Supporting Information for "Chemical and thermal impact of sprite streamers in the Earth mesosphere"

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3. Tables of statistical weights of CO_2, standard enthalpies of formation of the species and reaction rates of the processes

Introduction

This supporting information provides:

1. A bref description of the normal vibrational modes of the CO_2 molecule, the calculation and the values of the statistical weights of the first 28 vibrational levels of CO_2.

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2. A table with the stardard enthalpy of formation of the chemical species considered to calculate P$_{chem}$ as well as the sign criteria used.

3. The altitude-dependence of the correction factor used in the equation (3) of the main manuscript.

4. A set of tables with the chemical processes and its reaction rates employed in the model

Statistical weights of CO_2

CO_2 is a linear and triatomic molecule with three normal vibrational modes:

- Symmetric strech mode v_1 ($\hbar\omega_1 = 0.17$ eV)
- Double degenerate symmetric bending mode v_2 ($\hbar\omega_1 = 0.085$ eV)
- Asymmetric strech mode v_3 ($\hbar\omega_1 = 0.3$ eV)

The level of vibrational excitation of linear triatomic molecules can then be denoted as $CO_2(v_1\ v_2^{l_2}\ v_3)$ showing the number of quanta in each mode (see p. 268 *Fridman* [2008]).

To calculate the statistical weights of the vibrational levels of CO_2 (see p. 488-489 *Ochkin* [2009]), we need the required number of normal vibrations differing in frequency that are given for a linear molecule

$$n_v = 3N_a - 5 - l,$$

where N_a is the number of atoms in the molecule ($N_a(CO_2) = 3$) and l stands for the degenerate vibrations. In CO_2, we have $l = 1$, then $n_v = 3$. The normal vibration frequency v_2 is doubly degenerate, that is, $d_{v_2} = 2$ and for the rest we have $d_{v_1} = d_{v_3} = 1$. The statistical weight of the CO_2 vibrational state ($v_1\ v_2^{l_2}\ v_3$) is

$$g(v_1 v_2 v_3) = \prod_{n=1}^{n_v=3} \frac{(v_n + d_n - 1)!}{v_n!(d_n - 1)!},$$

with $l_2 = v_2$, v_2-2, v_2-4,...,1 or 0.

Table S1. *

Statistical weights of vibrational levels of the ground electronic state of CO_2

(v_1 v_2 v_3)	**g**
(0 0 0)	1
(0 1 0)	2
(0 2 0)	3
(1 0 0)	1
(0 3 0)	4
(1 1 0)	2
(0 0 1)	1
(0 4 0)	5
(1 2 0)	3
(2 0 0)	1
(0 1 1)	2
(0 2 1)	3
(1 0 1)	1
(0 3 1)	4
(1 1 1)	2
(0 0 2)	1
(0 4 1)	5
(1 2 1)	3
(2 0 1)	1

Standard Enthalpy of Formation

The potential energies ($Q_i = \Delta H_f$) of the species i required to calculate P_{chem} in the kinetic model are showed in the table below. These energies correspond with the standard enthalpy of formation of the neutral species. For the ionic species, the energies have been calculated as follows

$$\Delta H_f(M^+) = \Delta H_f(M) + IE,$$

$$\Delta H_f(M^-) = \Delta H_f(M) - EA,$$

where ΔH_f(M) is the standard enthalpy of formation of the neutral specie, IE is the ionization energy, EA is the electronic affinity and $\Delta H_f(M^+)$ and $\Delta H_f(M^-)$ are the standard enthalpies of formation of the positive and negative ions respectively. The ΔH_f of electronically, vibrationally and rotationally excited species is the addition of the potential energy of its ground neutral state to the excitation energy of the corresponding electronic, vibrational and rotational levels, respectively. If the standard enthalpy of formation of the species is negative, it indicates that the reaction of formation of the species is exothermic. The standard enthalpy of formation of the species will be positive for an endothermic reaction of formation. All species in their standard states (oxygen gas, nitrogen gas and argon gas) have a zero standard enthalpy of formation, as there is no change involved in their formation. The ΔH_f(M), IE and EA values have been obtained from *Manion et al.* [2013].

Table S2.1. *

Potential energies of the species i

i	$\mathbf{Q}_i$ **(eV)**
e^-	0.0
N	4.88
$N(^2D)$	7.264
$N(^2P)$	8.376
N^+	19.429
N_2(rot)	0.02
$N_2(X^1\Sigma_g^+)$	0.0
$N_2(A^3\Sigma_u^+)$	6.99
$N_2(B^3\Pi_g)$	7.35
$N_2(W^3\Sigma_g^+)$	7.36
$N_2(B'^3\Sigma_u^-)$	8.16
$N_2(a'^1\Sigma_u^-)$	8.4
$N_2(a^1\Pi_g)$	8.55
$N_2(w^1\Delta_u)$	8.89
$N_2(C^3\Pi_u)$	11.03
$N_2(E^3\Sigma_g^+)$	11.87
$N_2(a''^1\Sigma_g^+)$	12.25
$N_2(X^1\Sigma_g^+,v=1)$	0.291
$N_2(X^1\Sigma_g^+,v=2)$	0.59
$N_2(X^1\Sigma_g^+,v=3)$	0.88
$N_2(X^1\Sigma_g^+,v=4)$	1.17
$N_2(X^1\Sigma_g^+,v=5)$	1.47
$N_2(X^1\Sigma_g^+,v=6)$	1.76
$N_2(X^1\Sigma_g^+,v=7)$	2.06
$N_2(X^1\Sigma_g^+,v=8)$	2.35
N_2^+	15.6
$N_2^+(A^2\Pi_u)$	17.0
$N_2^+(B^2\Sigma_u^+)$	18.8
N_3^+	11.06
N_4^+	14.6
O	2.56
$O(^1D)$	4.527
$O(^1S)$	6.75
O^-	1.122
O^+	16.17

Table S2.2. *

Potential energies of the species i (cont.)

i	**Q_i (eV)**
$O_2(X^3\Sigma_g^-)$	0.0
$O_2(X^3\Sigma_g^-$,v=1)	0.19
$O_2(X^3\Sigma_g^-$,v=2)	0.38
$O_2(X^3\Sigma_g^-$,v=3)	0.57
$O_2(X^3\Sigma_g^-$,v=4)	0.75
O_2(rot)	0.02
$O_2(a^1\Delta_g)$	0.977
$O_2(b^1\Sigma_g^+)$	1.627
$O_2(A^3\Sigma_u^+)$	4.5
O_2^-	-0.448
O_2^+	12.06
O_3	1.478
O_3^-	-0.663
O_4^+	11.58
Ar	0.0
$Ar(^3P)$	11.55
Ar^+	15.759
NO	0.935
$NO(A^2\Sigma^+)$	6.39
NO^-	0.911
NO^+	10.195
NO_2	0.343
NO_2^-	-1.93
NO_2^+	10.093
NO_3	0.737
NO_3^-	-3.19
N_2O	0.85
N_2O^-	0.623
N_2O^+	13.74
N_2O_5	0.117
$N_2O_2^+$	11.82
CO	-1.145
$CO_2(00^00)$	-4.077
$CO_2(01^10)$	-3.997
$CO_2(02^00)$	-3.917
$CO_2(02^20)$	-3.911
$CO_2(10^00)$	-3.905
$CO_2(03^10)$	-3.836

Table S2.3. *

Potential energies of the species i (cont.)

i	**Q_i (eV)**
$CO_2(03^30)$	-3.827
$CO_2(11^10)$	-3.818
$CO_2(00^01)$	-3.784
$CO_2(04^00)$	-3.760
$CO_2(04^20)$	-3.755
$CO_2(12^00)$	-3.74479
$CO_2(04^40)$	-3.74471
$CO_2(12^20)$	-3.733
$CO_2(20^00)$	-3.729
$CO_2(01^11)$	-3.703
$CO_2(02^01)$	-3.681
$CO_2(02^21)$	-3.673
$CO_2(10^01)$	-3.6616
$CO_2(03^11)$	-3.6615
$CO_2(03^31)$	-3.648
$CO_2(11^11)$	-3.641
$CO_2(00^02)$	-3.627
$CO_2(04^01)$	-3.621
$CO_2(04^21)$	-3.615
$CO_2(04^41)$	-3.605
$CO_2(12^01)$	-3.601
$CO_2(12^21)$	-3.592
$CO_2(20^01)$	-3.586
CO_3^-	-5.077

The correction factor of $\mathbf{T}_{gas}$

Let's assume a collection of particles (atoms and/or molecules) in a radiation field characterized by the specific intensity I_ν. The specific intensity I_ν is related to the radiation energy density spectrum by

$$u_\nu = \frac{1}{c}\int_{4\pi} I_\nu d\Omega \tag{1}$$

with Ω being an element of solid angle about the direction Ω. The probability per unit time of induced emission into the solid angle $d\Omega$, corresponding to a transition from level i to level j is

$$B_{ij} I_{\nu_{ji}} d\Omega. \tag{2}$$

In a similar way, the probability per unit time of absorion from radiation propagating in the solid angle $d\Omega$ about the direction Ω, accompained by a $j \rightarrow i$ transition is

$$B_{ji} I_{\nu_{ji}} d\Omega. \tag{3}$$

If there are n_i and n_j particles per unit volume in levels i and j, respectively, then the condition for a steady state between (spontaneous + stimulated) emission and absortion is

$$n_i \left(\frac{A_{ij}}{4\pi} + B_{ij} I_{\nu_{ji}} \right) = n_j B_{ji} I_{\nu_{ji}}. \tag{4}$$

Obtaining $I_{\nu_{ji}}$ from equation (4),

$$I_{\nu_{ji}} = \frac{\frac{A_{ij} B_{ij}}{4\pi}}{\left(\frac{B_{ji}}{B_{ij}}\right)\left(\frac{n_j}{n_i} - 1\right)} \tag{5}$$

Assuming Boltzmann equilibrium for the populations of n_j and n_i, that is, assuming the particles are in thermodynamic equilibrium

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} \exp(-\epsilon_{ji}/k_B T_{gas}), \tag{6}$$

with $\epsilon_{ji} = |\epsilon_i - \epsilon_j|$. Then, the Boltzmann relation (6) is used as the condition for the radiation field to be in equilibrium with the matter. From (6) using (5), we obtain

$$I_{\nu_{ji}} = \frac{\frac{A_{ij}B_{ij}}{4\pi}}{\frac{g_j B_{ji}}{g_i B_{ij}} \exp(h\nu_{ji}/k_B T_{gas}) - 1}. \tag{7}$$

From equation (1)

$$I_{\nu_{ji}} = \frac{c}{4\pi} u_{\nu_{ji}}. \tag{8}$$

When the energy gap between levels i and j is much less than the thermal energy $k_B T_{gas}$, the value of $I_{\nu_{ji}}$ is given correctly classical theory (equiation (1)) with

$$u_{\nu_{ji}} = \frac{8\pi\nu_{ji}^2 k_B T_{gas}}{c^3}. \tag{9}$$

Then, for $h\nu_{ji}/k_B T_{gas} \ll 1$, we have from equations (1), (7) and (9) that

$$\frac{2\nu_{ji}^2}{c^2} k_B T_{gas} = \frac{\frac{A_{ij}B_{ij}}{4\pi}}{\frac{g_j B_{ji}}{g_i B_{ij}}(1 + h\nu_{ji}/k_B T_{gas}) - 1}. \tag{10}$$

For equation (10) to be valid for all the values of $k_B T_{gas}$, consistent with $h\nu_{ji}/k_B T_{gas} \ll 1$, Einstein found that it was needed that

$$g_i B_{ji} = g_i B_{ij} \tag{11}$$

and

$$\frac{A_{ij}}{B_{ij}} = \frac{8\pi h\nu_{ji}^3}{c^2}. \tag{12}$$

Substituting (11) and (12) in equation (7) given the equilibrium spectral distribution of specific intensity $I_{\nu_{ji}}$

$$I_{\nu_{ji}} = \frac{2h\nu_{ji}^3/c^2}{\exp(h\nu_{ji}/k_B T_{gas}) - 1}, \tag{13}$$

related to the blackbody radiation energy density spectrum $u_{\nu_{ji}}$ in an enclosure. The energy absorbed per unit time in all j to i transitions from radiation traveling in the solid angle $d\Omega$

about Ω is

$$h\nu_{ji}B_{ji}I_{\nu_{ji}}d\Omega. \tag{14}$$

If the Einstein spontaneous emission probabilities (A_{ij}) are known, then equation (12) with

$$B_{ij} = \frac{g_i}{g_j}B_{ji}, \tag{15}$$

with g_j and g_i being the degeneration (or statistical weights) of emitting/absorbing levels (in diatomic molecules, the statistical weights of vibrational levels are 1). From (12) and (15)

$$\frac{A_{ij}g_i}{g_jB_{ji}} = \frac{8\pi h\nu_{ji}^3}{c^2}, \tag{16}$$

then

$$B_{ji} = \frac{c^2}{8\pi h\nu_{ji}^3}A_{ij}\frac{g_i}{g_j}. \tag{17}$$

Thus, using equations (14)-(17), the power density absorbed from radiation is

$$P_{abs} = \sum_j n_j h\nu_{ji}B_{ji}I_{\nu_{ji}}, \tag{18}$$

with n_j being the lower absorbing level population in each transition considered. Substituting the equation (17) and (13) in (18), we obtain

$$P_{abs} = \sum_j n_j\frac{A_{ij}h\nu_{ji}}{4\pi}\frac{g_i}{g_j}\frac{1}{exp(h\nu_{ji}/k_BT_{gas})-1}. \tag{19}$$

The final expression for P_{abs} with the correction factor (k_{corr}) is given by

$$P_{abs} = k_{corr}\sum_j n_j\frac{A_{ij}h\nu_{ji}}{4\pi}\frac{g_i}{g_j}\frac{1}{exp(\frac{h\nu_{ji}}{k_bT_{gas}^{bg}})-1}, \tag{20}$$

where k_{corr} is an altitude-dependent factor obtained in the thermal relaxation of the model by imposing $T_{gas}(t = 0\text{ s}) = T_{gas}(t = 3\times10^4\text{ s})$ condition (see Figure S1).

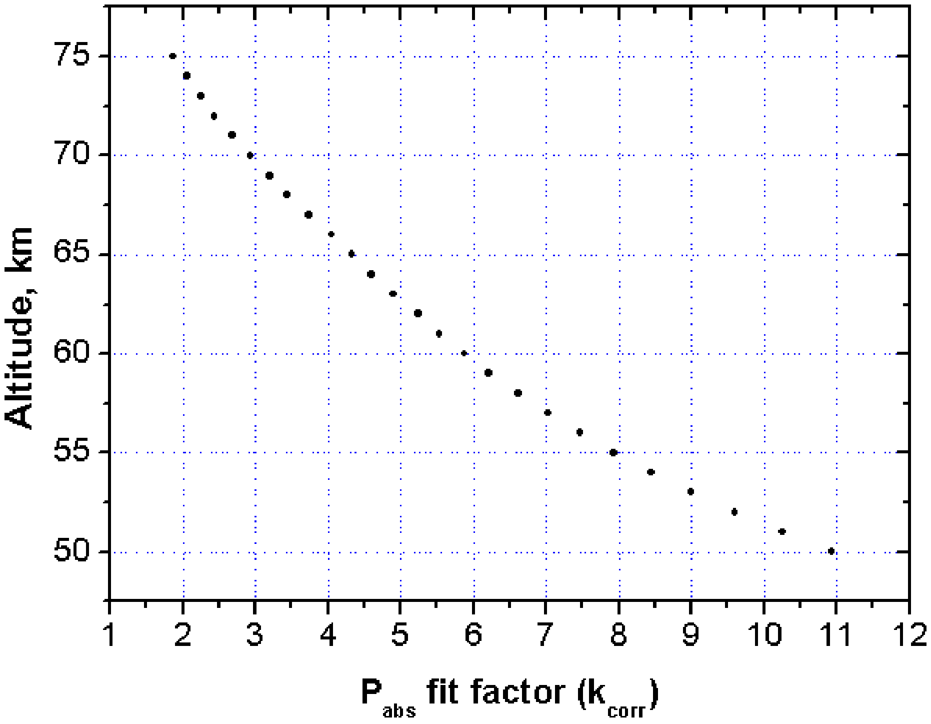

Figure S1. Variation of the correction parameter (k_{corr}) with altitude taken from the thermal relaxation stage of the model.

