2014

Crystals, Crystallography, the International Year of Crystallography and the Indian Institute of Science

Crystals – familiar to all in gemstones, snowflakes or grains of salt – are everywhere in nature. The study of their inner structure and properties gives us deep insights into the arrangements of atoms in the solid state. Crystallography has become the core of structural science and has led to many advances in the sciences of chemistry, physics, biology and mineralogy.

From the structure of diamond and rock salt to that of DNA and the ribosome, crystallography has enabled scientists to study the chemical bonds which draw one atom to another. A century ago, it was found that crystals diffract X-rays. This fundamental discovery opened up the subject of crystallography from one that pertained to the external study of crystals to one that is concerned with the internal structure of its constituents. In July 2012, noting this centennial of X-ray diffraction, the general assembly of the United Nations passed a resolution that 2014 should be the International Year of Crystallography. This is why the Indian Institute of Science has selected crystallography as the theme for the 2014 calendar.

The Indian Institute of Science has been one of the foremost academic institutions in the country where research in crystallography has been carried out in all aspects of the subject. The figures in this Calendar have been selected from crystallographic work that has actually been carried out in the Institute. This selection aims to cover all topics where the contribution of the Institute has been distinctive.

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Printed by:
Ravi Graphics, Bangalore

IISc Press
www.iiscpress.iisc.in

Indian Institute of Science, Bangalore, India
www.iisc.ernet.in

JANUARY 2014

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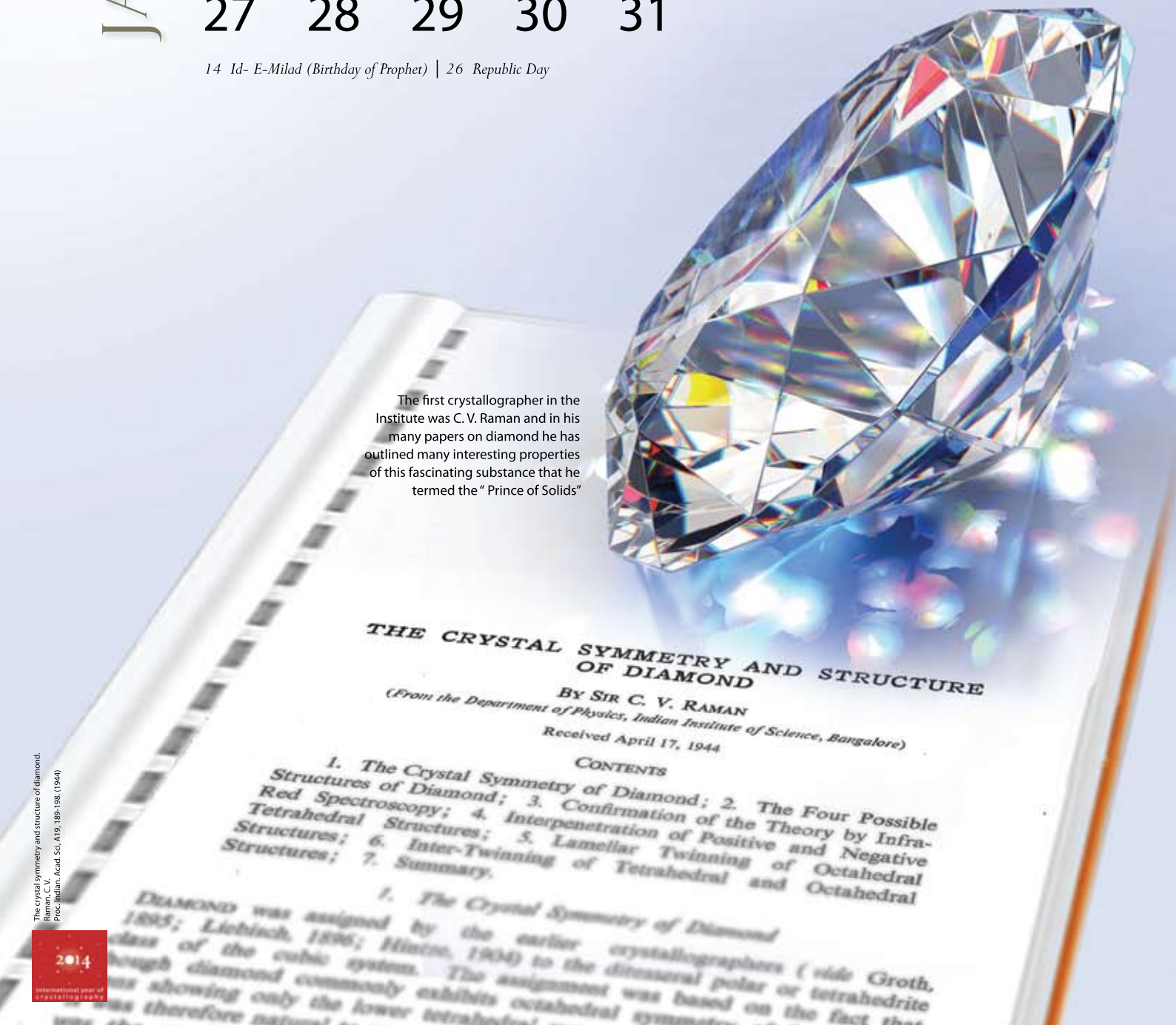
14 Id- E-Milad (Birthday of Prophet) | 26 Republic Day



