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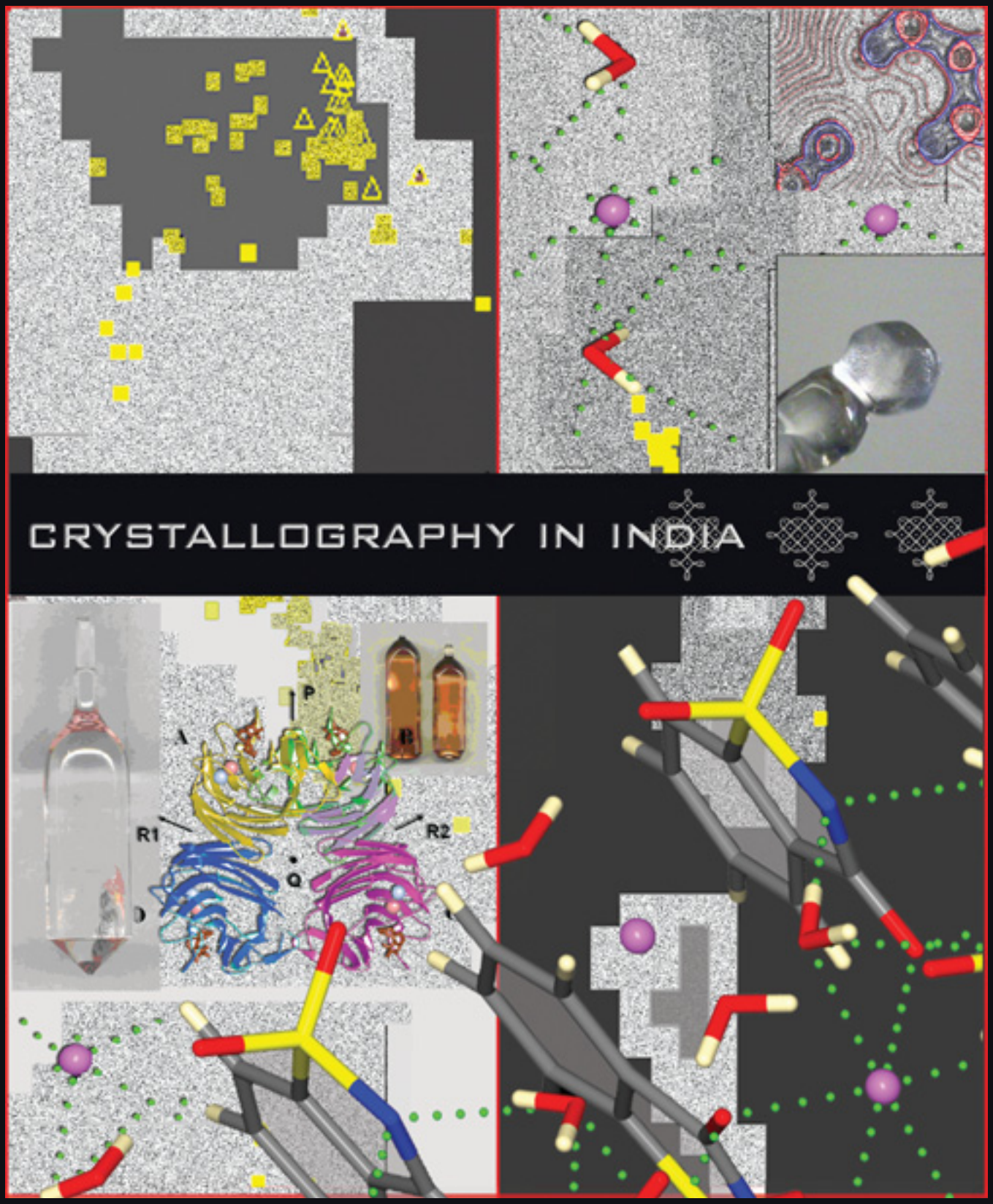
INTERNATIONAL UNION OF Crystallography

NEWSLETTER

Volume 15, Number 4 ♦ 2007



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The International Union of Crystallography Newsletter (ISSN 1067-0696; coden IUC-NEB) Volume 15, Number 4. Published quarterly (4x) by the International Union of Crystallography. Members receive the IUCr Newsletter by virtue of country membership in the IUCr. Periodical postage rates paid at Buffalo, NY and additional mailing offices. POSTMASTER: Please send changes of address to IUCr Newsletter Editorial Office, c/o Hauptman-Woodward Medical Research Inst., 700 Ellicott St., Buffalo, NY 14203 USA.

Yuji Ohashi

In this issue articles on Crystallography in India are included. I attended the 36th National Seminar on Crystallography in collaboration with the Indian Crystallographic Association (ICA) held at the University of Madras in Chennai, 22–24 January 2007, at the invitation of the organizer, Professor Ponnuswamy. More than 120 crystallographers attended the meeting. I was interviewed by a writer from the public newspaper, *The Hindu*, about the IUCr, because I was the first IUCr President to attend the Annual Meeting of the ICA. A large photograph of Professor Lal (President of ICA) and me appeared in the newspaper the next day. I was deeply impressed that many young students eagerly took part in the discussion. I am sure that crystallography in India will be developed more and more in the near future.

As I wrote in the letter of a previous issue (Vol. 15, No. 2), Dr Bernard Omondi has completed his PhD successfully under the direction of Professor Demi Levendis at the University of Witwaterstrand in Johannesburg, South Africa, with the support of an IUCr fund (Africa PhD Initiative). The Executive Committee approved continuation of this fund at its meeting held in Salt Lake City in July 2007 (Vol. 15, No. 3). However, the system was slightly modified so that the Professor responsible for hosting the student and administering the fund may come from any country in Africa although the fund should be limited to students from sub-Saharan African countries. Recently, we accepted two applications from Professor Trevor Sewell of the University of Cape Town in South Africa. The Executive Committee agreed that the fund should be awarded to two students, both of whom (Mr Ndoria Thuku and Ms Serah Kimani) come from Kenya, and they will start their doctors course at the University in 2008. We hope that they will complete their PhDs successfully after three years.

Recently I received a letter from my young friend in Ghana, Dr. Emmanuel Owusu-Marfo. He completed his PhD in a crystallographic laboratory of the Tokyo University of Agriculture and Technology in Tokyo and subsequently returned to Ghana; he is now a staff member of the Ghana Atomic Energy Commission. In Ghana he cannot teach crystallography since there is no diffractometer in Ghana. He asked me to introduce him to any crystallographer who has an old diffractometer not used in his or her laboratory. He promised that he will be able to arrange the transportation of the diffractometer to Ghana. I am now looking for such a Japanese crystallographer. If any reader has any information on the availability of a used diffractometer, please let me know. I hope that the IUCr will have some system for crystallographers in developing countries to obtain used diffractometers from developed countries in the near future.

Yuji Ohashi, yohashi@spring8.or.jp

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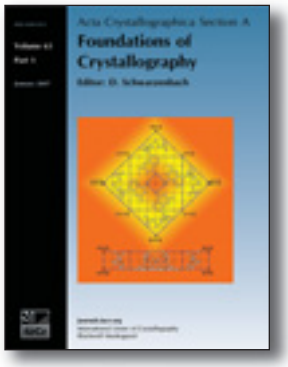


The crystallographic fast Fourier transform. Recursive symmetry reduction

A. Kudlicki, M. Rowicka and Z. Otwinowski

We present algorithms for non-redundant crystallographic fast Fourier transform (FFT), maximally reducing the computational complexity and memory usage for all 230 symmetry groups. Previously such algorithms have been known only in several cases. The central idea of our approach is to represent a symmetric Fourier transform as a series of transforms on grids with no special points. Such transforms are reduced to *P*1 FFTs in one step. We provide recipes for recursive decomposition for all symmetry groups and grids.

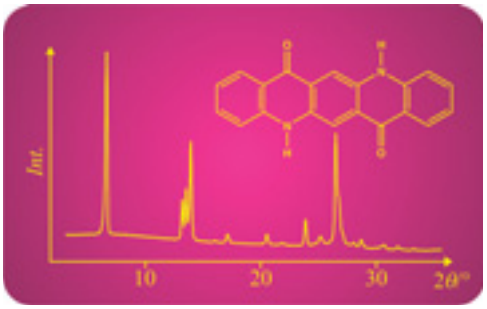
The fractal-like asymmetric unit for diagonal mirror symmetry. Color saturation depicts depth of recursion.

Acta Cryst. (2007). B**63**, 926–932 (doi.org/10.1107/S0108768107050823)

Rietveld refinement of a wrong crystal structure

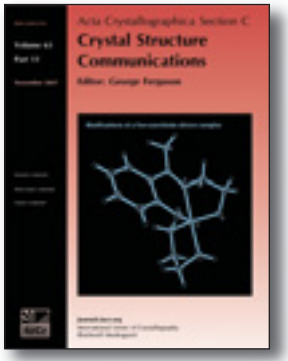
C. Buchsbaum and M.U. Schmidt

Rietveld refinements are used to confirm crystal structures solved from powder diffraction data. The Rietveld refinement of the X-ray powder pattern of γ-quinacridone with the crystal structure of β-quinacridone gives a good fit, and a reasonable looking crystal structure. However, the lattice parameters, molecular conformation and packing are wrong. This example shows that a successful Rietveld refinement is not always final proof of the correctness of a crystal structure.



Molecular formula of quinacridone and powder diagram of the γ phase.

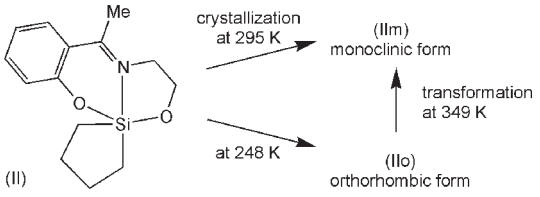
Acta Cryst. (2007). C**63**, o613–o616 (doi.org/10.1107/S0108270107045465)



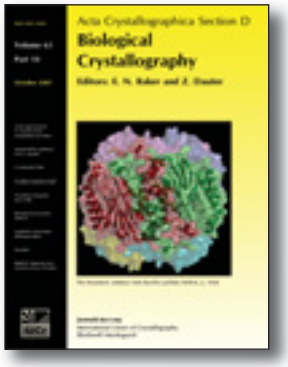
Structures of a dimorphic pentacoordinate silicon complex

U. Böhme and I.C. Foehn

The existence of polymorphs is of importance for many applications that depend on the solid state properties of a compound. TBPY-5-34-(Butane-1,4-diyl)(2-{[1-(2-oxidophenyl)ethylidene-κ*O*]amino-κ*N*}ethanolato-κ*O*)silicon, $C_{14}H_{19}NO_2Si$, crystallizes in two modifications. The monoclinic form, (IIm), was obtained by crystallization over a period of 2 days at room temperature; the orthorhombic form, (IIo), crystallized overnight at 248 K. According to thermal analysis it was concluded that (IIm) is the thermodynamically stable modification and (IIo) is a kinetically formed modification.



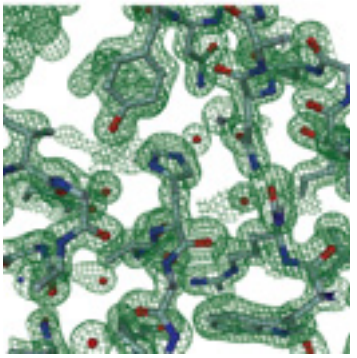
Acta Cryst. (2007). D**63**, 1069–1074 (doi.org/10.1107/S0907444907042230)



Structure determination of the *O*-methyltransferase NovP using the 'free lunch algorithm' as implemented in *SHELXE*

I. Usón, C.E.M. Stevenson, D.M. Lawson and G.M. Sheldrick

In an ideal world, all macromolecules should diffract to atomic resolution. Sadly, this is hardly ever the case. For the title protein native data to 1.35 Å resolution and a single mercury derivative to 2.45 Å did not yield an interpretable map with the available programs in the hands of the authors. It could only be solved after using main-chain tracing and data extrapolation to fill in missing reflections to extend data to 1 Å — the 'free lunch algorithm' — as implemented in the program *SHELXE*.

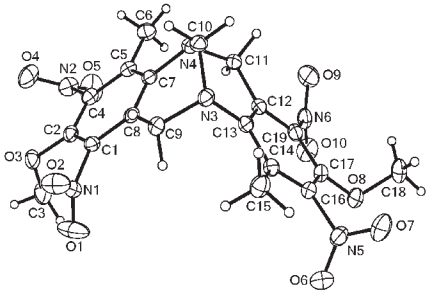


SIRAS combined with partial tracing and free lunch to 1 Å.

Acta Cryst. (2007). E**63**, o4393 (doi.org/10.1107/S1600536807050945)

2,8-Dimethoxy-4,10-dimethyl-1,3,7,9-tetranitro-6*H*,12*H*-5,11-methanodibenzo[*b*,*f*][1,5]diazocine

M.D.H. Bhuiyan, P. Jensen and A.C. Try

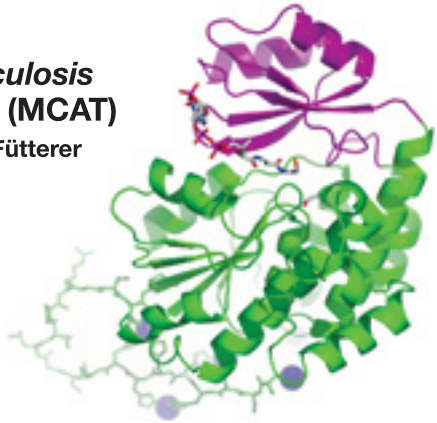


Tröger's base is a chiral, C_2-symmetric compound with a V-shaped geometry. Analogues of the compound are of interest in areas such as molecular recognition and asymmetric catalysis; however, applications have been limited by the type of substituents (generally electron-donating) that could be incorporated on the aryl rings. In this study the structure determination of a tetranitro analogue is reported, in which the dihedral angle between the two aromatic rings is 103.64 (5)°. The crystal chosen for analysis crystallised in enantiopure form from a racemic mixture.

