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Atmos. Chem. Phys., 5, 2395-2402, 2005

www.atmos-chem-phys.net/5/2395/2005/

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Kinetic isotope effects in the gas phase reactions of OH and Cl with CH₃Cl, CD₃Cl, and ¹³CH₃Cl

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Abstract. The kinetic isotope effects in the reactions of CH₃Cl, ¹³CH₃Cl and CD₃Cl with OH radicals and Cl atoms were studied in relative rate experiments at 298±2 K and 1013±10 mbar. The reactions were carried out in a smog chamber using long path FTIR detection and the spectroscopic data analyzed employing a non-linear least squares spectral fitting method using measured high-resolution infrared spectra as well as absorption cross sections from the HITRAN database. The reaction rates of ¹³CH₃Cl and CD₃Cl with OH and Cl were determined relative to CH₃Cl as:

$$k_{\text{OH}+\text{CH}_3\text{Cl}}/k_{\text{OH}+\text{CH}_3\text{Cl}}/k_{\text{OH}+^{13}\text{CH}_3\text{Cl}}/k_{\text{OH}+^{13}\text{CH}_3\text{Cl}}=1.059\pm 0.008,$$

$$k_{\text{OH}+\text{CH}_3\text{Cl}}/k_{\text{OH}+\text{CH}_3\text{Cl}}/k_{\text{OH}+\text{CD}_3\text{Cl}}/k_{\text{OH}+\text{CD}_3\text{Cl}}=3.9\pm 0.4,$$

$$k_{\text{Cl}+\text{CH}_3\text{Cl}}/k_{\text{Cl}+\text{CH}_3\text{Cl}}/k_{\text{Cl}+^{13}\text{CH}_3\text{Cl}}/k_{\text{Cl}+^{13}\text{CH}_3\text{Cl}}=1.070\pm 0.010 \text{ and}$$

$$k_{\text{Cl}+\text{CH}_3\text{Cl}}/k_{\text{Cl}+\text{CH}_3\text{Cl}}/k_{\text{Cl}+\text{CD}_3\text{Cl}}/k_{\text{Cl}+\text{CD}_3\text{Cl}}=4.91\pm 0.07.$$

The uncertainties given are 2σ from the statistical analyses and do not include possible systematic errors. The unexpectedly large ¹³C kinetic isotope effect in the OH reaction of CH₃Cl has important implications for the global emission inventory of CH₃Cl.

[Final Revised Paper](#) (PDF, 1392 KB) [Supplement](#) (39 KB) [Discussion Paper](#) (ACPD)Citation: Gola, A. A., D'Anna, B., Feilberg, K. L., Sellevåg, S. R., Bache-Andreassen, L., and Nielsen, C. J.: Kinetic isotope effects in the gas phase reactions of OH and Cl with CH₃Cl, CD₃Cl, and ¹³CH₃Cl, Atmos. Chem. Phys., 5, 2395-2402, 2005. [Bibtex](#) [EndNote](#) [Reference Manager](#)[Search ACP](#)

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