



INSTITUTE COLLOQUIUM

INDIAN INSTITUTE OF SCIENCE
BANGALORE

PROFESSOR J CHANDRASEKHAR
DEPARTMENT OF ORGANIC CHEMISTRY

Will deliver a lecture

on

CHEMICAL INSIGHTS FROM COMPUTATIONAL STUDIES

on Friday, the 13th November, 1998

at 4.00 PM in the Faculty Hall

PROFESSOR GOVERDHAN MEHTA

Director, will preside

All are cordially invited.

Coffee : 5.00 PM
Reception Hall

Prof. S S KRISHNAMURTHY
Convener

ABSTRACT

The inter-relationships between structure, bonding, energetics, reactivity and molecular properties represent recurrent themes in Chemistry. Computational methods, in particular, empirical molecular modelling techniques, quantum chemical methods and numerical simulations, offer an efficient means of identifying, isolating and quantifying several interesting connections. Specific examples of the insights obtained through such studies will be presented. These include electronic effects, such as distonic stabilization and captodative effect in radical ions, through-space and through-bond interactions, and negative hyperconjugation. Several unusual structural predictions and interpretations of subtle reactivity patterns will then be discussed. Finally, the possibility of designing molecular systems with specific electrical, magnetic and optical properties will be explored.