Acta Cryst. (2007). F**63**, 831–835 (doi.org/10.1107/S1744309107042455)

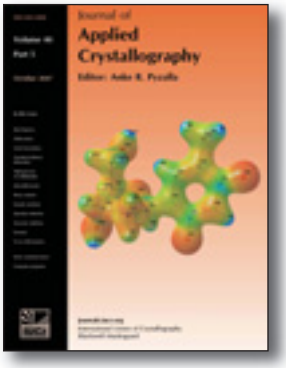
Crystal structure of *Mycobacterium tuberculosis* mtFabD, a malonyl-CoA:ACP transacylase (MCAT)

H. Ghadbane, A.K. Brown, L. Kremer, G.S. Besra and K. Fütterer



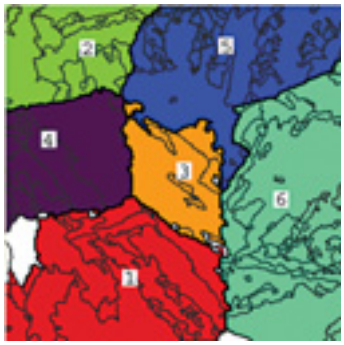
Mycolic acids — very long α-alkyl, β-hydroxylated fatty acids — are essential and characteristic components of the cell envelope of *Mycobacterium tuberculosis*, and are synthesised by the joint action of the type I and II fatty acid synthase (FAS) systems. The 3.0 Å crystal structure of *M. tuberculosis* FabD, which catalyses acyl transfer from coenzyme A to acyl carrier protein of FAS-II, was phased based on anomalous scattering of five ordered Ni^{2+} ions bound to the His_6-affinity tag of the recombinant enzyme.

J. Appl. Cryst. (2007). **40**, 1183–1188 (doi.org/10.1107/S0021889807048777)



ARPGE: a computer program to automatically reconstruct the parent grains from electron backscatter diffraction data

C. Cayron



Bainitic steel with the reconstruction of the austenitic grains.

A computer program called *ARPGE* automatically reconstructs the parent grains from EBSD data obtained on phase transition materials, with or without residual parent phase. The misorientations between the daughter grains are identified with operators, the daughter grains are identified with indexed variants, the orientations of the parent grains are determined and some statistics on the variants and operators can be established. Some examples with martensitic transformations in steels and titanium alloys have been treated. Variant selection phenomena have been revealed.

J. Synchrotron Rad. (2007). **14**, 453–470 (doi.org/10.1107/S0909049507037600)

Coherent X-ray scattering and lensless imaging at the European XFEL Facility

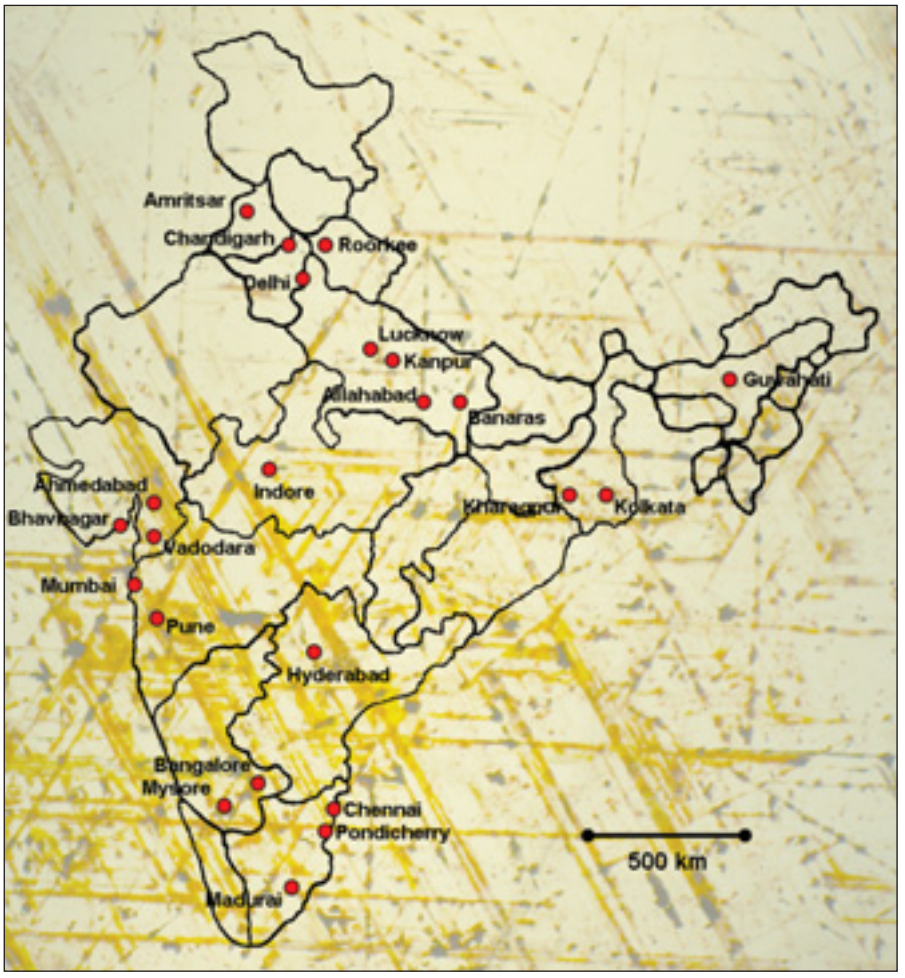
I.A. Vartanyants, I.K. Robinson, I. McNulty, C. David, P. Wochner and Th. Tschentscher

An artistic view of the experimental hall of the European XFEL and laboratory complex as viewed from the incoming photon tunnels.

Coherent X-ray diffraction imaging (CXDI) is a rapidly advancing form of lensless microscopy. The phase information of the diffraction pattern is embedded in a sufficiently sampled coherent diffraction pattern. Applying advanced computational methods based on iterative algorithms this diffraction pattern can be inverted to produce an image of a sample with diffraction-limited resolution. It is natural and highly attractive to use fully coherent X-ray beams produced by X-ray free-electron lasers (XFELs) for imaging nanoscale materials, magnetic domains and biological samples. In this article the scientific case, requirements and the possible realization of the coherent X-ray diffraction imaging experiments at the European XFEL Facility are discussed in detail.

Crystallography in India

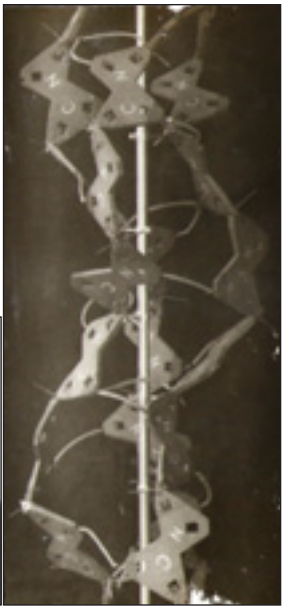
India has had an ancient tradition in science that spans many centuries. In the modern context, India entered the international scientific mainstream in the early 1900s and early activity was also connected with the freedom struggle—the setting up of the Indian Association for the Cultivation of Science (IACS) in Calcutta in 1905 was a purely indigenous move intended to indicate to the British authorities that original scientific research aiming at Western standards could be carried out in a colonial territory. Understandably, this was not entirely to the liking of the government. Serious research began in universities in the 1920s and 1930s (Allahabad, Dhaka, Punjab, Delhi, Mysore, Andhra, Banaras) pursuing the idea of teaching-cum-research institutions, in contrast to the purely teaching universities of Madras, Bombay and Calcutta set up by the British. The setting up of the national laboratory system (now called Council for Scientific and Industrial Research, CSIR), a few years before independence in 1947, was a major initiative. Important investments in science education and research were made by the government in the 1960s (Indian Institutes of Technology, IIT) and more recently, after 2000. Modern, that is post-diffraction, crystallography is therefore as young as the modern research tradition in India and it is interesting to trace the course of the subject in this vast country (see map), to see how we have developed and strengthened research in physical, chemical and biological crystallography. Attempting to do world class research, in a country that was geographically far removed from the major international scientific centres, a country which was grappling with tremendous problems as it made the transition from an older order into the modern world, was not easy. Today, time and distance scales have shrunk in all ways; globalization and the emergence of India as a major economic power have meant that Indian scientists have had to quickly readjust themselves, at least those who would like to project into a future in which India would provide international scientific leadership. The reader should note the equivalences of new and older place names in the text, such as Chennai (Madras), Mumbai (Bombay), Kolkata (Calcutta), New Delhi (Delhi) and Pune (Poona). Abbreviations are commonly used in India, for places and people, and they are invariably used here for institution names after the first appearance.



The background for the map is from a magnificent crystalline specimen (> 100 cm^2) of mica intergrown with haematite from the collection of C.V. Raman (courtesy Raman Research Inst., Bangalore).

Summary of activities between 1930 and 1980

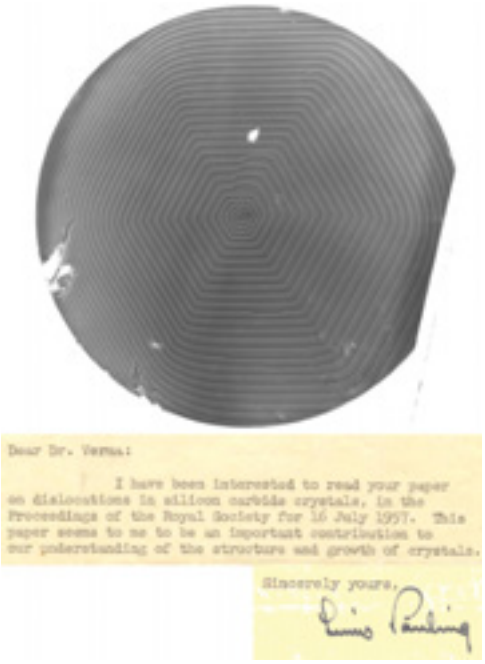
The earliest crystallographic activity in India was the determination of the crystal structures of naphthalene and anthracene by K. Banerjee at IACS (*Nature*, **125,** 456, 1930). IACS was the nucleus of crystallographic activity through the work of C.V. Raman, M.N. Saha, K.S. Krishnan, and S. Bhagavantam. These pioneers were physicists, and for decades, crystallography in India reflected a physics bias in the schools developed by G.N. Ramachandran in the U. of Madras, by A.R. Verma in Banaras Hindu U., (BHU), National Physical Lab. (NPL) and Delhi U., by S. Ramaseshan in National Aeronautical Lab., Bangalore and by R. Chidambaram in Bhabha Atomic Research Centre, Bombay, (BARC).



G.N. Ramachandran's original model of collagen triple helix.

G.N. Ramachandran, a student of C.V. Raman, and arguably the most distinguished scientist of independent India, worked on fibrous proteins and is recognized for the well known triple helical model for the structure of collagen (1954) and the now ubiquitous Ramachandran Plot for validation of protein structures (1963). Contact distances of non-bonded atom pairs obtained from the crystal structures of small organic molecules were used to delineate the conformational space that a polypeptide chain can occupy, leading in turn to the use of a plot of phi and psi conformational angles in a protein struc-

ture as a diagnostic tool in the evaluation of protein structures. The collagen structure was a very important ingredient in the development of the subject of structural biology. Influential books by him and his associates (R. Srinivasan, S. Parthasarathy) in 1970 and 1976 on methods of solving the phase problem and crystallographic statistics, are also noteworthy. Ramachandran was honored with the Ewald Prize, the highest recognition of the IUCr, in 1999. Anomalous dispersion as a structure solution tool was proposed by S. Ramaseshan and K.Venkatesan in Indian Institute of Science (IISc) Bangalore in 1957 and by S. Raman in Madras. The potential of this tool was, however, realised outside India only after the advent of synchrotron radiation and ultrafast computers, in the form of the well known MAD and SAD techniques in macromolecular crystallography.



Growth spiral on SiC surface (A.R. Verma) and extract of letter from L. Pauling

A.R. Verma and his students P. Krishna, K. Lal, O.N. Srivastava, G. Singh and G.C. Trigunayat initiated research in the area of crystal growth and imperfections in solids, using techniques of X-ray diffraction and optical as well as electron microscopy. He was the first to use multiple beam interferometry to directly observe a dislocation. His group studied the surfaces of single crystals using phase contrast microscopy and measured the observed step-heights using multiple-beam-interferometry. They took photographs of growth spirals on the surface of SiC and CdI_2 polytype crystals and determined their crystal structure using X-ray diffraction techniques. Many new polytype structures of SiC, CdI_2 and ZnS were identified. Several anomalous structures were observed whose growth could not be understood in terms of traditional models of spiral growth around screw dislocations. They therefore proposed an alternative faulted matrix model which gave a good agreement between theoretically predicted and observed structures. A well known monograph (Verma and Krishna, 1966) on polymorphism and polytypism continues to be well cited, and is relevant today given the current importance of polymorphs in pharmaceuticals.

