Appendix A: Expressions used for Cross Sections

The seven cross sections expressions for ionization (with or without dissociation) were taken from reference 6, except for $\mathbf{CH_4 + e_a^- \rightarrow C^+ + 2H_2 + e_a^- + e_b^-}$, which showed inconsistencies with experimental data so its model expression was taken from reference 7. The 11 photonic emission expressions were taken from reference 7.

Fourteen of these cross section expressions have the same functional form over their own energy range of E_{min} to E_{max} and is given by:

$$\sigma = f_3(E_1; a_1, a_2, a_3, a_4. a_5, a_6)$$

where:

$$f_3(x;\ c_1, c_2, c_3, c_4, c_5, c_6) = \frac{f_1(x; c_1, c_2)}{[1 + (x/c_3)^{(c_2+c_4)} + (x/c_5)^{(c_2+c_6)}]}$$

$$f_1(x; c_1, c_2) = \sigma_0 c_1 (x/E_R)^{c_2}$$

$$f_3(x;\ c_1, c_2, c_3, c_4, c_5, c_6) = \frac{f_1(x; c_1, c_2)}{[1 + (x/c_3)^{(c_2+c_4)} + (x/c_5)^{(c_2+c_6)}]}$$

such that:

$$\sigma = \frac{\sigma_0 a_1 (E_1/E_R)^{a_2}}{[1 + (E_1/a_3)^{(a_2+a_4)} + (E_1/a_5)^{(a_2+a_6)}]} \quad \text{A1}$$

where:
$\sigma_0 = 1 \text{ x } 10^{-16}$ cm^2
$E_R = 1.361 \text{ x } 10^{-2}$ keV (Rydberg constant)
$E_1 = E - E_{th}$

The remaining four cross sections have a different from given by:

$$\sigma = f_3(E_1; a_1, a_2, a_3, a_4. a_5, a_6) + a_7 f_3(E_1/a_8; a_1, a_2, a_3, a_4. a_5, a_6)$$

Such that:

$$\sigma = \frac{\sigma_0 a_1 (E_1/E_R)^{a_2}}{[1 + (E_1/a_3)^{(a_2+a_4)} + (E_1/a_5)^{(a_2+a_6)}]} + \frac{\sigma_0 a_1 a_7 (E_1/a_8 E_R)^{a_2}}{[1 + (E_1/a_8 a_3)^{(a_2+a_4)} + (E_1/a_8 a_5)^{(a_2+a_6)}]} \quad \text{A2}$$

Beyond E_{max}, the magnitude of all 18 cross sections were modeled linearly in a log-log representation consistent with Bethe-Born theory for inelastic processes, i.e.,

$$\mathbf{\ln(\sigma) = A \cdot \ln(E) + B} \quad \text{A3}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ were derived from slope and magnitude of the expressions at E_{max}.

Table C1 lists the coefficients used for these18 cross sections.

Table C1: Coefficients for equations C1-3

Event	$\rightarrow \mathbf{CH_4^+ + e_a^- + e_b^-}$	$\rightarrow \mathbf{CH_3^+ + H^* + e_a^- + e_b^-}$	$\rightarrow \mathbf{CH_2^+ + H_2 + e_a^- + e_b^-}$	$\rightarrow \mathbf{CH_3^* + H^+ + e_a^- + e_b^-}$
$\boldsymbol{E_{min}}$	1.50E-02	1.50E-02	1.75E-02	2.50E-02
$\boldsymbol{E_{max}}$	1	1	1	1
$\boldsymbol{E_{th}}$	1.26E-02	1.26E-02	1.26E-02	2.11E-02

