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TABULATIONS OF COLLISION CROSS SECTIONS AND CALCULATED TRANSPORT AND REACTION COEFFICIENTS FOR ELECTRON COLLISIONS WITH O_2

by

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Tabulations of collision cross sections and calculated transport and reaction coefficients for electron collisions with O_2

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This report contains a tabulation of the set of electron collision cross sections for O_2 initially developed in Appendix C of the paper "Excitation of the $b^1\Sigma_g^+$ state of O_2 by low energy electrons" by S. A. Lawton and A. V. Phelps, which was published in the Journal of Chemical Physics 69, 1055 (1978). This paper will be referred to as paper I. The present report replaces the JILA Data Center Memo No. 3 mentioned in I, which was never issued.

Table I lists the currently recommended cross sections for use in the calculation of electron transport coefficients and of attachment and ionization coefficients. Each table lists the electron energies in electron volts and the cross sections in 10^{-16} cm^2. A one line descriptor identifies the collision process. The reader is referred to I for further detail. The tabulated cross sections are significant to about 1%. The cross sections for electron excitation of the v = 1 level of O_2 are listed in two tables because of limitations set by our computer program and in order to different scaling factors to be applied to the input cross sections for the low energy resonances and for the 9 eV resonance. Similarly, for the cross sections for the v = 2 level.

Note that the "cross sections" listed under the heading of three-body attachment are expressed as equivalent cross sections for the attachment of monoenergetic electrons at an O_2 density of 1 molecule/cm^3. This means that the rate coefficients k and spatial attachment coefficients α/n calculated using our Boltzmann code[1] and the tabulated values must be multipled by the O_2 density to obtain the equivalent of the two-body rate coefficients used for other processes such as excitation. Multiplication by the square of the O_2 density yields the number of attachment events per second or per cm distance, respectively.

As discussed by Yamabe and Phelps[2] the relative magnitudes of the peak cross sections for vibrational excitation have been modified from those of I so as to agree better with theory. Note that in Table I the resonance cross sections for rotational and vibrational excitation and for three-body attachment have been represented by triangular functions as a consequence of the linear interpolation between tabulated points used in all of our tables. The widths of the "resonances" are chosen partly for computational convenience, although widths of the lower attachment resonances are in good agreement with the theory summarized in I. The areas under the resonances are chosen as discussed in I and in ref. 2.

Table II lists the transport and rate coefficients calculated using the cross sections listed in Table I. These calculations were made using the two-term spherical harmonic expansion for the electron energy distribution as discussed in I. The transport and rate coefficients listed are significant to about 1%. When applying the results of calculations made using this cross section set, it should be kept in mind that the discrepancy between electron induced dissociation coefficients inferred from the experiments of I and the values inferred from measurements of O_3 production rates is still unresolved. See I.

1. L. S. Frost and A. V. Phelps, Phys. Rev. 127, 1621 (1962); P. E. Luft, JILA Information Center Report No. 14, University of Colorado 1975 (unpublished).

2. C. Yamabe and A. V. Phelps, J. Chem. Phys. 78, 2984 (1983).

O_2 THREE-BODY ATTACHMENT, ENERGY LOSS = 0.00 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	.4700	0.0000
.0580	0.0000	.5600	0.0000
.0730	5.6(-21)	.5700	1.1(-21)
.0830	18.0(-21)	.5900	0.0000
.0890	4.2(-21)	.6800	0.0000
.0950	8.4(-21)	.6900	8.0(-22)
.1030	18.0(-21)	.7100	0.0000
.1090	0.0000	.7900	0.0000
.1500	0.0000	.8000	7.0(-22)
.1700	0.0000	.8200	0.0000
.2000	0.0000	.9000	0.0000
.2100	3.56(-21)	.9100	5.5(-22)
.2300	0.0000	.9300	0.0000
.3200	0.0000	1.0200	0.0000
.3300	2.30(-21)	1.0300	4.2(-22)
.3500	0.0000	1.0500	0.0000
.4400	0.0000	1.5000	0.0000
.4500	1.45(-21)	100.0000	0.0000

O_2 TWO-BODY ATTACHMENT, ENERGY LOSS = 0.00 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	7.5300	.0131
4.4000	0.0000	7.7700	.0110
4.9000	0.0000	8.0000	.0084
5.3800	.0023	8.2500	.0054
5.8600	.0072	8.7300	.0028
6.1000	.0108	9.2000	.0014
6.4800	.0138	9.6800	.0008
6.7700	.0152	10.1500	.0008
7.0500	.0156	11.3500	.0008
7.3000	.0148	100.0000	0.0000

