FIFTY SECOND ANNUAL MEETING OF THE INDIAN ACADEMY OF SCIENCES, HELD AT BANARAS HINDU UNIVERSITY, VARANASI – SUMMARIES OF LECTURES DELIVERED

2D NMR: Crystallography in Solution by
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Till about a few years ago, x-ray crystallography was the only method to determine the three-dimensional structures of biological macromolecules. The discovery of the two-dimensional (2D) NMR[1] has altered the situation. It is now possible to obtain detailed information on 3D structure and also of dynamics of biological macromolecules in aqueous solutions completely from NMR data. Thus one can compare the structures in solutions with those in the single crystals and derive useful information about the effects of environments on molecular conformations.

As against electrons, in x-ray crystallography, the information carriers in NMR are the magnetic nuclei such as ¹H. 'Different' protons in a molecule resonate at different frequencies when placed in a constant magnetic field. The protons also interact with each other and a knowledge of these interactions is the basis of the structure determination by NMR. In a conventional 1D NMR spectrum of a large molecule, the resonances overlap significantly and thus it is impossible to extract complete information about the various interactions. The power of 2D NMR lies in the fact that it enables spreading of the required information on to the plane and therefore it can be extracted.

There are a variety of 2D NMR experiments designed for different purposes and from the structural point of view, the ones of interest are those which depict the different interactions or the correlations. There are two types of interactions which need to be studied; these are: (i) *J*-coupling between protons which occurs through the electrons in the intervening bonds; and (ii) Dipolar coupling which occurs through the space. Corresponding to these the 2D NMR experiments are, Correlated Spectroscopy[1,2] (COSY) and Nuclear Over-hauser Enhanced Correlated Spectroscopy[3] (NOESY). Since the first publication of these two basic experiments, several modifications and improvements have appeared in the literature[4-9] for purposes of resolution and sensitivity enhancements.

A typical 2D ¹H–¹H correlated spectrum looks as shown in figure 1 The diagonal peaks essentially represent the 1D spectrum and the off-diagonal peaks or the cross peaks reflect the correlations. The COSY cross peaks allow identification of *J*-coupled spin systems and the NOESY cross peaks identify protons which are close by in space (< 5Å). The relative intensities of these peaks can be used to estimate distances between pairs of protons. A knowledge of a large number of such distances, even approximate values, allows reconstruction of the 3D structure in a fairly accurate manner Thus structure determination involves basically two stages (i) attach resonance labels to individual protons and (ii) estimate distances between assigned protons and reconstruct the structure.

While the principles of structure determination outlined above are applicable, in general, to all classes of biological macromolecules, the intricate details of workable strategies will be different for different classes, simply because of their different chemical structures. For example in nucleic acids there are larger dihedral angles per unit than in proteins, which determine the structure of the molecule. On the other hand nucleic acids are made up of only 4 types of units while proteins consist of about 20 types of amino acids The strategies for deter-
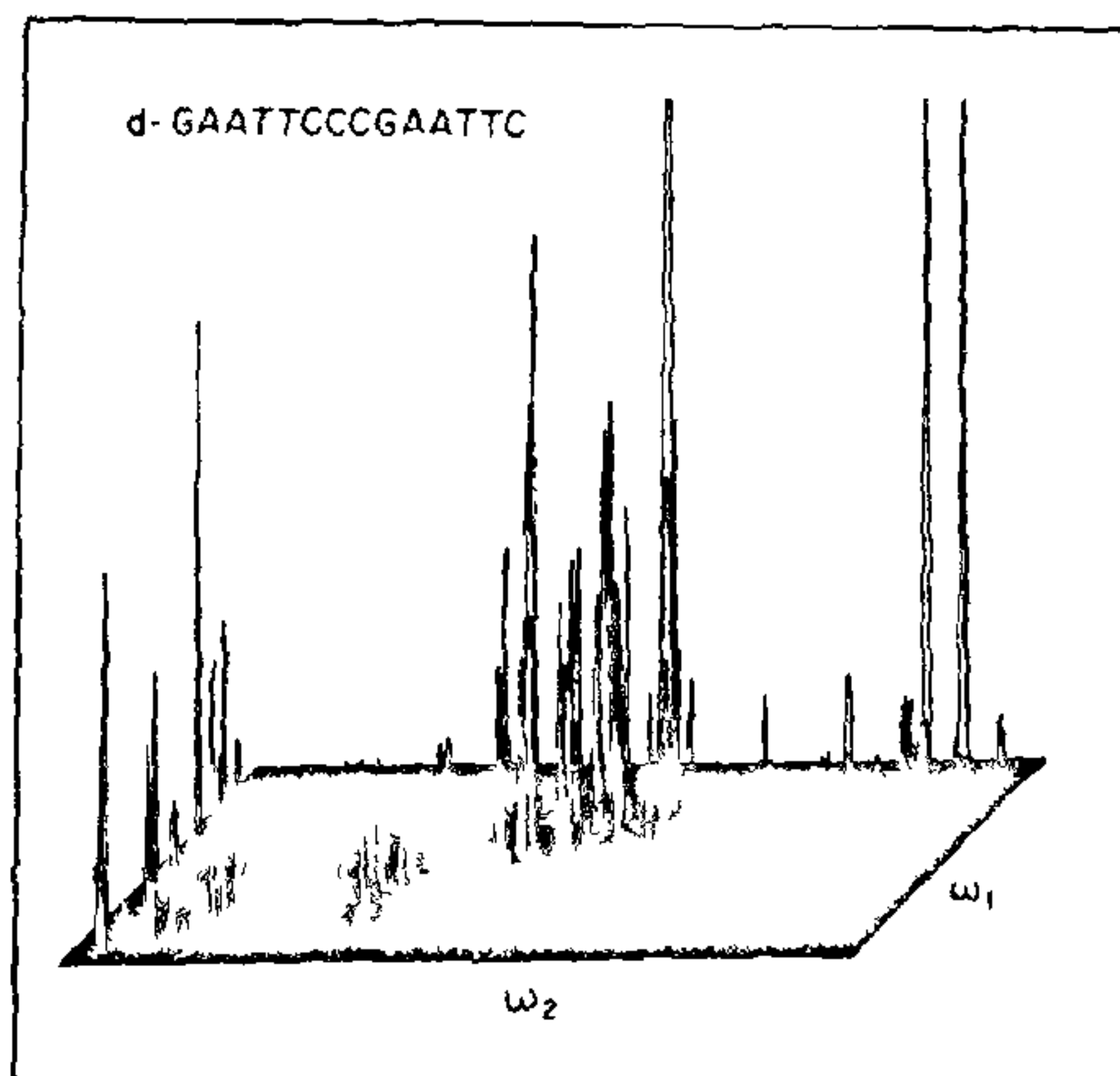
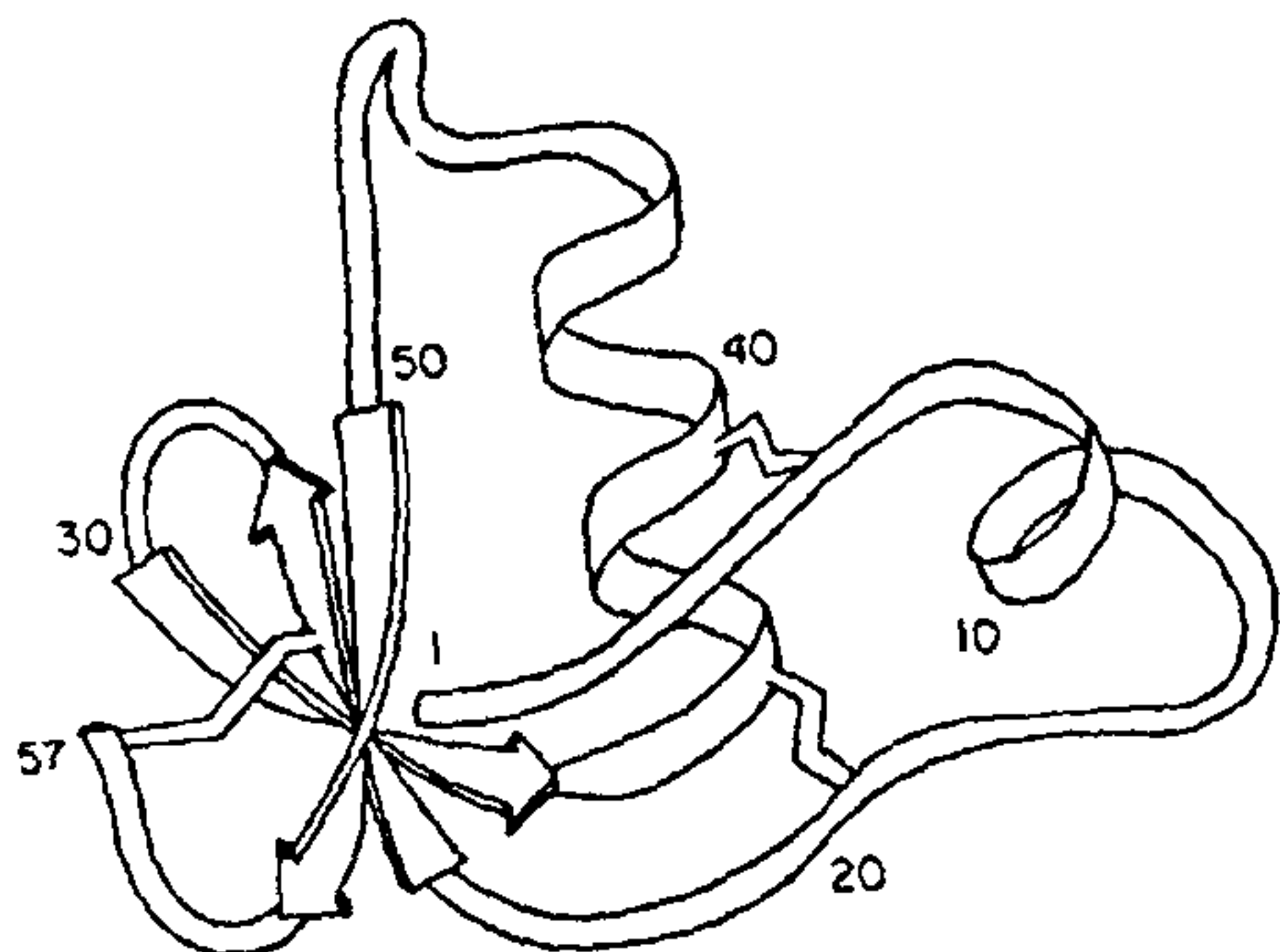

