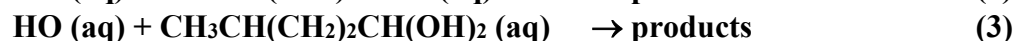
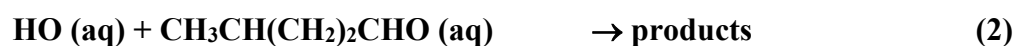


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_OH\_66

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This datasheet last evaluated: November 2019; last change in preferred values: June 2019



#### Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	T/K	pH	I / mol L <sup>-1</sup>	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
$3.0 \times 10^9$	294	2	-	Acero et al., 2001	Competition cinetics / HPLC (a)

The equilibrium constant for the hydration (1) is recommended as  $K_{298 \text{ K}} = 0.23$  by Doussin and Monod (2013).

$\Delta G_R^\circ$  (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data  $H_R^\circ$  (g) are not available.

#### Comments

(a) HO radicals were generated by addition of  $\text{O}_3$  ( $2 \times 10^{-5} \text{ M}$ ) to an aqueous  $\text{H}_2\text{O}_2$  (0.1 mM) solution; products analyzed by HPLC; Reference reaction:  $\text{HO} + \text{pCBA}$  with  $k(\text{HO} + \text{pCBA}) = 5 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$  (Buxton et al., 1988); the rate coefficient has been recalculated using the recommended value for the reference reaction  $k = 4.64 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$ ;  $c(2,2\text{-dimethylpropanal}) = 10^{-3} \text{ M}$ ,  $c(\text{pCBA}) = 10 \mu\text{M}$ ; Indigo method, as described by Bader and Hoigné (1981) was used for analyzing dissolved ozone; as no exact temperature is given,  $T = 294 \text{ K}$  is assumed for room temperature.

#### Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	$3.0 \times 10^9$	294
<i>Reliability</i> $\Delta \log k$	$\pm 0.15$	294

### *Comments on Preferred Values*

The rate coefficient determined by Acero et al. (2003) is the only one available so far. Therefore, it is suggested to follow this value. The uncertainty of this determination is estimated as  $\pm 33\%$  or  $\Delta \log k = 0.15$ . It should be noted that this rate coefficient refers to room temperature, which we estimate as  $T = 294 \text{ K}$ .

### **References**

- Acero, J. L., Haderlein, S. B., Schmidt, T. C., Suter, M. J. F. and von Gunten, U.: *Environ. Sci. Technol.*, 35(21), 4252-4259, 2001.
- Bader, H. and Hoigné, J.: *Water Res.*, 15(4), 449-456, 1981.
- Doussin, J. F., and Monod, A.: *Atmos. Chem. Phys.*, 13(23), 11625-11641, 2013.