

DEPARTMENT OF CHEMISTRY, IIT MADRAS

Ph. D. Colloquium

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Photo-oxidation studies initiated by OH radicals and Cl atoms on halogenated hydrocarbons, formates, and acrylates in the conditions relevant to the Earth's atmosphere.

Investigating the chemistry of Volatile Organic Compounds (VOCs) which are released into the Earth's atmosphere via both natural and anthropogenic processes has gained interest in the last few decades. The VOCs released into the atmosphere will be removed by several processes like chemical processes, dry and wet deposition, vegetation, photolysis, deposition on bio-matters and clouds. These VOCs have been verified to play a vital role in the formation of Secondary Organic Aerosols (SOAs) and secondary pollutants such as photochemical smog, acid rain and fog, which inimically affects the atmospheric composition. The formed SOAs are harmful to health and can also act as cloud condensation nuclei affecting cloud properties as well as the hydrological cycle in the atmosphere.¹ The kinetics data and complete mechanistic studies on all the important atmospheric degradation pathways of individual compounds are essential components, in any attempts to reliably assess the possible contribution of these compounds to the severe photo chemical air pollution which is frequently experienced in urban and regional areas.

The rate coefficients for the reactions of OH radicals and Cl atoms with halogenated hydrocarbons, saturated esters, fluorinated and non-fluorinated acrylates were experimentally determined in gas phase by employing relative rate technique in the temperature range of 268 – 363 K and at atmospheric pressure of 760 Torr using N₂/O₂ as bath gas.²⁻³ The OH radicals and Cl atoms were generated by photolysis of hydrogen peroxide (H₂O₂) and oxalyl chloride ((COCl)₂) at 248 nm by KrF excimer laser. The analytical techniques used to measure the concentration of the involved species and qualitative analysis of the formed end-products are Gas Chromatograph equipped with a Flame Ionization Detector (GC-FID), Mass Spectrometry (GC-MS) and Infrared Spectroscopy (GC-IR). Further to complement our experimentally obtained results, computational calculations were performed using Canonical Variational Transition State theory with Small Curvature Tunneling (CVT/SCT). To understand the environmental implications of these molecules in the Earth's atmosphere, the cumulative atmospheric lifetimes, radiative forcing, Global Warming Potentials (GWPs) and Ozone Formation Potentials (OFPs) were estimated for the chosen systems.

References

1. Harley, R.A.; Cass, G.R. *Atmos. Environ.* **1995**, *29*, 905-922.
2. Vijayakumar, S.; Kumar, A.; Rajakumar, B. *New J. Chem.* **2017**, *41*, 14299-14314.
3. Kumar, A.; Rajakumar, B. *J. Phys Chem A* 2019, *123*, 723-741.

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