#### TERRY THRELFALL

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#### CAREER HISTORY

## Senior Research Fellow, Crystallography Group, School of Chemistry 2003 - date

Research – investigating crystallisation and solid-solid transition processes, crystallizing samples for X-ray crystallographic studies, understanding the molecular solid state through structural systematics, spectral and thermal studies of polymorphs, solvates, hydrates and derivatives.

# Honorary Research Fellow, Department of Chemistry

1999 - 2003

Research – investigating polymorphism through spectral and structural investigation of the solid state forms of sulphadrugs.

# Industrial Liaison Executive, Department of Chemistry.

1991 - 1999

Responsible for organising Short Courses for Industry; setting up Multi-university Modular MSc.; External Analytical Services; Skills teaching

- Involved in skills based workshops for undergraduates
- Set up and tutored on "Problem Solving for Analytical Chemists" and "IR and Raman Spectroscopy" courses for industrial analysts.
- Joint author of 'A Question of Chemistry'. Now translated into French and Japanese.

# 29 years with Rhone Poulenc Rorer Ltd., formerly May & Baker Ltd, now Sanofi-Aventis.

**Consultant** 1990 - 1991

Responsible for providing technical support and data gathering for overseas tax litigation.

#### **Principal Scientist**

1987 **-** 1990

Responsible for maintaining patent monopoly worth £130 million per annum worldwide. Organised schools and academic liaison activities and acted as an internal scientific consultant.

• Negotiating skills, especially in Japan

#### **Process Research Manager**

1983 - 1987

Responsible for developing processes for whole of May and Baker Ltd. Facilities included pilot plant, pressure reactor and clean room. 28 scientific staff. Budget  $\pounds_{\frac{1}{2}}^{1}$  m.

- General management skills; also helped with management skills courses.
- Interviewing. Noted that many well qualified candidates did not interview well and that many well qualified appointees failed to apply their knowledge effectively.
- On Career Counselling Panel

### Departmental Head, Physical Chemistry

1976 - 1983

Providing a wide range of scientific services. Ran pigment development project. 22 staff.

- Organised technicians' development courses
- Presented successful cases for expansion, new laboratory and new equipment.

#### Section Head, Spectroscopy

1962 - 1976

Responsible for providing a spectroscopic service and for pearling agent research.

## **EARLIER HISTORY**

Mathematics Teacher 1962; NATO Research Student, Switzerland, 1959-1961; Part-time lecturer in Chemistry and Physics 1957-1959; Trainee in Electrical Engineering Industry 1955-1956.



**EDUCATION** 

B.Sc. Chemistry 1956; Ph.D. Organic Chemistry 1971; Ll.B. Law 1984.

**OTHER ACTIVITIES** 

Taught German part-time for ~ 25 years. Active member of many societies.

**PERSONAL** 

Aged 74 years, married with 2 grown-up children.

- 1. I am a Senior Research Fellow in the Department of Chemistry at the University of Southampton. My principal fields of interest are polymorphism and other aspects of solid state crystal structure and behaviour, and in understanding crystallization and transformation processes. My current research interests are in relating molecular structure to crystal structure using structural systematics and in applying spectroscopy and microscopy to crystallization and to solid-solid transition processes.
- 2. I received a Bachelor of Science degree in chemistry from London University in 1956, a Ph.D. in organic chemistry from London University in 1971 and a Batchelor of Law degree from the University of London in 1984.
- 3. In 1962, I was appointed Section Head of Spectroscopy at May & Baker Ltd., which later became known as Rhone Poulenc Rorer Ltd. Over the years at May & Baker, I introduced NMR, mass spectroscopy, preparative HPLC and chemical microscopy and electron microscopy to the company. As the Section Head, I was specifically responsible for the Pearling agent research program which presented substantial crystalline challenges. In 1976, I was appointed as the Department Head of Physical Chemistry. In this capacity, I was responsible for overseeing a substantial group of scientists, technical officers, and technicians in relation to the origin of samples, identity of samples, purity of samples, hydration, solvation, polymorphism, salt formation, crystal habit and amorphicity. In 1983, I was appointed as Process Research Manager and was responsible for scaling up synthetic routes, which involved consideration of the purity, purification, crystallisation, stability and filterability of samples. In 1987, I became a Principal Scientist, in which capacity I organized schools liaison and acted as an internal scientific consultant. Over my twenty-nine years at May & Baker, I gained considerable experience of a wide variety of situations and of problems associated with the identification, purification, crystallisation and separation of compounds of all kinds, but particularly with organic pharmaceuticals.



4. Prior to taking a position at the University of Southampton, I was the Industrial Liaison Executive in the Department of Chemistry at the University of York. Specifically, I joined the University of York faculty in 1991 and was later appointed a Research Fellow. At the University of York, I organized short courses for industry, participated in skills based workshops for undergraduates, and conducted research on polymorphism, instrumentation and molecular templates.

I currently conduct research relating to growing crystals large enough for single crystal diffraction work and for other studies. I personally carry out 500 crystallisations per year, particularly for the preparation of polymorphs, hydrates, solvates and co-crystals.



#### PUBLICATIONS BY TERRY THRELFALL

#### **BOOKS**

A Question of Chemistry: Creative Problems for Critical Thinkers. Garrett, J., Overton, T. and Threlfall, T., Longman, Harlow, UK, 1999. Now translated into French and Japanese.

