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**COMPUTATION OF RATE
COEFFICIENTS FOR ELECTRON
IMPACT COLLISIONS**

by

Thomas M. Philip

Memorandum No. UCB/ERL M98/43

10 July 1998

COVER

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ELECTRONICS RESEARCH LABORATORY

College of Engineering
University of California, Berkeley
94720

Abstract

Computation of Rate Coefficients for Electron Impact Collisions

by

T. M. Philip

**Department of Electrical Engineering and Computer Sciences
University of California at Berkeley**

The rate coefficients for electron impact collision reactions are required for a number of applications and in use in modelling. We employ two methods for the computation of these rate coefficients. In the method described in chapter 1, where cross sectional data is available for the reactions, we compute the rate coefficients by integrating over an assumed Maxwellian distribution. In chapter 2, we rely on a model developed by Clark et al. to approximate the rate coefficients for the electron impact excitations of light elements.

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Chapter 1

Electron Impact Collisions in a Boron Trifluoride Discharge

1.1 Introduction

The rate coefficient for an electron impact collision reaction can be obtained by integrating the cross sectional area over a Maxwellian velocity distribution, given the cross sectional area and the electron energy. In this chapter we describe such a computation for the electron impact collisions in a Boron Trifluoride Discharge.

1.2 Background

The rate coefficient for an electron impact collision is obtained by integrating the cross sections over an assumed Maxwellian distribution:

$$k = \langle \sigma v \rangle = 4\pi \int_0^{\infty} \sigma v^3 f(v) dv \quad (1.1)$$

where

$$f(v) = \left(\frac{m_e}{2eT_e} \right)^{3/2} \exp\left(-\frac{m_e v^2}{2eT_e} \right) \quad (1.2)$$

is the Maxwellian speed distribution, m_e is the electron mass, T_e is the electron temperature in equivalent voltage units, e is the electron charge, σ is the collision cross section, and v is the electron velocity¹. Using the relationship for the kinetic energy of a particle,

$$E = \frac{mv^2}{2e} \quad (1.3)$$

we can express the rate constant in terms of the electron temperature:

$$k = \int_0^{\infty} \left(\frac{8eT_e}{\pi m_e} \right)^{\frac{1}{2}} \sigma \frac{E}{T_e} \exp\left(-\frac{E}{T_e}\right) \frac{dE}{T_e} \quad (1.4)$$

The rate coefficients can then be fit to the Arrhenius form:

$$k = AT_e^B \exp\left(-\frac{C}{T_e}\right) \quad (1.5)$$

where A , B and C are constants.

1.3 Calculations

Based on the above expressions, we developed a MatLab program to compute the rate constants for a reaction given the cross-sectional area and electron energy, and to fit the generated data to the Arrhenius form (refer to Appendix A).

1.3.1 Dissociation Reactions

The rate constants for the following reactions were computed by first generating cross sections for given electron energies:

Table 1.1

| # | Reaction | #of binding electrons (B) |
|---|-------------------------------------|---------------------------|
| 1 | $e + BF_3 \rightarrow BF_2 + F + e$ | 3 |
| 2 | $e + BF_2 \rightarrow BF + F + e$ | 2 |
| 3 | $e + BF \rightarrow B + F + e$ | 1 |

The cross-sections were computed using a simple excitation model based on a Thomson cross section:

$$\sigma = \begin{cases} 0 & E < E_{diss} \\ B\pi\left(\frac{e}{4\pi\epsilon_0}\right)^2 \frac{1}{E} \left(\frac{1}{E_{diss}} - \frac{1}{E}\right) & E_{diss} < E < E_{iz} \\ B\pi\left(\frac{e}{4\pi\epsilon_0}\right)^2 \frac{1}{E} \left(\frac{1}{E_{diss}} - \frac{1}{E_{iz}}\right) & E > E_{iz} \end{cases} \quad (1.6)$$

where, E is the electron energy, E_{diss} is the dissociation energy, and E_{iz} is the ionization energy².

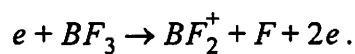
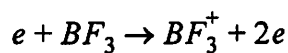
It was observed that while the theoretical dissociation energy for reaction 1 in Table 1 is 6.5 eV, the experimental value given by Kushner³ was 10.1 eV. In order to compensate for this discrepancy in energy, the dissociation energies of reactions 2 and 3 were approximated to be 2 eV higher than their theoretical values.

Table 1.2

| # | Reaction | Theoretical E_d (eV) | Experimental E_d (eV) | E_d Used (eV) |
|---|-------------------------------------|---------------------------|----------------------------|--------------------|
| 1 | $e + BF_3 \rightarrow BF_2 + F + e$ | 6.5 | 10.1 | 10.1 |
| 2 | $e + BF_2 \rightarrow BF + F + e$ | 5.9 | Not Available | 7.9 |
| 3 | $e + BF \rightarrow B + F + e$ | 8.1 | Not Available | 10.1 |

1.3.2 Ionization Reactions

The ionization of BF_3 includes the following two reactions:



Experimental data for the ionization of BF_3 did not differentiate between these reactions. Therefore, the reaction rate of the combined reaction from the experimental data was apportioned into a ratio equivalent to that based on a simple Thomson cross section estimate in order to obtain reaction rates for the individual reactions.

1.3.3 Normalization of Estimates

The estimates based on a simple Thomson cross section model were normalized by a scalar factor to agree with the experimental data. A summary of the normalization factors used is given in the table below:

Table 1.3

| Reaction | A (Estimated Value) | A (Value Used) | Normalization Factor |
|---|--------------------------|--------------------------|----------------------|
| $e + \text{BF}_3 \rightarrow \text{BF}_3^+ + 2e$ | 1.0640×10^{-14} | 3.5400×10^{-15} | 3.00 |
| $e + \text{BF}_3 \rightarrow \text{BF}_2^+ + \text{F} + 2e$ | 6.9500×10^{-14} | 2.3100×10^{-14} | 3.00 |
| $e + \text{BF}_3 \rightarrow \text{BF}_2 + \text{F} + e$ | 2.6207×10^{-13} | 8.7367×10^{-14} | 3.00 |
| $e + \text{BF}_2 \rightarrow \text{BF}_2^+ + 2e$ | 1.3000×10^{-13} | 1.7810×10^{-14} | 7.30 |
| $e + \text{BF}_2 \rightarrow \text{BF} + \text{F} + e$ | 1.6730×10^{-13} | 5.2280×10^{-14} | 3.20 |
| $e + \text{BF} \rightarrow \text{BF}^+ + 2e$ | 4.6700×10^{-14} | 4.6700×10^{-14} | 1.00 |
| $e + \text{BF} \rightarrow \text{B} + \text{F} + e$ | 3.8870×10^{-14} | 1.2140×10^{-14} | 3.20 |
| $e + \text{B} \rightarrow \text{B}^+ + 2e$ | 8.2600×10^{-14} | 2.6260×10^{-14} | 3.14 |
| $e + \text{F} \rightarrow \text{F}^+ + 2e$ | 9.4300×10^{-14} | 1.5700×10^{-14} | 6.00 |
| $e + \text{B}^+ \rightarrow \text{B}^{++} + 2e$ | 1.7600×10^{-14} | 2.4110×10^{-15} | 7.30 |

1.4 Results

The results are summarized in Table 4. These results are graphically depicted in Figures 1-19.

The figure numbers correspond to the reaction numbers of Table 4.

Table 4: Summary of Results

| Fig | Reaction | A | B | C | E_d (V) | E_{iz} (V) | Reference |
|------------|---|--------------------------|----------|----------|--------------------------|---------------------------|------------------|
| 1 | $e + BF_3 \rightarrow BF_3^+ + 2e$ | 1.0267x10 ⁻¹⁵ | 0.4449 | 15.3743 | 15.56 | 15.76 | 3 |
| | | 1.3630x10 ⁻¹⁵ | 0.3561 | 15.7143 | 15.56 | 15.76 | 4 |
| | | 3.54x10 ⁻¹⁵ | -0.5 | 15.60 | 15.56 | 15.76 | 2 |
| 2 | $e + BF_3 \rightarrow BF_2^+ + F + 2e$ | 6.7063x10 ⁻¹⁵ | 1.0559 | 15.9643 | | 15.76 | 3 |
| | | 8.9032x10 ⁻¹⁵ | 0.9671 | 16.3043 | | 15.76 | 4 |
| | | 2.31x10 ⁻¹⁴ | 0.111 | 16.19 | | 15.76 | 2 |
| 3 | $e + BF_3 \rightarrow BF_2 + F + e$ | 2.683x10 ⁻¹⁴ | 0.3532 | 10.46 | 10.10 | 15.56 | 3 |
| | | 8.7367x10 ⁻¹⁴ | -0.3026 | 11.11 | 10.10 | 15.56 | 2 |
| 4 | $e + BF_2 \rightarrow BF_2^+ + 2e$ | 2.229x10 ⁻¹⁵ | 1.371 | 8.367 | | 9.40 | 4 |
| | | 1.781x10 ⁻¹⁴ | 0.058 | 9.8 | | 9.40 | 2 |
| 5 | $e + BF_2 \rightarrow BF + F + e$ | 1.331x10 ⁻¹⁵ | -0.4054 | 6.768 | 5.90 | 9.40 | 2 |
| | | 5.228x10 ⁻¹⁴ | -0.481 | 8.488 | 7.90 | 9.40 | 2 |
| 6 | $e + BF \rightarrow BF^+ + 2e$ | 9.583x10 ⁻¹⁵ | 0.824 | 9.618 | | 11.12 | 4 |
| | | 4.67x10 ⁻¹⁴ | 0.040 | 11.5 | | 11.12 | 2 |
| 7 | $e + BF \rightarrow B + F + e$ | 3.728x10 ⁻¹⁴ | -0.4249 | 8.969 | 8.10 | 11.12 | 2 |
| | | 1.214x10 ⁻¹⁴ | -0.4936 | 10.55 | 10.10 | 11.12 | 2 |
| 8 | $e + B \rightarrow B^+ + 2e$ | 2.626x10 ⁻¹⁵ | 1.4073 | 6.9418 | | 8.29 | 5 |
| | | 2.429x10 ⁻¹⁴ | -0.02 | 8.8 | | 8.29 | 2 |
| 9 | $e + F \rightarrow F^+ + 2e$ | 1.30x10 ⁻¹⁴ | 0 | 16.50 | | 17.42 | 6 |
| | | 1.57x10 ⁻¹⁴ | 0.131 | 17.8 | | 17.42 | 2 |
| 10 | $e + BF_3^+ \rightarrow BF_2 + F$ | 4.353x10 ⁻¹² | -0.5 | 0 | | | 2 |
| 11 | $e + BF_2^+ \rightarrow BF + F$ | 4.398x10 ⁻¹⁵ | -1.44 | 6.16 | | | 2 |
| 12 | $e + BF^+ \rightarrow B + F$ | 1.301x10 ⁻¹⁴ | -1.47 | 4.26 | | | 2 |
| 13 | $e + B^+ \rightarrow B^{++} + 2e$ | 9.41x10 ⁻¹⁶ | 1.008 | 25.19 | | | 5 |
| | | 2.411x10 ⁻¹⁵ | 0.202 | 25.1 | | | 2 |
| 14 | $e + BF_3 \rightarrow BF_3 (\nu=1) + e$ | 1.573x10 ⁻¹⁵ | -0.4092 | 0.5662 | 5.89x10 ⁻² | | 3 |
| 15 | $e + BF_3 \rightarrow BF_3 (\nu=2) + e$ | 3.563x10 ⁻¹⁵ | -0.3533 | 0.5559 | 8.60x10 ⁻² | | 3 |
| 16 | $e + BF_3 \rightarrow BF_3 (\nu=3) + e$ | 3.329x10 ⁻¹⁴ | -0.2099 | 0.4195 | 1.80x10 ⁻¹ | | 3 |
| 17 | $e + BF_3 \rightarrow BF_3 + e$ | 6.866x10 ⁻¹⁴ | 0.4449 | 0.3893 | 2.42x10 ⁻⁵ | | 3 |