Figure 1. 500 MHz COSY[8] spectrum of d-GAATTCCCGAATTC

Figure 2. Structure of BUSI II A obtained from 2D NMR data (reproduced with permission from Williamson, et al 1985).

mining structures of small proteins using the 2D NMR methods are now very well established. Figure 2 shows as an illustration, the structure of a small protein, Bull Seminal Inhibitor II A, obtained using these methods[10].

In the case of nucleic acids, the strategies are still developing[11-14] and new 2D techniques are being developed to solve specific problems. However it is already evident that a stretch of DNA should be looked as a whole rather than as belonging to a particular type of DNA model such as A, B, Z etc.

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Vibrational Spectroscopic Studies on Structure of Liquid Water and Aqueous Solutions by Surjit Singh, Department of Chemistry, Indian Institute of Technology, Madras 600 036, India.

A lot of interest has been shown in the determination of structure of liquid water over the years using spectroscopic and non-spectroscopic methods as well as quantum and statistical mechanical calculations[1,2]. The microscopic properties of liquids are mainly related to the properties of molecules themselves, their dynamic behaviour and their arrangements in the liquid state. The problem of interpretations of macroscopic and microscopic properties, however, remains unsolved and because of this it is useful to gather more and more information about liquid structures. Although there are several other methods like x-ray and neutron scattering and computer simulation techniques, vibrational spectroscopy plays a useful role[3] in the determination of structure of liquids. Becasue of low time scale of vibrational transitions, associated molecular species with life-times of the order of 10^{-12} to 10^{-13} sec can be detected by IR and Raman spectroscopy.

It is well known that in ice at 0 C. Water molecules are arranged in hexagonal form with tetracoordinated oxygen atoms having C_2, symmetry. On the basis of the structure of ice two general models for liquid water, referred to as continuum and mixture models have been proposed by several investigators. In this connection vibrational spectroscopic in far, mid and near-IR regions have been reported for liquid water and its aqueous solutions over a wide temperature range. Raman spectra for the symmetric stretching (v_1) vibration of O D in dilute solutions of D_2O in H_2O show that the band contour is non-symmetrical and exhibits a shoulder on the high frequency side of the main peak. The asymmetry in the v_1 band (also

observed in the v_2 and v_1 bands) is interpreted in terms of the dual structural model for water[2] consisting of non-hydrogen bonded and hydrogen-bonded water molecules. The low frequency bands belonging to intermolecular vibrations are assigned to tetracoordinated water molecules exhibiting C_{2v} symmetry. Although, for the interpretation of the Raman spectra, the mixture model appears attractive, several physical properties as well as the computer simulation results do not support a dual structure model for water. Some recent investigations[4] on the second derivative analysis of the O—H stretching bands in Raman spectra and MO calculations show that the results can be explained on the basis of continuum model.

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Crystal Engineering a Solid State Diels-Alder Reaction by G. R. Desiraju, *School of Chemistry, University of Hyderabad, Hyderabad 500 134, India.*

The Diels–Alder reaction is one of the most versatile in organic synthesis and its extension to the domain of solid state chemistry is reported here. This is possible by using the principles of crystal engineering, that is, by a study of those intermolecular interactions which lead preferentially to certain geometrical motifs of molecules in the crystal. The key compound is 3,4-methylenedioxyphenylpropionic acid which was predicted to (and does in fact), crystallize with a short axis of 4 Å. Such a packing ensures that a triple bond of a molecule (dienophile) comes to within reacting distance (4 Å) of a conjugated triple bond (diene) translated neighbour. When the solid acid is heated, a Diels–Alder reaction takes place. This solid state reaction may have biosynthetic implications since the product is a well-known precursor in lignan synthesis.

The crystal structure of the closely related 3,4-methylene dioxycinnamic acid proved to be an effective starting point in this crystal engineering exercise

and two factors seem to be responsible for the 4 Å packing of the phenylpropionic acid mentioned above. C–H . . . O hydrogen bonding of the methylenedioxy groups favours the formation of a 'planar sheet' of molecules which may stack at van der Waals separation to generate the entire structure. Additionally, the high C:H ratio in the molecule ($C_{10}H_6O_4$) appears to direct the packing to a mode where such 'graphitic' stacking is preferred.

Structural Studies on Belladonna Mottle Virus by M. R. N. Murthy, S. K. Munshi, C. N. Hiremath, H. S. Savithri* and S. Suryanarayana*, *Molecular Biophysics Unit and *Department of Biochemistry, Indian Institute of Science, Bangalore 560 012, India.*

Belladonna mottle virus (BDMV) belongs to the tymogroup of sperical plant viruses. The virus particles contain 180 copies of identical protein subunits of MW 20,000, which encapulate a single-stranded, messenger sense RNA of molecular weight 2×10^6. The virus was propagated on *N. glutinosa* and purified from infected leaves by differential centrifugation. The purified virus contained in 0.1 M sodium citrate buffer of pH 5.6 (40 mg/ml) was crystallized by precipitation with 2.5% polyethelene glycol 6000. The crystals belong to rhombohedral space group R3 with cell edges of ~300 Å and interaxial angles of ~60°. Only one virus particle is compatible with the unit cell suggesting a particle 3-fold axis that is coincident with crystal 3-fold. Three-dimensional x-ray diffraction data from a complete asymmetric unit have been collected by screenless oscillation photography by rotating the crystal about its 3-fold axis. The oscillation angle was 1° with an overlap of 20% between consecutive films permitting measurement of reflections to a resolution of 5.5 Å[1] with marginal overlap at higher resolution. A rotating anode x-ray generator operating at 36 kV, 45 mA and equipped with a 200 μ focal cup provided the x-ray beam which was focussed with 2 perpendicular mirrors. The exposure time for each photograph was 40–50 hr and 15–20 hr for INDU and KODAK DEF-5 films, respectively. A total of 62 film pairs were recorded each containing 2500–3000 reflections. A and B films of a pair were scaled together with R factors varying from 7% to 11% with a mean of 9.5%. Scaling films together resulted in a total of 1,27,675 measurements of which 75,919 were unique. The post refinement procedure was carried out to

improve the cell dimensions and obtain a more precise estimation of partially estimated intensities. The post refined cell edge is 295.38 Å and the interaxial angle is 59.86°. The R-factor for reflections with $I/\sigma(I) \geqslant 2.0$ in the film-film scaling is 12.5%.

In order to determine the orientation of the virus particle in the unit cell, a rotation function[1] was computed using the data between 11 Å and 13 Å and a radius of integration of 50 Å. The function clearly reveals the icosahedral symmetry of the virus particle and also fixes the orientation of the virus particle in the unit cell. The rotation function peaks corresponding to 2,3 and 5 fold axes are 3–7σ above the mean background. The peak positions fit the corresponding positions of an idealized icosahedron to within 0.25° revealing that the data is of quality, comparable to those collected elsewhere. Attempts to determine phases of low resolution reflections ab initio using techniques of molecular replacement[2] are in progress.

In parallel with structural studies, the stability of BDMV was studied at elavated pH and with respect to freeze-thaw treatment. Contrary to earlier reports[3] the virus was found stable at alkaline pH. It was shown that this stability is due to the presence of 110 moles of spermidine, 25 moles of putrescine and 500–900 moles of calcium per mole of virus. The polyamines bound to BDMV are easily exchanged for other monovalent cations such as K^+ and Cs^+. In contrast, the cations bound to the related turnip yellow mosaic virus (TYMV) are removed only under more drastic conditions. Removal of intrinsic cations renders the virus particles unstable indicating that they play an important role in the integrity of the virus particles. RNA form virus particles are removed by freezing and subsequent thawing in a manner similar to that of TYMV. The influence of ionic strength, the presence and the concentration of different cations and anions on the effects of freeze-thaw treatment of BDMV also follow closely the effects observed for TYMV[4].

