

## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_OH\_47

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### HO (aq) + HO(CH<sub>2</sub>)<sub>5</sub>OH(aq) → products

#### 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>					
$3.6 \times 10^9$	294	9	-	Anbar et al., 1966	PR / UV-Vis (a)
$(4.2 \pm 0.7) \times 10^9$	298	7	-	Hoffmann et al., 2009	LF-LPA (b)
$1.38 \times 10^{11} \exp[-(1000 \pm 90)/T]$	278 - 318	7	-		LF-LPA (b1)

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

#### Comments

- (a) Reference reaction: HO + PNDA (p-nitrosodimethylaniline); reference rate constant was determined versus ethanol with  $k(\text{HO} + \text{ethanol}) = 1.10 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ ; recalculation of the rate coefficient was performed, using the selected value for the reference reaction ( $1.88 \times 10^9 \text{ M}^{-1} \text{ s}^{-1}$ ); no values given for initial concentrations; air saturated solutions; all experiments were repeated at least four times and the coefficient of variation was less than  $\pm 10\%$ ; as no temperature is given in their publication, for room temperature of  $T = 294 \text{ K}$  is assumed.
- (b) Radicals generated by laser flash photolysis of  $\text{H}_2\text{O}_2$  ( $c(\text{H}_2\text{O}_2) = 1 \times 10^{-4} \text{ M}$ ) at 248 nm (LF-LPA); Reference reaction: HO + SCN<sup>-</sup> with  $k(\text{HO} + \text{SCN}^-) = 1.24 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$  as reported by Chin and Wine (1992); the selected temperature dependence for the reference reaction by Zhu et al. (2003) was used for recalculation;  $c(\text{KSCN}) = 1.59 \times 10^{-5} \text{ M}$ . Arrhenius expression (b1) was calculated using the recalculated experimental data from Hoffmann et al. (2009).

#### Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	$4.10 \times 10^9$	298
$k / \text{L mol}^{-1} \text{s}^{-1}$	$1.47 \times 10^{11} \exp[-(1100)/T]$	278 – 318

### *Reliability*

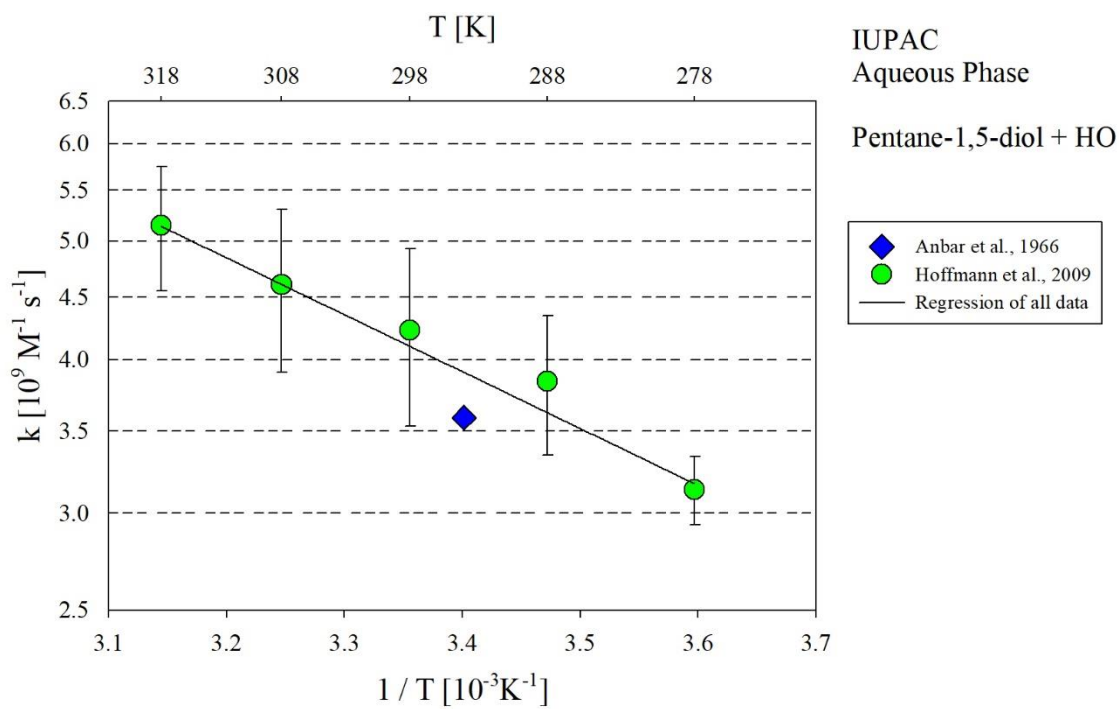
$\Delta \log k$	$\pm 0.15$	298
$\Delta E_A/R$	$\pm 150$	278 – 318

### *Comments on Preferred Values*

The available rate coefficient determined by Anbar et al. (1966) has been combined with the temperature dependent determination by Hoffmann et al. (2009). As the data agree well with each other within error limits, the result is the mean of them. The formerly recommended rate coefficient by Buxton et al. in 1988 ( $3.6 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ ) and Monod and Doussin in 2008 ( $3.81 \times 10^{10} \text{ M}^{-1} \text{ s}^{-1}$ ) are both slightly lower than the present recommendation after adjustment to the new reference rate constant by Zhou et al. (2003), but they still agree with it within error limits. The relative error of the recommended room temperature rate coefficient is estimated to be  $\pm 33\%$  or  $\Delta \log k = \pm 0.15$ .

### **References**

- Anbar, M., Meyerstein, D. and Neta, P.: *J. Chem. Soc. B*, 742-747, 1966.
- Buxton, G. V., Greenstock, C. L., Helman, W. P. and Ross, A. B.: *J. Phys. Chem. Ref. Data*, 12(2), 513 – 886, 1988.
- Hoffmann, D., Weigert, B., Barzaghi, P. and Herrmann, H.: *Phys. Chem. Chem. Phys.*, 11, 9351-9363, 2009.
- Kraljić, I. and Trumbore, C. N.: *J. Am. Chem. Soc.* 87(12), 2547-2550, 1965.
- Monod, A. and Doussin, J. F.: *Atmos. Environ.*, 42, 7611–7622, 2008.
- Zhu, L., Nicovich, J. M. and Wine, P. H.: *Aquat. Sci.*, 65(4), 425-435, 2003.



T-dependent rate constants for the reaction of pentane-1,5-diol with HO in aqueous solution. All available data have been used for regression.