

Number	Reaction	$A$	$n$	$E$	Ref.
N1f	$O + N_2 \rightleftharpoons NO + N$	1.470E+13	0.30	315	[1]
N2f	$N + O_2 \rightleftharpoons NO + O$	6.400E+09	1.00	26.3	[1]
N3f	$N + OH \rightleftharpoons NO + H$	3.800E+13	0.00	0	[1]
N4f	$N_2 + CH \rightleftharpoons HCN + N$	4.400E+12	0.00	92	[1]
N5f	$HCN + O \rightleftharpoons NCO + H$	1.400E+06	2.10	25.6	[1]
N6f <sup>a</sup>	$NCO + M^{(102)} \rightleftharpoons N + CO + M^{(102)}$	3.100E+16	-0.50	201	[1]
N7f	$NCO + H \rightleftharpoons CO + NH$	5.000E+13	0.00	0	[1]
N8f	$NCO + O \rightleftharpoons NO + CO$	4.700E+13	0.00	0	[1]
N9f	$NCO + H_2 \rightleftharpoons HNCO + H$	7.600E+02	3.00	16.7	[1]
N100f	$HCCO + NO \rightleftharpoons HNCO + CO$	2.350E+13	0.00	0	[2]
N10f <sup>a</sup>	$HNCO + M^{(102)} \rightleftharpoons NH + CO + M^{(102)}$	1.100E+16	0.00	360	[1]
N11f	$HNCO + H \rightleftharpoons NH_2 + CO$	2.200E+07	1.70	15.9	[1]
N12f	$HNCO + O \rightleftharpoons NCO + OH$	2.200E+06	2.11	47.9	[1]
N13f	$HNCO + O \rightleftharpoons NH + CO_2$	9.600E+07	1.41	35.7	[1]
N14f	$HNCO + OH \rightleftharpoons NCO + H_2O$	6.400E+05	2.00	10.7	[1]
N15f	$CN + H_2 \rightleftharpoons HCN + H$	3.600E+08	1.55	12.6	[1]
N16f	$CN + H_2O \rightleftharpoons HCN + OH$	7.800E+12	0.00	31.2	[1]
N17f	$CN + OH \rightleftharpoons NCO + H$	4.200E+13	0.00	0	[1]
N18f	$CN + O_2 \rightleftharpoons NCO + O$	7.200E+12	0.00	-1.75	[1]
N19f	$NH + H \rightleftharpoons N + H_2$	1.000E+13	0.00	0	[1]
N20f	$NH + O \rightleftharpoons NO + H$	9.200E+13	0.00	0	[1]
N21f	$NH + OH \rightleftharpoons HNO + H$	4.000E+13	0.00	0	[1]
N22f	$NH + OH \rightleftharpoons N + H_2O$	5.000E+11	0.50	8.37	[1]
N23f	$NH + O_2 \rightleftharpoons HNO + O$	4.600E+05	2.00	27.2	[1]
N24f	$NH + NO \rightleftharpoons N_2O + H$	3.200E+14	-0.45	0	[1]
N25f	$NH + NO \rightleftharpoons N_2 + OH$	2.200E+13	-0.23	0	[1]
N26f	$NH_2 + H \rightleftharpoons NH + H_2$	4.000E+13	0.00	15.3	[1]
N27f	$NH_2 + O \rightleftharpoons HNO + H$	9.900E+14	-0.50	0	[1]
N28f	$NH_2 + OH \rightleftharpoons NH + H_2O$	4.000E+06	2.00	4.19	[1]
N29f	$NH_2 + NO \rightleftharpoons N_2 + H_2O$	2.000E+20	-2.60	3.87	[1]
N30f	$NH_2 + NO \rightleftharpoons N_2H + OH$	9.300E+11	0.00	0	[1]
N31f <sup>a</sup>	$NH_3 + M \rightleftharpoons NH_2 + H + M$	2.200E+16	0.00	391	[1]
N32f	$NH_3 + H \rightleftharpoons NH_2 + H_2$	6.400E+05	2.39	42.6	[1]
N33f	$NH_3 + O \rightleftharpoons NH_2 + OH$	9.400E+06	1.94	27.1	[1]
N34f	$NH_3 + OH \rightleftharpoons NH_2 + H_2O$	2.040E+06	2.04	2.37	[1]
N35f	$N_2H \rightleftharpoons N_2 + H$	1.000E+08	0.00	0	[1]