The amino acid sequence of the coat protein of BDMV is required for x-ray structure determination. Also, the availability of the sequence provides a framework for understanding the stability properties, sites of protein-protein and protein-nucleic acid interactions. The sequence also provides information regarding evolution of tymoviruses. The amino acid sequence of TYMV[5] and another tymovirus, egg plant mosaic virus[6] (EMV) are known. We have initiated the determination of the amino acid sequence of BDMV coat protein. We have shown that the

amino terminal is blocked by an acetyl group. The fragments obtained by CNBr treatment of the coat protein show the size similarities to those anticipated from the known sequence of TYMV and EMV, suggesting that the methionines in these tymoviruses are similarly placed. The amino acid sequence of a 4K CNBr fragment has been determined by DABTIC/PITC manual sequencing of the fragment and its tryptic peptides. Alignment of the tryptic peptides was achieved by comparison with the sequences of TYMV and EMV. A preliminary comparison reveals that BDMV is evolutionarily closer to EMV than to TYMV. The sequence contains a highly conserved region which appears to be involved in the particle assembly. Quantitative analysis of the amino acid sequence homology, variation in the mutability of different segments of the coat protein and its implication to the structure and stability of tymoviruses may be carried out when the complete amino acid sequence of the coat protein and the three-dimensional structure of the virus become available.

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Gravitational Mirages by S. M. Chitre, Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400 005, India.

The mirage is a familiar sight to travellers in the scorching sun. It now appears that astronomers too have to be aware of cosmic illusions produced by the influence of gravity on light.

The gravitational bending of light is one of the classical tests of Einstein's General Theory of Relativity. The deflection of starlight by the gravitational influence of the sun was measured during the total

solar eclipse of 1919 and was indeed found to be in excellent agreement with the theoretical prediction of general relativity. Later, following the suggestion of a Czech electrical engineer Mandl, Einstein examined the possibility of the image of a distant star being split by the gravitational influence of a foreground star to conclude that the chance of observing such a phenomenon was extremely small. It was Zwicky who applied the concept of gravitational lenses to galaxies and suggested that a nearby galaxy along the sightline could create double images of a distant galaxy in the background and this might provide the simplest means of determining galaxy masses. It is perhaps extraordinary that the phenomenon of gravitational lenses, a direct consequence of general relativity was not widely appreciated until the appearance of quasars on the astronomical scene.

The long awaited discovery of a gravitational lens system came in 1979 when Walsh, Carswell and Weymann discovered the twin quasar 0957 + 561 comprising two quasars separated by 6.15 arc sec., with almost identical redshifts of 1.41. Since then, some half a dozen possible candidate lens systems have been reported in the literature and these have revealed optical illusions on a cosmic scale.

The original emphasis in gravitational lens theory centred around the imaging of a point source by a point mass lens. Recently, after the discovery of the gravitational lens systems, the interest has shifted to the imaging of a point source (e.g. quasar) by an extended lens like a galaxy or a cluster of galaxies. But there is another important aspect of lensing, namely the imaging of an extended source by a point mass lens, an effect which seems to work best within our own galaxy resulting in the production of "gravity rings". It seems almost certain that in the next several years when very long baseline interferometers provide detailed high resolution maps, the "gravity ring" will appear as a new type of astronomical image. This phenomenon will, hopefully, provide a new diagnostic tool for determining such astrophysical properties as masses of pulsars, mass-spectrum of stars in clusters, distances to galactic gas clouds.

There is another application of the lensing phenomenon. This arises in the context of the detection of two or more components, in the nuclear regions of some extragalactic radio sources, which were apparently separating at speeds exceeding that of light. This gravitational mirage, involving material components exhibiting faster than light motion, could be explained by invoking gravitational lenses. An inter-

vening galaxy acting as a gravitational lens can bend light rays coming from a background quasar. Thus, in place of the real separating components in the quasar, there may be seen images moving apart, so that they appear to have a much larger distance between them than what is actually covered in a given interval of time. This may very well mimic the apparent superluminal motion in quasi-stellar objects—a gigantic cosmic mirage!

Equatorial Heart by M. S. Valiathan, *Sree Chitra Tirunal Institute for Medical Sciences and Technology, Trivandrum 695 011, India.*

The heart evokes as many different images as varied moods in the human mind. The comparative anatomist, the embryologist, the physiologist and the engineer will have his own distinctive view of the heart. But a philosopher might claim that all these images are merely schema of the heart—produced by the distinctive tools of each discipline. When the schema are added, the total is less than the reality which stalks behind the organ—unknown and perhaps unknowable.

In the welter of cardiac images, what is missed is the sensitivity of the heart to the geographic environment. Geography conditions the heart in health and disease just as the drone of the tamboura conditions the music from the background. The heart responds to altitude, to climate, to the pull of the moon and sun and to the soil. But it is often a disease-or dysfunction which reveals to us the subtle link between the cardiac melody and the geographical drone. It is in this nontraditional context that one must view the geochemical intimations of endomyocardial fibrosis, a type of heart disease which characterizes the equatorial zone.

Endomyocardial fibrosis, which implies scarring of the inner lining of the heart constitutes a fatal cardiac muscle disease in Nigeria, Uganda, Ivory Coast, Tanzania, Kerala, Brazil and Venezuela—all within 12° of the equator. The clinical profile of the disease is dominated as much by the young age of the victim as by the symptoms and signs of heart failure. The onset is insidious and patients are generally unable to date their symptoms to any acute illness. The disease runs an invariably fatal course with only 25% alive, at the end of two years of medical treatment. The central problem in the disease is the growth of a fibrous layer which gradually obliterates

the pumping chambers of the heart. The fibrous mantle plasters the atrioventricular valves and restricts pumping function leading to intractable heart failure.

Laboratory investigations are necessary to confirm the diagnosis of endomyocardial fibrosis. Electrocardiogram while not specific may be marked by abnormal rhythms or diminished voltage. A far more important investigative method is ultrasonography which has revolutionized the office diagnosis of endomyocardial fibrosis. Apart from demonstrating the structural changes, the two-dimensional echocardiographic technique can also reveal wall motion abnormalities of the heart. However for a detailed demonstration of the anatomical lesions, cardiac catheterization and selective cardiac angiography continue to remain the best methods.

At the structural level the endocardium is replaced by an excessively thick collagenous layer in endomyocardial fibrosis. As the disease progresses, the fibrosis extends into the subjacent myocardium and distorts the myocardial architecture.

Medical treatment can offer very little in this situation except managing the consequences of severe heart failure. However, excising the fibrous tissue from the ventricular chambers and replacing the non-functioning valve does produce significant palliation and 70% survival at the end of 5 years.

In the absence of a cure for the disease, a probe into its cause is imperative. The cause of endomyocardial fibrosis has however been a matter of debate ever since its recognition and many theories on causation have surfaced over the years. A widely held view at the present time is that endomyocardial fibrosis in the equatorial zone is the terminal phase of a disease known as hypereosinophilic syndrome in the temperate zone. According to this view, an abnormal increase in the number of eosinophils in blood and their breakdown lead to the release of a toxic protein from their granules which injures the lining of the heart and triggers the fibrotic process. This theory however leaves several questions unanswered, particularly the difference in clinical features between endomyocardial fibrosis and hypereosinophilic syndrome. A viable hypothesis on endomyocardial fibrosis must account for three cardinal preferences which characterize the disease. These are the preference for the equator, for the poor socioeconomic class and for the heart.

The interesting overlap in the incidence of endomyocardial fibrosis and the distribution of latosolic soil in the equatorial zone prompted a recent search

for elements of laterite and monazite which might have replaced or displaced essential metal ions in the cardiac tissues of patients with endomyocardial fibrosis. A preliminary analysis showed that cardiac tissues of patients have less magnesium and more of calcium, sodium and thorium than the control samples[1]. While the excess of sodium and calcium could be explained on the basis of congestive cardiac failure and reciprocal movement of calcium in relation to magnesium, the deficiency of magnesium and the presence of thorium could not readily be explained.

Magnesium is an essential cation which has several functions including force development and relaxation, binding and release of calcium by sarcotubules and oxidative functions of the mitrochondria. Magnesium deficiency is known to produce a variety of pathological changes in several organs. As patients with endomyocardial fibrosis suffer from malnutrition which is often associated with magnesium deficiency, it is entirely possible that magnesium deficiency observed in endomyocardial fibrosis is not accidental. But the highly cardioselective lesions of endomyocardial fibrosis would suggest that the changes induced by magnesium deficiency are modified or overshadowed by another factor in endomyocardial fibrosis.

Thorium is present in the monazite sands of Kerala and the latosolic soils of several other tropical areas of the world. It has been shown to be present in water and is concentrated by tuber crops which form the staple food of poor people in Kerala. Surveys have also shown the presence of thorium in the urine samples of children in this region. While thorium has no physiological role, it is possible that due to its strong positive charge, it binds to the phosphate of the membrane phospholipid and lipid bilayer of the sarcolemma. Thorium might have several possible modes of action at myocardial level. It could affect the binding of MgATP complex to myosin, trigger interaction of lytic enzymes in the cell, produce superoxide anions and other free radicals or act as a substitute for magnesium in cellular processes. Any of these actions or interactions could initiate the cellular injury which results in endomyocardial fibrosis.

A hypothesis based on magnesium-thorium interaction has the merit of accounting for the three cardinal preferences of endomyocardial fibrosis referred to earlier. In our view endomyocardial fibrosis is an equatorial aberration which is geochemical in origin. While only experimental demonstration can confirm or refute the hypothesis, the present view also opens

up the exciting possibility of controlling or preventing the disease by simple means which are based on a fundamental understanding of the disease process.

