Effects of Solvation on Transition Metal Complexes

In solutions or on surfaces, the interactions of molecules with their chemical environment play an important role for the molecular properties one can observe. For example, the presence of solvent molecules or ions in the vicinity of a particular molecule will modify molecular electronic and geometric structure as well as molecular behavior, e.g. catalytic activity or photochemistry. However, these interactions are often ignored or accounted for in an averaged way (e.g. as a dielectric constant), since probing the molecular level details of such interactions in situ is very difficult. To use heterogeneous catalysis as an example, the complexity of the chemical environment, the multitude of possible interaction sites on many catalysts, and the lack of control over which and how many molecules are at a certain catalytic site at any given moment result in a very complicated response to many spectroscopic probes, hindering the development of a fundamental understanding of the intermolecular interactions that govern the function of catalysts.

The study of mass selected cluster ions provides a convenient way to circumvent such difficulties, because mass spectrometry techniques afford very good control over the composition of the sample under study. In combination with laser spectroscopic methods, mass selected cluster ions afford very good access to the details of intermolecular interactions. I will show several examples for the study of transition metal complexes by infrared and electronic spectroscopy.