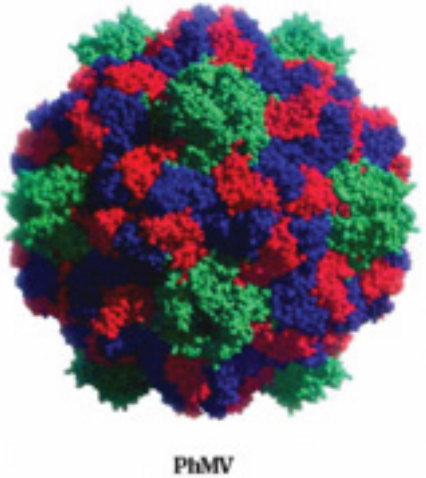
G.B. Mitra (Indian Inst. of Technology, IIT, Kharagpur) studied thermal expansion of crystals and the relationships between lattice defects and particle sizes. He established methods for classifying coal, estimating mineral contents and particle sizes of coal minerals using X-ray diffraction. He also developed a microwave analogue for the calculation of structure factors. R. Chidambaram began a program of neutron diffraction in BARC, Mumbai and carried out original studies on amino acids and hydrogen bonding. Nucleic acid crystallography was introduced by M.A. Viswamitra in IISc. The first oligonucleotide $dp(AT)_2$ structure solved by him, in collaboration with O. Kennard in Cambridge, gave the first view of a DNA duplex in atomic detail. Small molecule structure determinations were always being carried out in several groups, but the lack of proper instrumentation and computation was a definite handicap. Still, the early contributions of L. M. Pant (National Chemical Lab., NCL, Poona) on charge densities, H. Manohar (IISc) on topotactic reactions and natural products (*Z. Krist.*, 1962, **117**, 273), M.A. Viswamitra on nucleotides, and K. Venkatesan (IISc) on photochemical reactions in organic solids (*Chem. Rev.*, 1987, **87**, 433) are noteworthy.

Scientific communication with the international community was limited in those early years to leading personalities. Meetings conducted in Madras by G.N. Ramachandran in the 1960s attracted luminaries like W.L. Bragg, L. Pauling, D.C. Hodgkin, J.D. Bernal, J. M. Bijvoet, N.V. Belov, W. Cochran and A.I. Kitaigorodskii, while K. Lonsdale, F.C. Frank, P.L. Kapitza and F. Bertaut visited the laboratories of A.R. Verma in Delhi. Visits of Indians to foreign countries were even more limited. A.R. Verma and T.R. Anantharaman were trained abroad, but most others were homespun products, at the most spending a few years of post-doctoral studies abroad, mostly in the U.K.

Macromolecular Crystallography and Drug Design

Early attempts towards establishing macromolecular crystallographic studies in India were initiated at IISc (M. Vijayan) and BARC (K.K. Kannan), in the late 1970s and early 1980s. Crystallography of peanut lectin (*J. Mol. Biol.*, 1982, **154**, 177; *Proc. Natl. Acad. Sci.* USA, 1994, **91**, 227) at IISc marked the beginning of a very productive and scientifically rich protein crystallography program. The early focus of the BARC group was mainly on the crystallography of carbonic anhydrases (*J. Mol. Biol.*, 1986, **190**, 129; *J. Mol. Biol.*, 1994, **241**, 226). These two groups were working in geographical isolation, and special efforts were required for building necessary infrastructure and indigenous skills. Major infrastructural support provided by the Dept. of Science and Technology (DST) in 1983 to the Bangalore centre proved crucial in spurring subsequent growth and expansion of macromolecular crystallography in India. Macromolecular crystallography has now spread across the country, and more than 30 research groups in 15 institutions are now actively engaged in these efforts. Notable is the active participation of many groups in the international structural genomics initiatives (*Curr. Sci.*, 2003, **85**, 878). A large number of important protein structures from diverse organisms have been determined as a part of these efforts. Protein crystallography activities are marked by close collaborations between crystallographers, biochemists and molecular biologists.

The IISc has many independent groups active in the area. M. Vijayan (IISc) and his group has focussed on the crystallography of lectins and in addition to determining many novel structures and recognizing new folds, assemblies and quaternary structures, his



Subunit assembly of physallis mottle virus (M.R.N. Murthy).

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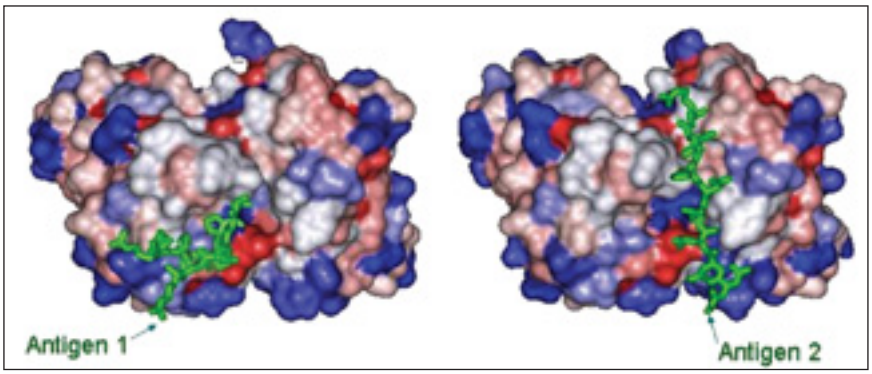
group has established a rich protein architectural database that may be correlated with the carbohydrate binding patterns (*Nat. Struct. Biol.*, 1996, **3**, 596; *Curr. Opin. Struct. Biol.*, 1999, **9**, 707). His group has also carried out innovative studies addressing protein hydration and associated phase transitions (*J. Biol. Chem.*, 1990, **265**, 16126). Also investigated are comparative crystal structure analyses of RecA and RuvA from *M tuberculosis* (*M TB*) and other bacteria providing elegant mechanistic insights regarding recombination (*J. Mol. Biol.*, 2007, **367**, 1130; *Tuberculosis* (Edinb), 2005, **85**, 357). Other protein structures that have been determined from *M TB* include the promoter recognition domain of the sigma factor from *M TB* by B. Gopal (*J. Biol. Chem.*, 2007, **282**, 4711). K. Suguna has determined structures from *P falciparum* including a complex of triose-phosphate isomerase-2-phosphoglycerate (*J. Biol. Chem.*, 2003, **278**, 52461) and FabZ (*Acta Cryst.*, 2007, D**63**, 458). M.R.N. Murthy has examined two viruses, sesbania mosaic virus and physalis mottle virus providing structural architectures and also mechanistic details of virus assembly (*Structure*, 1995, **3**, 1021; *Virology*, 2006, **346**, 440). S. Ramakumar has determined the structure of a thermostable xylanase from *T aurantiacus* at very high resolution (*J. Mol. Biol.*, 1999, **288**, 999).

D.M. Salunke (National Inst. of Immunology, NII, New Delhi) has addressed contemporary issues in immune mechanisms and elegant crystallographic experiments have been carried out by his group to discover novel mechanisms of antibody diversity with implications to affinity maturation, and analysis as to how the immune system reacts when encountered with antigens of changing shape (*Immunity*, 2006, **24**, 429; *J. Immunol.*, 2002, **168**, 2371). His group has also explored molecular mimicry in the physiological context, towards delineating the associated structural rules and possible molecular mechanism of a disease condition (*Biochemistry*, 2005, **44**, 5588; *J. Biol. Chem.*, 2001, *276*, 39277).



Differentially juxtaposed independent antigens on a germline antibody 36-65 to show a mechanism of generating diverse specificities (D.M. Salunke).

In Hyderabad, S.C. Mande (Center of DNA Fingerprinting and Diagnostics, CDFD) has actively pursued structural genomics of *M TB* and has determined the crystal structures of chaperonins, and chorismate mutase (*J. Bacteriol.*, 2004, **186**, 8105; *Biochemistry*, 2006, **45**, 6997). The latter structure has provided valuable insights regarding the role of this enzyme in host-pathogen interactions. Also in Hyderabad, R. Sankaranarayanan (Center for Cellular and Molecular Biology, CCMB) has contributed to the structural genomics of *M TB* and has determined the mycobacterial type III polyketide synthase structure, providing a structural basis for generating diverse metabolites (*Nat. Struct. Mol. Biol.*, 2004, **11**, 894). After determining the structure of threonyl-tRNA synthetase from archaea, his group deciphered an interesting D-amino acid editing module coupled to the translational apparatus (*Nat. Struct. Mol. Biol.*, 2005, **12**, 556).

The group at the International Center for Genetic Engineering and Biotechnology, ICGEB, in New Delhi (A. Sharma) is pursuing the structural basis of host cell receptor recognition by malarial parasite (*Nature*, 2006, **439**, 741). The structure of a gametocyte protein essential for sexual development in *P falciparum* has also been determined (*Nat. Struct. Biol.*, 2003, **10**, 197). S. Gourinath at the Jawaharlal Nehru U. (New Delhi) has determined the structure of a calcium binding protein from *E histolytica* (*Proteins*, 2007, **68**, 990).

J. K. Dattagupta in Saha Inst. of Nuclear Physics (Kolkata) carried out structural work on proteases and protease inhibitors (*Proteins*, 2003, **51**, 489; *Acta Cryst.*, 1996, D**52**, 521). This group has evolved into a centre for structural genomics. Recently, the structure of a DNA binding protein lambda CII was determined at Bose Inst., Kolkata (P. Parrack) providing insights into the recognition of direct-repeat DNA by an unusual tetrameric organization (*Proc. Natl. Acad. Sci.* USA, 2005, **102**, 11242). A.K. Das (IIT, Kharagpur) has initiated structural genomics studies and determined the crystal structure of a low-molecular-weight protein tyrosine phosphatase from *M TB* (*J. Bacteriol.*, 2005, **187**, 217581).

M.V. Hosur (BARC) is exploring


M. Vijayan

M. Vijayan is Honorary Professor at the Molecular Biophysics Unit, Indian Inst. of Science, Bangalore. He has played a major role in the establishment of macromolecular crystallography research in India. He obtained his Ph.D. from IISc in 1967 and did post-doctoral work with Dorothy Hodgkin on the structure determination of insulin. After returning to India, he established a very active school of macromolecular crystallography in IISc. Many of the over 50 students and post-doctoral fellows who trained with him during the past 35 years have now established frontline structural biology programs all over India. In his research contributions in lectin biology, he identified many novel folds and quaternary structural organizations. He analysed a large number of structures from peanut, winged bean, jackfruit, garlic, banana and snake gourd lectin. His analysis of the roles of water-bridges, post-translational modification, oligomerisation and variation in loop length led to strategies for generating carbohydrate specificity. He orchestrated a national programme on the structural genomics of microbial pathogens even while making his own contributions to the structural genomics of *M tuberculosis*. He provided fundamental insights into the relationship between hydration, molecular mobility and enzyme action using a novel approach involving water-mediated crystal transformations. He has been closely associated with the IUCr, AsCA and the ICA. He is the immediate past-president of AsCA. He founded the ICA in 2001 and was its president until 2004. He has been honored with Fellowships of the three most important science academies in India (INSA, IASc, NASc) and of TWAS (Academy of Science for the Developing World), with the Bhatnagar Prize in 1985 and with the Distinguished Biotechnologist Award for 2004. The President of India conferred the Padma Shri civilian award upon him in 2004. He has been recently elected as president of INSA which is the corresponding body in India for IUCr.

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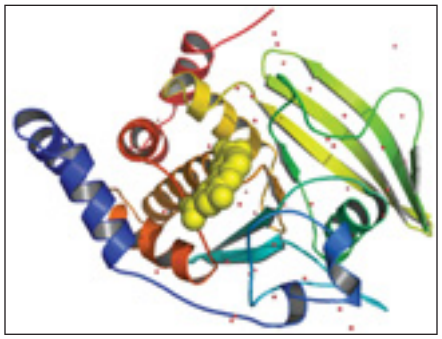
the structural biology of protease-inhibitor complexes towards rational design of HIV/AIDS drugs (*Proc. Natl. Acad. Sci.* USA, 2006, **103**, 18464) while V. Kumar has addressed structural enzymology of acid phosphatases (*Biochemistry*, 2007, **46**, 2079). C.G. Suresh (NCL) has determined the structures of penicillin V acylase and a conjugated bile salt hydrolase and has elucidated the evolutionary relationship between them (*Nat. Struct. Biol.*, 1999, **6**, 414; *J. Biol. Chem.*, 2006, **281**, 32516).

