new functional metal complexes but also contributes to the development of predictive strategies for tailoring their physicochemical and biomolecular properties.