

Structure Determinations by Powder X-ray Diffraction on 2,6-di(1H-tetrazol-5-yl)pyridine and its Related Complexes

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Abstract

Luminescence substance has potential to apply on modern manufacture with materials to be used in photoelectric, biomedicine, analyzing, and so on. If one substance has luminescence and other physical properties, such as magnetism, conductivity, or mechanical, which will be more useful in applications. In this report, 2,6-di(1H-tetrazol-5-yl)pyridine (**DITZP**), which has been reported as a tridentate ligand, has the maximum emission intensity around 350 nm ($\lambda_{\text{ex}} = 282$ nm). Therefore, we use **DITZP** to synthesize the iron complex **1** and complex **2** by using ethanol and dimethyl sulfoxide, respectively. The structure of these complexes are determined by powder x-ray diffraction (PXRD) and extended x-ray absorption fine structure (EXAFS). The cell constants are indexed by DICVOL and N-TREOR programs first. Second, we build a model to optimize in real space by using simulated annealing algorithm. After confirming the similarity between experimental and simulated X-ray diffraction patterns, we use Rietveld refinement to refine the geometric parameters and get the completed final structure. Based on PXRD results, complex **1** and complex **2** are not isostructures. The crystal system of complex **1** is monoclinic and the cell constants are $a = 13.8253(8)$ Å, $b = 9.1553(6)$ Å, $c = 8.8635(5)$ Å, $\alpha = 90^\circ$, $\beta = 97.809(5)^\circ$, $\gamma = 90^\circ$; the crystal system of complex **2** is also monoclinic and the cell constants are $a = 17.4427(2)$ Å, $b = 17.2021(3)$ Å, $c = 7.1092(2)$ Å, $\alpha = 90^\circ$, $\beta = 93.147(4)^\circ$, $\gamma = 90^\circ$. According to Rietveld refinement results, the local symmetry of Fe site in both complexes are octahedral. In equatorial positions of complex **1**, there are one oxygen atom from ethanol and three nitrogen atoms from **DITZP**. The axial positions are two nitrogen atoms from **DITZP**. In complex **2**, the Fe are bonded with four nitrogen atoms from **DITZP** in equatorial positions and the axial positions are bonded with two oxygen atoms from water.

Keywords : *PXRD, EXAFS*