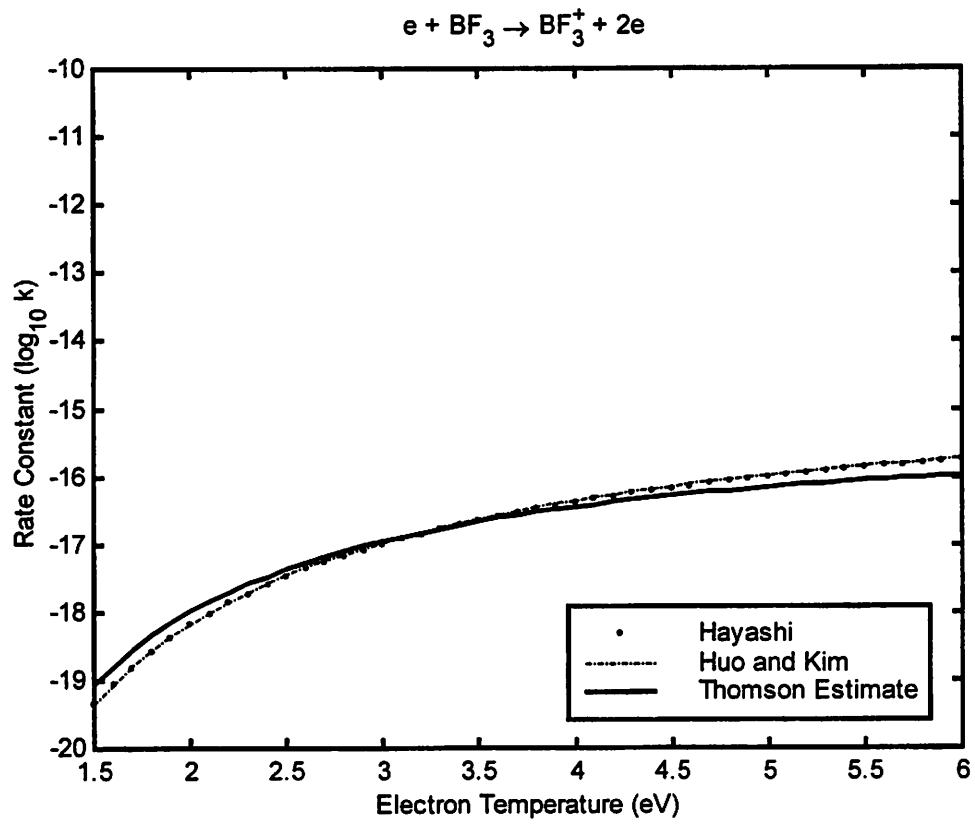


Figure 1.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3^+ + 2e$

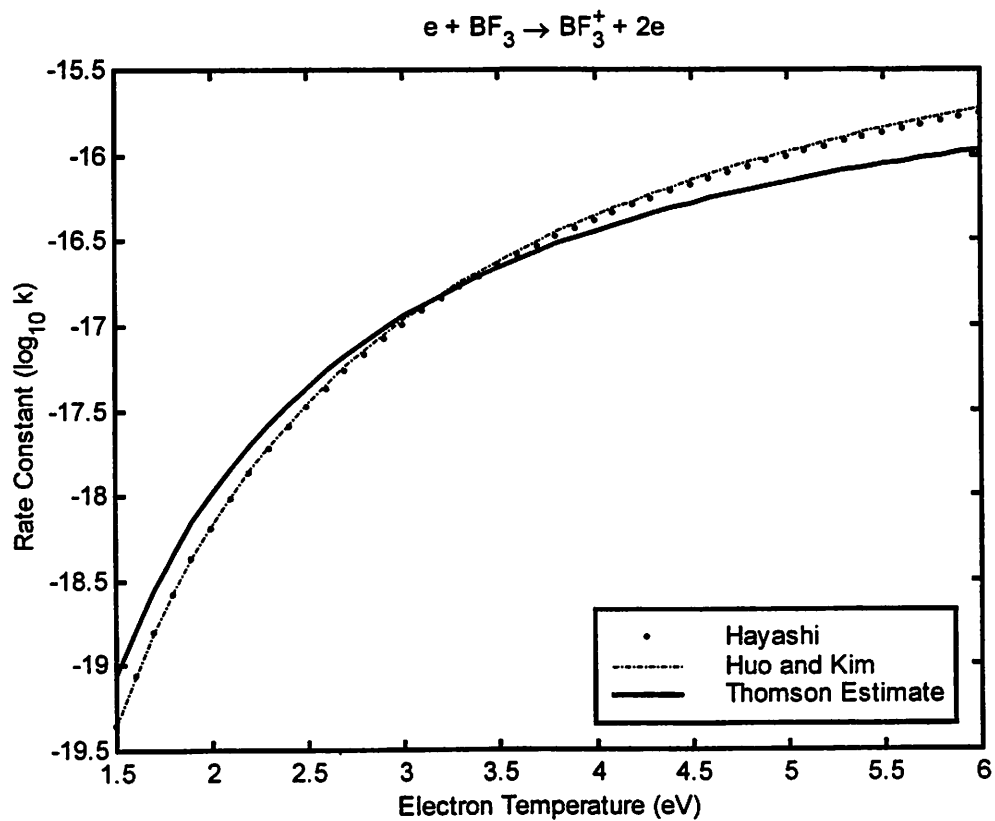


Figure 1.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3^+ + 2e$

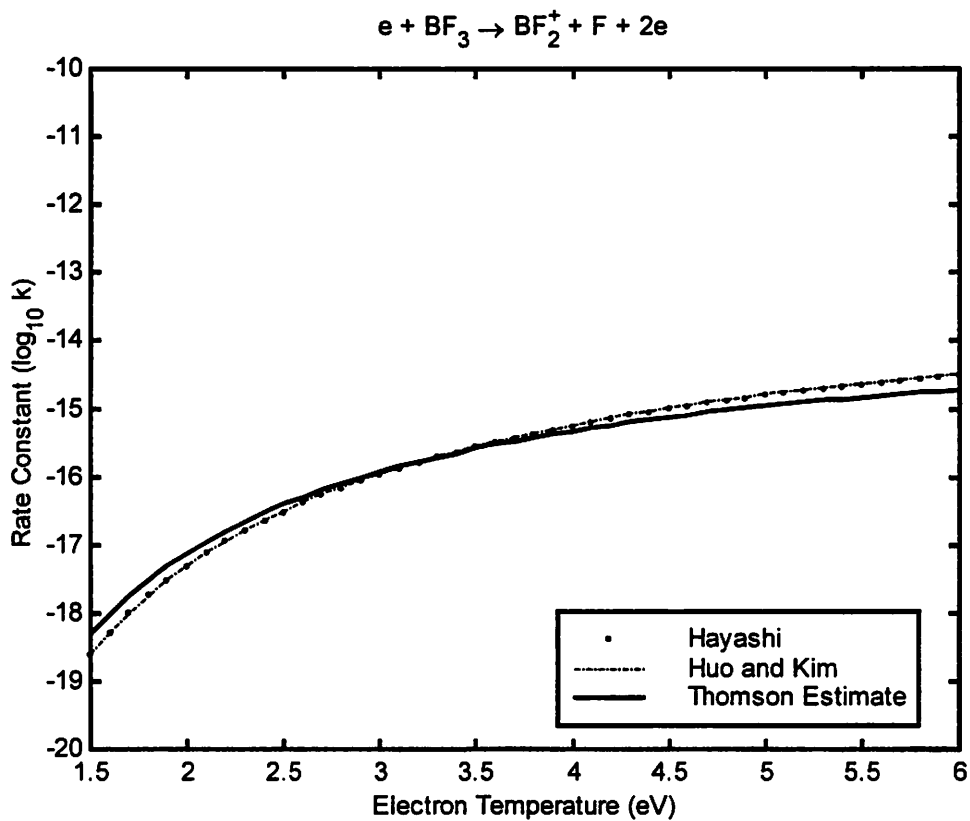


Figure 2.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_2^+ + \text{F} + 2e$

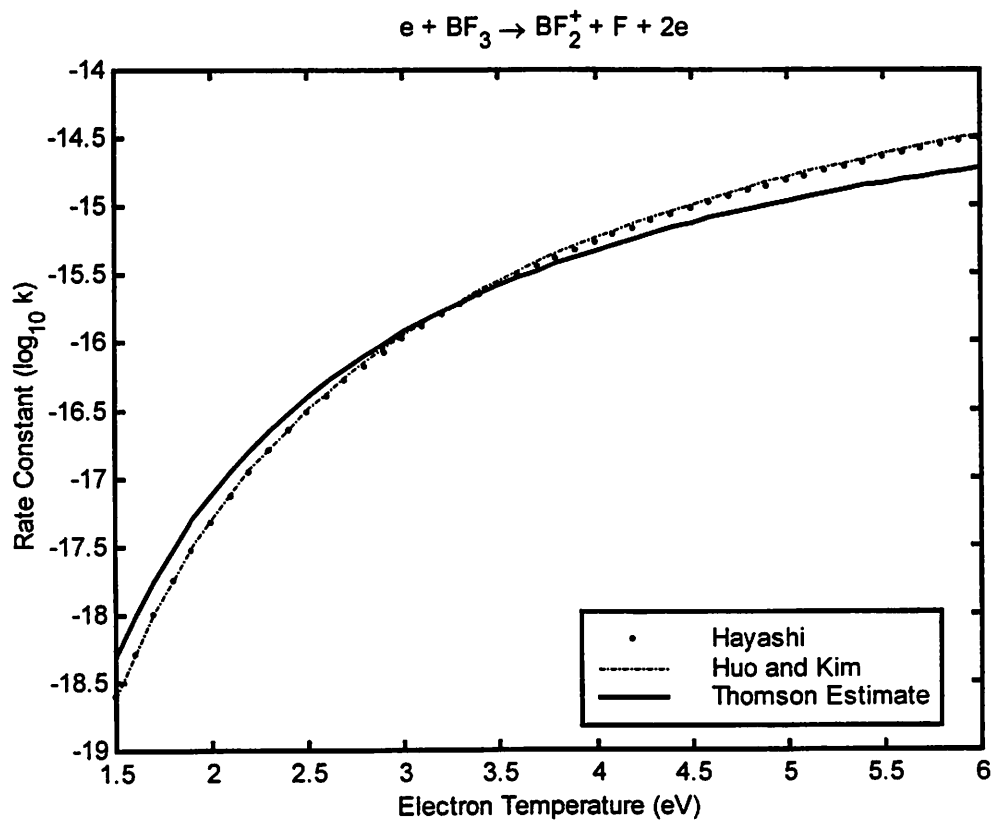


Figure 2.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_2^+ + \text{F} + 2e$

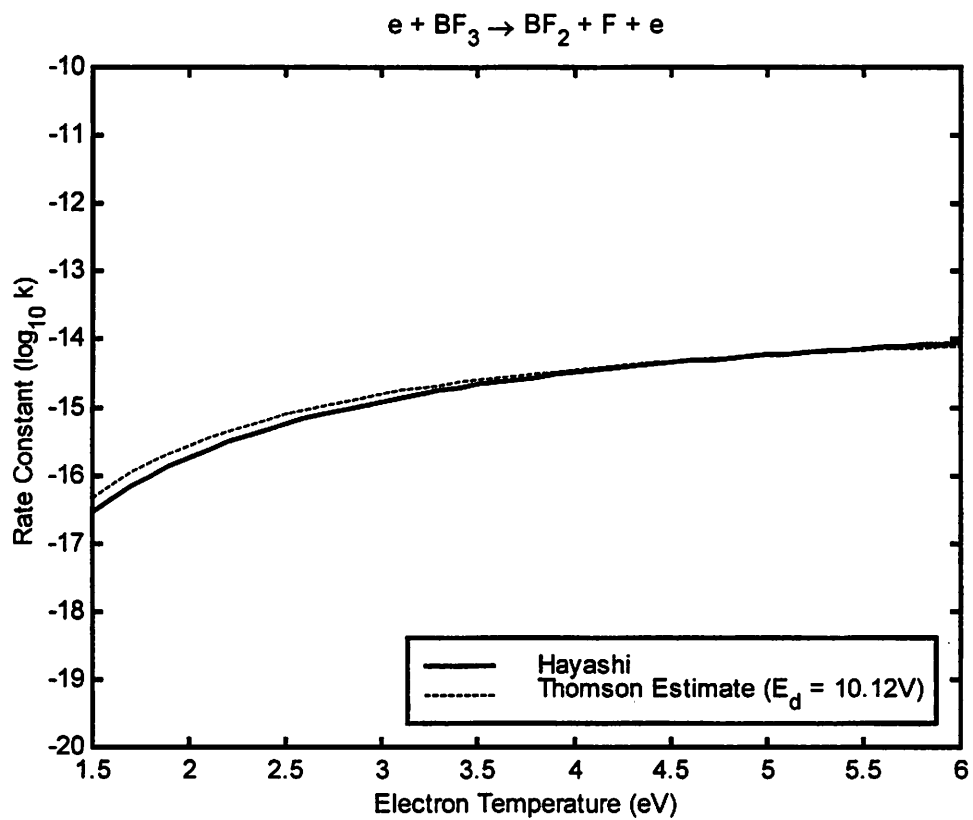


Figure 3.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_2 + \text{F} + e$

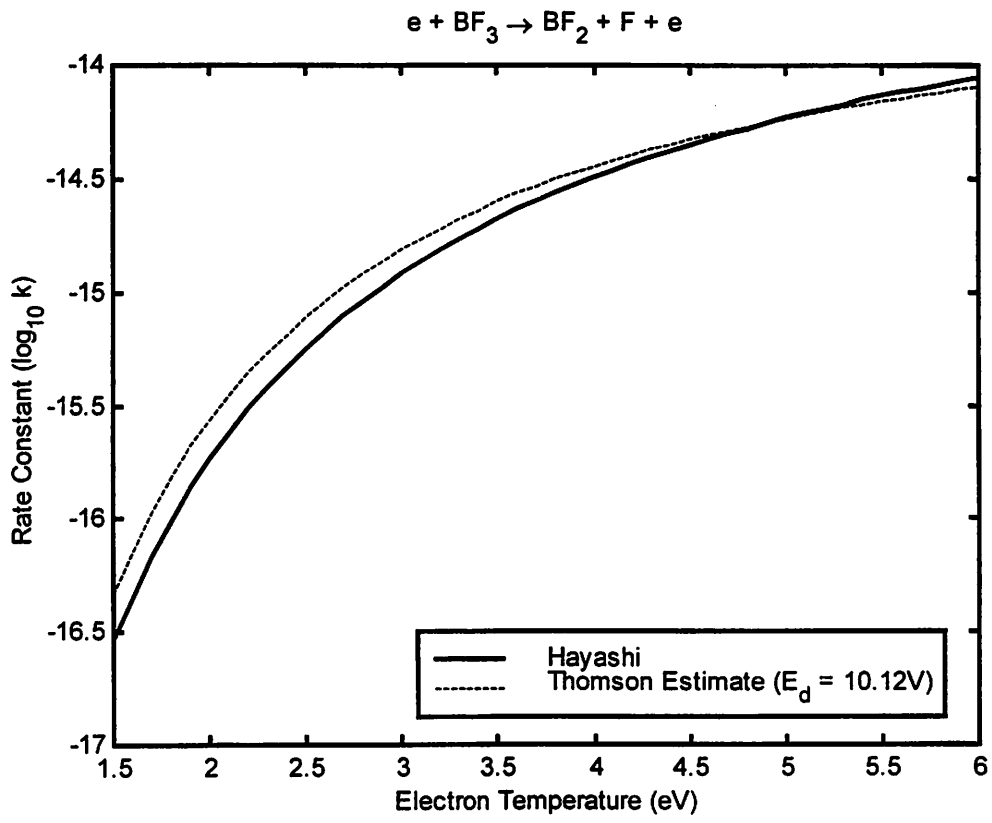


Figure 3.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_2 + \text{F} + e$

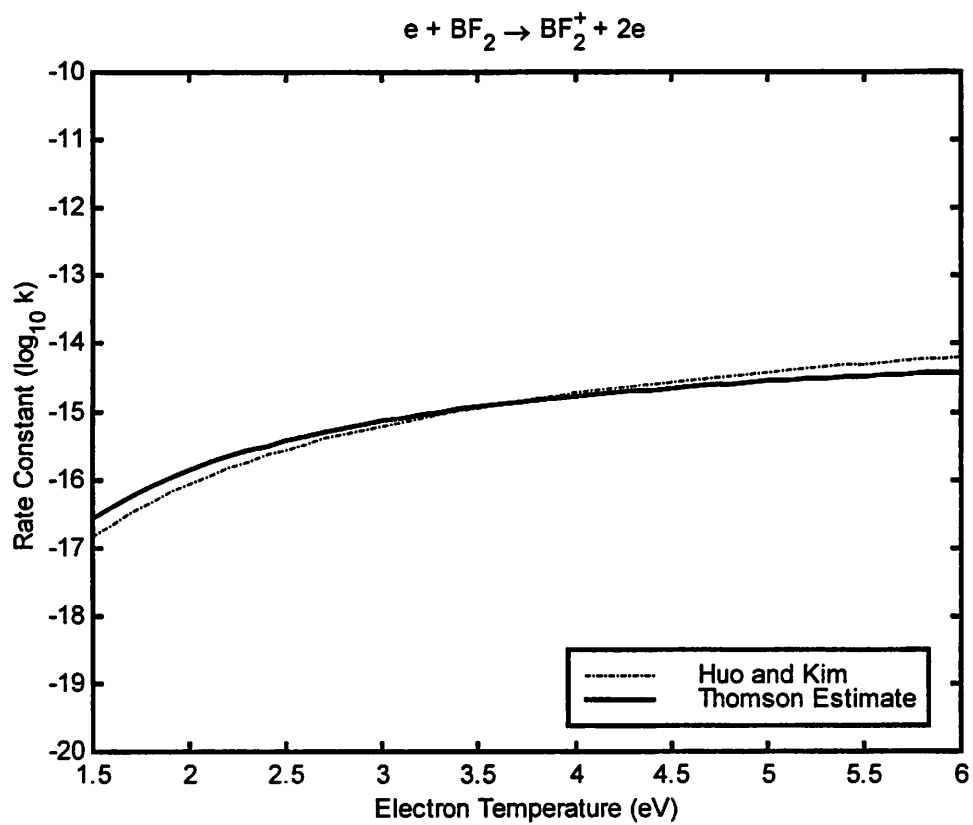


Figure 4.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2 \rightarrow \text{BF}_2^+ + 2e$

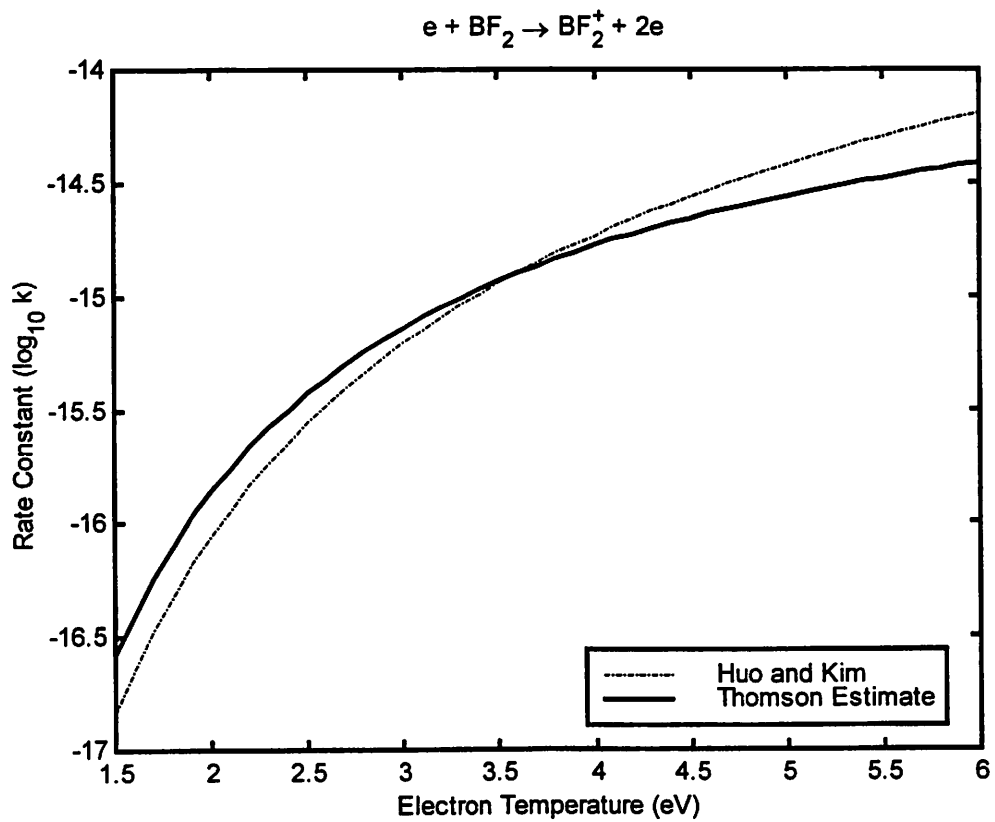


Figure 4.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2 \rightarrow \text{BF}_2^+ + 2e$

