

c full N2/O2/H2O/CO2 model; March 1994

c symbol	energy	yinit	MolWt	StatWt	Csubv	ion_Z	Q_flag
e	0.00	0.	0	1.	1.5	-1	F
N2	0.00	0.79	28	1.	2.5	0	T
N2v	0.29	0.	28	1.	2.5	0	F
N2A	6.17	0.0	28	1.	2.5	0	T
N2a	8.40	0.0	28	1.	2.5	0	T
N2+	15.60	0.0	28	1.	2.5	+1	F
N4+	15.60	0.0	56	1.	2.5	+1	F
O2	0.00	0.21	32	1.	2.5	0	T
O2v	0.00	0.0	32	1.	2.5	0	F
O2a1D	0.98	0.0	32	1.	2.5	0	T
O2B1S	1.63	0.0	32	1.	2.5	0	T
O2+	12.06	0.0	32	1.	2.5	+1	F
O4+	12.06	0.0	64	1.	2.5	+1	F
O2-	-0.43	0.0	32	1.	2.5	-1	F
O	5.15	0.0	16	1.	1.5	0	T
O1D	7.30	0.0	16	1.	1.5	0	F
O1S	9.10	0.0	16	1.	1.5	0	F
O+	13.66	0.0	16	1.	1.5	+1	F
O-	3.70	0.0	16	1.	1.5	-1	F
O3	1.51	0.0	48	1.	2.5	0	T
O3-	-0.60	0.0	48	1.	2.5	-1	F
O3+	14.31	0.0	48	1.	2.5	+1	F
O4-	0.	0.0	64	1.	2.5	-1	F
N	9.75	0.0	14	1.	1.5	0	F
NO	0.93	0.0	30	1.	2.5	0	F
NO+	9.28	0.0	30	1.	2.5	+1	F
NO-	0.91	0.0	30	1.	2.5	-1	F
NO2	0.37	0.0	46	1.	2.5	0	F
NO2-	-2.10	0.0	46	1.	2.5	-1	F
NO3	0.74	0.0	62	1.	2.5	0	F
NO3-	-2.00	0.0	62	1.	2.5	-1	F
N2O	0.88	0.0	44	1.	2.5	0	T
N2O3	0.86	0.0	76	1.	2.5	0	F
H2O	-2.51	0.025	18	1.	2.5	0	T
H	4.48	0.0	1	1.	1.5	0	F
H-	1.49	0.0	1	1.	1.5	-1	F
OH	5.12	0.0	17	1.	2.5	0	F
OH-	-1.43	0.0	17	1.	2.5	-1	F
H2	0.00	0.0	2	1.	2.5	0	F
H2O+	12.62	0.0	18	1.	2.5	+1	F
H3O+	4.80	0.0	19	1.	2.5	+1	F
OH+	12.94	0.0	17	1.	2.5	+1	F
HO2	0.217	0.0	33	1.	2.5	0	F
H2O2	-1.41	0.0	34	1.	2.5	0	F
H2O2-	2.9	0.0	34	1.	2.5	-1	F
H2O3-	-1.23	0.0	50	1.	2.5	-1	F
H2O4-	-1.4	0.0	66	1.	2.5	-1	F
H3O2-	-2.50	0.0	35	1.	2.5	-1	F

NO-w	0.28	0.0	48	1.	2.5	-1	F
NO2-w	-2.76	0.0	64	1.	2.5	-1	F
NH	0.00	0.0	15	1.	2.5	0	F
NH2	0.00	0.0	16	1.	2.5	0	F
HNO	-0.50	0.0	31	1.	2.5	0	F
HNO2	-0.79	0.0	47	1.	2.5	0	F
HNO3	-1.40	0.0	63	1.	2.5	0	F
CO2	-4.06	0.00	44	1.0	3.5	0	T
CO2v	-3.977	0.	44	1.0	3.5	0	F
CO	-1.18	0.	28	1.0	2.5	0	F
CO3-	0.	0.	60	1.0	2.5	-1	F
CO4-	0.	0.	76	1.0	2.5	-1	F
CN	0.	0.	26	1.0	2.5	0	F
HCO	0.	0.	29	1.0	2.5	0	F
Ar	0.0	0.0	40	1.0	1.5	0	T

End_List /

c Begining of Air Chemistry:

c Electron Processes:

c Processes involving solution of Boltzmann's eqn:

Boltz							/
	1 N2	+ 1 e	->	1 N2A	+ 1 e		/
	N2	N2A					/
Boltz							/
	1 N2	+ 1 e	->	1 N2a	+ 1 e		/
	N2	N2a					/
Boltz							/
	1 N2	+ 1 e	->	1 N2+	+ 2 e		/
	N2	N2+					/
Boltz							/
	1 O2	+ 1 e	->	1 O2+	+ 2 e		/
	O2	O2+					/
Boltz							/
	1 O2	+ 1 e	->	1 O2a1D	+ 1 e		/
	O2	O2a1D					/
Boltz							/
	1 O2	+ 1 e	->	1 O2B1S	+ 1 e		/
	O2	O2B1S					/
Boltz							/
	1 O2	+ 1 e	->	1 O	+ 1 O	+ 1 e	/
	O2	O+O					/
Boltz							/
	1 O2	+ 1 e	->	1 O-	+ 1 O		/
	O2	O+O-					/
Boltz							/
	1 O2	+ 1 e	->	1 O2-			/
	O2	O2-					/
Boltz							/
	1 O	+ 1 e	->	1 O+	+ 2 e		/
	O	O+					/

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Boltz      /
      1 O      + 1 e      -> 1 O1D      + 1 e      /
      O      O1D      /
Boltz      /
      1 O      + 1 e      -> 1 O1S      + 1 e      /
      O      O1S      /
Boltz      /
      1 N2a     + 1 e      -> 1 N2+     + 2 e      /
      N2a     N2+      /
Boltz      /
      1 N2A     + 1 e      -> 1 N2+     + 2 e      /
      N2A     N2+      /
Boltz      /
      1 O2a1D  + 1 e      -> 1 O      + 1 O      + 1 e      /
      O2a1D  O+O      /
Boltz      /
      1 O2a1D  + 1 e      -> 1 O2+     + 2 e      /
      O2a1D  O2+      /
Boltz      /
      1 O2B1S  + 1 e      -> 1 O      + 1 O      + 1 e      /
      O2B1S  O+O      /
Boltz      /
      1 O2B1S  + 1 e      -> 1 O2+     + 2 e      /
      O2B1S  O2+      /
Boltz      /
      1 N2O     + 1 e      -> 1 N2      + 1 O-     /
      N2O     N2+O-    /
Boltz      /
      1 O3      + 1 e      -> 1 O3+     + 2 e      /
      O3      O3+      /
Boltz      /
      1 H2O     + 1 e      -> 1 H      + 1 OH     + 1 e      /
      H2O     H+OH     /
Boltz      /
      1 H2O     + 1 e      -> 1 O1D     + 1 H2     + 1 e      /
      H2O     O*+H2    /
Boltz      /
      1 H2O     + 1 e      -> 1 H2O+    + 2 e      /
      H2O     H2O+     /
Boltz      /
      1 H2O     + 1 e      -> 1 OH-     + 1 H      /
      H2O     OH--+H    /
Boltz      /
      1 H2O     + 1 e      -> 1 H-      + 1 OH     /
      H2O     H--+OH    /
Boltz      /
      1 H2O     + 1 e      -> 1 H2      + 1 O-     /
      H2O     H2+O-    /