Reaction rates

The excitation/deexcitation rates for the electron impact processes are evaluated using the electron energy distribution function (EEDF) and their cross sections. When the cross sections are not available, the rates of electron driven mechanisms are calculated as

$$k_e = a \times T_e^b \times exp(-c/T_e)$$

where T$_e$ (in eV) is the electronic temperature. The excitation/deexcitation rates for the processes that include heavy species are parametrized as

$$k_h = d \times \left(\frac{300}{T_g}\right)^e \times exp(-f/T_g)$$

being T$_g$ (in K) the gas temperature. The k$_{e,h}$ units are cm^{3}s^{-1} and cm^{6}s^{-1} for two- and three-body processes, respectively. The general expression for the excitation/deexcitation rates of the VT1 and VT4 processes including collisions of electronically excited CO_2 with N_2 are

$$k_{co2} = g \times (h + i \times exp(-j/T_g^{1/3})).$$

For the VT1 and VV3 processes that include O, the reaction rates are parametrized as

$$k_{co2} = g \times h \times \left(\frac{T_g}{300}\right)^{1/2}.$$

As for the VV1, VV4 and VT2 processes that include O, and the VT3 processes that include N_2 and O_2, the reaction rates are parametrized as

$$k_{co2} = g \times h.$$

For the VT4 processes that include nitrogen oxides, the reaction rates are parametrized as

$$k_{co2} = g \times T_g,$$

and the reaction rates for other processes involving collisions of vibrationally excited CO_2 are parametrized as

$$k_{co2} = g \times h \times exp(i/T_g + j/T_g^2).$$

The k_{co2} units are cm^3 s^{-1}. The rates of the return (backward) reactions in processes VV1-VT1-VT4 and VV4 have been calculated multiplying the direct reaction rate by $exp(-E/k_B T_g)$, where E is the energy emitted/absorbed during the process depending on whether the process is exothermic or endothermic, and k_B is the Boltzmann constant.

The reaction rates of ionization due to cosmic rays are parametrized as

$$k_{cr} = k \times l,$$

where $l = crc$ is an altitude-dependent factor obtained in the model electronic relaxation stage imposing $n_e(t = 0$ s$) = n_e(t = 10^6$ s$)$ (see Figure S2). The units of k_{cr} are s^{-1}.

The reaction rates of the processes (695)-(711) including N^+ are parametrized as

$$k_{N+} = m \times \left(\frac{300}{T_e}\right)^n,$$

with the units of T_e in Kelvin and the k_{N+} in cm^3 s^{-1}. The rate of the process (698) is an exception that is parametrized as

$$k_{N+} = m \times exp\left(\frac{n}{T_g}\right),$$

with the units of T_g in Kelvin and the k_{N+} in cm^6 s^{-1}. The rates of the processes (712)-(718) are

$$k_{N+} = m \times \left(\frac{300}{T_g}\right)^n,$$

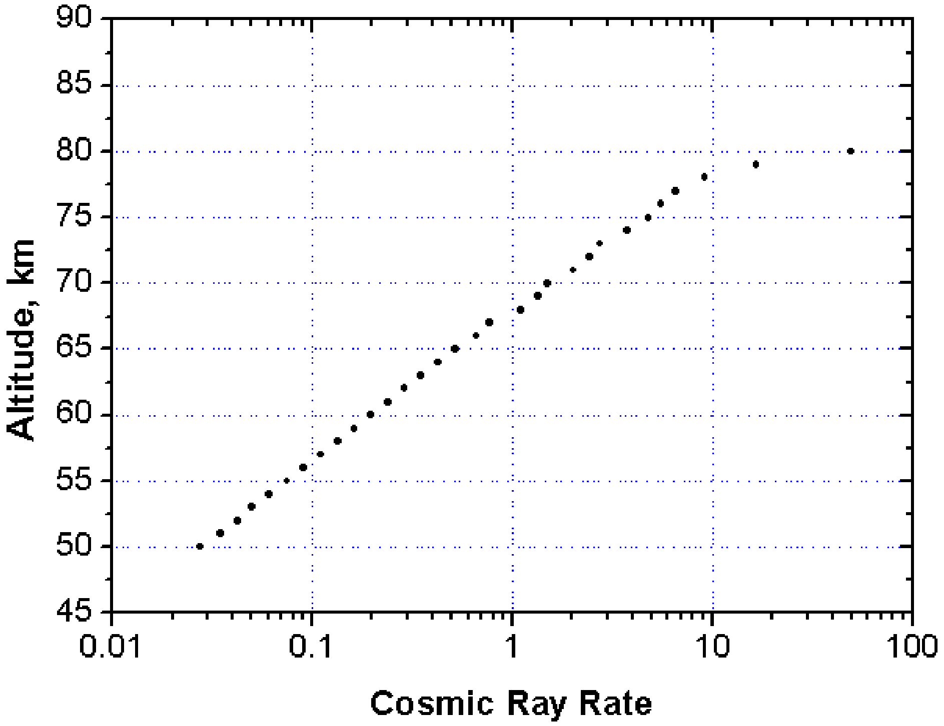

Figure S2. Variation of the cosmic rays constant (CRC) with altitude taken from the electronic relaxation stage of the model.

with the units of T_g in Kelvin and the k_{N+} in $cm^3\ s^{-1}$. The reaction rate of the process (80) have the expression

$$k_f = a \times \left(\frac{300}{T_g}\right)^b$$

with the units of T_g in Kelvin and the k_f in $cm^3\ s^{-1}$. The reaction rate of the process (369) is a polynomial fit performed on the *Rayment and Moruzzi* [1978] experimental data between 0 to 88 Td.

For the VT2 and VT3 processes of the type

$$N_2(v) + M \rightarrow N_2(v-1) + M,$$

with M = N, O; the reaction rates are parametrized using an Arrhenius-type approximation of the form

$$k_{N2} = d \times exp\left(\frac{-e}{T_g}\right) + f \times exp\left(\frac{-g}{T_g}\right)$$

with the units of T_g in Kelvin and the k_{N2} in $cm^3\ s^{-1}$.

The reaction rate of the process (86) is taken from *Kossyi et al.* [1992] and it is given by

$$k_{86} = 1.07 \times 10^{-31} \times \left(\frac{300}{T_e}\right)^2 \times exp\left(-\frac{70}{T_g}\right) \times exp\left(\frac{1500 \times (T_e - T_g)}{T_e \times T_g}\right),$$

with the units of T_g and T_e in Kelvin and the k_{86} in $cm^6\ s^{-1}$.

The reaction rates of the processes (153) is taken from *Capitelli et al.* [2000] and it is given by

$$k_{153} = 1.1 \times 10^{-12} \times T_g \times \left(\frac{-218}{T_g^{1/3}} + \frac{690}{T_g}\right) \times \left(1 - exp\left(-\frac{3375.19}{T_g}\right)\right)^{-1},$$

with the units of T_g in Kelvin and the k_{153} in $cm^3\ s^{-1}$.

The reaction rates of the processes (154) is taken from *Capitelli et al.* [2000] and it is given by

$$k_{154} = 3.2 \times 10^{-15} \times \left(\frac{T_g}{300}\right)^{2.5},$$

with the units of T$_g$ in Kelvin and the k$_{154}$ in cm^3 s^{-1}.

The reaction rates of the processes (155) is taken from *Capitelli et al.* [2000] and it is given by

$$k_{155} = 2.05 \times 10^{-20} \times exp\left(271 \times 10^{-4} \times T_g - 2.32 \times 10^{-5} \times T_g^2\right),$$

with the units of T$_g$ in Kelvin and the k$_{155}$ in cm^3 s^{-1}.

The reaction rates of the processes (159) is taken from *Capitelli et al.* [2000] and it is given by

$$k_{159} = 1.35 \times 10^{-12} \times T_g \times \left(\frac{-137.9}{T_g^{1/3}}\right) \times \left(1 - exp\left(-\frac{2203.76}{T_g}\right)\right)^{-1},$$

with the units of T$_g$ in Kelvin and the k$_{159}$ in cm^3 s^{-1}.

The reaction rates of the processes (160) is taken from *Capitelli et al.* [2000] and it is given by

$$k_{160} = 3.14 \times 10^{-12} \times T_g \times \left(\frac{-173.1}{T_g^{1/3}} + \frac{6.2 \times 10^5}{T_g^2}\right) \times \left(1 - exp\left(-\frac{2203.76}{T_g}\right)\right)^{-1},$$

with the units of T$_g$ in Kelvin and the k$_{160}$ in cm^3 s^{-1}.

The reaction rate of the process (346) is taken from *Rayment and Moruzzi* [1978] and it is given by

$$k_{346} = (1.156 \times 10^{-12} \times (E/N)^2)/(1892.2 + (E/N)^2)$$

with the units of E/N in Td and the k$_{346}$ in cm^3 s^{-1}.

Kinetic model

Table S3.1. *

EEDF and cross section dependent processes

No.	Reaction	Ref.
1	$Ar + e \rightarrow Ar(^3P_2) + e$	*Yamabe et al.* [1983]
2	$Ar + e \rightarrow Ar^+ + 2e$	*Yamabe et al.* [1983]
3	$N_2 + e \leftrightarrow N_2(v_1) + e$	*Phelps and Pitchford* [1985]
4	$N_2 + e \leftrightarrow N_2(v_2) + e$	*Phelps and Pitchford* [1985]
5	$N_2 + e \leftrightarrow N_2(v_3) + e$	*Phelps and Pitchford* [1985]
6	$N_2 + e \leftrightarrow N_2(v_4) + e$	*Phelps and Pitchford* [1985]
7	$N_2 + e \leftrightarrow N_2(v_5) + e$	*Phelps and Pitchford* [1985]
8	$N_2 + e \leftrightarrow N_2(v_6) + e$	*Phelps and Pitchford* [1985]
9	$N_2 + e \leftrightarrow N_2(v_7) + e$	*Phelps and Pitchford* [1985]
10	$N_2 + e \leftrightarrow N_2(v_8) + e$	*Phelps and Pitchford* [1985]
11	$N_2 + e \rightarrow N_2(A^3\Sigma_u^+) + e$	*Phelps and Pitchford* [1985]
12	$N_2 + e \rightarrow N_2(a^1\Pi_g) + e$	*Phelps and Pitchford* [1985]
13	$N_2 + e \rightarrow N_2(a'^1\Sigma_u^-) + e$	*Phelps and Pitchford* [1985]
14	$N_2 + e \rightarrow N_2(a''^1\Sigma_g^+) + e$	*Phelps and Pitchford* [1985]
15	$N_2 + e \rightarrow N_2(B^3\Pi_g) + e$	*Phelps and Pitchford* [1985]
16	$N_2 + e \rightarrow N_2(B'^3\Sigma_u^-) + e$	*Phelps and Pitchford* [1985]
17	$N_2 + e \rightarrow N_2(C^3\Pi_u) + e$	*Phelps and Pitchford* [1985]
18	$N_2 + e \rightarrow N_2(E^3\Sigma_g^+) + e$	*Phelps and Pitchford* [1985]
19	$N_2 + e \rightarrow N_2(W^3\Delta_u) + e$	*Phelps and Pitchford* [1985]
20	$N_2 + e \rightarrow N_2(w^1\Delta_u) + e$	*Phelps and Pitchford* [1985]
21	$N_2 + e \rightarrow N_2(rot) + e$	*Phelps and Pitchford* [1985]
22	$N_2 + e \rightarrow N_2^+ + 2e$	*Phelps and Pitchford* [1985]
23	$N_2 + e \rightarrow N_2^+(B^2\Sigma_u^+) + 2e$	*Phelps and Pitchford* [1985]
24	$N_2 + e \rightarrow N_2^+(A^2\Pi_u) + 2e$	*Shemansky and Broadfoot* [1971]
25	$N_2 + e \rightarrow N + N(^2D) + e$	*Phelps and Pitchford* [1985]
26	$O_2 + e \leftrightarrow O_2(v_1) + e$	*Lawton and Phelps* [1978]
27	$O_2 + e \leftrightarrow O_2(v_2) + e$	*Lawton and Phelps* [1978]
28	$O_2 + e \leftrightarrow O_2(v_3) + e$	*Lawton and Phelps* [1978]
29	$O_2 + e \leftrightarrow O_2(v_4) + e$	*Lawton and Phelps* [1978]
30	$O_2 + e \rightarrow O_2(A^3\Sigma_u^+) + e$	*Lawton and Phelps* [1978]
31	$O_2 + e \rightarrow O_2(a^1\Delta_g) + e$	*Lawton and Phelps* [1978]
32	$O_2 + e \rightarrow O_2(b^1\Sigma_g^+) + e$	*Lawton and Phelps* [1978]
33	$O_2 + e \rightarrow O_2^+ + 2e$	*Lawton and Phelps* [1978]

Table S3.2. *

EEDF and cross section dependent processes (cont.)