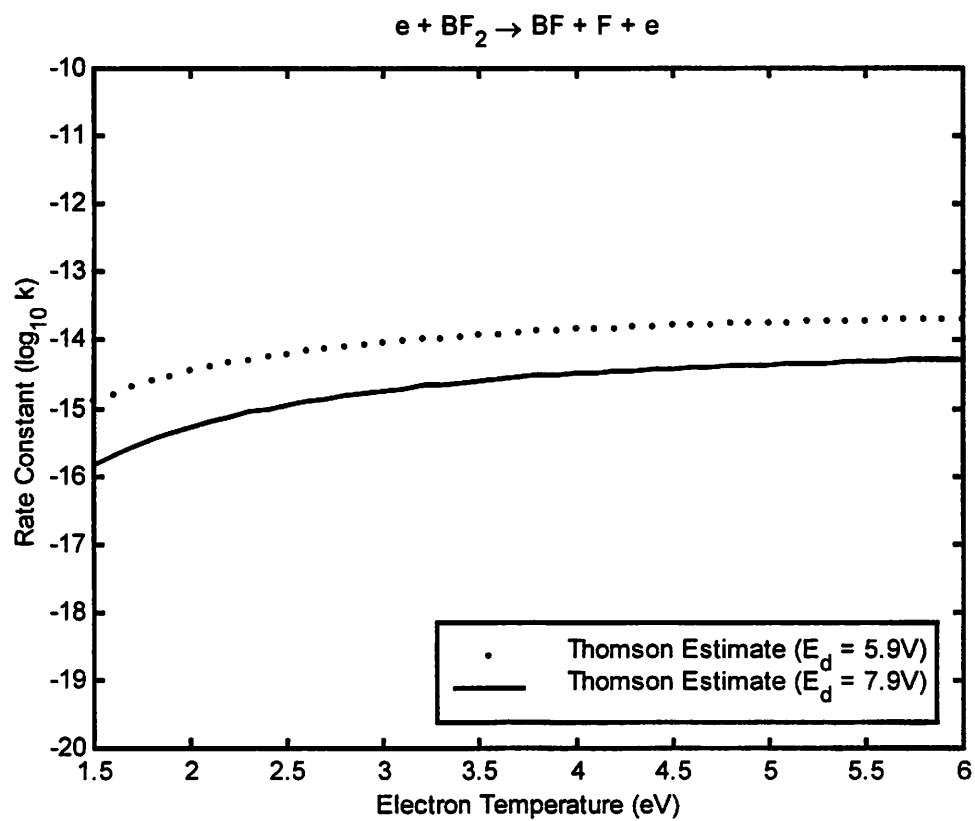


Figure 5.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2 \rightarrow \text{BF} + \text{F} + e$

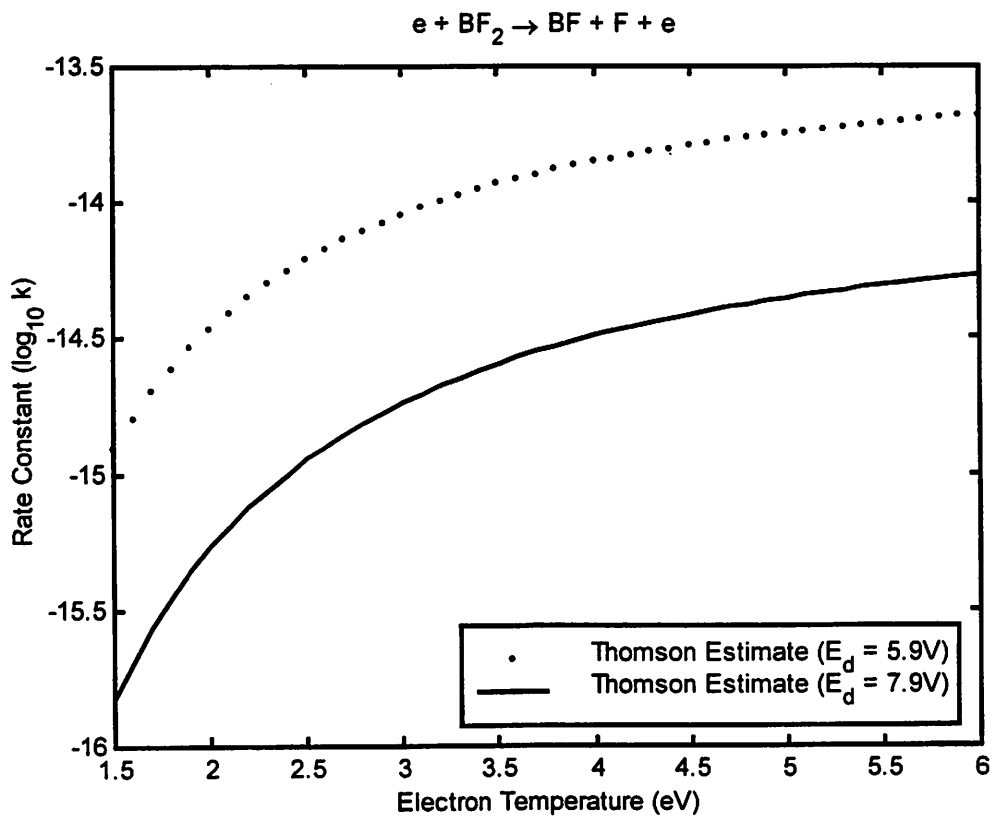


Figure 5.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2 \rightarrow \text{BF} + \text{F} + e$

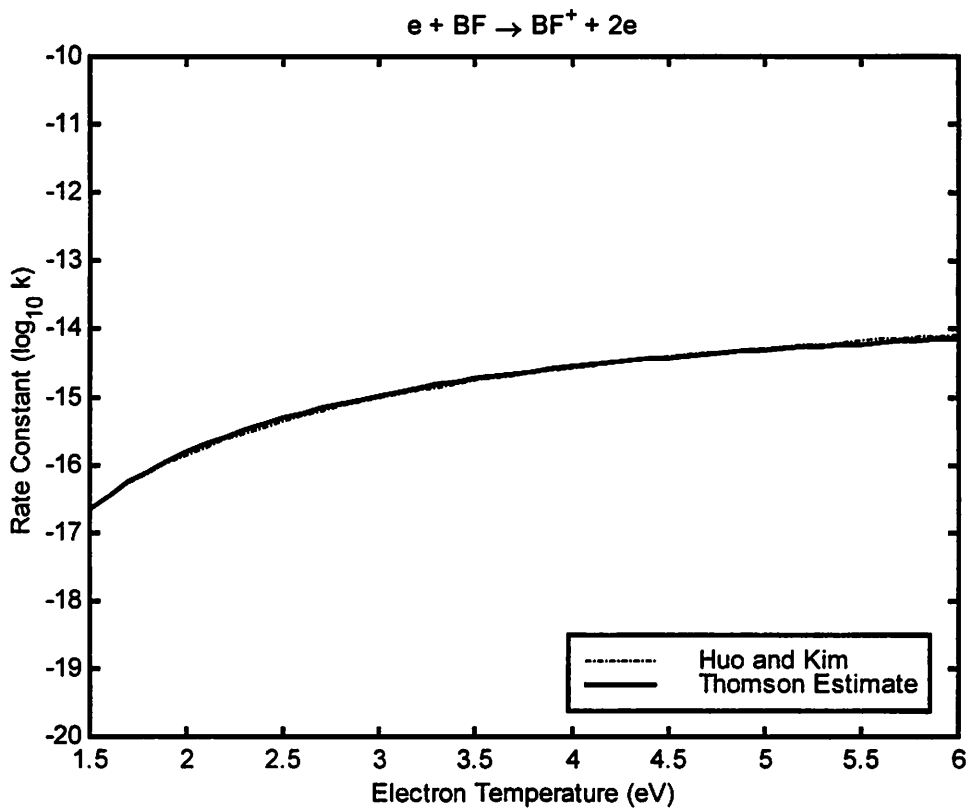


Figure 6.a: Rate Constant as a function of Electron Temperature for $e + \text{BF} \rightarrow \text{BF}^+ + 2e$

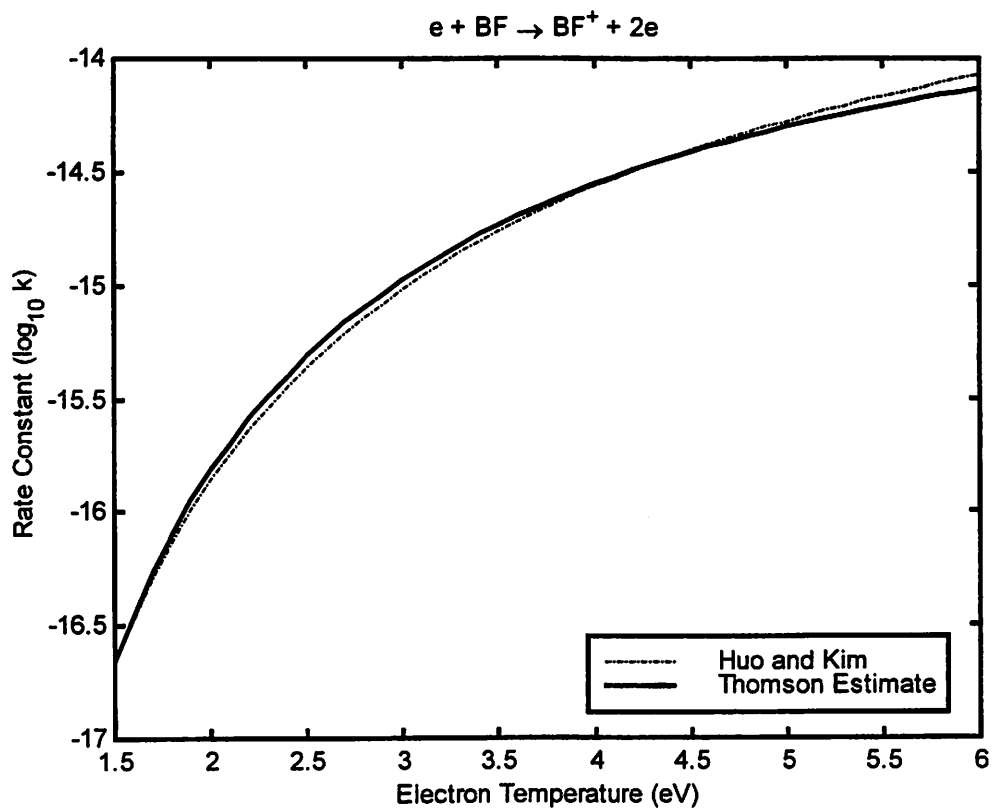


Figure 6.b: Rate Constant as a function of Electron Temperature for $e + \text{BF} \rightarrow \text{BF}^+ + 2e$

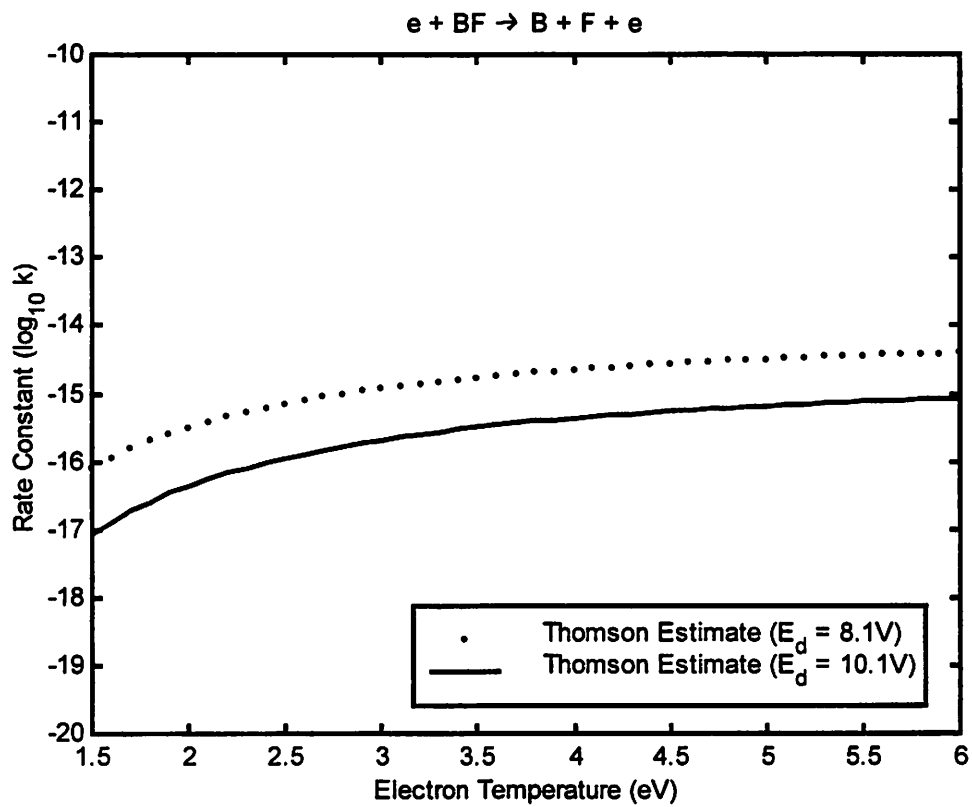


Figure 7.a: Rate Constant as a function of Electron Temperature for $e + BF \rightarrow B + F + e$

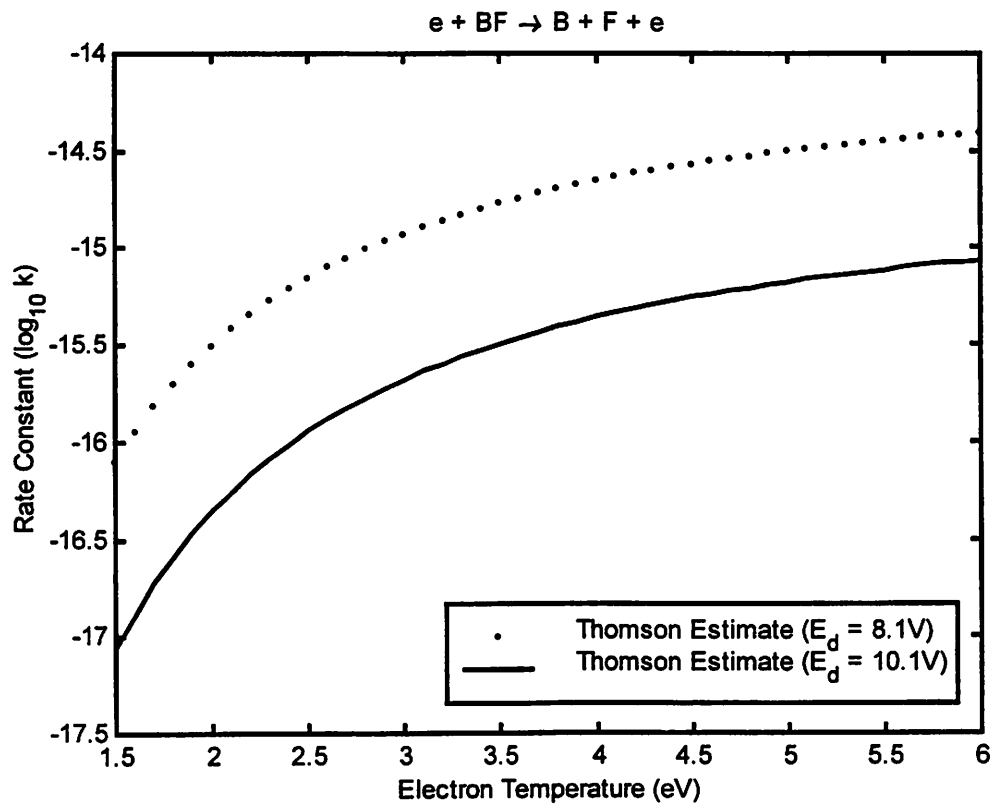


Figure 7.b: Rate Constant as a function of Electron Temperature for $e + BF \rightarrow B + F + e$

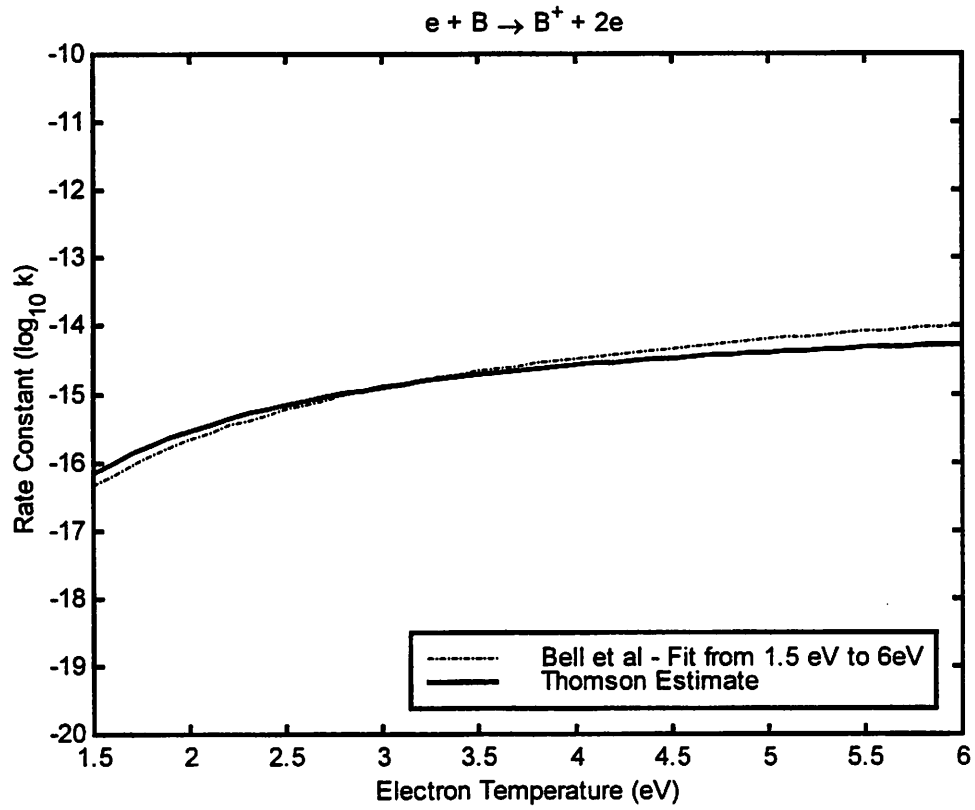


Figure 8.a: Rate Constant as a function of Electron Temperature for $e + B \rightarrow B^+ + 2e$