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c *****

c Electron "temperature" dependent processes: /

c Recombination:

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Etemp      /
      1 e      + 1 N2+     -> 1 N      + 1 N      /

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5.400e-08 -0.39 / 2.2e-7 @ 300K Biondi (76)
 Etemp 1 e + 1 N2+ + 1 O2 -> 1 N2 + 1 O2 /
 1.000e-26 /
 Etemp 1 e + 1 O2+ -> 1 O + 1 O /
 2.700e-08 -0.56 / 2.1e-7 @ 300K Biondi (76)
 Etemp 1 e + 1 O2+ -> 1 O + 1 O1D /
 1.950e-07 /
 Etemp 1 e + 1 O2+ + 1 O2 -> 1 O2 + 1 O2 /
 8.000e-29 /
 Etemp 1 e + 1 NO+ -> 1 N + 1 O /
 6.600e-08 -0.5 / 4.1e-7 @ 300K Biondi (76)
 Etemp 1 e + 1 NO+ + 1 O2 -> 1 NO + 1 O2 /
 3.100e-23 -1.5 /
 Etemp 1 e + 1 N4+ -> 1 N2 + 1 N + 1 N /
 2.000e-06 /
 Etemp 1 e + 1 O4+ -> 1 O2 + 1 O + 1 O /
 2.000e-06 /
 Etemp 1 e + 1 O4+ -> 1 O2 + 1 O2 /
 1.100e-07 /
 Etemp 1 e + 1 O+ + 1 e -> 1 O + 1 e /
 8.750e-27 -4.5 / CRR /
 Etemp 1 e + 1 O+ + 1 N2 -> 1 O + 1 N2 /
 5.600e-27 -4.5 / CRR /
 Etemp 1 e + 1 O+ + 1 O2 -> 1 O + 1 O2 /
 5.600e-27 -4.5 / CRR /
 Etemp 1 e + 1 H2O+ -> 1 H + 1 OH /
 1.100e-06 -0.5 / 6.6e-6 @ 300K /
 Etemp 1 e + 1 H2O+ -> 1 O + 1 H2 /
 3.800e-07 -0.5 / 2.4e-6 @ 300K /
 Etemp 1 e + 1 H2O+ -> 1 O + 1 H + 1 H /
 4.800e-07 -0.5 / 3.0e-6 @ 300K /
 Etemp 1 e + 1 H3O+ -> 1 H2O + 1 H /
 2.200e-06 -0.08 / 3.0e-6 @ 300K Biondi (82) value for
 H3O+*(H2O)2

c Attachment:

Etemp 1 e + 1 O2 + 1 O2 -> 1 O2- + 1 O2 /
 2.200e-30 /
 Etemp


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Chem
  1 O      + 1 O      + 1 N      -> 1 O2     + 1 N      /
6.498e-35  0. -1039.    / use the rate for M = N2
Chem
  1 O      + 1 O2     + 1 O2     -> 1 O3     + 1 O2     /
2.413e-34 -1.029    -238.9    / NIST fit 80-3000 K; K92 (#95) has
c          6.9e-34  -1.25  0.0
Chem
  1 O      + 1 O2     + 1 N2     -> 1 O3     + 1 N2     /
2.413e-34 -1.029    -238.9    / NIST fit 80-3000 K; K92 (#94) has
c          6.2e-34  -2.0   0.0
Chem
  1 O      + 1 O2     + 1 O3     -> 1 O3     + 1 O3     /
1.430e-33 -2.          / SGG87
Chem
  1 O      + 1 O2     + 1 O      -> 1 O3     + 1 O      /
2.150e-34 0.          -345.    / SGG87
Chem
  1 O      + 1 O3     -> 2 O2     /
1.529e-11 0. 2185.    / NIST fit 197-2000 K
c          K92 (#82): 2.0e-11  0. -2300.
Chem
  1 O      + 1 NO     + 1 N2     -> 1 NO2    + 1 N2     /
1.064e-31 -1.682    46.26    / NIST fit 200-3000 K; see also K92 (#96)
Chem
  1 O      + 1 NO     + 1 O2     -> 1 NO2    + 1 O2     /
1.064e-31 -1.682    46.26    / NIST fit 200-3000 K; see also K92 (#96)
Chem
  1 O      + 1 NO     -> 1 NO2    /
2.221e-11 0.459    -92.64    / NIST fit 200-1500 K
Chem
  1 O      + 1 NO     -> 1 O2     + 1 N      /
4.222e-11 0.0      23200.    / NIST fit 1500-5000 K
Chem
  1 O      + 1 NO     + 1 N2     -> 1 NO2    + 1 N2     /
1.064e-31 -1.682    46.26    / NIST fit 200-3000 K
Chem
  1 O      + 1 NO2    -> 1 O2     + 1 NO     /
9.090e-12 0.18          / K92 (#81)
c Chem
c  1 O      + 1 NO2    -> 1 NO3    /
c 2.200e-11          / NIST fit; 200-400 K
Chem
  1 O      + 1 NO2    + 1 N2     -> 1 NO3    + 1 N2     /
1.065e-31 -2.157    46.59    / NIST fit; 200-400 K
Chem
  1 O      + 1 NO2    + 1 O2     -> 1 NO3    + 1 O2     /
1.065e-31 -2.157    46.59    / NIST fit 200-400 K; see K92 (#97)
Chem
  1 O      + 1 NO2    + 1 N2     -> 1 NO3    + 1 N2     /
1.065e-31 -2.157    46.59    / NIST fit 200-400 K; see K92 (#97)
Chem
  1 O      + 1 NO3    -> 1 O2     + 1 NO2    /
1.000e-11          / K92 (#83); NIST