No.	Reaction	Ref.
34	$O_2 + e \rightarrow O_2(rot) + e$	*Lawton and Phelps* [1978]
35	$O_2 + e \rightarrow O^- + O$	*Lawton and Phelps* [1978]
36	$O_2 + e \rightarrow O + O + e$	*Lawton and Phelps* [1978]
37	$O_2 + e \rightarrow O + O(^1D) + e$	*Lawton and Phelps* [1978]
38	$O_2 + e \rightarrow O + O(^1S) + e$	*Lawton and Phelps* [1978]
39	$O_2 + O_2 + e \rightarrow O_2^- + O_2$	*Lawton and Phelps* [1978]
40	$O_3 + e \rightarrow O^- + O_2$	*Skalny et al.* [1996]
41	$O_3 + e \rightarrow O_2^- + O$	*Skalny et al.* [1996]
42	$O + e \rightarrow O(^1D) + e$	*Morgan* [2001]
43	$O + e \rightarrow O(^1S) + e$	*Morgan* [2001]
44	$N_2O + e \rightarrow N_2 + O^-$	*Hayashi* [1987]
45	$N_2O + e \rightarrow N_2O^+ + 2e$	*Hayashi* [1987]
46	$NO + e \rightarrow NO^+ + 2e$	*Phelps* [1969]
47	$CO_2 + e \leftrightarrow CO_2(01^10) + e$	*Phelps* [2010]
48	$CO_2 + e \leftrightarrow CO_2(00^01) + e$	*Phelps* [2010]
49	$CO_2 + e \leftrightarrow CO_2(02^00) + e$	*Phelps* [2010]
50	$CO_2 + e \leftrightarrow CO_2(02^20) + e$	*Phelps* [2010]
51	$CO_2 + e \leftrightarrow CO_2(10^00) + e$	*Phelps* [2010]
52	$CO_2 + e \leftrightarrow CO_2(03^10) + e$	*Phelps* [2010]
53	$CO_2 + e \leftrightarrow CO_2(03^30) + e$	*Phelps* [2010]
54	$CO_2 + e \leftrightarrow CO_2(11^10) + e$	*Phelps* [2010]
55	$CO_2 + e \leftrightarrow CO_2(04^00) + e$	*Phelps* [2010]
56	$CO_2 + e \leftrightarrow CO_2(04^20) + e$	*Phelps* [2010]
57	$CO_2 + e \leftrightarrow CO_2(12^00) + e$	*Phelps* [2010]
58	$CO_2 + e \leftrightarrow CO_2(04^40) + e$	*Phelps* [2010]
59	$CO_2 + e \leftrightarrow CO_2(12^20) + e$	*Phelps* [2010]
60	$CO_2 + e \leftrightarrow CO_2(20^00) + e$	*Phelps* [2010]
61	$CO_2 + e \leftrightarrow CO_2(01^11) + e$	*Phelps* [2010]
62	$CO_2 + e \leftrightarrow CO_2(02^01) + e$	*Phelps* [2010]
63	$CO_2 + e \leftrightarrow CO_2(02^21) + e$	*Phelps* [2010]
64	$CO_2 + e \leftrightarrow CO_2(10^01) + e$	*Phelps* [2010]
65	$CO_2 + e \leftrightarrow CO_2(03^11) + e$	*Phelps* [2010]
66	$CO_2 + e \leftrightarrow CO_2(03^31) + e$	*Phelps* [2010]
67	$CO_2 + e \leftrightarrow CO_2(11^11) + e$	*Phelps* [2010]
68	$CO_2 + e \leftrightarrow CO_2(00^02) + e$	*Phelps* [2010]
69	$CO_2 + e \leftrightarrow CO_2(04^01) + e$	*Phelps* [2010]
70	$CO_2 + e \leftrightarrow CO_2(04^21) + e$	*Phelps* [2010]
71	$CO_2 + e \leftrightarrow CO_2(04^41) + e$	*Phelps* [2010]
72	$CO_2 + e \leftrightarrow CO_2(12^01) + e$	*Phelps* [2010]
73	$CO_2 + e \leftrightarrow CO_2(12^21) + e$	*Phelps* [2010]
74	$CO_2 + e \leftrightarrow CO_2(20^01) + e$	*Phelps* [2010]
75	$CO_2 + e \rightarrow CO + O^-$	*Phelps* [2010]

Table S4. *

T_e dependent processes: ionization and dissociative ionization

No.	**Reaction**	**a**	**b**	**c**	**Ref.**
76	$NO_2 + e \rightarrow NO_2^+ + 2e$	2.6E-9	0.5	10.0	*Castillo* [2004]
77	$NO + e \rightarrow O^+ + N + 2e$	2.9E-9	0.5	21.0	*Castillo* [2004]
78	$NO_2 + e \rightarrow NO^+ + O + 2e$	8.1E-9	0.5	12.9	*Castillo* [2004]
79	$O_2 + e \rightarrow O^+ + O + 2e$	4.2E-9	0.5	23.0	*Castillo* [2004]

Table S5. *

T_e dependent processes: dissociation

No.	**Reaction**	**a**	**b**	**c**	**Ref.**
80	$e + O_3 \rightarrow O_2 + O + e$	1.0E-8			*Gudmundsson et al.* [2001]
81	$e + NO \rightarrow N + O + e$	7.4E-9		6.50	*Castillo* [2004]
82	$e + NO_2 \rightarrow NO + O + e$	5.6E-9		3.11	*Castillo* [2004]
83	$e + N_2O \rightarrow N_2 + O + e$	1.4E-9		1.67	*Castillo* [2004]
84	$e + N_2O \rightarrow N_2 + O(^1D) + e$	1.2E-9		3.64	*Castillo* [2004]
85	$e + N_2O \rightarrow NO + N + e$	1.0E-10		4.93	*Castillo* [2004]

Table S6. *

T_e dependent processes: attachment

No.	**Reaction**	**a**	**b**	**c**	**Ref.**
86	$e + O_2 + N_2 \rightarrow O_2^- + N_2$				
87	$e + O + O_2 \rightarrow O^- + O_2$	1.0E-31			*Capitelli et al.* [2000]
88	$e + O + N_2 \rightarrow O^- + N_2$	1.0E-31			*Capitelli et al.* [2000]
89	$e + NO_2 \rightarrow O^- + NO$	3.0E-11			*Kossyi et al.* [1992]
90	$e + NO_2 \rightarrow NO_2^-$	1.0E-11			*Kossyi et al.* [1992]
91	$e + O_3 + O_2 \rightarrow O_3^- + O_2$	1.0E-31			*Capitelli et al.* [2000]
92	$e + NO + N_2 \rightarrow NO^- + N_2$	1.0E-30			*Kossyi et al.* [1992]

Table S7. *

T_e dependent processes: recombination

No.	Reaction	a	b	c	Ref.
93	$e + N_2^+ \rightarrow N + N$	4.50E-8	-0.5		*Kossyi et al.* [1992]
94	$e + N_2^+ \rightarrow N + N(^2D)$	3.21E-8	-0.5		*Kossyi et al.* [1992]
95	$e + N_2^+ + O_2 \rightarrow N_2 + O_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
96	$e + O_2^+ \rightarrow O + O$	1.3006E-9	-0.7		*Peverall et al.* [2001]
97	$e + O_2^+ \rightarrow O + O(^1D)$	1.1334E-8	-0.7		*Peverall et al.* [2001]
98	$e + O_2^+ \rightarrow O(^1D) + O(^1D)$	4.645E-9	-0.7		*Peverall et al.* [2001]
99	$e + O_2^+ \rightarrow O(^1S) + O(^1D)$	1.3006E-9	-0.7		*Peverall et al.* [2001]
100	$e + NO^+ \rightarrow N + O$	1.66E-9	-1.5		*Kossyi et al.* [1992]
101	$e + NO^+ \rightarrow N(^2D) + O$	7.76E-9	-1.0		*Kossyi et al.* [1992]
102	$e + NO^+ + O_2 \rightarrow NO + O_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
103	$e + NO^+ + N_2 \rightarrow NO + N_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
104	$e + O_2^+ + O_2 \rightarrow O_2 + O_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
105	$e + N_4^+ \rightarrow N_2 + N + N$	3.13E-7	-0.41		*Whitaker et al.* [1981]
106	$e + N_4^+ \rightarrow N_2 + N_2$	3.21E-7	-0.5		*Kossyi et al.* [1992]
107	$e + O_4^+ \rightarrow O_2 + O + O$	2.30E-6			*Kruger and Olander* [1976]
108	$e + O_4^+ \rightarrow O_2 + O_2$	2.25E-7	-0.5		*Kossyi et al.* [1992]
109	$e + O^+ + N_2 \rightarrow O + N_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
110	$e + O^+ + e \rightarrow O + e$	7.18E-25	-4.5		*Kossyi et al.* [1992]
111	$e + O^+ + O_2 \rightarrow O + O_2$	2.49E-29	-1.5		*Kossyi et al.* [1992]
112	$e + N_2O^+ \rightarrow N_2 + O$	3.22E-8	-0.5		*Castillo* [2004]
113	$e + NO_2^+ \rightarrow NO + O$	3.22E-8	-0.5		*Castillo* [2004]
114	$e + N_2O_2^+ \rightarrow NO + NO$	3.61E-6	-0.5		*Starikovskaia et al.* [2001]
115	$e + N_2O_2^+ \rightarrow N_2 + O_2$	3.61E-6	-0.5		*Starikovskaia et al.* [2001]
116	$e + N_3^+ \rightarrow N_2 + N$	5.56E-7	-0.5		*Starikovskaia et al.* [2001]
117	$e + N_3^+ \rightarrow N_2(A^3\Sigma_u^+) + N$	6.91E-8	-0.5		*Starikovskaia et al.* [2001]
118	$e + N_3^+ \rightarrow N_2(B^3\Pi_g) + N$	6.91E-8	-0.5		*Starikovskaia et al.* [2001]
119	$e + e + N^+ \rightarrow e + N$	1.4E-8	-4.5		*Kossyi et al.* [1992]
120	$e + N^+ + O_2 \rightarrow N + O_2$	3.11E-23	-1.5		*Kossyi et al.* [1992]
121	$e + N^+ + N_2 \rightarrow N + N_2$	3.11E-23	-1.5		*Kossyi et al.* [1992]

Table S8. *

N_2 chemistry: vibrational-vibrational processes (VV1)

No.	Reaction	d	e	f	T_g(K)	Ref.
122	$N_2(v_1) + N_2(v_1) \leftrightarrow N_2(v_2) + N_2$	3.0E-14			200	*Cacciatore et al.* [2005]
123	$N_2(v_1) + N_2(v_2) \leftrightarrow N_2(v_3) + N_2$	4.0E-14			200	*Cacciatore et al.* [2005]
124	$N_2(v_1) + N_2(v_3) \leftrightarrow N_2(v_4) + N_2$	5.0E-14			200	*Cacciatore et al.* [2005]
125	$N_2(v_1) + N_2(v_4) \leftrightarrow N_2(v_5) + N_2$	5.6E-14			200	*Cacciatore et al.* [2005]
126	$N_2(v_1) + N_2(v_5) \leftrightarrow N_2(v_6) + N_2$	6.0E-14			200	*Cacciatore et al.* [2005]
127	$N_2(v_1) + N_2(v_6) \leftrightarrow N_2(v_7) + N_2$	5.6E-14			200	*Cacciatore et al.* [2005]
128	$N_2(v_1) + N_2(v_7) \leftrightarrow N_2(v_8) + N_2$	5.0E-14			200	*Cacciatore et al.* [2005]

Table S9. *

N_2 chemistry: vibrational-translational processes (VT1)

No.	Reaction	d	e	f	T_g(K)	Ref.
129	$N_2(v_1) + N_2 \leftrightarrow N_2 + N_2$	3.5E-21			500	*Kurnosov et al.* [2007]
130	$N_2(v_2) + N_2 \leftrightarrow N_2(v_1) + N_2$	6.5E-21			500	*Kurnosov et al.* [2007]
131	$N_2(v_3) + N_2 \leftrightarrow N_2(v_2) + N_2$	1.5E-20			500	*Kurnosov et al.* [2007]
132	$N_2(v_4) + N_2 \leftrightarrow N_2(v_3) + N_2$	2.5E-20			500	*Kurnosov et al.* [2007]
133	$N_2(v_5) + N_2 \leftrightarrow N_2(v_4) + N_2$	3.5E-20			500	*Kurnosov et al.* [2007]
134	$N_2(v_6) + N_2 \leftrightarrow N_2(v_5) + N_2$	7.0E-20			500	*Kurnosov et al.* [2007]
135	$N_2(v_7) + N_2 \leftrightarrow N_2(v_6) + N_2$	1.0E-19			500	*Kurnosov et al.* [2007]
136	$N_2(v_8) + N_2 \leftrightarrow N_2(v_7) + N_2$	1.0E-19			500	*Kurnosov et al.* [2007]

Table S10. *

N_2 chemistry: vibrational-translational processes (VT2)

No.	Reaction	d	e	f	g	T_g(K)	Ref.
137	$N_2(v_2) + O \leftrightarrow N_2(v_1) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
138	$N_2(v_3) + O \leftrightarrow N_2(v_2) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
139	$N_2(v_4) + O \leftrightarrow N_2(v_3) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
140	$N_2(v_5) + O \leftrightarrow N_2(v_4) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
141	$N_2(v_6) + O \leftrightarrow N_2(v_5) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
142	$N_2(v_7) + O \leftrightarrow N_2(v_6) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
143	$N_2(v_8) + O \leftrightarrow N_2(v_7) + O$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]

Table S11. *

N_2 chemistry: vibrational-translational processes (VT3)

No.	Reaction	d	e	f	g	T_g(K)	Ref.
144	$N_2(v_1) + N \leftrightarrow N_2 + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
145	$N_2(v_2) + N \leftrightarrow N_2(v_1) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
146	$N_2(v_3) + N \leftrightarrow N_2(v_2) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
147	$N_2(v_4) + N \leftrightarrow N_2(v_3) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
148	$N_2(v_5) + N \leftrightarrow N_2(v_4) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
149	$N_2(v_6) + N \leftrightarrow N_2(v_5) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
150	$N_2(v_7) + N \leftrightarrow N_2(v_6) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]
151	$N_2(v_8) + N \leftrightarrow N_2(v_7) + N$	2.3E-13	1280	2.7E-11	10840	300	*Capitelli et al.* [2000]

Table S12. *

N_2 chemistry: vibrational-translational processes (VT4)

No.	Reaction	d	e	f	T_g(K)	Ref.
152	$N_2(v_1) + CO_2 \leftrightarrow N_2 + CO_2$					*Capitelli et al.* [2000]
153	$N_2(v_1) + O \leftrightarrow N_2 + O$					*Capitelli et al.* [2000]
154	$N_2(v_1) + O_2 \leftrightarrow N_2 + O_2(v1)$					*Capitelli et al.* [2000]

Table S13. *

O_2 chemistry: vibrational-translational processes (VT5)

No.	Reaction	d	e	f	T_g(K)	Ref.
155	$O_2(v_1) + O \leftrightarrow O_2 + O$	4.5E-15				*Capitelli et al.* [2000]
156	$O_2(v_2) + O \leftrightarrow O_2(v_1) + O$	4.5E-15				*Capitelli et al.* [2000]
157	$O_2(v_3) + O \leftrightarrow O_2(v_2) + O$	4.5E-15				*Capitelli et al.* [2000]
158	$O_2(v_4) + O \leftrightarrow O_2(v_3) + O$	4.5E-15				*Capitelli et al.* [2000]

Table S14. *

O_2 chemistry: vibrational-translational processes (VT5)

No.	Reaction	d	e	f	T_g(K)	Ref.
159	$O_2(v_1) + O_2 \leftrightarrow O_2 + O_2$					*Capitelli et al.* [2000]
160	$O_2(v_1) + Ar \leftrightarrow O_2 + Ar$					*Capitelli et al.* [2000]

