

## Indo-French workshop on weak intermolecular interactions\*

About 12 scientists from France and 18 from India participated in the Indo-French workshop on weak intermolecular interactions. This meeting brought together chemists, crystallographers, physicists, biologists and theoreticians for an in-depth discussion of weak hydrogen bonds and other intermolecular interactions in the static and dynamic context (see Box 1). The breadth of topics covered was wide: two sessions on crystal engineering and one each on the physics of intermolecular interactions, theoretical and computational aspects, inorganic systems and biological aspects. A unique feature of the workshop was that a 20-min lecture was followed by a 20-min discussion section. Any misgivings about this format vanished quickly, as the duration of the discussion always exceeded the allotted time. C. N. R. Rao (Bangalore) inaugurated the proceedings with his lecture on the self-assembly of complex and exotic open-framework inorganic materials. He argued that mesoscopic assembly of 1D and 2D arrays and 3D superlattices in metal nanocrystals is governed by the Aufbau principle.

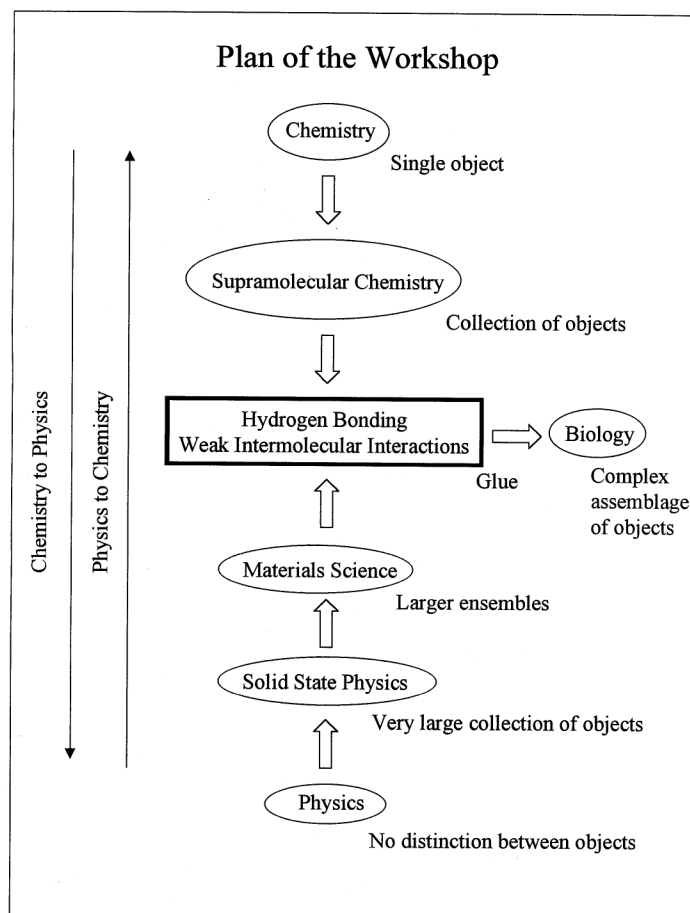
The first session on crystal engineering began with a lecture by G. R. Desiraju (Hyderabad) on the significance of multi-point recognition supramolecular synthons in solvates of gamboge pigments. M. W. Hosseini (Strasbourg) showed fascinating molecular networks assembled using programmed tectons and specific interaction patterns. A debate on the meaning of terms, tecton and synthon naturally followed: tecton is a molecule with potential hydrogen bonding sites in its periphery; synthon is an intermolecular interaction pattern constituted with functional groups and contains only parts of molecules. P. Ganguly (Pune) discussed the organization of

amphiphilic lipid molecules at the air-water interface and K. Boubekeur (Nantes) presented results on the dynamics of C-H...O interactions in trimethyl isocyanurate.

Physicists and computational chemists directed discussions in the next two sessions. J. Zyss (Paris) spoke about the new paradigm in nonlinear optics of multipolar engineering with 2D and 3D octupolar molecules. P. Levitz (Palaiseau) showed the effect of weak van der Waals interaction from the atomic to the mesoscopic scale. Molecular dynamics simulations on atomic argon at the solid-liquid transition temperature was presented by R. Ramaswamy (New Delhi) and the static and dynamics of cooperative phenomenon in neutral-ionic phase transitions was presented by H. Cailleau (Rennes). The presentation on exploring weak interactions based on topographical character-

istics of molecular electrostatic potential by S. R. Gadre (Pune) was followed by the lecture of E. Candell (Bellaterra, Spain; he has a French connection) on the relationship between crystal and electronic structure in BEDO-TTF salts. D. Mukherjee (Kolkata) proposed a method to treat inter-fragment interactions in the presence of valence fluctuations. B. Bagchi (Bangalore) spoke about dynamics of tagged water molecules and cesium ions at the aqueous micellar surface.

