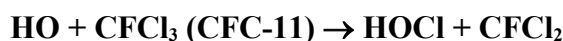


IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet oClOx44

Website: <http://iupac.pole-ether.fr>. See website for latest evaluated data. Data sheets can be downloaded for personal use only and must not be retransmitted or disseminated either electronically or in hardcopy without explicit written permission. The citation for this data sheet is: Atkinson, R., Baulch, D. L., Cox, R. A., Crowley, J. N., Hampson, R. F., Hynes, R. G., Jenkin, M. E., Rossi, M. J., Troe, J., and Wallington, T. J.: Atmos. Chem. Phys., 9, 4141, 2008; IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation, <http://iupac.pole-ether.fr>. This data sheet last evaluated: June 2015; last change in preferred values: December 2007.



$$\Delta H^\circ = 80.6 \text{ kJ mol}^{-1}$$

Rate coefficient data

$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	Temp./K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$<1 \times 10^{-15}$	296-424	Atkinson et al., 1975	FP-RF
$<5 \times 10^{-16}$	296 ± 2	Howard and Evenson, 1976	DF-LMR
$<5 \times 10^{-16}$	480	Chang and Kaufman, 1977	DF-RF
$<1 \times 10^{-15}$	293	Clyne and Holt, 1979	DF-RF
<i>Relative Rate Coefficients</i>			
$<4 \times 10^{-17}$	298	Cox et al., 1976	RR (a)

Comments

- (a) HO radicals were generated by the photolysis of HONO-air mixtures at 1.013 bar 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 CFCl_3 on NO formation and a rate coefficient for the reaction of HO radicals with CH_4 of $6.4 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ 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
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$<1 \times 10^{-24}$	298
$k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$<1 \times 10^{-10} \exp(-9695/T)$	220-480

Comments on Preferred Values

The studies of Atkinson et al. (1975), Cox et al. (1976), Howard and Evenson (1976), Chang and Kaufman (1977) and Clyne and Holt (1979) all observed no reaction of HO radicals with CFCl_3 . The preferred upper limit Arrhenius expression is obtained from an assumed Arrhenius pre-exponential factor of $1 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and equating the activation energy with the reaction endothermicity. The resulting upper limit Arrhenius expression yields upper limit rate coefficients at 298 K and 480 K which are consistent with the data of Atkinson et al. (1975), Cox et al. (1976), Howard and Evenson (1976), Chang and Kaufman (1977) and Clyne and Holt (1979).

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