Table S15.1. *

Heavy particle chemistry: electronically excited species

No.	Reaction	d	e	f	Ref.
161	$Ar(^3P_2) + N_2 \rightarrow Ar + N + N$	3.6E-11			*Piper et al.* [1973]
162	$Ar(^3P_2) + N_2 \rightarrow Ar + N_2(C^3\Pi_u)$	3.0E-11			*Bouróne and Le Calvé* [1973]
163	$Ar(^3P_2) + O_2 \rightarrow Ar + O + O$	2.1E-10			*Piper et al.* [1973]
164	$Ar(^3P_2) + CO_2 \rightarrow Ar + CO + O$	5.3E-10			*Piper et al.* [1973]
165	$Ar(^3P_2) + NO \rightarrow Ar + N + O$	2.2E-10			*Piper et al.* [1973]
166	$Ar(^3P_2) + N_2O \rightarrow Ar + NO + N$	4.4E-10			*Piper et al.* [1973]
167	$Ar(^3P_2) + N_2O \rightarrow Ar + N_2 + O$	4.4E-10			*Piper et al.* [1973]
168	$N(^2D) + O_2 \rightarrow NO + O$	1.5E-12	-0.5		*Kossyi et al.* [1992]
169	$N(^2D) + O_2 \rightarrow O(^1D) + NO$	6.0E-12	-0.5		*Kossyi et al.* [1992]
170	$N(^2D) + O \rightarrow N + O(^1D)$	4.0E-13			*Capitelli et al.* [2000]
171	$N(^2D) + N_2 \rightarrow N + N_2$	6.0E-15			*Capitelli et al.* [2000]
172	$N(^2D) + NO \rightarrow N_2 + O$	1.8E-10			*Capitelli et al.* [2000]
173	$N(^2D) + N_2O \rightarrow NO + N_2$	3.5E-12			*Capitelli et al.* [2000]
174	$N(^2P) + N \rightarrow N(^2D) + N$	1.8E-12			*Capitelli et al.* [2000]
175	$N(^2P) + O_2 \rightarrow NO + O$	2.6E-12			*Capitelli et al.* [2000]
176	$N(^2P) + N_2 \rightarrow N + N_2$	2.0E-18			*Capitelli et al.* [2000]
177	$N(^2P) + NO \rightarrow N_2 + O$	3.0E-11			*Capitelli et al.* [2000]
178	$N_2(a^1\Pi_g) + O_2 \rightarrow N_2 + O + O$	2.8E-11			*Kossyi et al.* [1992]
179	$N_2(a^1\Pi_g) + N_2 \rightarrow N_2 + N_2$	2.0E-13			*Kossyi et al.* [1992]
180	$N_2(a^1\Pi_g) + NO \rightarrow N_2 + N + O$	3.6E-10			*Kossyi et al.* [1992]
181	$N_2(a'^1\Sigma_u^-) + N_2 \rightarrow N_2(B^3\Pi_g) + N_2$	2.0E-13			*Kossyi et al.* [1992]
182	$N_2(a'^1\Sigma_u^-) + O_2 \rightarrow N_2 + O + O$	2.8E-11			*Kossyi et al.* [1992]
183	$N_2(a'^1\Sigma_u^-) + O_2 \rightarrow N_2 + O + O(^1D)$	2.8E-11			*Kossyi et al.* [1992]
184	$N_2(a'^1\Sigma_u^-) + NO \rightarrow N_2 + N + O$	3.6E-10			*Kossyi et al.* [1992]
185	$N_2(a'^1\Sigma_u^-) + N_2(a'^1\Sigma_u^-) \rightarrow N_4^+ + e$	2.0E-10			*Kossyi et al.* [1992]
186	$N_2(a'^1\Sigma_u^-) + N_2(A^3\Sigma_u^+) \rightarrow N_4^+ + e$	5.0E-11			*Kossyi et al.* [1992]
187	$N_2(C^3\Pi_u) + N_2 \rightarrow N_2(a'^1\Sigma_u^-) + N_2$	1.0E-11			*Kossyi et al.* [1992]
188	$N_2(C^3\Pi_u) + O_2 \rightarrow N_2 + O + O(^1S)$	3.0E-10			*Capitelli et al.* [2000]
189	$N_2(C^3\Pi_u) + N_2 \rightarrow N_2(B^3\Pi_g) + N_2$	1.0E-11			*Kossyi et al.* [1992]
190	$N_2(C^3\Pi_u) + O_2 \rightarrow N_2 + O + O(^1D)$	2.5E-10			*Capitelli et al.* [2000]
191	$N_2(B^3\Pi_g) + N_2 \rightarrow N_2 + N_2$	2.0E-12			*Capitelli et al.* [2000]
192	$N_2(B^3\Pi_g) + N_2 \rightarrow N_2(A^3\Sigma_u^+) + N_2$	1.0E-11			*Capitelli et al.* [2000]
193	$N_2(B^3\Pi_g) + O_2 \rightarrow N_2 + O + O$	3.0E-10			*Capitelli et al.* [2000]
194	$N_2(A^3\Sigma_u^+) + N_2 \rightarrow N_2 + N_2$	3.0E-18			*Kossyi et al.* [1992]
195	$N_2(A^3\Sigma_u^+) + O_2 \rightarrow N_2 + O + O$	2.54E-12			*Kossyi et al.* [1992]
196	$N_2(A^3\Sigma_u^+) + O_2 \rightarrow N_2O + O$	7.8E-14			*Kossyi et al.* [1992]
197	$N_2(A^3\Sigma_u^+) + O \rightarrow NO + N(^2D)$	7.0E-12			*Capitelli et al.* [2000]
198	$N_2(A^3\Sigma_u^+) + O \rightarrow N_2 + O(^1S)$	3.0E-11			*Kossyi et al.* [1992]
199	$N_2(A^3\Sigma_u^+) + N \rightarrow N_2 + N(^2P)$	5.0E-11			*Capitelli et al.* [2000]
200	$N_2(A^3\Sigma_u^+) + N_2O \rightarrow N_2 + N + NO$	1.0E-11			*Kossyi et al.* [1992]

Table S15.2. *

Heavy particle chemistry: electronically excited species (cont.)

No.	Reaction	d	e	f	Ref.
201	$N_2(A^3\Sigma_u^+) + N \rightarrow N_2 + N$	2.0E-11			*Capitelli et al.* [2000]
202	$N_2(A^3\Sigma_u^+) + NO \rightarrow N_2 + NO$	7.0E-11			*Kossyi et al.* [1992]
203	$N_2(A^3\Sigma_u^+) + NO \rightarrow N_2 + NO(A^2\Delta^+)$	8.75E-11			*Simek* [2003]
204	$N_2(A^3\Sigma_u^+) + N_2(A^3\Sigma_u^+) \rightarrow N_2(C^3\Pi_u) + N_2$	1.6E-10			*Kossyi et al.* [1992]
205	$N_2(A^3\Sigma_u^+) + N_2(A^3\Sigma_u^+) \rightarrow N_2(B^3\Pi_g) + N_2$	7.7E-11			*Kossyi et al.* [1992]
206	$N_2(A^3\Sigma_u^+) + O_2 \rightarrow N_2 + O_2(b^1\Sigma_g^+)$	7.5E-13			*Kossyi et al.* [1992]
207	$O(^1D) + N_2 \rightarrow O + N_2$	1.8E-11		-107	*Kossyi et al.* [1992]
208	$O(^1D) + N_2 \rightarrow O + N_2(v1)$	2.4E-11			*Capitelli et al.* [2000]
209	$O(^1D) + O_2 \rightarrow O + O_2(b^1\Sigma_g^+)$	2.56E-11		-67	*Kossyi et al.* [1992]
210	$O(^1D) + O_2 \rightarrow O + O_2$	6.4E-12		-67	*Kossyi et al.* [1992]
211	$O(^1D) + O_2 \rightarrow O + O_2(a^1\Delta_g)$	1.0E-12			*Capitelli et al.* [2000]
212	$O(^1D) + N_2O \rightarrow NO + NO$	7.2E-11			*Kossyi et al.* [1992]
213	$O(^1D) + N_2O \rightarrow N_2O + O$	1.0E-12			*Starikovskaia et al.* [2001]
214	$O(^1D) + N_2O \rightarrow N_2 + O_2$	4.9E-11			*Castillo* [2004]
215	$O(^1D) + NO_2 \rightarrow O_2 + NO$	3.0E-10			*Castillo* [2004]
216	$O(^1D) + NO \rightarrow O_2 + N$	1.7E-10			*Kossyi et al.* [1992]
217	$O(^1D) + O_3 \rightarrow O + O + O_2$	1.2E-10			*Kossyi et al.* [1992]
218	$O(^1D) + O_3 \rightarrow O + O_3$	2.41E-10			*Manion et al.* [2013]
219	$O(^1D) + O_3 \rightarrow O_2 + O_2$	2.4E-10			*Kossyi et al.* [1992]
220	$O(^1D) + CO_2 \rightarrow O + CO_2$	7.4E-11		-120	*Manion et al.* [2013]
221	$O(^1D) + CO \rightarrow CO_2$	7.3E-11			*Manion et al.* [2013]
222	$O(^1S) + NO \rightarrow O + NO$	2.9E-10			*Capitelli et al.* [2000]
223	$O(^1S) + NO \rightarrow O(^1D) + NO$	5.1E-10			*Capitelli et al.* [2000]
224	$O(^1S) + O_2 \rightarrow O_2 + O$	4.3E-12	0	850	*Kossyi et al.* [1992]
225	$O(^1S) + O_2 \rightarrow O_2 + O(^1D)$	1.3E-12	0	850	*Kossyi et al.* [1992]
226	$O(^1S) + O_2(a^1\Delta_g) \rightarrow O_2 + O(^1D)$	3.6E-11			*Kossyi et al.* [1992]
227	$O(^1S) + O_2(a^1\Delta_g) \rightarrow O + O + O$	3.4E-11			*Kossyi et al.* [1992]
228	$O(^1S) + O_2(a^1\Delta_g) \rightarrow O + O_2(b^1\Sigma_g^+)$	1.3E-10			*Kossyi et al.* [1992]
229	$O(^1S) + O \rightarrow O(^1D) + O$	5.0E-11	0	301	*Kossyi et al.* [1992]
230	$O(^1S) + O \rightarrow O(^1D) + O(^1D)$	5.0E-11	0	301	*Kossyi et al.* [1992]
231	$O(^1S) + O_3 \rightarrow O_2 + O + O(^1D)$	2.9E-10			*Kossyi et al.* [1992]
232	$O(^1S) + O_3 \rightarrow O_2 + O_2$	2.9E-10			*Kossyi et al.* [1992]
233	$O(^1S) + CO_2 \rightarrow O + CO_2$	3.09E-13			*Manion et al.* [2013]
234	$O_2(a^1\Delta_g) + N \rightarrow O + NO$	2.0E-14	0	600	*Kossyi et al.* [1992]
235	$O_2(a^1\Delta_g) + O \rightarrow O + O_2$	7.0E-16			*Kossyi et al.* [1992]
236	$O_2(a^1\Delta_g) + O_2 \rightarrow O_2 + O_2$	2.2E-18	0.8		*Kossyi et al.* [1992]
237	$O_2(a^1\Delta_g) + N_2 \rightarrow O_2 + N_2$	1.4E-19			*Atkinson et al.* [2003]
238	$O_2(a^1\Delta_g) + NO \rightarrow O + NO_2$	4.88E-18			*Manion et al.* [2013]
239	$O_2(a^1\Delta_g) + O_3 \rightarrow O_2 + O_2 + O$	5.2E-11	0	2841	*Manion et al.* [2013]
240	$O_2(a^1\Delta_g) + NO \rightarrow O_2 + NO$	2.5E-11			*Kossyi et al.* [1992]
241	$O_2(b^1\Sigma_g^+) + N_2 \rightarrow O_2(a^1\Delta_g) + N_2$	4.9E-15		253	*Kossyi et al.* [1992]

Table S15.3. *

Heavy particle chemistry: electronically excited species (cont.)

No.	Reaction	d	e	f	Ref.
242	$O_2(b^1\Sigma_g^+) + O_2 \rightarrow O_2(a^1\Delta_g) + O_2$	3.73E-16	2.4	241	*Kossyi et al.* [1992]
243	$O_2(b^1\Sigma_g^+) + O \rightarrow O_2 + O$	8.0E-14			*Kossyi et al.* [1992]
244	$O_2(b^1\Sigma_g^+) + O_3 \rightarrow O_2(a^1\Delta_g) + O_2(a^1\Delta_g) + O$	1.8E-11			*Kossyi et al.* [1992]
245	$O_2(b^1\Sigma_g^+) + NO \rightarrow O_2(a^1\Delta_g) + NO$	4.0E-14			*Kossyi et al.* [1992]
246	$NO(A^2\Sigma^+) + O_2 \rightarrow NO + O_2$	1.62E-10			*Simek* [2003]
247	$NO(A^2\Sigma^+) + N_2 \rightarrow NO + N_2(A^3\Sigma_u^+)$	5.0E-14			*Thoman et al.* [1992]
248	$N_2^+(A^2\Pi_u) + N_2 \rightarrow N_2^+ + N_2$	7.5E-10			*Piper et al.* [1985]
249	$N_2^+(A^2\Pi_u) + O_2 \rightarrow N_2^+ + O_2$	6.2E-10			*Piper et al.* [1985]
250	$N_2^+(B^2\Sigma_u^+) + N_2 \rightarrow N_2^+ + N_2$	7.5E-11			*Piper et al.* [1985]
251	$N_2^+(B^2\Sigma_u^+) + O_2 \rightarrow N_2^+ + O_2$	6.2E-10			*Piper et al.* [1985]

Table S16. *

Ionic chemistry: ion-ion recombination

No.	Reaction	d	e	f	Ref.
252	$N_2O_2^+ + O_2^- \rightarrow NO + NO + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
253	$N_2O_2^+ + O_2^- \rightarrow N_2 + O_2 + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
254	$N_2O_2^+ + O^- \rightarrow NO + NO + O$	1.0E-7			*Starikovskaia et al.* [2001]
255	$N_2O_2^+ + O^- \rightarrow N_2 + O + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
256	$N_2O_2^+ + O_3^- \rightarrow NO + NO + O_3$	1.0E-7			*Starikovskaia et al.* [2001]
257	$N_2O_2^+ + O_3^- \rightarrow N_2 + O_2 + O_3$	1.0E-7			*Starikovskaia et al.* [2001]
258	$N_2O_2^+ + NO^- \rightarrow NO + NO + NO$	1.0E-7			*Starikovskaia et al.* [2001]
259	$N_2O_2^+ + NO^- \rightarrow NO + N_2 + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
260	$N_2O_2^+ + NO_2^- \rightarrow NO + NO + NO_2$	1.0E-7			*Starikovskaia et al.* [2001]
261	$N_2O_2^+ + NO_2^- \rightarrow NO_2 + N_2 + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
262	$N_2O_2^+ + NO_3^- \rightarrow NO + NO + NO_3$	1.0E-7			*Starikovskaia et al.* [2001]
263	$N_2O_2^+ + NO_3^- \rightarrow NO_3 + N_2 + O_2$	1.0E-7			*Starikovskaia et al.* [2001]
264	$N_3^+ + O^- \rightarrow N + N_2 + O$	1.0E-7			*Starikovskaia et al.* [2001]
265	$N_3^+ + O_3^- \rightarrow N + N_2 + O_3$	1.0E-7			*Starikovskaia et al.* [2001]
266	$N_3^+ + NO^- \rightarrow N + N_2 + NO$	1.0E-7			*Starikovskaia et al.* [2001]
267	$N_3^+ + NO_3^- \rightarrow N + N_2 + NO_3$	1.0E-7			*Starikovskaia et al.* [2001]
268	$O^- + N^+ \rightarrow O + N$	2.0E-7	0.5		*Kossyi et al.* [1992]
269	$O^- + NO^+ + O_2 \rightarrow NO_2 + O_2$	2.0E-25	-2.5		*Capitelli et al.* [2000]
270	$O^- + O_2^+ \rightarrow O + O_2$	2.0E-7	-0.5		*Capitelli et al.* [2000]
271	$O^- + O_2^+ + O_2 \rightarrow O_3 + O_2$	2.0E-25	-2.5		*Capitelli et al.* [2000]
272	$O_2^- + O_2^+ \rightarrow O_2 + O_2$	2.0E-7	-0.5		*Capitelli et al.* [2000]
273	$O_2^- + N^+ \rightarrow N + O_2$	2.0E-7	0.5		*Kossyi et al.* [1992]
274	$O_2^- + NO^+ \rightarrow O_2 + N + O$	1.0E-7			*Capitelli et al.* [2000]
275	$O_2^- + NO^+ + O_2 \rightarrow O_2 + O_2 + NO$	2.0E-25	-2.5		*Capitelli et al.* [2000]
276	$O_3^- + O^+ \rightarrow O_3 + O$	2.0E-7	-0.5		*Capitelli et al.* [2000]
277	$O_3^- + N^+ \rightarrow O_3 + N$	2.0E-7	0.5		*Kossyi et al.* [1992]
278	$O_3^- + O_2^+ \rightarrow O_3 + O_2$	2.0E-7	-0.5		*Capitelli et al.* [2000]
279	$O_3^- + O_2^+ \rightarrow O + O + O_3$	1.0E-7			*Capitelli et al.* [2000]
280	$O_3^- + NO^+ \rightarrow O_3 + NO$	2.0E-7	-0.5		*Capitelli et al.* [2000]
281	$NO^- + N^+ \rightarrow NO + N$	2.0E-7	0.5		*Kossyi et al.* [1992]
282	$NO_2^- + N^+ \rightarrow NO_2 + N$	2.0E-7	0.5		*Kossyi et al.* [1992]
283	$NO_3^- + N^+ \rightarrow NO_3 + N$	2.0E-7	0.5		*Kossyi et al.* [1992]
284	$NO_3^- + NO^+ \rightarrow NO_3 + N + O$	1.0E-7			*Capitelli et al.* [2000]
285	$NO_3^- + O_2^+ \rightarrow NO_3 + O + O$	1.0E-7			*Capitelli et al.* [2000]
286	$N_2O^- + N^+ \rightarrow N_2O + N$	2.0E-7	0.5		*Kossyi et al.* [1992]

