Is the solid state structure of any help for the solution structure?

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Abstract: In his seminal case study on the relationships between solvation, aggregation and reactivity in organolithium chemistry Dave Collum stated "*X-ray crystallography provides little insight into the thermodynamics of aggregation and solvation*."[1] This is right for most chemical substances as the crystal structure is commonly believed to represent the least soluble derivative in the pot and not necessarily the most abundant, let alone the most reactive species. Moreover, the least populated species might represent the eye of the needle in the equilibrium the whole reaction goes through anyway on the course towards the overall product. Therefore it is an urgent aim of any chemist to get structural information on molecules in solution.

The talk will elucidate the interaction of X-ray structure analysis, spectroscopy and computational chemistry. We synthesised, crystallized and structurally characterized various thermolabile s-block organometallic aggregates and studied their behaviour in solution by 1 and 2-D heteronuclear NMR experiments[2] and computational chemistry[3] to start from firm ground and explore their constitution and behaviour in solution.

Unequivocally in this canon of methods X-ray structure analysis plays a leading role but all can learn from another:

- There are more beasts in the pot than those giving the nicest single crystals.[4]
- Without structural information it is impossible to get the intermediates.[5]
- Molecular weight determination from DOSY NMR spectroscopy provides new insights into the equilibrium in solution.[6]

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