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Significance of High Precision in Enzyme Structures†
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The catalytic activity of an enzyme in biochemical reactions is highly structure-specific. Single-crystal x-ray diffraction studies on a native enzyme and its inhibitor complexes at 2.5 to 2.0 Å resolution can provide adequate information on the biological function of the enzyme molecule. However, this information is usually qualitative and of uncertain precision. The use of high resolution x-ray data and the optimization of the molecular model of the enzyme provide more definitive and precise information about its molecular structure and function. During the past few years, many protein structures have been refined using various novel techniques of structure optimization. One such method and its application to an enzyme structure refinement are briefly described here.

In the method of stereochemically restrained least-squares (SRLSQ)[1,2] refinement, the positional and the thermal vibration parameters of the molecular model are optimized simultaneously with respect to the crystallographic and stereochemical data. Standard stereochemical parameters and the associated variances used in this method, can be obtained from the x-ray and neutron[3] studies on amino acids and small peptides. The structure of triclinic hen egg-white lysozyme[4] has recently been refined by SRLSQ method at 2 Å resolution. The refined structural model not only has a very small disagreement factor (R-factor) of 12.4% with respect to the diffraction

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data, but also has an excellent agreement with the standard stereochemical parameters. The refined B-values are relatively small and consistent with the structural features of the protein and the solvent molecules. A detailed analysis of this work will be published elsewhere. Some of the most importnat results are briefly discussed.

An optimal speed of convergence of the refinement process was achieved by scaling the relative weights associated with the restraints and the structure amplitudes on the basis of the numerical values of various kinds of residuals. Model corrections were applied after every few cycles of refinement with the help of Fourier maps on an interactive graphics system. Restraints on the peptide planarity were relaxed to some extent during the final cycles of refinement. This procedure, not only removed the strain on the polypeptide chain wherever the peptide linkages were significantly nonplanar, but also indicated the presence of model errors, which were not seen earlier. The final model contains 247 'solvent' molecules and 5 nitrate ions, in addition to the enzyme molecule. The distribution of B-values agrees well with the protein folding and the interatomic interactions. About a dozen side chains, mostly ARG (but some of them ASN, ASP, GLN and GLU types) are in poorer electron density regions, indicating their mobility. In addition, some GLY residues in the main chain also seem to have larger thermal motion or static disorder. Residues ASP-101, GLY-102, ASN-103 and GLY-104 were difficult to fit on the graphics system, since the density in that region was very poor. Three or four peptide linkages have nonplanar deviations of more than 10° Two of these are in the active site. Refinement of lysozyme at 1.5 Å resolution will be taken up soon. The pre-refinement R-factor at this resolution is as low as 19.9%. A copper complex of triclinic lysozyme[5] has also been refined at 2 Å resolution to an R-value of 16.9%. Further refinement of this complex is in progress.

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How Drugs Affect Enzyme Function? A Protein Crystallographic Approach† by K. K. Kannan*, Vinay Kumar*, K. Sankaran, Padma Sathyamurthy* and S. Chakravarthy*, *Neutron Physics Division and Food Technology and Enzyme Engineering Division, Bhabha Atomic Research Centre, Bombay 400 085, India.

Enzymes are the most important class of biological catalysts which make the life process possible. The turnover rates of many enzyme catalyzed reactions are several orders of magnitude higher than the uncatalyzed reactions. The function of the enzymes can be inhibited by different chemicals and transition state analogues.

Carbonic anhydrases are enzymes with a molecular weight of about 30,000 daltons consisting of about 260 amino acid residues and one essential Zn^{2+} ion, catalyzing the reversible hydration of CO_2. The carbonic anhydrases are widely distributed in nature and are found in bacteria, plants and animals. They are found in large quantities in the erythrocytes of animals, often as two isoenzyme forms with homologous amino acid sequence but different turnover rates and other physical properties. The muscle also contains a carbonic anhydrase, however with a considerably reduced catalytic activity as compared to the erythrocyte isozymes.

The enzyme-catalyzed reaction

$$CO_2 + H_2O <===== > HCO_3^- + H^+$$
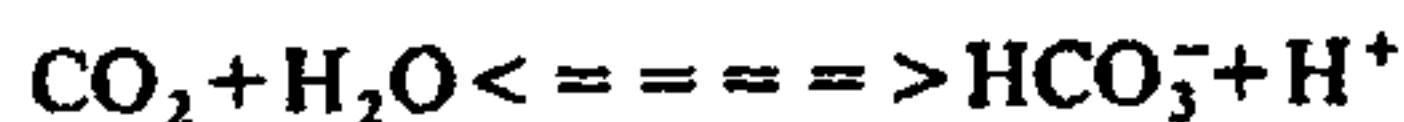
with a turnover rate of about 5 to 10×10^5 mole CO_2/enzyme/sec is one of the fastest enzyme-catalyzed reactions. The isoenzymes are inhibited by aromatic and heterocyclic sulphonamides very effectively. Heterocyclic sulphonamides, acetazolamide and methazolamide are often used as drugs in the treatment of glucoma, stomach and deodenal ulcers etc.

Protein crystallography is a very powerful method to explore enzyme structure, function and inhibition. The crystal structure of human erythrocyte carbonic anhydrase has been determined by protein crystallographic methods to 2.2 Å resolution[1,2]. The ellipsoidal shaped protein of dimension 42 Å × 45 Å × 55 Å is stabilized by extensive pleated sheet hydrogen bonding and hydrophobic interactions. The enzyme active site is a conical cavity with the essential Zn^{2+} ion anchored to the protein by three histidyl side chains, a water molecule forming the fourth ligand. The active site is divided into two halves, one containing predominantly hydrophilic residues and the other containing predominantly hydrophobic residues. The structure of the native enzyme has also been refined by the method of least-squares and computer graphics techniques using high resolution x-ray diffraction data[3,4] A large number of protein bound solvent molecules have been located, a number of which are involved in a network of hydrogen bond with protein side chains and Zn^{2+} ion liganded water molecule. This hydrogen bond network may be very important in the catalytic efficiency of this enzyme which requires fast proton transfer from the enzyme to the buffer and vice versa.

Drug interaction has been studied with the protein crystallographic technique for a number of carbonic anhydrase inhibitors/drugs such as *p*-nitro benzene sulphonamide, azetazolamide and methazolamide, which are sulphonamide inhibitors with differing inhibitory power[5]. The different inhibitors have been soaked into the crystals of the native carbonic anhydrase I isoenzyme, x-ray diffraction data collected on x-ray films and processed on a computer controlled microdensitometer. The structure of the drug molecules in the enzyme has been determined from difference Fourier synthesis and their interaction with the protein has been studied with the help of a 3D interactive graphics systems. The structure of azetazolamide (for e.g. in the enzyme active site) is found to be different as compared to that in the crystal structure of the drug molecule itself. There are differences in the interaction of the different inhibitors/drugs with the amino acid side chains in the active site of the enzyme, which would explain their different inhibitory power. The sulphamido group is also found to replace a catalytically important water molecule liganded to the essential Zn^{2+} ion. Methazolamide also binds in a similar way in the active site, except that there are more interactions with some other side chains also which indicate the higher inhibitory capacity.

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Structure, Transformation and Interaction of Proteins: an X-ray Study by M. Vijayan, *Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India.*

The protein crystallography programme in our laboratory is aimed at (i) determining the three-dimensional structures of proteins with receptor functions; and (ii) eliciting additional information, in terms of structural transformations and interactions, on proteins with known structures.

Quaternary structure of peanut lectin

As far as new proteins are concerned, the current efforts are primarily concerned with lectins, a relatively underexplored family of proteins involved in cell surface recognition through highly specific carbohydrate binding, with biochemical support and collaboration provided by Dr A. Surolia and his colleagues. As a part of these efforts, four different crystal forms, one orthorhombic, two monoclinic and one triclinic, of the tetrameric anti-T agglutinin from peanut have been grown[1,2]. All of them contain a tetrameric molecule, M. W. 1,10,000, in the asymmetric unit. Subsequently, x-ray intensity data from the orthorhombic crystals have been collected using oscillation photography. Rotation function studies using data up to a resolution of 4.5 Å indicate that the four subunits in the molecule are related to one another by three mutually perpendicular noncrystallographic two-fold axis.

Chemical crosslinking experiments in solution followed by SDS gel electrophoresis, carried out in parallel, suggest that there is more than one type of intersubunit approach in the molecule. Rotation function and crosslinking studies thus show that the tetrameric molecule of peanut lectin is a dimer of a dimer. The two monomers in a dimer are related by a two-fold axis. The two dimers are in turn related by another two-fold axis perpendicular to the one that relates the two monomers in the dimer, endowing the molecule with $222(D_2)$ symmetry[3].

Water-mediated transformations in protein crystals

Some progress has been made in our attempts to elicit more information on proteins with known structures. Following the accidental discovery of water-mediated transformations in some protein crystals[4], different crystal forms of bovine pancreatic ribonuclease A and hen egg white lysozyme, 2 Zn insulin, 4 Zn insulin and the crystals of Concanavalin A were examined under controlled environmental humidity in the relative humidity (r.h.) range[5] of 100% to 75%. Many of them, but not all, undergo reversible structural transformations as evidenced by discontinuous changes in the diffraction pattern, the unit cell dimensions and the solvent content. The results obtained so far indicate that the crystal structure has a definite influence on water-mediated transformations. The transformations do not appear to depend critically on the amount of solvent in the crystals, but the r.h. at which they occur is influenced by the composition of the solvent. The transformations appear to involve changes in crystal packing as well as conformational transitions in protein molecules. The present investigations and other related studies suggest that water-mediated transformations in protein crystals could be highly useful in exploring conformational transitions in and the hydration of proteins.