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c

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Chem
  1 N      + 1 N      + 1 N2   -> 1 N2   + 1 N2   /
  8.270e-34  0.      -500.      / K92 (#90)
c   NIST: ref 91PRA/SMI has k = 4.1e-34, 8.6e-34, 1.1e-33 for
c   M = He, Ar, Xe respectively @ 293 K
Chem
  1 N      + 1 N      + 1 N      -> 1 N2   + 1 N      /
  23.320e-34  0.      -500.      / use rate coefficient for M = N2
c   but multiplied by 2.82 to reflect the measurement of 1.25e-32
c   by ref 88KNI/RUB listed in the NIST database
Chem
  1 N      + 1 NO     -> 1 N2   + 1 O      /
  3.513e-11  0.      49.84      / NIST fit 196-3000 K; see K92 (#76)
Chem
  1 N      + 1 O2     -> 1 NO    + 1 O      /
  1.001e-11  0.      3473.      / NIST fit 200-1000 K; see K92 (#74)
Chem
  1 N      + 1 NO2    -> 1 N2O   + 1 O      /
  3.000e-12  0.      0.          / K92 (#79); NIST too
Chem
  1 N      + 1 O3     -> 1 NO    + 1 O2     /
  1.000e-16  0.      0.          / NIST; K92 (#75) has k <= 2.e-16
c
c -----
Chem
  1 NO     + 1 O3     -> 1 O2    + 1 NO2    /
  4.300e-12  0.      1560.      / K92 (#85)
c   the 195-500 K fit from the NIST database is 2.445e-12  0.  1446.
Chem
  1 NO2    + 1 O3     -> 1 NO3    + 1 O2     /
  1.893e-13  0.      2542.      / NIST fit 200-363 K; K92 (#87) has
Chem
  1 NO3    + 1 O3     -> 2 O2    + 1 NO2    /
  1.000e-17  0.      0.          / NIST
c
c -----
Chem
  1 NO     + 1 NO2    + 1 N2    -> 1 N2O3  + 1 N2    /
  9.110e-33  0.      0.          / NIST
c Chem
c   1 NO     + 1 NO2    -> 1 N2O3    /
c   3.400e-12  0.      0.          / NIST
Chem
  1 NO     + 1 NO3    -> 2 NO2    /
  1.113e-11  0.      -220.9     / NIST fit 200-1100 K; K92 (#86) has 1.7e-
11
c ----- Humid Air Chemistry Starts Here -----
c   Neutral Chemistry:
Chem
  1 H      + 1 O2     -> 1 O      + 1 OH     /

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1.168e-10	0.2789	7860.			/ NIST fit 250-5300 K
Chem					
1 H	+ 1 O2	+ 1 H2	-> 1 HO2	+ 1 H2	/
5.790e-32	-0.8	0.			/ NIST (84WAR) 300-2500 K
Chem					
1 H	+ 1 O2	+ 1 N2	-> 1 HO2	+ 1 N2	/
5.940e-32	-1.0	0.			/ NIST (86TSA/HAM) 300-2500 K
K					
Chem					
1 H	+ 1 O2	+ 1 O2	-> 1 HO2	+ 1 O2	/
5.940e-32	-1.0	0.			/ NIST use rate coeff for M = N2
c	note that the rate coefficient for M = Ar is lower: 2.032e-32 -0.8 0.				
Chem					
1 H	+ 1 OH	+ 1 N2	-> 1 H2O	+ 1 N2	/
6.880e-31	-2.	0.			/ NIST (86TSA/HAM) 300-3000 K
K					
Chem					
1 H	+ 1 OH	+ 1 O2	-> 1 H2O	+ 1 O2	/
6.880e-31	-2.	0.			/ use value for M = N2
Chem					
1 H	+ 1 OH	+ 1 H2O	-> 1 H2O	+ 1 H2O	/
4.360e-30	-2.	0.			/ NIST (84WAR) 1000-3000 K
Chem					
1 H	+ 1 NO2		-> 1 NO	+ 1 OH	/
2.200e-10	0.	182.			/ NIST (91KO/FON) 296-760 K
Chem					
1 H	+ 1 O3		-> 1 O2	+ 1 OH	/
7.788e-11	0.2551	327.8			/ NIST fit 196-2000 K
Chem					
1 H	+ 1 O3		-> 1 HO2	+ 1 O	/
7.500e-13					/ NIST (79FIN/KLE); k <= 7.5e-13
Chem					
1 H	+ 1 HO2		-> 1 H2	+ 1 O2	/
2.571e-11	0.5598	346.			/ NIST fit 245-2500 K
Chem					
1 H	+ 1 HO2		-> 1 OH	+ 1 OH	/
2.356e-10	0.	373.7			/ NIST fit 245-2500 K
Chem					
1 H	+ 1 HO2		-> 1 H2O	+ 1 O	/
9.180e-11	0.	971.9			/ NIST fit 245-773 K
c Chem					
c	1 H	+ 1 O2	-> 1 HO2		/
c	7.500e-11				/ NIST (87DEM/GOL)
c Chem					
c	1 H	+ 1 OH	-> 1 H2O		/
c	2.700e-14				/ NIST (77ZEL/ERL) @ 300 K; (72FRI/SUT) has 7.3e-14 @ 2130 K
2130 K					
Chem					
1 H	+ 1 HNO		-> 1 H2	+ 1 NO	/
4.270e-12	0.	-998.1			/ NIST fit 295-2100 K
Chem					
1 H	+ 1 HNO		-> 1 OH	+ 1 NH	/
2.410e-9	-0.5	9010.			/ NIST fit 359-3000 K
Chem					
1 H	+ 1 HNO		-> 1 O	+ 1 NH2	/
1.050e-9	-0.3	14730.			/ NIST (91COH/WES) 550-3000 K
K					

Chem	1 H	+ 1 NO		-> 1 NH	+ 1 O	/
	9.290e-10	-0.10	35220.			/ NIST (91COH/WES) 1300-3000
K						
Chem	1 H	+ 1 NO		-> 1 OH	+ 1 N	/
	2.111e-10	0.0	24330.			/ NIST fit 1750-4500 K
Chem	1 H	+ 1 NO	+ 1 N2	-> 1 HNO	+ 1 N2	/
	7.327e-32	-1.318	184.3			/ NIST fit 231-704 K
Chem	1 H	+ 1 NO	+ 1 O2	-> 1 HNO	+ 1 O2	/
	7.327e-32	-1.318	184.3			/ NIST fit 231-704 K
Chem	1 H	+ 1 NO3		-> 1 NO2	+ 1 OH	/
	1.100e-10					/ NIST (88BOO/CAN)
Chem	1 H	+ 1 H2O2		-> 1 OH	+ 1 H2O	/
	4.000e-11	0.	2000.			/ NIST (86TSA/HAM) 300-2500
K						
Chem	1 H	+ 1 H2O2		-> 1 H2	+ 1 HO2	/
	8.000e-11	0.	4000.			/ NIST (86TSA/HAM) 300-2500
K						
c						
Chem	1 OH	+ 1 OH		-> 1 H2O	+ 1 O	/
	1.549e-13	1.408	-267.3			/ NIST fit 200-2500 K
Chem	1 OH	+ 1 O		-> 1 O2	+ 1 H	/
	2.105e-11	-0.186	153.9			/ NIST fit 200-5000 K
Chem	1 OH	+ 1 H		-> 1 H2	+ 1 O	/
	1.123e-14	3.406	1233.			/ NIST fit 298-2500 K
Chem	1 OH	+ 1 H2		-> 1 H2O	+ 1 H	/
	2.313e-12	1.47	1761.			/ NIST fit 200-3000 K
Chem	1 OH	+ 1 O3		-> 1 HO2	+ 1 O2	/
	1.472e-12	0.	932.7			/ NIST fit 200-450 K
Chem	1 OH	+ 1 HO2		-> 1 H2O	+ 1 O2	/
	4.381e-11	0.	-110.9			/ NIST fit 200-2550 K
Chem	1 OH	+ 1 OH	+ 1 N2	-> 1 H2O2	+ 1 N2	/
	6.050e-31	-3.	0.			/ NIST (86TSA/HAM) 300-2500 K; the general fit is 1.543e-31 -2.021 -183.6 over 200-2500 K
c						
Chem	1 OH	+ 1 OH	+ 1 O2	-> 1 H2O2	+ 1 O2	/
	6.050e-31	-3.	0.			/ NIST (86TSA/HAM) 300-2500 K; same as M = N2
Chem	1 OH	+ 1 OH	+ 1 H2O	-> 1 H2O2	+ 1 H2O	/
	1.543e-31	-2.021	-183.6			/ use general fit from NIST; NIST ref 88ZEL/EWI have 4.e-30 at 300 K
c						
Chem						