Table S17.1. *

Ionic chemistry: positive ions

No.	Reaction	d	e	f	Ref.
287	$Ar^+ + N_2 \rightarrow Ar + N_2^+$	1.1E-11			*Lindinger et al.* [1981]
288	$Ar^+ + O_2 \rightarrow Ar + O_2^+$	4.6E-11			*Midey et al.* [2002]
289	$N^+ + N_2 + N_2 \rightarrow N_3^+ + N_2$	9.0E-30		-400	*Kossyi et al.* [1992]
290	$N^+ + O + N_2 \rightarrow NO^+ + N_2$	1.0E-29			*Kossyi et al.* [1992]
291	$N^+ + O + O_2 \rightarrow NO^+ + O_2$	1.0E-29			*Kossyi et al.* [1992]
292	$N^+ + N + N_2 \rightarrow N_2^+ + N_2$	1.0E-29			*Kossyi et al.* [1992]
293	$N^+ + N + O_2 \rightarrow N_2^+ + O_2$	1.0E-29			*Kossyi et al.* [1992]
294	$N^+ + O_2 \rightarrow O_2^+ + N$	2.8E-10			*Kossyi et al.* [1992]
295	$N^+ + O_2 \rightarrow NO^+ + O$	2.5E-10			*Kossyi et al.* [1992]
296	$N^+ + O_2 \rightarrow O^+ + NO$	2.8E-11			*Kossyi et al.* [1992]
297	$N^+ + O \rightarrow O^+ + N$	1.0E-12			*Kossyi et al.* [1992]
298	$N^+ + O_3 \rightarrow NO^+ + O_2$	5.0E-10			*Kossyi et al.* [1992]
299	$N^+ + NO \rightarrow NO^+ + N$	8.0E-10			*Kossyi et al.* [1992]
300	$N^+ + NO \rightarrow N_2^+ + O$	3.0E-12			*Kossyi et al.* [1992]
301	$N^+ + NO \rightarrow O^+ + N_2$	1.0E-12			*Kossyi et al.* [1992]
302	$N^+ + N_2O \rightarrow NO^+ + N_2$	5.5E-10			*Kossyi et al.* [1992]
303	$N_2^+ + N_2 + N \rightarrow N_3^+ + N_2$	9.0E-30		-400	*Capitelli et al.* [2000]
304	$N_2^+ + O \rightarrow N_2 + O^+$	1.0E-11	-0.2		*Kossyi et al.* [1992]
305	$N_2^+ + O \rightarrow NO^+ + N$	1.3E-10	-0.5		*Kossyi et al.* [1992]
306	$N_2^+ + O_2 \rightarrow N_2 + O_2^+$	6.0E-11	-0.5		*Kossyi et al.* [1992]
307	$N_2^+ + O_3 \rightarrow O_2^+ + O + N_2$	1.0E-10			*Capitelli et al.* [2000]
308	$N_2^+ + N_2O \rightarrow N_2O^+ + N_2$	5.0E-10			*Capitelli et al.* [2000]
309	$N_2^+ + N_2O \rightarrow NO^+ + N + N_2$	4.0E-10			*Capitelli et al.* [2000]
310	$N_2^+ + NO \rightarrow NO^+ + N_2$	3.3E-10			*Kossyi et al.* [1992]
311	$N_2^+ + N_2 + N_2 \rightarrow N_4^+ + N_2$	5.2E-29	-2.2		*Capitelli et al.* [2000]
312	$N_3^+ + N_2(A^3\Sigma_u^+) \rightarrow N_3^+ + N_2$	3.0E-10			*Starikovskaia et al.* [2001]
313	$N_3^+ + O_2 \rightarrow O_2^+ + N + N_2$	2.3E-11			*Kossyi et al.* [1992]
314	$N_3^+ + O_2 \rightarrow NO_2^+ + N_2$	4.4E-11			*Kossyi et al.* [1992]
315	$N_3^+ + N \rightarrow N_2^+ + N_2$	6.6E-11			*Kossyi et al.* [1992]
316	$N_3^+ + NO \rightarrow NO^+ + N + N_2$	7.0E-11			*Kossyi et al.* [1992]
317	$N_3^+ + NO \rightarrow N_2 + N_2O^+$	7.0E-11			*Starikovskaia et al.* [2001]
318	$N_4^+ + O_2 \rightarrow O_2^+ + N_2 + N_2$	2.5E-10			*Capitelli et al.* [2000]
319	$N_4^+ + O \rightarrow O^+ + N_2 + N_2$	2.5E-10			*Capitelli et al.* [2000]

Table S17.2. *

Ionic chemistry: positive ions (cont.)

No.	**Reaction**	**d**	**e**	**f**	**Ref.**
320	$O^+ + N_2 \rightarrow NO^+ + N$	3.0E-12			*Kossyi et al.* [1992]
321	$O^+ + O_2 \rightarrow O_2^+ + O$	2.0E-11	-0.5		*Capitelli et al.* [2000]
322	$O^+ + O_3 \rightarrow O_2^+ + O_2$	1.0E-10			*Capitelli et al.* [2000]
323	$O^+ + NO \rightarrow NO^+ + O$	2.4E-11			*Capitelli et al.* [2000]
324	$O^+ + NO \rightarrow O_2^+ + N$	3.0E-12			*Capitelli et al.* [2000]
325	$O^+ + N_2O \rightarrow NO^+ + NO$	2.3E-10			*Capitelli et al.* [2000]
326	$O^+ + N_2O \rightarrow O_2^+ + N_2$	2.0E-11			*Capitelli et al.* [2000]
327	$O^+ + N_2O \rightarrow N_2O^+ + O$	2.2E-11			*Capitelli et al.* [2000]
328	$O^+ + NO_2 \rightarrow NO_2^+ + O$	1.6E-9			*Capitelli et al.* [2000]
329	$O_2^+ + N \rightarrow NO^+ + O$	1.2E-10			*Kossyi et al.* [1992]
330	$O_2^+ + N_2 \rightarrow NO^+ + NO$	1.0E-17			*Kossyi et al.* [1992]
331	$O_2^+ + NO_2 \rightarrow NO^+ + O_3$	1.0E-11			*Capitelli et al.* [2000]
332	$O_2^+ + NO_2 \rightarrow NO_2^+ + O_2$	6.6E-10			*Capitelli et al.* [2000]
333	$O_2^+ + NO \rightarrow NO^+ + O_2$	4.4E-10			*Kossyi et al.* [1992]
334	$O_2^+ + O_2 + O_2 \rightarrow O_4^+ + O_2$	2.4E-30	-3.2		*Kossyi et al.* [1992]
335	$O_2^+ + N_2 + N_2 \rightarrow N_2O_2^+ + N_2$	9.0E-31	-2		*Kossyi et al.* [1992]
336	$O_4^+ + O_2(a^1\Delta_g) \rightarrow O_2^+ + O_2 + O_2$	1.0E-10			*Kossyi et al.* [1992]
337	$O_4^+ + O_2(b^1\Sigma_g^+) \rightarrow O_2^+ + O_2 + O_2$	1.0E-10			*Kossyi et al.* [1992]
338	$O_4^+ + N_2 \rightarrow N_2O_2^+ + O_2$	4.6E-12	2.5	2650	*Capitelli et al.* [2000]
339	$O_4^+ + NO \rightarrow NO^+ + O_2 + O_2$	1.0E-10			*Kossyi et al.* [1992]
340	$O_4^+ + O \rightarrow O_2^+ + O_3$	3.0E-10			*Kossyi et al.* [1992]
341	$O_4^+ + O_2 \rightarrow O_2^+ + O_2 + O_2$	3.3E-6	-4	5030	*Kossyi et al.* [1992]
342	$NO_2^+ + NO \rightarrow NO^+ + NO_2$	2.9E-10			*Capitelli et al.* [2000]
343	$N_2O^+ + NO \rightarrow NO^+ + N_2O$	2.9E-10			*Capitelli et al.* [2000]
344	$N_2O_2^+ + N_2 \rightarrow O_2^+ + N_2 + N_2$	1.1E-6	-5.3	2357	*Capitelli et al.* [2000]
345	$N_2O_2^+ + O_2 \rightarrow O_4^+ + N_2$	1.0E-10			*Capitelli et al.* [2000]

Table S18.1. *

Ionic chemistry: negative ions

No.	**Reaction**	**d**	**e**	**f**	**Ref.**
346	$O^- + N_2 \rightarrow N_2O + e$				*Rayment and Moruzzi* [1978]
347	$O^- + O_2 \rightarrow O_3 + e$	5.0E-15			*Kossyi et al.* [1992]
348	$O^- + O \rightarrow O_2 + e$	5.0E-10			*Kossyi et al.* [1992]
349	$O^- + N_2(A^3\Sigma_u^+) \rightarrow O + N_2 + e$	2.2E-9			*Kossyi et al.* [1992]
350	$O^- + O_2(a^1\Delta_g) \rightarrow O_3 + e$	3.0E-10			*Kossyi et al.* [1992]
351	$O^- + O_3 \rightarrow O_2 + O_2 + e$	5.3E-10			*Kossyi et al.* [1992]
352	$O^- + NO \rightarrow NO_2 + e$	2.6E-10			*Kossyi et al.* [1992]
353	$O^- + N_2O \rightarrow NO^- + NO$	2.1E-10			*Kossyi et al.* [1992]
354	$O^- + NO_2 \rightarrow NO_2^- + O$	1.2E-9			*Kossyi et al.* [1992]
355	$O^- + O_2 + O_2 \rightarrow O_3^- + O_2$	1.1E-30	-1		*Kossyi et al.* [1992]
356	$O^- + O_3 \rightarrow O_3^- + O$	5.3E-10			*Kossyi et al.* [1992]
357	$O^- + O_2(a^1\Delta_g) \rightarrow O_2^- + O$	1.0E-10			*Capitelli et al.* [2000]
358	$O^- + N_2(B^3\Pi_g) \rightarrow O + N_2 + e$	1.9E-9			*Capitelli et al.* [2000]
359	$O^- + CO \rightarrow CO_2 + e$	6.0E-10	-0.32		*Bortner and Baurer* [1972]
360	$O^- + CO_2 + Ar \rightarrow CO_3^- + Ar$	3.1E-28	-0.5		*Brasseur and Solomon* [1986]
361	$O^- + CO_2 + CO_2 \rightarrow CO_3^- + CO_2$	3.1E-28	-0.5		*Brasseur and Solomon* [1986]
362	$O_2^- + O \rightarrow O^- + O_2$	3.3E-10			*Kossyi et al.* [1992]
363	$O_2^- + O \rightarrow O_3 + e$	1.5E-10			*Kossyi et al.* [1992]
364	$O_2^- + O_2 \rightarrow O_2 + O_2 + e$	2.7E-18	0.5	5590	*Kossyi et al.* [1992]
365	$O_2^- + O_2(a^1\Delta_g) \rightarrow O_2 + O_2 + e$	2.0E-10			*Kossyi et al.* [1992]
366	$O_2^- + O_2(b^1\Sigma_g^+) \rightarrow O_2 + O_2 + e$	3.6E-10			*Kossyi et al.* [1992]
367	$O_2^- + N_2 \rightarrow O_2 + N_2 + e$	1.9E-12	0.5	4990	*Capitelli et al.* [2000]
368	$O_2^- + N \rightarrow NO_2 + e$	5.0E-10			*Kossyi et al.* [1992]
369	$O_2^- + NO_2 \rightarrow O_2 + NO_2^-$	8.0E-10			*Kossyi et al.* [1992]
370	$O_2^- + O_3 \rightarrow O_2 + O_3^-$	4.0E-10			*Kossyi et al.* [1992]
371	$O_2^- + N_2(A^3\Sigma_u^+) \rightarrow O_2 + N_2 + e$	2.1E-9			*Capitelli et al.* [2000]
372	$O_2^- + N_2(B^3\Pi_g) \rightarrow O_2 + N_2 + e$	2.5E-9			*Capitelli et al.* [2000]
373	$O_3^- + O \rightarrow O_2^- + O_2$	2.5E-10			*Kazil* [2002]
374	$O_3^- + O \rightarrow O_2 + O_2 + e$	1.4E-10			*Kossyi et al.* [1992]
375	$O_3^- + NO \rightarrow NO_3^- + O$	1.0E-11			*Kossyi et al.* [1992]
376	$O_3^- + NO_2 \rightarrow O_3 + NO_2^-$	7.0E-10			*Kossyi et al.* [1992]
377	$O_3^- + NO_2 \rightarrow NO_3^- + O_2$	2.0E-11			*Kossyi et al.* [1992]
378	$O_3^- + NO \rightarrow O_2 + NO_2^-$	2.6E-11			*Capitelli et al.* [2000]
379	$O_3^- + O_3 \rightarrow O_2 + O_2 + O_2 + e$	1.0E-10			*Kazil* [2002]
380	$O_3^- + CO_2 \rightarrow CO_3^- + O_2$	5.5E-10	0.5		*Brasseur and Solomon* [1986]

Table S18.2. *

Ionic chemistry: negative ions (cont.)

