IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

 – Data Sheet AQ\_OH\_84

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**H2O + (CH3)2CHCH2COCH3 (aq) → (CH3)2CHCH2C(OH)2CH3 (aq) (1)**

**HO (aq) + (CH3)2CHCH2COCH3 (aq) → (CH3)2CHCHCOCH3 (aq)+ H2O (2)**

*(product formation taken from Gligorovski et al., 2009)*

**Rate coefficient data**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| k/ L mol-1 s-1 | T/K | pH | I/ mol L-1 | Reference | Technique/ Comments |
| *Relative Rate Coefficients* |
| (2.9 ±0.7)  109 | 298 | 2 | - | Monod et al., 2005 | Dark Fenton / GC-FID (a) |
| 1.25  1012 exp[-(1700 ±330/T)] | 276 - 339 | 2 | - |  | Dark Fenton / GC-FID (a) |
| (4.41 ±1.5)  109 | 298 | 6 – 7 | - | Gligorovski et al., 2009 | LFP-LPA (b) |
| 5.0  1011 exp[-(1380 ±580/T)] | 278 - 308 | 6 – 7 | - |  | LFP-LPA (b1) |

The hydration of methyl isobutyl ketone has not been discussed in the above references, as the influence of hydration of higher carbonyls is neglectable. Following the calculated data of Raventos-Duran (2010) for ketone compounds, it is suggested to assume a value of KH ~ 10-3.

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

**Comments**

(a) Reference reaction: HO + 2-propanol; *k*(HO + 2-propanol) = 1.6  109 exp[-(5000/R)(1/T – 1/298)] M‑1s‑1 (Elliot and Simsons, 1984); for the Fenton-reaction, the initial concentrations of reactants were in the order of 1  10-3M; Arrhenius expression for HO + MIBK was given as: ln *k*(T) = 25.6(±1.0) – [1200(±300)]/T; all rate coefficients have been recalculated using the selected T dependence for the reference reaction *k*(T) = 1.17 × 1011 exp[-(1180 ±200/T)].

(b) Reference reaction: HO + SCN-, with ln *k*(HO + SCN-) = (29.614±0.636) – (1900±190)/TM‑1 s‑1 (Chin and Wine, 1992); for the Arrhenius expression (b1), the T-dependent rate constants were taken from the plotted data, as no specific values were given; all rate coefficients have been recalculated using the selected T dependence for the reference reaction by Zhu et al., 2003.

**Preferred Values**

|  |  |  |
| --- | --- | --- |
| **Parameter** | **Value** | ***T*/K** |
|  |  |  |
| *k* / L mol-1 s-1 | 4.39 × 109 | 298 |
|  |  |  |
| *k* / L mol-1 s-1 | 4.05 × 1011 exp[-(1300)/T] | 276 - 339 |
|  |  |  |

*Reliability*

|  |  |  |
| --- | --- | --- |
| Δ log *k* | ±0.24 | 298 |
| Δ EA/R | ±350 | 276 - 339 |
|  |  |  |

*Comments on Preferred Values*

There are two temperature dependent determinations available for the reaction of MIBK with HO from Monod et al. (2005) and Gligorovski et al. (2009). Both have been used for regression to obtain the preferred values. While the determination of Gligorovski et al. (2009) indicates a slightly higher room temperature rate coefficient, the mean of both data sets results in an Arrhenius expression, that correlates with both their data within error limits. The estimated uncertainty is given as Δ log *k* = ±0.24 or ±50%.

**References**

Chin, M. and Wine, P. H: J. Photochem. Photobiol., A, 69(1), 17-25, 1992.

Elliot, A. J. and Simsons, A. S.: Radiat. Phys. Chem. (1977), 24(2), 229-231, 1984.

Gligorovski, S., Rousse, D., George, C. H. and Herrmann, H.: Int. J. Chem. Kinet., 41(5), 309-326, 2009.

Monod, A., Poulain, L., Grubert, S., Voisin, D. and Wortham, H.: Atmos. Env., 39(40), 7667-7688, 2005.

Raventos-Duran, T., Camredon, M., Valorso, R., Mouchel-Vallon, C. and Aumont, B.: Atmos. Chem. Phys., 10(16), 7643-7654, 2010.

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T-dependent rate constants for the reaction of 4-methylpentan-2-one with HO radicals in aqueous solution. All data given in the plot have been used for regression.