The first crystallographer in the Institute was C. V. Raman and in his many papers on diamond he has outlined many interesting properties of this fascinating substance that he termed the " Prince of Solids"

THE CRYSTAL SYMMETRY AND STRUCTURE OF DIAMOND

BY SIR C. V. RAMAN

(From the Department of Physics, Indian Institute of Science, Bangalore)

Received April 17, 1944

CONTENTS

1. The Crystal Symmetry of Diamond; 2. The Four Possible Structures of Diamond; 3. Confirmation of the Theory by Infra-Red Spectroscopy; 4. Interpenetration of Positive and Negative Tetrahedral Structures; 5. Lamellar Twinning of Octahedral Structures; 6. Inter-Twinning of Tetrahedral and Octahedral Structures; 7. Summary.

1. The Crystal Symmetry of Diamond

DIAMOND was assigned by the earlier crystallographers (*vide* Groth, 1895; Liebisch, 1896; Hintze, 1904) to the ditesseral polar or tetrahedrite class of the cubic system. The assignment was based on the fact that ...ough diamond commonly exhibits octahedral symmetry ...ns showing only the lower tetrahedral ... was therefore natural ...

The crystal symmetry and structure of diamond.
Raman, C.V.
Proc. Indian. Acad. Sci. A19, 189-198. (1944)

2014
international year of crystallography

FEBRUARY 2014

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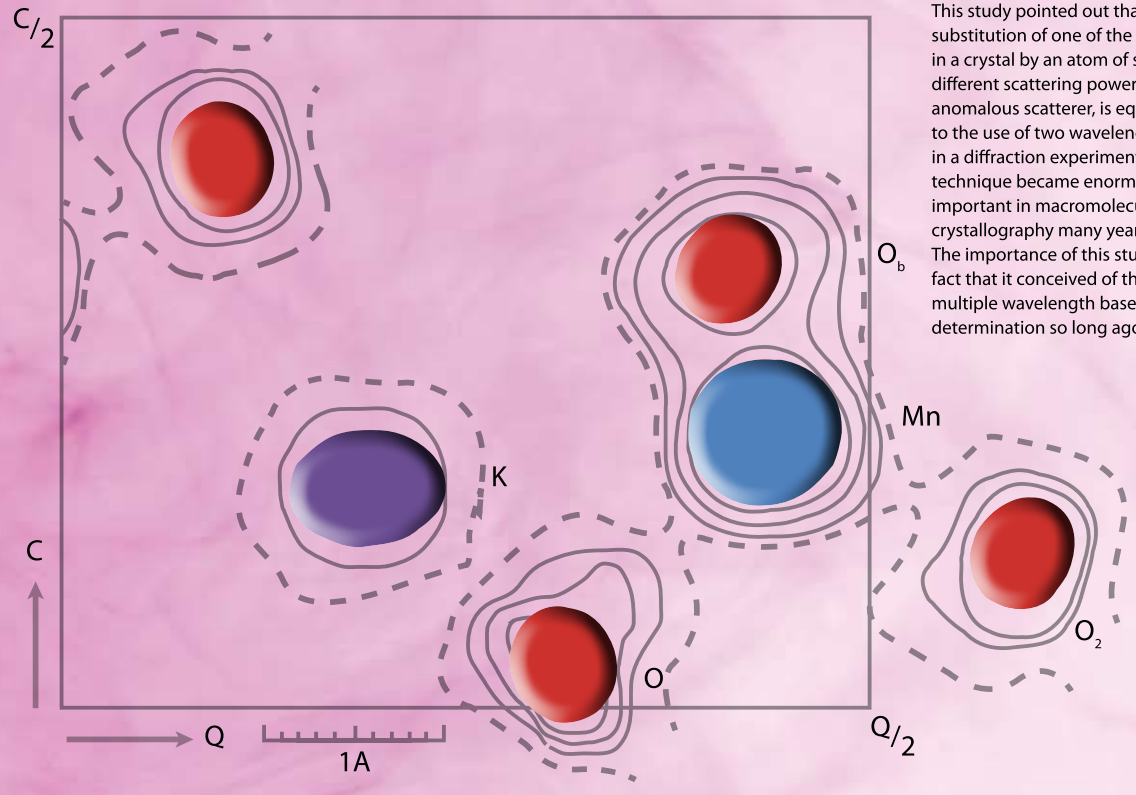
27 Maha Shivrathri



This study pointed out that the substitution of one of the atoms in a crystal by an atom of slightly different scattering power, the anomalous scatterer, is equivalent to the use of two wavelengths in a diffraction experiment. This technique became enormously important in macromolecular crystallography many years later. The importance of this study is the fact that it conceived of the idea of multiple wavelength based phase determination so long ago.

