DEPARTMENT OF CHEMISTRY, IIT MADRAS

Ph. D. Colloquium

Name: PARTH GUPTA (CY15D037) Date: 19.11. 2019

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Atmospheric chemistry of Volatile Organic Compounds (VOCs) initiated by atmospheric oxidizers: Kinetic and mechanistic aspects

Most of the Volatile Organic Compounds (VOCs) and non-carbon chemical compounds have low concentrations in the Earth's atmosphere. The emission of these compounds has significant influence on various environmental processes and health-related issues of both humans and animals. Various physical and chemical processes comprise the impact of all the processes in the Earth's atmosphere.[1] The complex chemistry contributes towards the chemical composition of the Earth's atmosphere. Based on the reaction kinetics of VOCs with various oxidizing agents, the impact of these molecules on the Earth's atmosphere can be elucidated, based on their residence times (τ), Radiative efficiencies (REs), Global Warming Potentials (GWPs), Ozone Creation and Depletion Potentials (OCP and ODP) respectively.

Over the years, theoretical methodologies have paved the way to understand the mechanistic complexities as well as the determination of the effect of organics emission onto the atmosphere. Various atmospheric cleansing agents such as OH radicals, Cl atoms, Criegee intermediates (CH_2OO), $XO^{\bullet}$ and phenyl radicals play key roles in providing information about the effect on the tropospheric environment via VOC degradation. Distinct categories of molecules such as hydrofluoroolefins[2,3] (HFOs), esters, alkanes, alkenes, and aldehydes react with atmospheric oxidants to generate a variety of stable secondary organics. The bimolecular degradation mechanism leads to photochemical smog formation, stratospheric ozone depletion, and Secondary Organic Aerosol (SOA) formation, which can influence the global climate by absorbing or scattering UV-radiations. This causes the formation of carcinogenic and mutagenic agents, which leads to harmful effects on human, animal health and plant growth. The kinetics of the reactions initiated by these oxidizing agents were evaluated over a wide range of temperature, covering both the tropospheric as well as stratospheric regimes. The effect of temperature on the kinetics was investigated using the well-known kinetic theories such as Conventional Transition State Theory (CTST), Canonical Variational Transition-State Theory (CVT), and Rice-Ramsperger-Kassel-Marcus (RRKM) theories, in conjunction with distinct multi-dimensional tunneling corrections like Eckart unsymmetrical tunneling, Zero-Curvature and Small-Curvature tunneling respectively.

References

1. Ravishankara, A.R. *Chem. Rev.* **2003**, *103*, 4505-4507.
2. Gupta, P.; Rajakumar, B. *J. Fluor. Chem.* **2019**, *222-223*, 31-45.
3. Gupta, P.; Rajakumar, B. *ChemistrySelect* **2019**, *4*, 4827-4838.

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Signature of Guide

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