American Crystallographic Association Annual Meeting 2013

Honolulu, Hawaii July 2013

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The American crystallographic associations (ACA) annual meeting was held in Honolulu, Hawaii, situated on the island of Oahu. The meeting not only attracted scientists based in the US and Canada but also other international leaders in the field of crystallography.

Over 750 participants from every corner of the world provided posters and talks, making the conference a diverse environment to not only discuss my current work, but also view cutting edge research from other institutions. Attendance at this conference allowed me to network with industrialists and academics and by talking about my work has given me some insight into a problem I am currently encountering with 'crystal twinning'.

The conference featured plenary lectures and over 30 different sessions which covered a range of topics, from general interest to supramolecular chemistry to structural enzymology. I particularly enjoyed the sessions on materials discovery, complementary methods in crystals and in solution and contemporary crystal engineering. These sessions involved the discovery of new functional materials. Notable talks were from Jack Gougoutas and Matt Peterson. Their talks discussed the recent developments across all aspects of the use of structural data in the understanding, design and prediction of condensed phase materials and included crystal engineering, polymorphism, structure/property relationships, drug development and structure-based drug design.

I presented a poster at the conference entitled "Concerning the crystal chemistry and enantiomer separation of TAK" (photo attached). My poster described how the use of crystallisation as a means of separating enantiomers of chiral molecules remains an area of active research as well as process development. In the research arena the relationship between molecular structure and phase behaviour is an outstanding problem which impacts on both product and process development. For example in racemic systems experiment shows that there is a great tendency (90%) to the formation of racemic crystals as opposed to conglomerates of single enantiomers. This situation hinders the use of crystallisation alone as a widespread separation technique and yet its molecular origins remain elusive. Thus while

the enhanced stability of the racemic compound may be understandable from the perspective of the entropy mixing (this imposes a free energy penalty of c.a.0.5kcalmol^{-1} on a conglomerate compared to a compound) in the world of polymorphism the existence of metastable forms is common and yet in chiral systems the existence of metastable conglomerates seems to be rare.

The crystallisation of a triazolylketone molecule first reported in 1989 to crystallise as a conglomerate was investigated in order to shed light on two features of the crystallisation process. First we reprised the crystal chemistry of the chloro TAK and dihalogenated 4chloro2fluoro derivatives, both in the Cambridge Structural Database (SEYPUH and DIVTEH respectively). Secondly we reported the binary and ternary phase diagrams of the TAK by way of confirming the conglomerate behaviour of this system. Thirdly we explored through computation the underlying reasons for the absence of a racemic compound in this system and the evident crystal twinning first reported, leading to crystals of almost racemic compositions but which retain the structure of the pure enantiomer.

The poster session allowed me to discuss my work with peers, generate new ideas and answer many questions that I had not thought of. I had a number of discussions about the objective of my project and whether using additives to control the enantiomeric outcome was feasible. Pharmaceuticals are perhaps the most valuable materials known to mankind and there are important intellectual property, regulatory and efficacy implications if one is able to discover new compositions of matter for active pharmaceutical ingredients (APIs). Generally I found my research to be well received and there was interest in the results I presented. I also had the opportunity to view other students' posters and discuss their research with them. I hope that I asked questions that will be useful for their future research.

Attendance at the ACA conference allowed me to present my research to an international audience and learn from the current work occurring in academia and industry. I had the chance to network and make a number of contacts. I also found the exhibitor stands interesting, not only for the new technology presented, but also for highlighting the range of jobs available in science.

I would sincerely like to thank the BACG for awarding me a travel bursary which has allowed me to attend such an informative conference with the opportunity of presenting my research to an international audience, in such a beautiful location!!!

Thank you,

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