Synthesis and spectroscopic characterization of a novel copper(II) complex with sulfathiazole and bipyridine

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Introduction

Copper(II) is present in many enzymes of the human body, acting mostly in redox reactions. Oxidative stress is one of the causes of many pathological processes, such as inflammatory damage, aging, and even some types of sclerosis. The copper(II) scavenging activity against free radicals is significant in avoiding oxidative stress and, therefore, many diseases.[1-2]

Copper(II) complexes and their biological properties have also been studied aiming the development of new metallodrugs. In the literature, it has been reported that copper(II) complexes with mixed ligands are more active when a nitrogen donor heterocyclic ligand is present, such as 2,2'-bipyridine.[3]

Sulfathiazole ($C_9H_9N_3O_2S_2$, SFT) is a sulfonamide used in humans. It has been used with other sulfonamides such as sulfabenzamide and sulfacetamide in preparations for the topical treatment of skin infections. Metal complexes with sulfathiazole have been reported in the literature. Recently a silver complex with SFT, which shows antibacterial activities over Gram-positive and Gram-negative bacterial strains, was prepared in our laboratory.[4] The present work deals with the synthesis and characterization of a novel copper(II) complex with sulfathiazole and bipyridine.

Results and Discussion

The synthesis of the copper(II) complex with sulfathiazole (SFT) and 2,2'-bipyridine (bipy) was carried out in methanol using 1.0 mmol of SFT, ammonium hydroxide, 0.50 mmol of bipy and 0.50 mmol of copper nitrate. The greenish obtained complex was shown to be soluble in dimethylsulfoxide (DMSO) and dimethylformamide (DMF). Elemental analysis for carbon, hydrogen and nitrogen was performed using a Perkin Elmer 2400 CHNS/O Analyser. The analysis led to a 1:1:1 metal/bipy/SFT composition. *Anal. Calc.* for $[Cu(bipy)(SFT)(OH)]\cdot H_2O$: C, 44.8; H, 3.76; N, 13.7. Found: C, 44.9; H, 3.35; N, 14.8.

Thermogravimetric analysis reinforces the molar composition proposed by elemental analysis. Thermal decomposition of the complex starts at 190 °C, with the formation of CuO as the final residue *Anal. Calc.* for loss of hydration water (25-82°C): 3.5%. Found 2.4%. *Anal. Calc.* for loss of ligands ($C_{19}H_{17}N_5O_3S_2$) (190-535°C): 83.6%. Found: 79.1%. *Anal. Calc.* for the formation of CuO (535°C): 15.5%. Found: 17.2%.

The mass spectrum was acquired on a Waters Quattro Micro API with direct infusion and operating in the positive mode. The complex was dissolved in DMSO and further diluted 100-fold in methanol. In the spectrum of the complex the peak at *m/z* 473.4 corresponds to the $[Cu(bipy)(SFT)]^+$ species, which confirms the 1:1:1 metal/bipy/SFT composition.

The infrared (IR) spectrum was obtained in KBr pellets using a Bomen MB-Series Model B100 FT-IR spectrophotometer in the range of 4000-400 cm^{-1} with resolution of 4 cm^{-1}. In the SFT spectrum the v(N-H) vibration band of the SO_2N-H group is observed at 3283 cm^{-1}, while in the complex this vibration band is no longer observed. This result indicates the loss of the hydrogen atom of the SO_2N-H group and suggests the coordination of the nitrogen atom of the sulfonamide group to the metal. The coordination mode of SFT is the same observed for the silver-sulfathiazole complex reported in the literature. [4]

Conclusions

Molar composition of the copper(II) complex with SFT and bipyridine was found to be 1:1:1 metal/bipy/SFT. Elemental, thermogravimetric and mass spectrometric analyses confirm the coordination formula $[Cu(bipy)(SFT)(OH)]\cdot H_2O$. Sulfathiazole coordinates to copper(II) by the nitrogen of the sulfonamide group. The compound is soluble in DMSO and DMF.

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