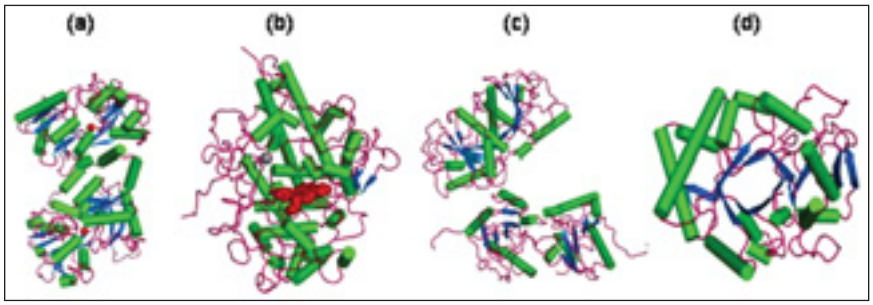
An active autolysate form of porcine alpha-trypsin was the first high resolution protein structure (1.8 Å) determined in Chennai by V. Pattabhi (*Acta Cryst.*, 1997, D**53**, 311). The Madras U. centre has also provided valuable insights with regard to sequence dependent features of DNA structure (N. Gautham) based on a series of designed oligonucleotide crystal structures (*Nucleic Acids Res.*, 2004, **32**, 5945). D. Velmurugan has contributed to the modern approaches of macromolecular structure determination (*J. Synchrotron Rad.*, 2004, **11**, 358).

Crystal structures of therapeutically important proteins in complexes with compounds that modulate their function are fundamental to the development of structure based strategies for new drug design. Significant experimental and computational activity in these areas is seen in the recently burgeoning corporate R&D sector. Notable among these are the groups in Aurigene Technologies, Bangalore (www.aurigene.com) and Jubilant Biosys Ltd, Bangalore (www.jubilantbiosys.com). Jubilant and Aurigene are drug discovery service organizations specializing in structural biology and structure based drug design. Hundreds of crystal structures of several therapeutically important classes of proteins incorporating many designed compounds have been determined at these organizations.



Crystal structure of protein tyrosine phosphatase-1B complex with an inhibitor (Aurigene)

T. P. Singh (All India Inst. of Medical Sciences, New Delhi) has contributed to the crystallography of mammary gland proteins, such as lactoferrins (*J. Mol. Biol.*, 2001, **309**, 751; *J. Biol. Chem.*, 2003, **278**, 14451). His group has been working on targets implicated in various disease areas including inflammation, cancer and infectious diseases. Several crystal structures of Phospholipase A_2 in complex with anti-inflammatory agents have provided valuable information towards design of therapeutically potent molecules (*Curr. Top. Med. Chem.*, 2007, **7**, 757).



Structures of proteins secreted during different phases of mammary gland function (T. P. Singh)

Central Drug Research Inst., Lucknow established a strong group dedicated to drug discovery utilizing rational structure based methods led by H. Subramanya and subsequently by R. Ramachandran. Novel inhibitors have been designed to target a DNA ligase and Lysine ε-aminotransferase from *M. TB* (*J. Biol. Chem.*, 2005, **280**, 30273; *J. Mol. Biol.*, 2006, **362**, 877; *Med. Chem. Res.*, 2007, **15**, 181) using the structural information as well as virtual screening techniques. This group successfully deciphered the function of a protein based on its crystal structure and showed that it is a SAM-dependent methyl transferase (*J. Mol. Biol.*, 2001, **312**, 381).

Other groups, in Madurai Kamaraj U. (S. Krishnaswamy), IITs in Roorkee (P. Kumar & A.K. Sharma), Chennai (N. Manoj) and Kanpur (B. Prakash) and Inst. of Microbial Technology, Chandigarh (S. Karthikeyan) are also actively pursuing structural biology programmes by multi-dimensional approaches that dominantly include crystallography. Other institutions such as National Centre for Biological Sciences (NCBS), Bangalore, Inst. of Genomics and Integrative Biology, Delhi, Panjab U. (Chandigarh) and Tata Memorial Centre (ACTREC), Navi Mumbai have recently initiated crystallography-based modern biology research activities. The protein folding problem has also been addressed through the design of structural motifs in oligopeptides (N. Shamala, S. Ramakumar, IISc; V. Pattabhi, Chennai). While macromolecular crystallography seems to have acquired the critical mass required for continued progress, keeping pace with future international developments in this field could be considerably limited due to lack of easy access to synchrotron radiation sources.

Crystal Engineering and Structural Chemistry

Till around 2000, chemical crystallographers in the country were struggling to get even the unit cell of a crystal and an ORTEP diagram because the scientific funding bodies of the government did not favour the general acquisition of state-of-the-art single crystal X-ray diffractometers. A change in this attitude resulted in a vastly improved situation for chemical crystallographers, indeed one wherein the Indian contribution to this global activity is represented by the deposit of over 2000 crystal structures in the Cambridge Structural Database (CSD) during the past seven years. Of these, about a third originate from the U. of Hyderabad where early work by G.R. Desiraju laid the foundations of the subject of crystal engineering worldwide (See box). The additional routine availability of low temperature equipment, powder diffractometers, automated structure solution software and inexpensive high performance computers is a further advantageous factor. Luckily, the hectic pace of research in small molecule crystallography in India also comes at a time when the subject of crystal engineering is growing rapidly, and the Indian contribution in the high impact journals *Crystal Growth & Design* (IF 4.37) and *CrystEngComm* (IF 3.71) is truly impressive. Several aspects of crystal engineering such as intermolecular interactions, crystal synthesis, crystal growth, polymorphism, and at a fundamental level, understanding the mechanism of crystallization, is being actively pursued by around 10 to 15 independent groups. One may confidently state that these groups are at the forefront of this innovative and outward-looking branch of the chemical sciences, which goes beyond traditional divisions of organic, inorganic and physical chemistry.

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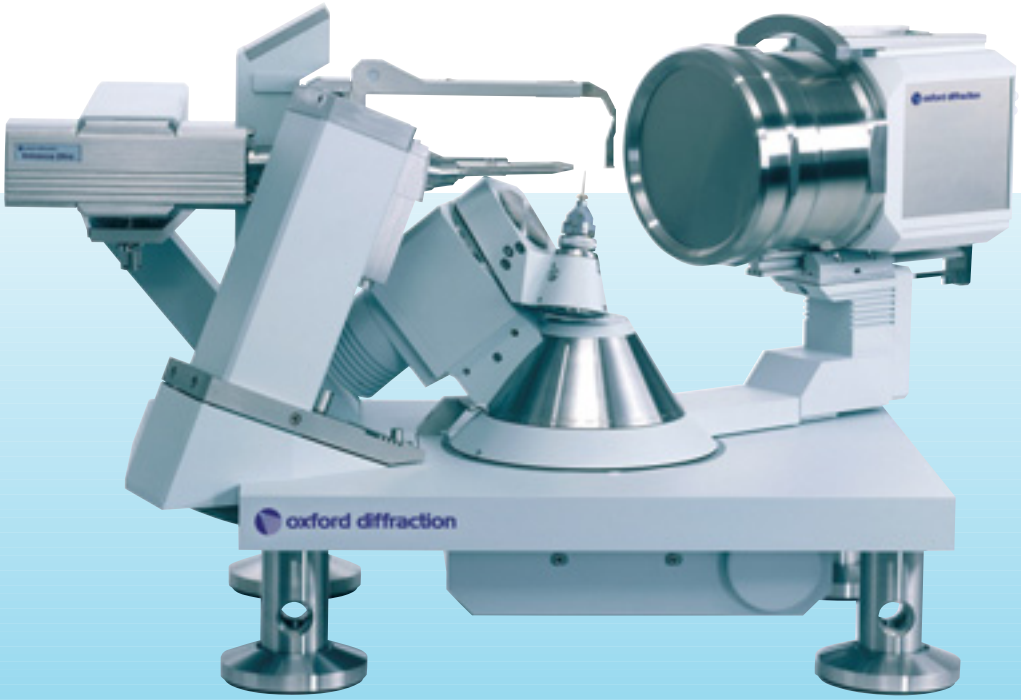

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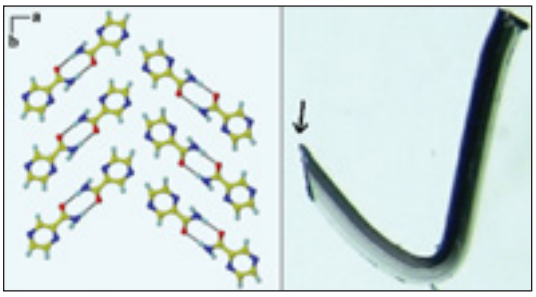


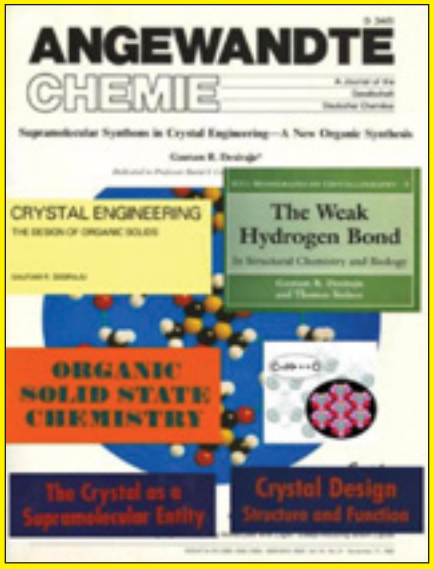
Bending of α-pyrazinamide crystal along the (100) crystal face (G.R. Desiraju).

Two papers are selected here from the 300 publications of Gautam Desiraju. In an interesting connection between intermolecular interactions, crystal packing and mechanical properties, it was shown that organic crystals where interactions along different directions are of different strengths are susceptible to anisotropic bending and shearing (*Chem. Eur. J.*, 2006, **12**, 2222), thereby affording a very dramatic way of comparing weak interactions. In another recent study, the hydration/dehydration behaviour of sodium saccharin was studied crystallographically, and a heavily hydrated large volume unit cell structure (15000 Å^3) was described as a model for a supramolecular transition state during crystallization (*Angew. Chem. Int. Ed.*, 2005, **44**, 2515). This result could have important implications in elucidating the mechanism of crystallization.

The ongoing activities within the Indian crystal engineering community and in related areas are now summarized for the IITs, the single largest category of institutions in this section, followed by the universities, and finally the Government laboratories of CSIR. The reader should note that there is also a great deal of crystal structure analysis of small molecule structures in other chemical and biological projects wherein crystal structure systematics was not the main aim, and in service crystallography groups, and that the number of 2000 structures in the CSD quoted above pertains largely to the activity in the crystal engineering field.

A. Ramanan at IIT, Delhi is developing chimie douce (soft chemistry) techniques such as hydrothermal, sol-gel and molten flux methods to isolate new hybrid materials with multi-dimensional structural features including nanomaterials. His objective is to establish reliable connections between molecular and supramolecular structures on the basis of intermolecular interactions, especially hydrogen bonding. A systematic investigation of crystal growth and influence of the solvent medium and reaction conditions (pH, temperature and hydrothermal/solvothermal) have enabled his group to recognize the building of molecular and hybrid solids in terms of supramolecular assembly of molecular species. The templating role of organic ligands and counter ions in helical structures, interpenetrating networks and pillared frameworks are demonstrated in vanadates, molybdates, MOFs, calcium phosphates and crystal hydrates. A theme paper elucidating the chemical events from molecular recognition and supramolecular assembly to metal–organic frameworks appeared as a Perspective in *Crystal Growth & Design* (2006, **6**, 2419). The synthesis of mononuclear, binuclear, trinuclear and polynuclear metal carboxylate complexes interests J.B. Baruah at IIT, Guwahati. Origins of polymorphism in aqua-bridged 2-nitrobenzoato cobalt(II) complexes have been ascribed to differences in the orientation of aromatic-ring substituent. Co-crystals of neutral transition metal complexes and crystal structures of phthalimide and 1,8-naphthalimide derivatives are systems of interest, the latter for their optical properties. M. Ray is assembling chiral molecules into cages and organized networks using metal complexes of amino acid derivatives. The metal provides the stability while the organic ligand directs the hydrogen bonding. His group synthesized and characterized a supramolecular capsule of L-histidine–Cu(II) and discovered an elegant way to reversibly disassemble the capsule via a molecular trigger. Helical channels of his-

Gautam R. Desiraju is Professor of Chemistry at the U. of Hyderabad. He received his B.Sc. at the U. of Bombay and was awarded a Ph.D. from the U. of Illinois at Urbana-Champaign in 1976. He has published 300 research papers in the areas of crystal engineering, solid-state supramolecular chemistry, organometallic crystal structures, database analysis, hydrogen bonding with special reference to weak hydrogen bonds, ligand–protein interactions, crystal structure prediction, polymorphism and pseudopolymorphism. The topic of crystal engineering would have remained a specialized chapter in structural chemistry dealing with solid-state topochemical reactions but for his single author monograph entitled, *Crystal Engineering: The Design of Organic Solids* in 1989. His broad definition of the term crystal engineering as "the understanding of intermolecular interactions in the context of crystal packing and the utilisation of such understanding in the design of new solids with desired physical and chemical properties" is now widely accepted in chemistry and materials science. Crystal engineering has grown very rapidly during the last decade. Following his keynote talk in the Seattle IUCr Congress in 1996, it became a microsymposium topic in these congresses. Two new journals were launched in the late 1990s—*CrystEngComm* in 1999 and *Crystal Growth & Design* in 2000—he being associated with both from their inception. Gautam Desiraju established the role of weak intermolecular interactions in crystals, such as C–H···O, C–H···N, N–H···π, halogen···halogen, in a series of reviews (*Acc. Chem. Res.*, 2002, **35**, 565; *Acc. Chem. Res.*, 1996, **29**, 441; *Acc. Chem. Res.* 1991, **24**, 290; *Acc. Chem. Res.* 1986, **19**, 222). He showed that what is often more significant for structure design and prediction are not the individual interactions but rather patterns composed of two or more interactions, often as cyclic motifs. Supramolecular synthons are structural units within supermolecules that can be formed or assembled by known or conceivable intermolecular interactions (*Angew. Chem. Int. Ed. Engl.* 1995, **34**, 2311). His innovative ideas and research over the last three decades (see selected highlights), often establishing connections between independent disciplines (*Chem. Commun.*, 2005, 2995), has opened new streams of thought and he has academically inspired a generation of young scientists. He has been honored with Fellowships of the three most important science academies in India. He is a fellow of the Academy of Science for the Developing World (TWAS) and the Royal Society of Chemistry. He is currently co-editor of *Acta Crystallographica* and a member of the Executive Committee of the IUCr. He is a recipient of the Humboldt Research Award, the TWAS Award for chemistry and the Michael Visiting Professorship of the Weizmann Inst. of Science. He is an honorary member of the Hungarian Chemical Society and was recognized as a Thomson Scientific Citation Laureate in 2006.



