IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet CGI_8

This datasheet updated: May 2015; .

$CH_2OO + CH_3(CO)CH_3 \rightarrow$ products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp /K	Reference	Technique/Comments
Absolute Rate Coefficients			
(2.3±0.3) x 10^{-13}	293	Taatjes et al., 2012	PLP-PIMS(a)

Comments

(a) CH_2OO (formaldehyde oxide) was produced by the reaction of $CH_2I + O_2$. CH_2I was generated by 248-nm laser photolysis of diiodomethane, CH_2I_2, at 293 K and 4 Torr total pressure in a large excess of O_2. The reacting mixture was monitored by tunable synchrotron photoionization mass spectrometry, which allowed characterisation of the PIMS for CH_2OO and its reaction products over the region 9.5 – 11.5 eV, and time-resolved direct detection of CH_2OO at m/z = 46 amu. The first order decay CH_2OO in the presence of excess known concentrations of acetone was used to determine the rate constants. The uncertainty limits are 95%, based on unweighted linear fit of [$CH_3(CO)CH_3$] dependence of decay lifetimes. Secondary ozonide (3,3-dimethyl-1,2,4-trioxalane) was identified as a reaction product from its PIMS aided by quantum chemical calculations.

Preferred Values

Parameter	Value	T/K
k /cm^3 molecule^{-1} s^{-1}	2.3 x 10^{-13}	298
Reliability		
$\Delta \log k$	± 0.3	298

Comments on Preferred Values

The direct photoionization mass spectrometric detection of formaldehyde oxide (CH_2OO) as a product of the photolysis of CH_2I_2 in the presence of O_2 (Welz et al., 2012) has allowed detailed investigation of the kinetics of the Criegee intermediates. including the reaction: $CH_2OO + CH_3(CO)CH_3 \rightarrow$ products. The rate measurements appear to be precise and consistent with the emerging reactivity pattern for CH_2OO reactivity. The higher uncertainty reflects the single investigation.

References

Taatjes, C.A., Welz, O., Eskola, A.K., Savee, J. D., Osborn, D. L., Lee, E.P.F., Dyke, J.M., Mok, D.W.K., Shallcross, D. E., and Percival, C. J., Phys Chem.Chem.Phys., 14, 10391, 2012.