Research Article

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Thermodynamics and kinetics of 1-fluoro-2-methoxypropane with Bromine monoxide radical ($BrO^{\bullet}$)

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ABSTRACT

CFCs containing volatile compounds are detrimental to atmospheric environment and to all living organisms. Their photodissociation reactions result to reasonable amount of Chlorine atoms formation in the stratospheric part of atmosphere.
In this work, an Insilco investigation was conducted on the thermochemistry, mechanism and kinetics of the Hydrogen abstraction reactions of partially fluorinated isopropyl methyl ether (1-fluoro-2-methoxypropane i.e. ($CH_2FCH(OCH_3)CH_3$)) with Bromine monoxide radical ($BrO^{\bullet}$) using the Density Functional Theory (DFT) based M06-2X/6-311++G^{**} strategy. To computationally refine the energy data, the single-point calculations (DFT/M06-2X/6-311++G(2df,2p) were immediately executed on the reacting species involved. The Monte Carlo search on the investigating $CH_2FCH(OCH_3)CH_3$ showed nine conformers with the global minimum configuration being studied.
The computed total theoretical rate of $7.95*10^{-11}$ M^{-1} sec^{-1} with atmospheric lifetime/global warming potential of $1.35*10^{-2}$ days/72.8 were also reported. The energy profile diagram of each reaction route with the $BrO^{\bullet}$ was sketched at absolute temperature of 298.15 K.

1. Introduction

The volatile organic compounds (VOCS) released into atmosphere often undergo primary degradation through oxidation with atmospheric radicals e.g. $^{\bullet}OH$, $ClO^{\bullet}$, $BrO^{\bullet}$, NO_3, $^{\bullet}OH_2$, RO_2 etc. [1-5]. Recently added knowledge by [6] on ozone chemistry revealed that aerosols: deodorant sprays, paint sprays, furniture polishes, refrigerators etc. cause environmental setback on ozone (O_3) due to usage of chlorofluorocarbons (CFCs) during their productions. They cause this environmental havoc by diffusing into O_3 layer and thus deplete it at a rate faster than it (ozone) can be replaced in the atmosphere [7-14]. For this reason, international warning and restrictions were placed on the application of CFCs as agreed upon in the Montreal Protocol [15-17]. Instead, alternative chemicals with zero or less posing ability on ozone were recommended as substantial substitutes for the CFCs [18-21]. Currently, oxygenated hydrofluoroethers (HFEs) [22], have been discovered as substantial substitutes for CFCs with numerous applications ranging from refrigerators, cleaning agents, propellants, painting, solvents, pesticides, varnishes in laboratories etc. [23-28]. The presence of $-O-$ linkage between these series increases their chemical reactivity in the atmosphere which account for the chemistry of their short lifetime and lesser atmospheric effects compared to CFCs [29-33].

An investigation of $CFH_2CH(OCH_3)CH_3$ with $BrO^{\bullet}$ radical is a vital atmospheric oxidation reaction that will helps in the provision of data regarding the tropospheric reactivity and degradation pathways of it in the atmosphere. Therefore, it is necessary to look into the atmospheric chemistry of it for proper understanding of this sample as a compound capable of replacing CFCs, and possibly estimate its atmospheric lifetime and global warming potentials.

Numerous wet laboratory studies investigated on the related study of this type only succeeded in providing

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