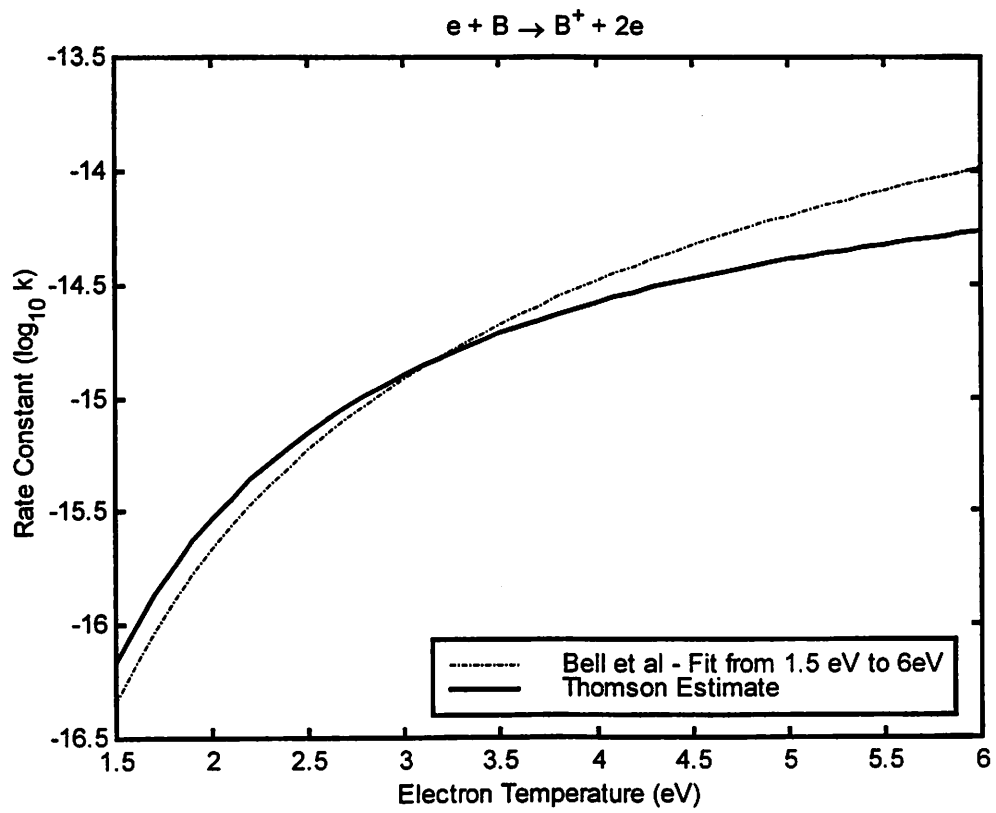


Figure 8.b: Rate Constant as a function of Electron Temperature for $e + B \rightarrow B^+ + 2e$

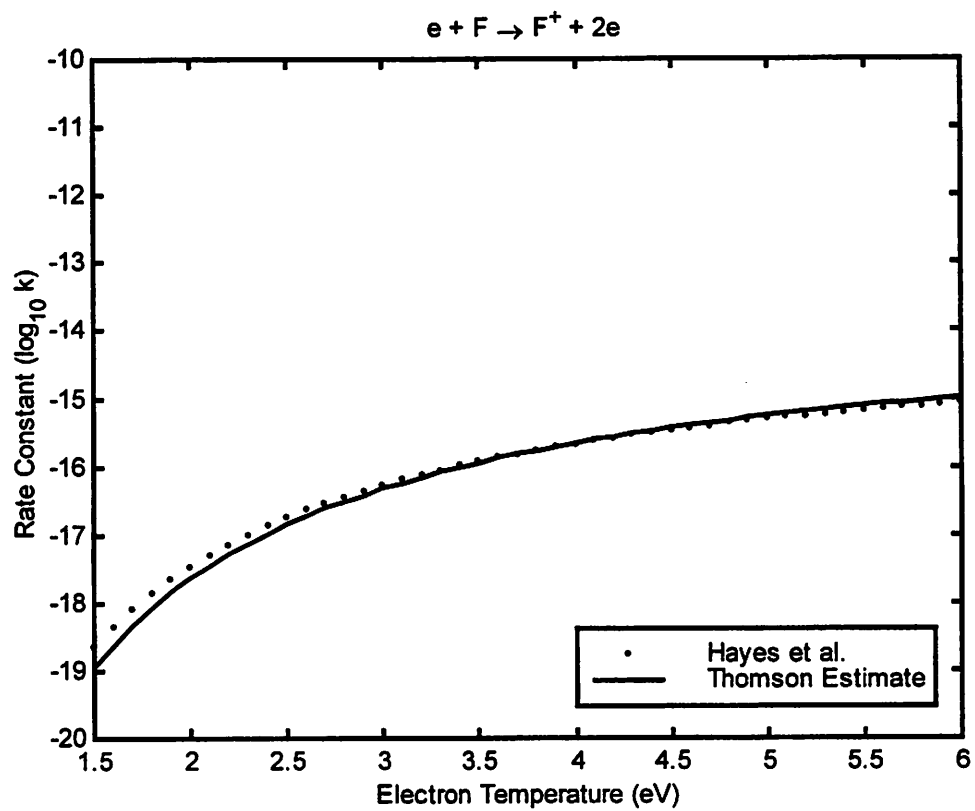


Figure 9.a: Rate Constant as a function of Electron Temperature for $e + F \rightarrow F^+ + 2e$

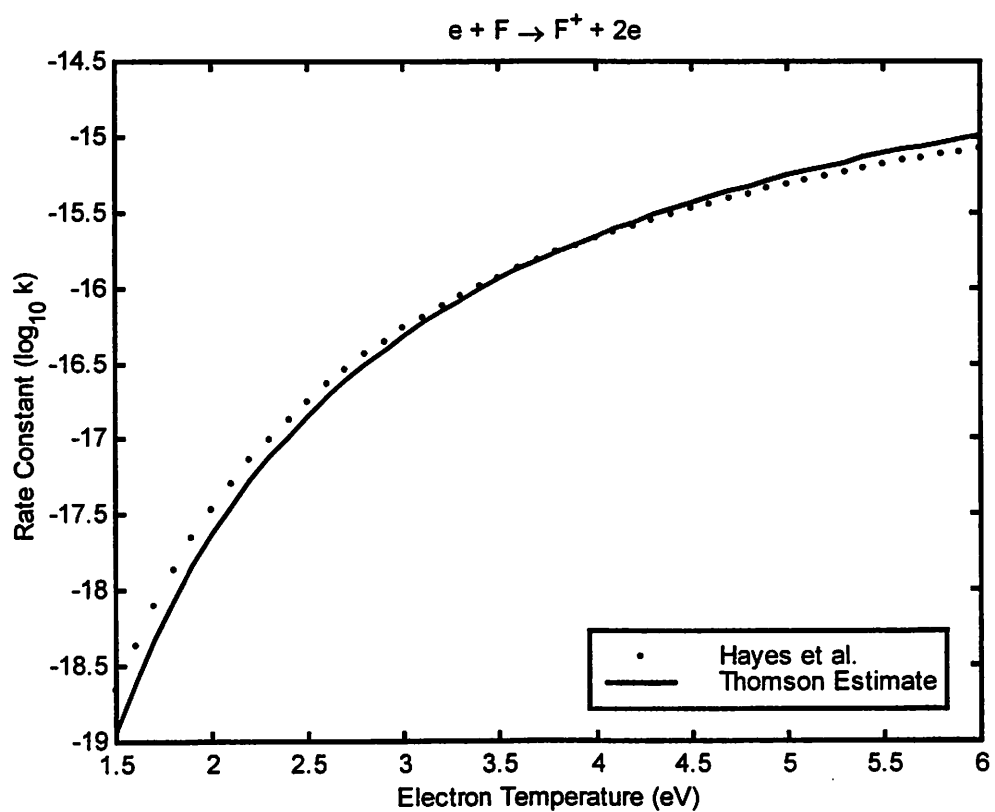


Figure 9.b: Rate Constant as a function of Electron Temperature for $e + F \rightarrow F^+ + 2e$

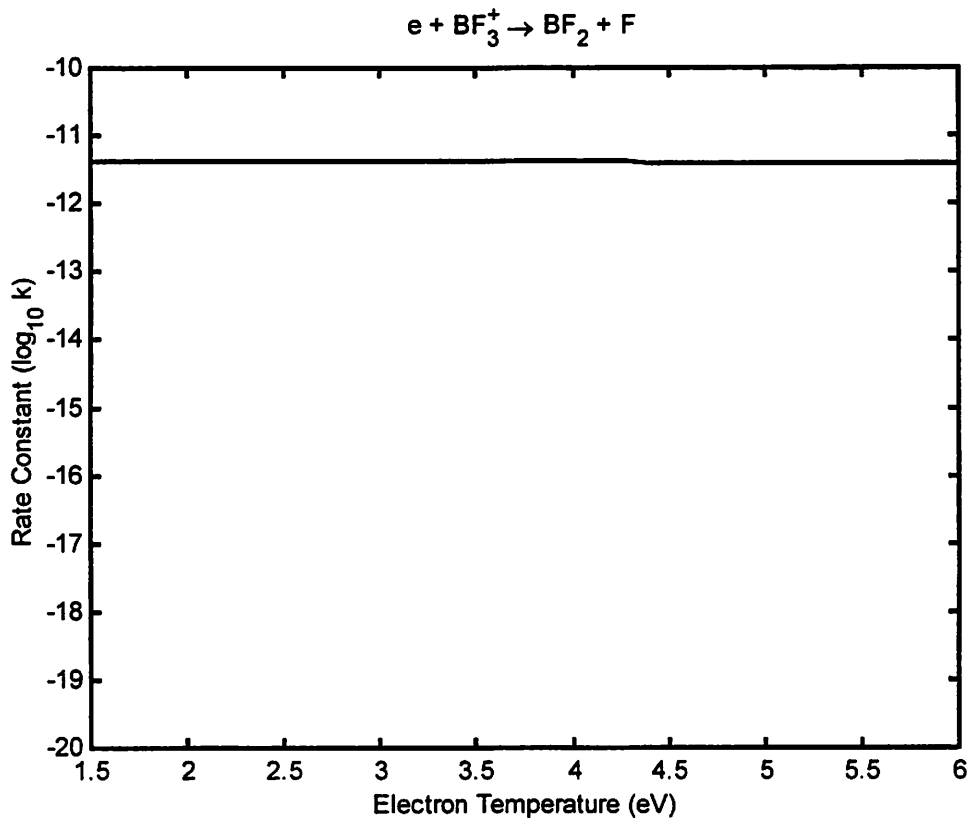


Figure 10.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3^+ \rightarrow \text{BF}_2 + \text{F}$

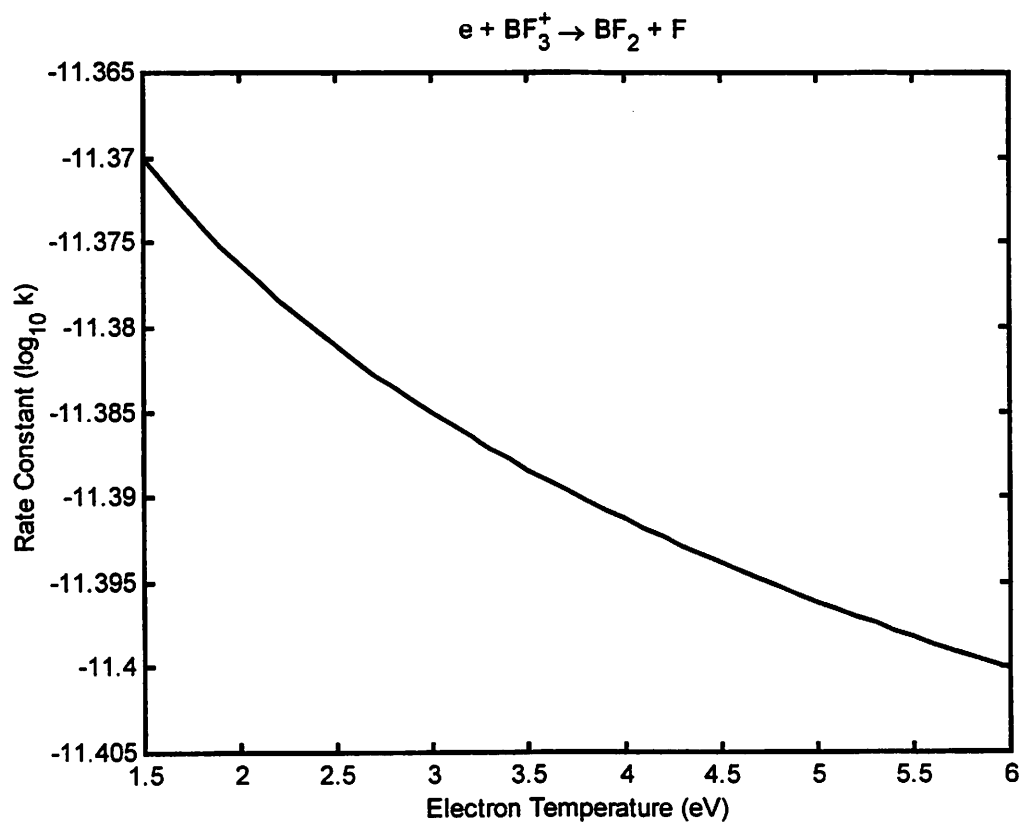


Figure 10.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3^+ \rightarrow \text{BF}_2 + \text{F}$

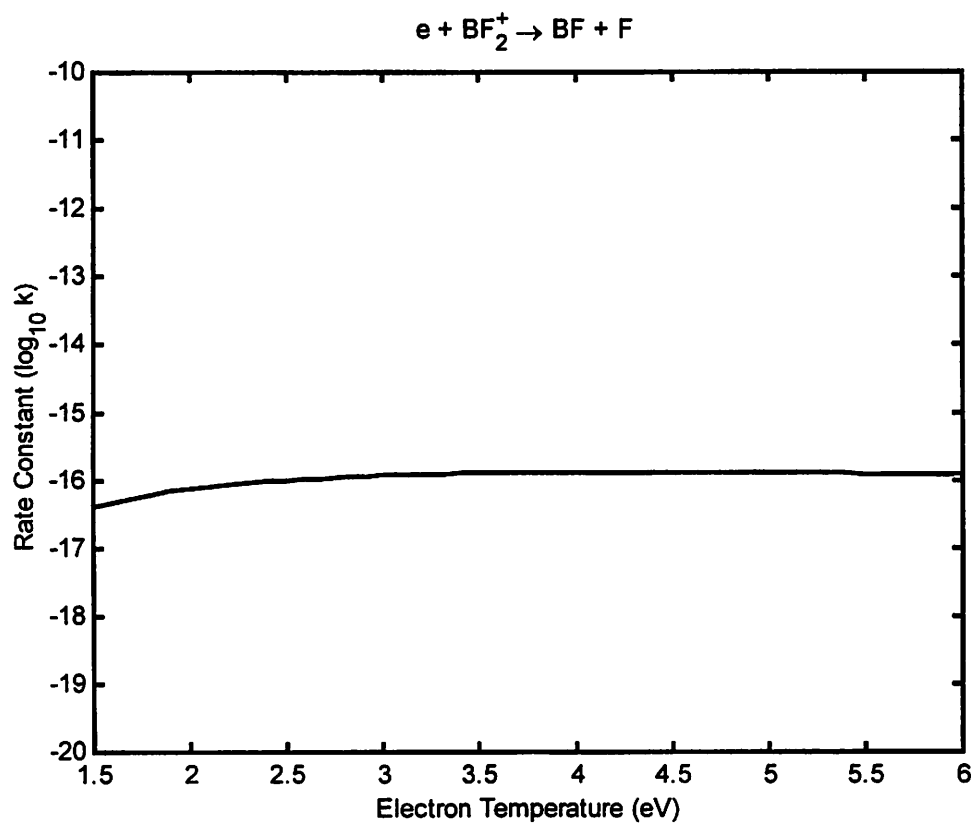


Figure 11.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2^+ \rightarrow \text{BF} + \text{F}$