A half-day sightseeing of 400-year-old sites and monuments (including the famous Charminar) was appropriately followed by the special lecture of G. Tsoucaris (Paris) on the chemistry of cosmetic materials in ancient civilizations. From the Greco-Roman texts and powder X-ray diffraction pattern analysis at the Louvre Museum, it appears that laurionite (PbOHCl) and phosgenite



**Box 1.**

\*A report on the Indo-French workshop on 'Static and dynamic aspects of weak intermolecular interactions' held at Hyderabad from 17 to 21 February 2001, organized by G. R. Desiraju (Hyderabad) and P. Batail (Nantes) and sponsored by the Indo-French Centre for the Promotion of Advanced Research (CEFIPRA).



**Figure 1.** Cosmetics in ancient Egypt. Chemistry as a subject is a lot older than one might think and there is now definite evidence that the ancient Egyptians were proficient in synthetic techniques enabling them to make lead compounds which they then used for eye make-up (Courtesy: Prof. G. Tsoucaris, Louvre Museum, Paris).

( $\text{Pb}_2\text{Cl}_2\text{CO}_3$ ) were synthesized by the Egyptians using 'wet' chemistry as long ago as 2000 BC! These materials were used as eye make-up and their significance apparently went beyond the cosmetic to the religious context (see Figure 1).

The focus of the meeting returned to crystal engineering on the third day. The session was kicked-off by P. Batail (Nantes) with a discussion on the interplay of hydrogen bonding and redox state in EDT-TTF-amides. Interactions of halogens were discussed in the next two lectures: A. Nangia (Hyderabad) showed that the halogen $\cdots\pi$  synthon induces crystallization in polar, non-centrosymmetric space groups, while M. Fourmigué (Nantes) discussed the interplay of halogen and hydrogen bonding in TTF molecules. The discussion revolved around the theme: What

controls crystal packing—shape or interaction? R. Ziessel (Strasbourg) correlated ferromagnetic interactions in nitroxide radicals with C—H $\cdots$ O hydrogen bonds in their crystal structures. K. N. Ganesh (Pune) showed intricate hydrogen bond patterns in crystalline adducts of cyanuric acid and adenine derivatives.

In the session on inorganic systems, J. Gopalakrishnan (Bangalore) described  $d^0$  transition metal oxides with unique structures and properties and M. V. Rajasekaran (Hyderabad) spoke about weak interactions in copper and silver coordination complexes. G. Cerveau (Montpellier) presented examples of hydrolytic polycondensation materials from *bis*-trialkoxysilylated precursors. J. A. R. P. Sarma (Hyderabad) showed a Monte Carlo simulation film on the dynamics of aromatic guest in zeolite channel.

Macromolecular structures of nucleotides, proteins and enzymes are the most complex systems to study weak hydrogen bonds. M. A. Viswamitra (Bangalore) started the last session on biological aspects by highlighting the role of C—H $\cdots$ O and C—H $\cdots\pi$  interactions in stabilizing enzyme crystal structures. P. Chakrabarti (Kolkata) discussed the geometrical approaches of aromatic residues in protein complexes. C. Mioskowski (Illkirch) described a novel method for the fixation and crystallization of proteins on carbon nanotubes. B. Jayaram (New Delhi) has developed a computational atlas of free-energy contributions to binding in about 50 proteins that can be applied to study DNA–protein and drug–protein binding. B. Gopalakrishnan (Chandigarh) presented an overview on enthalpy–entropy balance in ligand–receptor interactions.

All in all, the atmosphere was lively and informal, the younger participants had an opportunity to make short presentations [V. R. Pedireddi, (Pune), G. U. Kulkarni and S. Natarajan (Bangalore)]. The discussion prompted all of us to think more seriously about the static and dynamic consequences of weak intermolecular interactions. The meeting succeeded in bringing together differing views on weak interactions and will foster stronger scientific collaboration between the two countries.

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