

Preface

Spectroscopy of cold molecules, in particular *cold, isolated* molecules, has long been an interesting and powerful tool in the hands of chemists and physicists to understand many of the phenomena involving structure and bonding in molecules. The cold ambience provided in these experiments allows for only a few quantum states to be populated, thus relieving spectral congestion often seen at room and higher temperatures. In addition, it also allows for performing state selective chemistry and spectroscopy, which has led to many interesting experimental schemes. The low temperatures and chemically inert environment (achieved due to isolation) also allow weak intermolecular interactions to survive and be studied. We know today how important weak intermolecular interactions are in the context of biochemical and biophysical phenomenon; studies on cold, isolated molecules, therefore, need little justification or apology.

Studies on cold molecules have received a tremendous impetus due to the advances made in the field of theoretical chemistry. High-level *ab-initio* computations have come to the desktop of most experimentalists, who now use it to great advantage to corroborate their experimental findings, as some of the articles in this issue will demonstrate. The synergy between experiments and theory has driven research to new heights, as the article on molecular dynamics simulation by Prof. Haas from The Hebrew University of Jerusalem will highlight. This is a delightful review that discusses the various issues involved in the trapping of molecules in inert gas matrices.

There also exist a wide range of interesting games that researchers play using cold molecules. Cold, isolated gas phase experiments, using supersonic beams, are as popular as their condensed phase counterparts, using the technique of matrix isolation. Likewise, a range of detection schemes involving microwave, infrared, fluorescence, magnetic circular dichroism and photoelectrons are used, each probing different aspects of molecular properties. The articles in this issue serve to showcase this range of flavour. The work of Prof. Arunan's group, from the Indian Institute of Science, on Ar-(H₂S)₂ clusters uses microwave spectroscopy coupled to a supersonic beam to understand weak intermolecular interactions; studies which highlight the role of dispersive forces in chemistry. Using supersonic beams and fluorescence spectroscopy, Prof. Tapas Chakraborty's group from the Indian Institute of Technology (IIT), Kanpur, has presented its work on the adducts of acetic acid and fluorobenzoic, discussing both the structures and hydrogen-bonded interactions in this system. Prof. Sanjay's group at the Tata Institute of Fundamental Research (TIFR) has combined the supersonic beam technique with zero kinetic energy photoelectron spectroscopy (ZEKE) and to study the vibrational spectroscopy and ionization energies of hydroquinone. Magnetic circular dichroism has been used to study the SH radicals in inert gas matrices by Prof. Bryce Williamson and his group from the University of Canterbury, New Zealand; studies that are important as these and other related radicals are important intermediate species in tropospheric and combustion chemistry. Dr Viswanathan's group from the Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam, has studied triethyl phosphate using matrix isolation spectroscopy and has unraveled the conformational picture in this system, with possible directions to the study of tributyl phosphate, a molecule of great in-

terest to the nuclear industry. It cannot escape one's attention that every work presented in this issue highlights the synergy that exists between experiments and theory.

No compilation of such excellent research work will be possible without the ready and enthusiastic contributions from the various research groups, to all whom I am grateful. I must also thank the large number of reviewers who have meticulously gone through the manuscripts and made their critical and incisive comments.

With advances in experimental techniques and computational methods, coupled with the leaps that computing technology is making, we certainly look forward to this field rising to new heights and seeing new panoramas in the coming decades. This growth will be fueled not just by our scientific curiosity but also by the demands that modern biology and material science is making towards understanding systems at the molecular level.

Director,
Indira Gandhi Centre for Atomic Research,
Kalpakkam, India
e-mail: dmg@igcar.ernet.in; dir@igcar.ernet.in

(Baldev Raj)
Guest Editor