

Linking structure to activity in Ni(II) complexes with {NiN₂O₄} geometry via spectroscopic analysis

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Streszczenie

This study presents the synthesis, structural characterization, and biological evaluation of three nickel(II) complexes containing bioactive ligands: two bidentate pyridyl alcohols (2-pymetH and 2-pyethH) and a mixed-ligand system with memantine and acetylacetone. Single-crystal X-ray diffraction revealed that all complexes adopt a distorted octahedral geometry with a {NiN₂O₄} coordination core, differing in ligand orientation, symmetry, and supramolecular packing. Complementary spectroscopic techniques, including FT-IR, Raman, and UV–Vis, confirmed successful ligand coordination and complex integrity. Fluorescence studies indicated comparable photophysical properties among the complexes, with emission lifetimes of approximately 8ns. Thermal and solution stability studies demonstrated greater structural robustness for the monoligand complexes (**1** and **2**), whereas partial ligand dissociation was observed in the mixed-ligand complex **3**. Antimicrobial testing revealed that complex **3** exhibited enhanced activity against resistant Gram-negative bacteria (including *A. baumannii*, *S. maltophilia*), while complexes **1** and **2** demonstrated notable antifungal activity against *Candida albicans* (MIC₅₀=64µg/mL). These findings underscore the importance of ligand identity, coordination geometry, and complex stability on the biological and photophysical performance of Ni(II) complexes. Collectively, the findings support the potential of these systems as scaffolds for development of novel Ni-based antimicrobial agents.

Słowa kluczowe

Ni(II) complexes, Pyridyl alcohol ligands, Memantine, Antimicrobial activity, Spectroscopic study

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