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$$N(^4S) + NO_2(X^2A_1) \rightarrow N_2(X^1\Sigma^+_g) + O_2(X^3\Sigma_g) \quad (1)$$
$$\rightarrow 2\ NO(X^2\Pi) \quad (2)$$
$$\rightarrow N_2O(^1\Sigma^+) + O(^3P) \quad (3)$$
$$\rightarrow N_2(X^1\Sigma^+_g) + 2\ O(^3P) \quad (4)$$

Thermodynamic Data from Baulch *et al.*[1]

$\Delta H^o_{298}(1) = -505.77$ kJ mol^{-1} $\Delta H^o_{298}(2) = -325.19$ kJ mol^{-1}

$\Delta H^o_{298}(3) = -174.56$ kJ mol^{-1} $\Delta H^o_{298}(4) = -7.45$ kJ mol^{-1}

Rate Coefficient Data

k / cm^3 molecule^{-1} s^{-1}	T / K	Reference	Comments
Rate Coefficient Measurements			
$\Sigma\ k = 5.8\times10^{-12}$ exp(+220/T)	213 – 369	Wennberg *et al.*, 1994[2]	(a)
$k_3 / \Sigma\ k = 100$ %			
Reviews and Evaluations			
$k = k_3 = 5.8\times10^{-12}$ exp(+220/T)	N/A	JPL Publication, 2006[3]	(*)

Comments

This atomic radical-molecule reaction has been mainly studied at room temperatures[4-7] and up to 700 K.[8]

(*) Evaluation of literature data up to 1994. Recommendation mainly based on the temperature dependence and product branching ratios of Wennberg *et al.*[2]

(a) Discharge flow of trace N_2 in He and resonance fluorescence using a gas filter scheme. Product branching ratio determination from comparison of atomic oxygen production of N + NO and N + NO_2. The atomic oxygen atom is the principal reaction product, in agreement with Clyne and McDermid.[6]

Preferred Values

$k_3(T) = 1.1\times10^{-11}$ cm^3 molecule^{-1} s^{-1}
in T=10-400K range
with $F_0 = 1.4$ and $g = 10$

Comments on Preferred Values

An *ab initio* study[9] of the potential energy surface of this reaction confirms that the reaction proceeds via an initial barrier-free addition process. The reaction leads mainly to O + N_2O, but the channel O_2 + N_2 is also energetically accessible. The N_2 + 2O channel should not occur (non-conservation of spin multiplicity).

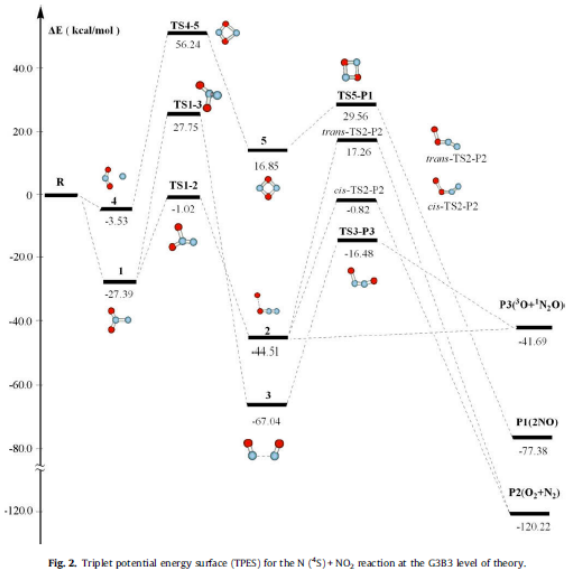
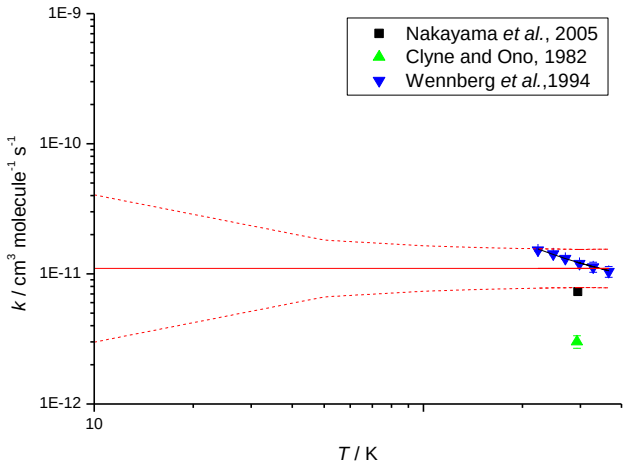


Fig. 2. Triplet potential energy surface (TPES) for the N (^{4}S) + NO_2 reaction at the G3B3 level of theory.

From Zuo et al, *Chem. Phys.* **2009**, *358*, 80-84.

The submerged barrier is known to produce negative temperature dependence at low temperature, in agreement with the experimental results of Wenberg *et al.*[2]

However, the extrapolation at 10 K of the small temperature dependence of Wennberg *et al.*[2] leads to a value not reasonable. Moreover, the preferred attack on the nitrogen atom of NO_2 should produce a bottleneck which thus could reduce the rate coefficient at low temperature: an average value of the experimental measurements is thus recommended (calculations at low temperatures might be worthwhile).



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