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Coordination chemistry in pyridine and imidazole compounds containing gem-diol moieties: solidstate NMR and X-Ray studies

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The need for clean technology either for fine chemistry or for waste treatment leads to the replacement of traditional \mathbf{I} inorganic oxidants such as K₂Cr₂O₇ and KMnO₄ by benign, easy-to-handle oxidants, such as H₂O₂ and O₂. The activation of H₂O₂ can be achieved by transition-metal ion complexes with organic ligands. Particularly, H₂O₂ can produce OH• via the Cu(II)/Cu(I) cycle involving different reaction pathways. A high number of metal complexes bearing gem-diols has been reported, in which the presence of these moieties is generally demonstrated by single-crystal X-ray diffraction. As a rule, the stability of this functional group is not studied in the free ligand before the preparation of the metal complex. Understanding the chemistry of gem-diols is crucial for the development of synthetic methods to obtain new organic ligands, which are often used for the design of metal complexes with catalytic activity. In this context, solid-state NMR (ss-NMR) is a useful methodology to elucidate the chemical composition of mixtures in which both gem-diol and carbonyl forms are present in cases where the single-crystal cannot be obtained for X-ray studies. Additionally, the ¹H-MAS ss-NMR spectra (@60 kHz) can also bring structural information about the ligands surrounding the paramagnetic center. To have an insight into the chemistry of gem-diol compounds, the aim of this work is to study the gem-diol generation and copper coordination properties in imidazole- and pyridinecarboxaldehydes through the combination of ss-NMR and single-crystal X-ray diffraction techniques. Complementary analyses were performed by solution-state NMR, high-resolution mass spectrometry (HRMS), and ¹H ss-NMR. These studies allow us to expand the chemistry in metal complexes in terms of structural diversity of the ligands at the same time that new Cu(II)-homogenous catalyst towards the activation of H₂O₂ will be explored.



Recent Publications:

- Lázaro Martínez et al. (2016) New insights about the selectivity in the activation of hydrogen peroxide by cobalt or copper hydrogel heterogeneous catalysts in the generation of reactive oxygen species. J. Phys. Chem. C. 120(51):29332-29347.
- 2. Lombardo Lupano et al. (2014) synthesis, characterization, and catalytic properties of cationic hydrogels containing copper (II) and cobalt (II) ions. Langmuir. 30(10):2903-2913.
- 3. Lázaro Martínez et al. (2010) NMR Characterization of hydrate and aldehyde forms of imidazole-2-carboxaldehyde and derivates. J. Org. Chem. 75(10):3208-3213.

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4. Crespi A F et al. (2016) gem-Diol and hemiacetal forms in formylpyridine and vitamin-B6 related compounds: solidstate NMR and single crystal X-ray diffraction studies. J. Phys. Chem. A. 120(39):7778-7785.

Biography

Juan M Lazaro Martinez obtained his PhD in Organic Chemistry from University of Buenos Aires (UBA) in 2011. His work is based on the development, characterization and applications of hydrogel materials has received two important mentions: "Dr. Luis Federico Leloir 2012 Prize" (UBA), "SAIQO 2013 Prize" to the best PhD thesis in the area of organic synthesis (SAIQO -Argentine Society of Research in Organic Chemistry). He was a Postdoctoral fellow at the Enrique Gaviola Institute of Physics of National University of (UNC), Argentina. Currently, he is an Assistant Professor of Organic Chemistry at UBA. He is a Member of the Institute of IQUIMEFA-CONICET as a Researcher. His areas of research are focused on the synthesis and crystalline properties of poly(ethylenimine) polymers with biotechnology applications and structural elucidation in Cu- and Co-complexes studied by solid-state NMR and single-crystal X-ray techniques with environmental and synthetic applications.

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