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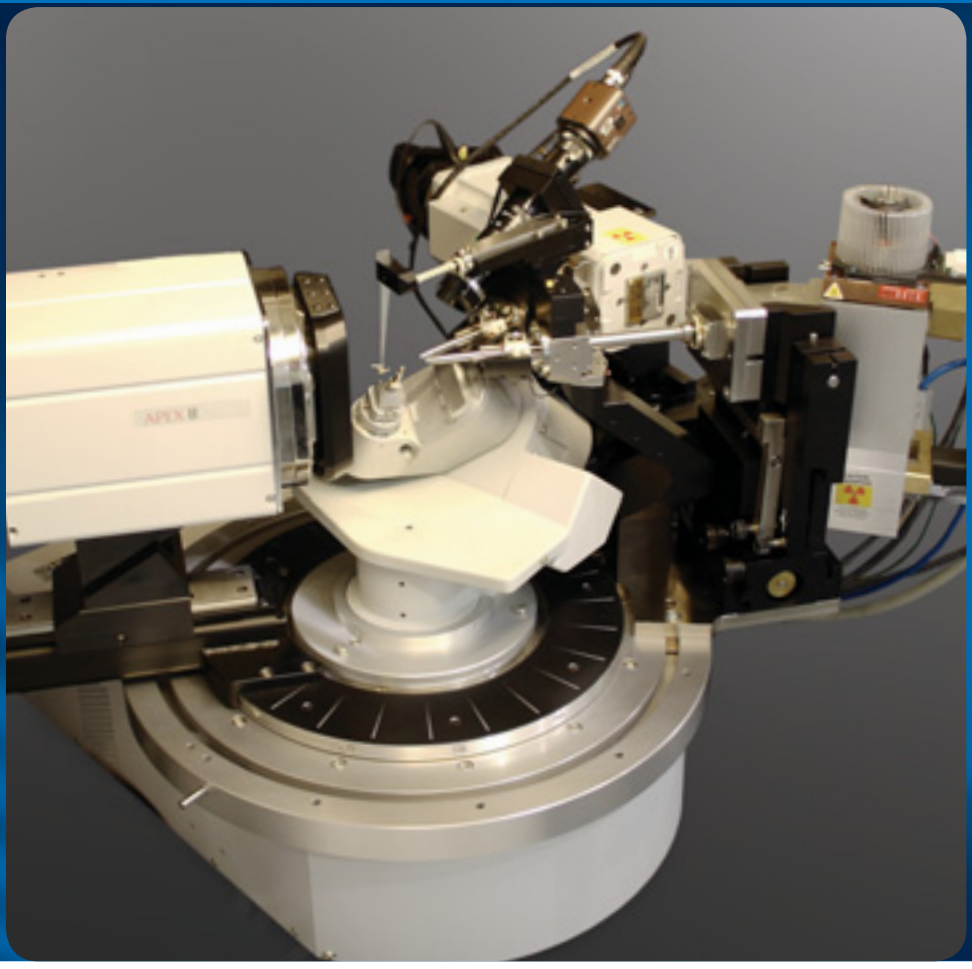

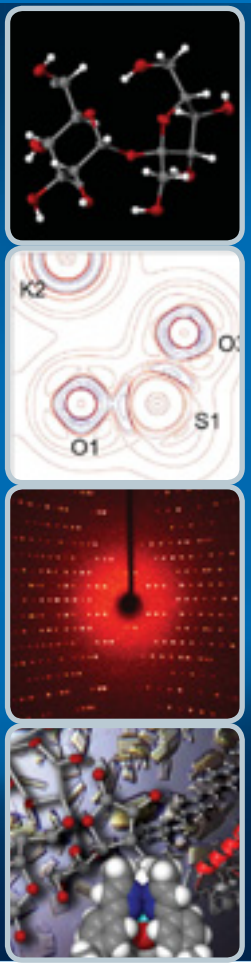

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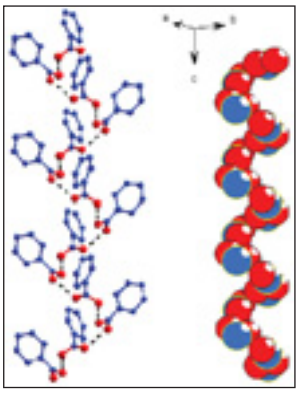
tidine ligand with Fe(III) can be emptied and refilled with iodine (*Angew. Chem. Int. Ed.*, 2003, **42**, 1940).

R. Mukherjee's research at IIT, Kanpur covers coordination chemistry, biomimetic inorganic chemistry and inorganic crystal engineering (*Dalton Trans.*, 2006, 1611). He is working on the synthesis, characterization, properties and interactions of (i) coordination compounds of varying nuclearity with novel electronic, magnetic and redox properties; (ii) bio-inspired coordination compounds, e.g. low-molecular-weight representations of metallo-biomolecules using tailor-made organic ligands of Mn, Fe, Ni, Cu and Zn-containing non-heme proteins; (iii) radical-coordinated transition metal complexes and half-sandwich organometallic complexes of pyridyl/ pyrazole/ imidazole/ aliphatic amine/ phenol-containing bidentate/tridentate chelating ligands, the latter to investigate nucleophilic addition reactions with Ru(II)-coordinated benzene; (iv) coordination polymers including homochiral metal–organic frameworks; (v) water oxidation relevant to photosystem II, aromatic ring hydroxylation for tyrosinase-like activity, fixation of atmospheric carbon dioxide to carbonate; (vi) study of noncovalent interactions, such as, C–H···Cl, N–H···Cl, O–H···Cl, π···π, C–H···π etc. J. N. Moorthy in the same department is using intermolecular interactions to control molecular reactivity in the solid state, and to develop crystalline materials that exhibit unique properties. Based on crystal structures of aromatic carboxylic acids and amides, he argues that "the presence of weakly interacting groups can decisively modify the molecular association of strongly interacting functional groups" (*J. Am. Chem. Soc.*, 2002, **124**, 6530). Weak C–H···O/X interactions direct the conformation and photoreactivity in the solid state of *o*-alkylaldehydes.

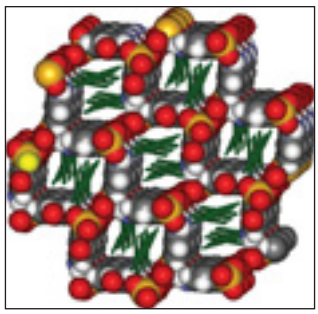
Several of the above themes are reflected in the research program of K. Biradha at IIT, Kharagpur. His group has built MOF's (metal-organic frameworks) of exotic topologies, such as one-dimensional chains with cavities, two-dimensional open and interpenetrated (4,4)-networks, and three-dimensional networks of $6^5 8$ and quartz topologies (*Chem. Comm.*, 2005, 2229). Porosity, guest/ ion exchange, network transformations give an idea of the stability and robustness of these frameworks assembled *via* metal–ligand and amide–amide bonds. What is the effect of a particular functional group when it is present in the presence of several others? He examines "structural interference" between supramolecular synthons to correlate molecular



Weak interactions direct the uncommon helical catemer of carboxyl groups in halogenated mesitoic acids (J.N. Moorthy)

and crystal structure. In crystal structures of diamides containing the pyridine group, interference from pyridyl N is minimal in the formation of N–H···O bonded β-sheet and 2D-layers (*Cryst. Growth Des.*, 2007, **7**, 1318). The synthesis of co-crystals via heterosynthons is another project in his group. Co-crystals of 4,4'-bipyridine with chiral or racemic bis-β-naphthols include guest molecules. Extending these ideas, aryl sulfonates make synthons similar to carboxylic acids with pyridine partners.

P. Mathur's research in IIT Mumbai is on the synthesis of organometallic and mixed-metal clusters and of metal ion complexes of carbohydrates and calixarenes. He works on the designed construction of metal cluster compounds by using lone pairs of single atom ligands for addition to coordinatively unsaturated metal carbonyl fragments. He studies nonlinear optical activity of novel mixed-metal and mixed-chalcogen clusters. This methodology is extended to the incorporation of organic fragments in chalcogen-bridged metal carbonyl clusters for reactivity modulation. Biomimetic chemistry of essential metal ions provides means to design systems for ion and molecular recognition in C.P. Rao's group, in this institute. Understanding the binding of small molecules to proteins, e.g. lectins, and their inhibitory role towards glycosidases is

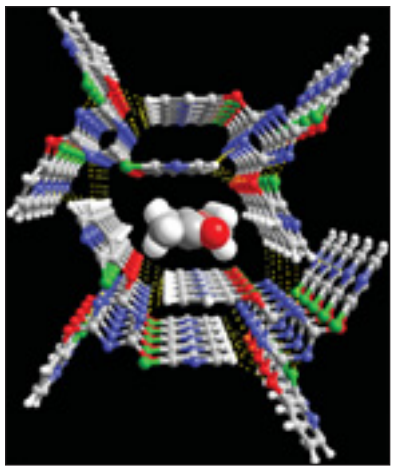


Honeycomb network of pyridinium and sulfonate synthons in sulfanilate. 4,4'-bipyridinium.$2H_2O$ (K. Biradha)

one of their goals.

At the U. of Hyderabad, A. Nangia is pursuing studies in crystal engineering and polymorphism. Inter-halogen interactions and the Piedfort Unit trigonal symmetry are matched to construct tubular and cage architecture for guest inclusion (*Cryst. Growth Des.*, 2007, **7**, 393). Guest-free forms of host materials, which infrequently yield single crystals for X-ray diffraction, were crystallized by solvent-free melt and sublimation procedures. Extending the utility of crystallization at high temperature his group discovered a novel, stable polymorph of venlafaxine hydrochloride (Effexor, Wyeth), a top-selling anti-depressant drug, by solid-to-solid phase transition at ca. 180 ºC. To understand the origin of high Z' in crystal structures, Nangia's group analyzed O–H···O and C–H···O hydrogen bond geometry in polymorphic crystals of variable Z' and found that there is a 70% correlation between high Z' and stronger H bonds (*CrystEngComm* 2007, **9**, 980-983). Apart from the acid–pyridine synthon mentioned earlier, co-crystals of amide type drugs with pyridine-N-oxide partners were shown to form reproducibly.

In IISc, T. N. Guru Row has established a program for mapping of electron densities in crystals to obtain insights into the nature of chemical bonding. This development has



2-Butanone guest in the carbon-walled nanotube of lattice inclusion host (A. Nangia)

been possible only because of the increasing number and availability of CCD detectors and low temperature facilities. The significance of charge density results have been analysed to obtain insights into the nature of intermolecular contacts such as C-H···O, C-H···π, π···π, C-H···S and S···S (*Cryst. Rev.*, 2005, 11, 199; *Acta Cryst.* B., 2006, **62**, 118). The appearance of a "region of overlap" to segregate hydrogen bonds from van der Waals interactions has been identified.

