



«ETTORE MAJORANA» FOUNDATION AND CENTRE FOR SCIENTIFIC CULTURE
TO PAY A PERMANENT TRIBUTE TO GALILEO GALILEI, FOUNDER OF MODERN SCIENCE
AND TO ENRICO FERMI, THE "ITALIAN NAVIGATOR", FATHER OF THE WEAK FORCES



Thirty Years of the INTERNATIONAL SCHOOL OF CRYSTALLOGRAPHY

35th Course: DIVERSITY AMIDST SIMILARITY: A MULTIDISCIPLINARY APPROACH TO POLYMORPHS, SOLVATES AND PHASE RELATIONSHIPS

A EuroSummerSchool and a Nato Advanced Study Institute

ERICE-SICILY: 9 - 20 JUNE 2004

Sponsored by the Italian Ministry of Education, University and Scientific Research, the Sicilian Regional Government, the European Commission, DG Research, the International Union of Crystallography and Sanofi-Chimie

PROGRAMME AND LECTURERS

Historical background

Fundamentals

Thermodynamics

Phase diagrams and energy/temperature diagrams

Kinetics of crystallization

Controlling the polymorph obtained

Seeding

Disappearing and reappearing polymorphs

Concomitant polymorphs

In situ crystallization

Analytical methods for characterizing polymorphs

Hot stage microscopy

DSC/TGA methods

X-ray diffraction

IR spectroscopy

Raman spectroscopy

Solid state NMR

Electron crystallography

Quantitative analysis

Computational approaches to polymorphs/solvates

Computation of lattice energies – general principles

Practical aspects of lattice energy calculations and “polymorph prediction”

Polymorphism and the study of structure/property relations

Polymorphism and pharmaceuticals

Polymorphism and pigments

Polymorphism and high energy materials (including chocolate)

Polymorphism and patents

- R. BOESE, University of Essen, D
- T. BRILL, University of Delaware, Newark, DE, USA
- D.E. BUGAY, Analytical Chemistry, SSCI, Inc., West Lafayette, IN, USA
- S. BYRN, Purdue University, West Lafayette, IN, USA
- R.J. DAVEY, University of Manchester, UK
- P. ERK, BASF AG, Ludwigshafen am Rhein, D
- K.D.M. HARRIS, University of Birmingham, UK
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- J.-O. HENCK, Bayer AG, Leverkusen, D
- F. HERBSTEIN, Israel Institute of Technology, Haifa, IL
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- F. GREPIONI, University of Sassari, I
- U. GRIESSER, University of Innsbruck, A
- A. KATRUSIAK, University of Poznan, PL
- L. LEISEROWITZ, Weizmann Institute of Sciences, Rehovot, IL
- H. LEVINE, Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P., Washington, D.C., USA
- S.L. MORISSETTE, TransForm Pharmaceuticals, Inc., Lexington, MA, USA
- T.M. NIEMCZYK, University of New Mexico, Albuquerque, NM, USA
- S.L. PRICE, University College, London, UK
- S.M. REUTZEL-EDENS, Eli Lilly & Company, Indianapolis, IN, USA
- M.A. SPACKMAN, University of New England, NSW, AUS
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- M.D. WARD, University of Minnesota, Minneapolis, MN, USA

PURPOSE OF THE COURSE

This event is designed to provide a sound background on the phenomenon of crystallization – a technique of purification used by chemists for generations. The existence of the diversity of polymorphs and solvates can wreak havoc in the practice of that technique. The Course will provide:

- a. the theoretical basis for the existence of these diverse structural forms;
- b. the methodology to control the form, from the nucleation to macroscopic growth;
- c. the techniques used to characterize the variety of products obtained;
- d. the advantages resulting by this way of surveying structure/property relations for the design and preparation of new materials.

