

Pyrones and related ligand analogues in applied inorganic chemistry.

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3-Hydroxypyrones, and their corresponding analogues 3-hydroxypyridinones are a versatile range of ligands, and both groups of compounds contain several classes of compounds.[1]

The commercially available pyrones: 3-hydroxy-2-methylpyran-4-one (1) and 3-hydroxy-2-ethylpyran-4-one (2) were functionalised to yield the respective 3-hydroxy-2-methylpyrid-4-one (3) and 3-hydroxy-2-ethylpyrid-4-one (4) derivatives. These ligands were then coordinated to an array of metals to form the corresponding complexes. A total of eight bidentate ligands were used in this study with different electronic and steric demands. These ligands are explored for: (i) the potential beneficiation of Hafnium and Zirconium for the nuclear industry, (ii) application as model complexes for diagnostic and therapeutic radiopharmaceuticals in studies using the fac-ReI(CO)₃⁺ core and (iii) exploiting as model Rhodium(I) homogeneous catalysts.[2][3]

In all the respective sub-sections of this study solid state systematic structural characterisation of crystalline products of the above mentioned compounds, intended on revealing the coordination modes that can be observed, were extensively evaluated by means of single crystal X-Ray Diffraction (XRD), and will be given.

Thus, this presentation will cover a detailed structural discussion of the in-depth analysis and comparison with similar Zr(IV), Hf(IV), Re(I) and Rh(I) compounds which could yield valuable insight into physical and/or chemical state differences to be exploited for purification/separation techniques, diagnostic and therapeutic endeavours and catalytic processes respectively.

Finally, structure/ reactivity relationships will be attempted to assist in future prediction of relevant characteristics of these compounds.

[1] Xu , L. et al. (2015). J. Nucl. Mater. 466, 21-28.

[2] Alberto, R. et al. (1999). Coord. Chem. Rev. 190–192, 901–919.

[3] Roodt, A. et al. (2003). Coord. Chem. Rev. 245, 121–137.

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