IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx45

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This data sheet last evaluated: June 2015; last change in preferred values: December 2007.

$HO + CCl_4 \rightarrow HOCl + CCl_3$

$\Delta H^o = 51.7$ kJ mol^{-1}

Rate coefficient data

k/cm^3 molecule^{-1} s^{-1}	Temp./K	Reference	Technique/Comments
Absolute Rate Coefficients			
$<4 \times 10^{-15}$	296 ± 2	Howard and Evenson, 1976	DF-LMR
$<1 \times 10^{-15}$	293	Clyne and Holt, 1979	DF-RF
Relative Rate Coefficients			
$<9 \times 10^{-17}$	298	Cox et al., 1976	RR (a)

Comments

(a) HO radicals were generated by the photolysis of HONO-air mixtures at 1013 mbar pressure. Relative rate coefficients were obtained from measurements of the rates of NO formation as a function of the HONO and organic concentrations. Based on the lack of effect of CCl_4 on NO formation and a rate coefficient for the reaction of HO radicals with CH_4 of 6.4×10^{-15} cm^3 molecule^{-1} s^{-1} at 298 K (Atkinson et al., 2006), the upper limit to the rate coefficient cited in the table is obtained.

Preferred Values

Parameter	Value	*T*/K
k /cm^3 molecule^{-1} s^{-1}	$<1 \times 10^{-19}$	298
k /cm^3 molecule^{-1} s^{-1}	$<1 \times 10^{-10} \exp(-6220/T)$	220-300

Comments on Preferred Values

The studies of Cox et al. (1976), Howard and Evenson (1976) and Clyne and Holt (1979) all observed no reaction of HO radicals with CCl_4. The preferred upper limit Arrhenius expression is obtained by equating the activation energy with the reaction endothermicity and assuming an Arrhenius pre-exponential factor of 1×10^{-10} cm^3 molecule^{-1} s^{-1}. The preferred upper limit Arrhenius expression is consistent with the experimental results of Cox et al. (1976), Howard and Evenson (1976) and Clyne and Holt (1979).

References

Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., and Troe, J.: Atmos. Chem. Phys., 6, 3625, 2006; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, http://iupac.pole-ether.fr

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