An additional binding site in lysozyme

Another interesting result we have obtained pertains to an additional binding site in lysozyme. Following the lead from solution studies[6], x-ray studies on the binding of indicator dyes such as bromophenol red (BPR) to lysozyme were taken up. They bind to the enzyme and inhibits its activity against bacterial cell wall, but not against the polysaccharide component of the peptidoglycan. The binding site of BPR in the enzyme has been chara-

cterized by the x-ray analysis of the complex at 5.5 Å resolution[7]. The new binding site, which is outside the cleft close to subsite F and contains well-conserved residues, is presumably involved in interactions with the peptide component of the peptidoglycan, in the action of lysozyme against bacterial cell wall. This result appears to mark a significant departure from the conventional wisdom on lysozyme action.

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Dynamics of Atoms and Molecular Clusters in Complex Crystals by K. R. Rao, *Nuclear Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400 085, India.*

Study of dynamics of atoms and 'molecular' clusters in solids theoretically and experimentally has been an active area over several decades. Although the study of organic crystals has been in vogue for quite sometime, the study of ionic systems has been in vogue mostly over the past ten years. The organics had attracted the attention mainly because of the inherent simple basic interactions involving only a few species of atoms mostly carbon, oxygen and nitrogen. Using thermodynamic information like virial coefficient, melting point etc these interaction 'force constants' were parametrized and one could transfer these parameters from system to system. On the other hand, the ionic systems consist of a large variety of atoms and the nature of interactions involve electrostatic forces in addition to other short range interactions. Till about 1970, one knew how to determine the Coulomb coefficients needed for the study of lattice dynamics of ionic atomic systems in cubic and hexagonal crystals based on the famous Ewald summation. The classic paper of Venkataraman and Sahni[1] dealt with the details of evaluating such Coulomb coefficients in ionic systems containing atoms and 'molecules' in crystals of any symmetry; in other words, this paper provides the formalism essential for the lattice dynamical studies of ionic 'molecular' systems involving rotational degrees of freedom. However, this work lay dormant for the next five or six years. The paper dealing with neutron investigations of lattice dynamics of α-KNO_3 by Rao et al[2] is the first work that deals with calculation of the detailed dispersion relation of phonons making use of the formalism of ref. 1. This paper[2] details the application of group theoretical formalism for external modes in this complex crystal and provides theoretical results on phonon dispersion curves well within 10-15% of the available experimental data. The program written by Chaplot[3] was used in this analysis. Ever since, the Trombay group has made extensive studies of a variety of complex systems like $KNbO_3$, $LiNbO_3$, $(NH_4)_2CuCl_4 \cdot 2H_2O$, $K_2CuCl_4 \cdot 2H_2O$, Sb_2S_3, $SbSI$, $LiKSO_4$, Mg_2SiO_4 etc to understand the dynamics of atoms and 'molecules' in various phases of these systems. The phonon dispersion relation and the frequency distribution of phonons are the basic results obtained in most of these cases to make suitable comparison, assignments and analysis of x-ray, neutron and/or laser Raman scattering data. In some cases, information concerning phonons responsible for successive phase transitions, partial density of states, anharmonic phonon renormalization, specific heat as a function of temperature, thermal expansion, compressibility etc have been obtained and compared with experimental data. The neutron scattering cross-sections obtained using the eigenvectors of lattice modes have helped in planning neutron inelastic scattering experiments.

The crystal potential used in these studies is still a parametrized one. However, it is noted that some of these parameters are transferable from system to system as in the case of organic systems. Secondly since these potentials are appropriate to the equilibrium structure of the crystals and also since they lead to results in agreement with a variety of experi-

mental data, they can be used in 'computer simulation experiments' to obtain dynamical information about these systems at a variety of temperatures and pressures. Such computer experiments have been carried out by the Trombay group in mixed inert systems, NH_4-halides and $LiKSO_4$. In addition to providing useful dynamical information which cannot easily be derived by experiments, these studies have also led to suggestions for new experiments.

In conclusion, it may be stated that these studies are somewhat unique in the sense that the formalism, the program and the systems studied have had a very local flavour.

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Corrugated Wave Fronts by R. Nityananda, *Raman Research Institute, Bangalore 560 080, India.*

The propagation of radio waves through the plasma in the Galaxy, the solar system, and immediately surrounding the earth is strongly influenced by the fluctuations in the refractive index associated with the density inhomogeneities. Related theoretical problems are encountered in the study of the propagation of laser beams through the atmosphere and sound through the ocean. The essential common features are: (i) inhomogeneities on scales which are much larger than the wavelength, and (ii) path differences which are also much larger than a wavelength introduced over the wavefront.

It is interesting that the archetypal problem for this currently very active field is the diffraction of light by ultrasonic waves, studied experimentally by Debye and Sears more than fifty years ago. Experience with diffraction gratings and x-ray diffraction from crystals led people to expect a small number of diffraction orders. The rich diffraction pattern actually observed was explained by Raman and Nath with the physical concept of a *corrugated wave front.* In addition, these authors introduced a system of differential equations which describe the spreading of the wave amplitude from order to order.

These two basic concepts underlie the early work in the case of a random medium as well. A generalization of the Raman-Nath work by Rytov has been widely used, but breaks down for propagation distances so large that focussing of rays can occur. Well beyond this distance, the number of rays is so large that Gaussian statistics can be applied. The difficult problems which remain open in spite of much work are: (i) a proper description of the intermediate region where strong focussing sets in and (ii) the effect of inhomogeneities on a whole range of scales, which do not simply add but interact with each other. A useful framework for answering these questions is provided by the Markov approximation, which can be regarded as a kind of "embedding". The change in the statistical properties of the wavefield caused by a thin layer is a tractable problem. The cumulative effect of the whole medium must then be obtained by solving a differential equation.

In dealing with the effect of different scales, it appears that there are two distinct physical regimes, in one of which the short scales are the most important while in the other the large scales dominate. Observations of the intensity fluctuations (scintillations) of pulsars as a function of frequency and time suggest a case very close to the borderline between these two situations. There are tantalizing but largely unexplored parallels with the theory of phase transitions. An interesting aspect is that the process of ensemble averaging implicit in any statistical theory may be misleading when applied to the large scales, because the variations from one random realization to the other may be large. Very recent observations seem to suggest such a picture.

The Raman-Nath regime of wave propagation phenomena was first revealed by their theory of ultrasonic diffraction of light. Over the years the case of a random medium has excited great interest, both because of its wide application and because of the theoretical challenges that it poses.

Chaotic Behaviour in the Eigenstates of Molecular Systems by R. Ramaswamy, *School of Physical Sciences, Jawaharlal Nehru University, New Delhi 110 067, India.*

Classical dynamical systems have been studied in detail in recent years, and in some sense, they are well

understood. One reason for this is the existence of precise mathematical statements and theorems that pertain to the differential equations that govern classical motion, e.g. the KAM theorem regarding Hamiltonian systems. Thus it is known that both regular (periodic or quasiperiodic), and chaotic (aperiodic) motions can exist, and that the purely deterministic equations of classical mechanics can give rise to complicated, unpredictable and seemingly probabalistic motions.

An important and unresolved matter is the relevance of such classical behaviour in a quantal world—the so-called question of quantum chaos. One area where this is of relevance is in molecular physics. Small molecules are well-described as Hamiltonian systems with a few degrees of freedom, and thus are amenable to both a classical and quantal study, in order to elucidate the connections between classical and any possible quantum chaotic behaviour.

Conjectures have dealt with the properties of the so-called regular and irregular eigenstates, as analogues and consequences of regular and chaotic motions. These can be distinguished as those that relate to eigenvalues or eigenfunctions. For regular states, for example, the eigenvalues are stable under small perturbations, and the eigenstates are well-characterized by a set of good quantum numbers. Irregular states, on the other hand, cannot be ascribed to any set of quantum numbers and the eigenvalues are very sensitive to perturbations. The eigenfunctions are of different types as well, having well-defined nodal patterns in the former case, and being "random" in the latter. In fact it may be possible to associate a statistically fractal character with irregular wavefunctions. Eigenvalue spacing statistics are also very different: Poisson for regular states and Wigner for irregular levels.

Using high resolution infrared spectroscopy, it is possible to study the high energy vibrational levels of small molecules. Some recent experimental results suggest that the chaotic eigenstates of molecules (such as acetylene) have been observed.

The Metallurgical Synthesis of Titanium Alloys by D. Banerjee, *Defence Metallurgical Research Laboratory, Hyderabad 500 258, India.*

The mechanical properties of current commercial titanium alloys depend on the distribution, strength and morphology of the hexagonal closed packed (α) and body-centred cubic (β) allotropic forms of titanium. The rationale used to alloy and heat treat titanium, so as to arrive at the appropriate structural synthesis of the α and β phases has been derived from a wide variety of studies on phase transformations and the relationship between microstructure and properties in various titanium based alloy systems. The role of the specific alloying additions, in strengthening and stabilizing these and other metastable phases is described, followed by a description of the manner in which microstructure controls deformation behaviour as represented by the motion of crystal defects such as dislocations. Control of atomistic or micromechanisms of deformation through microstructural modification is utilized to achieve the desired property levels—titanium and its alloys are known for their outstanding strength/weight ratios, intermediate temperature properties and corrosion resistance. It is then emphasized that the synthesis of shape to obtain a desired engineering product cannot be delinked from synthesis of structure to achieve a given set of properties. The strain energy stored, in imparting a given shape to an alloy interacts with thermodynamic and kinetic parameters which control the evolution of microstructure to significantly affect the nature of the final product. This interaction is briefly described for titanium alloys.