No.	Reaction	d	e	f	Ref.
381	$NO^- + O_2 \rightarrow O_2^- + NO$	5.0E-10			*Kossyi et al.* [1992]
382	$NO^- + NO_2 \rightarrow NO_2^- + NO$	7.4E-16			*Kossyi et al.* [1992]
383	$NO^- + N_2O \rightarrow NO_2^- + N_2$	2.8E-14			*Kossyi et al.* [1992]
384	$NO^- + CO_2 \rightarrow NO + CO_2 + e$	8.3E-12			*Albritton* [1978]
385	$NO^- + CO \rightarrow NO + CO + e$	5.0E-13			*Albritton* [1978]
386	$NO^- + N_2O \rightarrow NO + N_2O + e$	5.1E-12			*Albritton* [1978]
387	$NO^- + NO \rightarrow NO + NO + e$	5.0E-12			*Albritton* [1978]
388	$NO_2^- + O_3 \rightarrow O_2 + NO_3^-$	1.8E-11			*Kossyi et al.* [1992]
389	$NO_2^- + NO_2 \rightarrow NO_3^- + NO$	4.0E-12			*Capitelli et al.* [2000]
390	$NO_2^- + NO_3 \rightarrow NO_2 + NO_3^-$	5.0E-10			*Capitelli et al.* [2000]
391	$NO_3^- + NO \rightarrow NO_2^- + NO_2$	3.0E-15			*Capitelli et al.* [2000]
392	$CO_3^- + O \rightarrow O_2^- + CO_2$	1.1E-10	0.5		*Brasseur and Solomon* [1986]
393	$CO_3^- + NO \rightarrow NO_2^- + CO_2$	1.1E-11	0.5		*Brasseur and Solomon* [1986]
394	$CO_3^- + NO_2 \rightarrow NO_3^- + CO_2$	2.0E-10	0.5		*Brasseur and Solomon* [1986]

Table S19.1. *

Heavy particle chemistry: ground neutrals

No.	**Reaction**	**d**	**e**	**f**	**Ref.**
395	$N + O_2 \rightarrow NO + O$	1.0E-11	0	3473	*Kossyi et al.* [1992]
396	$N + NO_2 \rightarrow O + O + N_2$	9.1E-13			*Capitelli et al.* [2000]
397	$N + NO_2 \rightarrow O + N_2O$	3.0E-12			*Capitelli et al.* [2000]
398	$N + NO_2 \rightarrow O_2 + N_2$	7.0E-13			*Capitelli et al.* [2000]
399	$N + NO_2 \rightarrow NO + NO$	2.3E-13			*Capitelli et al.* [2000]
400	$NO_2 + NO_3 + O_2 \rightarrow N_2O_5 + O_2$	5.9E-29	-1.27		*Starikovskaia et al.* [2001]
401	$NO_2 + NO_3 + N_2 \rightarrow N_2O_5 + N_2$	5.9E-29	-1.27		*Starikovskaia et al.* [2001]
402	$NO_2 + NO_3 + NO \rightarrow N_2O_5 + NO$	5.9E-29	-1.27		*Starikovskaia et al.* [2001]
403	$NO_2 + NO_3 + N_2O_5 \rightarrow N_2O_5 + N_2O_5$	5.9E-29	-1.27		*Starikovskaia et al.* [2001]
404	$N_2O_5 + N_2 \rightarrow NO_2 + NO_3 + N_2$	2.1E-11	-4.4	11080	*Capitelli et al.* [2000]
405	$N_2O_5 + O_2 \rightarrow NO_2 + NO_3 + O_2$	2.1E-11	-4.4	11080	*Capitelli et al.* [2000]
406	$N_2O_5 + Ar \rightarrow NO_2 + NO_3 + Ar$	2.1E-11	-4.4	11080	*Capitelli et al.* [2000]
407	$N_2O_5 + O \rightarrow N_2 + O_2 + O_2 + O_2$	3.0E-16	0.5		*Kossyi et al.* [1992]
408	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13	0	2450	*Capitelli et al.* [2000]
409	$O + NO_2 + N_2 \rightarrow NO_3 + N_2$	8.9E-32	-2.0		*Capitelli et al.* [2000]
410	$O + NO_2 + O_2 \rightarrow NO_3 + O_2$	8.9E-32	-2.0		*Capitelli et al.* [2000]
411	$O + NO_3 \rightarrow NO_2 + O_2$	1.0E-11			*Kossyi et al.* [1992]
412	$NO + NO_3 \rightarrow NO_2 + NO_2$	1.11E-11			*Capitelli et al.* [2000]
413	$O + NO_2 \rightarrow O_2 + NO$	9.09E-12	0.18		*Kossyi et al.* [1992]
414	$N + O_3 \rightarrow NO + O_2$	2.0E-16			*Kossyi et al.* [1992]
415	$O + NO + N_2 \rightarrow NO_2 + N_2$	1.2E-31	-1.682		*Capitelli et al.* [2000]
416	$O + NO + O_2 \rightarrow NO_2 + O_2$	9.3E-32	-1.682		*Capitelli et al.* [2000]
417	$O + NO \rightarrow O_2 + N$	8.93E-13	1	19494.5	*Manion et al.* [2013]
418	$O_3 + NO \rightarrow O_2 + NO_2$	4.3E-12	0	1560	*Kossyi et al.* [1992]
419	$N + N + N_2 \rightarrow N_2 + N_2$	8.27E-34	0	500	*Kossyi et al.* [1992]
420	$N + N + N \rightarrow N_2 + N$	3.31E-27	-1.5		*Starikovskaia et al.* [2001]

Table S19.2. *

Heavy particle chemistry: ground neutrals (cont.)

No.	Reaction	d	e	f	Ref.
421	$O + O + N_2 \rightarrow O_2 + N_2$	6.49E-35	0	1039	*Capitelli et al.* [2000]
422	$O + O + N \rightarrow O_2 + N$	3.2E-33	-0.41		*Capitelli et al.* [2000]
423	$O + O_2 + O_2 \rightarrow O_3 + O_2$	7.6E-34	-1.9		*Capitelli et al.* [2000]
424	$O + O_2 + N_2 \rightarrow O_3 + N_2$	5.8E-34	-2.8		*Capitelli et al.* [2000]
425	$O + O_2 + O_3 \rightarrow O_3 + O_3$	1.5E-34	0	750	*Starikovskaia et al.* [2001]
426	$O + O_2 + O \rightarrow O_3 + O$	2.15E-34	0	345	*Capitelli et al.* [2000]
427	$O + O_3 \rightarrow O_2 + O_2$	2.0E-11	0	2300	*Kossyi et al.* [1992]
428	$N + O + N_2 \rightarrow NO + N_2$	1.0E-32	-0.5		*Capitelli et al.* [2000]
429	$N + O + O_2 \rightarrow NO + O_2$	1.0E-32	-0.5		*Capitelli et al.* [2000]
430	$NO_2 + N_2 \rightarrow NO + O + N_2$	6.8E-6	-2	36180	*Capitelli et al.* [2000]
431	$NO_2 + O_2 \rightarrow NO + O + O_2$	5.3E-6	-2	36180	*Capitelli et al.* [2000]
432	$NO_2 + NO \rightarrow NO + NO + O$	5.3E-5	-2	36180	*Capitelli et al.* [2000]
433	$NO_2 + NO_2 \rightarrow NO + O + NO_2$	4.0E-5	-2	36180	*Capitelli et al.* [2000]
434	$NO_2 + Ar \rightarrow NO + O + Ar$	4.0E-6	-2	36180	*Capitelli et al.* [2000]
435	$NO_3 + N_2 \rightarrow NO_2 + O + N_2$	3.1E-5	-2	25000	*Capitelli et al.* [2000]
436	$NO_3 + O_2 \rightarrow NO_2 + O + O_2$	3.1E-5	-2	25000	*Capitelli et al.* [2000]
437	$NO_3 + NO \rightarrow NO_2 + O + NO$	3.1E-5	-2	25000	*Capitelli et al.* [2000]
438	$NO_3 + N \rightarrow NO_2 + O + N$	3.1E-4	-2	25000	*Capitelli et al.* [2000]
439	$NO_3 + O \rightarrow NO_2 + O + O$	3.1E-4	-2	25000	*Capitelli et al.* [2000]
440	$NO_3 + Ar \rightarrow NO_2 + O + Ar$	3.72E-5	-2	25000	*Capitelli et al.* [2000]
441	$NO_3 + N_2 \rightarrow NO + O_2 + N_2$	6.2E-5	-2	25000	*Capitelli et al.* [2000]
442	$NO_3 + O_2 \rightarrow NO + O_2 + O_2$	6.2E-5	-2	25000	*Capitelli et al.* [2000]
443	$NO_3 + NO \rightarrow NO + O_2 + NO$	6.2E-5	-2	25000	*Capitelli et al.* [2000]
444	$NO_3 + N \rightarrow NO + O_2 + N$	7.44E-4	-2	25000	*Capitelli et al.* [2000]
445	$NO_3 + O \rightarrow NO + O_2 + O$	7.44E-4	-2	25000	*Capitelli et al.* [2000]
446	$NO_3 + Ar \rightarrow NO + O_2 + Ar$	7.44E-5	-2	25000	*Capitelli et al.* [2000]
447	$CO_2 + O \rightarrow CO + O_2$	2.81E-11	0	26474	*Manion et al.* [2013]
448	$CO + O + N_2 \rightarrow CO_2 + N_2$	1.7E-33	0	1510	*Manion et al.* [2013]
449	$CO + O_2 \rightarrow CO_2 + O$	4.2E-12	0	24000	*Manion et al.* [2013]
450	$CO + NO_2 \rightarrow CO_2 + NO$	1.48E-10	0	16967	*Manion et al.* [2013]

Table S20. *

CO_2 chemistry: vibrational-translational processes (VT1)

No.	Reaction	g	h	i	j	Ref.
451	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(02^00) + CO_2$	0.18	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
452	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(02^20) + CO_2$	0.18	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
453	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(10^00) + CO_2$	0.18	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
454	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(03^10) + CO_2$	0.82	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
455	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(03^30) + CO_2$	0.82	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
456	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(11^10) + CO_2$	0.82	7.3E-14	-850.3	86523	*Lepoutre et al.* [1977]
457	$CO_2(00^01) + N_2 \leftrightarrow CO_2(02^00) + N_2$	0.1	2.2E-15	1.14E-10	-76.75	*Taine and Lepoutre* [1980]
458	$CO_2(00^01) + N_2 \leftrightarrow CO_2(02^20) + N_2$	0.1	2.2E-15	1.14E-10	-76.75	*Taine and Lepoutre* [1980]
459	$CO_2(00^01) + N_2 \leftrightarrow CO_2(10^00) + N_2$	0.1	2.2E-15	1.14E-10	-76.75	*Taine and Lepoutre* [1980]
460	$CO_2(00^01) + N_2 \leftrightarrow CO_2(03^10) + N_2$	0.9	7.3E-14	-850.3	86523	*Taine and Lepoutre* [1980]
461	$CO_2(00^01) + N_2 \leftrightarrow CO_2(03^30) + N_2$	0.9	7.3E-14	-850.3	86523	*Taine and Lepoutre* [1980]
462	$CO_2(00^01) + N_2 \leftrightarrow CO_2(11^10) + N_2$	0.9	7.3E-14	-850.3	86523	*Taine and Lepoutre* [1980]
463	$CO_2(00^01) + CO \leftrightarrow CO_2(03^10) + CO$	1.0	1.7E-14	-448.3	53636	*Starr and Hankock* [1975]
464	$CO_2(00^01) + CO \leftrightarrow CO_2(03^30) + CO$	1.0	1.7E-14	-448.3	53636	*Starr and Hankock* [1975]
465	$CO_2(00^01) + CO \leftrightarrow CO_2(11^10) + CO$	1.0	1.7E-14	-448.3	53636	*Starr and Hankock* [1975]
466	$CO_2(00^01) + O \leftrightarrow CO_2(02^00) + O$	0.1	2.0E-13			*Buchwald and Hunten* [1975]
467	$CO_2(00^01) + O \leftrightarrow CO_2(02^20) + O$	0.1	2.0E-13			*Buchwald and Hunten* [1975]
468	$CO_2(00^01) + O \leftrightarrow CO_2(10^00) + O$	0.1	2.0E-13			*Buchwald and Hunten* [1975]
469	$CO_2(00^01) + O \leftrightarrow CO_2(03^10) + O$	0.9	2.0E-13			*Buchwald and Hunten* [1975]
470	$CO_2(00^01) + O \leftrightarrow CO_2(03^30) + O$	0.9	2.0E-13			*Buchwald and Hunten* [1975]
471	$CO_2(00^01) + O \leftrightarrow CO_2(11^10) + O$	0.9	2.0E-13			*Buchwald and Hunten* [1975]

Table S21. *

CO_2 chemistry: vibrational-translational processes (VT2)