O_2 SINGLE LEVEL APPROXIMATION TO PEAKED ROTATIONAL CROSS SECTION
FOR USE AT T_g = 300 K, ENERGY LOSS = .020 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	.9100	.0840
.0067	0.0000	.9300	0.0000
.0700	0.0000	1.0200	0.0000
.0800	.0054	1.0300	.0720
.1000	0.0000	1.0500	0.0000
.2000	0.0000	1.1300	0.0000
.2100	.0216	1.1400	.0465
.2200	0.0000	1.1600	0.0000
.3200	0.0000	1.2300	0.0000
.3300	.0384	1.2300	.0600
.3500	0.0000	1.2600	0.0000
.4400	0.0000	1.3400	0.0000
.4500	.0540	1.3500	.0360
.4700	0.0000	1.3700	0.0000
.5600	0.0000	1.4400	0.0000
.5700	.0672	1.4500	.0240
.5900	0.0000	1.4700	0.0000
.6800	0.0000	1.5400	0.0000
.6900	.0804	1.5500	.0120
.7100	0.0000	1.5700	0.0000
.7900	0.0000	1.6400	0.0000
.8000	.0936	1.6500	.0048
.8100	0.0000	1.6700	0.0000
.9000	0.0000	100.0000	0.0000

O_2 v=1 WITH SPLIT PEAK, ENERGY LOSS = 0.19 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	1.0300	.2850
.1900	0.0000	1.0500	0.0000
.2000	.0010	1.1300	0.0000
.2100	.0010	1.1400	.1125
.2300	0.0000	1.1600	0.0000
.3200	0.0000	1.2300	0.0000
.3300	.4150	1.2400	.0475
.3500	0.0000	1.2600	0.0000
.4400	0.0000	1.3400	0.0000
.4500	1.3500	1.3500	.0165
.4700	0.0000	1.3700	0.0000
.5600	0.0000	1.4400	0.0000
.5700	1.8500	1.4500	.0055
.5900	0.0000	1.4700	0.0000
.6800	0.0000	1.5400	0.0000
.6900	1.6500	1.5500	.0020
.7100	0.0000	1.5700	0.0000
.7900	0.0000	1.6300	0.0000
.8000	1.0000	1.6500	.0007
.8200	0.0000	1.6700	0.0000
.9000	0.0000	3.5000	0.0000
.9100	.6000	4.0000	0.0000
.9300	0.0000	5.0000	0.0000
1.0200	0.0000	100.0000	0.0000

O_2 v=2, ENERGY LOSS = .380 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	1.1400	.2000
.3800	0.0000	1.1600	0.0000
.4400	0.0000	1.2300	0.0000
.4500	.0000	1.2400	.0950
.4700	0.0000	1.2600	0.0000
.5600	0.0000	1.3400	0.0000
.5700	.1400	1.3500	.0400
.5900	0.0000	1.3700	0.0000
.6800	0.0000	1.4400	0.0000
.6900	.4150	1.4500	.0185
.7100	0.0000	1.4700	0.0000
.7900	0.0000	1.5400	0.0000
.8000	.5350	1.5500	.0085
.8200	0.0000	1.5700	0.0000
.9000	0.0000	1.6300	0.0000
.9100	.4650	1.6500	.0034
.9300	0.0000	1.6700	0.0000
1.0200	0.0000	3.5000	0.0000
1.0300	.3150	4.0000	0.0000
1.0500	0.0000	5.0000	0.0000
1.1300	0.0000	100.0000	0.0000

O_2 v=3 WITH 9EV RESONANCE, ENERGY LOSS = .570 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	1.4500	.0300
.5700	0.0000	1.4700	0.0000
.6800	0.0000	1.5400	0.0000
.6900	.0037	1.5500	.0165
.7100	0.0000	1.5700	0.0000
.7900	0.0000	1.6300	0.0000
.8000	.0215	1.6500	.0080
.8200	0.0000	1.6700	0.0000
.9000	0.0000	3.5000	0.0000
.9100	.0900	4.0000	0.0000
.9300	0.0000	5.0000	0.0000
1.0200	0.0000	6.0000	.0125
1.0300	.1200	7.0000	.0363
1.0500	0.0000	8.0000	.0588
1.1300	0.0000	9.0000	.0750
1.1400	.1150	10.0000	.0675
1.1600	0.0000	11.0000	.0563
1.2300	0.0000	12.0000	.0475
1.2400	.0950	13.0000	.0300
1.2600	0.0000	14.0000	.0175
1.3400	0.0000	15.0000	.0088
1.3500	.0550	20.0000	0.0000
1.3700	0.0000	45.0000	0.0000
1.4400	0.0000	100.0000	0.0000