Use of anomalous scattering for the determination of crystal structures – potassium permanganate
Ramaseshan, S., Venkatesan, K. and Mani, N.V.
Proc. Indian Acad. Sci. A46, 95-111 (1957)

2014 international year of crystallography

MARCH 2014

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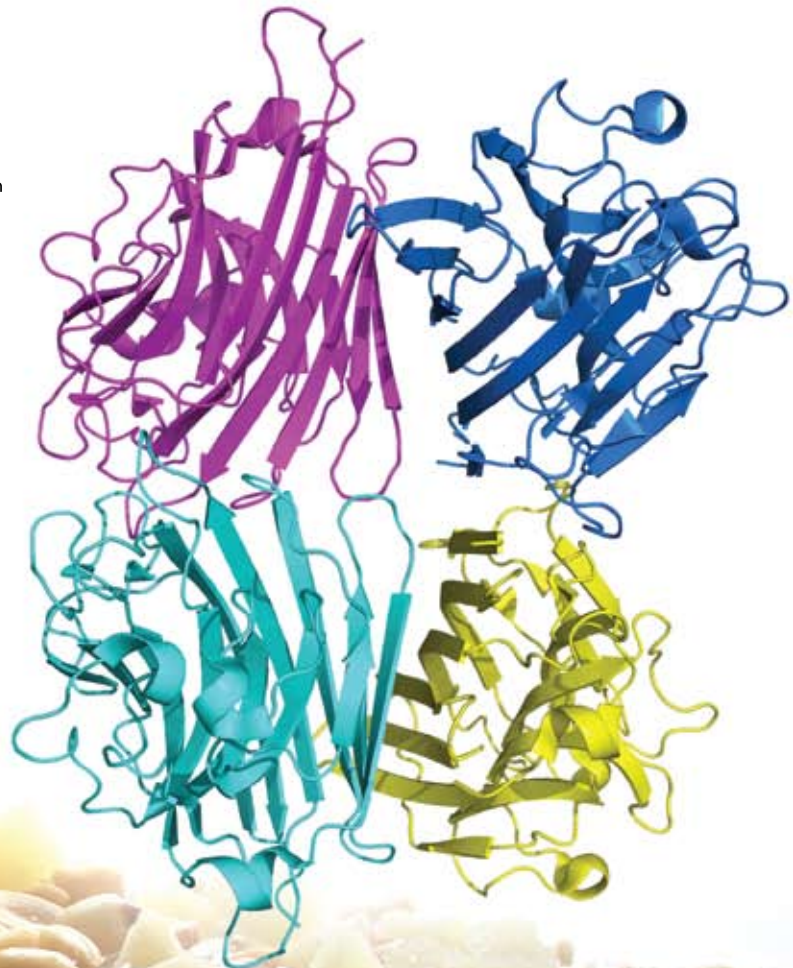
31 Ugadi

The crystal structure of peanut lectin revealed an unorthodox quartenary structure. This protein specifically binds the tumor associated T-antigen.



Crystal Structure of peanut lectin, a protein with an unusual quaternary structure
Banerjee, R., Mande, S. C., Ganesh, V., Das, K., Dhanaraj, V., Mahanta, S. K., Suguna, K., Surolia, A. and Vijayan, M.
Proc. Natl. Acad. Sci. (U.S.A.), 91, 227-231. (1994)

