Structure and Luminescence Studies on 2-(2-(4-((5-(pyridin-2-yl)-1H-tetrazol-1-yl)methyl)benzyl)-2H-tetrazol-5-yl)pyridine and it's chelating FeII Metal Complex

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Abstract

Compounds with fluorescence characters are often used as sensing devices in various fields. The conjugation property of chemical bonds is easier to cause the compound fluorescent, so we choose compounds containing benzene ring for synthesis. We synthesized a series of ligands based on 5-(2-Pyridyl)-1H-tetrazole and 1,4-bis(bromomethyl)benzene. They are 1,4-bis((5-(pyridin-2-yl)-1H-tetrazol-1-yl)methyl)benzene (**PPB1**), 2-(2-(4-((5-(pyridin-2-yl)-1H-tetrazol-1-yl)methyl)benzyl)-2H-tetrazol-5-yl)pyridine (**PPB2**), and 1,4-bis((5-(pyridin-2-yl)-2H-tetrazol-2-yl)methyl)benzene (**PPB3**). The powder x-ray diffraction (PXRD), extended x-ray absorption fine structure (EXAFS), ultraviolet-visible (UV-vis), and photoluminescence (PL) spectroscopies are used to characterize the geometric and electronic structures of these compounds. First, the cell parameters of these compounds are obtained by DICVOL and N-TREOR program based on the PXRD data. Then the global optimization was used to get the best model for Rietveld refinement based on simulated annealing algorithm. The cell constants of **PPB1** are a = 13.2931(8) Å , b = 15.240(1) Å , c = 9.3891(5) Å , α = 90°, β = 96.742(2) °, γ = 90 °, and its space group is P 2_1/n. The cell constants of **PPB2** are a = 4.6 Å , b = 14.32 Å , c = 28.65 Å , α = 90°, β = 90 °, γ = 90 °, and its space group is P bcn. The cell constants of **PPB3** are a = 35.301(1) Å , b = 8.3868(2) Å , c = 6.2858(2) Å , α = 90°, β = 94.2810(3) °, γ = 90 °, and its space group is P 2_1/a. The **PPB1** and **PPB2** display luminescence characters at emission wavelength 394 nm and 435 nm by the excitation wavelength at 350 nm and 370 nm respectively. Furthermore, Iron(II) perchlorate hydrate was used to synthesize a new complex, $Fe^{II}(H_2O)_2(PPB2)_2(ClO_4)_2$. The cell constants are a = 29.38 Å , b = 9.8041 Å , c = 9.917 Å , α = 90°, β = 90 °, γ = 90 °. According to EXAFS results, the averaged Fe-N and Fe-O distances are 2.12(1) Å , and the center metal is hexa-coordinate octahedron.

Keywords : Fluorescence , Powder x-ray diffraction, Rietveld refinement