No.	Reaction	g	h	i	j	Ref.
472	$CO_2(01^10) + CO_2 \leftrightarrow CO_2 + CO_2$	1.0	4.2E-12	-2988	303930	*López-Valverde* [1980]
473	$CO_2(02^00) + CO_2 \leftrightarrow CO_2(01^10) + CO_2$	2.5	4.2E-12	-2988	303930	*López-Valverde* [1980]
474	$CO_2(02^20) + CO_2 \leftrightarrow CO_2(01^10) + CO_2$	2.5	4.2E-12	-2988	303930	*López-Valverde* [1980]
475	$CO_2(10^00) + CO_2 \leftrightarrow CO_2(01^10) + CO_2$	2.5	4.2E-12	-2988	303930	*López-Valverde* [1980]
476	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
477	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(02^20) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
478	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(10^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
479	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(02^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
480	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(02^20) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
481	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(10^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
482	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
483	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(02^20) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
484	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(10^00) + CO_2$	3.75	4.2E-12	-2988	303930	*López-Valverde* [1980]
485	$CO_2(01^10) + N_2 \leftrightarrow CO_2 + N_2$	1.0	2.1E-12	-2659	223052	*López-Valverde* [1980]
486	$CO_2(02^00) + N_2 \leftrightarrow CO_2(01^10) + N_2$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
487	$CO_2(02^20) + N_2 \leftrightarrow CO_2(01^10) + N_2$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
488	$CO_2(10^00) + N_2 \leftrightarrow CO_2(01^10) + N_2$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
489	$CO_2(03^10) + N_2 \leftrightarrow CO_2(02^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
490	$CO_2(03^10) + N_2 \leftrightarrow CO_2(02^20) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
491	$CO_2(03^10) + N_2 \leftrightarrow CO_2(10^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
492	$CO_2(03^30) + N_2 \leftrightarrow CO_2(02^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
493	$CO_2(03^30) + N_2 \leftrightarrow CO_2(02^20) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
494	$CO_2(03^30) + N_2 \leftrightarrow CO_2(10^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
495	$CO_2(11^10) + N_2 \leftrightarrow CO_2(02^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
496	$CO_2(11^10) + N_2 \leftrightarrow CO_2(02^20) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
497	$CO_2(11^10) + N_2 \leftrightarrow CO_2(10^00) + N_2$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
498	$CO_2(01^10) + CO \leftrightarrow CO_2 + CO$	1.0	2.1E-12	-2659	223052	*López-Valverde* [1980]
499	$CO_2(02^00) + CO \leftrightarrow CO_2(01^10) + CO$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
500	$CO_2(02^20) + CO \leftrightarrow CO_2(01^10) + CO$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
501	$CO_2(10^00) + CO \leftrightarrow CO_2(01^10) + CO$	2.5	2.1E-12	-2659	223052	*López-Valverde* [1980]
502	$CO_2(03^10) + CO \leftrightarrow CO_2(02^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
503	$CO_2(03^10) + CO \leftrightarrow CO_2(02^20) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
504	$CO_2(03^10) + CO \leftrightarrow CO_2(10^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
505	$CO_2(03^30) + CO \leftrightarrow CO_2(02^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
506	$CO_2(03^30) + CO \leftrightarrow CO_2(02^20) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
507	$CO_2(03^30) + CO \leftrightarrow CO_2(10^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
508	$CO_2(11^10) + CO \leftrightarrow CO_2(02^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
509	$CO_2(11^10) + CO \leftrightarrow CO_2(02^20) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
510	$CO_2(11^10) + CO \leftrightarrow CO_2(10^00) + CO$	3.75	2.1E-12	-2659	223052	*López-Valverde* [1980]
511	$CO_2(01^10) + O \leftrightarrow CO_2 + O$	1.0	3.0E-12			*López-Valverde* [1980]
512	$CO_2(02^00) + O \leftrightarrow CO_2(01^10) + O$	2.0	3.0E-12			*López-Valverde* [1980]
513	$CO_2(02^20) + O \leftrightarrow CO_2(01^10) + O$	2.0	3.0E-12			*López-Valverde* [1980]
514	$CO_2(10^00) + O \leftrightarrow CO_2(01^10) + O$	2.0	3.0E-12			*López-Valverde* [1980]
515	$CO_2(03^10) + O \leftrightarrow CO_2(02^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]
516	$CO_2(03^10) + O \leftrightarrow CO_2(02^20) + O$	3.4	3.0E-12			*López-Valverde* [1980]
517	$CO_2(03^10) + O \leftrightarrow CO_2(10^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]
518	$CO_2(03^30) + O \leftrightarrow CO_2(02^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]
519	$CO_2(03^30) + O \leftrightarrow CO_2(02^20) + O$	3.4	3.0E-12			*López-Valverde* [1980]
520	$CO_2(03^30) + O \leftrightarrow CO_2(10^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]
521	$CO_2(11^10) + O \leftrightarrow CO_2(02^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]
522	$CO_2(11^10) + O \leftrightarrow CO_2(02^20) + O$	3.4	3.0E-12			*López-Valverde* [1980]
523	$CO_2(11^10) + O \leftrightarrow CO_2(10^00) + O$	3.4	3.0E-12			*López-Valverde* [1980]

Table S22. *

CO_2 chemistry: vibrational-translational processes (VT3)

No.	Reaction	g	h	i	j	Ref.
524	$CO_2(10^01) + CO_2 \leftrightarrow CO_2(02^01) + CO_2$	1.0	1.6E-12			*Orr and Smith* [1987]
525	$CO_2(10^01) + N_2 \leftrightarrow CO_2(02^01) + N_2$	1.0	1.6E-12			*Orr and Smith* [1987]
526	$CO_2(10^01) + CO_2 \leftrightarrow CO_2(02^21) + CO_2$	1.0	5.0E-12			*Orr and Smith* [1987]
527	$CO_2(10^01) + N_2 \leftrightarrow CO_2(02^01) + N_2$	1.0	5.0E-12			*Orr and Smith* [1987]
528	$CO_2(02^20) + CO_2 \leftrightarrow CO_2(02^01) + CO_2$	1.0	5.0E-12			*Orr and Smith* [1987]
529	$CO_2(02^20) + N_2 \leftrightarrow CO_2(02^01) + N_2$	1.0	5.0E-12			*Orr and Smith* [1987]

Table S23. *

CO_2 chemistry: vibrational-vibrational processes (VV1)

No.	Reaction	g	h	i	j	Ref.
530	$CO_2(02^00) + CO_2 \leftrightarrow CO_2(01^10) + CO_2(01^10)$	1.0	2.5E-11			*Orr and Smith* [1987]
531	$CO_2(02^20) + CO_2 \leftrightarrow CO_2(01^10) + CO_2(01^10)$	1.0	2.5E-11			*Orr and Smith* [1987]
532	$CO_2(10^00) + CO_2 \leftrightarrow CO_2(01^10) + CO_2(01^10)$	1.0	2.5E-11			*Orr and Smith* [1987]
533	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
534	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(02^20) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
535	$CO_2(03^10) + CO_2 \leftrightarrow CO_2(10^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
536	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
537	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(02^20) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
538	$CO_2(03^30) + CO_2 \leftrightarrow CO_2(10^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
539	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
540	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]
541	$CO_2(11^10) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	6.0	2.5E-11			*López-Valverde* [1980]

Table S24. *

CO_2 chemistry: vibrational-vibrational processes (VV2)

No.	Reaction	g	h	i	j	Ref.
542	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(02^00) + CO_2(01^10)$	1.0	3.6E-13	-1660	176948	*Lepoutre et al.* [1977]
543	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(02^20) + CO_2(01^10)$	1.0	3.6E-13	-1660	176948	*Lepoutre et al.* [1977]
544	$CO_2(00^01) + CO_2 \leftrightarrow CO_2(10^00) + CO_2(01^10)$	1.0	3.6E-13	-1660	176948	*Lepoutre et al.* [1977]

Table S25. *

CO_2 chemistry: vibrational-vibrational processes (VV3)

No.	Reaction	g	h	i	j	Ref.
545	$CO_2(01^11) + N_2 \leftrightarrow N_2(v_1) + CO_2(01^10)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
546	$CO_2(02^01) + N_2 \leftrightarrow N_2(v_1) + CO_2(02^00)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
547	$CO_2(02^21) + N_2 \leftrightarrow N_2(v_1) + CO_2(02^20)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
548	$CO_2(10^01) + N_2 \leftrightarrow N_2(v_1) + CO_2(10^00)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
549	$CO_2(03^11) + N_2 \leftrightarrow N_2(v_1) + CO_2(03^10)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
550	$CO_2(03^31) + N_2 \leftrightarrow N_2(v_1) + CO_2(03^30)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
551	$CO_2(11^11) + N_2 \leftrightarrow N_2(v_1) + CO_2(11^10)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
552	$CO_2(00^02) + N_2 \leftrightarrow N_2(v_1) + CO_2(00^01)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
553	$CO_2(04^01) + N_2 \leftrightarrow N_2(v_1) + CO_2(04^00)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
554	$CO_2(04^21) + N_2 \leftrightarrow N_2(v_1) + CO_2(04^20)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
555	$CO_2(04^41) + N_2 \leftrightarrow N_2(v_1) + CO_2(04^40)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
556	$CO_2(12^01) + N_2 \leftrightarrow N_2(v_1) + CO_2(12^00)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
557	$CO_2(12^21) + N_2 \leftrightarrow N_2(v_1) + CO_2(12^20)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]
558	$CO_2(20^01) + N_2 \leftrightarrow N_2(v_1) + CO_2(20^00)$		5.0E-13	0.5		*Inoue and Tsuchiya* [1975]

Table S26. *

CO_2 chemistry: vibrational-translational processes (VT4)

No.	Reaction	g	h	i	j	Ref.
559	$CO_2(10^01) + O_2 \leftrightarrow O_2 + CO_2(02^01)$	1.0	2.0E-11			*López-Puertas and Taylor* [1989]
560	$CO_2(10^01) + O_2 \leftrightarrow O_2 + CO_2(02^21)$	2.0	2.4E-12			*López-Puertas and Taylor* [1989]
561	$CO_2(02^21) + N_2 \leftrightarrow O_2 + CO_2(02^01)$	1.0	2.4E-12			*López-Puertas and Taylor* [1989]
562	$CO_2(02^21) + O_2 \leftrightarrow O_2 + CO_2(02^01)$	1.0	2.4E-12			*López-Puertas and Taylor* [1989]
563	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(03^10)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
564	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(03^30)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
565	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(11^10)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
566	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(02^00)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
567	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(02^20)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
568	$CO_2(00^01) + O_2 \leftrightarrow O_2 + CO_2(10^00)$	1.0	2.3E-15	1.54E-10	-76.75	*López-Puertas et al.* [1986]
569	$CO_2(00^01) + NO \leftrightarrow NO + CO_2(11^10)$	1.09E-16				*Bauer et al.* [1987]
570	$CO_2(00^01) + N_2O \leftrightarrow N_2O + CO_2(11^10)$	6.34E-16				*Bauer et al.* [1987]

Table S27. *

CO_2 chemistry: vibrational-vibrational processes (VV4)

No.	Reaction	g	h	i	j	Ref.
571	$CO_2 + N_2(v_1) \leftrightarrow N_2 + CO_2(00^01)$	3.96E-13				*Moore et al.* [1967]
572	$CO_2 + N_2(v_2) \leftrightarrow N_2(v_1) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
573	$CO_2 + N_2(v_3) \leftrightarrow N_2(v_2) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
574	$CO_2 + N_2(v_4) \leftrightarrow N_2(v_3) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
575	$CO_2 + N_2(v_5) \leftrightarrow N_2(v_4) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
576	$CO_2 + N_2(v_6) \leftrightarrow N_2(v_5) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
577	$CO_2 + N_2(v_7) \leftrightarrow N_2(v_6) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]
578	$CO_2 + N_2(v_8) \leftrightarrow N_2(v_7) + CO_2(00^01)$	3.96E-13	1.0			*Moore et al.* [1967]

Table S28.1. *

Radiative decay processes

No.	**Reaction**	**A**(s^{-1})	**Ref.**
579	$CO_2(01^10) \rightarrow CO_2 + h\nu$	1.564	*García-Comas* [2010]
580	$CO_2(02^00) \rightarrow CO_2(01^10) + h\nu$	1.21	*García-Comas* [2010]
581	$CO_2(02^20) \rightarrow CO_2(01^10) + h\nu$	3.153	*García-Comas* [2010]
582	$CO_2(10^00) \rightarrow CO_2(01^10) + h\nu$	2.08	*García-Comas* [2010]
583	$CO_2(03^10) \rightarrow CO_2(02^00) + h\nu$	2.052	*García-Comas* [2010]
584	$CO_2(03^10) \rightarrow CO_2(02^20) + h\nu$	0.529	*García-Comas* [2010]
585	$CO_2(03^10) \rightarrow CO_2(10^00) + h\nu$	0.0302	*García-Comas* [2010]
586	$CO_2(03^10) \rightarrow CO_2 + h\nu$	9.644E-4	*García-Comas* [2010]
587	$CO_2(03^30) \rightarrow CO_2(02^20) + h\nu$	4.778	*García-Comas* [2010]
588	$CO_2(03^30) \rightarrow CO_2 + h\nu$	2.381E-7	*García-Comas* [2010]
589	$CO_2(11^10) \rightarrow CO_2 + h\nu$	6.6E-3	*García-Comas* [2010]
590	$CO_2(11^10) \rightarrow CO_2(02^00) + h\nu$	0.0152	*García-Comas* [2010]
591	$CO_2(11^10) \rightarrow CO_2(02^20) + h\nu$	1.202	*García-Comas* [2010]
592	$CO_2(11^10) \rightarrow CO_2(10^00) + h\nu$	2.547	*García-Comas* [2010]
593	$CO_2(00^01) \rightarrow CO_2(02^00) + h\nu$	0.2	*García-Comas* [2010]
594	$CO_2(00^01) \rightarrow CO_2 + h\nu$	450.0	*García-Comas* [2010]
595	$CO_2(00^01) \rightarrow CO_2(10^00) + h\nu$	0.35	*García-Comas* [2010]
596	$CO_2(04^00) \rightarrow CO_2(01^10) + h\nu$	8.866E-4	*García-Comas* [2010]
597	$CO_2(04^00) \rightarrow CO_2(03^10) + h\nu$	2.746	*García-Comas* [2010]
598	$CO_2(04^00) \rightarrow CO_2(11^10) + h\nu$	5.03E-3	*García-Comas* [2010]
599	$CO_2(04^00) \rightarrow CO_2(00^01) + h\nu$	3.073E-6	*García-Comas* [2010]
600	$CO_2(04^20) \rightarrow CO_2(01^10) + h\nu$	1.469E-3	*García-Comas* [2010]
601	$CO_2(04^20) \rightarrow CO_2(03^10) + h\nu$	3.472	*García-Comas* [2010]
602	$CO_2(04^20) \rightarrow CO_2(03^30) + h\nu$	4.982E-1	*García-Comas* [2010]
603	$CO_2(04^20) \rightarrow CO_2(01^11) + h\nu$	1.575E-2	*García-Comas* [2010]
604	$CO_2(12^00) \rightarrow CO_2(01^10) + h\nu$	2.275E-4	*García-Comas* [2010]
605	$CO_2(12^00) \rightarrow CO_2(03^10) + h\nu$	1.343	*García-Comas* [2010]
606	$CO_2(12^00) \rightarrow CO_2(11^10) + h\nu$	7.013E-1	*García-Comas* [2010]
607	$CO_2(12^00) \rightarrow CO_2(00^01) + h\nu$	1.878E-4	*García-Comas* [2010]
608	$CO_2(04^40) \rightarrow CO_2(03^30) + h\nu$	5.866	*García-Comas* [2010]
609	$CO_2(12^20) \rightarrow CO_2(01^10) + h\nu$	2.293E-2	*García-Comas* [2010]
610	$CO_2(12^20) \rightarrow CO_2(03^10) + h\nu$	6.103E-2	*García-Comas* [2010]
611	$CO_2(12^20) \rightarrow CO_2(03^30) + h\nu$	9.958E-2	*García-Comas* [2010]
612	$CO_2(12^20) \rightarrow CO_2(11^10) + h\nu$	3.949	*García-Comas* [2010]

Table S28.2. *

Radiative decay processes (cont.)

