DEPARTMENT OF CHEMISTRY, IIT MADRAS
Ph. D. Colloquium

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Venue: CB310

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Kinetics and mechanistic investigations on OH radicals, Cl atoms and CH_2OO initiated photo-oxidation reactions of saturated methyl alkyl esters, unsaturated fluorinated esters and carbonyl compounds under tropospheric pertinent conditions.

The theme of atmosphere chemistry emphasizes on the chemical configuration of the Earth's atmosphere and the underlying chemical and physical progressions regulating the sources and fortune of Oxygenated Volatile Organic compounds (OVOCs) emitted from the anthropogenic and biogenic sources. These emitted OVOCs play an important role in the formation of tropospheric ozone, Secondary Organic Aerosol (SOAs) and photochemical smog in the urban environments. These formed SOAs stimulates the climate by either absorbing or scattering solar radiation or by acting as cloud condensation nuclei (CCN), which affect the cloud precipitation. This affects the global climate change and leads to a negative impact on the plant growth, human and animal health.[1] The kinetics and mechanistic investigations on the reactions of the emitted OVOCs in the gas phase are of central importance to understand the impact of the anthropogenic emissions on air quality and global climate.

In the Earth's atmosphere, the photo-oxidation of OVOCs get initiated mainly by their reactions with atmospheric oxidants (such as OH radicals, Cl atoms and Criegee intermediate (CH_2OO)).[2] Based on this knowledge, the rate coefficients for the reactions of saturated methyl alkyl esters, unsaturated fluorinated alkyl esters were experimentally investigated using Relative rate technique coupled with Gas Chromatography/Flame Ionization detector (RR-GC-FID) in the temperature of 268-363 K and at 760 Torr of N_2/O_2 as bath gas. Furthermore, the product analysis for the degradation of the chosen compounds in the presence of O_2 were studied using Gas Chromatograph with Mass Spectrometry (GC-MS) and Gas Chromatograph with Infrared Spectroscopy (GC-IR). Moreover, to further understand the mechanistic pathways, computational calculations were performed using Canonical Variational Transition State theory in conjunction with Small Curvature Tunneling (CVT/SCT). To further understand the atmospheric fate of the chosen OVOCs, atmospheric lifetimes, Radiative Forcing (RF), Global Warming Potentials (GWPs) and Ozone Formation Potentials (OFPs) were estimated.

References

1. Mellouki, A., Wallington, T.J. and Chen, *Chemical reviews.* **2015**, *115*, 3984-4014.
2. Kaipara, R. and Rajakumar, B. *J. Phys Chem A.* **2018**, *122*, 8433-8445.

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