2014 international year of crystallography

APRIL 2014

MON	TUE	WED	THU	FRI	SAT	SUN
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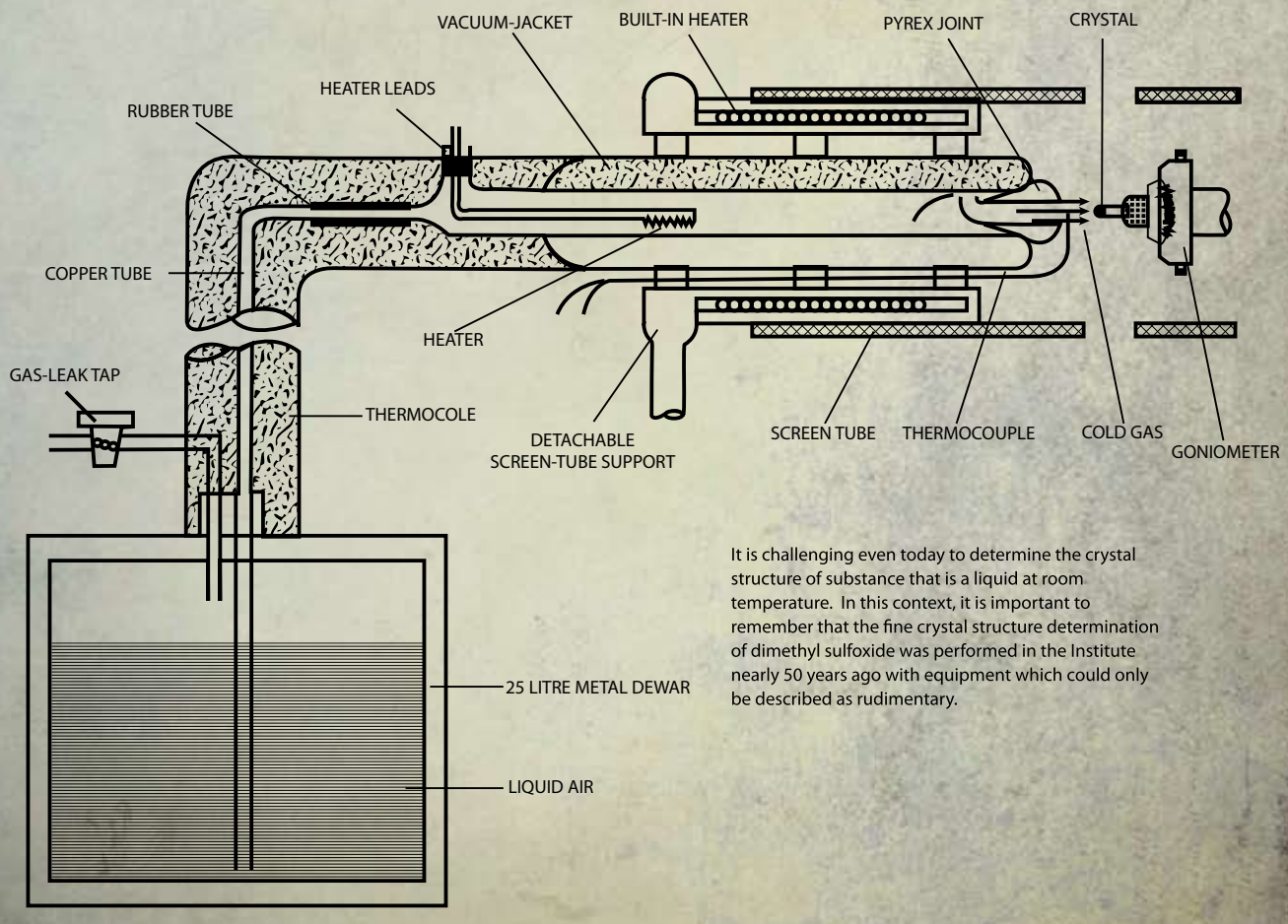
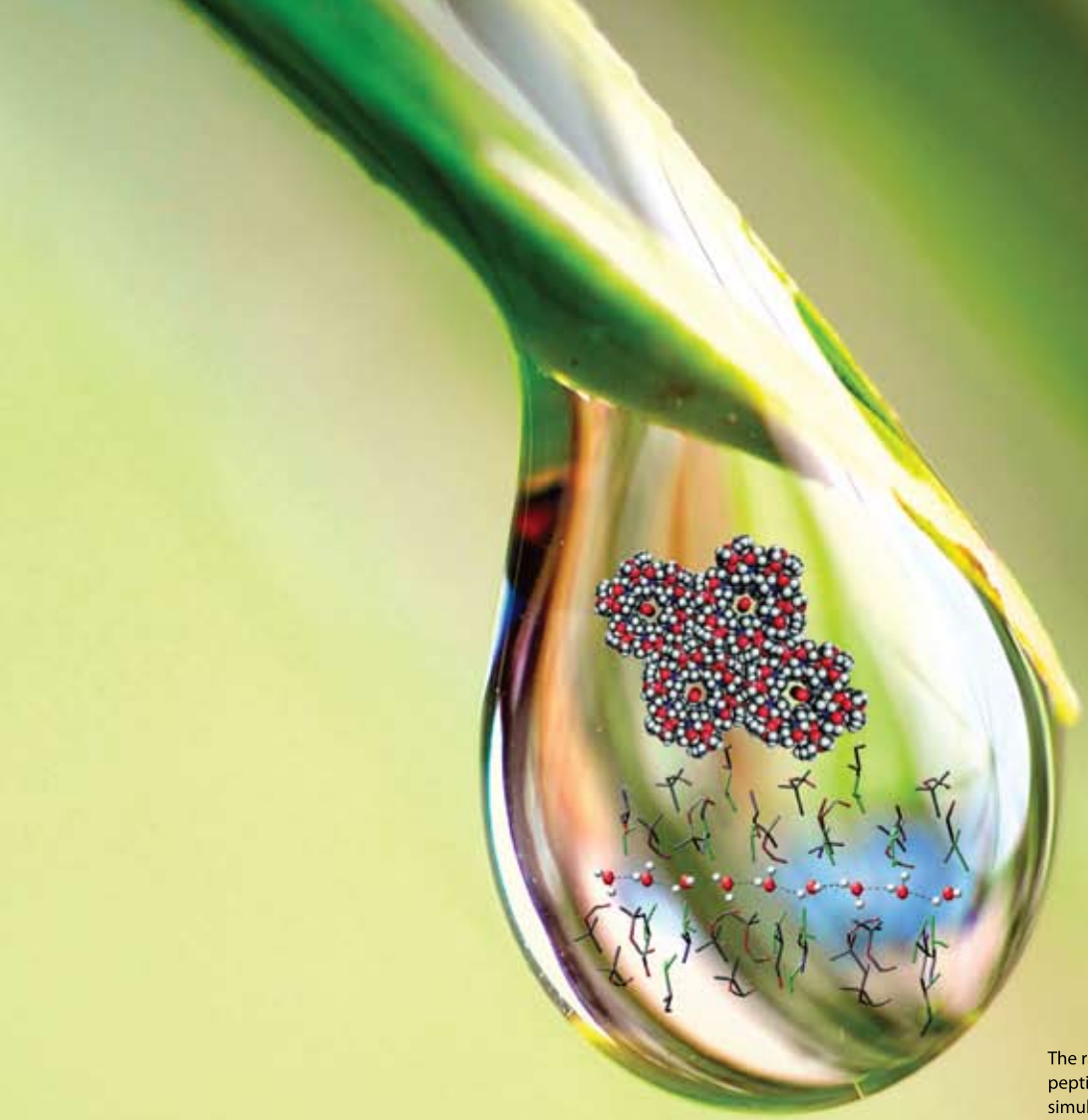
13 Mahavir Jayanthi | 18 Good Friday



It is challenging even today to determine the crystal structure of substance that is a liquid at room temperature. In this context, it is important to remember that the fine crystal structure determination of dimethyl sulfoxide was performed in the Institute nearly 50 years ago with equipment which could only be described as rudimentary.

