

Experimental and computational gas phase kinetic investigations on the chlorine atom initiated photo-oxidization reactions with a series of butenes

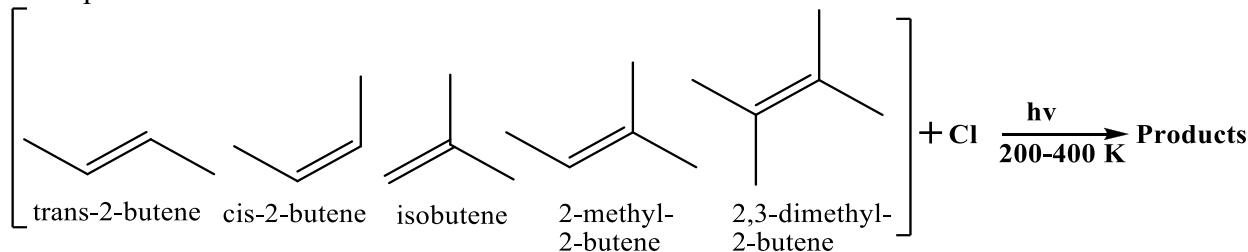
S. Vijayakumar and B. Rajakumar*

Department of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India.

*Address for correspondence: rajakumar@iitm.ac.in

Abstract:

The chemistry of unsaturated hydrocarbons plays an important role in troposphere as they contribute quite significant in the formation of Secondary Organic Aerosols (SOAs) ^[1]. Because of the presence of double bond and the dramatic variations in the energies of C-H bonds across the various reaction sites. Among them, C₄ stream is an important raw material to produce fuel additives and highly useful for the synthesis of heavy alkylates in petrochemical industry which are being released into the Earth's atmosphere. Therefore, it is essential to know the atmospheric life times and global warming potentials of these compounds in the Earth's atmosphere. These parameters can be estimated with the measured or computed kinetic parameters of their reactions with the oxidizing species such as OH radicals, Cl atoms, O₃ and NO₃ radicals in the Earth's atmosphere.



Temperature dependent rate coefficients for the chlorine atom reactions with trans-2-butene and isobutene were measured in our laboratory over the temperature range of 269-363K by using relative rate experimental technique with reference to isoprene and 1-pentene compounds, whose kinetic parameters for their reaction with Cl atoms are known [2,3]. To have deeper insight into the reaction mechanism and to complement our experimental results, theoretical calculations were performed for chlorine atom reactions with trans-2-butene, cis-2-butene, isobutene, 2-methyl-2-butene and 2,3-dimethyl-2-butene using canonical variational transition state theory (CVT/SCT) in combination with MP2/6-31G(d,p) level of theory. Rate coefficients, thermodynamic parameters and atmospheric implications will be discussed in detailed in the conference.

References:

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