Table 1:

Short-lived species:	O_3, HO_2, OH, H_2^+, H_3^+, $O^+(2P)$, $O^+(2D)$, N_2^+, CO^+, CO_2^+, O_2^+, NO^+, OH^+, N(2D), O(1D), H_2O_2, $O_2(^1\sum_g)$, $O_2(^1\Delta_g)$												
Long-lived species	O	O_2	N_2	H_e	H	H_2	CO_2	CO	N(4S)	NO	H_2O	O^+	N^+	H^+
Upper boundary condition	0	1	1	0	0	0	1	1	0	1	1	0	0	0
Lower boundary condition	Fixed mixing ratio													

0: effusion velocity
1: zero flux

A. Roble et al. 1987
B. Roble 1995
C. Rees 1989
D. Smithtro and Sojka 2005a
E. JPL 1994
F. Yelle 2004
G. Kasting and Pollack 1983
H. Schunk and Nagy 2000
I. Fox and Dalgarno 1979
J. Nagy et al. 1983
K. Kumar et al. 1983
L. Barth et al. 1992
M. Yung and DeMore 1999

Table 2: chemical reactions, reaction rates, energy associated, and the references

	Reaction										Reaction Rate ($cm^3\ s^{-1}$)	Reference
1	N(4S)	+	O_2	=	NO	+	O	+	1.40	eV	4.4e-12*EXP(-3220./T)	A
2	N(4S)	+	NO	=	N_2	+	O	+	2.68	eV	1.6E-10*EXP(-460/T)	B
3	N(2D)	+	O	=	N(4S)	+	O	+	2.38	eV	6.90E-13	C
4	N(2D)	+	O_2	=	NO	+	O(1D)	+	1.84	eV	6.2E-12*SQRT(T/300.)*0.1	Estimated
5	N(2D)	+	O_2	=	NO	+	O	+	3.76	eV	6.2E-12*SQRT(T/300.)*0.9	Estimated

6	N(2D)	+	NO			=	N_2	+	O	+			5.63	eV	7E-11	B
7	N(2D)					=	N(4S)	+	HV						1.06E-05	B
8	O(1D)	+	N_2			=	O	+	N_2	+			1.96	eV	1.8E-11*EXP(107./T)	B
9	O(1D)					=	O	+	HV						8.33E-03	D
10	O(1D)	+	H_2O			=	OH	+	OH	+			1.23	eV	2.20E-10	B
11	O	+	O	+	M	=	O_2	+	M	+			5.10	eV	9.59E-34*EXP(480/T)*[M]	B
12	O	+	O_2	+	M	=	O3	+	M	+			1.10	eV	6E-34*(300./T)**2.3*[M]	E
13	O	+	O3			=	O_2	+	O_2	+			4.06	eV	8E-12 * EXP(-2060./T)	B
14	CO	+	O	+	M	=	CO_2	+	M	+			5.51	eV	6.6E-33*EXP(-1103./T)*[M]	B
15	H_2	+	O(1D)			=	H	+	OH	+			1.88	eV	1E-10	B
16	H_2	+	O			=	H	+	OH	+			0.08	eV	1.6E-11*EXP(-4570./T)	B
17	H_2	+	M			=	H	+	H	+	M	+	-4.52	eV	1.5E-9*EXP(-4.8E4/T)	F
18	H	+	O_2			=	O	+	OH	+			-0.72	eV	3.7E-10*EXP(-8450./T)	G
19	H	+	O3			=	OH	+	O_2	+			3.34	eV	1.4E-10*EXP(-470./T)	B
20	H	+	H	+	M	=	H_2	+	M	+			4.52	eV	$5.7E-32*(300./T)^{1.6}$*[M]	B
21	H	+	H_2O			=	H_2	+	OH	+			-0.65	eV	1.5E-10*EXP(-10250./T)	G
22	OH	+	N(4S)			=	NO	+	H	+			2.10	eV	5E-11	B
23	OH	+	O			=	H	+	O_2	+			0.72	eV	2E-11*EXP(117./T)	B
24	OH	+	CO			=	CO_2	+	H	+			1.07	eV	1.5E-13 * (1. + 0.6*PATM)	E
25	OH	+	H_2			=	H_2O	+	H	+			0.65	eV	7.7E-12*EXP(-2100./T)	B
26	OH	+	OH			=	H_2O	+	O	+			0.73	eV	4.2E-12*EXP(-240./T)	B
27	OH	+	H	+	M	=	H_2O	+	M	+			5.17	eV	$6.1E-26*T^{-2}$ *[M]	G
28	OH	+	H			=	H_2	+	O	+			0.08	eV	1.4E-14*T*EXP(-3500./T)	G
29	N_2^+	+	O_2			=	O_2^+	+	N_2	+			3.52	eV	5E-11*(300./Ti)	D
30	N_2^+	+	O			=	NO^+	+	N(2D)	+			0.70	eV	k33	B
31	N_2^+	+	O			=	O^+	+	N_2	+			1.96	eV	k34	D
32	N_2^+	+	NO			=	NO^+	+	N_2	+			6.25	eV	4.1E-10	H
33	N_2^+	+	CO_2			=	CO_2^+	+	N_2	+			1.81	eV	8E-10	H
34	N_2^+	+	CO			=	CO^+	+	N_2	+			1.57	eV	7.40E-11	I
35	N^+	+	O_2			=	O^+	+	NO	+			1.28	eV	4.60E-10	H
36	N^+	+	O_2			=	O_2^+	+	N(2D)	+			0.10	eV	3.07E-10*0.66	C