Number	Reaction	$A$	$n$	$E$	Ref.	
N36f	$\text{N}_2\text{H} + \text{H} \rightleftharpoons \text{N}_2 + \text{H}_2$	1.000E+14	0.00	0	[1]	
N37f	$\text{N}_2\text{H} + \text{O} \rightleftharpoons \text{N}_2\text{O} + \text{H}$	1.000E+14	0.00	0	[1]	
N38f	$\text{N}_2\text{H} + \text{OH} \rightleftharpoons \text{N}_2 + \text{H}_2\text{O}$	5.000E+13	0.00	0	[1]	
N39f <sup>a</sup>	$\text{HNO} + \text{M}^{(101)} \rightleftharpoons \text{H} + \text{NO} + \text{M}^{(101)}$	1.500E+16	0.00	204	[1]	
N40f	$\text{HNO} + \text{H} \rightleftharpoons \text{NO} + \text{H}_2$	4.400E+11	0.72	2.72	[1]	
N41f	$\text{HNO} + \text{OH} \rightleftharpoons \text{NO} + \text{H}_2\text{O}$	3.600E+13	0.00	0	[1]	
N42	$\text{NO} + \text{CH}_3 \rightarrow \text{HCN} + \text{H}_2\text{O}$	8.300E+11	0.00	67.3	[1]	
N43f	$\text{NO} + \text{T-CH}_2 \rightleftharpoons \text{HNCO} + \text{H}$	2.900E+12	0.00	-2.5	[1]	
N44f	$\text{NO} + \text{CH} \rightleftharpoons \text{HCN} + \text{O}$	1.100E+14	0.00	0	[1]	
N45f	$\text{N}_2\text{O} \rightleftharpoons \text{N}_2 + \text{O}$	$k_0$	2.000E+14	0.00	237	[1]
		$k_\infty$	8.000E+11	0.00	262	
N46f	$\text{N}_2\text{O} + \text{H} \rightleftharpoons \text{N}_2 + \text{OH}$	2.230E+14	0.00	70.1	[1]	
N47f	$\text{N}_2\text{O} + \text{O} \rightleftharpoons 2 \text{NO}$	2.900E+13	0.00	96.9	[1]	
N48f	$\text{N}_2\text{O} + \text{OH} \rightleftharpoons \text{N}_2 + \text{HO}_2$	2.000E+12	0.00	41.8	[1]	
N49f <sup>a</sup>	$\text{NO}_2 + \text{M} \rightleftharpoons \text{NO} + \text{O} + \text{M}$	1.000E+16	0.00	276	[1]	
N50f	$\text{NO} + \text{HO}_2 \rightleftharpoons \text{NO}_2 + \text{OH}$	2.100E+12	0.00	-2.01	[1]	
N51f	$\text{NO}_2 + \text{H} \rightleftharpoons \text{NO} + \text{OH}$	3.500E+14	0.00	6.28	[1]	
N52f	$\text{NO}_2 + \text{O} \rightleftharpoons \text{NO} + \text{O}_2$	1.000E+13	0.00	2.51	[1]	

Units are mol, cm<sup>3</sup>, kJ, K.

The backward rates for all reversible reactions can be calculated from thermodynamic data.

<sup>a</sup>Third-body efficiencies are:

$$[\text{M102}] = 1.5 [\text{N}_2] + 1.5 [\text{O}_2] + 18.6 [\text{H}_2\text{O}] + 1 [\text{other}].$$

$$[\text{M}] = 1 [\text{other}].$$

$$[\text{M101}] = 2 [\text{N}_2] + 2 [\text{O}_2] + 2 [\text{H}_2] + 10 [\text{H}_2\text{O}] + 1 [\text{other}].$$

<sup>b</sup>Pressure dependent reactions are described by the TROE-formulation [3]. The centering parameters are given by:

$$F_{c,N45f} = 1.$$

## References

- [1] J. C. Hewson and M. Bollig. Reduced mechanisms for NO<sub>x</sub> emissions from hydrocarbon diffusion flames. In *Twenty-Sixth Symposium (International) on Combustion*, pages 2171–2179, Pittsburgh, Pennsylvania, 1996. The Combustion Institute.
- [2] C. T. Bowman, R. K. Hanson, D. F. Davidson, Jr. W. C. Gardiner, V. Lissianski, G. P. Smith, D. M. Golden, M. Frenklach, and M. Goldenberg. Gri-mech 2.11. [http://www.me.berkeley.edu/gri\\_mech/](http://www.me.berkeley.edu/gri_mech/).

- [3] R. G. Gilbert, K. Luther, and J. Troe. Theory of thermal unimolecular reactions in the fall-off range. ii. weak collision rate constants. *Ber. Bunsenges. Phys. Chem.*, 87:169–177, 1983.