Dynamics on Homogenous Spaces and Diophantine Approximation by S. G. Dani, *Tata Institute of Fundamental Research, Homi Bhabha Road, Bombay 400 005, India.*

We consider flows, namely one-parameter groups of transformations of a space X, where the space X is a homogeneous space of a Lie group G and the flow arises from a one-parameter subgroup (g_t). Then we may write $X = G/C$, where C is a closed subgroup of G and the flow is given by $x C \rightarrow g_t x C$ for all x in G. We assume further that G/C admits a finite measure invariant under the action of G. In this case, satisfactory necessary and sufficient conditions are known for 'ergodicity' of the (g_t)-action; 'ergodicity' implies, in particular, that *for almost all x in G* C the orbit of x, namely the set $\{g_t x | t$ a real number$\}$ is dense in G/C and uniformly distributed over the space. In particular when $G = SL(n, R)$ and $C = SL(n, Z)$, in which case G/C may be viewed as the space of lattices

in the n-dimensional euclidean space, with a prescribed descriminant, a one-parameter subgroup acts ergodically if and only if it is not contained in a compact subgroup.

In general, however, it is a hard problem to determine for a *given* x in G/C, whether its orbit is dense, uniformly distributed etc. This is of interest both in terms of dynamics, where x corresponds to initial conditions and also in various problems in geometry and diophantine approximation. We discuss various results in the nature of partial answers to the above problem and their application to various problems including finding integral solutions of systems of linear inequalities, estimating the number of lattice points in long and narrow triangles, studying the behaviour of fractional parts of multiples of irrational numbers, the behaviour of geodesics and horospheres on manifolds of constant negative curvature etc.

In the particular case when $G = SL(2, \mathbf{R})$, $C = SL(2, \mathbf{Z})$ and $g_t = \left(\begin{smallmatrix} 1 & t \\ 0 & 1 \end{smallmatrix}\right)$ it turns out that the orbit of $x\,C$, where $x = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$, is dense and uniformly distributed when c/d is irrational and periodic when c/d is either infinite (that is, $d = 0$) or rational. Similar results also hold for other subgroups C of $SL(2, \mathbf{R})$ satisfying the assumption of finite invariant measure made earlier. We indicate the ideas involved in proving these results and their geometric meaning. We shall also discuss the behaviour of orbits of the flow induced by the one-parameter subgroup $\left(\begin{smallmatrix} e^t & 0 \\ 0 & e^{-t} \end{smallmatrix}\right)$; this corresponds to studying the unit speed flow along geodesics on certain surfaces of negative curvature.

Microbial Degradation of Pesticides: Prospects and Problems by N. Sethunathan, *Division of Soil Science and Microbiology, Central Rice Research Institute, Cuttack 753 006, India.*

From the standpoint of environmental safety, a pesticide should disappear from the environment after its desired period of pesticidal activity. The bulk of the pesticides applied in agriculture, forestry and public health eventually reaches the soil as residues. In the complex and dynamic soil system, pesticides are subjected to degradation by physical, chemical and/or biological processes. It is now well established that microbial degradation is the major or probably the only means of detoxification for many pesticides in the soil and water environments. Information on the biodegradability of a potential pesticide is a major pre-requisite for its registration in most countries.

Microbial degradation has several advantages over physical and chemical means of degradation. Degradation in physical and chemical processes is seldom complete and the degradation products may accumulate in the environment. In contrast, microbial degradation especially in a complex ecosystem such as soil with its mixed microflora would lead to more complete and extensive mineralization of a pesticide molecule often to innocuous inorganic end products. Moreover, ring cleavage of aromatic compounds is not chemically feasible and is mediated only by microorganisms through oxygenases. Stepwise degradation of the pesticide to the inorganic end product can be effected by an individual microorganism or a group of microorganisms indigenously present in the soil. Of applied interest is the fact that the cultural practices used in agriculture such as flooding (in rice culture) and organic amendment hasten the activity of these indigenous microorganisms. Microbes are highly versatile and easily adapt to a changing environment (for instance chemicals, through mutation and induction).

Microbial degradation of pesticides need not always be beneficial. Certain pesticides are transformed biologically to compounds, equally or more toxic and persistent than the parent molecules as, for instance, conversion of DDT to TDE in anaerobic ecosystems. Likewise, very rapid degradation of a pesticide by microorganisms before effecting control of target pests can have disastrous consequence of the build-up of these pests and total destruction of agricultural crops. There are reports of decreased efficacy of diazinon against brown planthoppers in rice and of carbofuran against root worm in corn. Evidence suggested that this phenomenon, generally noticed in areas of intensive use of the same pesticide year after year, was due to the build-up of pesticide-degrading microorganisms that undermine the efficacy of these pesticides. Formation of soil-bound residues of xenobiotic pollutants and their metabolites and remobilization of bound residues from soil humus are, at least in part, microbially mediated. The toxicological significance of such bound residues is, however, not clearly understood.

The Nature of Crust-mantle Boundary and Compositional Variation of Magma in the Light of Experimental Evidence by Alok K. Gupta,

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Mohorovicic discontinuity between the crust and the mantle is related to the phase transformation from gabbro/basalt to eclogite[1-3]. Subsequent experimental studies[4-6] show that basaltic rocks are converted to eclogites at pressures above 20 ± 3 kb. Thus there is experimental evidence in favour of the hypothesis put forward by Fermor[1], Lovering[2] and Kennedy[3].

The density of upper mantle materials (3.4-3.95 g/cm^3) as demanded by the propagation of P and S waves through this section of the earth agrees with that of eclogite (3.55-3.8 g/cm^3). Thus, generation of basaltic liquid from eclogites appears at first sight to be a viable hypothesis. Since the mohorovicic discontinuity below the ocean floor occurs only at a depth of 10-15 km, the presence of eclogite at such a depth is questionable. Besides, the complete melting of eclogite is necessary to generate a basalt magma. There is geophysical evidence to suggest that only partial melting of the earth's upper mantle takes place in the low velocity zone within the earth (80-150 km).

Garnet peridotite/lherzolite (containing olivine and pyroxene with or without garnet) is considered by many to constitute the upper mantle. Kushiro[7] made melting studies of garnet lherzolite at high pressures and noted that partial melting of such lherzolites under pressures of 10 and 20 kb produced tholeiitic and alkali basalt melts, respectively.

Meteorites are considered to be parts of disrupted planets and hence analogy of their compositions with certain segments of the earth is obvious. Chemistry of stoney meteorites is similar to that of peridotites rather than eclogites. Experimental studies[8] on carbonaceous condrites from Allende showed that a liquid produced by partial melting under MW and IW buffers have the composition similar to that of some ferro basalts from the moon.

Fayalite (α olivine, orthorhombic structure) is converted to β olivine (spinel structure) under 53 kb at 1000°C, whereas more magnesian olivine (forsterite$_{50}$, fayalite$_{50}$, wt%) is transformed to β phase under 112 kb at 1000 C. At higher pressures (i.e. greater depth) the conversion should take place at higher temperatures. This change in olivine structure adequately explains the change in the depth versus velocity profiles of P and S waves in the transition zone between lower and upper mantle.

Experimental studies[9,10] on the system forsterite-kalsilite-SiO_2 under variable pressures with or without volatiles (H_2O and/or CO_2) show that the invariant point involving olivine-orthopyroxene and kalsilite (K-feldspar in case of isobaric sections at 20 kb or below) shifts more and more towards the alkali-rich side of the system. Comparison of the study[9] on the system forsterite-nepheline-SiO_2 under 28 kb with that of others also show that the invariant point involving olivine, orthopyroxene and an alkali phase (nepheline or jadeite, depending on pressure) also shifts towards more alkali-rich side of the system under higher pressures. These observations suggest that the composition of the first batch of melts produced from all these systems (corresponding to the invariant point) are a function of depth of melting. The initial melts produced under hydrous conditions at shallow depths are more silica-rich and alkali-poor, whereas those formed at greater depths under dry conditions or in presence of CO_2 are more alkalic and silica-poor. These findings confirm Kuno's[10] observation that while the basalts generated at shallow depths are silica-saturated, those coming from greater depths are more alkalic and silica-poor.

Study on the kalsilite-forsterite-SiO_2 system under 28 kb showed that from certain compositions under dry conditions olivine appeared as the first crystalline phase, the same compositions yielded orthopyroxene or phlogopite under CO_2 or hydrous conditions, respectively. Thus the composition of the residual liquid is greatly controlled by the fluid phase in presence of which melting takes place.

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Precambrian Crustal Evolution in the Indian Subcontinent by R. K. Lal, *Department of Geology, Banaras Hindu University, Varanasi 221 005, India.*

The Southern Indian Shield which represents one of the classic terranes of the early crust, has been considered here as a model for the Precambrian crustal evolution in the Indian Sub-continent. The Shield consists of Precambrian rocks (3.8–0.57 billion years) and can be divided into three belts: (i) the Dharwar craton, (ii) the Southern granulite belt, and (iii) the Eastern Ghats belt.