Molecular dimensions and crystal structure of dimethyl sulphoxide at -60°C
Viswamitra, M.A. and Kannan, K.K.
Nature 209, 1016-1017, (1966)

A low temperature Weissenberg Camera
Viswamitra, M. A.
J. Sci. Instrum. 39:381-383, (1962)



The rational design of tubular peptide structures can aid in simulations of the structure and dynamics of water wires in confined environments

MAY 2014

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14 Buddha Poornima

Characterization of water wires inside hydrophobic tubular peptide structures
Raghavender, U.S., Aravinda, S., Shamala, N., Rai R., Kantharaju, R. and Balaram, P.
J Am Chem Soc. 131, 15130-32. (2009)

JUNE 2014

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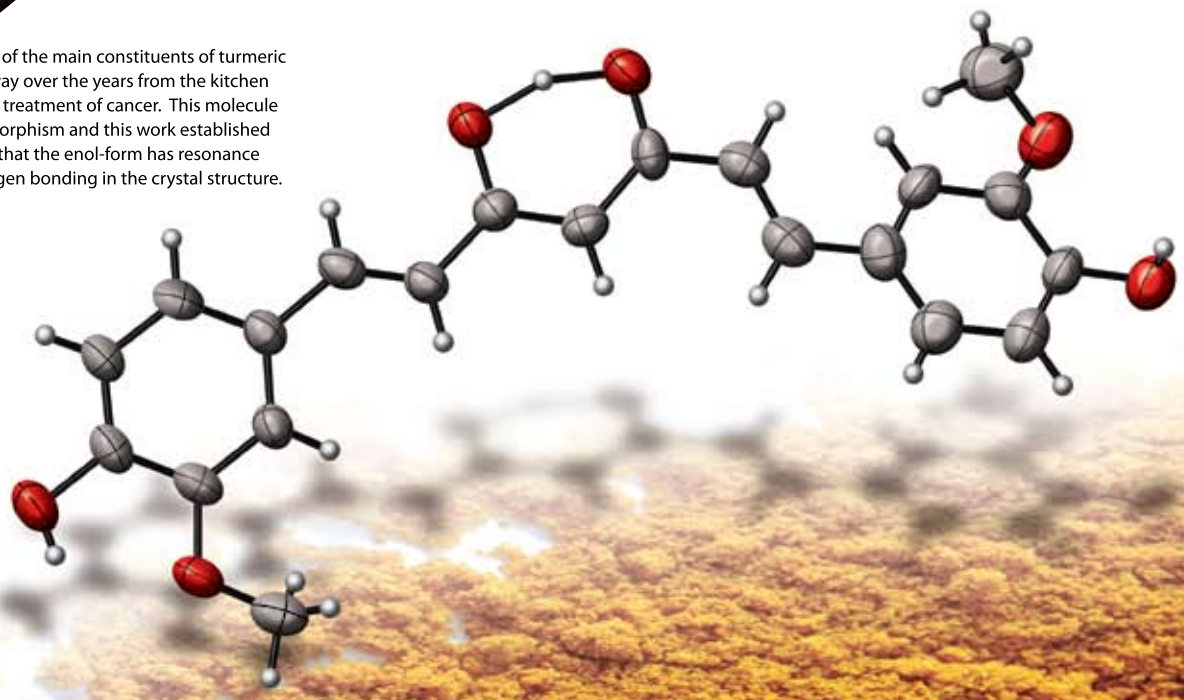
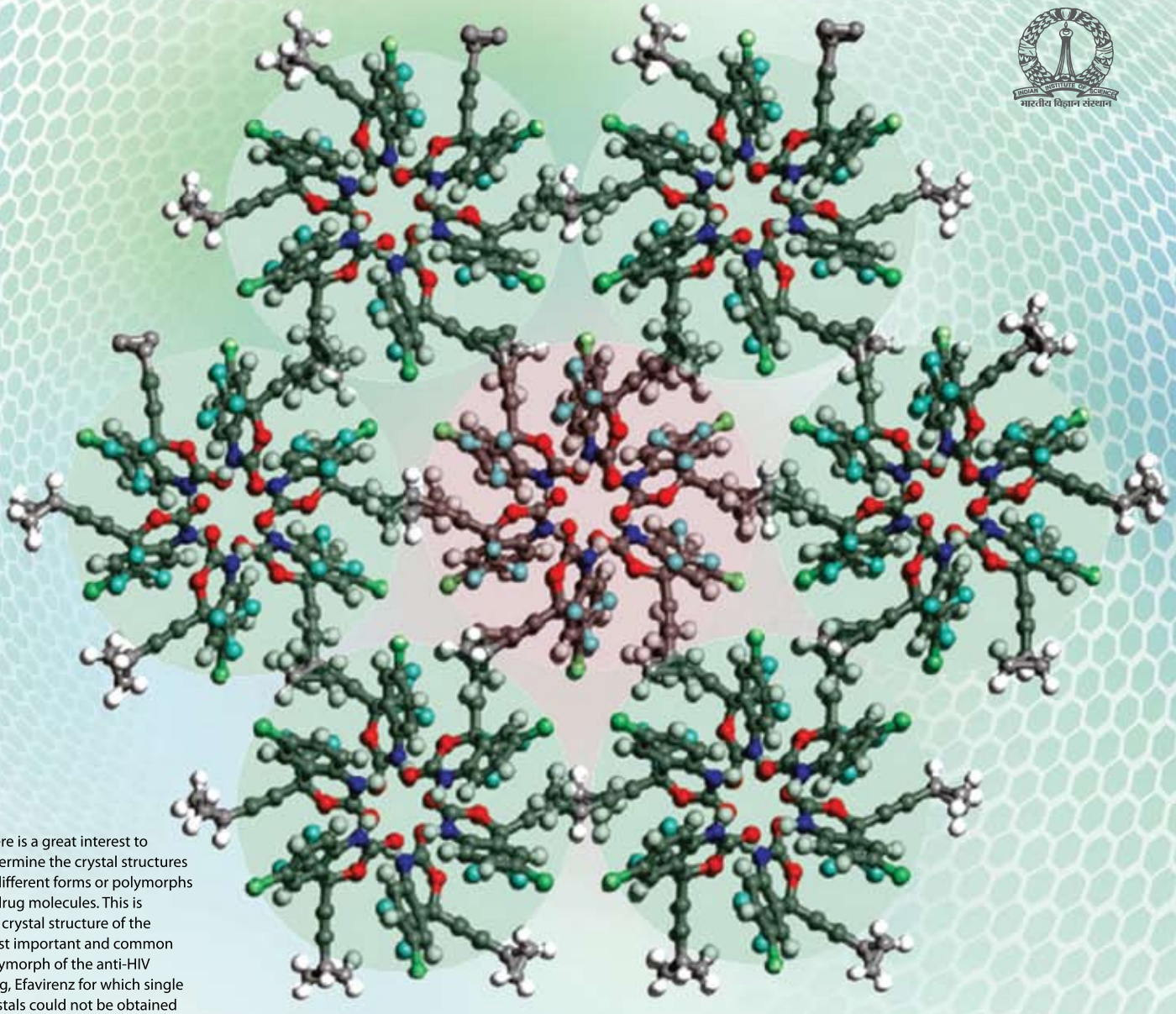
Curcumin, one of the main constituents of turmeric has found its way over the years from the kitchen to modern day treatment of cancer. This molecule exhibits polymorphism and this work established unequivocally that the enol-form has resonance assisted hydrogen bonding in the crystal structure.



