University of Birmingham

Dr Maryjane Tremayne BSc(Hons), PhD

Lecturer in Structural Chemistry

School of Chemistry (/schools/chemistry/index.aspx)

Contact details

Telephone +44 (0) 121 414 3201 (tel:+44 121 414 3201)

Email m.tremayne@bham.ac.uk (mailto:m.tremayne@bham.ac.uk)

School of Chemistry
University of Birmingham
Edgbaston
Birmingham
B15 2TT
UK

About

Maryjane Tremayne is a Lecturer of Structural Chemistry and has research interests in organic solid state chemistry, molecular crystallography, powder diffraction and evolutionary algorithms.

Maryjane has published over 40 research papers in scientific journals and books, and solved over 50 molecular crystal structures from powder diffraction data following the development of new techniques for determination. She has given presentations around the world on both structure solution from powder diffraction data and the application of evolutionary algorithms to crystallography.

Qualifications

- PhD in Chemistry, University of St.Andrews, 1995
- BSc(Hons) in Chemistry and Mathematics, University of St.Andrews, 1992

Biography

Maryjane Tremayne was awarded a BSc joint honours degree in chemistry and mathematics from the University of St.Andrews in 1992 and remained there for her PhD studies in *Ab initio* structure determination from powder diffraction data, awarded in 1995. Following postdoctoral research in 'direct-space' structure solution methods at University College London and the development of crystallographic software at the University of Glasgow, she was awarded a Royal Society University Research Fellowship held initially at the University of St.Andrews and then at the University of Birmingham (from 2000) before taking up a Lectureship position there in 2007.

Her research interests centre on the structural behaviour of organic solid state materials and the application of evolutionary optimisation techniques in chemistry and materials science, with an emphasis on polymorphic behaviour, cocrystals and the application of new structure determination methods from powder diffraction data.

Her work was recognised by the award of the 2004 British Crystallographic Association CCDC Younger Scientist Chemical Crystallography Prize for 'Original research in the field of chemical crystallography or the application of crystallographic information to structural chemistry'. She has served on the editorial and advisory board for crystallographic journals and continues to act as a consultant and expert advisor on powder diffraction in the pharmaceutical area.

Maryjane teaches physical chemistry at all degree levels and is undergraduate Year 3 and Year 4 research project coordinator.

Postgraduate supervision

Teaching Programmes

- Year 2 Computational Chemistry
- Year 3 Physical Chemistry - Techniques for the Solid State
- Year 3 Advanced Computational Chemistry
- Year 4 Physical Chemistry – Molecular Solids

Research

STRUCTURAL STUDIES IN THE ORGANIC SOLID STATE

Organic crystalline materials play many important roles as pharmaceuticals, pigments, agrochemicals, organic conductors or non-linear optics, to name just a few. As the bulk properties of these crystalline solids are dictated by crystal and molecular structure, a knowledge of both is crucial so that the properties of these chemical systems are fully understood. The rationalisation of a structure-property relationship is even more vital when the design of solid state materials is required to fulfil a particular application.

Our research encompasses aspects from all these areas: from the design and synthesis of new molecular cocrystals, the investigation of polymorphic behaviour of pharmaceuticals to the development of new computational algorithms for the determination of crystal structure.

STRUCTURE SOLUTION FROM POWDER DIFFRACTION DATA

Many important crystalline materials cannot be prepared in the form of single crystals of sufficient quality for conventional single-crystal diffraction studies. It is therefore essential that reliable structural information can be obtained from other sources such as powder diffraction data or by crystal structure prediction on the basis of molecular structure. We are currently developing new more sophisticated approaches to the process of structure determination from powder diffraction data. This research involves both the development of structure solution software utilising powerful computational techniques and the application of this software to important structural problems including many taken from organic and biological chemistry. Our work on 'direct-space' structure solution methods has enabled the structural characterisation of relatively complex structures from powder diffraction data and opened up the field to a wider scientific community, initially through the use of global optimization techniques based on Monte Carlo methods, and more recently by the development of evolutionary algorithms.

Our research is also focussed on the complementary use of theoretical crystal structure prediction techniques and experimental diffraction methods. This combination of techniques is vital in cases where either structure determination from powder diffraction data is not possible, or there are many possible predicted structures that are not easily distinguished by theoretical methods.

EVOLUTIONARY ALGORITHMS IN CRYSTALLOGRAPHY

Evolutionary algorithms are powerful global optimisation techniques that can be used to solve complex multi-dimensional problems. These algorithms mimic natural evolutionary behaviour using the principles of mutation, mating and natural selection to evolve a population until the fittest and best individuals dominate the population and provide the optimal solution.

We develop and utilise the differential evolution technique to solve complex structural problems primarily from powder diffraction data. Our work has resulted in the development of other highly efficient algorithms such as cultural differential evolution which based on a hybrid of natural evolution and human social behaviour. The combination of these contrasting evolutionary dictates has resulted in efficiency gains of up to 50% over pure biological evolutionary computation. Our first paper on this work was highlighted as a 'Hot Paper' in *Chem.Comm*. and was the focus of highlights in *Nature*, *MRS Bulletin* and other RSC publications.

CRYSTAL ENGINEERING AND THE DESIGN OF MOLECULAR COCRYSTALS

An understanding of intermolecular interactions in the solid state and its utilisation in the design of new materials is one of the most important areas in chemistry. As such, crystal engineering continues to attract both academic and commercial attention. There are many examples of multi-dimensional aggregates that have been assembled through a perceptive use of hydrogen bonds and these have shown that the selectivity of such interactions can be employed in the deliberate design of reproducible structural motifs. The incorporation of specific structural units in the design of a crystal will result in materials with desirable chemical and physical properties.

