

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet HO<sub>x</sub>\_VOC66

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### HO + CH<sub>3</sub>C(O)C(O)CH<sub>3</sub> → products

#### Rate coefficient data

<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	<i>T</i> /K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
(2.4 <sup>+0.8</sup> <sub>-0.6</sub> ) × 10 <sup>-13</sup>	298	Darnall et al., 1979	FP-RF (a)
(1.12 ± 0.65) × 10 <sup>-12</sup> exp[-(450 ± 90)/ <i>T</i> ]	240-440	Dagaut et al., 1988	FP-RF (b)
(2.3 ± 0.2) × 10 <sup>-13</sup>	298		

#### Comments

- (a) HO radicals were generated by the vacuum ultraviolet ( $\lambda \geq 105$  nm) photolysis of H<sub>2</sub>O and monitored as function of time under pseudo-first order conditions by resonance fluorescence.
- (b) HO radicals were generated by the vacuum ultraviolet ( $\lambda \geq 165$  nm) photolysis of H<sub>2</sub>O and monitored as function of time under pseudo-first order conditions by resonance fluorescence.

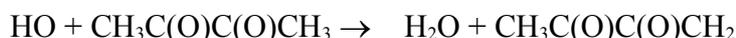
#### Preferred Values

Parameter	Value	<i>T</i> /K
<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	2.3 × 10 <sup>-13</sup>	298
<i>k</i> /cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup>	5.25 × 10 <sup>-13</sup> exp(-243/ <i>T</i> )	240-350
<i>Reliability</i>		
Δ log <i>k</i>	± 0.10	298
Δ <i>E</i> / <i>R</i>	± 50	

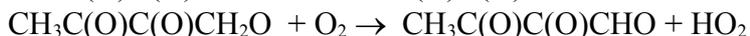
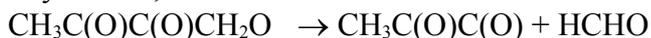
#### Comments on Preferred Values

The 298 K rate coefficient from the study of Darnall et al. (1979) is in excellent agreement with that of Dagaut et al. (1988). The combined data set of Darnall et al. at 298 K and those of Dagaut et al. below 350 K are used to derive the preferred values for the temperature dependence for atmospheric purposes.

The reaction of OH with 2,3-butanedione is assumed to proceed via H-atom abstraction from one of the methyl groups:



leading to a peroxy radical after reaction with O<sub>2</sub> which can at least partly react with NO to form an alkoxy radical, that can either dissociate or react with O<sub>2</sub>:



Christensen et al. (1998) have reported that the atmospheric fate of CH<sub>3</sub>C(O)C(O)CH<sub>2</sub>O formed from the Cl-initiated oxidation of 2,3-butanedione is decomposition to give HCHO, CO, and CH<sub>3</sub>C(O) radicals. Hence, it is expected that the products of the reaction of OH with 2,3-butanedione under atmospheric conditions are CH<sub>3</sub>C(O)O<sub>2</sub>, HCHO and CO.

### References

Christensen, L. K., Sehested, J., Nielsen, O. J., Wallington, T. J., Guschin, A., and Hurley, M.D.: J. Phys. Chem. A, 102, 8913, 1998.

Dagaut, P., Wallington, T. J., Liu, R., and Kurylo, M. J.: J. Phys. Chem. 92, 4375, 1988.

Darnall, K. R., Atkinson, R., and Pitts Jr., J. N.: J. Phys. Chem. 83, 1943, 1979.

