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On conformational isomerism of a Ru(II) complex and potential anticancer activities to its derivatives.

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Palavras Chave: *Ruthenium complexes, Fluorescent complexes, 1,4-Bis(diphenylphosphino)butane, Isomerism.*

Highlights

Biphosphine complexes of ruthenium(II); Fluorescent complexes of ruthenium(II); Probable conformational isomerism of ruthenium(II) complex; Solid state NMR of ruthenium(II) complexes to evaluate conformational isomerism.

Abstract

Ruthenium complexes have been excelled for demonstrating potential activity against cancer and against infectious diseases.[1] Thus, one approach in the field of cancer is related to the target of the agent on study. In this case, should be good to know how the drug, or the potential drug, interacts with the target, by which mecanism, and to know if the compound acts inside, or outside the cell, for instance. Trying to answer some of these questions, in this work new ruthenium complexes with fluorescence properties, were synthesized, and for this a pyrene(py) derivative, a quimiosensor specie, was used as ligand.[2] The new ruthenium complexes have in their coordination sphere, basically, the 1,4-bis(diphenylphosphino)butane, 2-(1-pyrenil)1*H*-imidazo[4,5-*f*][1,10]-phenantroline (pyphen), using the chloride complex as precursor (see Fig. 1). To complete the coordination sphere of the metal, mercapto ligands were used (Complex A2, Fig. 2). It is interesting to mention that the $^{31}P\{^{1}H\}$ NMR spectrum of the precursor showed a complex pattern, different of the expected for a AX system, suggesting that more than one specie was in solution, according Fig. 3. Also, the spectra of the complex are a little different, depending of the solvent used in the experiment. The hypothesis of the presence of more than one compound in solution was discarded by cyclic voltammetry experiments, where only one oxidation process, Ru(II)→Ru(III), was observed, which was supported by mass spectra data. In order to evaluated the presence of possible isomers of the precursor, in solution, NMR spectra, in solid state, were undertaken, and the results suggest the presence of conformational isomers, which was confirmed by $^{31}P\{^{1}H\}$ experiments, where at least five signals were observed. Additionally, worth it to mention that the reaction of the precursor with the mercapto ligand (complex A2), only one complex was obtained, again, suggesting that in the precursor solution only one specie was present. Worth it to mention that, the obtained complexes are fluorescent, and can be used as probe to study the mechanism of their interaction with the cancer cells.

Fig.1- Precursor

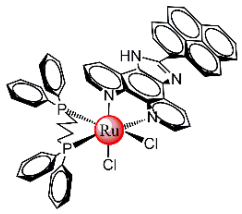


Fig. 2- Complex A2

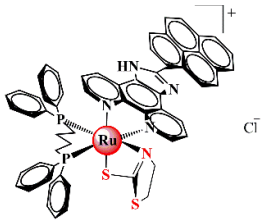


Fig. 3- NMR ^{31}P spectra to precursor and complex A2 in CH_2Cl_2/D_2O

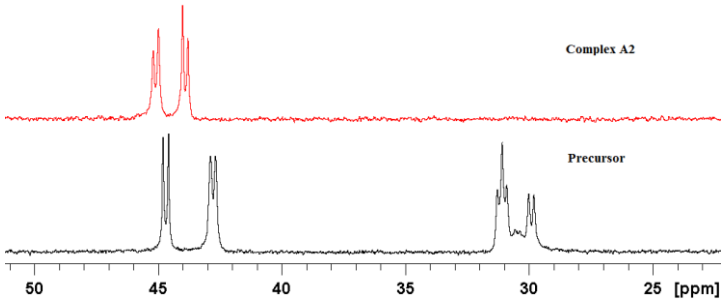
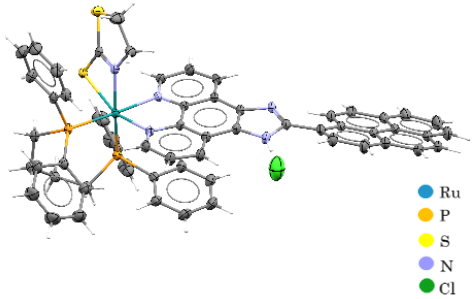


Fig. 4- X-ray diffraction to complex A2



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