No.	**Reaction**	**A**(s^{-1})	**Ref.**
613	$CO_2(20^00) \rightarrow CO_2(01^10) + h\nu$	2.948E-2	*García-Comas* [2010]
614	$CO_2(20^00) \rightarrow CO_2(03^10) + h\nu$	3.272E-2	*García-Comas* [2010]
615	$CO_2(20^00) \rightarrow CO_2(11^10) + h\nu$	4.266	*García-Comas* [2010]
616	$CO_2(01^11) \rightarrow CO_2(01^10) + h\nu$	4.117E+2	*García-Comas* [2010]
617	$CO_2(01^11) \rightarrow CO_2(03^10) + h\nu$	4.398E-1	*García-Comas* [2010]
618	$CO_2(01^11) \rightarrow CO_2(11^10) + h\nu$	3.565E-1	*García-Comas* [2010]
619	$CO_2(01^11) \rightarrow CO_2(00^01) + h\nu$	1.451	*García-Comas* [2010]
620	$CO_2(02^01) \rightarrow CO_2 + h\nu$	1.088E+1	*García-Comas* [2010]
621	$CO_2(02^01) \rightarrow CO_2(02^00) + h\nu$	4.008E+2	*García-Comas* [2010]
622	$CO_2(02^01) \rightarrow CO_2(10^00) + h\nu$	4.008E-1	*García-Comas* [2010]
623	$CO_2(02^01) \rightarrow CO_2(04^00) + h\nu$	7.379E-1	*García-Comas* [2010]
624	$CO_2(02^01) \rightarrow CO_2(12^00) + h\nu$	4.318E-1	*García-Comas* [2010]
625	$CO_2(02^01) \rightarrow CO_2(20^00) + h\nu$	9.068E-3	*García-Comas* [2010]
626	$CO_2(02^01) \rightarrow CO_2(01^10) + h\nu$	1.263	*García-Comas* [2010]
627	$CO_2(02^21) \rightarrow CO_2 + h\nu$	3.963E-4	*García-Comas* [2010]
628	$CO_2(02^21) \rightarrow CO_2(02^20) + h\nu$	3.989E+2	*García-Comas* [2010]
629	$CO_2(02^21) \rightarrow CO_2(04^20) + h\nu$	4.325E-1	*García-Comas* [2010]
630	$CO_2(02^21) \rightarrow CO_2(12^20) + h\nu$	3.262E-1	*García-Comas* [2010]
631	$CO_2(02^21) \rightarrow CO_2(01^11) + h\nu$	2.877	*García-Comas* [2010]
632	$CO_2(10^01) \rightarrow CO_2 + h\nu$	1.735E+1	*García-Comas* [2010]
633	$CO_2(10^01) \rightarrow CO_2(02^00) + h\nu$	1.704E-1	*García-Comas* [2010]
634	$CO_2(10^01) \rightarrow CO_2(10^00) + h\nu$	3.98E+2	*García-Comas* [2010]
635	$CO_2(10^01) \rightarrow CO_2(04^00) + h\nu$	9.511E-4	*García-Comas* [2010]
636	$CO_2(10^01) \rightarrow CO_2(12^00) + h\nu$	6.237E-1	*García-Comas* [2010]
637	$CO_2(10^01) \rightarrow CO_2(20^00) + h\nu$	5.543E-1	*García-Comas* [2010]
638	$CO_2(10^01) \rightarrow CO_2(01^11) + h\nu$	1.639	*García-Comas* [2010]
639	$CO_2(03^11) \rightarrow CO_2(01^10) + h\nu$	1.008E+1	*García-Comas* [2010]
640	$CO_2(03^11) \rightarrow CO_2(03^10) + h\nu$	3.907E+2	*García-Comas* [2010]
641	$CO_2(03^11) \rightarrow CO_2(11^10) + h\nu$	1.988E-1	*García-Comas* [2010]
642	$CO_2(03^11) \rightarrow CO_2(00^01) + h\nu$	9.012E-4	*García-Comas* [2010]
643	$CO_2(03^11) \rightarrow CO_2(02^01) + h\nu$	1.91	*García-Comas* [2010]
644	$CO_2(03^11) \rightarrow CO_2(02^21) + h\nu$	5.551E-1	*García-Comas* [2010]
645	$CO_2(03^11) \rightarrow CO_2(10^01) + h\nu$	2.827E-2	*García-Comas* [2010]
646	$CO_2(03^31) \rightarrow CO_2(03^30) + h\nu$	3.847E+2	*García-Comas* [2010]
647	$CO_2(03^31) \rightarrow CO_2(02^21) + h\nu$	4.135	*García-Comas* [2010]
648	$CO_2(11^11) \rightarrow CO_2(01^10) + h\nu$	1.752E+1	*García-Comas* [2010]
649	$CO_2(11^11) \rightarrow CO_2(03^10) + h\nu$	4.651E-2	*García-Comas* [2010]
650	$CO_2(11^11) \rightarrow CO_2(11^10) + h\nu$	3.869E+2	*García-Comas* [2010]

Table S28.3. *

Radiative decay processes (cont.)

No.	**Reaction**	**A**(s^{-1})	**Ref.**
651	$CO_2(11^{1}1) \rightarrow CO_2(00^{0}1) + h\nu$	6.242E-3	*García-Comas* [2010]
652	$CO_2(11^{1}1) \rightarrow CO_2(02^{0}1) + h\nu$	1.063E-1	*García-Comas* [2010]
653	$CO_2(11^{1}1) \rightarrow CO_2(02^{2}1) + h\nu$	2.987E-1	*García-Comas* [2010]
654	$CO_2(11^{1}1) \rightarrow CO_2(10^{0}1) + h\nu$	2.104	*García-Comas* [2010]
655	$CO_2(00^{0}2) \rightarrow CO_2(01^{1}0) + h\nu$	7.307E-4	*García-Comas* [2010]
656	$CO_2(00^{0}2) \rightarrow CO_2(00^{0}1) + h\nu$	4.126E+2	*García-Comas* [2010]
657	$CO_2(00^{0}2) \rightarrow CO_2(02^{0}1) + h\nu$	4.109E-1	*García-Comas* [2010]
658	$CO_2(00^{0}2) \rightarrow CO_2(10^{0}1) + h\nu$	4.063E-1	*García-Comas* [2010]
659	$CO_2(04^{0}1) \rightarrow CO_2 + h\nu$	1.567E-1	*García-Comas* [2010]
660	$CO_2(04^{0}1) \rightarrow CO_2(02^{0}0) + h\nu$	1.705E+1	*García-Comas* [2010]
661	$CO_2(04^{0}1) \rightarrow CO_2(10^{0}0) + h\nu$	1.498E-1	*García-Comas* [2010]
662	$CO_2(04^{0}1) \rightarrow CO_2(04^{0}0) + h\nu$	3.814E+2	*García-Comas* [2010]
663	$CO_2(04^{0}1) \rightarrow CO_2(12^{0}0) + h\nu$	4.571E-1	*García-Comas* [2010]
664	$CO_2(04^{0}1) \rightarrow CO_2(20^{0}0) + h\nu$	1.056E-2	*García-Comas* [2010]
665	$CO_2(04^{0}1) \rightarrow CO_2(01^{1}1) + h\nu$	1.242E-3	*García-Comas* [2010]
666	$CO_2(04^{0}1) \rightarrow CO_2(03^{1}1) + h\nu$	2.768	*García-Comas* [2010]
667	$CO_2(04^{0}1) \rightarrow CO_2(11^{1}1) + h\nu$	4.822E-3	*García-Comas* [2010]
668	$CO_2(04^{2}1) \rightarrow CO_2 + h\nu$	3.247E-5	*García-Comas* [2010]
669	$CO_2(04^{2}1) \rightarrow CO_2(02^{2}0) + h\nu$	9.901	*García-Comas* [2010]
670	$CO_2(04^{2}1) \rightarrow CO_2(04^{2}0) + h\nu$	4.774E+2	*García-Comas* [2010]
671	$CO_2(04^{2}1) \rightarrow CO_2(12^{2}0) + h\nu$	1.129E-1	*García-Comas* [2010]
672	$CO_2(04^{2}1) \rightarrow CO_2(01^{1}1) + h\nu$	1.006E-3	*García-Comas* [2010]
673	$CO_2(04^{2}1) \rightarrow CO_2(03^{1}1) + h\nu$	3.351	*García-Comas* [2010]
674	$CO_2(04^{2}1) \rightarrow CO_2(03^{3}1) + h\nu$	4.968E-1	*García-Comas* [2010]
675	$CO_2(04^{2}1) \rightarrow CO_2(11^{1}1) + h\nu$	1.382E-2	*García-Comas* [2010]
676	$CO_2(04^{4}1) \rightarrow CO_2(04^{4}0) + h\nu$	3.695E+2	*García-Comas* [2010]
677	$CO_2(04^{4}1) \rightarrow CO_2(03^{3}1) + h\nu$	5.664	*García-Comas* [2010]
678	$CO_2(12^{0}1) \rightarrow CO_2 + h\nu$	7.169E-1	*García-Comas* [2010]
679	$CO_2(12^{0}1) \rightarrow CO_2(02^{0}0) + h\nu$	2.138E+1	*García-Comas* [2010]
680	$CO_2(12^{0}1) \rightarrow CO_2(10^{0}0) + h\nu$	1.486E+1	*García-Comas* [2010]
681	$CO_2(12^{0}1) \rightarrow CO_2(04^{0}0) + h\nu$	1.347E-1	*García-Comas* [2010]
682	$CO_2(12^{0}1) \rightarrow CO_2(12^{0}0) + h\nu$	3.75E+2	*García-Comas* [2010]
683	$CO_2(12^{0}1) \rightarrow CO_2(20^{0}0) + h\nu$	4.229E-1	*García-Comas* [2010]
684	$CO_2(12^{0}1) \rightarrow CO_2(03^{1}1) + h\nu$	1.194	*García-Comas* [2010]
685	$CO_2(12^{0}1) \rightarrow CO_2(11^{1}1) + h\nu$	7.268E-1	*García-Comas* [2010]
686	$CO_2(12^{2}1) \rightarrow CO_2 + h\nu$	3.97E-5	*García-Comas* [2010]
687	$CO_2(12^{2}1) \rightarrow CO_2(02^{2}0) + h\nu$	1.801E+1	*García-Comas* [2010]
688	$CO_2(12^{2}1) \rightarrow CO_2(04^{2}0) + h\nu$	1.308E-2	*García-Comas* [2010]
689	$CO_2(12^{2}1) \rightarrow CO_2(12^{2}0) + h\nu$	3.747E+2	*García-Comas* [2010]
690	$CO_2(12^{2}1) \rightarrow CO_2(01^{1}1) + h\nu$	2.426E-2	*García-Comas* [2010]

Table S28.4. *

Radiative decay processes (cont.)

No.	**Reaction**	**A**(s^{-1})	**Ref.**
691	$CO_2(12^21) \rightarrow CO_2(03^11) + h\nu$	6.489E-2	*García-Comas* [2010]
692	$CO_2(12^21) \rightarrow CO_2(03^31) + h\nu$	9.08E-1	*García-Comas* [2010]
693	$CO_2(12^21) \rightarrow CO_2(11^11) + h\nu$	3.76	*García-Comas* [2010]
694	$CO_2(20^01) \rightarrow CO_2 + h\nu$	2.363E-1	*García-Comas* [2010]
695	$CO_2(20^01) \rightarrow CO_2(02^00) + h\nu$	3.832E-1	*García-Comas* [2010]
696	$CO_2(20^01) \rightarrow CO_2(10^00) + h\nu$	2.877E+1	*García-Comas* [2010]
697	$CO_2(20^01) \rightarrow CO_2(12^00) + h\nu$	1.128E-1	*García-Comas* [2010]
698	$CO_2(20^01) \rightarrow CO_2(20^00) + h\nu$	3.749E+2	*García-Comas* [2010]
699	$CO_2(20^01) \rightarrow CO_2(01^11) + h\nu$	3.261E-2	*García-Comas* [2010]
700	$CO_2(20^01) \rightarrow CO_2(03^11) + h\nu$	3.443E-2	*García-Comas* [2010]
701	$CO_2(20^01) \rightarrow CO_2(11^11) + h\nu$	3.433	*García-Comas* [2010]
702	$N_2(A^3\Sigma_u^+) \rightarrow N_2(X^1\Sigma_g^+) + h\nu$	0.5	*Capitelli et al.* [2000]
703	$N_2(B^3\Pi_g) \rightarrow N_2(A^3\Sigma_u^+) + h\nu$	1.34E+5	*Capitelli et al.* [2000]
704	$N_2(C^3\Pi_u) \rightarrow N_2(B^3\Pi_g) + h\nu$	2.45E+7	*Capitelli et al.* [2000]
705	$N_2(W^3\Delta_u) \rightarrow N_2(X^1\Sigma_g^+) + h\nu$	0.154	*Capitelli et al.* [2000]
706	$N_2(B'^3\Sigma_u^-) \rightarrow N_2(B^3\Pi_g) + h\nu$	3.4E+4	*Capitelli et al.* [2000]
707	$N_2(E^3\Sigma_g^+) \rightarrow N_2(A^3\Sigma_u^+) + h\nu$	1.2E+3	*Capitelli et al.* [2000]
708	$N_2(E^3\Sigma_g^+) \rightarrow N_2(B^3\Pi_g) + h\nu$	3.46E+2	*Capitelli et al.* [2000]
709	$N_2(E^3\Sigma_g^+) \rightarrow N_2(C^3\Pi_u) + h\nu$	1.73E+3	*Capitelli et al.* [2000]
710	$N_2(a''^1\Sigma_g^+) \rightarrow N_2(X^1\Sigma_g^+) + h\nu$	2.86E+5	*Kam and Pipkin* [1991]
711	$N_2(a'^1\Sigma_u^-)) \rightarrow N_2(X^1\Sigma_g^+) + h\nu$	1.0E+2	*Capitelli et al.* [2000]
712	$N_2(a^1\Pi_g) \rightarrow N_2(X^1\Sigma_g^+) + h\nu$	8.55E+3	*Capitelli et al.* [2000]
713	$N_2(a^1\Pi_g) \rightarrow N_2(a'^1\Sigma_u^-)) + h\nu$	1.3E+2	*Capitelli et al.* [2000]
714	$N_2(w^1\Delta_u) \rightarrow N_2(a^1\Pi_g) + h\nu$	1.51E+3	*Capitelli et al.* [2000]
715	$N_2^+(A^2\Pi_u) \rightarrow N_2^+(X^2\Sigma_g^+) + h\nu$	4.64E+4	*Gilmore et al.* [1992]
716	$N_2^+(B^2\Sigma_u^+) \rightarrow N_2^+(X^2\Sigma_g^+) + h\nu$	1.14E+7	*Gilmore et al.* [1992]
717	$NO(A^2\Sigma^+) \rightarrow NO(X^2\Pi_r) + h\nu$	5.0E+6	*Radzig and Smirnov* [1985]
718	$O(^1D) \rightarrow O + h\nu$	5.1E-3	*Wiese et al.* [1966]
719	$O(^1S) \rightarrow O(^1D) + h\nu$	1.34	*Wiese et al.* [1966]
720	$O_2(A^3\Sigma_u^+) \rightarrow O_2(X^3\Sigma_g^-) + h\nu$	1.1E+1	*Bates* [1988]
721	$O_2(a^1\Delta_g) \rightarrow O_2(X^3\Sigma_g^-) + h\nu$	3.307E-4	*Krupenie* [1972]
722	$O_2(b^1\Sigma_g^+) \rightarrow O_2(X^3\Sigma_g^-) + h\nu$	8.2E-2	*Krupenie* [1972]
723	$O_2(b^1\Sigma_g^+) \rightarrow O_2(b^1\Sigma_g^+) + h\nu$	1.7E-3	*Krupenie* [1972]

Table S29. *

Ionization processes due to galactic cosmic rays

No.	Reaction	k	l	Ref.
724	$N_2 + h\nu \rightarrow N_2^+ + e$	5.85E-18	crc	*Yelinov et al.* [2009]
725	$O_2 + h\nu \rightarrow O_2^+ + e$	1.54E-18	crc	*Yelinov et al.* [2009]
726	$N_2 + h\nu \rightarrow N^+ + N + e$	1.85E-18	crc	*Yelinov et al.* [2009]
727	$O_2 + h\nu \rightarrow O^+ + O + e$	7.6E-19	crc	*Yelinov et al.* [2009]

Table S30. *

Rotational deexcitation processes

No.	Reaction	k	l	Ref.
728	$N_2(rot) + N_2 \rightarrow N_2 + N_2$	1.02E-10		*Capitelli et al.* [2000]
729	$O_2(rot) + O_2 \rightarrow O_2 + O_2$	5.35E-10		*Capitelli et al.* [2000]

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