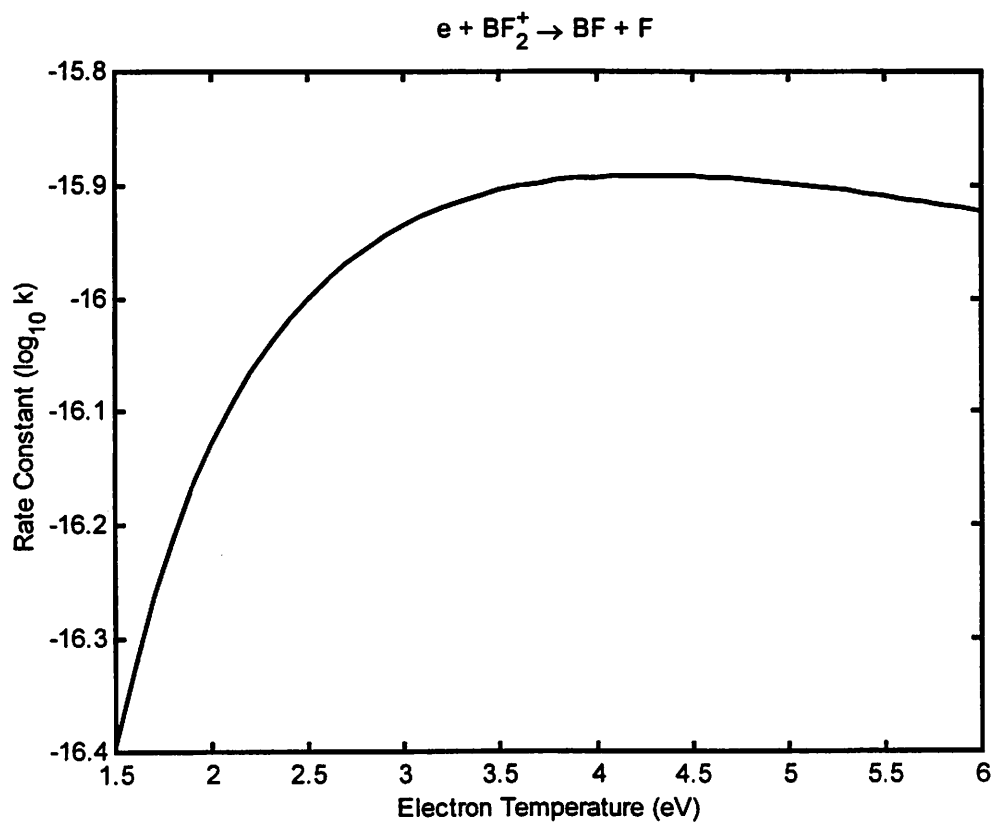


Figure 11.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_2^+ \rightarrow \text{BF} + \text{F}$

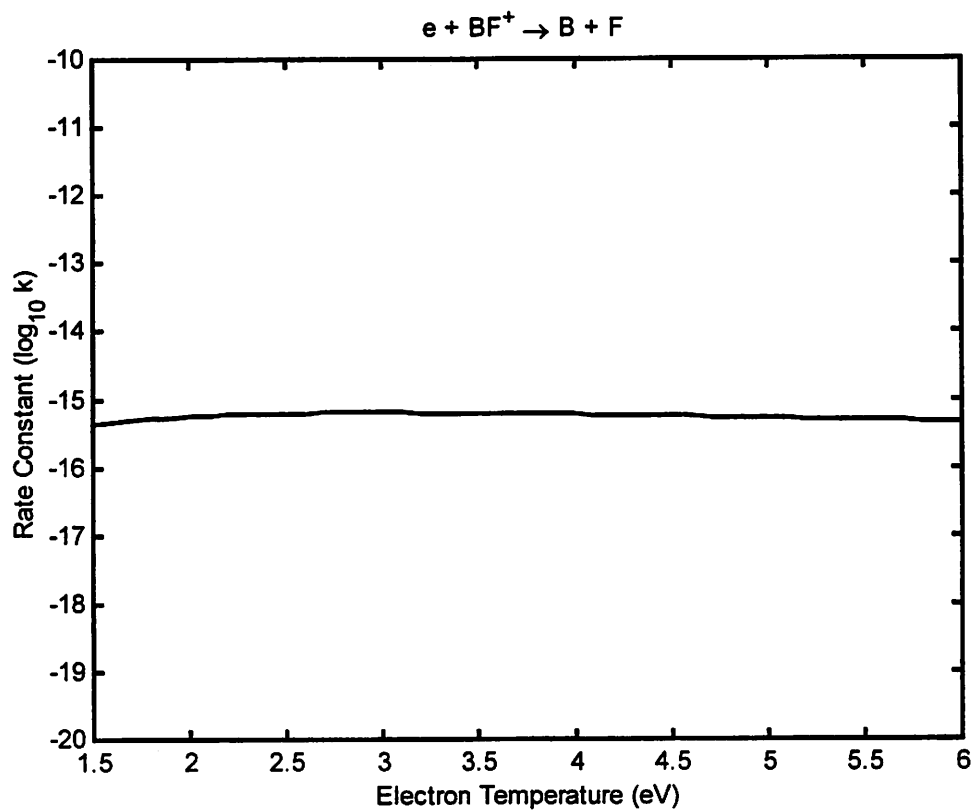


Figure 12.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}^+ \rightarrow \text{B} + \text{F}$

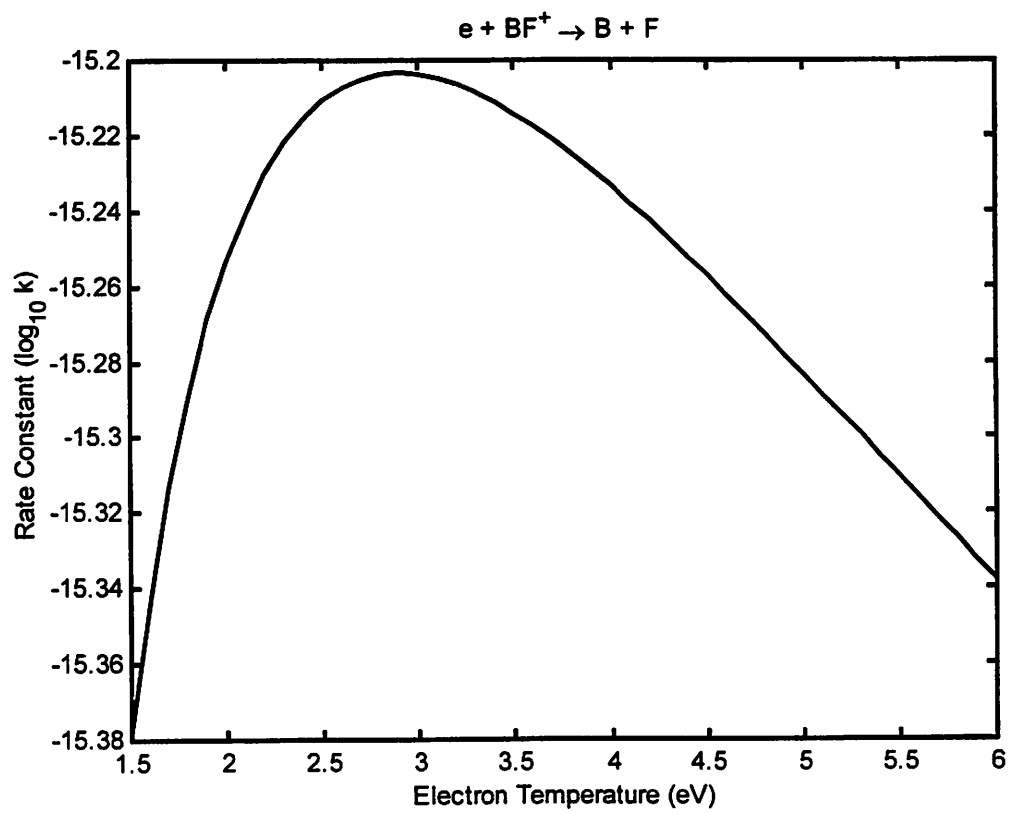


Figure 12.b: Rate Constant as a function of Electron Temperature for $e + BF^+ \rightarrow B + F$

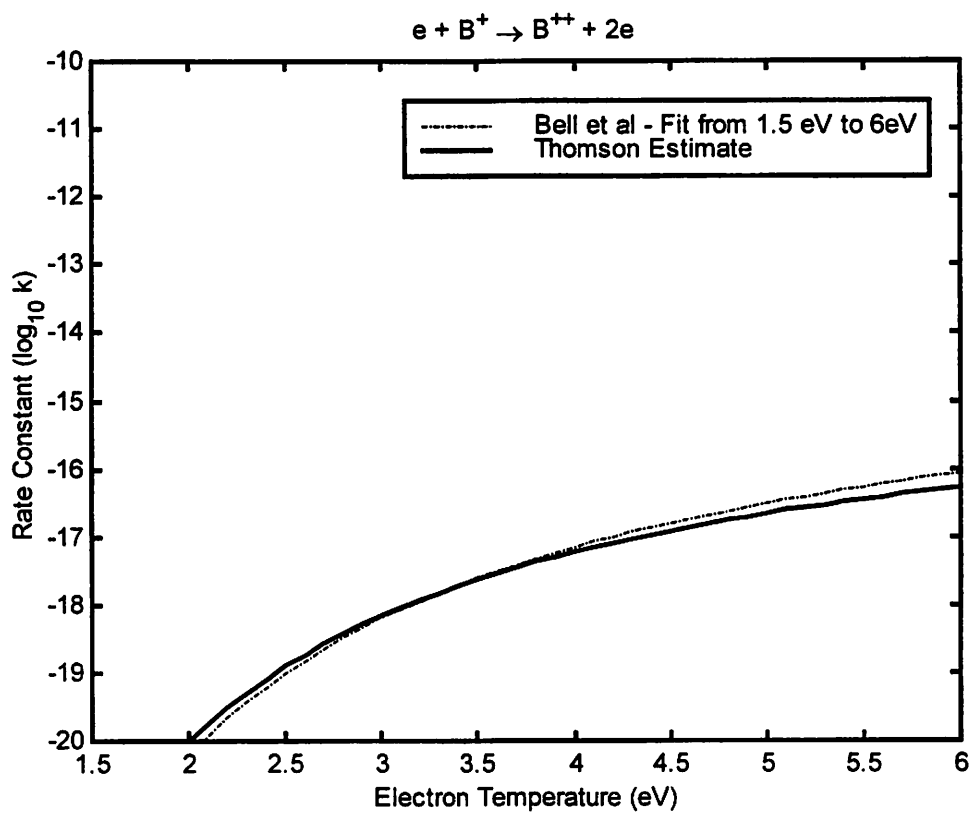


Figure 13.a: Rate Constant as a function of Electron Temperature for $e + B^+ \rightarrow B^{++} + 2e$

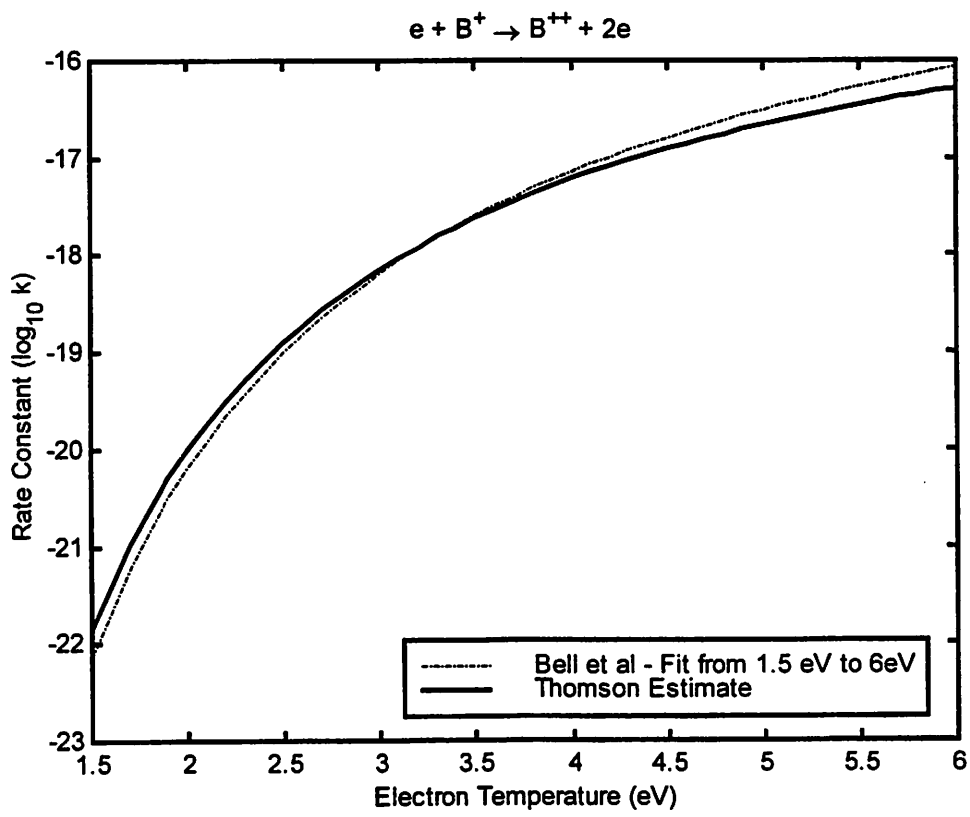


Figure 13.b: Rate Constant as a function of Electron Temperature for $e + B^+ \rightarrow B^{++} + 2e$