a_1	9.66E+00	7.13E+00	2.06E-01	4.97E-02
a_2	2.32E+00	2.26E+00	3.29E+00	3.51E+00
a_3	5.60E-03	5.60E-03	1.50E-02	2.24E-02
a_4	-2.08E-01	-2.34E-01	-3.13E-01	-8.22E-01
a_5	1.87E-02	1.92E-02	2.87E-02	3.90E-02
a_6	9.10E-01	9.08E-01	1.01E+00	1.04E+00
A	-0.74434	-0.75386	-0.91907	-1.0325
B	-32.444	-32.592	-33.237	-32.365
Event	$\rightarrow \mathbf{CH^+ + H_2 + H^* + e_a^- + e_b^-}$	$\rightarrow \mathbf{CH_2^* + H_2^+ + e_a^- + e_b^-}$	$\rightarrow \mathbf{C^+ + 2H_2 + e_a^- + e_b^-}$	
E_{min}	2.50E-02	2.50E-02	3.00E-02	
E_{max}	1	1	1	
E_{th}	2.22E-02	2.23E-02	0.0282	
a_1	4.54E-01	6.30E-03	0.064	
a_2	2.80E+00	5.20E+00	1.43	
a_3	2.00E-02	1.74E-02	0.0133	
a_4	1.00E+00	-7.78E-01	-0.33	
a_5	7.90E-03	2.72E-02	0.0424	
a_6	-5.22E-01	1.04E+00	1.181	
A	-0.9829	-1.0363	-1.1594	
B	-33.6774	-34.873	-33.686	
Event	Ly-$\boldsymbol{\alpha}$ line: 121.567 nm	Ly-$\boldsymbol{\beta}$ line: 102.572 nm	Ly-$\boldsymbol{\gamma}$ line: 97.254 nm	**H**-$\boldsymbol{\alpha}$ line: 656.28 nm
E_{min}	2.06E-02	2.03E-02	2.15E-02	2.16E-02
E_{max}	9.86E-01	9.88E-01	9.84E-01	6.00E+00
E_{th}	1.47E-02	1.66E-02	1.73E-02	1.66E-02
a_1	8.54E-03	5.21E-02	2.24E-02	1.33E-02
a_2	2.82E+00	4.65E+00	4.21E+00	2.41E+00
a_3	2.72E-02	5.91E-03	5.80E-03	1.04E-02
a_4	-1.90E-01	-1.24E+00	-1.12E+00	-1.19E+00
a_5	5.95E-02	1.66E-02	1.78E-02	3.35E-02
a_6	1.60E+00	1.10E+00	1.16E+00	1.04E+00
A	-1.5044	-1.1107	-1.1703	-1.0436
B	-31.591	-35.694	-36.075	-35.305
Event	H-$\boldsymbol{\beta}$ line: 486.13 nm	H-$\boldsymbol{\gamma}$ line: 434.05 nm	H-$\boldsymbol{\delta}$ line: 410.17 nm	
E_{min}	2.07E-02	1.88E-02	2.02E-02	
E_{max}	6.00E+00	6.00E+00	6.00E+00	
E_{th}	1.73E-02	1.76E-02	1.76E-02	
a_1	1.55E-02	1.33E-03	4.05E-04	
a_2	3.54E+00	1.98E+00	2.31E+00	
a_3	6.40E-03	2.30E-02	2.49E-02	

a_4	-1.06E+00	-4.00E-01	-3.20E-01	
a_5	1.90E-02	4.08E-02	4.06E-02	
a_6	1.05E+00	1.08E+00	1.11E+00	
A	-1.0557	-1.0848	-1.1058	
B	-36.695	-37.261	-38.033	
Event	CH G-band: ~430 nm	**C I** line: 165.7 nm	**C III** line: 190.9 nm	**C IV** line: 151.1 nm
E_{min}	1.46E-02	2.75E-02	2.43E-02	2.62E-02
E_{max}	5.00E+00	4.00E-01	9.80E-01	1.00E+00
a_1	1.22E-02	2.35E-02	1.57E-02	2.50E-02
a_2	1.07E+00	1.08E-02	6.88E-04	1.82E-03
a_3	1.60E+01	4.35E+00	6.55E+00	2.20E+00
a_4	8.40E-03	8.08E-03	1.72E-02	1.16E-02
a_5	-1.19E+00	-2.30E-01	2.10E-01	9.50E-01
a_6	1.18E-02	1.37E-02	2.50E-02	1.87E-02
a_7	9.09E-01	1.81E+00	1.80E+00	9.50E-01
a_8	3.27E+00	1.75E+00	1.22E+00	1.82E+00
A	-0.91092	-1.3889	-1.4876	-0.97797
B	-36.036	-35.749	-34.29	-38.783

The remaining 10 cross sections were constructed as piece-wise polynomials over the available range of published data, and given by:

$$\sigma = a_4E^4 + a_3E^3 + a_2E^2 + a_1E + a_0 \qquad \text{A4}$$

Above the maximum of those data, the cross sections were modeled linearly in a log-log representation consistent with Bethe-Born theory for inelastic processes according to equation

C3. Table C2 lists the coefficients used for these 10 cross sections.