37	N^+	+	O_2	=	O_2^+	+	N(4S)	+	2.49	eV	3.07E-10*0.33	C
38	N^+	+	O_2	=	NO^+	+	O	+	6.70	eV	2.32E-10	D
39	N^+	+	O	=	O^+	+	N(4S)	+	0.98	eV	1E-12	B
40	N^+	+	NO	=	NO^+	+	N(4S)	+	5.29	eV	9E-10	J
41	N^+	+	CO_2	=	CO_2^+	+	N(4S)	+	0.78	eV	9.2E-10	H
42	N^+	+	CO_2	=	CO^+	+	NO	+	1.57	eV	2E-10	H
43	N^+	+	CO	=	CO^+	+	N(4S)	+	0.54	eV	4E-10	J
44	N^+	+	H	=	H^+	+	N(4S)	+	0.90	eV	3.6E-12	C
45	O_2^+	+	N_2	=	NO^+	+	NO	+	0.93	eV	5E-16	D
46	O_2^+	+	N(4S)	=	NO^+	+	O	+	4.21	eV	1.5E-10	H
47	O_2^+	+	NO	=	NO^+	+	O_2	+	2.81	eV	4.4E-10	B
48	O^+	+	NO	=	NO^+	+	O	+	4.36	eV	8E-13	H
49	O^+	+	CO_2	=	O_2^+	+	CO	+	1.20	eV	1.1E-09	H
50	OI	+	H_2	=	OH^+	+	H	+	0.36	eV	2E-09	B
51	O^+	+	H	=	H^+	+	O	+	0.02	eV	6E-10	B
52	O^+	+	N_2	=	NO^+	+	N(4S)	+	1.09	eV	K56	B
53	O^+	+	O_2	=	O_2^+	+	O	+	1.56	eV	K57	B
54	O^+	+	N(2D)	=	N^+	+	O	+	1.45	eV	1.3E-10	B
55	O^+(2P)	+	N_2	=	N_2^+	+	O	+	3.02	eV	4.8E-10	C
56	O^+(2P)	+	N_2	=	N^+	+	NO	+	0.70	eV	1E-10	C
57	O^+(2P)	+	O	=	O^+	+	O	+	5.20	eV	5.2E-11	C
58	O^+(2P)			=	O^+	+	HV				0.047	C
59	O^+(2P)			=	O^+(2D)	+	HV				0.171	C
60	O^+(2D)	+	N_2	=	O^+	+	N_2	+	3.31	eV	8E-10	C
61	O^+(2D)	+	N_2	=	N_2^+	+	O	+	1.33	eV	1E-10	C
62	O^+(2D)	+	O	=	O^+	+	O	+	3.31	eV	1E-11	C
63	O^+(2D)	+	O_2	=	O_2^+	+	O	+	4.87	eV	7E-10	C
64	O^+(2D)			=	O^+	+	HV				7.7E-05	C
65	H_2^+	+	O	=	OH^+	+	H	+	2.17	eV	1.5E-09	K
66	H_2^+	+	H_2	=	$H3^+$	+	H	+	1.70	eV	2E-09	F
67	H_2^+	+	H	=	H^+	+	H_2	+	1.83	eV	6.4E-10	F

