IUPAC Subcommittee on Gas Kinetic Data Evaluation – Data Sheet CGI_17
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CH_3CHOO (*syn and anti*) + NO_2 → CH_3CHO + NO_3 (1)

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp /K	Reference	Technique/Comments
Absolute Rate Coefficients			
$(2.0 \pm 0.3) \times 10^{-12}$ *(syn)* $(3.1 \pm 1.1) \times 10^{-12}$ *(anti)*	298	Taatjes et al., 2013	PLP-PIMS(a)

Comments

(a) CH_3CHOO (acetaldehyde oxide) was produced by the reaction of CH_3CHI + O_2. CH_3CHI was generated by 248-nm laser photolysis of 1,1-diiodoethane, $CH_3CH_2I_2$, at 293 K and 4 torr, in a large excess of O_2. The reacting mixture was monitored by tunable synchrotron photoionization mass spectrometry, which allowed characterisation of the PIMS. Both conformers of CH_3CHOO (*syn*- and *anti*-) are produced, which could be distinguished by the difference in ionisation energy of the two conformers. The first order decay plots of *syn*- and *anti*-CH_3CHOO in the presence of excess known concentrations of NO_2 was used to determine the rate constants.

Preferred Values

Parameter	Value	T/K
k_{syn} /cm^3 molecule^{-1} s^{-1}	2 x 10^{-12}	298
k_{anti}/cm^3 molecule^{-1} s^{-1}	2 x 10^{-12}	298
Reliability		
$\Delta \log k_{syn}$	0.3	298
$\Delta \log k_{anti}$	0.3	298

Comments on Preferred Values

The only reported measurements on the overall reaction of *syn*- and *anti*-CH_3CHOO with NO_2 suffer from reduced signal-to-noise ratio compared to SO_2 but show a rate coefficient that is substantially smaller than that for CH_2OO reacting with NO_2, $k(CH_2OO + NO_2) = 7 \times 10^{-12}$ cm^3 s^{-1}. The cited values were given by unweighted fits of the data, with

uncertainty limits of 95%; returns from weighted fits gave *k* values lower by 30% but also indicated a slightly larger value for anti-conformer. However, the substantial difference between the weighted and unweighted fits may reflect some systematic inaccuracy. Although a small (statistically significant at 1σ level) conformer dependence was reported, the preferred recommendation is simply an overall $k(NO_2) = (2 \pm 1) \times 10^{-12}$ cm^3 $molecule^{-1}$ s^{-1}, for both conformers. The products of the reactions of Criegee intermediates with NO_2 are usually presumed to be NO_3 and a carbonyl compound (in this case CH_3CHO). however there are several possible association channels, not all of which may lead to NO_3 formation. Product studies are required

References

Taatjes, C. A. , Welz, C. A.; Eskola, A. J. , Savee, J. D. , Scheer, A. M., Shallcross, D. E., Rotavera, B., Lee, E. P. F., Dyke, J. M., Mok, D. K. W., Osborn, D. L. and Percival, C. J.: Science, 340, 171, 2013.