O_2 v=4 WITH 9EV RESONANCE, ENERGY LOSS = .750 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	1.4400	0.0000
.7500	0.0000	1.4500	.0285
.7900	0.0000	1.4700	0.0000
.8000	.0015	1.5400	0.0000
.8200	0.0000	1.5500	.0215
.9000	0.0000	1.5700	0.0000
.9100	.0055	1.6300	0.0000
.9300	0.0000	1.6500	.0165
1.0200	0.0000	1.6700	0.0000
1.0300	.0004	6.0000	0.0000
1.0500	0.0000	7.0000	.0275
1.1300	0.0000	8.0000	.0350
1.1400	.0165	9.0000	.0413
1.1600	0.0000	10.0000	.0463
1.2300	0.0000	11.0000	.0313
1.2400	.0315	12.0000	.0250
1.2600	0.0000	13.0000	.0175
1.3400	0.0000	14.0000	.0088
1.3500	.0335	15.0000	0.0000
1.3700	0.0000	100.0000	0.0000

O_2 SING DELTA, ENERGY LOSS = 0.977 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	7.6100	.0891
.9770	0.0000	7.8900	.0863
1.5000	.0058	8.9600	.0768
2.0000	.0153	10.0400	.0679
3.0000	.0380	13.0000	.0527
3.5000	.0490	15.1000	.0455
4.0000	.0570	17.5000	.0387
5.0000	.0740	20.5000	.0324
5.6200	.0825	24.9000	.0256
5.9100	.0862	30.9000	.0196
6.1900	.0888	41.0000	.0137
6.5300	.0908	45.0000	.0120
6.9900	.0914	100.0000	0.0000

O_2 B SINGLET SIGMA, ENERGY LOSS = 1.627 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	13.0000	.0131
1.6270	0.0000	14.9000	.0117
2.0000	.0026	17.0000	.0103
3.0000	.0097	19.4000	.0092
3.5000	.0133	20.7000	.0086
4.0000	.0149	22.5000	.0080
5.0000	.0182	24.0000	.0072
5.6900	.0194	28.0000	.0061
6.5400	.0194	35.1000	.0047
7.3400	.0191	41.9000	.0034
8.4100	.0183	45.1000	.0031
9.2600	.0174	100.0000	0.0000
10.0000	.0160		

O_2 v=1 9V RESONANCE, ENERGY LOSS = .190 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	11.0000	.1860
4.0000	0.0000	12.0000	.1430
5.0000	.0420	13.0000	.1020
6.0000	.1000	14.0000	.0710
7.0000	.1760	15.0000	.0400
8.0000	.2310	20.0000	.0100
9.0000	.2470	45.0000	0.0000
10.0000	.2340	100.0000	0.0000

O_2 v=2 9V RESONANCE, ENERGY LOSS = .380 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	11.0000	.0930
4.0000	0.0000	12.0000	.0730
5.0000	.0280	13.0000	.0510
6.0000	.0400	14.0000	.0280
7.0000	.0730	15.0000	.0130
8.0000	.0940	20.0000	.0050
9.0000	.1100	45.0000	0.0000
10.0000	.1090	100.0000	0.0000

O_2 4.5 EV LOSS, ENERGY LOSS = 4.50 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	7.5000	.1000
4.5000	0.0000	8.0000	.1000
4.8000	.0030	9.0000	.0850
5.0000	.0090	10.0000	.0700
5.5000	.0300	12.0000	.0450
6.0000	.0650	15.0000	0.0000
6.5000	.0850	50.0000	0.0000
7.0000	.0950	100.0000	0.0000

O_2 6.0 EV LOSS, ENERGY LOSS = 6.00 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	12.0000	.1650
6.0000	0.0000	15.0000	.1050
7.0000	.1500	17.0000	.0650
7.8000	.2300	20.0000	.0475
9.0000	.2300	45.0000	.0190
10.0000	.2100	100.0000	0.0000

O_2 8.4 EV LOSS, ENERGY LOSS = 8.40 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	30.0000	1.2000
8.4000	0.0000	50.0000	1.1700
9.4000	1.0000	100.0000	.9400

O_2 9.97 EV LOSS, ENERGY LOSS = 10.0 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	50.0000	.0500
10.0000	0.0000	60.0000	.0600
20.0000	.0130	70.0000	.0650
30.0000	.0260	80.0000	.0700
40.0000	.0400	100.0000	.0700

