

**MS29-P10** Halogen-halogen, halogen-oxygen, and dipolar interactions in a series of  $\text{Re(I)}(\text{CO})_3$  complexes with halogen-substituted nitrogen-donor ligands

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Intermolecular interactions are of significant interest in chemistry, mainly because they are responsible for stabilization of many important molecules such as DNA and proteins [1]. They have also important roles in the arrangement of molecular species in crystal packing. Therefore, they are one of the main foci in the field of crystal engineering because of their structural role on the physical properties of crystalline materials such as nonlinear optics, electrical, and magnetic properties [2]. In this study, the effect of different intermolecular interactions such as halogen-halogen, halogen-oxygen, and  $\pi$ - $\pi$  interactions has been investigated on the crystal packing of  $\text{Re}(\text{CO})_3$  complexes with halogen-substituted nitrogen-donor ligands.

References

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**MS29-P11** Insights into solution and solid-state coordinative properties of tantalum(V) and niobium(V) metal centres.

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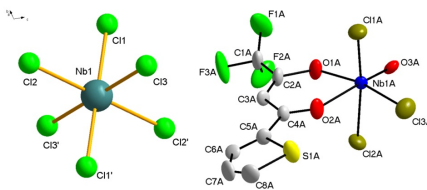
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Tantalum(V) and niobium(V) are two transition metals found in the vanadium triad in the periodic table, with very similar chemical properties, and always occur together in nature. Both elements have hard metal centres and the halido species are known to readily hydrolyse to form relatively unreactive oxido species, which severely inhibit bidentate ligand coordination to these metal centres.[1] Accordingly, in-depth investigations of the coordinative preferences of these elements remain elusive.

In this present investigation of tantalum(V) and niobium(V) complexes, a range of functionalized mono-charged bidentate ligands (*L,L'-Bid*) has been used in synthesis, in an attempt to study the variation in activity and selectivity of coordination of *L,L'-Bid* to the metal halides in both solid- and solution state. [*L,L'-Bid*H = functionalized acetylaceton- (acacH), 8-hydroxyquinoline- (oxH) and tropolone (tropH) derivatives].

Two new stable (relatively hydrolysis resistant) synthons  $(\text{Et}_3\text{N})[\text{NbCl}_6]$  (see Figure 1 a) and  $(\text{Et}_3\text{N})[\text{TaCl}_6]$  have been instrumental in the success of  $\beta$ -diketone and tropolone ligand coordination to tantalum and niobium metal centres.[2] Crystal structures have been obtained for numerous complexes, with examples including:  $[\text{Nb}(\text{trop})_2\text{Cl}]$ ,  $[\text{Ta}(\text{trop})_2\text{Cl}]$ ,  $(\text{Et}_3\text{N})[\text{NbOCl}_2(\text{tfa})]$  (see Figure 1 b),  $(\text{Et}_3\text{N})[\text{NbOCl}_2(\text{hfaa})]$  and  $(\text{Et}_3\text{N})[\text{NbOCl}_2(\text{bfa})]$ , where tropH = tropolone, tfaH = thenoyltrifluoroacetone, hfaaH = hexafluoroacetylacetonone, bfaH = benzoyltrifluoroacetone and tffaH = trifluorofurylacetonone. Differences in coordination modes and crystal packing of these isostructural complexes have been identified in an attempt to gain insight into these compounds to assist in predictions of properties for future use.

Additionally, to further evaluate the electronic environment experienced by the niobium(V) and tantalum(V) centres in these complexes, a solution-state kinetic study of the substitution reactions of  $[\text{NbCl}_6]^-$  and  $[\text{TaCl}_6]^-$  with a range of  $\beta$ -diketones as entering ligands was undertaken. These results will also be reported and correlated to entering ligand electronic characteristics.



**Figure 1.** (a) Ball-and-stick representation of  $(\text{Et}_3\text{N})[\text{NbCl}_6]$  (tetraethylammonium counter-ion omitted) (b) Ball-and-stick