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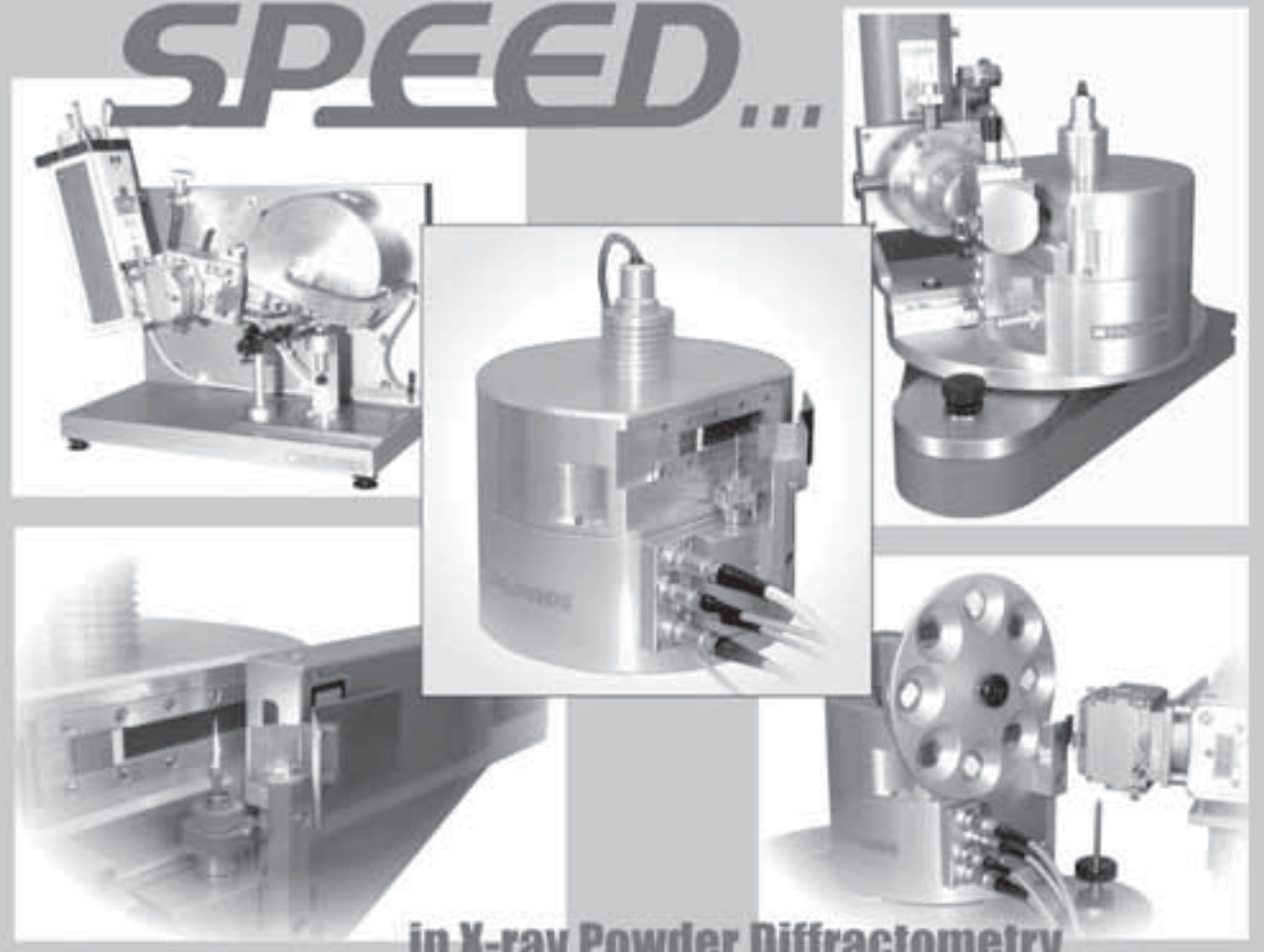

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In the CSIR labs, P. Dastidar, formerly at the Central Salt and Marine Chemicals Research Inst., Bhavnagar (now at IACS) has been working on the crystal engineering of organic and inorganic materials. The goal is to understand the structural basis of gelation by studying supramolecular synthons in crystals. Organic gelators have potential application in containing oil spills. They demonstrate supramolecular and structural diversities in metal-organic frameworks (MOFs) as a function of the ligating topology and the hydrogen bonding backbone and its use in anion control and recognition. In a remarkable discovery last year, near-spherical crystals of common salt, NaCl, were grown by an ingenious method of recycling glycine, a crystal habit modifier. Their research paper in *Cryst. Growth Des.* 2007, **7**, 205 was listed in the section "Year in Ideas – 2006" by *The New York Times*.

In NCL, Pune, M.M. Bhadbhade is studying hydrogen bonding, crystal packing and polymorphism in inositols. Diastereomers of 2,4(6)-di-*O*-benzoyl–6(4)-*O*-[(1*S*)-10-camphorsulfonyl]-*myo*-inositol 1,3,5-orthoformate associate via C–H···O interactions and do not leave voids for guest inclusion whereas association via S=O···C=O bridges produced pseudopolymorphs. A guest-free form I ($P2_1$) and solvated forms II and III ($P2_1$ and $C2$) were crystallized and characterized by X-ray diffraction. Selective inclusion in channels is of potential application in separation science (*Cryst. Growth Des.*, 2005, **5**, 833; see also Aitipamula and Nangia, *Chem. Eur. J.*, 2005, **11**, 6727). S=O···C=O dipolar short contacts, a persistent interaction in these structures, is relevant to the binding of sulfonyl drugs to the C=O moiety of receptor proteins. Continuing in the same series, myo-inositol hexabenzoate of meso configuration gave a resolved polymorph (Form I, $P6_1$) when crystallized rapidly but yielded a centrosymmetric polymorph (Form II, *P*-1) by slow crystallization (*Chem. Commun.*, 2004, 2530). Additionally, Bhadbhade has begun analysis of halogen bonding by charge density. Using a patented technology developed by V. Puranik, Asomex-2.5, the first chirally pure anti-hypertensive drug was launched in the Indian market by Emcure Pharmaceuticals.

Apart from the groups mentioned above, M.S. Hundal at Guru Nanak Dev U., Amritsar is studying hydrogen bonding between metal-organic frameworks and anions in helical chains, staircase coordination polymers, and self-assembled supramolecular structures. Additionally, structural chemistry is being pursued at Pondicherry U. and Panjab U., Chandigarh. It is believed that the quantity and quality of work in crystal engineering from India will increase greatly in the coming years.

Bioinformatics, Database Development and Drug Discovery

A natural inclination of the Indian mind is to try to find common threads linking diverse facets of life, and from the earliest days of the Ramachandran plot this inclination has led to India being a fertile ground for attempts to decipher patterns hidden in the vast amounts of data generated by crystallography. The concept of weak hydrogen bonding, exemplified by interactions such as C–H···O and X–H···π, was greatly extended by G.R. Desiraju (U. of Hyderabad; *Chem. Comm.*, 1989, 179) using the CSD, and is now being applied to understand the stability of protein folds and their interactions with ligands (V. Pattabhi, Chennai, *Acta Cryst.*, 1997, D**53**, 316; P. Chakrabarti, Bose Inst., Kolkata, *J. Mol. Biol.*, 1998, **284**, 867; S. Ramakumar, IISc, *Acta Cryst.*, 1990, A**46**, 455). Likewise, the concept of aromatic···aromatic interactions has been invoked to understand the relative orientations between planar side chains in proteins. With the increasing availability of high resolution structures in the Protein Data Bank there are many groups pursuing structural bioinformatics to understand the structure and function of macromolecules at the molecular level. The topics include analysis of side chain rotamers (V. Sasisekharan, M. Vijayan, IISc), local structures in proteins (C. Ramakrishnan, IISc), side chain influence on main chain conformation (P. Chakrabarti, *Prog. Biophys. Mol. Biol.*, 2001, **76**, 1), clustering of residues and its implication in protein thermostability (S. Vishveshwara, IISc). The stereochemical modeling of disulfide bridges (C. Ramakrishnan, P. Balaram, *Protein Eng.*, 1993, **6**, 873) is now an important component of strategies to enhance protein stability. In addition, other databases like PALI, SUPFAM (IISc), DDBase, SMoS (NCBS), porins and prophages (S. Krishnaswamy, MKU), lectins (IISc), conformational angles (IISc), and secondary structural motifs (Bose Inst., NII, CCMB) facilitate efficient analysis. New algorithms and machine learning approaches have been explored in a variety of situations: application of mutually orthogonal Latin square sampling in protein structure prediction (N. Gautham, Chennai) and graph theoretical approaches for understanding and classifying protein structure networks (IISc and IIT, Mumbai).

At the DNA level, the variations in oligonucleotide crystals (M. Bansal, IISc), and the location of water molecules and their implication for DNA function (B. Jayaram, IIT, Delhi) have been rationalized. A. S. Kolaskar in U. of Poona has designed selective inhibitors for *P. Falciparum* aspartic proteases through in silico approaches (*Frontiers Biophys.*, 2005, **168**). In Hyderabad, modelling tools such as virtual screening, pharmacophore generation, molecular dynamics and QSAR have been used to understand the binding of drugs to macromolecules by G.R. Desiraju, U. of Hyderabad, J.A.R.P. Sarma, GVKBio, and B. Gopalakrishnan, Tata Consultancy Services, TCS, (*J. Chem. Inf. Model.*, 2005, **45**, 725). A software package has been developed to analyze weak hydrogen bonds in biological structures (*Proteins*, 2007, **67**, 128). A recent exercise

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sponsored by the CSIR involved TCS (M. Vidyasagar, S. Mande) with more than 20 academic partners, and resulted in an entire software platform (Bio-suite) which is now being successfully marketed by TCS (*Curr. Sci.*, 2007, **29**). Bio-suite provides tools for predicting biological activities, and for studying binding energy patterns among functionalities. There are now specialized webservers and databases dealing with protein domain superfamilies and spatially interacting motifs, (R. Sowdhamini, NCBS, N. Srinivasan, IISc).

Crystallography introduced the Indian scientific community to the "database culture". During the last decade, India has witnessed a rapid growth in the pharmaceutical sector because of off-shoring from abroad. Besides helping organizations like Chemical Abstracts Services (CAS) and Beilstein in creating and managing their databases, many smaller players in India have started developing their own databases. GVK Biosciences in Hyderabad (J.A.R.P. Sarma, www.gvkbio.com) is notable in this regard and has captured much information, which exists in a more or less disorganized fashion in the public domain, converting them into value added databases for the international pharmaceutical industry (MediChem, kinases, toxicity, clinical candidates, metabolism toxicities, natural products). Multiple advantages may be envisaged from these databases. In particular, they may be used in virtual screening in drug discovery. Strategic and committed collaborations from companies abroad (DuPont, Wyeth, Novartis) ensure that these early initiatives will succeed and much further progress is expected.

Dr. Krishan Lal (National Physical Lab, Delhi), is one of the leaders of physical crystallography in India, and he has established a very active laboratory for growth of well characterized high quality single crystals and investigations of real structure of single crystals, thin films, interfaces and devices. He has contributed significantly to the design of new instrumentation for high resolution work, studies of electric field induced microstructural changes in crystals and accurate measurements of crystal surfaces and interiors. He obtained his early training with A. R. Verma and went on to establish his independent research in NPL. Among the highlights of his work is the crystal growth of nearly perfect crystals using the Czochralski technique. He developed very accurate techniques for measurement of dielectric constants and dielectric loss of single crystals. By using these, effect of impurities and defects on dielectric constants of sapphire and gadolinium gallium garnet crystals could be experimentally demonstrated. Under Dr. Lal's leadership a co-ordinated project with 30 national laboratories has successfully planned, prepared and distributed Indian Certified Reference Materials. Already, 25 CRMs have been prepared in this strategically important initiative. Dr. Lal has been deeply involved at the national and the international levels in activities related to high quality data for science and technology. He is presently President of CODATA the Committee for Data in Science and Technology of ICSU for 2006-2010. He served as President of the Indian Crystallographic Assn (2004-07) and as an editor of *Z. Krist.* between 1997-2003.

F. C. Frank in the laboratory of K. Lal. In the background is A. R. Verma

Powder Diffraction and Industrial Crystallography

Applications of X-ray diffraction in the Indian pharmaceutical industry began in the early 1990s. With the current extreme interest in solid forms of active pharmaceutical ingredients (API), especially with the application of crystal engineering methods to polymorphs, pseudopolymorphs, multi-component crystals ("co-crystals"), mixed phases and amorphous forms, it is no wonder that several academic and industrial groups are seriously engaged in development and application of the powder diffraction techniques (PXRD). Different polymorphs exhibit different physical and/or chemical properties such as solubility, bioactivity, bioavailability, physicochemical, formulation and processing parameters as well as the shelf life of the drug substance and formulated product. Therefore, understanding and controlling the solid-state properties of APIs, both as pure drug substances and in formulated products, is an important aspect of the drug development process. The enforcement of TRIPS (trade related aspects of intellectual property rights) agreements since 2005 has caused a paradigm shift in India's bulk and formulation oriented pharmaceutical industry. Indian generic companies will now need to compete with the multinationals by focusing on drug development and produce their own patented products. It is realized that intellectual property issues can only be addressed by careful screening of drugs for the absence of forms patented by other companies. Another important aspect in this area is the determination of crystal structures from PXRD data because growing single crystals has been difficult for some APIs. For example, T. N. Guru Row (IISc) and A. Mukherjee (Jadavpur) are collaborating with Dr. Reddy's Laboratories (K. Vyas; Hyderabad) to develop methodologies for *ab initio* structure solution packages from PXRD data. A. Nangia (in collaboration with G. Kruger in South Africa) has made interesting contributions pertaining to discovery of new drug polymorphs and co-crystals using variable temperature PXRD (*Chem. Asian. J.*, 2007, **2**, 505). Other Indian pharmaceutical companies such as Alembic (Vadodara), Orchid, Shasun (Chennai), Sun (Vadodara), Torrent (Ahmedabad), Ranbaxy (Delhi), Lupin (Pune), Cadila (Bangalore) and Aurobindo, Suven, Matrix, Hetero (Hyderabad) are actively involved in these efforts. A measure of the success of the Indian pharmaceutical industry in this area may be seen in the increasing number of Para IV filings that are being concluded successfully in the U.S. law courts.

