IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet RO_8

This data sheet updated: 12th June 2003.

$CH_3COCH_2O + O_2 \rightarrow CH_3COCHO + HO_2$ **(1)**

$CH_3COCH_2O + M \rightarrow CH_3CO + HCHO + M$ **(2)**

Rate coefficient data

$k_1 \cdot k_2^{-1}$/ cm^3 molecule^{-1}	Temp./K	Reference	Technique/ Comments
$k_1[O_2] << k_2$(1 bar, air)	298	Jenkin *et al*., 1993[1]	RR (a)
$k_1[O_2] << k_2$(1 bar, air)	298	Bridier *et al*., 1993[2]	RR (b)
$k_1[O_2] << k_2$(1 bar, O_2/N_2)	225-298	Orlando *et al*., 2000[3]	S-FTIR (c)

Comments

(a) Steady-state photolysis of Cl_2-CH_3COCH_3-O_2-N_2 mixtures at 930 mbar (700 Torr) with long-path FTIR and long-path UV visible diode array spectroscopy analyses of products. Data indicate that reaction (2) predominated over reaction (1) under the conditions of the experiments.

(b) Flash photolysis of Cl_2-CH_3COCH_3-air mixtures at 1 bar pressure with UV absorption monitoring of $CH_3COCH_2O_2$ radicals. Data indicate that reaction (2) predominated over reaction (1) under the conditions of the experiments.

(c) Mixtures of Cl_2/acetane/O_2 balanced to 1 atm with N_2 with and without NO_x were irradiated in a static chamber using a filtered . .. Xe-arc lamp. The diagnostic products CH_2O and methylglycerol ($CH_3C(O)CHO$) and others were monitored using in situ long pathlength FTIR absorption. The independence of CH_2O and $CH_3C(O)CHO$ yields on the O_2 partial pressure varied from 66 to 865 mbar was taken as an indication of the predominance of (2) over (1) across the entire temperature range 225-298 K, even at 1 atm of O_2: $k_2/k_1 = 1.5 \times 10^{20}$ and 1.0×10^{20} molecule cm^{-3} at 298 and225 K, respectively.

Preferred Values

No quantitative recommendations.

Comments on Preferred Values

Although the results listed above for the reactions of the CH_3COCH_2O radical are not quantitative, for the purposes of atmospheric modelling studies it is recommended that the above qualitative information on the ratios k_1/k_2 be used to decide if one or the other of the alkoxy radical reaction pathways predominates, or if both pathways should be considered. All three studies listed above point towards the predominance of the decomposition pathway under atmospheric conditions down to 225 K.

References

[1] M. E. Jenkin, R. A. Cox, M. Emrich, and G. K. Moortgat, J. Chem. Soc. Faraday Trans. **89**, 2983 (1993).

[2] I. Bridier, B. Veyret, R. Lesclaux, and M. E. Jenkin, J. Chem. Soc. Faraday Trans. **89**, 2993 (1993).

[3] J. Orlando, G. S. Tyndall, L. Vereecken, and J. Peeters, J. Phys. Chem. A **104**, 11578 (2000).