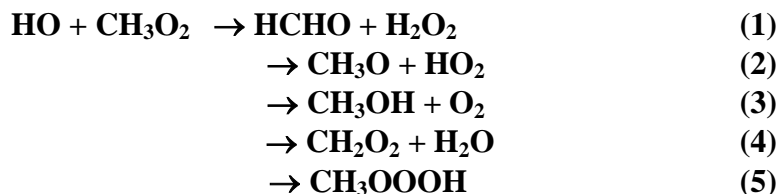


## Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HOx\_VOC95

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The citation for this data sheet is: IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, (<http://iupac.pole-ether.fr>), 2015

This datasheet last evaluated: November 2015; last change in preferred values: June 2015



$$\Delta H^\circ(1) = -291 \text{ kJ mole}^{-1}$$

$$\Delta H^\circ(2) = -13 \text{ kJ mole}^{-1}$$

$$\Delta H^\circ(3) = -248 \text{ kJ mole}^{-1}$$

### Rate coefficient data ( $k = k_1 + k_2 + k_3 + k_4$ )

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$(2.8 \pm 1.4) \times 10^{-10}$	294	Bossolasco et al., 2014	LP-LIF/CRD (a)

### Comments

- (a) HO was generated by the 248 nm photolysis of  $\text{H}_2\text{O}_2$  or  $\text{O}_3 / \text{H}_2\text{O}$ , and detected by LIF.  $\text{CH}_3\text{O}_2$  (excess reactant) was generated by the photolysis of  $\text{CH}_3\text{I}$  in the presence of  $\text{O}_2$  and detected by CW- CRDS. Bath gas was He and no pressure dependence (67 or 133 mbar) was observed.

### Preferred Values

#### Preferred Values

Parameter	Value	T/K
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$2 \times 10^{-10}$	298
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.3$	298

#### Comments on Preferred Values

There is only one experimental study of this reaction. The uncertainty in the rate constant reported by Bossolasco et al. (2014) stems mainly from uncertainty in the  $\text{CH}_3\text{O}_2$  cross section at  $7489 \text{ cm}^{-1}$  which was derived from an analysis of  $\text{CH}_3\text{O}_2$  self-reaction kinetics. The

authors assessed the role of I, IO and O(<sup>3</sup>P) reactions via numerical simulation using an assumed reaction scheme. The complexity of the chemical system used, significant divergence (factor three) in the literature values for the cross section of CH<sub>3</sub>O<sub>2</sub> at ~7489.16 cm<sup>-1</sup> and the fact that this is the only study to date, lead us to prefer a rate constant of  $2 \times 10^{-10}$  cm<sup>3</sup> molecule<sup>-1</sup> s<sup>-1</sup> with extended error limits. There are no published experimental data on the products of this reaction.

A theoretical study (Bian et al, 2015) indicates that CH<sub>3</sub>O and HO<sub>2</sub> (channel 2) are the favoured products on a singlet PES, with formation of CH<sub>2</sub>O<sub>2</sub> + H<sub>2</sub>O (channel 4) being formed via a triplet PES. In supplementary information to their calculations on CH<sub>2</sub>O<sub>2</sub> formation in a related chemical system, Nguyen et al (2015) present a potential energy surface and reaction mechanism that indicates that the trioxide (channel 5) is expected to be the dominant product under atmospheric conditions.

### References

- Bian, H., Zhang, S. G., and Zhang, H. M., *Int. J. Quantum Chem.*, 115, 1181-1186, 2015.  
Bossolasco, A., Farago, E. P., Schoemaeker, C., and Fittschen, C., *Chem. Phys. Lett.*, 593, 7-13, 2014.  
Nguyen, T. L., McCarthy, M. C., and Stanton, J. F., *J. Phys. Chem. A*, 119, 7197-7204, 2015.