Redetermination of curcumin; (1E,4Z,6E)-5-hydroxy-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,4,6-trien-3-one
Parimita, S. P., Ramshankar, Y. V., Suresh, S. and Guru Row, T. N.
Acta Cryst. E63, 0860-0862. (2007)



There is a great interest to determine the crystal structures of different forms or polymorphs of drug molecules. This is the crystal structure of the most important and common polymorph of the anti-HIV drug, Efavirenz for which single crystals could not be obtained initially, before this study was carried out.

JULY 2014

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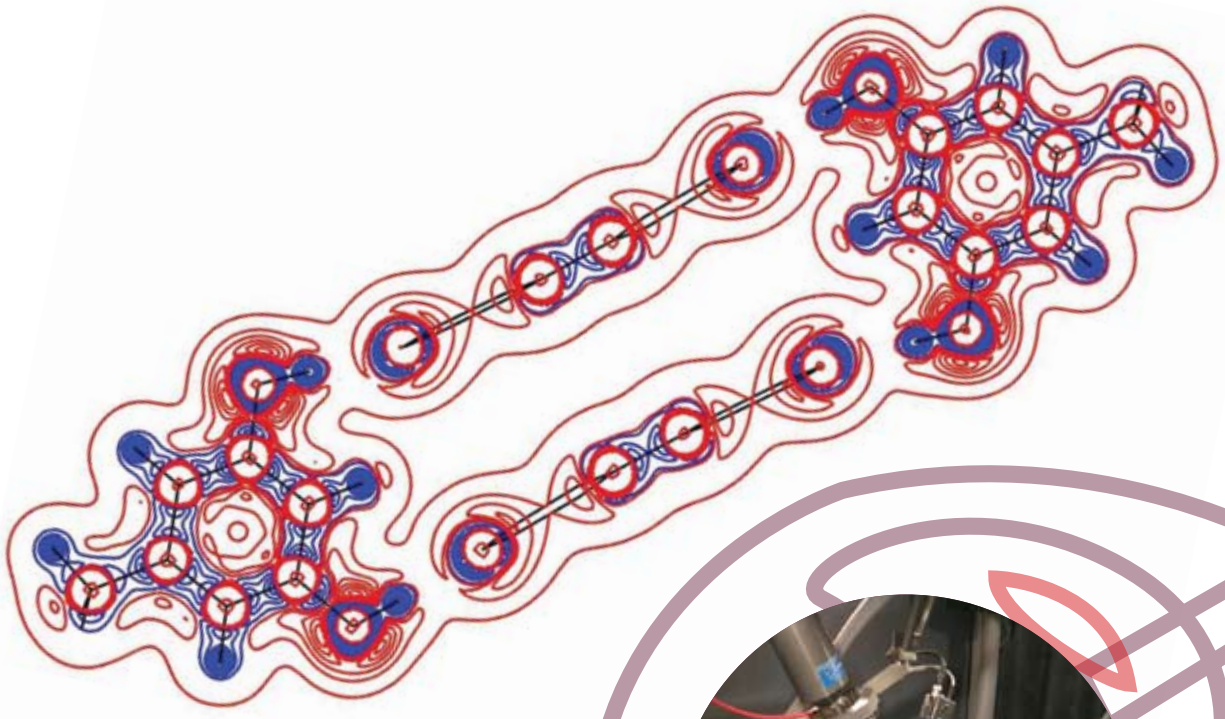
29 Idu'l Fitr

