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Research Interests: Metal-mediated chemistry, mass spectrometry, computational chemistry, functionalised materials.



Materials Mass Spectrometry

Research in the Duncombe group includes instrument and strategy development in order to overcome the common problems of air-sensitivity, high ion concentration, and molecule thermal lability thus enabling systems to be investigated using the analytical strengths of mass spectrometry. This is leading to innovative approaches to investigate functionalised materials in order to direct material design for a variety of applications.

Metal-Mediated Chemistry

The focus of our research is to use the dilute environment afforded by a mass spectrometer to investigate molecular factors that influence the structure and thus function of metal complexes and functionalised materials. A particular focus is the development of experimental methodology to transfer labile, non-covalent interactions from solution into a controlled-solvent environment. Secondary interactions, such as ligand-ligand & hydrogen-bonding play an important rôle in the determination of preferred structure (stability) and thus greatly influence reactivity. For example, the function of a significant number of metal complexes is associated with the outer- rather than inner-sphere coordination. Studying the outer-sphere configuration of such complexes will not only help recognize its influence on the function of these species but also help guide the design of new reagents for chemical processes. Employing the EaStCHEM computational research facility, accompanying theoretical work focuses on probing the influence of molecular parameters such as molecular dipole moment & polarisability on both the immediate & extended structure around metal centres, particularly, in mixed ligand systems.

Ionic Liquids

These liquids are increasingly important solvents and catalysts in many industrial processes and water contamination, for example, has a strong influence on their solvating properties. One possibility to investigate the impact of water is to exploit the analytical strengths of mass spectrometry, its ability to size select ions and investigate different types of ions for trends such as solvation structure or common dissociation pathways. However, the very nature of ionic liquids makes this problematic, since the most popular method of transfer, electrospray ionisation, is exceptionally sensitive and pmol/L concentrations can be detected. Conversely, high ion concentration, such as that found in ionic liquids, 3 - 4 mol/L, is likely to lead to significant instrument contamination and ion signal instability. On-going source development focuses on overcoming these problems allowing analysis of undiluted ionic liquids, their hydration, and functionality.

SELECTED RECENT PUBLICATIONS

1. The solvation of Cu^{2+} with gas-phase clusters of water and ammonia. B. J. Duncombe, K. Duale, A. Buchanan-Smith, & A. J. Stace, *Journal of Physical Chemistry A*, **2007**, 111, 5158.
2. Fragmentation pathways of $[\text{Mg}(\text{NH}_3)_n]^{2+}$ complexes: electron capture versus charge separation. B. Wu, B. J. Duncombe, A.J. Stace, *Journal of Physical Chemistry A*, **2006**, 110, 8423.
3. Gas-phase experiments on the chemistry and coordination of Zn(II) by aprotic solvent molecules. B. J. Duncombe, L. Puškar, B. Wu, A. J. Stace, *Canadian Journal of Chemistry*, **2005**, 83, 1994.
4. What is required to stabilize Al^{3+} ? A gas-phase perspective. L. Puškar, K. Tomlins, B. Duncombe, H. Cox, A. J. Stace, *Journal of the American Chemical Society*, **2005**, 127, 7559.