Our research involves the study of systems in which the primary interest centres on the intermolecular aggregation of often well-defined molecular building blocks. The investigation of pure compounds teaches us much about strong intermolecular interactions that can then be applied to the design and synthesis of multi-component hydrogen-bonded materials such as molecular cocrystals. These materials are becoming increasingly important within the pharmaceutical industry as an alternative formulation source with optimal physical properties. We are investigating the predictability of synthon formation, the crystal structures and tunability of physicochemical properties of new molecular cocrystals using both single-crystal and powder diffraction techniques.

POLYMORPHISM

Powder diffraction and crystal structure prediction techniques are key to the study of materials that display polymorphism - the existence of more than one crystalline form of the same chemical compound. Compounds from a wide range of fields exhibit polymorphism, with different forms often obtained from only slight variations in reaction conditions (e.g. temperature or pressure, or by crystallisation from different solvents). Despite this, polymorphs often display distinct differences in their physical properties arising from their differing crystal structures. The phenomenon of polymorphism is still not fully understood and the occurrence of polymorphic behaviour still not predictable.

STRUCTURAL STUDIES OF PHARMACEUTICALS

The majority of pharmaceutical substances are processed in the form of crystalline powders and many exhibit polymorphism. This raises various problems as both physical properties such as stability, dissolution rate, and bioavailability of the substance, and processing properties such as crystal shape, compressibility and particle size, vary between polymorphs and formulations. Patenting and life cycle management of pharmaceuticals are also critical to the modern pharmaceutical and agrochemical industries, and recent cases have demonstrated the possibility of patenting known drugs in new formulations such as novel crystal forms. Detailed study of crystal structure and polymorphic behaviour of these materials is essential for a rational control of the crystallisation process and solid state properties, and for patenting and registration purposes. Our structure determination techniques and synthesis of new cocrystal materials can be used to investigate these rationalise these aspects.

Other activities

- Member of the British Crystallographic Association
- Member of the International Centre for Diffraction Data

Publications

- Thompson, L.J., Voguri, R.S., Male, L., Tremayne, M., (2011), The crystal structures and melting points properties of isonicotinamide cocrystals with alkanediacids $HO_2C(CH_2)_{n-2}CO_2H$ n=7-9., CrystEngComm, 13: 4188
- Thompson, L.J., Voguri, R.S., Cowell, A., Male, L., Tremayne, M., (2010), The cocrystal nicotinamide-succinic acid (2/1)., Crystal Growth and Design, 9:853, Acta Crystallographica, C66: o421.
- Maclean, E.J., Tremayne, M., Kariuki, B.M., Cameron, J.R.A., Roberts, M.A., Harris, K.D.M., (2009), Lessons on the discovery and assignment of polymorphs, highlighted by the case of the latent pigment DPP-Boc., Crystal Growth and Design, 9:853.
- Chong, S., Tremayne, M. (2006), Combined optimization using cultural and differential evolution, application to crystal structure solution from powder diffraction data., Chemical Communications, 4078.
- Chong, S., Seaton, C.C., Kariuki, B.M., Tremayne, M. (2006), Molecular versus crystal symmetry in tr-substituted triazine, benzene and isocyanurate derivatives., Acta Crystallographica, B62: 864.
- Grover, L.M., Gbureck, U., Wright, A.J., Tremayne, M., Barralet, J.E. (2006), Biologically mediated resorption of brushite cement in vitro., Biomaterials, 27: 2178.
- Modi, R., Hix, G.B., Tremayne, M., MacLean, E. (2005), Polymorphism in nickel phosphonates: synthesis of layered and microporous $Ni(O_3PCH_2C(O)NH_2).H_2O$., New Journal of Chemistry, 29: 427.
- Tremayne, M. (2004), The impact of powder diffraction on the structural study of organic materials., Philosophical Transactions of the Royal Society of London Series A: Chemistry and Life Sciences Triennial Issue, 362: 2691.
- Tremayne, M., Grice, L., Pyatt, J.C., Seaton, C.C., Kariuki, B.M., Tsui, H.Y., Price, S.L., Cherryman, J.C., (2004), Characterization of complicated new polymorphs of chlorothalonil by X-ray diffraction and computer crystal structure prediction., Journal of the American Chemical Society, 126:7071.
- Tremayne, M., Seaton, C.C., Glidewell, C., (2002), Structures of three substituted arenesulfonamides from X-ray powder diffraction data using the differential evolution technique., Acta Crystallographica, B58:823.
- Seaton, C.C., Tremayne, M., (2002), Differential evolution: Crystal structure determination of a triclinic polymorph of adipamide from powder diffraction data., Chemical Communications, 880.
- Harris, K.D.M., Tremayne, M., Kariuki, B.M., (2001), Contemporary advances in the use of powder X-ray diffraction for structure determination., Angewandte Chemie International Edition in English, 40:1626.
- Glidewell, C., Tremayne, M., (2000), Direct-space structure solution from laboratory powder diffraction data of an organic cocrystal 1,2,3-trihydroxybenzene-HMTA (1/1)., Chemical Communications, 2425.

- Tremayne, M., Kariuki, B.M., Harris, K.D.M., (1997), Structure determination of a complex organic solid from X-ray powder diffraction data by a generalised Monte Carlo method: The crystal structure of red fluorescein., Angewandte Chemie International Edition in English, 36:770

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