IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation

– Data Sheet AQ_OH_66

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

$H_2O + CH_3CH(CH_2)_2CHO\ (aq) \rightarrow CH_3CH(CH_2)_2CH(OH)_2\ (aq)$ (1)

$HO\ (aq) + CH_3CH(CH_2)_2CHO\ (aq) \rightarrow$ products (2)

$HO\ (aq) + CH_3CH(CH_2)_2CH(OH)_2\ (aq) \rightarrow$ products (3)

Rate coefficient data

k/ L mol^{-1} s^{-1}	T/K	pH	I/ mol L^{-1}	Reference	Technique/ Comments
Relative Rate Coefficients					
3.0×10^9	294	2	-	Acero et al., 2001	Competition cinetics / HPLC (a)

The equilibrium constant for the hydration (1) is recommended as $K_{298\,K} = 0.23$ by Doussin and Monod (2013).

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

Comments

(a) HO radicals were generated by addition of O_3 (2×10^{-5} M) to an aqueous H_2O_2 (0.1 mM) solution; products analyzed by HPLC; Reference reaction: HO + pCBA with k(HO + pCBA) = 5×10^9 M^{-1}s^{-1} (Buxton et al., 1988); the rate coefficient has been recalculated using the recommended value for the reference reaction $k = 4.64 \times 10^9$ M^{-1}s^{-1}; c(2,2-dimethylpropanal) = 10^{-3} M, c(pCBA) = 10 µM; Indigo method, as described by Bader and Hoigné (1981) was used for analyzing dissolved ozone; as no exact temperature is given, T = 294 K is assumed for room temperature.

Preferred Values

Parameter	Value	T/K
k / L mol^{-1} s^{-1}	3.0×10^9	294
Reliability		
$\Delta \log k$	±0.15	294

Comments on Preferred Values

The rate coefficient determined by Acero et al. (2003) is the only one available so far. Therefore, it is suggested to follow this value. The uncertainty of this determination is estimated as ±33% or $\Delta \log k = 0.15$. It should be noted that this rate coefficient refers to room temperature, which we estimate as T = 294 K.

References

Acero, J. L., Haderlein, S. B., Schmidt, T. C., Suter, M. J. F. and von Gunten, U.: Environ. Sci. Technol., 35(21), 4252-4259, 2001.

Bader, H. and Hoigné, J.: Water Res., 15(4), 449-456, 1981.

Doussin, J. F., and Monod, A.: Atmos. Chem. Phys., 13(23), 11625-11641, 2013.