	1 OH	+ 1 H2O2		-> 1 H2O	+ 1 HO2	/
	4.529e-12	0.	288.9			/ NIST fit 200-2500 K
Chem						
	1 OH	+ 1 HNO2		-> 1 H2O	+ 1 NO2	/
	1.800e-11	0.	390.			/ NIST (89ATK/BAU) 280-430 K
Chem						
	1 OH	+ 1 N2O		-> 1 HO2	+ 1 N2	/
	3.696e-13	0.	2740.			/ NIST fit 298-2700 K
c Chem						
c	1 OH	+ 1 OH		-> 1 H2O2		/
c	1.510e-11	-0.37	0.			/ NIST (87BRO/COB) 200-1500 K
K Chem						
	1 OH	+ 1 NO	+ 1 N2	-> 1 HNO2	+ 1 N2	/
	3.924e-32	0.	-794.2			/ NIST fit 200-505 K
Chem						
	1 OH	+ 1 NO	+ 1 O2	-> 1 HNO2	+ 1 O2	/
	3.924e-32	0.	-794.2			/ NIST fit 200-505 K
Chem						
	1 OH	+ 1 NO2		-> 1 HO2	+ 1 NO	/
	3.300e-11	0.	3360.			/ NIST (80HOW) 452-1115 K
Chem						
	1 OH	+ 1 NO2	+ 1 N2	-> 1 HNO3	+ 1 N2	/
	8.378e-30	-3.878	409.3			/ NIST fit 200-1200 K
Chem						
	1 OH	+ 1 NO2	+ 1 O2	-> 1 HNO3	+ 1 O2	/
	8.378e-30	-3.878	409.3			/ NIST fit 200-1200 K
Chem						
	1 OH	+ 1 NO3		-> 1 HO2	+ 1 NO2	/
	2.300e-11					/ NIST (89ATK/BAU)
Chem						
	1 OH	+ 1 HNO		-> 1 H2O	+ 1 NO	/
	1.266e-11	0.9904	334.2			/ NIST fit 298-4000 K
Chem						
	1 OH	+ 1 HNO3		-> 1 H2O	+ 1 NO3	/
	4.006e-14	0.	-317.6			/ NIST fit 200-1100 K
c						

Chem						
	1 HO2	+ 1 O3		-> 1 OH	+ 2 O2	/
	1.752e-15	0.	-628.3			/ NIST fit 200-413 K
Chem						
	1 HO2	+ 1 HO2		-> 1 H2O2	+ 1 O2	/
	3.000e-12					/ NIST (86TSA/HAM) 300-2500 K
Chem						
	1 HO2	+ 1 O		-> 1 OH	+ 1 O2	/
	2.900e-11	0.	-200.			/ NIST (86TSA/HAM) 300-2500 K
K Chem						
	1 HO2	+ 1 NO		-> 1 OH	+ 1 NO2	/
	3.600e-12	0.	-240.			/ NIST (89ATK/BAU) 230-500 K & (84HAN/SAL) 1000-2000 K
c Chem						
	2 HO2	+ 1 N2		-> 1 H2O2	+ 1 O2 + 1 N2	/
	1.900e-33	0.	-980.			/ NIST (89ATK/BAU) 230-420 K
Chem						

1 HO2 + 1 HO2 + 1 O2 -> 1 H2O2 + 2 O2 /
 1.900e-33 0. -980. / use rate coeff for M = N2
 Chem

1 HO2 + 1 NO -> 1 O2 + 1 HNO /
 9.100e-19 0. -2819. / NIST (79HOW) 271-303 K
 Chem

1 HO2 + 1 NO -> 1 OH + 1 NO2 /
 3.500e-12 0. -240. / NIST (89ATK/BAU) 230-2000
 K
 Chem

1 HO2 + 1 NO2 -> 1 HNO2 + 1 O2 /
 1.200e-13 / NIST (75COX)
 c Chem

1 HO2 + 1 NO -> 1 HNO3 /
 c 1.400e-13 / NIST (75COX/DER)
 Chem

1 HO2 + 1 N -> 1 OH + 1 NO /
 2.200e-11 / NIST (83BRU/SCH2); 1 entry
 Chem

1 HO2 + 1 NO3 -> 1 HNO3 + 1 O2 /
 9.210e-13 / NIST; for O2 + prod on RHS, k=4.3e-12 (89ATK/BAU)

c -----

Chem

1 N + 1 OH -> 1 NO + 1 H /
 3.917e-11 0. -72.36 / NIST fit 250-515 K
 Chem

1 N + 1 OH -> 1 O + 1 NH /
 1.880e-11 0.1 10700. / NIST (91COH/WES) 500-3000
 K
 Chem

1 O + 1 H2 -> 1 OH + 1 H /
 1.501e-13 2.844 2834. / NIST fit 293-3532 K
 Chem

1 O + 1 H2O2 -> 1 OH + 1 HO2 /
 1.792e-13 2.919 1394. / NIST fit 200-2500 K
 Chem

1 N2O3 + 1 H2O -> 2 HNO2 /
 6.300e-11 0. 4468. / NIST (75ENG/COR) 298-323 K
 Chem

1 HNO2 + 1 O -> 1 OH + 1 NO2 /
 1.000e-15 / NIST (78KAI/JAP2) k <= 1.e-15
 Chem

1 HNO3 + 1 O -> 1 OH + 1 NO3 /
 3.000e-17 / NIST; k<= 3.e-17
 Chem

1 HNO2 + 1 NO3 -> 1 HNO3 + 1 NO2 /
 2.000e-15 / NIST (1 entry); k<= 2.e-15
 Chem

1 H2O2 + 1 NO3 -> 1 HO2 + 1 HNO3 /
 2.000e-15 / NIST (1 entry); k<= 2.e-15

c Excited State Chemistry:

