# Kinetic study on the reaction of $CF_3CH=CH_2$ with Cl atoms in a smog chamber

María Rosario Martín-Luengo,[1] Bernabé Ballesteros,[1,2*] Thomas M. Townsend,[2] Elena Jiménez,[2] and José Albaladejo[2*]

[1] Instituto de Combustión y Contaminación Atmosférica. Universidad de Castilla – La Mancha. Camino Moledores s/n, 13071 Ciudad Real. Spain.
[2] Departamento de Química Física. Facultad de Ciencias y Tecnologías Químicas. Universidad de Castilla – La Mancha. Avenida Camilo José Cela, s/n. 13071 Ciudad Real. Spain.
* Corresponding authors: Jose.Albaladejo@uclm.es, Bernabe.Ballesteros@uclm.es



Recognition of the adverse environmental impact of chlorofluorocarbons (CFCs) released into the atmosphere [1,2] has led to an international effort to replace these compounds with environmentally acceptable alternatives. Saturated hydrofluorocarbons (HFCs) have become widely used CFC replacements. Unsaturated hydrofluorocarbons are a class of compounds, which are potential replacements for CFCs and saturated HFCs in air conditioning units.
In this work, the rate coefficient, $k_{Cl}$, for the reaction of $CF_3CH=CH_2$ with Cl atoms at room temperature and 720 Torr of air is measured using a relative kinetic technique:

$$Cl + CF_3CH=CH_2 \rightarrow \text{Products} \qquad k_{Cl} \qquad (1)$$

Chlorine atoms are generated by UV photolysis of $Cl_2$ and the loss of $CF_3CH=CH_2$ and the reference compound (propene or 1,3-butadiene) and are monitored by both FTIR and GC-FID.
Two kinetic studies of reaction (1) were found in the literature. Sulbaek Andersen et al. [3] reported a relative rate coefficient of $(9.07 \pm 1.08) \times 10^{-11}$ $cm^3molecule^{-1}s^{-1}$ in 700 Torr of $N_2$ or $N_2/O_2$ at $296 \pm 1$ K. These authors also used FTIR spectroscopy as a detection technique. Takahashi et al. [4] employed the pulsed laser photolysis/ vacuum ultraviolet laser-induced fluorescence techniques to study the kinetics of reaction (1) at low pressure (9.1 Torr of $CF_4$) at 295±2 K. The absolute $k_{Cl}$ reported by Takahashi et al., $(4.49 \pm 0.64) \times 10^{-11}$ $cm^3molecule^{-1}s^{-1}$, was found to be half of that reported by Sulbaek Andersen et al. [3].
Additionally, in this work the products of the reaction are investigated by GC-MS and SPME. The atmospheric implications of the Cl reactivity are also discussed in terms of its lifetime and detected products.

**References**

(1) Molina, M.J., Rowland, F.S., *Nature* **1974**, 249, 810-812.
(2) Farman, J.D., Gardiner, B.G., Shanklin, J.D., *Nature* **1985**, 315, 207-210.
(3) Sulbaek Andersen, M.P., Nielsen, O.J., Toft, A., Nakayama, T., Matsumi, Y., Waterland, R.L., Buck, R.C., Hurley, M.D., Wallington, T.J., *J. Photochem. Photobiol. A: Chem.* **2005**, 176, 124-128.
(4) Takahashi, K., Iwasaki, E., Nakayama, T., Matsumi, Y., Wallington, T.J., *Int. J. Chem. Kinet.* **2007**, 39, 328-332.