X-ray Diffraction Studies on the Binding Affinity of Solvent Molecules in Co/Ni Metal Complexes

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Abstract

Solvent molecules or counter anions often affect the molecular structure or conformation. In metalloenzyme research, such changes can even influence its normal function. In this work, two series of Co/Ni complexes with octahedral local structure are designed to study the solvent molecules and counter anions bonding effects on axial positions by controlling 2-(1-benzyl-1H-tetrazol-5-yl)pyridine) (1BTP) as equatorial bonding ligands. Based on the *ab* initio structure determination from powder x-ray diffraction (PXRD) and single crystal x-ray diffraction (SXRD) analysis, we have obtained the structures of $[Co^{II}(1BTP)_2(EtOH)_2](ClO_4)_2$ (**1**), $[Co^{II}(1BTP)_2(H_2O)_2](ClO_4)_2$ (**2**), $[Ni^{II}(1BTP)_2(EtOH)_2](ClO_4)_2$ (**3**), $[Ni^{II}(1BTP)_2(H_2O)_2](ClO_4)_2$ (**4**), $Co^{II}(1BTP)_2(NO_3)_2$ (**5**), and $Ni^{II}(1BTP)_2(NO_3)_2$ (**6**). The coordination environment at equatorial positions of these complexes are four nitrogen atoms derived from two tetrazole and pyridine in 1BTP ligands. The axial sites of complex **5** and **6** are oxygen atoms of both nitrate ligands. Those become oxygen atoms of ethanol in complex **1** and **3**. However, the axial positions are replaced by H_2O in complex **2** and **4**. Based on these results, we propose that the binding affinities are $H_2O > C_2H_5OH$ and $NO_3^- > ClO_4^-$. The analysis process of PXRD and the detailed bond distances, angles and conformations of these complexes will also be discussed in this poster.

Keywords : High Resolution Powder X-ray Diffraction, Rietveld refinement, metal complex