Chem

	1 N2A	+ 1 H2O	-> 1 H2	+ 1 N	+ 1 NO	/
	1.000e-10					/
Chem	1 N2a	+ 1 H2O	-> 1 H2	+ 1 N	+ 1 NO	/
	1.000e-10					/
c	-----					
Chem	1 O1D	+ 1 H2O	-> 1 OH	+ 1 OH		/
	2.000e-10				/ A89	
Chem	1 O1D	+ 1 H2	-> 1 OH	+ 1 H		/
	1.000e-10			/ NIST; no T dependence 200-350 K		
Chem	1 O1D	+ 1 H2O	-> 1 H2	+ 1 O2		/
	2.300e-10			/ NIST		
Chem	1 O1D	+ 1 H2O2	-> 1 H2O	+ 1 O2		/
	5.200e-10			/ NIST (76FLE/HUS)		
c	-----					
Chem	1 O1S	+ 1 H2O	-> 1 O	+ 1 H2O		/
	3.000e-10			/ S&B78		
Chem	1 O1S	+ 1 H2O	-> 1 OH	+ 1 OH		/
	5.000e-10			/ S&B78		
Chem	1 O1S	+ 1 H2O	-> 1 H2	+ 1 O2		/
	5.000e-10			/ S&B78		
c	-----					
Chem	1 O2a1D	+ 1 H2O	-> 1 O2	+ 1 H2O		/
	5.000e-18					/
Chem	1 O2B1S	+ 1 H2O	-> 1 O2	+ 1 H2O		/
	4.000e-12					/
c	Ion - Molecule:					
c	Positive Ion					
Chem	1 O+	+ 1 H2	-> 1 OH+	+ 1 H		/
	1.000e-10			/ A93		
Chem	1 O+	+ 1 H2O	-> 1 H2O+	+ 1 O		/
	2.600e-09			/ A93		
Chem						

	1 O2+	+ 2 H2O	->	1 H3O+	+ 1 OH	+ 1 O2	/
	2.000e-28						/
Chem	1 O4+	+ 2 H2O	->	1 H3O+	+ 1 OH	+ 2 O2	/
	2.000e-28						/
Chem	1 N2+	+ 1 H2O	->	1 H2O+	+ 1 N2		/
	2.200e-09					/ A93	
Chem	1 H2O+	+ 1 O2	->	1 H2O	+ 1 O2+		/
	3.300e-10					/ A93	
Chem	1 H2O+	+ 1 H2O	->	1 H3O+	+ 1 OH		/
	1.850e-09					/ A93	
Chem	1 OH+	+ 1 O2	->	1 OH	+ 1 O2+		/
	3.800e-10					/ A93	
Chem	1 NO+	+ 2 H2O	->	1 H3O+	+ 1 HNO2		/
	2.000e-28						/
c Negative Ion							
Chem	1 O-	+ 1 H2	->	1 H2O	+ 1 e		/
	6.500e-10						/
Chem	1 O2-	+ 1 H2O	->	1 O2	+ 1 H2O	+ 1 e	/
	5.000e-9	0.	5000.			/ DNA (10-7)	
Chem	1 OH-	+ 1 O3	->	1 OH	+ 1 O3-		/
	5.000e-10						/
Chem	1 OH-	+ 1 O3	->	1 O2-	+ 1 HO2		/
	1.000e-11						/
Chem	1 H-	+ 1 H2O	->	1 OH-	+ 1 H2		/
	1.000e-09						/
c Ionic Recombination:							
Chem	1 H3O+	+ 1 NO2-	->	1 H2O	+ 1 OH	+ 1 NO	/
	1.890e-06						/
Chem	1 H3O+	+ 1 O3-	->	1 H2O	+ 1 OH	+ 1 O2	/
	1.000e-06						/

c Electron temperature:

Etemp
1 H2O + 1 O2 + 1 e -> 1 O2- + 1 H2O /
1.400e-29 /

c -----

c Atomic & Molecular Reactions: Excited State Chemistry

Chem
1 N2a + 1 N2a -> 1 N2 + 1 N2+ + 1 e /
1.000e-10 /
Chem
1 N2a + 1 O2 -> 1 N2 + 2 O /
2.800e-11 / K92 (#115)
Chem
1 N2a + 1 N2 -> 1 N2 + 1 N2 /
2.000e-13 / K92 (#114)
Chem
1 N2a + 1 NO -> 1 N2 + 1 N + 1 O /
3.600e-10 / K92 (#116)

c -----

Chem
1 N2A + 1 N2 -> 1 N2 + 1 N2 /
3.000e-18 / K92 (#105)
Chem
1 N2A + 1 O2 -> 1 N2 + 2 O /
1.290e-12 / K92 (#106)
Chem
1 N2A + 1 O2 -> 1 N2O + 1 O /
7.800e-14 /
Chem
1 N2A + 1 NO -> 1 N2 + 1 NO /
7.000e-11 / K92 (#109)
Chem
1 N2A + 1 O -> 1 NO + 1 N /
7.000e-12 / DNA72 (#32-22)
Chem
1 N2A + 1 O -> 1 N2 + 1 O1S /
2.100e-11 / K92 (#108)
Chem
1 N2A + 1 N -> 1 N2 + 1 N /
5.000e-11 / K92 (#107)
Chem
1 N2A + 1 N2O -> 1 N2 + 1 N + 1 NO /
1.000e-11 /

c -----

Chem
1 O1D + 1 N2 -> 1 O + 1 N2 /
1.800e-11 0. -107. / K92 (#144)

Chem	1 O1D	+ 1 O2		-> 1 O	+ 1 O2B1S	/
	2.560e-11	0.	-67.		/ K92 (#145)	/
Chem	1 O1D	+ 1 O2		-> 1 O	+ 1 O2a1D	/
	1.000e-12					/
Chem	1 O1D	+ 1 NO		-> 1 O2	+ 1 N	/
	1.700e-10			/ K92 (#149);	NIST has 8.5e-11	/
Chem	1 O1D	+ 1 NO2		-> 1 O2	+ 1 NO	/
	3.000e-10				/ NIST	/
Chem	1 O1D	+ 1 N2O		-> 1 NO	+ 1 NO	/
	7.200e-11			/ K92 (#150);	NIST has 6.7e-11	/
Chem	1 O1D	+ 1 N2O		-> 1 N	+ 1 NO2	/
	2.450e-13			/ NIST;	0.005 x rate with N2 + O2 products	/
Chem	1 O1D	+ 1 N2O		-> 1 N2	+ 1 O2	/
	4.900e-11			/ NIST;	K92 (#151) has 4.4e-11	/
Chem	1 O1D	+ 1 O3		-> 2 O	+ 1 O2	/
	1.200e-10			/ K92 (#147) &	NIST; little T	/
dependence						
Chem	1 O1D	+ 1 O3		-> 2 O2		/
	2.400e-10			/ K92 (#148) &	NIST; little T	/
dependence						
Chem	1 O1D	+ 1 O3		-> 1 O	+ 1 O3	/
	2.400e-10				/ B82	/
c Chem						
c	1 O1D	+ 1 O3		-> 1 O2B1S	+ 1 O2	/
c	3.600e-11					/
c						
Chem	1 O1S	+ 1 NO		-> 1 O2	+ 1 N	/
	5.000e-10					/
Chem	1 O1S	+ 1 O2		-> 1 O2	+ 1 O	/
	4.300e-12	0.	850.		/ K92 (#153, 154)	/
Chem	1 O1S	+ 1 O3		-> 1 O2	+ 1 O	/
	2.900e-10				+ 1 O1D	/
					/ K92 (#155)	/
Chem	1 O1S	+ 1 O3		-> 2 O2		/
	2.900e-10				/ K92 (#156)	/
Chem	1 O1S	+ 1 O2a1D		-> 1 O2	+ 1 O1D	/
	3.600e-11				/ K92 (#161)	/
Chem	1 O1S	+ 1 O2a1D		-> 3 O		/
	3.400e-11				/ K92 (#162)	/
Chem						

