

Gordon Conference on Crystal Engineering, New Hampshire, June 6th - 11th 2010

Report by Prof. Roger Davey

The first Gordon Conference on Crystal Engineering was held in the Waterville Valley Resort in New Hampshire from June 6th -11th 2010. The chairman was Professor Gautam Desiraju, world famous crystallographer and author of the classic 1989 book 'Crystal Engineering' and the co-chair Professor Robin Rogers, editor of the ACS journal 'Crystal Growth and Design'. At 170 attendees this was the largest 'first' Gordon conference ever and it is, evidently, almost certain that there will now be a series, one every two years. The Gordon Conference format is classic and well known to many scientists – speakers and poster presenters are encouraged to present unpublished work. Afternoons are free for fun: tennis, hiking, canoeing, whatever takes your fancy. The focus is on discussion and nothing is recorded. Attendees were warned that taking photos of presenters' slides or posters was punishable by immediate ejection from the conference and that nothing disclosed in the scientific sessions could be recorded outside the meeting. This makes writing a report somewhat problematic but I can tell you that in the best of BACG traditions, there was a free bar every evening.

The attendees seemed to come from two schools of crystal growth and design. Firstly, the organic solid state – from the UK, myself, Sally Price, Colin Pulham, Janet Scott, Neil Champness, Aurora Cruz, Peter Wood, Bill Jones, Graeme Day- with a fair representation from the international Pharma industry. Secondly from the coordination polymers and metal organic framework community (MOFs) represented from the UK by Matt Rosseinsky. I will just mention some of the talks that I personally enjoyed and found relevant. Jim Wuest from Montreal enlightened me about the design of materials that won't crystallise (JACS 2006, 128, 10372) and in particular the use of crystallisation rates from amorphous phases as a means of comparing the relative difficulty of crystallisation of a series of molecules. Lourdes Infantes, who I know from her work on hydrates with Sam Motherwell, gave more insights into hydrogen bonding group preferences, in particular showing from crystallographic database analysis the validity of Etter's rules.

There were a couple of talks (Richard Robson, Shilun Qui) on metal organic framework materials (also known as co-ordination polymers) in which the goal appeared to be the synthesis of as many variants as possible. Nobody is evidently interested in the crystal growth or nucleation of these materials despite that fact that the metal content may make them ideal vehicles for in situ x-ray studies. Christian Serre's talk on applications of some of these coordination polymers to drug delivery made me wonder about potential toxicity of such materials containing, as they do, copper and zinc. Colin Pulham and Adam Matzger gave quite different perspectives in polymorphism. Colin reviewed some of the Edinburgh Group's studies on hydrates of paracetamol formed by crystallisation from solution at high pressure and went on to show some of his new work on energetic materials. It is well known that many of these compounds are polymorphic (eg TNT, pentaerythritoltetranitrate) and the potential application of high pressure to the discovery of new forms was clear. Matzger spoke about polymorph screening and the armoury of high throughput methodologies to the

discovery of all polymorphs of a given material. His particular emphasis is on the use of polymeric substrates as heterogeneous seeds to aid nucleation of novel forms. The success of the technique was obvious but again I noted little interest in exploring underlying mechanisms.

I always enjoy an update on structure prediction and energy landscapes from Sally Price and indeed as another Database blind test is due it seems that progress continues. I was talking on nucleation in the same session as Peter Vekilov. It was good to hear his latest thinking and to discuss the role of liquid – liquid phase separation in nucleation kinetics. There were two excellent sessions focussed on applications and future needs. The first of these really dealt with pharmaceutical materials and included an inspirational talk by Pat Connelly on the need to match molecular discovery with the needs of formulation together with talks from Matt Peterson and Magali Hickey dealing with specific problems of quaternary ammonium salts and cocrystals. The second session took a broader view exploring problems and opportunities associated with ionic liquids, cocrystals and organic semiconductors. The latter talk from Peter Erk of BASF brought the conference to an end.

This was undoubtedly a very special meeting. The discussion in all sessions was lively and not, as can so often be the case, dominated by one or two questioners. The poster sessions (there were 110 posters) which ran every day from 4 to 6pm were very busy and organised on a repeating basis – half the posters were on display on Monday and the other half on Tuesday. This was repeated on Wednesday and Thursday so that you could have two shots at getting around each poster set. This worked very well and all the sessions were very busy. My students reported lots of interest in their work and that this was the best conference they had been to yet. For me it was of course a chance to meet up with old friends as well as meeting new people. On my afternoons off I played tennis. Orn Almarsson hammered me 6-1 and from then on we played tag doubles – much more relaxing particularly on the moist clay court with its bounce deadening properties. We had fun.