IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_81

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

**H2O + CH3CH2COCH3 (aq) → CH3CH2C(OH)2CH3 (aq) (1)**

**HO (aq) + CH3CH2COCH3 (aq) → CH3CHCOCH3 (aq) + H2O (2)**

*(product formation taken from Mezyk, 1994)*

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| 9.0  108 | 294 | 6-7 | - | Adams et al., 1965 | PR / UV-Vis (a) |
| (7.17 ±0.08)  108 | 297.4 | 5.2 | - | Mezyk, 1994 | PR / UV-Vis (b) |
| 4.77  1010 exp [- (1250 ±40)/T] | 275 - 340 | 5.2 | - |  | PR / UV-Vis (b) |
| (1.4 ±0.7)  109 | 298 | - | - | Gligorovski and Herrmann, 2004 | LP-LPA (c) |
| 3.0  1011 exp [- (1660 ±380)/T] | 278 - 348 | - | - |  | LP-LPA (c) |
| (8.1 ±0.8)  108 | 298 | 2 | - | Monod et al., 2005 | Dark Fenton / GC-FID (d) |
| 1.55  1010 exp [- (900 ±240)/T] | 276 - 339 | 2 | - |  | Dark Fenton / GC-FID (d1) |

The equilibrium constant for the hydration (1) has been estimated to be K298 K = 3.8 × 10-3 by Raventos-Duran et al. (2010).

*GR* (aq): Aqueous phase thermochemical data not available. As well, gas phase thermochemical data *R* (g) are not available.

**Comments**

(a) Reference reaction: HO + SCN- with *k*(HO + SCN-) = 6.6  109 M‑1s‑1; recalculation has been performed using the selected value for the reference reaction (1.10  1010 M‑1s‑1); no exact value is given for the initial concentrations of the reactants; as no exact temperature is given, for room temperature T = 294 K is assumed.

(b) Reference reaction: HO + SCN‑ with *k*(HO + SCN‑) = 1.22  1010 M‑1s‑1 according to Chin and Wine (1992); recalculation has been performed using the selected T dependence for the reference reaction by Zhu et al. (2003); experiments were performed in deoxygenated N2O / N2 saturated solutions

(c) Radicals generated by excimer laser flash photolysis of H2O2 at 248 nm; reactions were investigated by laser flash photolysis long path absorption relative to *k*(HO + SCN-) = 1.24  1010M‑1s‑1 as determined by Chin and Wine (1992); recalculation has been performed using the selected T dependence for the reference reaction by Zhu et al. (2003).

(d) Radicals generated by dark Fenton reaction, products analysed by GC-FID; Reference reactions:·HO + ethanol with ln *k*(T) = (24.2 ±0.4)-(830 ±140)/T (from data of Monod, 2005 and Ervens et al., 2003); HO + 1-propanol with ln *k*(T) = (24.5 ±0.6)-(780 ±200)/T (from data of Monod, 2005 and Ervans et al., 2003); HO + formaldehyde; *k*(T) = exp[-1020±90 (1/T)] (Chin and Wine, 1994); For the Fenton-reaction, the initial concentrations of reactants were in the order of 1  10-3M; Arrhenius expression (d1) is calculated from experimental data of Monod (2005), but given as: ln *k*(T) = (26.2±1.0) – [(1600±300)]/T in their work, resulting from the combined data of Monod (2005), Adams et al. (1965), Mezyk et al. (1994) and Gligorowski et al. (2009); no recalculation has been done on the T-dependent rate coefficients, as four out of seven determinations are given as mean values referring to two different reference reactions.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 9.77 × 108 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 2.35 × 1011 exp [-(1630)/T] | 274 - 348 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.24 | 298 |
| Δ EA/R | ±350 | 274 - 348 |
|  |  |  |

*Comments on Preferred Values*

Since the recommendation of Buxton et al. in 1988 with *k* = 9.0  108 M‑1s‑1, three temperature dependent determinations became available. As the publication by Monod (2005) does not provide information about the individually determined rate coefficients, a possible reevaluation of these values could not be performed. Therefore, this determination was not taken into consideration for the final regression. While the temperature dependent studies by Mezyk (1994) and Monod et al. (2005) are in good agreement with each other, the results of Gligorovski and Herrmann (2004) indicate a higher rate constant for the reaction. Therefore, the preferred room temperature rate coefficient is suggested to be slightly higher than in the publications mentioned before with an estimated uncertainty of ±50% or Δ log *k* = ±0.24.

**References**

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T-dependent rate constants for the reaction of 2-Butanone with HO in aqueous solution. Data from Adams et al. (1965), Mezyk (1994) and Gligorovski and Herrmann (2004) were used for the regression.