Event	$\rightarrow \mathbf{CH_3^* + H^* + e_a^-}$	$\rightarrow \mathbf{CH_2^* + H_2 + e_a^-}$	$\rightarrow \mathbf{CH^* + H_2 + H^* + e_a^-}$	$\rightarrow \mathbf{CH_3^* + H^-}$
E_{min} (eV)	7.5	7.5	13	6
E_{max} (eV)	17	22	90	8
a_0	1.7536E-16	2.1296E-16	-4.4972E-18	3.8263E-20
a_1	-5.3092E-17	-7.9147E-17	4.5944E-19	-8.5858E-19
a_2	5.0307E-18	9.7273E-18	-8.8557E-21	6.9593E-18
a_3	-1.511E-19	-4.4331E-19	8.2949E-23	-2.3656E-17
a_4	-3.2217E-25	6.8159E-21	1.402E-21	2.7270E-17
E_{min} (eV)	17	22	-	8
E_{max} (eV)	40	40	-	12
a_0	-1.1553E-15	1.2817E-16	-	6.7363E-17
a_1	1.6685E-16	-3.555E-18	-	-3.5794E-17
a_2	-7.8001E-18	1.1875E-20	-	6.5238E-18
a_3	1.5689E-19	0	-	-4.9237E-19

a_4	-1.156E-21	0	-	1.3212E-20
E_{min} (eV)	40	-	-	-
E_{max} (eV)	100	-	-	-
a_0	2.0729E-16	-	-	-
a_1	-2.1828E-18	-	-	-
a_2	-7.6710E-22	-	-	-
a_3	7.2059E-23	-	-	-
a_4	0	-	-	-
E_{min} (eV)	100	40	90	12.5
E_{max} (eV)	100000	100000	100000	100000
A	-1.1196	-8.636	-0.8511	-15.944
B	-32.335	-7.9828	-36.077	-2.7595
Event	mode v_1	mode v_2	mode v_3	mode v_4
E_{min} (eV)	1	1	1	1
E_{max} (eV)	5	5	5	5
a_0	9.5775E-18	1.1232E-17	2.3026E-17	2.7555E-17
a_1	-8.9135E-18	-6.0423E-18	-1.2559E-17	-1.004E-17
a_2	3.3126E-18	2.2599E-18	3.3263E-18	2.1595E-18
a_3	-2.1225E-19	-1.008E-19	-1.2141E-19	-9.2766E-20
a_4	0	0	0	0
E_{min} (eV)	5	5	5	5
E_{max} (eV)	10	10	10	10
a_0	1.2176E-16	2.5438E-16	2.8946E-16	2.33E-16
a_1	-8.6348E-17	-1.618E-16	-1.8694E-16	-1.3779E-16
a_2	2.2772E-17	3.8308E-17	4.4288E-17	3.0494E-17
a_3	-2.2987E-18	-3.622E-18	-4.1437E-18	-2.7257E-18
a_4	7.8662E-20	1.1914E-19	1.344E-19	8.6051E-20
E_{min} (eV)	10	10	10	10
E_{max} (eV)	17	17	17	17
a_0	1.9796E-16	1.5228E-16	1.3383E-16	3.5303E-17
a_1	-3.4049E-17	-1.9841E-17	-1.149E-17	3.2174E-18
a_2	2.0965E-18	1.0086E-18	3.2806E-19	-3.7628E-19
a_3	-4.3665E-20	-1.8137E-20	-2.3848E-21	9.5309E-21
a_4	0	0	0	0
E_{min} (eV)	17	17	17	17
E_{max} (eV)	100000	100000	100000	100000
A	-0.76715	-1.3092	-1.5041	-0.76174
B	-36.926	-34.883	-34.149	-35.94
Event	$\mathcal{J}=0$ to $\mathcal{J}=3$	$\mathcal{J}=0$ to $\mathcal{J}=4$		
E_{min} (eV)	1	1		
E_{max} (eV)	7.5	7.5		

a_0	4.0187E-17	-1.4292E-18		
a_1	-3.4332E-17	4.8739E-18		
a_2	9.5048E-18	-3.8881E-18		
a_3	-5.8352E-19	1.276E-18		
a_4	0	-8.8977E-20		
E_{min} (eV)	7.5	7.5		
E_{max} (eV)	30	30		
a_0	3.8926E-17	-5.9277E-16		
a_1	3.3496E-18	1.577E-16		
a_2	1.8872E-19	-1.1631E-17		
a_3	-6.3879E-21	3.5567E-19		
a_4	0	-3.9501E-21		
E_{min} (eV)	30	30		
E_{max} (eV)	100000	100000		
A	-0.75386	-1.2547		
B	-33.963	-32.873		