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Atmospheric and environmental chemistry

Atmospheric chemistry is a branch of atmospheric science where major focus is the composition of the Earth's atmosphere. Knowledge of atmospheric composition is essential due to its interaction with (solar and terrestrial) radiation and interactions of atmospheric species (gaseous and particulate matter) with living organisms. Since atmospheric chemistry covers a vast range of topics, in this article (page 426) focus is on the chemistry of atmospheric aerosols with special emphasis to Indian region. Even though information on aerosol chemical composition over India is available from a few measurements as part of national field campaigns or as part of fixed sites, the database is not adequate to develop a comprehensive aerosol model for India. Scarcity of nationwide information on aerosol chemical composition, their vertical distribution demands a national effort in this direction. Establishment of a network of aerosol mass spectrometers nationwide is one option to address these issues and thereby carefully to answer crucial questions related to the role of aerosol chemistry on regional climate. No doubt, there is still a great degree of uncertainty about the role of aerosol chemistry on climate. Here, Sathesh presents a review of current state of knowledge of aerosol chemistry in India and propose future directions.

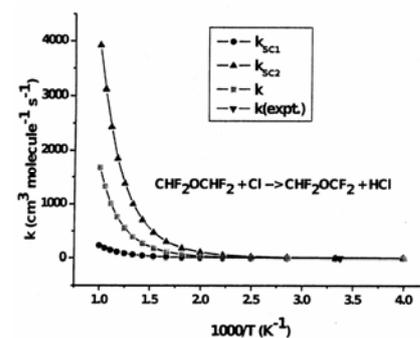
Atmospheric aerosols are important from a perspective of ambient air pollution and health to humans and other biological receptors as well as for potential effects on local weather and global climate. Ravi Krishna (page 440) attempts to

account for the different research efforts of academic research groups and regulatory agencies in India on the issue of atmospheric aerosols and their effects. The review highlights representative studies on the report of physical characterization (size), chemical composition (organic and inorganic), radiative forcing effects and health effects of ambient atmospheric aerosols. The review also presents a view of several studies reporting source apportionment studies identifying sources of aerosols and some focus on specific issues. The review also points out a significant need for more data with a greater spatial and temporal resolution for better understanding of the dynamics of atmospheric aerosols in the Indian context.

The diverse environmental problems faced today, such as stratospheric ozone depletion, photochemical smog, etc. emphasize the detrimental role of different chemical species released into the troposphere, as a result of intensified human activities. The environmental impact of various chemical species present in industrial and vehicular emission is influenced by their reactions with tropospheric oxidants (OH, Cl, O₃ and NO₃) along with other parameters such as solubility in water, photodissociation, etc. Hence, understanding and modelling their impact requires kinetic parameters of their reactions with these oxidants. Dhanya *et al.* (page 452) describes the experimental methods for measuring these parameters and highlight the importance of such measurements. Fluorocompounds (potential CFC alternatives) with long tropospheric lifetimes (days) and unsaturated/heterocyclic molecules with short tropospheric lifetimes (hours) are considered and

the atmospheric implications of the results are also discussed. The laboratory measurements provide the base for developing predictive structure–activity relationships and for validating theoretical methods for calculations of rate coefficients.

Theoretical studies are carried out on the mechanism, kinetics and thermochemistry of the gas-phase reactions between CHF₂OCHF₂ (HFE-134) and Cl atom using the high-level *ab initio* G2(MP2) and hybrid density functional model MPWB1K methods. As two conflicting experimental results are reported for this reaction, a detailed theoretical studies of the titled reaction was attempted. The hydrogen abstraction pathway for the reactions of the



two lower energy conformers of CHF₂OCHF₂ with Cl atom are studied and the rate constants are reported in a wide temperature range of 250–1000 K. The G2(MP2) calculated total rate constant value of $5.9 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 296 K is found to be in good agreement with the most recent experimental value of $(5.7 \pm 1.5) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at $296 \pm 1 \text{ K}$. The heats of formation for the CHF₂OCHF₂ molecule and CHF₂OCF₂ radical and the atmospheric lifetime of CHF₂OCHF₂ are also reported. See page 470.