

Interesting coordination chemistry of Ni(II) complexes with redox non-innocent pyridylpyrrolide ligands

René W. Buell, Nikolay Tsvetkov, José G. Andino, Maren Pink, Chun-Hsing Chen, Ashley R. Head, Dennis L. Lichtenberger, and Kenneth G. Caulton

A new class of redox non-innocent ligands with tunable electronic properties is being studied for possible use as catalytic agents when complexed with metals. These pyridylpyrrolides have the ability to bind transition metals to make low oxidation state and unsaturated complexes. This study focuses on the chemistry of nickel (II) pyridylpyrrolide complexes including structural, binding, and reactivity properties. Density functional theory show the HOMOs of $\text{Ni}(\text{L}^{0-2})_2$ are ligand based, which supports the idea that low valent NiL_2 complexes can be oxidized at the ligands themselves, increasing the reducing agent power of these species. The Lewis acidity of the Ni(II) species was tested by addition of both redox and non-redox agents including H_2O , THF, CO, I_2 , and Br_2 .