O_2 IONIZATION, ENERGY LOSS = 12.06 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	48.0000	2.0700
12.0600	0.0000	58.0000	2.4100
13.0000	.0250	68.0000	2.6100
18.0000	.2500	78.0000	2.8100
28.0000	1.0240	88.0000	2.8400
38.0000	1.7750	100.0000	2.9000

O_2 130 NM LINE EXCITATION, ENERGY LOSS = 14.70 EV

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	0.0000	40.0000	.0280
14.7000	0.0000	60.0000	.0370
20.0000	.0085	70.0000	.0380
25.0000	.0160	80.0000	.0390
30.0000	.0225	100.0000	.0380

MOMENTUM-TRANSFER CROSS SECTION

ENERGY EV	CROSS SECTION 10^{-16} CM^2	ENERGY EV	CROSS SECTION 10^{-16} CM^2
0.0000	.3500	1.3000	7.9000
.0010	.3500	1.5000	7.6000
.0020	.3600	1.7000	7.3000
.0030	.4000	1.9000	6.9000
.0050	.5000	2.1000	6.6000
.0070	.5800	2.2000	6.5000
.0085	.6400	2.5000	6.1000
.0100	.7000	2.8000	5.8000
.0150	.8700	3.0000	5.7000
.0200	.9900	3.3000	5.5000
.0300	1.2400	3.6000	5.4500
.0400	1.4400	4.0000	5.5000
.0500	1.6000	4.5000	5.5500
.0700	2.1000	5.0000	5.6000
.1000	2.5000	6.0000	6.0000
.1200	2.8000	7.0000	6.6000
.1500	3.1000	8.0000	7.1000
.1700	3.3000	10.0000	8.0000
.2000	3.6000	12.0000	8.5000
.2500	4.1000	15.0000	8.8000
.3000	4.5000	17.0000	8.7000
.3500	4.7000	20.0000	8.6000
.4000	5.2000	25.0000	8.2000
.5000	5.7000	30.0000	8.0000
.7000	6.1000	50.0000	7.7000
1.0000	7.2000	75.0000	6.8000
1.2000	7.9000	100.0000	6.5000

Table II. Transport and reaction coefficients for electrons in O_2 at 300 K. Calculated using two-term approximation using the current modifications of BACKPRO, but with no exponential growth of electron density. The three-body attachment was calculated for an O_2 density of 1 molecule/m^3. 1E-21 = 10^{-21}.

E/N (Td=10^{-21} Vm^2)	5	8	10	15	25	40	80	100	120	150	250
W (m/s)	26948	29122	32647	43502	63447	91891	157040	184340	208790	241350	322380
D/μ (eV)	.5186	.9691	1.2014	1.5654	2.0185	2.4035	3.0762	3.373	3.662	4.087	5.551
$\langle\varepsilon\rangle$ (eV)	.7294	1.3985	1.7087	2.1944	2.7194	3.1719	3.973	4.333	4.694	5.2402	7.184
ν_m/n (m^3/s)	3.26E-14	4.83E-14	5.39E-14	6.06E-14	6.93E-14	7.66E-14	8.96E-14	9.54E-14	1.01E-13	1.09E-13	1.36E-13
ν^m/n (m^3/s)	2.73E-16	2.47E-16	2.78E-16	4.24E-16	7.96E-16	1.55E-15	4.12E-15	5.51E-15	6.89E-15	8.91E-15	1.46E-14
$(\dot{E}_{PL}-\dot{E}_{PG})$(eV-$m^3$/s)	1.23E-18	2.82E-18	3.60E-18	4.93E-18	6.61E-18	8.39E-18	1.23E-17	1.44E-17	1.67E-17	2.05E-17	3.59E-17
EN. BALANCE (%)*	.32	.22	.23	.4	.38	.35	.44	.36	.31	.43	.34
SUM VIB QUANT (m^2)	5.33E-16	4.17E-16	3.90E-16	5.10E-16	7.42E-16	1.23E-15	2.51E-15	3.03E-15	3.50E-15	4.08E-15	5.17E-15
SUM TO BISIGMA (m^2)	4.42E-18	2.46E-17	4.24E-17	9.64E-17	2.48E-16	5.58E-16	1.74E-15	2.48E-15	3.29E-15	4.57E-15	9.02E-15
SUM DISSOCIATION (m^2)	1.69E-21	1.43E-19	5.70E-19	3.26E-18	1.89E-17	1.02E-16	7.57E-16	1.27E-15	1.87E-15	2.89E-15	6.76E-15
α/n VIBRATION (m^2)	1.98E-20	1.43E-20	1.19E-20	1.17E-20	1.17E-20	1.34E-20	1.60E-20	1.65E-20	1.68E-20	1.69E-20	1.60E-20
α/n BISIGMA (m^2)	1.64E-22	8.45E-22	1.30E-21	2.22E-21	3.90E-21	6.07E-21	1.11E-20	1.35E-20	1.57E-20	1.89E-20	2.80E-20
α/n DISSOCIATION (m^2)	6.26E-26	4.92E-24	1.74E-23	7.50E-23	2.97E-22	1.11E-21	4.82E-21	6.89E-21	8.97E-21	1.20E-20	2.10E-20
α/n NET IONIZ. (m^2)	-1.7E-21	-1.4E-19	-5.7E-19	-3.1E-18	-1.1E-17	-2.2E-17	-3.3E-17	-2.7E-17	-7.3E-18	5.64E-17	7.10E-16

