## Mechanism, kinetics, and environmental assessment of CTDE during OH-oxidation in the presence of NO and O2

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## Abstract

The transformation mechanism and kinetics of 2-chloro-1,1,2-trifluoroethyl-difluoromethyl-ether (CTDE, CHF2OCF2CHFCl) triggered by OH radicals were researched by DFT methods and canonical variational transition state theory. The computational rate constant including small-curvature tunneling correction was in commendable agreement with the experimental data. Two hydrogen abstraction channels to form the alkyl radicals of C·F2OCF2CHFCl and CHF2OCF2C·FCl were observed, and the formation of CHF2OCF2C·FCl was more favorable than C·F2OCF2CHFCl in kinetics and thermodynamics. Subsequent evolution of CHF2OCF2C·FCl in the presence of NO and O2 indicated that the organic nitrate (CHF2OCF2CONO2FCl) was the stable product. The dechlorinate of alkoxy radical (CHF2OCF2C(O·)FCl) was the most favorable degradation channel and the estimated ozone depletion potential for CTDE relative to CFC-11 was 0.0204, which could lead to a consequence of ozone depletion. Computed atmospheric lifetime for CTDE was 3.69 years by considering the combined contributions from OH radicals and Cl atoms. The total radiative forcing and global warming potential of CTDE were respectively 0.547 W m-2 ppbv and 628.58 (100 years) at 298 K, suggesting that the contribution of CTDE to the greenhouse effect is moderate.

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