

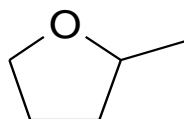
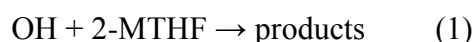
# Rate coefficient for the reaction of OH radical with 2-Methyltetrahydrofuran

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The growing criticism of the sustainability of the first generation biofuels has raised attention to the second generation (2G) biofuels. The cyclic ether 2-methyltetrahydrofuran, 2-MTHF, is one of the most promising renewable biomolecules. It can be produced from biomass with high yields, for example, through levulinic (LA) acid by using homogeneous and heterogeneous catalytic processes.

Some release of 2-MTHF into the atmosphere is inevitable during its use as a biofuel in transportation or as a solvent in organic synthesis. Thus, we strongly believe that it is of vital importance to make reliable assessment of the atmospheric chemistry and environmental impact of this renewable chemical before its widespread use, as it should be in the case of any other industrial chemicals, or alternative fuels proposed in recent years. Rate parameters for the reactions of OH with 2-MTHF are needed in a wide range of temperature and pressure for the development of predictive chemical kinetic models for combustion applications. Therefore, we have decided to carry out a detailed kinetic study of this reaction reporting here the first results obtained at room temperature.



2-methyltetrahydrofuran, 2-MTHF

The low pressure discharge flow (DF) method coupled with OH-resonance fluorescence detection (RF) has been applied to carry out the experiments. OH radicals were produced by the reaction  $\text{H} + \text{NO}_2 \rightarrow \text{OH} + \text{NO}$ , H atoms were generated by microwave-discharge dissociation of  $\text{H}_2$ . The experiments were performed under pseudo-first order condition in large excess of 2-MTHF over OH.

The following rate coefficient has been determined:  $k_1$  (300 K, 2.6 mbar He) =  $(1.18 \pm 0.16 (2\sigma)) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ .

To our knowledge, a single other rate coefficient has been published in the literature so far. Wallington et al. [1] have reported about two times higher rate coefficient determined also at room temperature. The study of these authors was performed at higher pressure (above 32 mbar) which might indicate a possible pressure dependence of the reaction. The pressure dependence would be possible if the pre-reaction complex reported by a theoretical study [2] could be stabilized by collisions. Survey experiments, using the relative-rate method have been underway to address the question of this possible pressure dependence.

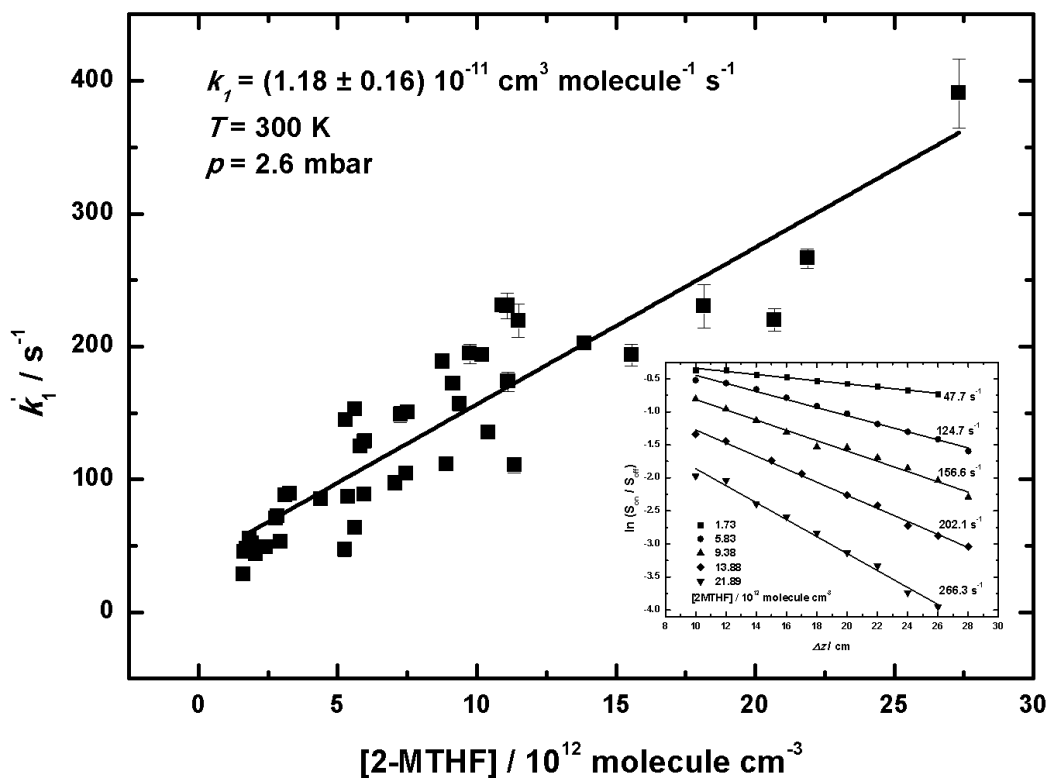


Fig.1. Plot of pseudo-first order rate coefficient against the 2-methyltetrahydrofuran concentration. The slope provides  $k_1$ . The figure in the inset shows typical semi-logarithmic OH decay plots.  $\Delta z$  is the length of the reaction zone,  $S_{on}$  and  $S_{off}$  are the RF signal strengths with 2-MTHF flow 'on' and 'off', respectively.

- [1] T. J. Wallington, W. O. Siegl, R. Liu, Z. Zhang, R. E. Hule, M. J. Kurylo, Environ. Sci. Technol., 1990, 24, 1596-1599.
- [2] J. M. Simmie, J. Phys. Chem. A, 2012, 116, 4528-4538.