

## Coordination preferences of Schiff base ligands with transition metals: DFT study

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The chemistry of the first-row transition metals is highly diverse, with a multitude of different reactivity and property patterns. This richness results from a wide range of ligands and coordination flexibility around the central metal ion. Still, it results from the partial occupation of the metal d-orbitals, which leads to different oxidation and spin states.<sup>1</sup> For the past years, our research has focused on investigating transition metal complexes with hydrazone-based ligands and studying their catalytic<sup>2</sup>, magnetic<sup>3</sup>, and biological activities.<sup>4</sup> We have studied a series of tridentate NNO/NNS and pentadentate NNNNO/NNNSS ligands obtained by condensation reactions of 2-acetylpyridine, 2-quinolinecarboxaldehyde, 2-acetylthiazole, or 2,6-diacetylpyridine and Girard's reagents (N-substituted glycine hydrazides) or thiosemicarbazide, and their mono- and binuclear complexes with various transition metal ions (Fe<sup>2+</sup>, Fe<sup>3+</sup>, Co<sup>2+</sup>, Co<sup>3+</sup>, Ni<sup>2+</sup>, Cu<sup>2+</sup>).

To rationalize coordination preferences of the ligands to form mono- or binuclear complexes and coordinate differently, together with the electronic structure of transition metal ions, we performed Density Functional Theory (DFT) calculations accompanied by the Energy Decomposition Analysis and Ligand Field Theory. The results explain the different ways of ligand binding and how the electronic structure of the central metal ion and the spin state affect the coordination pattern. Our results pave the way for the rational design of transition-metal complexes.

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