68	H^+	+	O	=	O^+	+	H	+		-0.02	eV	k72	B
69	H^+	+	NO	=	NO^+	+	H	+		4.34	eV	1.9E-09	J
70	H^+	+	H_2	=	H_2^+	+	H	+		-1.83	eV	1E-9*EXP(-2.19E4/T)	F
71	H_3^+	+	H	=	H_2^+	+	H_2	+		-1.70	eV	K75	F
72	CO_2^+	+	O	=	O_2^+	+	CO	+		1.33	eV	1.6E-10	I
73	CO_2^+	+	O	=	O^+	+	CO_2	+		0.13	eV	1E-10	I
74	CO_2^+	+	NO	=	NO^+	+	CO_2	+		4.51	eV	1.2E-10	I
75	CO_2^+	+	H	=	H^+	+	CO_2	+		0.17	eV	1E-10	J
76	CO^+	+	O	=	O^+	+	CO	+		0.39	eV	1.4E-10	J
77	CO^+	+	NO	=	NO^+	+	CO	+		4.75	eV	3.3E-10	J
78	CO^+	+	CO_2	=	CO_2^+	+	CO	+		0.24	eV	1.1E-09	I
79	N_2^+	+	e	=	N(4S)	+	N(4S)	+		5.82	eV	$2.2E-7*(300./Te)^{0.39}*0.1$	D
80	N_2^+	+	e	=	N(4S)	+	N(2D)	+		3.44	eV	$2.2E-7*(300./Te)^{0.39}*0.9$	D
81	N^+	+	e	=	N(4S)	+	HV					$3.6e-12*(250./Te)^{0.7}$	H
82	O_2^+	+	e	=	O	+	O	+		6.99	eV	k86	D
83	O_2^+	+	e	=	O	+	O(1D)	+		5.02	eV	k87	D
84	O_2^+	+	e	=	O(1D)	+	O(1D)	+		3.06	eV	k88	D
85	O^+	+	e	=	O	+	HV					$3.7e-12*(250./Te)^{0.7}$	H
86	NO^+	+	e	=	N(4S)	+	O	+		2.75	eV	$4.2E-7*(300./Te)^{0.85}*0.2$	B
87	NO^+	+	e	=	N(2D)	+	O	+		0.38	eV	$4.2E-7*(300./Te)^{0.85}*0.8$	B
88	H^+	+	e	=	H	+	HV					$4.2e-7*(300./Te)^{0.64}$	F
89	H_2^+	+	e	=	H	+	H	+		10.91	eV	$2.4E-8*(300./Te)^{0.4}$	F
90	H_3^+	+	e	=	H_2	+	H	+		9.21	eV	$2.9E-8*(300./Te)^{0.65}$	F
91	H_3^+	+	e	=	H	+	H	+	H	+	4.69	eV	$8.6E-8*(300./Te)^{0.65}$	F
92	OH^+	+	e	=	O	+	H	+			8.74	eV	2E-07	K
93	CO_2^+	+	e	=	CO	+	O	+			4.56	eV	1.4E-4/Te	L
94	N(2D)	+	e	=	N(4S)	+	e	+			2.38	eV	$5.5E-10*(300./Te)^{0.5}$	C
95	O^+(2P)	+	e	=	O^+	+	e	+			5.00	eV	$4E-8*(300./Te)^{0.5}$	C
96	O^+(2P)	+	e	=	O^+(2D)	+	e	+			1.69	eV	$1.5E-7*(300./Te)^{0.5}$	C
97	O^+(2D)	+	e	=	O^+	+	e	+			3.31	eV	$7.8E-8*(300./Te)^{0.5}$	C

