Strueture and physical properties study on $[Fe(2BTP)(bpy)_2](ClO_4)_2$

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Abstract

In recent years, the capability of applying the intrinsic bistability of spin crossover(SCO) materials for data storage, switchable or sensing devices has been demonstrated. In general, tetrazoles, pyridines, and their derivatives are often used to synthesize new SCO compounds. In this work, we successfully synthesize two bidentate ligands which are 2-(1-benyl-1H-tetrazol-5-yl)pyridine(1BTP) and 2-(2-benyl-2H-tetrazole-5-yl)prydine(2BTP). In addition, we also synthesize an iron(II) coordination polymer with formula $[Fe(2BTP)(bpy)_2](ClO_4)_2$ (**1**) (bpy=4,4'-bipyridine). Based on X-ray single crystal analysis, the structure is crystallized in monoclinic system. The cell constants of **1** are a = 21.796(1) Å, b = 11.1621(5) Å, c = 16.3743(7) Å, α = 90.00 °, β = 93.466(2)°, γ = 90.00° and space group is C 2/c. The Fe is located on 2-fold rotation axis and coordinated by one 2BTP and two bpy ligands, so that the local pseudo symmetry of Fe site is octahedral. The averaged distance of six Fe-N bonds is Fe-N=1.99(2) Å. Moreover, the Fe K-edge extend absorption fine structure (EXAFS) analysis indicated that the Fe of **1** is coordinated by six atoms with averaged distance Fe-N = 1.98(2) Å. These bond distances indicated that complex **1** is at low spin state at room temperature.

Keywords: EXAFS、PXRD、SCO