Authors:

Astrid Bergeat and Kevin M. Hickson (Univ. Bordeaux, France)

$$N(^4S) + OH(X^2\Pi) \rightarrow H(^2S) + NO(X^2\Pi) \quad (1)\ \Delta H^o_{298}(1) = -201.59 \text{ kJ mol}^{-1}$$

$$\rightarrow O(^3P) + NH(X^3\Sigma^-) \quad (2)\ \Delta H^o_{298}(2) = +95.8 \text{ kJ mol}^{-1}$$

Thermodynamic Data from (Baulch *et al.*, 2005)

Rate Coefficient Data *k*

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
	50 – 294	Daranlot *et al.*, 2011	[2]
$k_1 = 2.0\times10^{-10}\ (T/298)^{-0.17}\times3/[4*(2+\exp(-205/T))]$	103 – 294	Smith and Stewart, 1994	[3]
$k_1 = (4.2\pm0.8)\times10^{-11}$	298	Brune *et al.*, 1983	[4]
$k_1 = (2.21\pm0.18)\times10^{-10}\ T^{-0.25\pm0.17}$	250 – 515	Howard and Smith, 1981	[5]
Theory			
	5 – 500	Daranlot *et al.*, 2012	[6]
	5 – 500	Li *et al.*, 2011	[7]
	5 – 500	Jorfi *et al.*, 2009	[8]
	5 – 500	Ge *et al.*, 2008	[9]
	5 – 515	Edvardsson *et al.*, 2006	[10]
	300 – 500	Chen *et al.*, 2003	[11]
$8.41\times10^{-12}\ T^{0.30}$	5 – 200	Cobos, 1995	[12]
Reviews and Evaluations			
$k_1 = 1.8\times10^{-10}\ T^{-0.2}$	100-2500	Baulch *et al.* 2005	[1]
Preferred value			
4.5×10^{-11}	100 – 500		

Comments

[1] Evaluation of literature data up to 1994. Recommendation mainly based on the two experimental temperature dependences.

[2] Experiments in a continuous supersonic flow reactor. N atoms were produced by microwave discharge upstream of the Laval nozzle OH radicals produced by pulsed laser photolysis of H_2O_2 and probed by laser-induced fluorescence.

[3] OH radicals produced by pulsed laser photolysis of HNO_3 and probed by laser-induced fluorescence. N atoms produced by microwave discharge and titrated by NO. Cryogenically cooled flow tube. Errors quoted as single standard deviations.

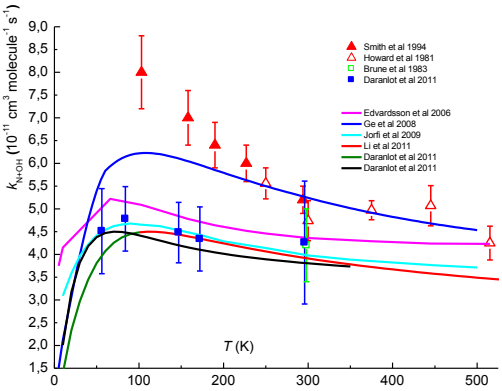
[4] OH radicals produced by the reaction F + H_2O and N atoms produced by microwave discharge. Radical concentrations were determined by a variety of techniques and titration: laser magnetic resonance, resonance fluorescence and resonance absorption.

[5] OH radicals produced by flash photolysis of H_2O and probed by resonance fluorescence with a lamp. N atoms produced by microwave discharge and titrated by NO in Ar. Cooled or heated flow tube. Cited uncertainties are 95% confidence limits.

[6] Calculations: (1) time-independent quantum mechanical (TIQM) method and J-shifting approach and (2) time-dependent quantum method (TDQM) including contributions from all angular momenta J on the high-quality potential energy surface (PES) of the a^3A'' state

(the lowest triplet electronic state of HNO) of Li *et al*. 2011.
[7] PES and all *J* TDQM calculations down to 100 K.
[8] Quasi-classical trajectory (QCT) calculations on an *ab initio* global PES X^3A'' of Guadagnini *et al*. 1995.
[9] TDQ wave packet (WP) method, on the same PES (Guadagnini *et al*. 1995) under both coupled-state or centrifugal sudden (CS) approximation and Coriolis-coupled or close-coupling (CC) approach.
[10] Calculations using the rotationally adiabatic capture centrifugal sudden approximation (ACCSA) in combination with *ab initio* electronic structure theory. For 103 K $\leq T$, $k_, = (4.03\pm0.02) \times 10^{-11}$ exp((25±1)/*T*) cm^3 $molecule^{-1}$ s^{-1}.
[11] Three-dimensional TDQWP calculations on the potential energy surface of Guadagnini *et al*. 1995.
[12] Statistical adiabatic channel model (SACM) on a PES based on ab initio quantum chemical data of Pauzat *et al.* 1993.

This atom-radical reaction has been studied up to 3000 K.



Preferred Values

Rate coefficient (10 – 300 K)
k (T) = 5×10^{-11} exp(-6/T) cm^3 $molecule^{-1}$ s^{-1}

Reliability
F_0 = 1.4 ; g = 7

Comments on Preferred Values

References

D. L. Baulch, C. T. Bowman, C. J. Cobos, R. A. Cox, T. Just, J. A. Kerr, M. J. Pilling, D. Stocker, J. Troe, W. Tsang, R. W. Walker, J. Warnatz, J. Phys. Chem. Ref. Data **34**, 757-1397 (2005).
J. Daranlot, M. Jorfi, C. Xie, A. Bergeat, M. Costes, P. Caubet, D. Xie, H. Guo, P. Honvault, K. M. Hickson, Science, 334, 1538-1541 (2011).
I. W. M. Smith, D. W. A. Stewart, J. Chem. Soc. Faraday Trans., **90**, 3221-3227 (1994).
W. H. Brune, J. J. Schwab, J. G. Anderson, J. Phys. Chem., **87**, 4503-4514 (1983).
M. J. Howard, I. W. M. Smith, J. Chem. Soc. Faraday Trans. 2, **77**, 997-1008 (1981).
A. Li, C. Xie, D. Xie, H. Guo, J. Chem. Phys. 134, 194309 (2011).
M. Jorfi, P. Honvault, P. Halvick, Chem. Phys. Lett., **471**, 65-70 (2009).
M.-H Ge, T.-S. Chu, K.-L. Han, J. Theor. Comput. Chem., **7**, 607-613 (2008).
D. Edvardsson, C. F. Williams, D. C. Clary, hem. Phys. Lett., 431, 261-266 (2006).
M.-D. Chen, B.-Y. Tang, K.-L. Han, N.-Q. Lou, J. Z. H. Zhang, J. Chem. Phys., **118**, 6852-6857 (2003).
C. J. Cobos, Int. J. Chem. Kinet., **27**, 219-233 (1995).
R. Guadagnini, G. C. Schatz, S. P. Walch, *J.* Chem. Phys., **102**, 784-791 (1995).
F. Pauzat, Y. Ellinger, G. Berthier, M. Gérin, Y. Viala, Chem. Phys., **174**, 71-79 (1993).
C. Morley, 18th Symp. (Int.) on Combust., 23-32 (1981).
A. Khachatrian, P. J. Dagdigian, J. Phys. Chem. A, **110**, 3388-3392 (2006).