



REGIONAL CENTRE FOR BIOTECHNOLOGY

Seminar series

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## Application of Quantum Mechanics in Atmospheric Chemistry, and Radiation Chemistry of Biomolecules

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11:00 AM  
Seminar Room

The greenhouse gases (GHG) in the Earth's atmosphere play a central role in global warming. Carbon dioxide, methane, water and halocarbons are the main greenhouse gases. Some molecules are inherently more potent than others. For example, the global warming potential (GWP) of hydrofluorocarbon HFC-23 (CHF<sub>3</sub>) is 14800, i.e., it is almost fifteen thousand times more potent as a greenhouse gas compared to carbon dioxide, and the GWP of SF<sub>6</sub> is 22800. Halocarbons are in general extremely potent greenhouse gases. In this study we investigate the physical characteristics of greenhouse gases to understand the key molecular properties that govern their potency as global warming agents. We find that their molecular radiative efficiency - ability to absorb infrared radiation - is the most important factor. Long lifetime and concentration in the atmosphere also contribute. In our studies a molecular radiative efficiency, or effectiveness of absorption of IR radiation, was developed by means of systematic theoretical quantum mechanical calculations. The origin of large radiative efficiency and large IR absorption for several classes of molecules was traced to their large bond dipole derivatives. Polarity of the bonds inside the GHGs and unique position of these absorption bands in the electromagnetic spectrum are major contributing factors. Subsequently, we proposed a design strategy to screen the industrially used halocarbons. We investigated various classes of halocarbons, including hydrofluorocarbons, perfluorocarbons, fluoro-ethers, thioethers, and olefins, and we found significant differences in their infrared absorption abilities. Perfluoroethers are most intense absorbers followed by perfluorothioethers, sulfur fluorides and perfluorocarbons. Even within the same class of molecules, a strategic design can reduce the radiative efficiencies of fluorocarbons by a factor of two. Finally, we propose a group increment scheme for estimating molecular radiative efficiencies.

Towards the end I will talk about radiation-induced damage to biomolecules, specially damage to components of DNA and RNA. Biomolecular degradation has been reported to cause various diseases. Complete understanding of biochemistry of DNA damage will be obtained by exploring the processes of damage in full range of conditions, i.e. in isolated gas phase, in micro-solvated condition and in fully solvated condition to understand the role of solvation. Our research explores the physical chemistry of biomolecular degradation in the gas phase at the highest level using state-of-the-art ab initio quantum chemical methods. The role of local solvation in influencing excitation, ionization, dissociative attachment, and fate of excited states can then be understood well. Our effort will be invested in understanding the above-mentioned processes in both the gas phase and the solvated conditions.