This data sheet updated: 9th August 2002.

$HO_2 + HCHO \rightarrow HOCH_2OO$
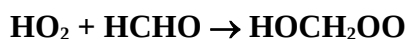
$\Delta H° = -68.1$ kJ·mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/ Comments
Absolute Rate Coefficients			
(1.1 ± 0.4) x 10^{-13}	273	Barnes *et al.*, 1985[1]	S-FTIR (a)
7.7 x 10^{-15} exp[(625 ± 550)/T]	275-333	Veyret *et al.*, 1989[2]	FP-AS (b)
(6.0 ± 0.7) x 10^{-14}	295		

Comments

(a) FTIR spectroscopic study in a 420 L reaction chamber. HO_2 radicals were generated from the thermal decomposition of HO_2NO_2 in the presence of HCHO, NO_2 and synthetic air at a total pressure of 530 mbar (400 Torr). The rate coefficient, k, was obtained from a computer simulation of the rates of decay of HCHO and rates of formation of HC(O)OH and $HOCH_2O_2NO_2$, based on a reaction scheme consisting of nine elementary reactions.

(b) Flash photolysis of Cl_2 in the presence of HCHO or CH_3OH and O_2 with long-path absorption measurements of HO_2 and $HOCH_2O_2$ radicals at total pressures of 110 mbar to 230 mbar (85 Torr to 170 Torr). The rate coefficient, k, was obtained from a computer simulation of the absorption profiles based on a mechanism of five elementary reactions.

Preferred Values

$k = 7.9$ x 10^{-14} cm^3 molecule^{-1} s^{-1} at 298 K.
$k = 9.7$ x 10^{-15} exp(625/T) cm^3 molecule^{-1} s^{-1} over the temperature range 275 K to 333 K.

Reliability
    Δlog $k = \pm0.3$ at 298 K.
    $\Delta(E/R) = \pm600$ K.

Comments on Preferred Values
    The studies of Barnes *et al.*[1] and of Veyret *et al.*[2] are in excellent agreement regarding this rate coefficient, and both are in good agreement with the earlier data of Veyret *et al.*[3] The preferred expression for the rate coefficient is derived by taking an average value of the rate coefficients of Barnes *et al.*[1] [k(273 K) = 1.1 x 10^{-13} cm^3 molecule^{-1} s^{-1}] and Veyret *et al.*[2] [k(275 K) = 8.0 x 10^{-14} cm^3 molecule^{-1} s^{-1}] together with the value of E/R determined by Veyret *et al.*[2]
    This reaction is believed to proceed via the initial formation of the adduct radical, HO_2CH_2O,

which rapidly isomerizes to the product radical, $HOCH_2OO$ via H-atom transfer.

References

[1] I. Barnes, K. H. Becker, E. H. Fink, A. Reimer, F. Zabel, and H. Niki, Chem. Phys. Lett. **115**, 1 (1985).

[2] B. Veyret, R. Lesclaux, M.-T. Rayez, J.-C. Rayez, R. A. Cox, and G. K. Moortgat, J. Phys. Chem. **93**, 2368 (1989).

[3] B. Veyret, J.-C. Rayez, and R. Lesclaux, J. Phys. Chem. **86**, 3424 (1982).