Differences in OH Reactivity Between the (*E*)- and (*Z*)-Isomers of $CF_3CH=CHCF_3$

Munkhbayar Baasandorj,[1,2] A.R. Ravishankara,[1] and James B. Burkholder[1]*

[1] Earth System Research Laboratory, Chemical Sciences Division, National Oceanic and Atmospheric Administration, 325 Broadway, Boulder, CO, USA
[2] Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, CO, USA
* Corresponding author: James.B.Burkholder@noaa.gov

Unsaturated hydrofluorocarbons (hydrofluoroolefins, HFO) are currently being considered as potential replacements for hydrochlorofluorocarbons (HCFCs) and saturated-hydrofluorocarbons (HFCs) in various commercial applications. (*E*)- and (*Z*)- $CF_3CH=CHCF_3$ are replacement candidates but before used commercially their atmospheric fate and potential impacts on the environment need to be fully assessed. A significant atmospheric loss process for these compounds is expected to be their gas-phase reaction with the OH radical.

A study of the OH reaction kinetics of (*Z*)-$CF_3CH=CHCF_3$ was recently reported from our laboratory.[1] The reaction rate coefficient, *k*, has a non-Arrhenius behavior with a negative temperature dependence at temperatures <300 K. The rate coefficient for the OH + (*E*)-$CF_3CH=CHCF_3$ reaction was measured in this study using pulsed laser photolysis–laser induced fluorescence (PLP–LIF) and relative rate techniques. Rate coefficients were measured over a range of temperature (212 – 373) K and total pressure (20 – 600 Torr; He, N_2). The rate coefficient was found to be independent of pressure and showed Arrhenius behavior over the temperature range of the measurements. The profound differences in the reactivity of the (*E*)- and (*Z*)- isomers are discussed.

References

(1) Baasandorj, M; A.R. Ravishankara, and J. B. Burkholder, J. Phys. Chem. A 2012, 115, 10539-10549.