RATE COEFFICIENTS (m^3/s) FOR INDIVIDUAL PROCESSES

PROCESS	E/N(Td) EN. LOSS (eV)	5	8	10	15	25	40	80	100	120	150	250
3BOD.ATTACH./N		1.05E-42	5.26E-43	3.80E-43	2.85E-43	1.92E-43	1.51E-43	1.30E-43	1.14E-43	1.02E-43	1.36E-43	3.76E-44
2BOD.ATTACH.		1.69E-21	1.43E-19	5.69E-19	3.14E-18	1.13E-17	2.21E-17	3.76E-17	4.18E-17	4.47E-17	4.74E-17	4.91E-17
ROTATION	.02	2.39E-17	1.86E-17	1.63E-11	1.70E-17	1.25E-17	1.03E-17	1.16E-17	1.04E-17	9.33E-18	5.97E-18	4.46E-18
v= 0-1	.19	3.38E-16	1.98E-16	1.74E-16	2.75E-16	3.08E-16	4.68E-16	8.56E-16	1.01E-15	1.14E-15	1.33E-15	1.62E-15
v= 0-2	.38	7.15E-17	7.28E-17	7.13E-17	8.05E-17	1.30E-16	2.02E-16	3.75E-16	4.44E-16	5.05E-16	5.91E-16	7.14E-16
v= 0-3	.57	1.31E-17	1.79E-17	1.77E-17	1.64E-17	3.62E-17	7.18E-17	1.72E-16	2.15E-16	2.54E-16	2.97E-16	4.02E-16
v= 0-4	.75	3.18E-18	4.94E-18	5.01E-18	6.25E-18	1.62E-17	3.69E-17	9.74E-17	1.23E-16	1.46E-16	1.71E-16	2.30E-16
a_1	.977	2.41E-17	1.05E-16	1.58E-16	2.59E-16	3.81E-16	4.85E-16	6.40E-16	6.94E-16	7.40E-16	7.96E-16	9.12E-16
b_1	1.627	4.40E-18	2.30E-17	3.64E-17	6.17E-17	9.07E-17	1.14E-16	1.49E-16	1.61E-16	1.72E-16	1.85E-16	2.14E-16
4.5LOSS	4.5	2.38E-20	1.44E-18	5.13E-18	2.49E-17	8.47E-17	1.72E-16	3.40E-16	4.02E-16	4.53E-16	5.12E-16	6.00E-16
6 LOSS	6	3.05E-22	1.27E-19	8.50E-19	9.65E-18	6.46E-17	1.91E-16	5.31E-16	6.89E-16	8.36E-16	1.03E-15	1.50E-15
8.4LOSS	8.4		8.62E-24	5.52E-22	1.20E-19	7.59E-18	8.02E-17	7.19E-16	1.23E-15	1.82E-15	2.83E-15	6.67E-15
9.97 LOSS	10				2.42E-25	2.41E-22	1.36E-20	6.25E-19	1.59E-18	3.17E-18	6.86E-18	3.18E-17
IONIZATION	12.06						1.63E-20	4.10E-18	1.47E-17	3.74E-17	1.04E-16	7.59E-16
DIS.EXCIT.	14.7							2.64E-20	1.32E-19	4.12E-19	1.39E-18	1.30E-17

1. See JILA Information Center Report 26 for a summary of recent calculation procedures.

* See S. Yoshida, A. V. Phelps and L. C. Pitchford, Phys. Rev. A 27, 2858 (1983) for the calculation of the contribution of ionization to the energy balance. The calculation for attachment is similar. In the energy balance attachment results in a term equal to the negative of average electron energy times the attachment rate coefficient and a term equal to the average of the energy times the energy dependent attachment frequency.