(i) *Dharwar craton*: In the Dharwar craton the oldest rock identified till date is the tonalitic gneiss from Hassan, Karnataka (3.4 b.y.) which presumably formed the basement for the older supracrustals (more than 3.0 b.y. old). The older supracrustal rocks occur as narrow belts or enclaves within the Peninsular gneisses (3.2–3.0 b.y. old) and are characterized by metamorphosed shelf facies orthoquartzite-shale-carbonate association with variable amounts of mafic/ultramafic flows and intrusives e.g. the high-grade schists of the Sargur belt and the older greenstones of Holenarsipur, Nuggihalli, Hutti etc. The Peninsular gneisses and the older supracrustals have been affected by a high-grade upper amphibolite facies metamorphic event (M I) at about 3.0 b.y. ago. The Peninsular gneisses are overlained unconformably by the younger supracrustals (younger greenstones) represented by the Dharwar Supergroup (less than 3.0–2.6 b.y. old). The conglomerates at the base of the Dharwar Supergroup contain pebbles of the Peninsular gneisses (tonalitic gneiss, 3.2 b.y. old), folded banded iron-formation and fuchsite quartzites belonging to the older supracrustals. The Dharwar Supergroup includes shallow water platformal association of orthoquartzite, mafic/ultramafic flows, banded iron-formation and minor black shales (Bababudan Group and Kolar Group in the western and eastern Dharwar craton respectively, the latter predominantly of mafic flows) overlained unconformably by geosynclinal sequence of meta-greywacks and andesitic to basaltic meta-volcanics (Chitradurga Group). Closepet granites (2.6–2.4 b.y.), Chitradurga-Hyderabad-Karimnagar granites (2.6 b.y.) and dolerites (2 1–1.7 b.y.) are intrusives into the Dharwar Supergroup and the basement Peninsular gneisses. The whole sequence of the basement and supracrustals is affected by three-phases of deformations involving mainly horizontal compression and regional metamorphism (M II) during a second major tectonothermal event around 2.6/2.5 b.y. ago. The M II event displays prograde greenschist (425°C) to granulite (730°C) facies of metamorphism from the north to the south of the craton merging into the Southern granulite belt. Two baric types of metamorphism have been recognized demarcated by a prominent northerly trending thrust located a few kilometers west of the curvilinear Closepet granites: (a) low-medium pressure (3 kb in the greenschist facies to 6.5 kb in the granulite facies) andalusite-sillimanite type with cordierite and andalusite—bearing pelitic rocks in the Eastern Dharwar craton, and (b) medium-high pressure (5 kb in the greenschist to 7.6 kb in the granulite facies) kyanite-sillimanite type with kyanite and staurolite in the pelitic rocks in the Western Dharwar craton.

(ii) *Southern granulite belt*: This is essentially a high-grade charnockite-khondalite terrane constituted of granulite facies rocks. The khondalite suites are characterized by metamorphosed shallow water shelf facies orthoquartzite-shale-carbonate-evaporite association. The presence of minor amounts of mafic and ultramafic rocks distinguishes the khondalite suites from the older supracrustals of the Dharwar craton. The charnockites (also the older supracrustals of the Dharwar craton) are intruded by peridotite, gabbro and anorthosites that occur as dykes, sills, laccoliths and layered igneous complex. Preliminary radiometric age data of the khondalite (3.1 b.y.) from Kerala and widespread 2.6–2.5 b.y. ages of the charnockites are comparable respectively to age of the older supracrustals and the major M II event of the Dharwar craton.

Geothermobarometric estimates of the granulites suggest temperature of 730–800°C; and pressure of 6.0–6.5 kb (low to medium-pressure granulites and

6.6–9.3 kb (medium to high-pressure granulites). The two baric types are located respectively towards the south (also Arcot District of Tamil Nadu) and north of the Novil-Cauvery shear zone/lineament. Considering the average thickness of 35 km of the Precambrian crust preserved in the Southern Indian Shield at present, as revealed by the seismic and gravity data, the estimated pressure conditions of metamorphism during the M II episode suggest crustal thickness of 52 to 68 km in the Dharwar craton and Southern granulite belt during 2.6/2.5 b.y. age.

A third minor tectonothermal event of probably Proterozoic age is restricted to several major E–W and northerly trending shear zones/lineaments along which retrogression took place during the M III event.

(iii) *Eastern Ghats belt*: This belt displays low-grade greenstone belt (Nellore belt) towards the west grading into gneisses containing the Sargur types of high-grade enclaves of amphibolite facies (Nellore–Khammam belt, similar to the western Dharwar craton) and granulite belt towards the east. The whole sequence is thrusted over the Eastern Dharwar craton towards the west. Radiometric age data e.g. 3.1 b.y. of khondalite, 2.5 to 2.7 b.y. of khondalites and charnockites and 2.4 b.y. of intrusive granites correspond to the age of the older supracrustals (more than 3.0 b.y.), M II event (2.6/2.5 b.y.) of the Dharwar craton and the Southern granulite belt, and the age of the Closepet granite (2.6–2.4 b.y.) respectively. Besides this significantly younger ages, ranging between 2.1 and 1.0 b.y., have also been reported for the Eastern Ghats granulites. This presumably reflects resetting of the radiometric clock during the later thermal events due to several phases of igneous activity in this terrane viz granite (2.1–1.0 b.y.), anorthosite (1.4 b.y.), etc.

The different tectono-thermal events during the Precambrian crustal evolution in the Southern Indian Shield are summarized below:

(a) *4.6 to 3.4 b.y. events*: Frequent meteoritic impact, analogous to the Moon. Formation of differentiated ultramafic-mafic-anorthosite/tonalite crust. No evidence preserved possibly due to reworking during later superposed events.

(b) *3.4 to 3.0 b.y. events*: (i) Mantle plume/hot spot activity, down-sagging of the mafic/ultramafic crust in regions of descending currents, conversion of mafic/ultramafic crust to amphibolites and partial melting of the latter to form tonalitic intrusives rising to higher crustal levels as diapires. (ii) Development of basins, in regions of collapsed domes formed due to ascending currents, in which the older supracrustals viz greenstone belts of Holenarsipur, Nuggihalli, Hutti etc., Sargur belt, and Khondalite suites evolved in mainly ensimatic, partly ensimatic to sialic and essentially sialic environment respectively. (iii) Partial melting of the mafic/ultramafic basement of the older greenstones and simatic crust and emplacement of second generation of tonalite-trondhjemite diapirs (3.1 to 3.0 b.y.). Widespread tectonothermal event, deformation (probably mostly diapiric), migmatization and regional metamorphism (M I) with vertical zonation of greenschist to amphibolite facies with depth during 3.0 b.y. Uplift and complete erosion of the upper crustal level greenschist facies rocks, thus exposing high-grade amphibolite facies rocks of the older supracrustals and the Peninsular gneisses to the surface.

(c) *3.0 to 2.4 b.y. events*: Plate tectonics regime analogous to the Phanerozoic Circum-Pacific belts e.g. Andes Mountains. Formation of the younger greenstones in the marginal basins/back-arc basins on the sialic basement of the Peninsular gneisses with enclaves of the older supracrustals. Deformation due to horizontal compression, microcontinent–arc (arcs) collision, thrusting of the Eastern Dharwar block over the Western block, and regional metamorphism (M II, 2.6/2.5 b.y.) accompanied by widespread influx of CO_2 along the shears at deeper crustal level with development of vertical metamorphic zonation from greenschist to granulite facies with increase in depth. Late K-granites (granodiorite to granite) emplacement derived from partial melting of the thickened sialic crust (2.6 to 2.4 b.y.). Rapid uplift and erosion followed by tilting of the crustal rocks towards the north thus exposing the granodiorite representing the 'root' of the andesitic arc, two baric types of domains of the Dharwar craton of different crustal levels of regional metamorphism, and prograde increase in metamorphic grade (both *P* and *T*) from the greenschist to granulite facies from north to south in the Dharwar craton and the Southern granulite belt.

(d) *2.4 to 0.57 b.y. events (Proterozoic)*: Mainly reactivation of the crustal rocks formed between 3.4 and 2.4 b.y. ago. Hot-spot activity in the region towards the east of the Dharwar craton, development of faults with triple junction, abortive attempt in disrupting the Dharwar craton with possible formation of small mid-oceanic ridge, followed by subduction and obduction of the proto-oceanic

crust, latter possibly represented by ultramafic-mafic suites of the Sukinda towards the north of the Eastern Ghats, and collision of the two disrupted micro-continents followed by thrusting. Emplacement of granites (2.1 to 1.0 b.y.), anorthosite suites (1.4 b.y.) in the thickened crust in the Eastern microcontinent (Eastern Ghats) accompanied by reworking of the older crustal rocks formed during the 3.4 to 2.4 b.y. events as evident from relict and discordant radiometric age data. Simultaneously in the Western micro-continent (Eastern Dharwar craton) cratonic basin developed in which the Proterozoic rocks Cuddapah Group (about 1.6 to 1.0 b.y.) were deposited. The Godavary and Mahanadi rifts may represent failed rifts or aulacogenes in which sedimentation of the fresh water Gondawana rocks occurred during Phanerozoic.

The Southern granulite belt disrupted by several E–W trending shear zones/lineaments thus exposing granulites of the two baric types. Local retrogression of the charnockites to gneisses during the M III event (probably Proterozoic) along the Shear Zones.

The whole-rocks and mineral ages ranging between 0.9 to 0.4 b.y. possibly represent the Indian Oceanic cycle which affected the Southern granulites and the Eastern Ghats belts.