1 O1S + 1 O2a1D -> 1 O + 1 O2B1S /
1.300e-10 / K92 (#163)
Chem

1 O1S + 1 O -> 1 O + 1 O1D /
5.000e-11 0. 301. / K92 (#164)

c -----

Chem 1 O2a1D + 1 N -> 1 O + 1 NO /
2.000e-14 0. 600. / K92 (#121)
Chem

1 O2a1D + 1 O -> 1 O + 1 O2 /
7.000e-16 / K92 (#124)
Chem

1 O2a1D + 1 NO -> 1 NO + 1 O2 /
2.500e-11 / K92 (#126)
Chem

1 O2a1D + 1 O3 -> 2 O2 + 1 O /
6.239e-11 0. 2876. / NIST fit 283-360 K;
c K92 (#119) has 9.7e-13 0. 1564.

Chem 1 O2a1D + 1 O2 -> 1 O2 + 1 O2 /
2.200e-18 0.8 / K92 (#123)
Chem

1 O2a1D + 1 N2 -> 1 O2 + 1 N2 /
1.400e-19 / A89; K92 (#122) has 3.e-21
Chem

1 O2a1D + 1 NO -> 1 O + 1 NO2 /
4.880e-18 / NIST

c -----

Chem 1 O2B1S + 1 N2 -> 1 O2a1D + 1 N2 /
4.900e-15 0. 253. / K92 (#127)
Chem

1 O2B1S + 1 O2 -> 1 O2a1D + 1 O2 /
3.730e-16 2.4 241. / K92 (#128); A89 has 4.0e-17 @ 298 K
Chem

1 O2B1S + 1 O3 -> 2 O2a1D + 1 O /
1.800e-11 / K92 (#126)
Chem

1 O2B1S + 1 O -> 1 O2 + 1 O /
8.000e-14 / K92 (#129)
Chem

1 O2B1S + 1 NO -> 1 O2a1D + 1 NO /
4.000e-14 / K92 (#131)

c -----

c Ion - Molecule Reactions:

c Positive Ions

Chem 1 O+ + 1 N2 -> 1 NO+ + 1 N /

3.000e-12 / K92 (#187)

Chem
 1 O2+ + 1 NO -> 1 O2 + 1 NO+ /
 4.400e-10 / K92 (#208)

Chem
 1 O2+ + 1 O2 + 1 N2 -> 1 O4+ + 1 N2 /
 2.400e-30 -3.2 / K92 (#167) [O2]

Chem
 1 O2+ + 1 O2 + 1 N -> 1 O4+ + 1 N /
 2.400e-30 -3.2 / use the rate for M = O2

Chem
 1 O2+ + 1 N -> 1 NO+ + 1 O /
 1.200e-10 / K92 (#207)

Chem
 1 O2+ + 1 N2 -> 1 NO+ + 1 NO /
 1.000e-17 / K92 (#206)

Chem
 1 O3+ + 1 O2 -> 1 O2+ + 1 O3 /
 1.000e-11 /

Chem
 1 O4+ + 1 O2a1D -> 1 O2+ + 1 O2 + 1 O2 /
 1.000e-10 / K92 (#228)

Chem
 1 O4+ + 1 O2B1S -> 1 O2+ + 1 O2 + 1 O2 /
 1.000e-10 / K92 (#228)

Chem
 1 O4+ + 1 NO -> 1 NO+ + 1 O2 + 1 O2 /
 1.000e-10 / K92 (#230)

Chem
 1 O4+ + 1 O -> 1 O3 + 1 O2+ /
 3.000e-10 / K92 (#229); DNA (14-22)

Chem
 1 O4+ + 1 O -> 1 O3+ + 1 O2 /
 3.000e-10 /

Chem
 1 O4+ + 1 O -> 1 O2+ + 1 O3 /
 3.000e-10 /

Chem
 1 O4+ + 1 O2 -> 1 O2+ + 1 O2 + 1 O2 /
 2.000e-13 /

c -----

Chem
 1 N2+ + 1 O -> 1 N2 + 1 O+ /
 1.000e-11 -0.2 / K92 (#199)

Chem
 1 N2+ + 1 O -> 1 NO+ + 1 N /
 1.300e-10 -0.5 / K92 (#198)

Chem
 1 N2+ + 1 O2 -> 1 N2 + 1 O2+ /
 6.000e-11 -0.5 / K92 (#197)

Chem
 1 N2+ + 1 NO -> 1 N2 + 1 NO+ /

3.300e-10 / K92 (#203)
 Chem 1 N2+ + 1 N2 + 1 N2 -> 1 N4+ + 1 N2 /
 5.000e-29 -1. / DNA72 (#19-6); also K92 (#165) w/o T
 dependence
 Chem 1 N2+ + 1 N2 + 1 N -> 1 N4+ + 1 N /
 5.000e-29 -1. / use the rate for M = N2
 Chem 1 N4+ + 1 O2 -> 1 O2+ + 1 N2 + 1 N2 /
 2.500e-10 /
 Chem 1 N4+ + 1 O -> 1 O+ + 1 N2 + 1 N2 /
 2.500e-10 /

c Negative Ions

Chem 1 O- + 1 N2 -> 1 N2O + 1 e /
 1.000e-12 /
 Chem 1 O- + 1 O2 -> 1 O3 + 1 e /
 5.000e-15 / K92 (#72)
 Chem 1 O- + 1 O -> 1 O2 + 1 e /
 5.000e-10 / K92 (#68)
 Chem 1 O- + 1 N -> 1 NO + 1 e /
 2.600e-10 / K92 (#69)
 Chem 1 O- + 1 N2A -> 1 O + 1 N2 + 1 e /
 2.200e-9 / K92 (#64)
 Chem 1 O- + 1 O2a1D -> 1 O3 + 1 e /
 3.000e-10 / K92 (#62)
 Chem 1 O- + 1 O3 -> 2 O2 + 1 e /
 5.300e-10 / K92 (#243)
 Chem 1 O- + 1 NO -> 1 NO2 + 1 e /
 2.600e-10 / K92 (#73)
 Chem 1 O- + 1 N2O -> 1 NO- + 1 NO /
 2.100e-10 / K92 (#245)
 Chem 1 O- + 1 NO2 -> 1 O + 1 NO2- /
 1.200e-09 / K92 (#244)
 Chem 1 O- + 1 NO2 -> 1 O2- + 1 NO /
 2.000e-11 /
 Chem 1 O- + 1 O2 + 1 O2 -> 1 O3- + 1 O2 /
 1.100e-30 / K92 (#235)
 Chem 1 O- + 1 O3 -> 1 O3- + 1 O /
 5.500e-10 / SGG87; K92 (#243) has 5.3e-10

