Gas-Phase Kinetics and Atmospheric Implications of the Photo-oxidation Reactions of 2-methyl tetrahydrofuran with Cl atoms in the Troposphere

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Abstract

The ongoing use of fossil fuels has led to a substantial rise in atmospheric CO_2 levels, speeding up global warming and causing significant harm to the environment[1]. 2-methyl tetrahydrofuran shows great promise as a renewable energy source biofuel[1]. The relative-rate method was employed to measure temperature-dependent rate coefficients for the reactions between Cl atoms and 2-methyl tetrahydrofuran (MTHF) across the temperature span of 268-343 K under atmospheric pressure conditions. A KrF excimer laser operating at 248 nm was employed to photo-dissociate $(COCl)_2$, resulting in the generation of Cl atoms. A gas chromatograph coupled with a flame ionization detector (GC-FID) was utilized for quantitative analysis, while qualitative analysis was performed using a gas chromatograph connected to a mass spectrometer (GC-MS). The derived Arrhenius expression for the title reaction is represented by the equation $cm^3\,molecule^{-1}\,s^{-1}$. Alongside our experimental results, we conducted computational calculations using the CCSD(T)//BHandHLYP/6-31+G(d,p) level of theory to enhance and support our study. The rate coefficients were calculated for temperatures ranging from 250 to 400 K and at a pressure of 760 Torr using the canonical transition state theory (CTST). Under conditions of 298 K and 760 Torr with oxygen present, the sole product observed from the degradation of MTHF was 5-methyl-2,3-dihydrofuran. The calculated value for the photochemical ozone creation potential (POCP) of MTHF was approximately 56 and Cumulative lifetime () was found to be 4.93 hours (MBL condition) 10.40 hours (AMB condition) respectively.

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