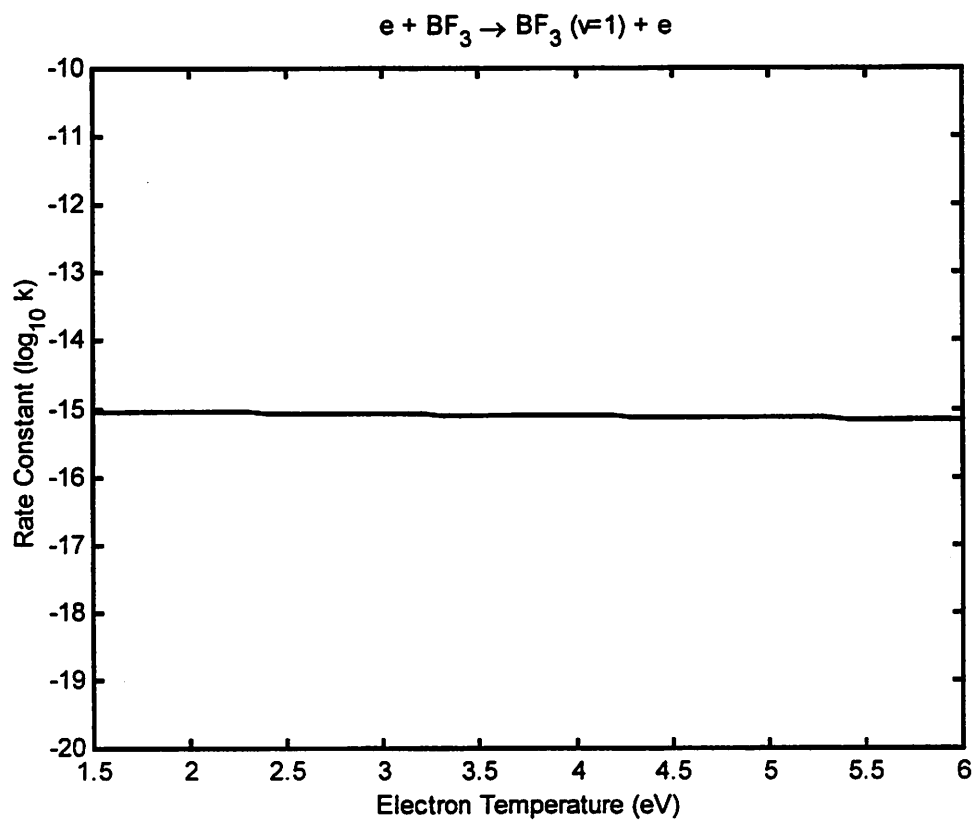


Figure 14.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=1) + e$

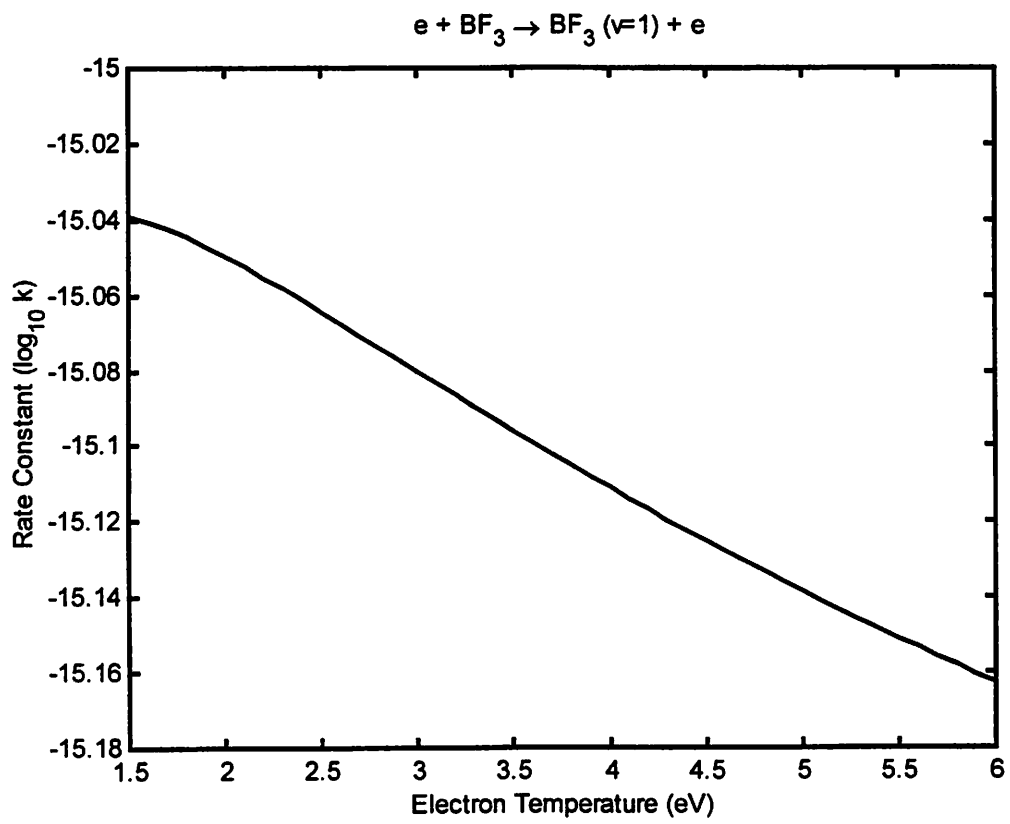


Figure 14.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=1) + e$

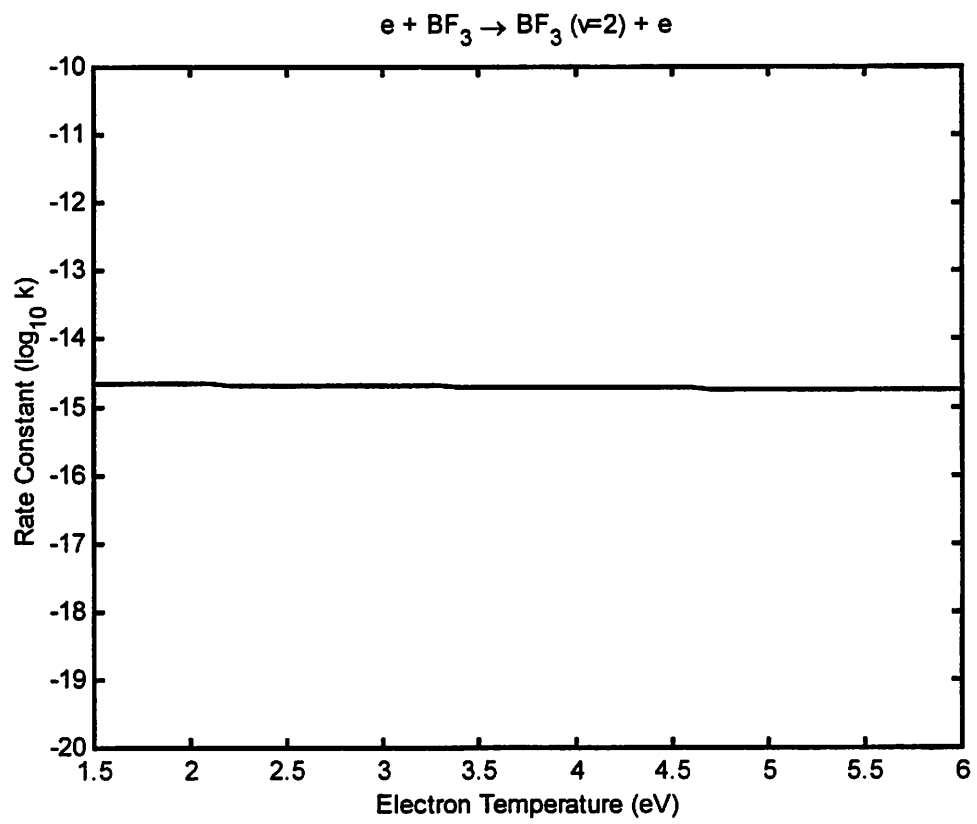


Figure 15.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=2) + e$

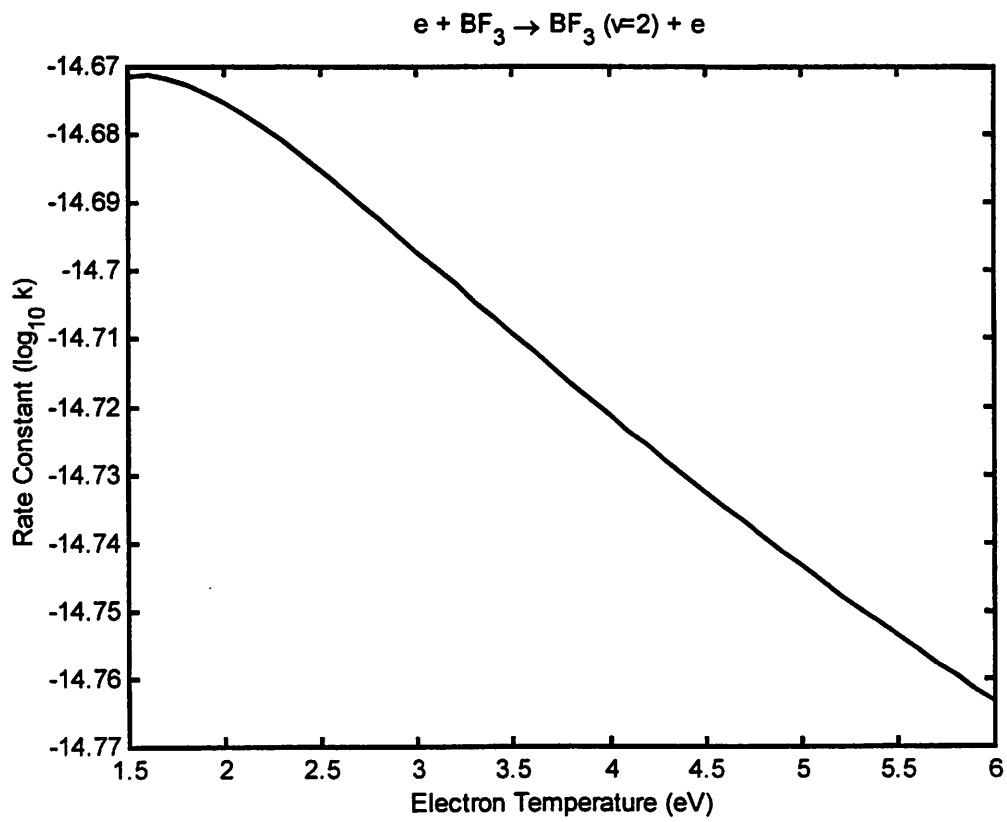


Figure 15.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=2) + e$

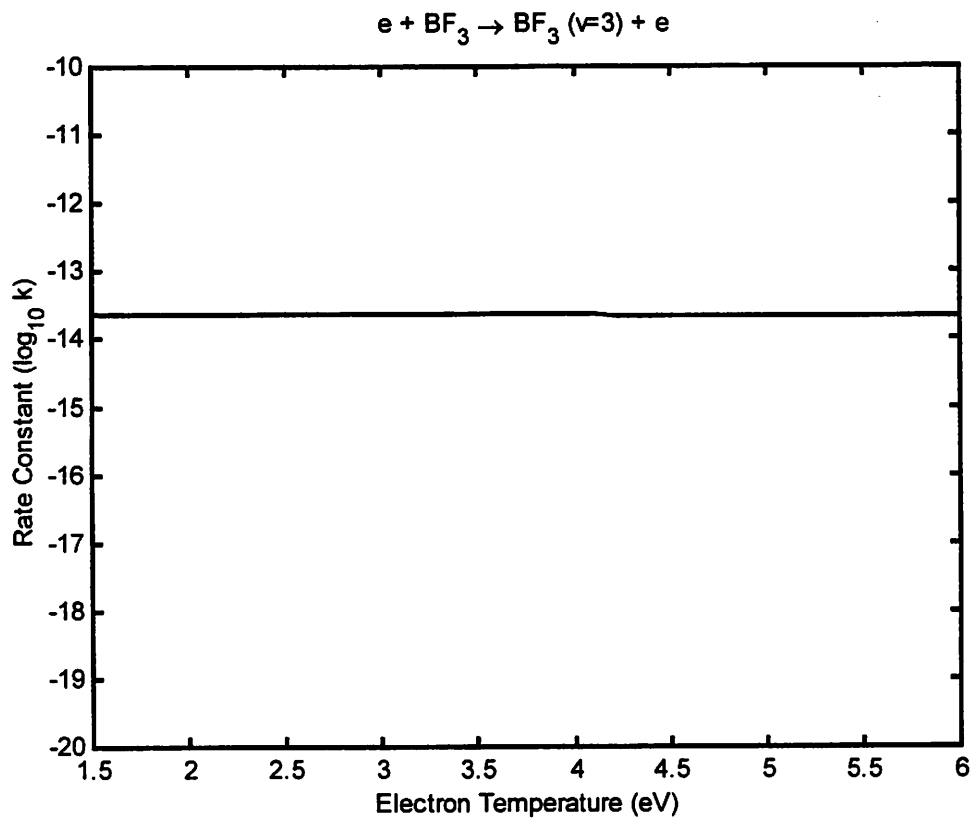


Figure 16.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=3) + e$

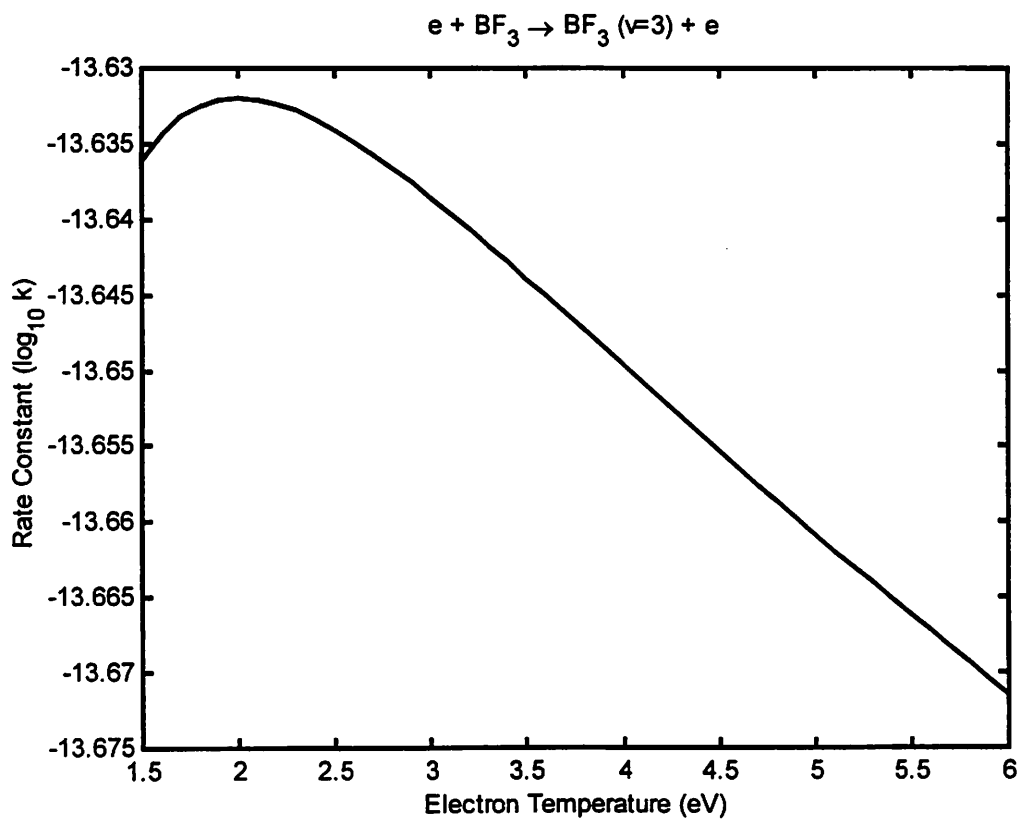


Figure 16.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 (\nu=3) + e$

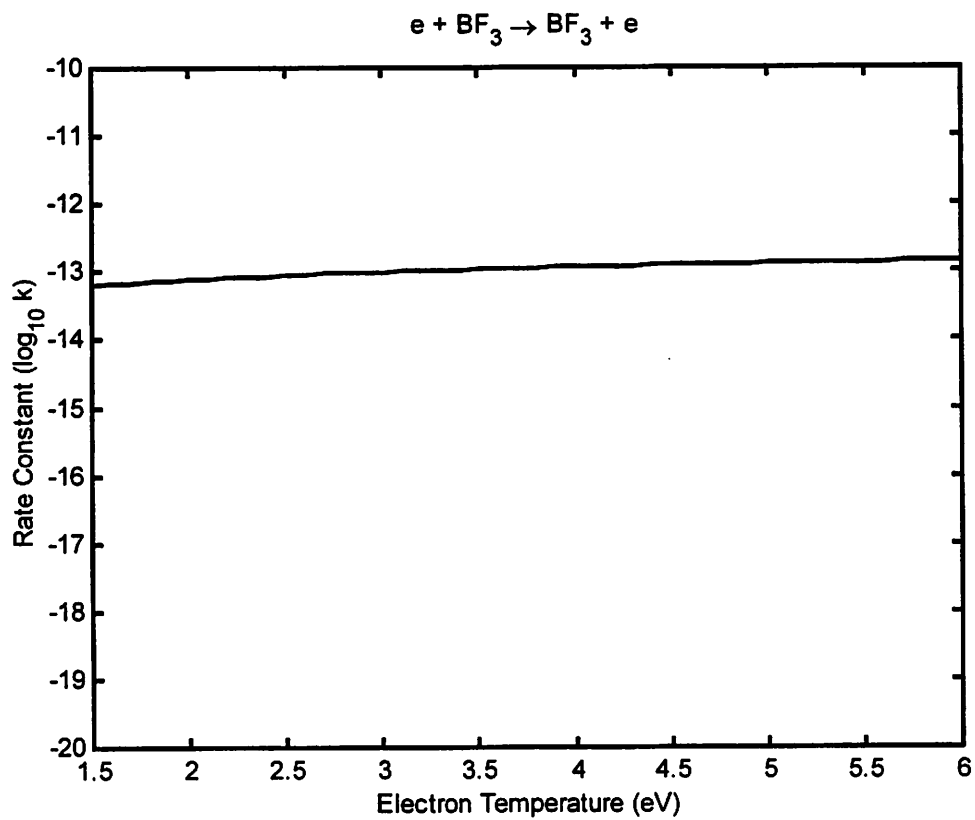


Figure 17.a: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 + e$

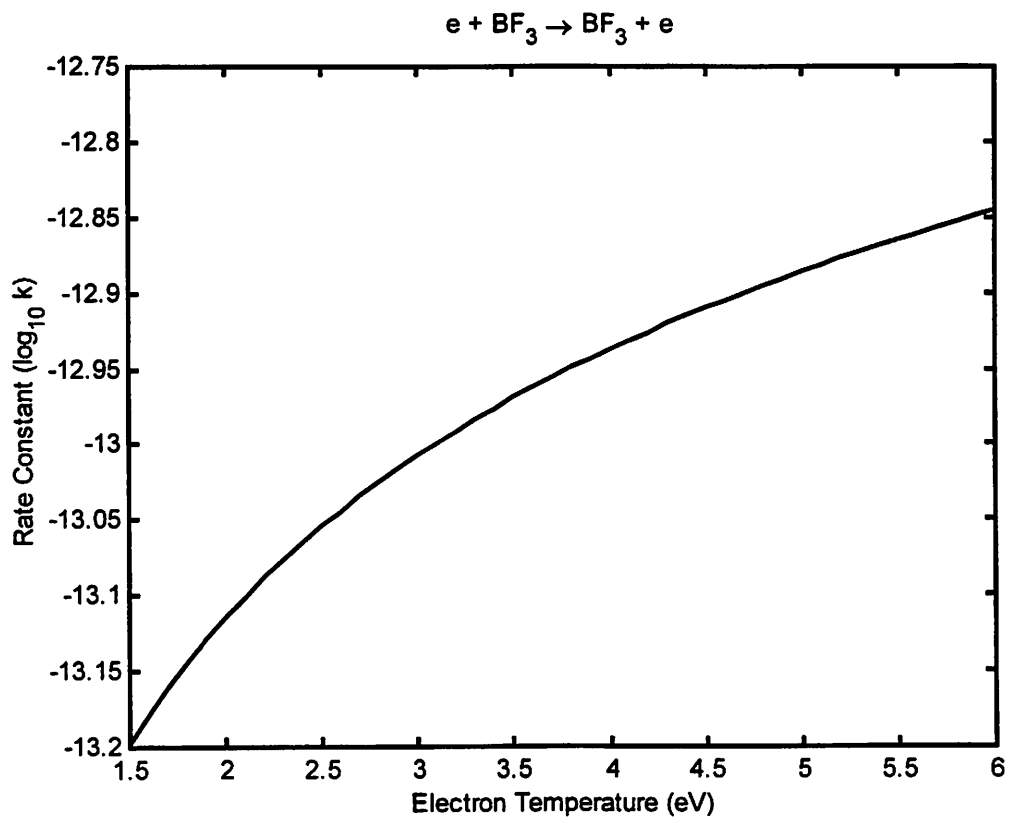


Figure 17.b: Rate Constant as a function of Electron Temperature for $e + \text{BF}_3 \rightarrow \text{BF}_3 + e$

Chapter 2

Excitation Rates for Atomic Boron

2.1 Introduction

It is often desirable to approximate the rate coefficients for an electron impact excitation, particularly when actual data are not available or when one only requires a simple estimate. Clark et al.⁷ provide a mathematical model to calculate the rate coefficients for the electron impact excitations of hydrogen, helium, lithium, beryllium, boron, sodium and magnesium. In this chapter we compute the rate coefficients for an electron impact excitation of atomic boron based on the above model.

