Exploring The Scope of Transition Metal Complexes Bearing Imidazol(in)ium-2-dithiocarboxylate Ligands

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Despite the widespread use of N-heterocyclic carbenes (NHCs) as neutral, twoelectron donors in organic synthesis and in organometallic chemistry, only a modest number of reports have looked at their potential to generate other ligand systems. Yet, the facile reaction of NHCs with heteroallenes X=C=Y such as COS, CS₂, or RNCS to afford the corresponding betaines in high yields and purities provides a convenient starting point to generate new heteroatom-based ligands with tailored binding modes.¹

In particular, the reaction of preformed or *in situ* generated NHCs with carbon disulfide affords stable, crystalline adducts that can act as κ^2 -*S*,*S'* chelating or bridging ligands toward various transition metals. Thus, in 2009 our group reported the formation of cationic ruthenium - arene complexes bearing imidazol(in)ium-2-dithiocarboxylate ligands.² In collaboration with James Wilton-Ely at Imperial College, the coordination chemistry of NHC•CS₂ zwitterions was further extended to various other complexes of ruthenium,^{3,4} osmium,⁴ palladium,⁵ and gold.⁶ We also demonstrated that NHC•CS₂ betaines were suitable ligands for the stabilization of gold nanoparticles.⁶

The potential of NHC•CS₂ zwitterions to generate new molecular architectures prompted us to further investigate the preparation of a large family of mono- and polynuclear complexes based on transition metals from groups 6 to 8 bearing these ligands. In this presentation, we shall discuss the coordination mode of NHC•CS₂ zwitterions in a series of new transition metal carbonyl complexes, on the basis of X-ray diffraction analysis and spectroscopic characterization techniques. We will also discuss their potential applications in catalysis.

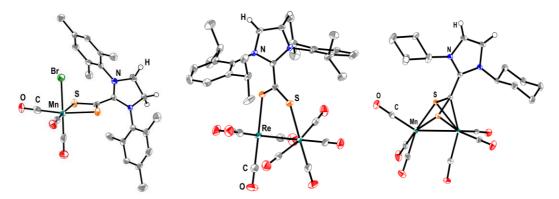


Figure 1. ORTEP representations of $[MnBr(CO)_3(S_2C \cdot SIMes)]$ (left), $[Re_2(CO)_8 \cdot (S_2C \cdot IDip)]$ (center) and $[Mn_2(CO)_6(S_2C \cdot ICy)]$ (right).

References

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