IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet oFOx76; VII.A1.5

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$HO + CF_3CH_2CF_2CH_3$ (HFC-365mfc) $\rightarrow CF_3CHCF_2CH_3 + H_2O$ (1)

$\rightarrow CF_3CH_2CF_2CH_2 + H_2O$ (2)

Rate coefficient data ($k = k_1 + k_2$)

k/cm^3 molecule^{-1} s^{-1}	T/K	Reference	Technique/ Comments
Absolute Rate Coefficients			
$1.68 \times 10^{-12} \exp[-(1585 \pm 80)/T]$	269-370	Mellouki et al. (1995)	PLP-LIF (a)
8.69×10^{-15}	298		
Relative Rate Coefficients			
$1.39 \times 10^{-12} \exp[-1651/T]$	278-323	Barry et al. (1997)	RR (b)
5.46×10^{-15}	298		

Comments

(a) HO radicals were produced by the 248 nm photolysis of H_2O_2. Experiments were performed in 100 Torr (133 mbar) of helium diluent.

(b) HO radicals were produced by the 254 nm photolysis of O_3 in the presence of H_2O. Experiments were performed in 1 bar of air diluent. Rate coefficient ratios were placed on an absolute basis using $k(OH+CH_3CCl_3) = 1.2 \times 10^{-12} \exp(-1440/T)$ cm^3 molecule^{-1} s^{-1} (Atkinson et al., 2006).

Preferred Values

Parameter	Value	T/K
k	7.1×10^{-15} cm^3 molecule^{-1} s^{-1}	298
k	$1.6 \times 10^{-12} \exp(-1620/T)$ cm^3 molecule^{-1} s^{-1}	270-380
Reliability		
$\Delta \log k$	0.2	298
$\Delta E/R$	$\pm$ 200	270-380

Comments on Preferred Values

The rate coefficient at 298 K reported in the absolute rate study by Mellouki et al. (1995) is approximately 60% greater than that measured in the relative rate study by Barry et al. (1997). A possible explanation for this discrepancy is the presence of reactive impurities in the sample used by Mellouki et al. (1995). This explanation should lead to an increasing discrepancy between the two studies with decreasing temperature, but no such trend is evident. The temperature dependencies of the rate coefficients reported in the two studies are in good agreement. There being no obvious reason to prefer either study we recommend an average of the k(298K) values and temperature dependencies from the two studies with the pre-exponential A factor chosen for consistency with the k(298K). As discussed by Barry et al. (1997) and Inoue et al. (2008), the OH radical initiated atmospheric oxidation of $CF_3CH_2CF_2CH_3$ is expected to lead to the formation of $CF_3CH_2CF_2CHO$ as the main primary product.

Oxidation of $CF_3CH_2CF_2CHO$ will generate CF_3CHO and COF_2 as secondary products. Oxidation of CF_3CHO will produce COF_2.

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 8, 4141, 2008.
Barry, J., Locke, G., Scollard, D., Sidebottom, H. W., Treacy, J., Clerbaux, C., Colin, R., and Franklin, J.: Int. J. Chem. 29, 607, 1997.
Inoue, Y., Kawasaki, M., Wallington, T. J., and Hurley M. D.: Chem. Phys. Lett., 462, 164, 2008.
Mellouki, A., Téton, S., and Le Bras, G.: Geophys. Res. Lett., 22, 389, 1995.