

Poster Presentations

[MS37-P09] **An in-depth crystallographic study of tantalum(V) and niobium(V) complexes utilizing various mono- and bidentate ligands.**

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The separation of niobium and tantalum has always been a complicated process, particularly due to their near identical chemical properties. Niobium(V) and tantalum(V) are both hard metal centres and the halido species are known to readily hydrolyse.[1] In this present investigation of tantalum(V) and niobium(V) complexes, different mono-(carbene) and bidentate ligands (*L,L'*-*Bid*) have been used in synthesis, in an attempt to study the variation in activity and selectivity of coordination of *L,L'*-*Bid* to tantalum-halides, -methoxides. (*L,L'*-*BidH* = acacH, tfaaH, hfaaH and tropH). Different synthetic procedures and characterization methods of these complexes will be discussed. Tantalum(V) and niobium(V) complexes of the type [Ta(X)₄(*L,L'*-*Bid*)] (X = halides, OMe and OEt; examples of *L,L'* = acetylacetonato (acac), dibenzoylmethanato (dbm) and tetramethylheptanedionato (thmd)), were synthesized and characterized by nuclear magnetic resonance spectroscopy (NMR) and infrared (IR).[2] Moreover, single crystal X-ray diffraction was used to evaluate the characteristics of a range of complexes, and the results of the obtained structures containing mono-(halido and pseudo halido) and bidentate hard ligands *O,O'*- and *N,O*-donor atoms will be presented and discussed.[3] A kinetic investigation of acacH coordination to solvated TaCl₅ is also presented. The reaction is defined by limiting kinetic behaviour and is indicative of a two-step process. This involves the rapid formation of a proposed *trans*-[TaCl₂(OMe)₃(η¹-acacH)]-intermediate. Comparison of the forward rate constants for the two steps, *k*₁ and *k*₂ indicates

that the first reaction is approximately six orders of magnitude (10⁶) faster than the second slower, rate determining step.

[1] J. B. Lambert. *Kirk-Othmer Encyclopedia of Chemical Technology*. 2011, John Wiley & Sons, Inc., 1-23.

[2] N.N. Greenwood, A. Earnshaw, *Chemistry of the Elements*, 1997, 976.

[3] S. Basson, *Transition Met. Chem.*, 1982, **7**, 207-209.

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