

# Study of the structural and spectroscopic properties of Cu(I) and Ag(I) isothiocyanate complexes containing neutral ligands

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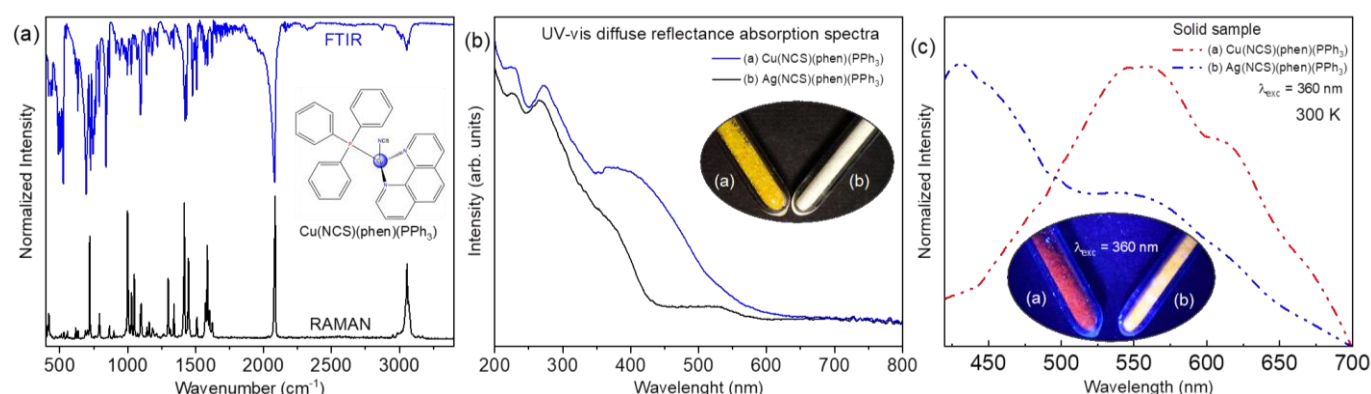
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## Highlights

Cu(I) and Ag(I) complexes with luminescence in wide range of the visible spectrum. Structural influence on luminescence properties.

## Resumo/Abstract

Coordination compounds containing Cu(I) and Ag(I) are among the most studied in the field of luminescent materials. One of the most interesting features, which has attracted attention to these compounds, is the possibility of emitting different colors in the visible region (blue to red) [1]. In this way, one of the main challenges is the preparation of compounds that present thermal and photophysical stability and high emission quantum yield, mainly for application in luminescent devices [2]. Herein, we synthesized, characterized and studied the photophysical properties of coordination compounds based on Cu(I) and Ag(I), containing isothiocyanate (NCS<sup>-</sup>) as an anionic ligand, also nitrogenous neutral ligands (LN) and triphenylphosphine (PPh<sub>3</sub>), with the general formula [M(NCS)(LN)(PPh<sub>3</sub>)] in which M: Cu(I) or Ag(I) and LN: pyridine, 2,2'-bipyridine, 1,10-phenanthroline, 5-nitro-1,10-phenanthroline and 1,10-phenanthroline-5,6-dione. Furthermore, in this work we investigate the influence of these different neutral ligands coordinated to the metal center on the metal–ligand charge transfer (MLCT) state. The FTIR, Raman spectra (Figure 1a), TGA/DTA, elemental analysis, diffuse reflectance (UV-vis), and emission were carried out, indicating the formation of the complexes. Thus, the thermal stability of the compounds was analyzed by TGA/DTA, the onset of decomposition varied within a range of 150-200°C. According to UVvis absorption spectra by diffuse reflectance the M'(NCS)(phen)(PPh<sub>3</sub>) shows an absorption range from 200 to 600nm, the Cu(I) complex presenting low LMCT states (Figure 1b). The Cu(I) and Ag(I) complexes presented distinct characteristics regarding the emitting properties, displaying red and yellow color emission, as presented in Figure 1c.



**Figura 1.** a) Infrared and Raman spectra of the Cu'(NCS)(phen)(PPh<sub>3</sub>), b) UV-vis diffuse reflectance spectra and inserted photographs (under daylight) of the Cu'(NCS)(phen)(PPh<sub>3</sub>) and Ag'(NCS)(phen)(PPh<sub>3</sub>), and c) Emission spectra and photographs (under 360 nm UV light) of the Cu'(NCS)(phen)(PPh<sub>3</sub>) and Ag'(NCS)(phen)(PPh<sub>3</sub>) complexes at 300 K.

## Reference

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