XXI Brazilian Meeting on Inorganic Chemistry
X Brazilian Meeting on Rare Earths
III Workshop on Theoretical Bioinorganic Chemistry
Belo Horizonte, September 12 - 15th 2024

Spectroscopic studies in Sb(III) alkyl xanthate complexes

Maria A. Oliveira (IC); Daniella B. Miranda (PG)[a] ; Glaucio B. Ferreira (PQ)[a,b], Susana Quintal* (PQ)[b]

[a] Universidade Federal Fluminense, PPGQ, Niterói, RJ, Brasil
[b] Universidade Federal Fluminense, GQI, Niterói, RJ, Brasil
E-mail: * squintal@id.uff.br

Thematic Area: Main group

Keywords: Xanthate, Sb(III) complexes, UV-Vis spectroscopy

Antimony is a semimetal belonging to group 15 of the periodic table, with industrial applications in the production of semiconductors, infrared detectors, and diodes.[1] Biologically, antimony compounds have been used as drugs since their introduction in the 14th century, in the treatment of two parasitic diseases: leishmaniasis and schistosomiasis.[2] In this work, the synthesis of distorted octahedral antimony(III) complexes containing three isopropyl, isobutyl, methyl or ethyl xanthate bidentade ligands, [Sb(alkyl xanthate)$_3$], and their respective spectroscopic characterizations will be presented: Infrared, UV-Vis, Raman and NMR spectra. The infrared spectra of the complexes show the presence and slight displacement of the xanthate bands at approximately 1270, 1100, 1060, and 690 cm^{-1}, assigned to the ν_{as}C-O-C, νC=S, ν_sC-O-C and νC-S vibrational modes, respectively. The formation of the complexes was further corroborated by the far-infrared spectrum, which exhibited the Sb-S stretching mode at 318 cm^{-1}. The UV-Vis spectra (acetonitrile, 10^{-4} M) showed the characteristic bands of the xanthate group, assigned to the n→π* and π→π* transitions, at *ca.* 220 and 300 nm, respectively. TD-DFT and population analysis theoretical calculations were performed at the B3LYP level with 6-311++G** basis set. Bands at 224 and 247 nm were assigned to the n→π* and π→π* electronic transitions, respectively. The orbitals involved on the transitions were determined by population analysis (Figure 1).

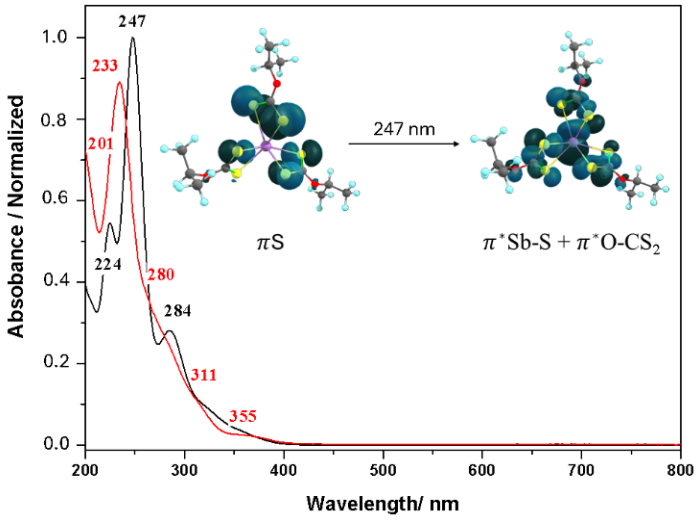

Figure 1. Electronic spectra of [Sb($S_2COCH(CH_3)_2$)$_3$]: black - theoretical (B3LYP/6-311++G**/acetonitrile) and red - experimental (acetonitrile, 10^{-4} M) and orbitals involved on the π→π* transition.

Acknowledgments: CNPq, CAPES, FAPERJ, LDRX, LMQC, LAME and PROPPi UFF.

References

[1] S. Sundar, J. Chakravarty, Int. J. Environ. Res. Public Health. **7**, 4267 (2010).
[2] E. Moore, *et al*., Bulletin of the WHO. **79**, 388 (2001).