#### **BOOK CHAPTERS**

"Vibrational Spectroscopy of Solid-State Forms – Introduction, Principles and Overview" T.L, Threlfall and J.M. Chalmers in "Applications of Vibrational Spectroscopy in Pharmaceutical Research and Development" Ed. D.E. Pivonka, J.M. Chalmers and P.R. Griffiths, J. Wiley, New York and Chichester

"Polymorphs, Solvates and Amorphous Compounds" in the "Wiley Handbook of Vibrational Spectroscopy", Ed. Griffiths, P. and Chalmers, J. Wiley, New York and Chichester 2001

"Instrument Design Considerations" in <u>Standards and Best Practice in Absorption</u> <u>Spectrometry.</u> Ed. Burgess, C. and Frost, T., Blackwell Science, Oxford, UK 1999

"Colour Measurement" in <u>Practical Absorption Spectrometry</u> Ed. Burgess, C., Russell, M. and Frost, T., Chapman and Hall, London, UK, 1996

"Structure-Spectral Relationships" in <u>Practical Absorption Spectrometry</u> Ed. Burgess, C., Russell, M. and Frost, T., Chapman and Hall, London, UK, 1996

### **ARTICLES**

- 35. A Systematic Study of the Crystallisation Products of a Series of Dicarboxylic Acids with Imidazole Derivatives. S. Callear, M.B. Hursthouse and T. Threlfall, CrystEngComm., 2010. 12, 898-908
- 34. Why do organic compounds crystallise well, badly or ever so slowly? Why is crystallisation nevertheless such a good purification technique? M.B. Hursthouse, L.S. Huth and T.L. Threlfall, Org. Proc. Res. Dev., 2009, 13, 1231-40
- 33. Turning DSC Charts of Polymorphs into Phase Diagrams: A Tutorial Paper. T. Threlfall, Org. Proc. Res. Dev., 2009, <u>13</u>, 1224-1230
- 32. The Elusive High-Temperature Solid-State Structure of D,L-Norleucine. S.J. Coles, T. Gelbrich, U.J. Greisser, M.B. Hursthouse, M. Pitak and T. Threlfall, Cryst. Growth. Des., 2009, 9, 4610-12
- 31. Co-crystallisation of organic α,ω-dicarboxylic acids with the cyclic amides 2-pyrrolidine and 2-imidazoline. S. Callear, M.B. Hursthouse and T.L. Threlfall, CrystEngComm., 2009, 11, 1609-14
- 30. *Packing Similarity in Polymorphs of Sulfathiazole*, T. Gelbrich, D. S. Hughes, M.B. Hursthouse and T.L. Threlfall, CrystEngComm. 2008, 10, 1328



- 29. *Delta-Sulfanilamide* T. Gelbrich, A. Bingham, T. Threlfall, M. Hursthouse, Acta Cryst.C 2008, <u>C64</u>, o205-o207
- 28. Polymorph VI of sulfapyridine: interpenetrating two- and three-dimensional hydrogen-bonded nets formed from two tautomeric forms, T. Gelbrich and T. Threlfall, Acta Cryst. C 2007, C63, o323-o326
- 27. T. Gelbrich, M.B. Hursthouse and T.L. Threlfall, *Structural Systematics: Crystal structures of para, para-disubstitured benzenesulfonamides: Part 1, Overview and the isostructural dimers.* Acta Cryst. B, 2007, <u>63B</u>, 621-632.
- 26. T.L. Threlfall and T. Gelbrich, *The structure of methylparaben at 118K does not represent a new polymorph*, Cryst. Growth and Design, 2007, 7, 2297
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  Furosemide and Finasteride. Acta Cryst., 2006, B62, 689-91
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- 20. Threlfall, T.L., *The Structural and Thermodynamic Basis of Ostwald's Rule*. Org. Proc. Res. Dev., 2003, <u>7(6)</u>, 1017-1027
- 21. Portieri, A., Harris, R.K., Fletton, R.A, Lancaster, R.W. and Threlfall, T.L. *Effects of Polymorphic Differences for Sulfanilamide, as seen through 13C and 15N solid-state NMR, together with shielding calculations.* Org. Magn. Resonance, 2003
- 19. Bingham, A., Hughes, D.S., Hursthouse, M., Lancaster, R.W., Tavener, S., Threlfall, T. *Over one hundred solvates of Sulfathiazole*. Chem. Commun. 2001, 603-604
- 18. Threlfall, T.L, Crystallisation of Polymorphs: Thermodynamic Insight into the Role of Solvent, Org. Process Res. Dev. 2000, 4, 384-390
- 17. Apperley, D.C., Fletton, R.A., Harris, R.K., Lancaster, R.W., Tavener, S. and Threlfall, T.L., *Sulfathiazole Polymorphism Studied by Magic Angle Spinning NMR Spectroscopy*, J. Pharm. Sci., 1999, <u>88</u>, 1275-1280
- 16. Hughes, D.S., Hursthouse, M.B., Threlfall, T. and Tavener, S. *A New Polymorph of Sulfathiazole*, Acta Cryst. 1999, <u>C55</u>, 1831-1833
- 15. Hughes, D., Hursthouse, M., Lancaster, R., Tavener, S., Threlfall, T. and Turner, P, How Many Polymorphs has Sulphathiazole? Proposals for reporting Crystallographic Data of Polymorphs, J. Pharm. Pharmacol.,1997, 49, (S4) p.20
- 14. Threlfall, T.L. *Analysis of Organic Polymorphs A Review*, Analyst, 1995, <u>120</u>, 2435-2460
- 13. Windram, V.A. and Threlfall, T.L. *Chemical Microscopy in the Pharmaceutical Industry*, Analytical Proceedings, 1992, 29, 108-110
- 12. Deeley, C.M., Spragg, R.A. and Threlfall, T.L. A Comparison of Fourier Transform Infrared and Fourier Transform Raman Spectroscopy for Quantitative



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