INSTITUTE COLLOQUIUM

INDIAN INSTITUTE OF SCIENCE

Prof. T.N. Guru Row

Solid State and Structural Chemistry Unit

will deliver a lecture

on

Intermolecular interactions, polymorphism and charge density in molecular crystals

on Monday, 10th October 2005
at 4.00 p.m. in the Faculty Hall

THE DIRECTOR
will preside.

All are cordially invited

Coffee/Tea: 5.00 p.m.
Venue: Reception Hall

ABSTRACT

X-ray diffraction has remained the mainstay of structure determination of crystalline solids and the recent developments in technology and computing have paved the way for unequivocal determination of macromolecular structures with remarkable accuracy. On the other hand, extremely fine features related to structures of small molecules, like for example mapping of charge densities, have allowed the results from high resolution X-ray data to be compared with highest levels of theory in chemistry. The understanding of the nature of a chemical bond, the features of hydrogen bonds and the validity of van der Waals interactions in crystalline substances are now becoming clear with the mapping of charge densities and evaluating the associated relevant parameters. Polymorphism, the ability of molecules to crystallize in more than one form has risen to prominence in applications related to drug development and design. Recently attempts to obtain the subtle differences in energy causing the crystallization of polymorphs in molecular crystals have been made in terms of plotting energy surfaces of molecules in different crystalline environments. Starting from the basic principles, I attempt to give an overview of the progress made in this area highlighting the contributions made by us in recent years.