Crystal Growth and Diffraction Physics

A centre for crystal growth was established in NPL (K. Lal) in the 1970s and continues to make several contributions. Many whisker crystals were grown and investigated with a high resolution X-ray Laue technique. X-ray diffraction topography was used to confirm the absence of screw dislocations in ZnS whiskers. Also studied were Al_2O_3, garnet and semiconductors. Also developed was a new high-resolution technique and a three-crystal X-ray diffractometer to investigate diffuse X-ray scattering from nearly perfect single crystals very close to reciprocal lattice points. With this set up it was possible for the first time, to make diffuse X-ray scattering (DXS) measurements on Si single crystals very close to the diffraction peaks having a half width of only ~ 5 arc sec. This DXS technique is now a powerful non-destructive tool to characterize point defects and their clusters in nearly perfect crystals. High resolution methods were also used to study thin diamond crystals having varying degrees of perfection. It was shown that point defect clusters are obtained with sizes in the range 40-190 nm. Techniques of defect measurement are closely related to crystal growth methods, and naturally these methodologies have developed in parallel in the NPL group. Crystal growth facilities have also been established in Mysore (K. Byrappa) where there is a focus on hydrothermal methods and in BARC (J.S. Yakhmi) where large alkali halide crystals have been grown for applications in nuclear radiation detection.

T.R. Anantharaman (BHU), with his students P. Rama Rao and S. Lele, established an active school in the field of X-ray line profile analysis in the 1960s. This technique may be used to study the diffuse streaking which is observed in the X-ray diffraction of materials which have random distributions of stacking faults (*J. Appl. Cryst.*, 1987, **20**, 84). The presence of such faults leads to characteristic peak broadening and/or peak shifts of powder diffraction profiles (G.B. Mitra, IIT Kharagpur; S.P. Sen Gupta, IACS). Indian contributions to the theoretical aspects of this field (S. Lele, D. Pandey, BHU), especially the introduction of the concept of non-random faulting when stacking faults bring about phase transformation from one layer stacking to another, are noteworthy. Other contributions by D. Pandey are the use of X-ray diffraction in the field of doped quantum paraelectrics, morphotropic phase transitions and ferroelectric transitions.

Quasicrystals

The advent of quasicrystals as an ordered but aperiodic arrangement of atoms in the solid state saw several innovative research results originating from India. K. Chattopadhyay and S. Ranganathan (IISc) discovered a new type of quasicrystalline phase known as the decagonal phase (*Acta Metall.*, 1987, **35**, 727). Together with S. Lele (BHU) they analyzed vacancy ordered phases as an example of one dimensional quasicrystals. P Ramachandra Rao and G.V. S. Sastry (BHU) blazed a new path in the synthesis of quasicrystals by rapid solidification of Mg-Zn-Al alloy. C. Suryanarayana (BHU) discovered polytypism in quasicrystals. S. Lele and R.K. Mandal (BHU) were the first to postulate the existence of pentagonal quasicrystals. Using Pettifor maps, Ranganathan also provided new insight by demonstrating that all quasicrystals are either binary or pseudobinary. Other notable contributions came from J.A. Sekhar and T. Rajasekharan (Defence Metallurgical Research Lab., Hyderabad), and from S. Banerjee, G.K. Dey, U.D. Kulkarni and R. Chidambaram in BARC.

However, India missed some opportunities in this area. Early work of T.R. Anantharaman on Mn-Ga alloys and G. V.S. Sastry and C. Suryanarayana (BHU) on Al-Pd alloys came tantalizingly close to the discovery of quasicrystals.

On the Cover

The design for the cover (courtesy Sita Lakshminarayan), has been inspired by the Ramachandran plot. Its classic quadrants contain and constrain illustrations (clockwise from top right) of the most accurate charge density measurement of a C–H···O interaction done in India, a recent hot result (spherical salt), our most complex small molecule structure to date (sodium saccharin dihydrate, V=15000 Å^3), one of our first protein structures (peanut lectin, 1980) and one of the larger crystals grown in India (for radiochemical purposes). The intricate motifs on the horizontal axis are *kolam* (Tamil), auspicious threshold designs that welcome a guest into an Indian home. Each pattern is drawn in a continuous line incorporating symmetry and infinity, themes dear to crystallographers. This particular image is known as Brahma's knot, in itself supposed to be the ultimate in complexity, but now a recurring topic in contemporary scientific thought. The title is in Bank Gothic font, in use since the 1930's, that is, as long as crystallography has been practised in India. For information please contact the artist at sita_lakshminarayan@yahoo.com.

Liquid crystals

S. Chandrasekhar (RRI, Bangalore) made a seminal discovery in 1977 on a new type of liquid crystal made of stacked disc-like molecules (*Pramana*, 1977, **9**, 471). These columnar or discotic liquid crystals have since become an important branch of research, and 2D lattices with hexagonal, and different types of rectangular arrangements have been found. X-ray scattering studies have been useful in identifying these phases and also other smectic and nematic phases. Studies by N. Madhusudana and R. Pratibha in RRI (*Curr. Sci.*, 1997, **73**, 761) and by C. Manohar in BARC have delineated the transformations between these phases. A very unusual skew-cybotactic (smecticC-like) arrangement which exhibits fibre-like patterns of molecules tilted with respect to the local layer-normal have been discovered in some special compounds (U. Deniz, BARC). If the molecules are chiral, the liquid crystalline compound often exhibits a superstructure at the micrometer scale. Many mesogenic rod-like and disk-like compounds can also be crystallised from solution and V.A. Raghunathan (RRI) has found new types of molecular organisation based on such systematic X-ray studies.

ICA Council members and special invitees at a meeting in INSA, New Delhi on August 9, 2007. From left: N. Goswami (Joint Secretary), J.K. Dattagupta (President), Rajnikant, K. Lal, M. Vijayan, T.N. Guru Row (Vice-President), D.M. Salunke, K. Sekar (Treasurer), N. Gautham (Secretary), G.R. Desiraju, M.V. Hosur, B. Das, A. Nangia (Editor).

Neutron Scattering Facilities

A national facility for neutron beam research, designed and developed indigenously is operated in BARC, Mumbai (R. Mukhopadhyay; S.L. Chaplot). The facility has been built around the research reactor Dhruva that uses natural uranium as fuel and heavy water as both moderator and coolant. At present, a four-circle single-crystal diffractometer, three powder diffractometers, a high-Q diffractometer, a polarization analysis spectrometer, a triple-axis spectrometer, a filter detector spectrometer, and a quasi-elastic scattering spectrometer are located inside the reactor hall on various beam ports. Two neutron guide tubes, G1 and G2 with characteristic wavelengths 3.0 Å and 2.2 Å respectively, transport neutron beams into the Guide-Tube Lab. from the reactor hall. The average flux at the breaks, provided on the guides to accommodate various instruments, is ~10^7 neutrons/cm^2/s. Two small-angle neutron scattering instruments and a polarized neutron reflectometer are operational at G2 one after another. A spin-echo cum polarised neutron small-angle instrument has also been commissioned recently at G1.

Synchrotron facilities

Two synchrotron sources, Indus-1 (450MeV) and Indus-2 (2.5 GeV), were planned and designed by the Atomic Energy Commission Govt of India as national facilities at Raja Ramanna Centre for Advanced Technology at Indore. Of these, Indus-1 with a critical wavelength of 61 Å has been commissioned and is routinely operated at the design current of 100 mA. The beam lifetime achieved at 100 mA is 75 minutes. This vacuum ultraviolet/ soft x-ray source is used by various research groups in the country. Indus-2 with a critical wavelength of ~2 Å is in the process of being made operational. The Indian effort to acquire indigenous synchrotron capabilities has been long and arduous, even as it has been well-meaning. With rapid changes in the international scientific scenario, there is a real sense of urgency in having ready access to state-of-the-art synchrotron facilities by macromolecular, small molecule and industrial crystallographers. Reference has already been made to the fact that a whole generation of Indian crystallographers were enfeebled in the past because of the general absence of single crystal diffractometers between 1975 and 1995. It is sincerely hoped that the same scenario will not be repeated in another context.

National Committee for Crystallography

ICSU activities in India were brought under the banner of the Indian National Science Academy, INSA (then known as National Inst. of Science India) in 1968. The first and second National Committees appointed by INSA were chaired by G.N. Ramachandran. Subsequent chairs were A.R. Verma, S. Ramaseshan, N.N. Saha, R. Chidambaram, M.A. Viswamitra, S.P. Sen Gupta, K.K. Kannan, K. Lal, O.N. Srivastava and S.K. Sikka. In 2004, the National Committees of IUCr and IUPAB were merged on an experimental basis with M. Vijayan as chair. This committee will be demerged in 2008, and a new National Committee for Crystallography with P. Chakrabarti as chair (members K. Byrappa, S. K. Halder, A. Nangia, C. G. Suresh) will assume responsibility in January 2008. The National Committee has consistently played a major role in the collective activities of the crystallographic community in India and in its liaison with the IUCr.

Recognition by IUCr to the Indian crystallographic community has come in the form of the Ewald Prize to G.N. Ramachandran, the elections of S. Ramaseshan and R. Chidambaram as vice-presidents, and of G.R. Desiraju as a member of the current executive committee. P. Krishna, has been a former Chairman of the Commission on Crystallographic Teaching. M. Vijayan, a former Chairman of the Commission on Biological Macromolecules is president of the Asian Crystallographic Association (AsCA) till the end of 2007. G.R. Desiraju, M.R.N. Murthy, D. Pandey and M. Vijayan have served as past or present co-editors of *Acta Cryst.*

Indian Crystallographic Association

The Indian Crystallographic Association (ICA) was established in 2000-2001, fulfilling a long-felt need in the Indian crystallographic community for a professional association. One of its first activities was to organise the AsCA meeting in Bangalore in 2001. The ICA (iris.physics.iisc.ernet.in/ica/) currently comprises more than 350 members, whose research interests cover the entire gamut of crystallography-related disciplines. These include materials science, biology, chemistry, mathematics, and physics. Geographically, the ICA membership covers the entire country. Historically, and in the absence of a crystallographic association, the National Committee of Crystallography was responsible for

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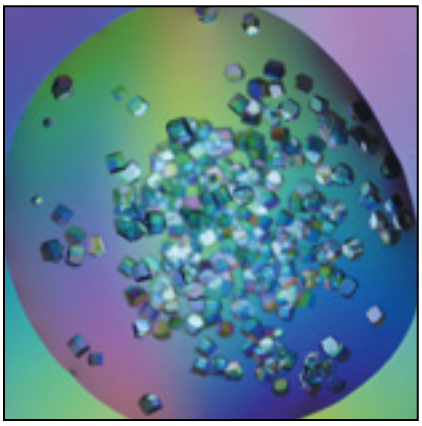

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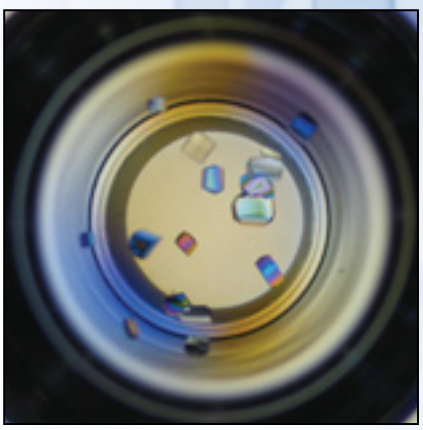

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all collective activity. Increasingly now, the ICA is co-ordinating academic and scientific activities, while the national committee, in its capacity as the accredited body of INSA, is liaising with the IUCr. Accordingly, the national meetings, which evolved from the Madras meetings, are now the responsibility of the ICA rather than of the national committee. The ICA council of 15 members (see photograph) is elected by the general body for a three-year term.

Comings and goings

The past 60 years have seen several interesting trends with respect to students and scientists moving between India and foreign countries, notably the USA and the UK. These events also convey much information with respect to the Indian presence, or the lack of it, in the international context. Crystallographers settled in India have obtained their doctoral degrees both in India and abroad, but the former group predominates numerically. Large numbers of Indian students emigrate to the USA either before or just after their Ph.D.; a few have made a distinct mark in their country of adoption: G. Kartha (Roswell Park), J. Kuriyan (U.C. Berkeley), V. Ramakrishnan (MRC Cambridge). In an interesting aside, S.N. Rao (U. of Central Oklahoma) is widely acknowledged as one of the most successful treasurers of the American Crystallographic Association. More in the context of times to come, a number of youngsters from foreign countries have pursued doctoral and post-doctoral studies in India. Stefka Peneva, from Sofia, Bulgaria received her Ph.D. in 1970 from U. of Delhi, working with K. Lal, while Michael Kirchner from Essen, Germany, who was the recipient of the prestigious Lynen fellowship of the Alexander von Humboldt foundation, carried out post-doctoral work with G.R. Desiraju in Hyderabad in 2003-04. The growing academic significance of Indian laboratories, coupled with the rapid improvements in the economic conditions in India, ensure that the number of foreign scholars in India will increase significantly. Already, there are initiatives through government sponsored projects and organisations like the Academy of Sciences for the Developing World (TWAS) and Human Frontiers of Science Program (HFSP) to aid in the movement of young crystallographers from anywhere in the world to India.

Pleased editors of the special issue at the end of their assignment in Hyderabad. From left: A. Nangia, G.R. Desiraju and V. Pattabhi. The fourth editor D.M. Salunke was not present on this occasion.

Contributors to this article:
K. Biradha, P. Chakrabarti, N. Chandra, J. K. Datta Gupta, N. Gautham, T.N. Guru Row, K.V.R. Kishan, P. Krishna, K. Lal, S.C. Mande, N. Madhusudana, D. Pandey, S. Ranganathan, S.N. Rao, J.A.R.P. Sarma, M. Vijayan, K. Vyas and V.K. Wadhawan, Edited by: A. Nangia, D.M. Salunke, V. Pattabhi and G.R. Desiraju.

