[MS37-P09] An in-depth crystallographic study of tantalum(v) and niobium(v) complexes utilizing various mono- and bidentate ligands. Renier Koen\textsuperscript{a}, Hendrik Visser\textsuperscript{a} and Andreas Roodt\textsuperscript{a}

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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 \((L,L'\textsuperscript{-Bid})\) have been used in synthesis, in an attempt to study the variation in activity and selectivity of coordination of \(L,L'\textsuperscript{-Bid}\) to tantalum -halides, -methoxides. \((L,L'\textsuperscript{-BidH})=\text{acacH, tfaaH, hfaaH and tropH}\). Different synthetic procedures and characterization methods of these complexes will be discussed. Tantalum(V) and niobium(V) complexes of the type \([\text{Ta}(X)\text{}\text{(L,L'\textsuperscript{-Bid})}]\) \((X=\text{halides, OMe and OEt}; \text{examples of L,L' = acetylacetonato (acac), dibenzoylmethanato (dbm) and tetramethylheptanedionato (thmd)})\), 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 \(\text{trans-[TaCl}_2(\text{OMe})_2(\eta\text{-acacH})}\)-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 \((10^6)\) faster than the second slower, rate determining step.


\textbf{Keywords:} tantalum, niobium, separation, bidentate ligands.