

The 2008 BCA CCG Autumn meeting took place at Newcastle University on Wednesday the 12th of November. The meeting, “**New Methods in Chemical Crystallography**” was chaired by **Dr Andrew Bond** and featured six speakers presenting current research in crystallographic techniques.



Natalie Fey, Lynne Thomas, Susanne Huth, Trixie Wagner, Sarah Lister & Rob Hooft

The first lecture, “**Advancing into higher dimensions: a practical approach to modulated structures**”, was given by **Dr Trixie Wagner** (Novartis). In this very engaging talk, Trixie gave an introduction to what modulated structures are, and how they can be dealt with in practice using a reciprocal lattice viewer and the program Jana to refine the necessary extra parameters associated with this type of problem.

Next to speak was **Dr Rob Hooft**, (Bruker AXS) who gave a lecture on “**Reliable Determination of Absolute Structure Using Small Bijvoet Differences**”. Within the lecture he argued that Gaussian distribution does not fully account for legitimate outliers, and instead showed that by using Student t-distribution, the determination of absolute structure using Molybdenum radiation can be made more reliable.

After lunch **Dr Lynne Thomas** (University of Glasgow) spoke about thermal diffuse scattering in the lecture “**Bragg Scattering and Beyond... Getting More From Diffraction Patterns**”. She described the process in which observed scattering patterns are compared with those calculated from a simulated model in order to determine the most likely model for the disorder present in a structure.

Sarah Lister gave some nice examples of how techniques other than diffraction have been used to gain insight into unknown phases in a talk entitled “**The Use of**

Complementary Techniques in Structure Solution from Powders". Solid state NMR, IR and thermal gravimetric analysis proved invaluable to her in determining the behaviour of molybdenum phosphate.

Susanne Huth (University of Southampton) gave a talk about "**Understanding the Crystal Chemistry of Organic Solids**". She showed how she has used structural systematics to study the 1, 2 and 3 dimensional similarities and differences of families of compounds. The molecular packing motifs and hydrogen bonding of substituted anilides and anthraquinones were examined in detail. Susanne pointed out that structural systematics can be used to select samples on which to perform charge density experiments, often resulting in chemically interesting results.

"**Building Knowledge Bases from Structural Data**" was the final talk of the meeting, given by **Dr Natalie Fey** (University of Bristol). The talk highlighted some of the challenges and opportunities that arise when combining results from experimental crystallography and computational chemistry. Searches through databases reveal compounds that are outliers in terms of expected structural features. These outliers often can be either rationalised through combining these complimentary approaches, or improved to become more accurate.

Helena Shepherd, Durham University