2.2 Background

Clark et al. assume a Maxwellian distribution and predict the rate coefficients to be:

$$R = F_1(Z)C_E \left[\frac{c_0 e^{-y}}{y} + c_1 E_1(y) + c_2 E_2(y) \right] + F_2(Z)C_E \left[\frac{c_3}{y} E_1(y) + \frac{c_4 e^{-y}}{y} \right] cm^3 s^{-1} \quad (2.1)$$

where,

$$y = E_t/T,$$

$E_n(y)$ = exponential integral of order n,

T = electron temperature (eV)

E_t = threshold energy (eV)

$$C_e = \frac{8.010 \times 10^{-8} y}{[(2L + 1)(2S + 1)T^{1/2}]}$$

L, S = ground state orbital and spin angular momentum quantum numbers

$$F_1(Z) = (Z + b_1 + d_1/Z)^{-2}$$

$$F_2(Z) = (Z + b_2 + d_2/Z)^{-2}$$

$$E_t = a_0 + a_1Z + a_2Z^2 + a_3Z^3 + a_4Z^4 .$$

The parameters $a_0, a_1, a_2, a_3, a_4, b_1, b_2, c_0, c_1, c_2, c_3, c_4, d_1,$ and d_2 are fit parameters given by Clark et al.

2.3 Calculations

We developed a MatLab program to compute the rate coefficients for the electron impact reactions modeled by Clark et al (refer to Appendix C).

The following approximation was used for the exponential integral of order n:

$$E_{n+1}(z) = \frac{1}{n} [e^{-z} + zE_n(z)] \quad \text{for } n = 1, 2, 3, \dots \quad (2.2)$$

The rate coefficients for the electron impact excitation of boron was calculated by summing the rate coefficients for each transition of boron. The results were fitted to the Arrhenius form using the MatLab utility FitDat (refer to Appendix A).

2.4 Results

The calculated rate coefficient for the electron impact excitation of boron was

$k = 6.497 \times 10^{-14} T^{0.4589} \exp\left(\frac{-5.338}{T}\right)$, where T is the electron temperature in electron volts. The

results are graphically depicted below in Figure 18.

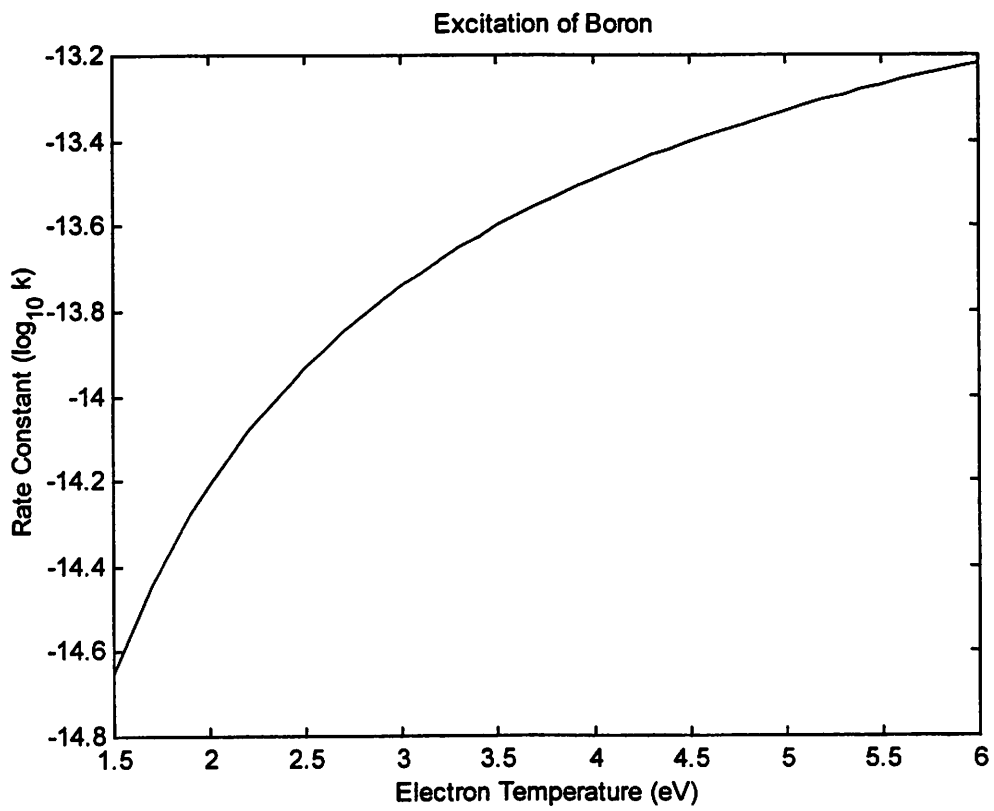


Figure 18: Rate Constant as a function of Electron Temperature for the Excitation of Atomic Boron

Appendix A

A.1 Rate.m

```
% This function computes the rate constant for an electron impact
% collision reaction as a function of electron temperature (Te),
% given the cross-sectional area and the electron energy.
% The input should be a 2 column matrix with the energy in the
% first column and the cross sectional area in the second column.
% The energy should be in electron volts. The normalization factor
% ensures the areas are in square meters.
function d = rate()

% Normalization Factor to make xsectional area into square meters
NF = input(' Please enter normalization factor (default = 1): ');

% Get Data
inData = getvar;

% Quit if no data
if inData == 0
    break
end

% Assign Variables, normalize xsectional area
Energy = inData(:,1);
Sigma = inData(:,2)*NF;

% Assign lower and upper bounds of integration to lower and upper
% values of Energy data
lower = min(Energy);
upper = max(Energy);

% Compute rate constants for 1.5 < Te < 6 eV.
% The function to be integrated is in integrand.m
i = 1;
for Te=1.5:.1:6
    k(i) = quad8 ('integrand', lower, upper, [], [], Energy, Sigma, Te);
    t(i) = Te;
    i = i + 1;
    Te
end

% Create matrix with electron temperature as the first column and the
% corresponding rate as the second column.
outData = [t' k'];

% Save data is necessary
choice = input(' Save rate constants? (y/n): ', 's');
if strcmp(choice, 'y')
    putvar(outData);
end
```

A.2 Rate_2.m

```

% This function computes the rate constant for an electron impact
% collision reaction as a function of electron temperature (Te),
% given the cross-sectional area and the electron energy.
% The input should be a 2 column matrix with the energy in the
% first column and the cross sectional area in the second column.
% The energy should be in electron volts. The normalization factor
% ensures the areas are in square meters.
% rate_2.m can be used in preference to rate.m when writing automated
% scripts.
function rate_2(infile, name, outfile, NF)

% load infile
eval(['load ('' infile '')']);

% Get Data
Data = eval(name);

% Assign Variable, normalize xsectional area
Energy = Data(:,1);
Sigma = Data(:,2)*NF;

% Assign lower and upper bounds of integration to lower and upper
% values of the Energy data
lower = min(Energy);
upper= max(Energy);

% Compute rate constants for 1.5 < Te < 6 eV.
i = 1;
for Te=1.5:.1:6
    k(i) = quad8 ('integrand', lower, upper, [], [], Energy, Sigma, Te);
    t(i) = Te;
    i = i + 1;
    Te;
end

% Create matrix with electron temperature as the first column and
% the corresponding rate as the second column.
d = [t' k'];

% Save data
eval(['save '' outfile '' d -ascii']);

```

A.3 Integrand.m

```

% This function is the function to be integrated in rate.m. The result of
% the integration is the rate coefficient for a given electron temperature,
% a data of energies vs. cross sections. The variable of integration is E.
function F = integrand(E, Energy, Sigma, Te)

% Define electron charge and mass
ee = 1.6022e-19;
me = 9.1094e-31;

% Interpolate Sigma for a set of E
S = interp1 (Energy, Sigma, E, 'linear');

% Function to be integrated. E is the variable of integration

```

```
F = sqrt(8*ee/(pi*me)) .* (Te .^ (-1.5)) .* S .* E .* exp(-E ./ Te);
```

A.4 Getvar.m

```
% This function uses a graphical interface to load a
% matrix stored in ascii format.
function data = getvar()

% Get file name and path
[datafile, datapath] = uigetfile('*.txt', 'Data File');

% Exit if the user pressed Cancel
if datafile == 0
    data = 0;
    return;
end

% Strip the extension from the filename to
% get the variable name
name = strtok(datafile, '.');

% Load the file
eval(['load -ascii('' datapath datafile '')']);

% Assign return value
data = eval(name);
```

A.5 Putvar.m

```
% This function uses a graphical interface to save a
% matrix in ascii format.
function putvar(data)

% Assign path and filename
[datafile, datapath] = uiputfile('*.txt', 'Save Rates');

% Exit if user pressed Cancel
if datafile == 0
    disp(' Data not saved');
    break;
end

% Save file
eval(['save '' datapath datafile '' -ascii data']);
```

A.6 Fitdata.m

```
% This function fits data to the form  $k = A(t^B) \cdot \exp(-C/t)$ 
% where  $t$  is the first column of Data and  $k$  is the second
% column of Data.
function fitdata(Data)
```

```

t = Data(:,1);
k = Data(:,2);

% Find an initial estimate for A, B, C. Note linearization
% of logarithmic function.
X = [ones(size(t)) log(t) (-1 ./ t)];
k_ln = log(k);
lam = X\k_ln;
lam(1) = exp(lam(1));

OPTIONS(5) = 1;
OPTIONS(2) = 1e-8;

% Find least squares fit using fiterr.
[lam,OPTIONS]=leastsq('fiterr', lam, OPTIONS, [], t, k);

% K is the fitted data
K = lam(1) .* (t .^ lam(2)) .* exp (- lam(3) ./ t);

% Plot results
plot(t, log10(K), t, log10(k), 'o')
ylabel('Rate Constant (log10 k)');
xlabel('Electron Temperature (eV)');

% Add legend with A, B, C
xt = 2*max(t)/3;
yt = (max(log10(k)) - min(log10(k))) / 10;
text(xt,min(log10(k)) + 3*yt,['A' = ' num2str(lam(1))])
text(xt,min(log10(k)) + 2*yt,['B' = ' num2str(lam(2))])
text(xt,min(log10(k)) + 1*yt,['C' = ' num2str(lam(3))])

% Display values of A, B, C
lam(1)
lam(2)
lam(3)

```

A.7 Fiterr.m

```

% This function return the difference between k and
%  $K = A*(T^B)*exp(-C/T)$ , where lam = [A B C]
function f = fiterr(lam, t, k)

K = lam(1) .* (t .^ lam(2)) .* exp (- lam(3) ./ t);

f = K - k;

```

Appendix B

B.1 Kushner Data

BF3-MOMENTUM TRANSFER

THRESHOLD= 0.0000E+00 eV

CHANGE IN $\epsilon = 0$

(>0 = IONIZATION, <0 = LOSS)

NUMBER POINTS= 200

ENERGY (eV), XSECTION (cm**2)

5.0000E-02 3.4078E-15
5.1766E-02 3.3669E-15
5.3595E-02 3.3245E-15
5.5488E-02 3.2824E-15
5.7448E-02 3.2478E-15
5.9477E-02 3.2119E-15
6.1578E-02 3.1748E-15
6.3753E-02 3.1364E-15
6.6004E-02 3.0976E-15
6.8336E-02 3.0583E-15
7.0750E-02 3.0176E-15
7.3249E-02 2.9755E-15
7.5836E-02 2.9353E-15
7.8514E-02 2.9052E-15
8.1288E-02 2.8739E-15
8.4159E-02 2.8416E-15
8.7132E-02 2.8082E-15
9.0209E-02 2.7759E-15
9.3396E-02 2.7432E-15
9.6695E-02 2.7092E-15
1.0011E-01 2.6741E-15
1.0365E-01 2.6399E-15
1.0731E-01 2.6051E-15
1.1110E-01 2.5690E-15
1.1502E-01 2.5317E-15
1.1908E-01 2.4928E-15
1.2329E-01 2.4522E-15
1.2765E-01 2.4101E-15
1.3215E-01 2.3666E-15
1.3682E-01 2.3215E-15
1.4165E-01 2.2718E-15
1.4666E-01 2.2101E-15
1.5184E-01 2.1462E-15
1.5720E-01 2.0801E-15
1.6275E-01 2.0162E-15
1.6850E-01 1.9510E-15
1.7446E-01 1.8795E-15
1.8062E-01 1.7775E-15
1.8700E-01 1.6720E-15
1.9360E-01 1.5827E-15
2.0044E-01 1.4924E-15
2.0752E-01 1.4094E-15
2.1485E-01 1.3245E-15
2.2244E-01 1.2184E-15
2.3030E-01 1.1060E-15
2.3843E-01 1.0514E-15
2.4685E-01 9.9496E-16
2.5557E-01 9.3650E-16
2.6460E-01 8.8056E-16
2.7395E-01 8.2472E-16
2.8362E-01 7.6474E-16
2.9364E-01 6.8375E-16
3.0401E-01 6.5029E-16
3.1475E-01 6.1978E-16
3.2587E-01 5.8872E-16
3.3738E-01 5.5760E-16
3.4929E-01 5.3051E-16
3.6163E-01 5.1477E-16
3.7441E-01 4.9847E-16
3.8763E-01 4.8563E-16
4.0132E-01 4.7408E-16
4.1550E-01 4.6212E-16
4.3017E-01 4.5604E-16
4.4537E-01 4.5195E-16
4.6110E-01 4.4772E-16
4.7739E-01 4.4333E-16
4.9425E-01 4.3881E-16
5.1171E-01 4.4176E-16

