HO + 1-C$_3$H$_7$ONO$_2$ → products

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
5.0 x 10^{-13} exp[(140 ± 144)/T]	298-368	Nielsen et al., 1991	PR-RA (a)
(8.2 ± 0.8) x 10^{-13}	298 ± 2		
Relative Rate Coefficients			
(7.2 ± 2.3) x 10^{-13}	303 ± 2	Kerr and Stocker, 1986	RR (b)
(5.8 ± 1.0) x 10^{-13}	298 ± 2	Atkinson and Aschmann, 1989	RR (c)
(7.0 ± 0.8) x 10^{-13}	298 ± 2	Nielsen et al., 1991	RR (d)

Comments

(a) Carried out in 1 bar Ar.

(b) HO radicals were generated by the photolysis of HONO-air mixtures at atmospheric pressure. The decay rates of 1-propyl nitrate and ethene (the reference organic) were measured by GC and rate coefficient ratio k(HO + 1-propyl nitrate)/k(HO + ethene) = 0.086 ± 0.027 is placed on an absolute basis by use of a rate coefficient of k(HO + ethene) = 8.32 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 303 K and atmospheric pressure of air (Atkinson, 1997).

(c) HO radicals were generated by the photolysis of CH$_3$ONO at ~1 bar air at >300 nm. Experiments were carried out in a 6400 liter Teflon chamber. The concentrations of 1-propyl nitrate and cyclohexane (the reference organic) were measured by GC, and irradiations in the absence of CH$_3$ONO allowed the photolysis of 1-propyl nitrate to be accurately taken into account in the data analysis. The measured rate coefficient ratio of k(HO + 1-propyl nitrate)/k(HO + cyclohexane) = 0.083 ± 0.013 is placed on an absolute basis by use of a rate coefficient of k(HO + cyclohexane) = 6.97 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson, 2003).

(d) HO radicals were generated from the photolysis of CH$_3$ONO in 1 bar air at >290 nm. The concentrations of 1-propyl nitrate and 2-methylpropane (the reference organic) were measured by GC. The measured rate coefficient ratio k(HO + 1-propyl nitrate)/k(HO + 2-methylpropane) is placed on an absolute basis by use of a rate coefficient of k(HO + 2-methylpropane) = 2.12 x 10^{-12} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson, 2003).

Preferred Values

k = 5.8 x 10^{-13} cm^3 molecule^{-1} s^{-1} at 298 K and 1 bar air.

Reliability

Δlog k = ± 0.3 at 298 K (1 bar).

Comments on Preferred Values

The absolute and relative rate coefficients of Kerr and Stocker (1986), Atkinson and Aschmann (1989) and Nielsen et al. (1991) are in reasonable agreement at room temperature. All studies have been carried out at ~1 bar pressure.

The absolute rate coefficient study of Talukdar et al. (1997) for the HO radical reactions with CH_3ONO_2 and $C_2H_5ONO_2$ is in serious disagreement (by a factor of 13-16 for CH_3ONO_2 and a factor of 2.3-2.9 for $C_2H_5ONO_2$) with the rate coefficients from the studies of Kerr and Stocker (19869 and Nielsen et al. (1991), while for $2\text{-}C_3H_7ONO_2$ the 298 K rate coefficients of Talukdar et al. (1997) and Atkinson and Aschmann (1989) disagree by 33% (suggesting for one that the discrepancies decrease as the reactivity of the alkyl nitrate increases). Accordingly, the 298 K rate coefficient of Atkinson and Aschmann (1989) is used for the preferred value, and no temperature dependence is recommended (note that by analogy with the reaction of the HO radical with 2-propyl nitrate (IUPAC, 2007), the temperature dependence of the rate coefficient is likely to be small). That 1-propyl nitrate is more reactive than 2-propyl nitrate is expected from structure-reactivity relationships (Atkinson and Aschmann, 1989) based on assuming that the reaction proceeds by H-atom abstraction, as concluded by Talukdar et al. (1997) for methyl nitrate, ethyl nitrate and 2-propyl nitrate.

References

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