Photomovement of Cyanobacteria by Wilhelm Nultsch, *Botanisches Instituts, Fachbereich Biologie der Universität, Karl-v.-Frisch-Straße, D-3550 Marburg 1, FRG.*

The antecedents of the cyanobacteria (=cyanophyceae=blue-green algae) arose on earth about 2.3 billion years ago. Up to this time, the atmosphere was reducing i.e. free from molecular oxygen. The cyanobacteria, however, invented the oxygenic photosynthesis, in which water serves as electron and proton donor for CO_2-reduction. Since the second product of water splitting is molecular oxygen, the cyanobacteria are mainly responsible for the generation of an oxidizing atmosphere in the early history of life.

The development of an oxygen-rich atmosphere created two serious problems for the cyanobacteria themselves as for other organisms. On the one hand, the fixation of molecular hydrogen (N_2) necessary for protein synthesis is inhibited because of the high oxygen sensitivity of nitrogenase, the main enzyme

of N_2 fixation. On the other hand, energy-rich oxygen species such as singlet molecular oxygen ($^1O_2$), superoxide (O_2^-), hydrogen peroxide (H_2O_2) and the hydroxyl radical (OH) can be formed inside reactions of photosynthesis. As these oxygen species are aggressive and, in higher concentrations, cytotoxic, cells capable of oxygenic photosynthesis would be photodamaged or even photokilled in strong light, if no photoprotective mechanisms were developed. This photo-protection has been achieved in different ways: $^1O_2$ is quenched by carotenoids, and O_2^- is made innoxious by superoxide dismutase. At high fluence rates, however, these protective mechanisms may be insufficient for photosynthetic organisms which are adapted to low fluence rates. Therefore, motile forms of algae and cyanobacteria have developed photosensing systems coupled to the movement apparatus which enable them to avoid areas of bright light and to search out areas of those light conditions in the biotope which are favourable for photosynthesis but do not cause photodamage.

Two different types of photosensory motor responses were developed during the evolution in cyanobacteria as in many other organisms: Phototaxis which denotes the orientation of movement with respect to the light conditions and photophobic responses which are caused by sudden changes in the photon fluence rates. In addition, light can also influence the speed of movement. This phenomenon is called photokinesis.

Photokinesis

The photokinetic effect of light on cyanobacteria is mostly positive i.e. movement is accelerated or even caused by light. In this case, light serves as an energy source of movement. The energy is supplied either from the cyclic phosphorylation (Oscillatoriaceae, Nultsch 1970)[1] or from the pseudocyclic phosphorylation (Nostocaceae, Nultsch and Hellmann 1972)[2].

Phototaxis

Phototaxis i.e. a movement either toward the light source (positive) or away from it (negative), can either be brought about by a change of the autonomous rhythm of reversal on exposure to unilateral light or by an active steering mechanism.

The first type is realized in Phormidium and some other genera of the Oscillatoriaceae. The organisms

which rotate about their long axis during movement, display an alternative forward and backward movement without preferring any direction. Under unilateral illumination, movement toward the light source is prolonged, while movement away is shortened in those individuals which are in a more or less parallel position to the light beam. However, the trichomes are not able to change the movement direction actively.

In the Nostocaceae which do not rotate during gliding movement, such as *Anabaena variabilis*, both positive and negative phototaxis are the result of an active steering mechanism. Once a trichome is irradiated from the side, it bends toward the light source at low but away from it at high fluence rates. Only at the transition point from positive to negative phototaxis the trichomes display a random orientation. As a result even a population moves either toward the light source or away from it, or spreads circularly at the transition point[3].

The action spectra of positive phototaxis measured with *Ph. uncinatum* and *A. variabilis* show striking differences. In *Ph. uncinatum* near UV and visible light up to 640 nm are active. Although the strong effectiveness of light between 450 and 510 nm points to yellow pigments and the peak in the UV favours flavins being the photoreceptors, the maximum around 560 nm and the shoulder at 620 nm clearly indicate that the phycobiliproteins C-phycoerythrin and C-phycocyanin are involved in photoperception, while chlorophylla is not active as photoreceptor. Since red light above 640 nm is entirely ineffective[4].

In *A. variabilis*, which lacks C-phycoerythrin, the maximum in the phototactic action spectrum coincides with the absorption maximum of C-phycocyanin. Unlike *Ph. uncinatum*, even light absorbed by chlorophylla is active, as indicated by the red maximum around 675 nm and a small but significant peak at 440 nm. Thus, in *A. variabilis* the phototacically effective radiation is absorbed by the photosynthetic pigments with the exception of carotenoids. This is true also for negative phototaxis, but in addition light between 500 and 560 nm and above 700 nm causes negative phototaxis, indicating that another photoreceptor of unknown nature is also involved.

It appears that the trichomes make use of the so-called one instant mechanism to detect the spatial light absorption gradient between the irradiated and the shaded side. Since this gradient exists at any fluence rate, a second mechanism is necessary to recognize high and low fluence rates. Therefore, the

existence of a hypothetical sign reversal generator has been postulated which is under the control of a highly active oxygen species, probably singlet molecular oxygen $^1O_2$ which is produced in photosynthesis at high fluence rates[5]. This is confirmed by experiments with chemicals which quench $^1O_2$ and, hence, reverse the phototactic reaction sign from negative to positive at high fluence rates, such as sodium azide, imidazole, carotenoids and others. These findings can be interpreted from an ecological point of view: at low fluence rates the Anabaena trichomes move into illuminated areas, whereas at high fluence rates which cause photodamage they reverse the phototactic reaction sign to "negative" and this way withdraw from the surface and move into the soil.

Photo-phobic responses

In cyanobacteria, the photo-phobic response is simply a stop of movement which is normally followed by a resumption of movement in the opposite direction, irrespective of whether it is caused by a decrease (step-down) or an increase (step-up) of the fluence rate.

In Phormidium uncinatum and other Oscillatoriaceae it has been shown that the photo-phobically active radiation is absorbed by the photosynthetic pigments, though the effectiveness of blue light is far out of the proportion to its absorption by the Soret band of chlorophyll[6]. Therefore, it has been concluded[7] that photo-phobic responses are caused by a sudden change in the steady state of the photosynthetic electron transport.

Recently, similar results have been found for the Nostocaceae *A. variabilis* in so far as the action spectrum which indicates that even in this organism the photo-phobically active radiation is absorbed by the photosynthetic pigments and, hence, is coupled to the non-cyclic electron transport. Unlike Phormidium, however, the fluence rate response curve looks as a saturation curve rather than an optimum curve, i.e. only step down responses are observed. This points to a different mechanism of the photo-phobic responses of Anabaena as compared to Phormidium.

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Biological Implications of Soil Solarization by D. K. Arora, *Centre of Advanced Study in Botany, Banaras Hindu University, Varanasi 221 005, India.*

Soil solarization is a method of hydrothermal disinfestation accomplished by covering moist soil with transparent polyethylene films during summer. Effective solarization process depends on climatic factors (solar radiation and air-temperature; humidity and velocity), soil characteristics and polyethylene properties (e.g. transmissivity to short and long-wave atmospheric infrared radiation). By appropriate knowledge gained in the changes in microbial ecology of solarized soil and technology of application, "solarization" is the most suitable technique to control soilborne plant diseases, weeds, mites and insects.

Direct thermal effects are probably the major phenomenon implicated in the death of soilborne pathogens during the process of solarization. Besides pest control, soil solarization may cause: (a) shift in non-thermophillic microbial population, (b) physico-chemical properties of soil, and (c) increase in the activity of various resistant saprophytes and antagonistic microorganisms. In a solarized soil partial nullification of fungistasis and reduced viability of heat sensitive fungal propagules may occur. Such propagules may also consequently become more sensitive for parasitism and lysis by antagonistic microorganisms.

In a solarized soil, sub-lethal temperature (35–45° C) causes delay in germination of fungal spores, depending on the temperature and the duration of exposure. In general, less viable "heat stressed" propagules possess lower inoculum potential and shorter longevity. Solarized "heat stressed" microorganisms revealed some changes like inactivation of enzymes, phase changes in fatty acids and membrane components and slow turnover of heat sensitive protein.

The process of increased plant growth response (IGR) in solarized soil denotes the improvement in plant growth. The mechanisms for explaining IGR are either chemical (release of nutrients or growth factors; nullification of toxins) or biological (elimination of minor or unknown pathogens; stimulation of beneficial microorganisms).

"Solarization" technique may widely be used to eradicate several important soilborne diseases in summer in most of the eastern-central parts of India. Successful application of this technique will not only depend on effectiveness, but also on a competitive cost with conventional pesticides, and this technique has no long-term side effects. Further investigations are, therefore, needed to develop a cost-effective programme to use this novel technology for Indian farmers.

ANNOUNCEMENT

SEVENTH INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC) CONFERENCE ON ORGANIC SYNTHESIS

The seventh IUPAC Conference on Organic Synthesis will be held in Nancy during July 4 to 7, 1988. The meeting will consist of about eighteen lectures and poster sessions. About eighty of the posters will be selected for short oral presentations.

The following topics will be covered: 1. New reagents for organic synthesis, 2. Single electron transfer and radical chemistry in synthesis, 3. Asymmetric synthesis, 4. Automation and computer in synthesis.

Further particulars may be had from: Prof. P. Caubere, Chairman, IUPAC, Universite de Nancy I, Faculte des Sciences, B.P. 239, 54506 Vandoeuvre Les Nancy Cedex, France.