Ljubo Golic (1932-2007)

Sadly Ljubo Golic came to the end of his very fruitful life in July 2007 just after his 75th birthday. He was a first-class scientist, who was highly respected in the international scientific and crystallographic community, and who persistently promoted the development of chemical and structural crystallography, not only in Slovenia. Through his scientific work he had a great impact on neighbouring university centres. Almost forty years ago he was a founder of regular annual crystallographic conferences, organized by the Yugoslav Centre of Crystallography, under the auspices of the Yugoslav Academy of Sciences and Arts in Zagreb, Croatia. He attended most of the meetings, vigorously discussing crystallographic matters, as well as many other topics, including mountain climbing in the Alps.

In 1974 Golic obtained an automatic X-ray diffractometer, built a modern X-ray lab and gathered a group of young coworkers in Ljubljana. This was the first instrument of its kind in Southeast Europe outside the Iron Curtain, and it had a tremendeous impact on the development of crystallography in Slovenia and neighbouring countries.

The crystallographic accomplishments and conferences held annually in Yugoslavia led to the selection of Ljubljana as the venue of the 13th European Crystallographic Meeting in 1991. Golic was the Chair of the Organizing Committee for that Meeting, and the Secretariat of the Meeting operated out of Ljubljana. Due to the outbreak of civil war in Yugoslavia the venue had to be moved to Trieste. The change of the venue on such short notice was a very difficult challenge for Golic, Boris Kamenar (Zagreb) and their colleagues on the Organizing Committee, but with tremendeous effort and the generous help of Italian friends ECM-13 was successfully held in Trieste.

After the desintegration of Yugoslavia, Ljubo Golic, Boris Kamenar, Stanko Popovic and I gathered in the spring of 1992 in the castle of Mokrice, Slovenia, and decided to continue annual crystallographic gatherings, as bilateral Slovenian-Croatian meetings (when the venue was in Slovenia) or Croatian-Slovenian meetings (when the venue was in Croatia). This year we had the 16th CRO-SLO meeting in Petrcane, near Zadar, Croatia. Ljubo Golic's name will live on in these annual meetings.

He was a cheerful person, but a strict and fair teacher, who was diligent and precise in his work. He received the highest scientific awards in Slovenia for his scientific and teaching activities. He was very helpful to his co-workers and had a major role in my academic career and my study in England. In the 1970s we collected multilayer film data on Weissenberg and precession cameras in Ljubljana and estimated intensities by eye. It took six months to collect the data that had to be punched onto cards. Golic made his own Patterson -Tunnell strips and it was very exciting to see the atomic structures drawn on equally spaced glass plates. He was technically gifted and had a large collection of precision tools. There was always a small screw driver in the pocket of his gown in case something should go wrong. He was often able to repair our diffractometers, which was critically important because the service visits to our country in those days were quite expensive.

Crystallographers, scientists in related fields, colleagues and friends will long remember Ljubo Golic. His coworkers and students, inspired by his love of crystallography, will continue his work. All of us miss him and his inspiring leadership very much.

Ivan Leban with coworkers
Fac. of Chemistry and Chem. Technology, U. of Ljubljana, Slovenia

It is an intention of *Acta Chimica Slovenica* (http://acta.chem-soc.si/) to dedicate one of the forthcoming issues in late 2008 to his memory. Therefore we would like to invite you to contribute the results of your research to the memory of Prof. Golic, respecting fully the Editorial policy of *Acta Chimica Slovenica*. All the contributions will undergo the usual peer review.

The deadline for contributions is March 31, 2008. Complete contributions should be sent to ACSi@fkkt.uni-lj.si. A note about the submission should be sent also to ivan.leban@fkkt.uni-lj.si.

The guest editors for this issue are Slavko Kaucic, National Inst. of Chemistry (slavko.kaucic@KI.si) and Ivan Leban, UL, Ljubljana, Slovenia (ivan.leban@fkkt.uni-lj.si).

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About Incoatec: Incoatec was incorporated in 2002 by former members of the GKSS research center in Geesthacht near Hamburg and the Bruker AXS GmbH. Incoatec has more than 10 years of experience in X-ray optics based on thin film technology. Incoatec develops and produces all products directly in-house – Made in Germany. Incoatec Optics are used in X-ray diffractometry, spectrometry and at synchrotron beamlines all over the world.

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A selection of future meetings. A more complete list is available at www.iucr.org. Corrections and new listings are invited by the Editor.

MARCH 2008

28-29 ♦ II Int'l Workshop on Layered Materials: Structure and Properties. Vercelli, Italy. www.layeredmaterials.mfn.unipmn.it/

APRIL 2008

7-3 ♦ Summer School on Mathematical and Theoretical Crystallography. Garda Lake, Italy. www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.

MAY 2008

29-8 ♦ From Molecules to Medicine. Integrating Crystallography in Drug Discovery. Erice, Italy. www.crystalerice.org/erice2008/2008.htm.

31-5 ♦ ACA 2008. Knoxville, TN, USA. www.amercrystalassn.org.

JULY 2008

21-26 ♦ XRM2008 - 9th Int'l Conf. on X-ray Microscopy. ETH Zurich, Switzerland. xrm2008.web.psi.ch/.

AUGUST 2008

23-31 ♦ IUCr 2008 - XXI General Assembly and Congress of the IUCr. Osaka, Japan. www.iucr2008.jp.

JUNE 2009

4-14 ♦ High Pressure Crystallography: From Novel Experimental Approaches to Applications in Cutting-Edge Technology. Erice, Italy. www.crystalerice.org/erice2009/2009.htm.

JULY 2009

25-30 ♦ ACA 2009. Toronto, ONT, Canada. www.amercrystalassn.org.

AUGUST 2009

9-14 ♦ ECM-25. Istanbul Turkey. www.ecm25.org/.

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FUTURE MEETINGS

Summer School

Garda Lake, Italy
April 7 -May 3,2008

The Commission on Mathematical and Theoretical Crystallography (MaThCryst) of the IUCr, in cooperation with the Commission on Crystallographic Teaching (CTC) is organizing a summer school at the Palazzo Feltrinelli of Gargnano, on the Italian Garda Lake, April 27 - May 3, 2008. The school will consist of lectures and practical sessions from invited lecturers. Poster presentations by the participants are welcome.

After an introduction to crystallographic symmetry and exercises on the International Tables Volume A and a dimension-independent approach to crystallographic symmetry, application to concrete problems in three-dimensional space, group-subgroup relations, Bärnighausen trees (on the International Tables Volume A1), crystallographic tools for inorganic and organic crystal-chemistry will be presented. Lecturers include Mois I. Aroyo, Michele Catti, Angelo Gavezzotti, Ulrich Müller, Massimo Nespolo and Bernd Souvignier.

Limited financial support for PhD students and post-doctoral fellows is available. Further information is available at www.lcm3b.uhp-nancy.fr/mathcryst/gargnano2008.htm For general inquiries contact mathcryst.satellite@lcm3b.uhp-nancy.fr.

Statement of Ownership, Management, and Circulation

1. Publication Title: International Union of Crystallography Newsletter
2. Publication Number: 1067-0696
3. Filing Date: October 31, 2007
4. Issue Frequency: Quarterly
5. Number of Issues Published Annually: 4
6. Annual Subscription Price: $0.00
7. Complete Mailing Address of Known Office of Publication: IUCr Newsletter, c/o Hauptman-Woodward Medical Research Inst., 700 Ellicott Avenue, Buffalo, NY, 14203-1102, Erie County
8. Complete Mailing Address of Headquarters or General Business Office of Publisher: Same as above
9. Full Names and Complete Mailing Addresses of Publisher and Editor: Publisher: International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK; Editor: Judith Flippen-Anderson, 3521 Lancelot Way, Annandale, VA 22003
10. Owner: International Union of Crystallography, 2 Abbey Square, Chester CH1 2HU, UK
11. Known Bondholders, Mortgagees, and Other Security Holders Owning or Holding 1 Percent or More of Total Other Securities: None
12. Tax Status: Not Changed During Preceding 12 Months
13. Publication Title: International Union of Crystallography Newsletter
14. Issue Date for Circulation Data Below: July 2007

15. Extent and Nature of Circulation			Average No. Copies Each Issue During Preceding 12 Months	No. Copies of Single Issue Published Nearest to Filing Date
a. Total Number of Copies (Net press run)			18,675	18,300
b. Paid and/or Requested Circulation	(1)	Paid/Requested Outside-County Mail Subscriptions Stated on Form 3541	7,579	7,547
	(2)	Paid In-County Subscriptions Stated on Form 3541	0	0
	(3)	Sales Through Dealers and Carriers, Street Vendors, Counter Sales, and Other Non-USPS Paid Distribution	10,234	9,933
	(4)	Other Classes Mailed Through the USPS	0	0
c. Total Paid and/or Requested Circulation [Sumof15b.(1),(2),(3), and(4)]			17,813	17,480
d. Free Distribution by Mail	(1)	Outside-County as Stated on Form 3541	225	223
	(2)	In-County as Stated on Form 3541	0	0
	(3)	Other Classes Mailed Through the USPS	0	0
e. Free Distribution Outside the Mail			343	341
f. Total Free Distribution (Sum of 15d. and 15e.)			568	564
g. Total Distribution (Sum of 15c. and 15f.)			18,381	18,044
h. Copies not Distributed			294	256
i. Total (Sumof15g.andh.)			18,675	18,300
j. Percent Paid and/or Requested Circulation			97%	97%

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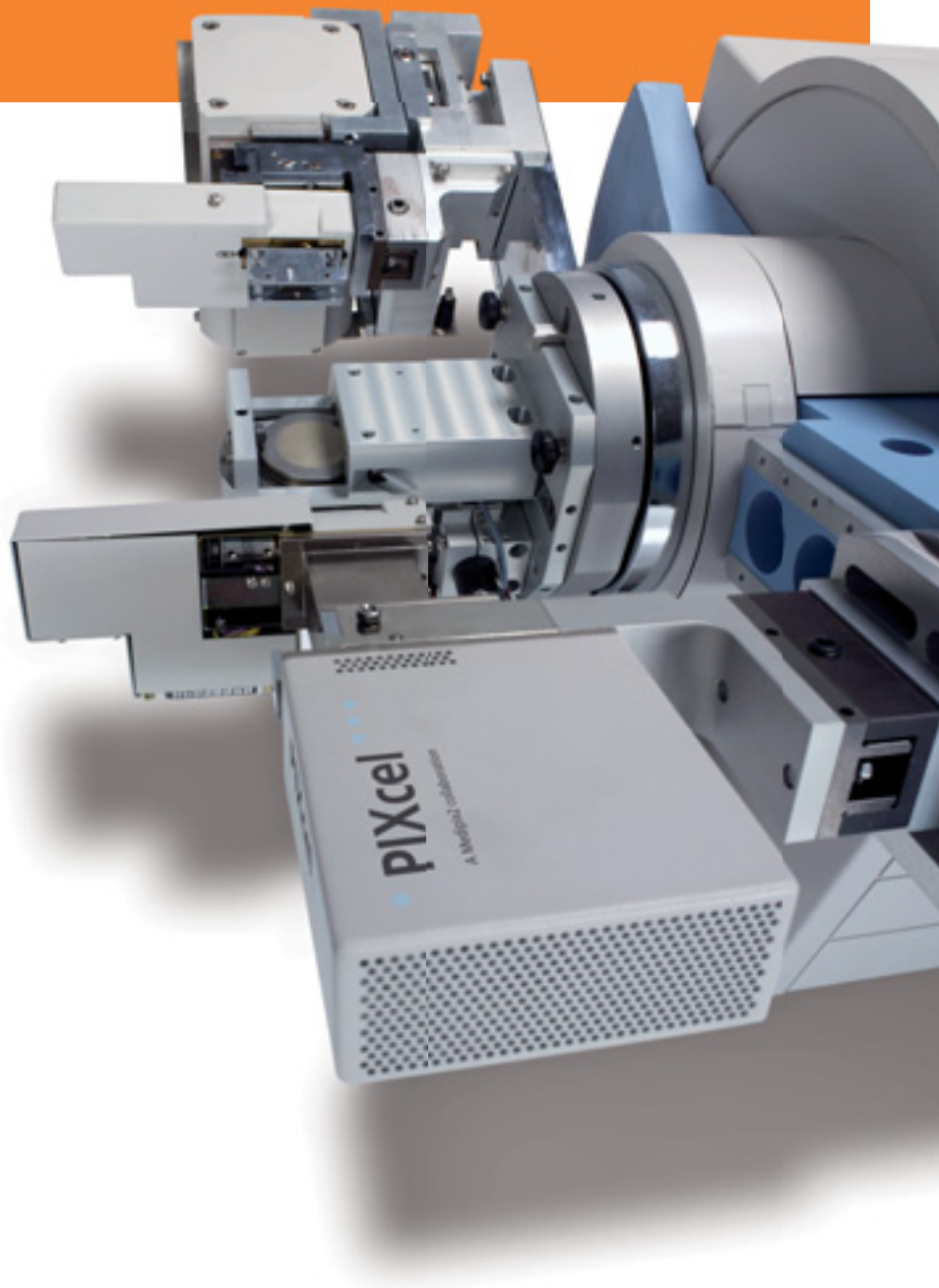

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