New solid state forms of the anti-HIV drug Efavirenz. Conformational flexibility and high Z' issues
Mahapatra, S., Thakur, T. S., Joseph, S., Varughese, S. and Desiraju, G. R.
Cryst. Growth Des., 10, 3191-3202. (2010)



To celebrate the International Year of Crystallography, the International Union of Crystallography has launched a new scientific journal called IUCrJ. The structural study in this illustration pertains to the very first paper that was accepted for publication in this new journal.

AUGUST 2014

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8 Varamahalaxmi Vratha | 15 Independence Day | 29 Ganesh Chaturthi

Crystal landscape in the orcinol-4,4′-bipyridine system: synthon modularity, polymorphism and transferability of multiple charge density parameters
Dubey, R., Pavan, M. S., Guru Row, T. N. and Desiraju, G. R.
IUCrJ, 1, 000-000, 2014

B-DNA, the genetic material of all living cells, is usually a double helix with 10 residues per turn and raise per residues of 3.3 Å. On theoretical grounds, this paper clearly demonstrated that the DNA double helix could have considerable evidence for polymorphism.

SEPTEMBER 2014

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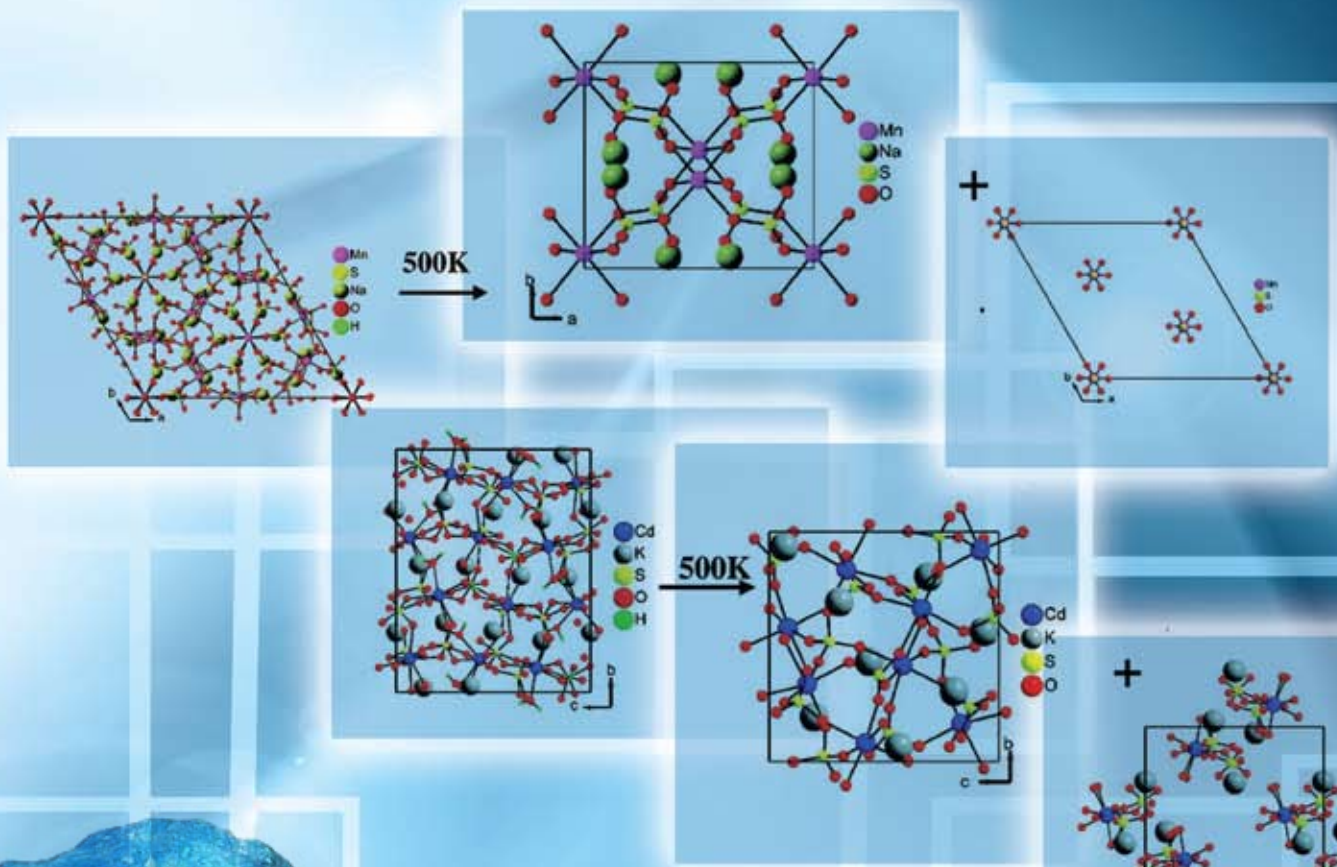
Double standard polynucleotides: two typical alternative conformations for nucleic acids
Sasisekharan, V. and Pattabiraman, N.
Curr Sci. 45, 779-83. (1976)



Variable temperature X-ray diffraction studies on hydrated minerals provide evidence for phase separation on dehydration leading to single crystal- single crystal transitions. This suggests a possible pathway for mineral evolution.