Chem
 1 NO- + 1 O2 -> 1 O2- + 1 NO /
 5.000e-10 / K92 (#253)

Chem
 1 NO- + 1 NO2 -> 1 NO2- + 1 NO /
 7.400e-16 / K92 (#254)

Chem
 1 NO- + 1 N2O -> 1 NO2- + 1 N2 /
 2.800e-14 / K92 (#255)

Chem
 1 NO2- + 1 O3 -> 1 O2 + 1 NO3- /
 9.000e-11 / SGG87; K92 (#256) has 1.8e-11

c -----

c Negative Ion Clusters:

Chem
 1 O- + 1 H2O + 1 N2 -> 1 H2O2- + 1 N2 /
 1.300e-28 /

Chem
 1 O- + 1 H2O + 1 O2 -> 1 H2O2- + 1 O2 /
 1.300e-28 /

Chem
 1 O2- + 1 H2O + 1 N2 -> 1 H2O3- + 1 N2 /
 2.200e-28 /

Chem
 1 O2- + 1 H2O + 1 O2 -> 1 H2O3- + 1 O2 /
 2.200e-28 /

Chem
 1 O3- + 1 H2O + 1 N2 -> 1 H2O4- + 1 N2 /
 2.700e-28 /

Chem
 1 O3- + 1 H2O + 1 O2 -> 1 H2O4- + 1 O2 /
 2.700e-28 /

Chem
 1 OH- + 1 H2O + 1 N2 -> 1 H3O2- + 1 N2 /
 2.500e-28 /

Chem
 1 OH- + 1 H2O + 1 O2 -> 1 H3O2- + 1 O2 /
 2.500e-28 /

Chem
 1 NO- + 1 H2O + 1 N2 -> 1 NO-w + 1 N2 /
 1.000e-28 /

Chem
 1 NO- + 1 H2O + 1 O2 -> 1 NO-w + 1 O2 /
 1.000e-28 /

Chem
 1 NO2- + 1 H2O + 1 N2 -> 1 NO2-w + 1 N2 /
 1.600e-28 /

Chem
 1 NO2- + 1 H2O + 1 O2 -> 1 NO2-w + 1 O2 /
 1.600e-28 /

c -----

c Ionic Recombination of + & - Clusters:

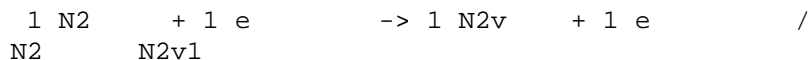
Chem							/
	1 H3O+	+ 1 H2O2-	->	2 H2O	+ 1 OH		/
	1.000e-06						/
Chem							/
	1 H3O+	+ 1 H2O3-	->	2 H2O	+ 1 HO2		/
	1.000e-06						/
Chem							/
	1 H3O+	+ 1 H2O4-	->	2 H2O	+ 1 OH	+ 1 O2	/
	1.000e-06						/
Chem							/
	1 H3O+	+ 1 H3O2-	->	3 H2O			/
	1.000e-06						/
Chem							/
	1 H3O+	+ 1 NO-w	->	2 H2O	+ 1 HNO		/
	1.000e-06						/
Chem							/
	1 H3O+	+ 1 NO2-w	->	2 H2O	+ 1 HNO2		/
	1.000e-06						/
c							/
Chem							/
	1 OH+	+ 1 H2O2-	->	1 H2O	+ 1 HO2		/
	1.000e-06						/
Chem							/
	1 OH+	+ 1 H2O3-	->	1 H2O	+ 1 OH	+ 1 O2	/
	1.000e-06						/
Chem							/
	1 OH+	+ 1 H2O4-	->	1 H2O	+ 1 HO2	+ 1 O2	/
	1.000e-06						/
Chem							/
	1 OH+	+ 1 H3O2-	->	2 H2O	+ 1 O		/
	1.000e-06						/
Chem							/
	1 OH+	+ 1 NO-w	->	1 H2O	+ 1 HNO2		/
	1.000e-06						/
Chem							/
	1 OH+	+ 1 NO2-w	->	1 H2O	+ 1 HNO3		/
	1.000e-06						/
c							/
Chem							/
	1 O2+	+ 1 H2O2-	->	1 H2O	+ 1 O3		/
	1.000e-06						/
Chem							/
	1 O2+	+ 1 H2O3-	->	1 H2O	+ 2 O2		/
	1.000e-06						/
Chem							/
	1 O2+	+ 1 H2O4-	->	1 H2O	+ 1 O3	+ 1 O2	/
	1.000e-06						/
Chem							/
	1 O2+	+ 1 H3O2-	->	1 H2O2	+ 1 HO2		/
	1.000e-06						/
Chem							/
	1 O2+	+ 1 NO-w	->	1 H2O	+ 1 NO3		/
	1.000e-06						/
Chem							/
	1 O2+	+ 1 NO2-w	->	1 H2O	+ 1 NO2	+ 1 O2	/

1.000e-06							/
c							/
Chem							/
1.000e-06	1 NO+	+ 1 H2O2-	-> 1 H2O	+ 1 NO2			/
Chem							/
1.000e-06	1 NO+	+ 1 H2O3-	-> 1 H2O	+ 1 NO3			/
Chem							/
1.000e-06	1 NO+	+ 1 H2O4-	-> 1 H2O	+ 1 NO2	+ 1 O2		/
Chem							/
1.000e-06	1 NO+	+ 1 H3O2-	-> 1 H2O	+ 1 HNO2			/
Chem							/
1.000e-06	1 NO+	+ 1 NO-w	-> 1 H2O	+ 2 NO			/
Chem							/
1.000e-06	1 NO+	+ 1 NO2-w	-> 1 H2O	+ 1 NO2	+ 1 NO		/
Chem							/
1.000e-06							/
Chem							/
1.000e-07	1 O2-	+ 1 NO+	-> 1 O2	+ 1 N	+ 1 O		/
Chem							/
2.000e-07	1 O3-	+ 1 O+	-> 1 O3	+ 1 O			/
Chem							/
2.000e-07	1 O3-	+ 1 O2+	-> 1 O3	+ 1 O2			/
Chem							/
1.000e-07	1 O3-	+ 1 O2+	-> 2 O	+ 1 O3			/
Chem							/
2.000e-07	1 O3-	+ 1 NO+	-> 1 O3	+ 1 NO			/
Chem							/
1.000e-07	1 NO3-	+ 1 NO+	-> 1 NO3	+ 1 N	+ 1 O		/
Chem							/
1.000e-07	1 NO3-	+ 1 O2+	-> 1 NO3	+ 1 O	+ 1 O		/
Chem							/
2.000e-07	1 O-	+ 1 O2+	-> 1 O	+ 1 O2			/
Chem							/
2.000e-25	1 O-	+ 1 O2+	+ 1 O2	-> 1 O3	+ 1 O2		/
Chem							/
2.000e-25	1 O-	+ 1 NO+	+ 1 O2	-> 1 NO2	+ 1 O2		/
Chem							/
4.200e-07	1 O2-	+ 1 O2+	-> 1 O2	+ 1 O2			/
Chem							/
2.000e-25	1 O2-	+ 1 NO+	+ 1 O2	-> 2 O2	+ 1 NO		/

c *****

c Electron Collisions:

