Complexation of Molybdenum(VI) by *O,S*-Donor Ligands. Solution and X-ray Studies

Marco Gil[a], Sílvia Chaves[a], Ratomir Jelic[a], M. João Romão[b], José Trincão[b], Eberhardt Herdtweck[c], and M. Amélia Santos[a*].

[a] Centro de Química Estrutural, Instituto Superior Técnico, Portugal. [b] REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Portugal. [c] Technische Universität München, Department Chemie, Germany.
[*] masantos@ist.utl.pt.

The biological relevance of molybdenum is well known and is related to the fact that it is part of a cofactor called molybdopterin, where the Mo atom is coordinated to the dithiolene group of the organic cofactor. The molybdopterin is present in a large range of redox enzymes, such as xanthine oxydase.

Mo complexes with 3-hydroxy-4-pyridinones (*N*-heterocyclycic *O,O*-bidentate ligands) have been studied in solid state and in solution, by several groups including ours, and also bioassayed in animal models for the treatment of cardiac dysfunction associated with diabetes. Since in biology, the Mo-coordination usually involves S-donor atoms, we have decided to study the Mo-complexation with two model molecules containing *O,S*-donor atoms, namely thiopyrone and a 3-hydroxy-4-thiopyridinone derivative. We report herein the X-ray crystal structure of Mo-thiopyrone complex and the solution equilibrium studies of the Mo-complexation for both ligands. The crystal structure determination revealed that the complex possesses two Mo atoms bridged by an oxygen atom, each coordinated to a thiopyrone and by two additional oxo groups.

The molecular structure of $[MoO_2(thiopyrone)]_2(\mu\text{-}O)$ with ellipsoids at 30% probability, at 177K.