OCTOBER 2014

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2 Mahatma Gandhi's Jayanthi | 3 Dussehra (Maha Saptami) | 6 Idu'l Zuha (Bakrid) | 23 Deepawali

In situ phase separation following dehydration in bimetallic sulfates: A variable-temperature X-Ray diffraction study
Swain, D. and Guru Row, T. N.
Inorg. Chem., 48, 7048–7058. (2009)

NOVEMBER 2014

MON	TUE	WED	THU	FRI	SAT	SUN
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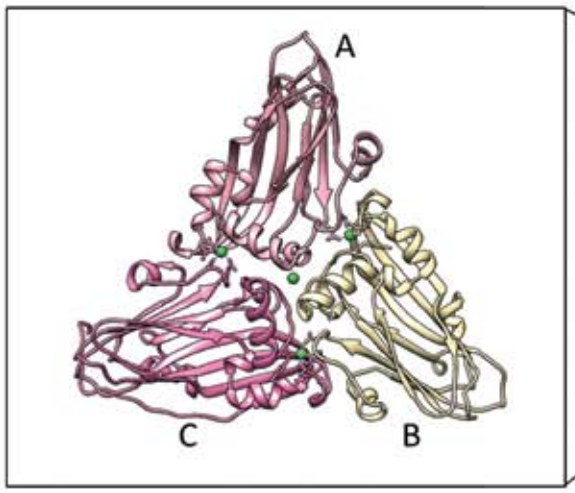
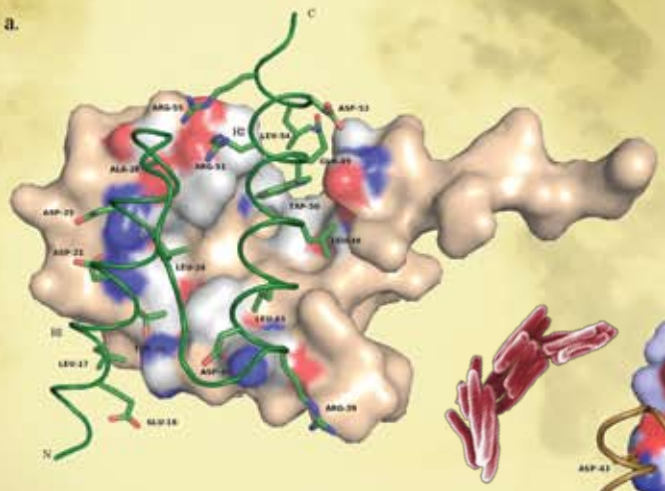
4 Muharram | *6 Guru Nanak's Birthday*

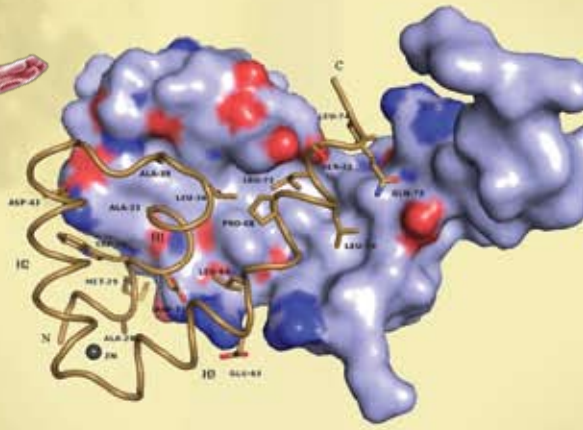


The *Sesbania* Mosaic Virus is a plant virus that was isolated from *Sesbania grandiflora* plants in fields near Tirupati, India. The virus capsid consists of sixty icosahedral asymmetric units, each comprising three copies of a chemically identical coat protein subunit.

Structure of sesbania mosaic virus at 3 Å resolution
Bhuvaneshwari, M., Subramanya, H. S., Gopinath, K., Savithri, H. S., Nayudu, M. V. and Murthy, M. R. N.
Structure 3,1021-1030. (1995)



The environmental triggers that allow persistent *Mycobacterium tuberculosis* cells to reactivate is crucial to understand why only a fraction of humans infected with *Mycobacterium tuberculosis* actually develop the active disease. Studies on transcription factors, such as the sigma factors, provide a basis for understanding the bacterial response to diverse micro-environments in the human host.



DECEMBER 2014

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Mycobacterium tuberculosis RsdA provides a conformational rationale for selective regulation of sigma-factor activity by proteolysis
Jaiswal, R. K., Suryaprabha, T., Manjeera, G. and Gopal, B.
Nucleic Acids Res. 41, 3414-23. (2013)

25 *Christmas*