

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet of FOx77; VII.A1.6

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This datasheet last evaluated: June 2015; last change in preferred values: June 2009.



Rate coefficient data (*k*)

<i>k</i> /cm ³ molecule ⁻¹ s ⁻¹	<i>T</i> /K	Reference	Technique/ Comments
<i>Absolute Rate Coefficients</i>			
$2.94 \times 10^{-12} \exp[-(1734 \pm 87)/T]$	260-365	Zhang et al. (1994)	FP-RF (a)
$(8.17 \pm 1.04) \times 10^{-15}$	296		
$(6.73 \pm 0.14) \times 10^{-15}$	296	Nelson et al. (1995)	DF-LIF (b)

Comments

- (a) HO radicals were produced by photolysis of H₂O using a xenon flash lamp at $\lambda > 165$ nm. Experiments were performed in 35 Torr (47 mbar) of argon diluent.
- (b) HO radicals were produced by the reaction of H atoms with NO₂. Experiments were performed in 2.0 Torr (2.7 mbar) of helium diluent.

Preferred Values

Parameter	Value	<i>T</i> /K
<i>k</i>	$7.8 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	298
<i>k</i>	$2.6 \times 10^{-12} \exp(-1734/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	260-370
<i>Reliability</i>		
$\Delta \log k$	0.10	298
$\Delta E/R$	± 300	260-370

Comments on Preferred Values

There is good agreement in the rate coefficients reported by Zhang et al. (1994) and Nelson et al. (1995) at 296 K. Adjusting these rate coefficients to 298 K using the temperature dependence reported by Zhang et al. (1994) and taking an average gives our recommended rate coefficient at 298 K. Taking the temperature dependence reported by Zhang et al. (1994) and choosing a pre-exponential A-factor to be consistent with the rate coefficient at 298 K gives the recommended Arrhenius expression.

References

- Nelson Jr., D.D., Zahniser, M.S, Kolb, C.E, and Magid, H.: J. Phys. Chem., 99 16301, 1995.
Zhang, Z., Padmaja, S., Saini, R.D., Huie, R.E., and Kurylo, M.J.: J. Phys. Chem., 98, 4312, 1994.

