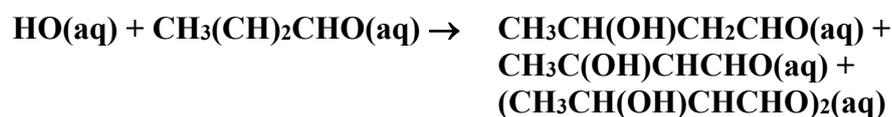


## IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

### – Data Sheet AQ\_OH\_72

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



(Product distribution taken from Lilie and Henglein, 1970)

#### 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>					
$5.8 \times 10^9$	294	-	-	Lilie and Henglein, 1970	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) HO radicals were generated by irradiation of N<sub>2</sub>O saturated solutions;  $c(\text{N}_2\text{O}) = 2.5 \times 10^{-2} \text{ M}$ , concentration of the carbonyl compounds was given as “some  $10^{-4}$  molar”, concentration of the compound radicals was calculated to be around  $10^{-5} \text{ M}$ ; Lilie and Henglein determined the rate constant to be  $3.5 \times 10^9 \text{ M}^{-1}\text{s}^{-1}$ , referring to the reference reaction  $\text{HO} + \text{SCN}^-$  with  $k(\text{HO} + \text{SCN}^-) = 6.6 \times 10^9 \text{ M}^{-1} \text{s}^{-1}$ ; the selected reference rate constant  $k = 1.10 \times 10^{10} \text{ M}^{-1}\text{s}^{-1}$  was used for recalculation; analysis was performed within a buffered pH range from 5 to 13; Lilie and Henglein determined, that 86% of the nonhydrated compound radical disproportionated to yield the enol and  $\beta$ -alcohol while the rest forms a dimer from radical recombination; as no exact temperature is given, T = 294 K is assumed for room temperature.

#### Preferred Values

Parameter	Value	T/K
$k / \text{L mol}^{-1} \text{s}^{-1}$	$5.8 \times 10^9$	294
<i>Reliability</i>		
$\Delta \log k$	$\pm 0.15$	294

### *Comments on Preferred Values*

The only available determination of the rate constant has been performed by Lilie and Henglein (1970). That value has been recalculated, using the newly recommended constant for the reference reaction. The error of this determination is estimated as  $\pm 33\%$  or  $\Delta \log k = 0.15$ . This rate coefficient refers to room temperature, which we estimate as  $T = 294 \text{ K}$ .

### **References**

Lilie, J. and Henglein, A.: Ber. Bunsen-Ges. Phys. Chem., 74(4), 388-393, 1970.