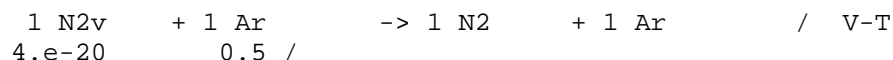
Boltz



c -----

c the V-T rates are V-scaled based on the P(1,0) transition
c probability shown by Center & Caledonia (1971)

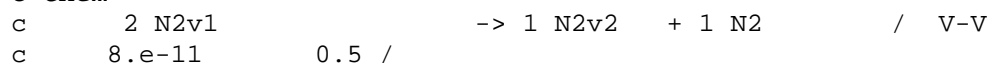
Chem



c -----

c the following all use the same V-V rate coefficient based on
c the canonical P(1,0;0,1) V-V transition probability of 10⁻³
c from Center & Caledonia (1971)

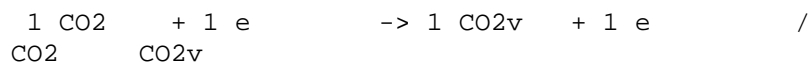
c Chem



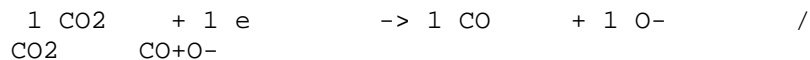
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c CO2 chemistry

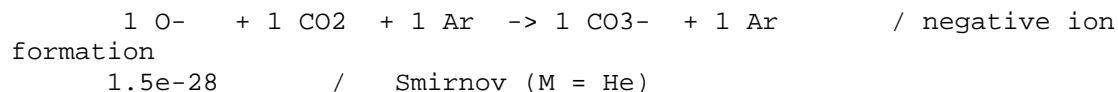
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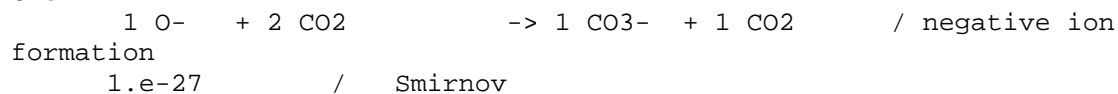
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Chem



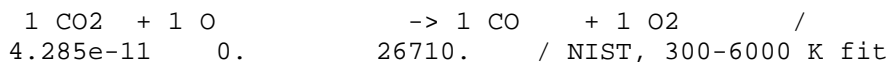
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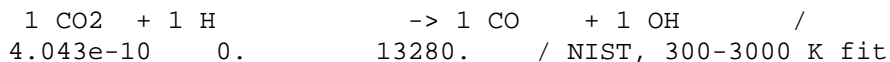
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c CO2 chemistry

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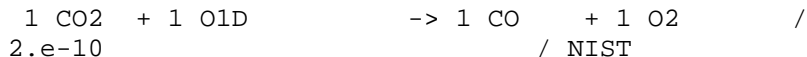


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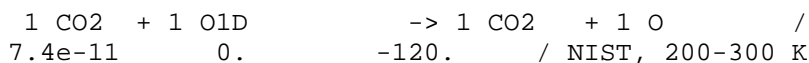


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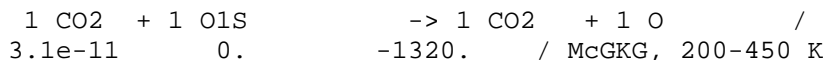
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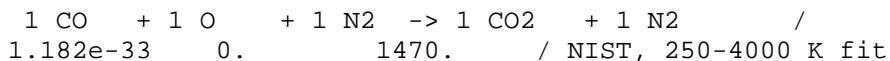


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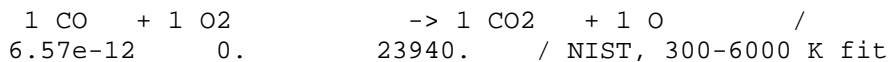


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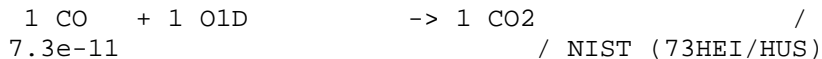
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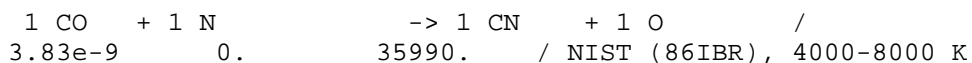
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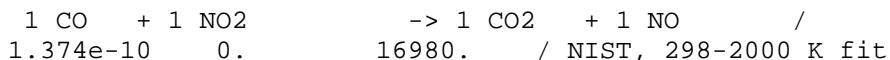
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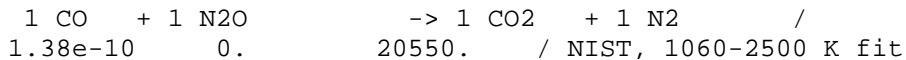
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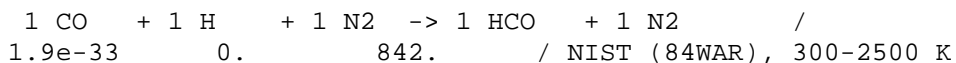
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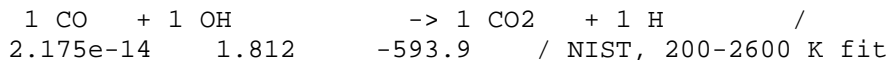
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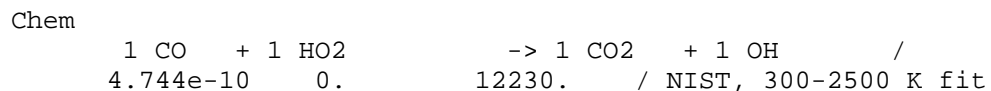


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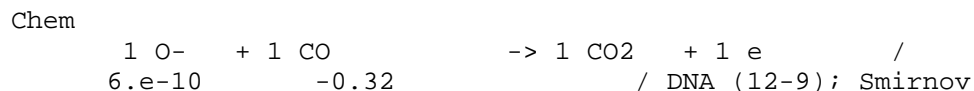


Chem





c Negative Ion chemistry



End_List /