98	H	+	O_2	+	M	=	HO_2	+	M	+			2.11	eV	$5.5E\text{-}32*(300/T)^{1.6}*[M]$	B
99	HO_2	+	H			=	H_2O	+	O	+			2.34	eV	8.1E-11*0.02	E
100	HO_2	+	H			=	H_2	+	O_2	+			2.41	eV	8.1E-11*0.08	E
101	HO_2	+	H			=	OH	+	OH	+			1.61	eV	8.1E-11*0.9	E
102	HO_2	+	OH			=	H_2O	+	O_2	+			3.06	eV	4.8E-11*EXP(250./T)	E
103	OH	+	O_3			=	HO_2	+	O_2	+			1.73	eV	1.6E-12*EXP(-940./T)	E
104	HO_2	+	O			=	OH	+	O_2	+			2.33	eV	3E-11*EXP(200./T)	E
105	HO_2	+	O_3			=	OH	+	O_2	+	O_2	+	1.23	eV	1.1E-14*EXP(-500./T)	E
106	HO_2	+	HO_2			=	H_2O_2	+	O_2	+			1.71	eV	2.3E-13*EXP(600./T)	E
107	H_2O_2	+	OH			=	HO_2	+	H_2O	+			1.35	eV	2.9E-12*EXP(-160./T)	E
108	H_2O_2	+	O			=	HO_2	+	OH	+			3.44	eV	1.4E-12*EXP(-2000./T)	E
109	O(1D)	+	O_2			=	$O_2(^1\sum_g)$	+	O	+			0.33	eV	3.2E-11*EXP(70/T)*0.75	E
110	O(1D)	+	O_2			=	O2	+	O	+			1.96	eV	3.2E-11*EXP(70/T)*0.25	E
111	O(1D)	+	O			=	O	+	O	+			1.96	eV	8E-12	B
112	O(1D)	+	H_2			=	H	+	OH	+			1.88	eV	1E-10	B
113	O(1D)	+	CO_2			=	O	+	CO_2	+			1.96	eV	7.4E-11*EXP(120/T)	E
114	O(1D)	+	O_3			=	O_2	+	O_2	+			6.03	eV	1.2E-10	E
115	O(1D)	+	O_3			=	O_2	+	O	+	O	+	0.87	eV	1.2E-10	E
116	N(2D)	+	CO_2			=	NO	+	CO	+			3.41	eV	3.5E-13	M
117	N(2D)	+	N_2			=	N(4S)	+	N_2	+			2.38	eV	1.7E-14	M
118	$O_2(^1\sum_g)$	+	N_2			=	$O_2(^1\Delta_g)$	+	N_2	+			0.65	eV	2.1E-15	E
119	$O_2(^1\sum_g)$	+	CO_2			=	$O_2(^1\Delta_g)$	+	CO_2	+			0.65	eV	4.2E-13	E
120	$O_2(^1\sum_g)$	+	O_3			=	$O_2(^1\Delta_g)$	+	O_3	+			0.65	eV	2.2E-11	E
121	$O_2(^1\sum_g)$	+	O			=	$O_2(^1\Delta_g)$	+	O	+			0.65	eV	8E-14	E
122	$O_2(^1\sum_g)$	+	O_2			=	$O_2(^1\Delta_g)$	+	O_2	+			0.65	eV	3.9E-17	E
123	$O_2(^1\Delta_g)$	+	O_2			=	O_2	+	O_2	+			0.98	eV	3.6E-18*EXP(-220/T)	E
124	$O_2(^1\Delta_g)$	+	N_2			=	O_2	+	N_2	+			0.98	eV	1E-20	E
125	$O_2(^1\Delta_g)$	+	O			=	O_2	+	O	+			0.98	eV	1.3E-16	E
126	$O_2(^1\Delta_g)$					=	O_2	+	HV						$2.58E\text{-}4\ s^{-1}$	B
127	$O_2(^1\sum_g)$					=	O_2	+	HV						$0.085\ s^{-1}$	B
128	N_2	+	HV			=	N(4S)	+	N(2D)							

129	O_2	+	HV	=	O	+	O(1D)		
130	O_2	+	HV	=	O	+	O		
131	O_3	+	HV	=	O_2	+	O(1D)		
132	O_3	+	HV	=	O_2	+	O		
133	NO	+	HV	=	N(4S)	+	O		
134	CO_2	+	HV	=	CO	+	O		
135	CO_2	+	HV	=	CO	+	O(1D)		
136	H_2O	+	HV	=	H	+	OH		
137	H_2O	+	HV	=	H_2	+	O		
138	H_2O_2	+	HV	=	OH	+	OH		
139	O_3	+	HV	=	$O_2(^1\Delta_g)$	+	O(1D)		
140	N_2	+	HV	=	N_2^+	+	e		
141	N_2	+	HV	=	N^+	+	N(4S)	+	e
142	N_2	+	HV	=	N^+	+	N(2D)	+	e
143	N(4S)	+	HV	=	N^+	+	e		
144	O_2	+	HV	=	O_2^+	+	e		
145	O_2	+	HV	=	O^+	+	O	+	e
146	O_2	+	HV	=	O^+(2P)	+	O	+	e
147	O_2	+	HV	=	O^+(2D)	+	O	+	e
148	O	+	HV	=	O^+	+	e		
149	O	+	HV	=	O^+(2P)	+	e		
150	O	+	HV	=	O^+(2D)	+	e		
151	NO	+	HV	=	NOI	+	e		
152	H_2	+	HV	=	H_2^+	+	e		
153	H_2	+	HV	=	H^+	+	H	+	e
154	H	+	HV	=	H^+	+	e		

k33=5.2E-11*(Tr/300.)$^{0.2}$ Tr>1500

$k33=1.4E-10*(300/Tr)^{0.44}$ Tr<1500

$k34=3.62E-12*(Ti/300.)^{0.41}$ Ti>1500
$k34=1E-11*(300/Tr)^{0.23}$ Ti<1500

$k56=1.533E-12-5.92E-13*b+8.6E-14*b^2$
where b=T2/300, T2=0.6363*Ti+0.3637*T (300<T2<1700K)

$k57=2.82E-11-7.74E-12*a+1.073E-12*a^2-5.17E-14*a^3+9.65E-16*a^4$
where a=T1/300 and T1=0.667*Ti+0.333*T (300<T1<6000K)

k72=k55*8/9*SQRT((Ti+T/16.)/(T+Ti/16.))

k75 estimated to be the same as k70 in F

k86=c*0.22, k87=c*0.42, k88=c*0.36,
$c=7.38E-8*(1200./Te)^{0.56}$ Te>1200K, $c=1.95E-7*(300./Te)^{0.7}$ Te<1200K