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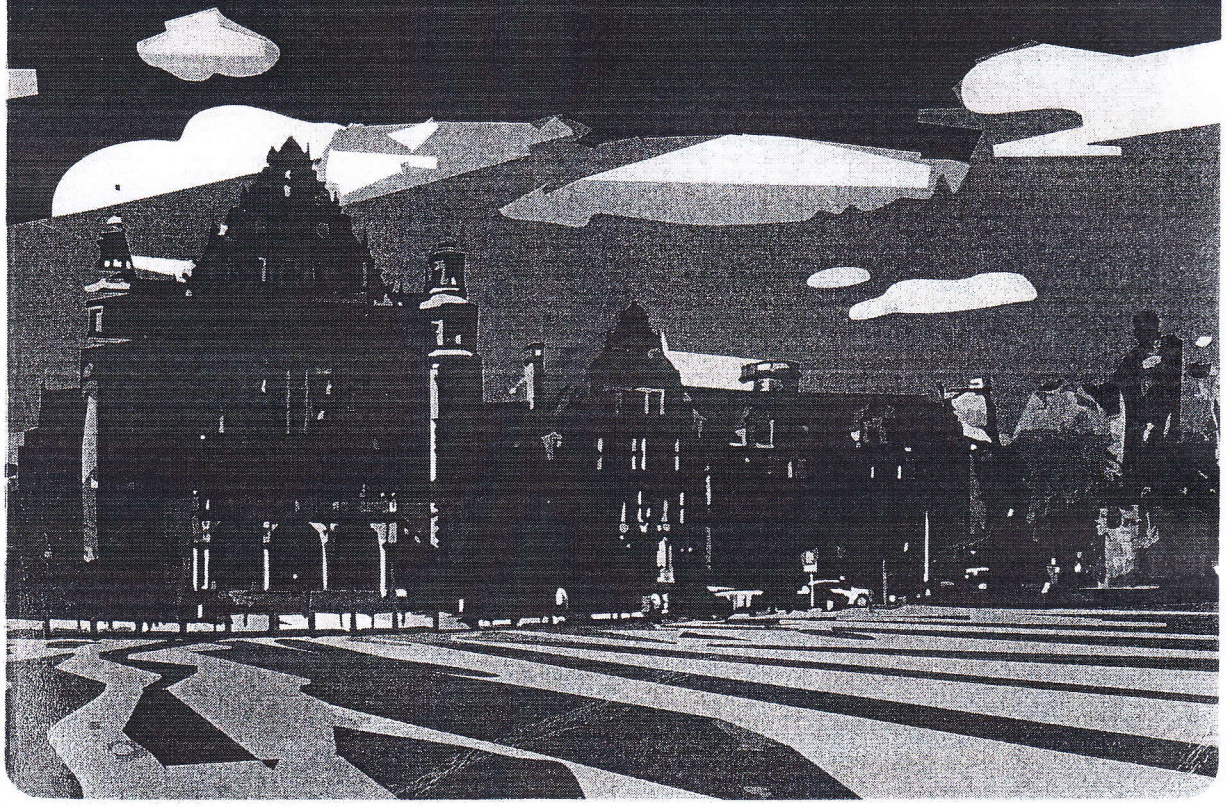
Book of Abstracts



Chiral Molybdenum and Tungsten Complexes Bearing Oxazoline-Derived Cyclopentadienyl Ligands

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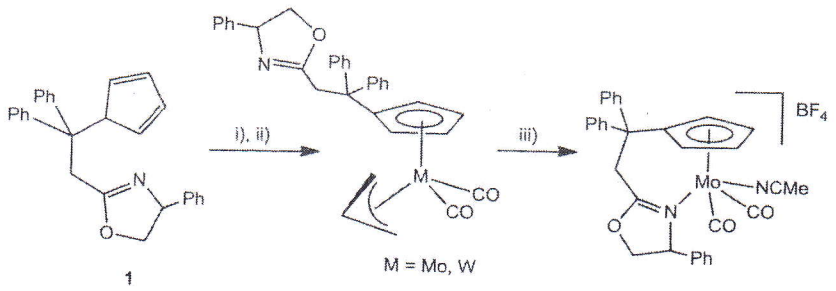
In the last years, $CpMO_2R$ compounds (M = Mo, W; R = halogen, alkyl) and their carbonyl precursors $CpM(CO)_3R$ have shown to be excellent catalysts for the epoxidation of olefins with *tert*-butylhydroperoxide (TBHP) [1] and for the oxidation of sulfides with TBHP and H_2O_2.[2] Based on these results, we became interested in developing effective chiral cyclopentadienyl-based catalysts for their use in the asymmetric version of these oxidation reactions. We envisaged that the synthesis of a cyclopentadienyl ring functionalized with an oxazoline group might provide a chiral chelate ligand capable to increase the stability of their metal complexes and favour the rigidity required for the preparation of effective asymmetric catalysts.
Here we report the synthesis of the novel cyclopentadienyl-oxazoline hybrid ligand **1** and their coordination to molybdenum and tungsten metals. A series of molybdenum and tungsten species bearing **1** have been synthesized and fully characterized by NMR (^1H, ^{13}C, ^{95}Mo) and IR spectroscopy, mass spectrometry, elemental analyses and X-ray diffraction studies. These species displayed high activity in the epoxidation of *cis*-cyclooctene and limonene. Their performance in asymmetric epoxidation of olefins will be discussed.



Reaction conditions: i) BuLi/THF; ii) $M(\eta^3\text{-}C_3H_5)Cl(CO)_2(NCMe)_2$; iii) HBF_4

References:
[1] Abrantes, M.; Santos, A.M.; Mink; J.; Kühn, F.E.; Romão, C.C. *Organometallics* **2003**, *22*, 2112 and references therein. [2] Gamelas, C.A.; Lourenço, T.; da Costa, A.P.; Simplicio, A.L.; Royo, B.; Romão, C.C. *Tetrahedron Lett.* **2008**, *49*, 4708.