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Rate Coefficient Data k

| $k / \text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ | T / K | Reference | Comments |
|---|------------------|-------------------------------|----------|
| <i>Rate Coefficient Measurements</i> | | | |
| $(2.8 \pm 0.1) \times 10^{11} (T/300)^{-0.40, 0.15}$ | 196 – 370 | Lee <i>et al.</i> , 1978 | [3] |
| $(2.2 \pm 0.2) \times 10^{11} \exp\{(160 \pm 50) / T\}$ | 213 – 369 | Wennberg <i>et al.</i> , 1994 | [4] |
| $(3.2 \pm 0.6) \times 10^{11} \exp\{(25 \pm 16) / T\}$ | 48 – 211 | Bergeat <i>et al.</i> , 2009 | [5] |
| <i>Theory</i> | | | |
| $3.4 \times 10^{11} \exp(-24.8 / T)$ | 100 – 1000 | Duff <i>et al.</i> , 1996 | [6] |
| | 10 – 500 | Jorfi <i>et al.</i> , 2009 | [7] |
| | 10 – 5000 | Gamallo <i>et al.</i> , 2010 | [8] |
| <i>Reviews and Evaluations</i> | | | |
| 3.5×10^{11} | 210 – 3700 | Baulch <i>et al.</i> , 2005 | [1] |
| $2.1 \times 10^{11} \exp(+100 / T)$ | all temperatures | JPL Publication, 2006 | [2] |
| $3.75 \times 10^{11} \exp(-26 / T)$ | 100 – 4000 | UMIST database, 2006 | |
| $3.0 \times 10^{11} (T/300)^{0.6}$ | all temperatures | OSU website, 2008 | |

Comments

There are numerous studies at room temperatures and at higher temperatures (up to 3660 K).

[1] Evaluation of literature data up to 1996. Recommendation mainly based on the temperature independence at high temperatures and the small one at low temperature, which is consistent within the fairly substantial scatter in the measurements.

[2] Based on the temperature dependence of Wennberg *et al.* 1994 and measurements of Lee *et al.* 1978

[3] Discharge flow-filtered resonance fluorescence (DF-RF) and flash photolysis-resonance fluorescence. However, N_2O photolysis is known to produce excited N atoms. The data obtained with this technique are thus not reported here and the other data (DF-RF) were corrected for axial diffusion and fitted by weighted least squares analysis.

[4] N atoms produced by microwave discharge of trace N_2 in He and monitored by

atomic resonance fluorescence using a gas filter scheme.

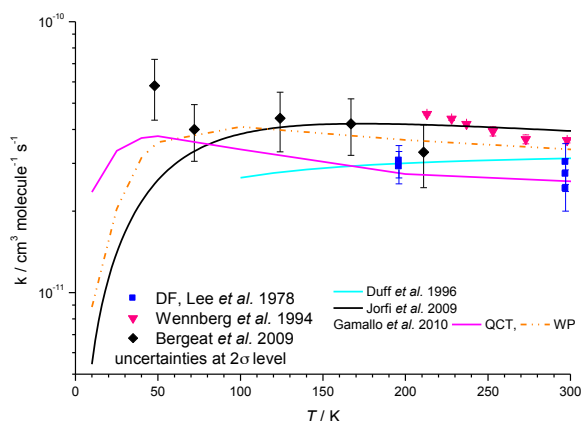
[5] Experiments in a continuous supersonic flow reactor. N atoms were produced by microwave discharge upstream of the Laval nozzle and were probed in the vacuum ultraviolet by resonance fluorescence.

[6] Quasiclassical trajectory calculations on the $^3\text{A}''$ surface of Walch *et al.* 1987 which presents a small energy barrier (in the uncertainty). The temperature dependence of the spin-orbit coupling effect was not taken into account.

[7] Time-independent quantum mechanical calculation with J -shifting approximation. Potential energy surfaces (PES) from Gamallo *et al.* 2010

[8] Time-dependent real wave-packet (WP) quantum dynamics rate constants on the $1^3\text{A}''$ and $1^3\text{A}'$ analytical PES and quasiclassical trajectory (QCT) method. The $^3\text{A}''$ PES is barrierless along the minimum energy path, while the analytical $^3\text{A}'$ excited PES presents an energy barrier of $36.57 \text{ kJ mol}^{-1}$, including zero point energy. The WP rate constant values

are in good agreement with the laboratory values.



Preferred Values

Rate coefficient (10 – 300 K)

$$k(T) = 4 \times 10^{-11} (T/300)^{-0.2} \exp(-20/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

Reliability

$$F_0 = 1.4 ; g = 10$$

Comments on Preferred Values

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