By its very nature this event requires the involvement of a broad spectrum of practitioners from a variety of fields. Occurrence of polymorphs and solvates have had an increasing impact and influence on product development and on the protection of intellectual property rights particularly in the pharmaceutical field over the past two decades. Developments in other areas such as pigments, fats, high energy materials, organic magnets and high temperature superconductors have also been influenced by the discovery, investigation, understanding and utilization of the multiplicity of structures for a single chemical entity.

There has been a number of symposia covering research and development issues on these topics; however there has not yet been a comprehensive course to introduce the variety of issues involved to new practitioners in the field – from graduate students to experienced scientists from other fields.

The organizers are aware that the subject of Polymorphism is also of wide interest to the inorganic and mineral world. However, given the major impact of recent scientific, legal and economic (new and spectacular) developments in the realm of molecular crystals, in particular different crystal forms on the pharmaceutical front, it has been decided to place the emphasis for the current teaching event on molecular crystals.

APPLICATIONS

Interested candidates should register by 30 November 2003 using the format available at <http://www.chfi.unipd.it/home/chor/erice> or write to the Executive Secretary of the International School of Crystallography:

- Professor Paola SPADON - Executive Secretary
International School of Crystallography
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specifying:

- i) full name(s), age, sex, citizenship;
- ii) postal address, phone, fax, electronic mail;
- iii) present academic position and scientific interests;
- iv) the title or abstract of a scientific contribution to the poster session(s) which might be included in the programme.

Young researchers please add a list of no more than five scientific publications and a letter of recommendation from the group leader or a senior scientist, where the amount of support, if needed, is justified. In order to reflect the multi-disciplinary nature of the Course, attendance will be encouraged on the basis of the scientific discipline, publication record and the correspondence between the current research of the applying scientists and the listed topics.

POETIC TOUCH

According to legend, Erice, son of Venus and Neptune, founded a small town on top of a mountain (750 metres above sea level) more than three thousand years ago. The founder of modern history — i.e. the recording of events in a methodic and chronological sequence as they really happened without reference to mythical causes — the great Thucydides (~500 B.C.), writing about events connected with the conquest of Troy (1183 B.C.), says: «After the fall of Troy some Trojans on their escape from the Achaei arrived in Sicily on boats and as they settled near the border with the Sicilians all together they were named Elymi: their towns were Segesta and Erice.» This inspired Virgil to describe the arrival of the Trojan royal family in Erice and the burial of Anchise, by his son Enea, on the coast below Erice. Homer (~1000 B.C.), Theocritus (~300 B.C.), Polybius (~200 B.C.), Virgil (~50 B.C.), Horace (~20 B.C.), and others have celebrated this magnificent spot in Sicily in their poems. For seven centuries (XIII-XIX) the town of Erice was under the leadership of a local oligarchy, whose wisdom assured a long period of cultural development and economic prosperity which in turn gave rise to the many churches, monasteries and private palaces which you see today.

In Erice you can admire the Castle of Venus, the Cyclopean Walls (~800 B.C.) and the Gothic Cathedral (~1300 A.D.). Erice is at present a mixture of ancient and medieval architecture. Other masterpieces of ancient civilization are to be found in the neighbourhood: at Motya (Phoenician), Segesta (Elymian), and Selinunte (Greek). On the Aegadian Islands — theatre of the decisive naval battle of the first Punic War (264-241 B.C.) — suggestive neolithic and paleolithic vestiges are still visible: the grottoes of Favignana, the carvings and murals of Levanzo.

Splendid beaches are to be found at San Vito Lo Capo, Scopello, and Cornino, and a wild and rocky coast around Monte Cofano: all at less than one hour's drive from Erice.

More information about the International School of Crystallography can be found on the WWW at the following address:
<http://www.crystalerice.org>

PLEASE NOTE

Participants must arrive in Erice on June 9, not later than 5 p.m.

More information about the activities of the Ettore Majorana Centre
can be found on the WWW at the following address:
<http://www.ccsem.infn.it>