

SOLID-STATE MOLECULAR ORGANOMETALLIC CHEMISTRY: SIGMA ALKANE COMPLEXES, C-H ACTIVATION AND CRYSTALLINE MOLECULAR FACTORIES

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Abstract: Organometallic synthesis and catalysis are normally performed in the homogeneous solution state, where the advantages of metal/ligand catalyst design provide exquisite control over fundamental mechanistic steps. Such control, through precise atomic precision, is more challenging for heterogeneous systems. Bridging the gaps between the two areas are highly-active supported molecular catalysts (surface organometallic catalysis) that lead to very active catalysts, but still present challenges in precise catalyst speciation and mechanistic elucidation. We have been developing an alternative approach to, so-called, solid-state molecular organometallic chemistry (SMOM), where we study synthesis and reactivity in crystallo using well-defined organometallic complexes. These studies have focused on the synthesis and characterisation of highly reactive species that can be isolated using “crystalline matrix isolation methods”. Consideration of the likely surfaces of such molecular organometallic crystals as single atom catalytic sites offers possibilities and opportunities for catalysis.

In this presentation I discuss our approach to organometallic chemistry in single-crystals (SMOM) by outlining the synthesis and reactivity of complexes that are almost impossible to prepare stable in solution (e.g. sigma-alkane complexes), and their use in industrially-relevant catalysis such as ethene to propene (ETP) or the catalytic generation hyperpolarised gases for potential imaging applications.