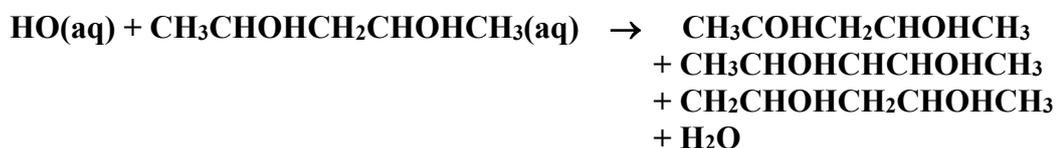


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_OH\_48

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



(Product distribution given by Ulanski et al. (1994))

#### Rate coefficient data

$k / \text{L mol}^{-1} \text{s}^{-1}$	$T/\text{K}$	$pH$	$I / \text{mol L}^{-1}$	Reference	Technique/ Comments
<i>Relative Rate Coefficients</i>					
$2.3 \times 10^9$	294	6.5	-	Ulanski et al., 1994	PR / UV-Vis (a)

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

#### Comments

- (a) The rate constant was determined to be  $2.3 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$  relative to  $k(\text{HO} + \text{SCN}^-) = 1.1 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$ ;  $c(\text{pentan-2,4-diol}) = 10^{-3} \text{ M}$ , the concentration of  $\text{SCN}^-$  varied from  $2.1 \times 10^{-5}$  to  $1.2 \times 10^{-4} \text{ M}$ , absorbance of  $\text{SCN}^-$  was measured at 480 nm. It was shown that a tertiary  $\alpha$ -hydroxyalkyl radical is formed with a yield of 74%; as no temperature is given, for room temperature  $T = 294 \text{ K}$  is assumed.

#### Preferred Values

Parameter	Value	$T/\text{K}$
$k / \text{L mol}^{-1} \text{s}^{-1}$	$2.3 \times 10^9$	294
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.15$	294

#### Comments on Preferred Values

The kinetic data by Ulanski et al. (1994) are the only available ones for the aqueous phase reaction of pentane-2,4-diol with the HO radical in aqueous solution. As the rate coefficient of

the reference reaction is identical to the recommended value, no recalculation was necessary. The uncertainty is estimated to  $\pm 33\%$  or  $\Delta \log k = 0.15$ . It should be noted that this rate coefficient refers to room temperature, which is estimated as  $T = 294 \text{ K}$

### References

Ulanski, P., Bothe, E., Rosiak, J. M. and von Sonntag, C.: *Macromol. Chem. Phys.*, 195, 1443–1461, 1994.