5.2978E-01 4.4481E-16
5.4849E-01 4.4797E-16
5.6787E-01 4.5124E-16
5.8792E-01 4.5560E-16
6.0869E-01 4.6109E-16
6.3019E-01 4.6677E-16
6.5245E-01 4.7266E-16
6.7550E-01 4.7875E-16
6.9936E-01 4.8505E-16
7.2406E-01 4.9158E-16
7.4963E-01 4.9968E-16
7.7611E-01 5.0809E-16
8.0353E-01 5.1680E-16
8.3191E-01 5.2581E-16
8.6129E-01 5.3456E-16
8.9172E-01 5.4323E-16
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9.5582E-01 5.6151E-16
9.8958E-01 5.7113E-16
1.0245E+00 5.8080E-16
1.0607E+00 5.9051E-16
1.0982E+00 6.0056E-16
1.1370E+00 6.1097E-16
1.1771E+00 6.2173E-16
1.2187E+00 6.3135E-16
1.2618E+00 6.4131E-16
1.3063E+00 6.5161E-16
1.3525E+00 6.6228E-16
1.4003E+00 6.7333E-16
1.4497E+00 6.8183E-16
1.5009E+00 6.8860E-16
1.5539E+00 6.9562E-16
1.6088E+00 7.0288E-16
1.6656E+00 7.1040E-16
1.7245E+00 7.1938E-16
1.7854E+00 7.2890E-16
1.8485E+00 7.3874E-16
1.9137E+00 7.4894E-16
1.9813E+00 7.5950E-16
2.0513E+00 7.7004E-16
2.1238E+00 7.8094E-16
2.1988E+00 7.9223E-16
2.2765E+00 8.0286E-16
2.3569E+00 8.0594E-16
2.4401E+00 8.0913E-16
2.5263E+00 8.1244E-16
2.6155E+00 8.1586E-16
2.7079E+00 8.1940E-16
2.8036E+00 8.2466E-16
2.9026E+00 8.3011E-16
3.0051E+00 8.3575E-16
3.1113E+00 8.4159E-16
3.2212E+00 8.4763E-16
3.3350E+00 8.5389E-16
3.4528E+00 8.5663E-16
3.5747E+00 8.5907E-16
3.7010E+00 8.6159E-16
3.8317E+00 8.6420E-16
3.9670E+00 8.6602E-16
4.1072E+00 8.6745E-16
4.2522E+00 8.6893E-16
4.4024E+00 8.7046E-16
4.5579E+00 8.7204E-16
4.7189E+00 8.7369E-16
4.8856E+00 8.7724E-16
5.0582E+00 8.8119E-16
5.2369E+00 8.8528E-16
5.4218E+00 8.8952E-16
5.6133E+00 8.9391E-16
5.8116E+00 8.9715E-16
6.0169E+00 8.9925E-16
6.2294E+00 9.0142E-16
6.4495E+00 9.0367E-16
6.6773E+00 9.0600E-16
6.9131E+00 9.0842E-16
7.1573E+00 9.0905E-16
7.4101E+00 9.0897E-16
7.6718E+00 9.0889E-16
7.9428E+00 9.0880E-16
8.2234E+00 9.0945E-16
8.5138E+00 9.1014E-16
8.8146E+00 9.1086E-16

9.1259E+00 9.1161E-16
9.4483E+00 9.1232E-16
9.7820E+00 9.1252E-16
1.0128E+01 9.1273E-16
1.0485E+01 9.1295E-16
1.0856E+01 9.1317E-16
1.1239E+01 9.1340E-16
1.1636E+01 9.1364E-16
1.2047E+01 9.1147E-16
1.2473E+01 9.0847E-16
1.2913E+01 9.0537E-16
1.3369E+01 9.0216E-16
1.3841E+01 9.0063E-16
1.4330E+01 9.0297E-16
1.4837E+01 9.0540E-16
1.5361E+01 9.0791E-16
1.5903E+01 9.0815E-16
1.6465E+01 9.0601E-16
1.7046E+01 9.0378E-16
1.7649E+01 9.0148E-16
1.8272E+01 8.9909E-16
1.8917E+01 8.9441E-16
1.9586E+01 8.8353E-16
2.0277E+01 8.7227E-16
2.0994E+01 8.6060E-16
2.1735E+01 8.4853E-16
2.2503E+01 8.3926E-16
2.3298E+01 8.3199E-16
2.4121E+01 8.2446E-16
2.4973E+01 8.1666E-16
2.5855E+01 8.0638E-16
2.6768E+01 7.9410E-16
2.7713E+01 7.8317E-16
2.8692E+01 7.7512E-16
2.9706E+01 7.6678E-16
3.0755E+01 7.5729E-16
3.1841E+01 7.4275E-16
3.2966E+01 7.2769E-16
3.4130E+01 7.1210E-16
3.5336E+01 6.9895E-16
3.6584E+01 6.8895E-16
3.7876E+01 6.7861E-16
3.9214E+01 6.6790E-16
4.0599E+01 6.5749E-16
4.2033E+01 6.5091E-16
4.3518E+01 6.4409E-16
4.5055E+01 6.3704E-16
4.6647E+01 6.2974E-16
4.8294E+01 6.1965E-16
5.0000E+01 6.0909E-16

BF3-DIS ATTACHMENT

THRESHOLD= 1.0700E+01 eV

CHANGE IN $\epsilon = -1$

(>0 = IONIZATION, <0 = LOSS)

NUMBER POINTS= 200

ENERGY (eV), XSECTION (cm**2)

5.0000E-02 0.0000E+00
5.1766E-02 0.0000E+00
5.3595E-02 0.0000E+00
5.5488E-02 0.0000E+00
5.7448E-02 0.0000E+00
5.9477E-02 0.0000E+00
6.1578E-02 0.0000E+00
6.3753E-02 0.0000E+00
6.6004E-02 0.0000E+00
6.8336E-02 0.0000E+00
7.0750E-02 0.0000E+00
7.3249E-02 0.0000E+00
7.5836E-02 0.0000E+00
7.8514E-02 0.0000E+00
8.1288E-02 0.0000E+00
8.4159E-02 0.0000E+00
8.7132E-02 0.0000E+00
9.0209E-02 0.0000E+00
9.3396E-02 0.0000E+00
9.6695E-02 0.0000E+00
1.0011E-01 0.0000E+00
1.0365E-01 0.0000E+00
1.0731E-01 0.0000E+00
1.1110E-01 0.0000E+00
1.1502E-01 0.0000E+00

| | | | | | |
|------------|------------|------------|------------|---|----------------------|
| 1.1908E-01 | 0.0000E+00 | 2.0513E+00 | 0.0000E+00 | 3.5336E+01 | 0.0000E+00 |
| 1.2329E-01 | 0.0000E+00 | 2.1238E+00 | 0.0000E+00 | 3.6584E+01 | 0.0000E+00 |
| 1.2765E-01 | 0.0000E+00 | 2.1988E+00 | 0.0000E+00 | 3.7876E+01 | 0.0000E+00 |
| 1.3215E-01 | 0.0000E+00 | 2.2765E+00 | 0.0000E+00 | 3.9214E+01 | 0.0000E+00 |
| 1.3682E-01 | 0.0000E+00 | 2.3569E+00 | 0.0000E+00 | 4.0599E+01 | 0.0000E+00 |
| 1.4165E-01 | 0.0000E+00 | 2.4401E+00 | 0.0000E+00 | 4.2033E+01 | 0.0000E+00 |
| 1.4666E-01 | 0.0000E+00 | 2.5263E+00 | 0.0000E+00 | 4.3518E+01 | 0.0000E+00 |
| 1.5184E-01 | 0.0000E+00 | 2.6155E+00 | 0.0000E+00 | 4.5055E+01 | 0.0000E+00 |
| 1.5720E-01 | 0.0000E+00 | 2.7079E+00 | 0.0000E+00 | 4.6647E+01 | 0.0000E+00 |
| 1.6275E-01 | 0.0000E+00 | 2.8036E+00 | 0.0000E+00 | 4.8294E+01 | 0.0000E+00 |
| 1.6850E-01 | 0.0000E+00 | 2.9026E+00 | 0.0000E+00 | 5.0000E+01 | 0.0000E+00 |
| 1.7446E-01 | 0.0000E+00 | 3.0051E+00 | 0.0000E+00 | | |
| 1.8062E-01 | 0.0000E+00 | 3.1113E+00 | 0.0000E+00 | | |
| 1.8700E-01 | 0.0000E+00 | 3.2212E+00 | 0.0000E+00 | | |
| 1.9360E-01 | 0.0000E+00 | 3.3350E+00 | 0.0000E+00 | | |
| 2.0044E-01 | 0.0000E+00 | 3.4528E+00 | 0.0000E+00 | | |
| 2.0752E-01 | 0.0000E+00 | 3.5747E+00 | 0.0000E+00 | | |
| 2.1485E-01 | 0.0000E+00 | 3.7010E+00 | 0.0000E+00 | | |
| 2.2244E-01 | 0.0000E+00 | 3.8317E+00 | 0.0000E+00 | | |
| 2.3030E-01 | 0.0000E+00 | 3.9670E+00 | 0.0000E+00 | | |
| 2.3843E-01 | 0.0000E+00 | 4.1072E+00 | 0.0000E+00 | | |
| 2.4685E-01 | 0.0000E+00 | 4.2522E+00 | 0.0000E+00 | | |
| 2.5557E-01 | 0.0000E+00 | 4.4024E+00 | 0.0000E+00 | | |
| 2.6460E-01 | 0.0000E+00 | 4.5579E+00 | 0.0000E+00 | | |
| 2.7395E-01 | 0.0000E+00 | 4.7189E+00 | 0.0000E+00 | | |
| 2.8362E-01 | 0.0000E+00 | 4.8856E+00 | 0.0000E+00 | | |
| 2.9364E-01 | 0.0000E+00 | 5.0582E+00 | 0.0000E+00 | | |
| 3.0401E-01 | 0.0000E+00 | 5.2369E+00 | 0.0000E+00 | | |
| 3.1475E-01 | 0.0000E+00 | 5.4218E+00 | 0.0000E+00 | | |
| 3.2587E-01 | 0.0000E+00 | 5.6133E+00 | 0.0000E+00 | | |
| 3.3738E-01 | 0.0000E+00 | 5.8116E+00 | 0.0000E+00 | | |
| 3.4929E-01 | 0.0000E+00 | 6.0169E+00 | 0.0000E+00 | | |
| 3.6163E-01 | 0.0000E+00 | 6.2294E+00 | 0.0000E+00 | | |
| 3.7441E-01 | 0.0000E+00 | 6.4495E+00 | 0.0000E+00 | | |
| 3.8763E-01 | 0.0000E+00 | 6.6773E+00 | 0.0000E+00 | | |
| 4.0132E-01 | 0.0000E+00 | 6.9131E+00 | 0.0000E+00 | | |
| 4.1550E-01 | 0.0000E+00 | 7.1573E+00 | 0.0000E+00 | | |
| 4.3017E-01 | 0.0000E+00 | 7.4101E+00 | 0.0000E+00 | | |
| 4.4537E-01 | 0.0000E+00 | 7.6718E+00 | 0.0000E+00 | | |
| 4.6110E-01 | 0.0000E+00 | 7.9428E+00 | 0.0000E+00 | | |
| 4.7739E-01 | 0.0000E+00 | 8.2234E+00 | 0.0000E+00 | | |
| 4.9425E-01 | 0.0000E+00 | 8.5138E+00 | 0.0000E+00 | | |
| 5.1171E-01 | 0.0000E+00 | 8.8146E+00 | 0.0000E+00 | | |
| 5.2978E-01 | 0.0000E+00 | 9.1259E+00 | 0.0000E+00 | | |
| 5.4849E-01 | 0.0000E+00 | 9.4483E+00 | 0.0000E+00 | | |
| 5.6787E-01 | 0.0000E+00 | 9.7820E+00 | 0.0000E+00 | | |
| 5.8792E-01 | 0.0000E+00 | 1.0128E+01 | 0.0000E+00 | | |
| 6.0869E-01 | 0.0000E+00 | 1.0485E+01 | 0.0000E+00 | | |
| 6.3019E-01 | 0.0000E+00 | 1.0856E+01 | 1.1976E-18 | | |
| 6.5245E-01 | 0.0000E+00 | 1.1239E+01 | 2.0933E-18 | | |
| 6.7550E-01 | 0.0000E+00 | 1.1636E+01 | 2.1960E-18 | | |
| 6.9936E-01 | 0.0000E+00 | 1.2047E+01 | 7.8811E-19 | | |
| 7.2406E-01 | 0.0000E+00 | 1.2473E+01 | 0.0000E+00 | | |
| 7.4963E-01 | 0.0000E+00 | 1.2913E+01 | 0.0000E+00 | | |
| 7.7611E-01 | 0.0000E+00 | 1.3369E+01 | 0.0000E+00 | | |
| 8.0353E-01 | 0.0000E+00 | 1.3841E+01 | 0.0000E+00 | | |
| 8.3191E-01 | 0.0000E+00 | 1.4330E+01 | 0.0000E+00 | | |
| 8.6129E-01 | 0.0000E+00 | 1.4837E+01 | 0.0000E+00 | | |
| 8.9172E-01 | 0.0000E+00 | 1.5361E+01 | 0.0000E+00 | | |
| 9.2321E-01 | 0.0000E+00 | 1.5903E+01 | 0.0000E+00 | | |
| 9.5582E-01 | 0.0000E+00 | 1.6465E+01 | 0.0000E+00 | | |
| 9.8958E-01 | 0.0000E+00 | 1.7046E+01 | 0.0000E+00 | | |
| 1.0245E+00 | 0.0000E+00 | 1.7649E+01 | 0.0000E+00 | | |
| 1.0607E+00 | 0.0000E+00 | 1.8272E+01 | 0.0000E+00 | | |
| 1.0982E+00 | 0.0000E+00 | 1.8917E+01 | 0.0000E+00 | | |
| 1.1370E+00 | 0.0000E+00 | 1.9586E+01 | 0.0000E+00 | | |
| 1.1771E+00 | 0.0000E+00 | 2.0277E+01 | 0.0000E+00 | | |
| 1.2187E+00 | 0.0000E+00 | 2.0994E+01 | 0.0000E+00 | | |
| 1.2618E+00 | 0.0000E+00 | 2.1735E+01 | 0.0000E+00 | | |
| 1.3063E+00 | 0.0000E+00 | 2.2503E+01 | 0.0000E+00 | | |
| 1.3525E+00 | 0.0000E+00 | 2.3298E+01 | 0.0000E+00 | | |
| 1.4003E+00 | 0.0000E+00 | 2.4121E+01 | 0.0000E+00 | | |
| 1.4497E+00 | 0.0000E+00 | 2.4973E+01 | 0.0000E+00 | | |
| 1.5009E+00 | 0.0000E+00 | 2.5855E+01 | 0.0000E+00 | | |
| 1.5539E+00 | 0.0000E+00 | 2.6768E+01 | 0.0000E+00 | | |
| 1.6088E+00 | 0.0000E+00 | 2.7713E+01 | 0.0000E+00 | | |
| 1.6656E+00 | 0.0000E+00 | 2.8692E+01 | 0.0000E+00 | | |
| 1.7245E+00 | 0.0000E+00 | 2.9706E+01 | 0.0000E+00 | | |
| 1.7854E+00 | 0.0000E+00 | 3.0755E+01 | 0.0000E+00 | | |
| 1.8485E+00 | 0.0000E+00 | 3.1841E+01 | 0.0000E+00 | | |
| 1.9137E+00 | 0.0000E+00 | 3.2966E+01 | 0.0000E+00 | | |
| 1.9813E+00 | 0.0000E+00 | 3.4130E+01 | 0.0000E+00 | | |
| | | | | BF3-VIB 1 (NU 4) | |
| | | | | THRESHOLD= | 5.8970E-02 eV |
| | | | | CHANGE IN e= | 0 |
| | | | | (>0 = IONIZATION, <0 = LOSS) | |
| | | | | NUMBER POINTS= | 200 |
| | | | | ENERGY (eV), XSECTION (cm**2) | |
| | | | | 5.0000E-02 | 0.0000E+00 |
| | | | | 5.1766E-02 | 0.0000E+00 |
| | | | | 5.3595E-02 | 0.0000E+00 |
| | | | | 5.5488E-02 | 0.0000E+00 |
| | | | | 5.7448E-02 | 0.0000E+00 |
| | | | | 5.9477E-02 | 2.3185E-18 |
| | | | | 6.1578E-02 | 7.9571E-18 |
| | | | | 6.3753E-02 | 1.0203E-17 |
| | | | | 6.6004E-02 | 1.1344E-17 |
| | | | | 6.8336E-02 | 1.2397E-17 |
| | | | | 7.0750E-02 | 1.3452E-17 |
| | | | | 7.3249E-02 | 1.4145E-17 |
| | | | | 7.5836E-02 | 1.4776E-17 |
| | | | | 7.8514E-02 | 1.5429E-17 |
| | | | | 8.1288E-02 | 1.5932E-17 |
| | | | | 8.4159E-02 | 1.6280E-17 |
| | | | | 8.7132E-02 | 1.6640E-17 |
| | | | | 9.0209E-02 | 1.7013E-17 |
| | | | | 9.3396E-02 | 1.7394E-17 |
| | | | | 9.6695E-02 | 1.7721E-17 |
| | | | | 1.0011E-01 | 1.8060E-17 |
| | | | | 1.0365E-01 | 1.8410E-17 |
| | | | | 1.0731E-01 | 1.8773E-17 |
| | | | | 1.1110E-01 | 1.9034E-17 |
| | | | | 1.1502E-01 | 1.9076E-17 |
| | | | | 1.1908E-01 | 1.9119E-17 |
| | | | | 1.2329E-01 | 1.9164E-17 |
| | | | | 1.2765E-01 | 1.9210E-17 |
| | | | | 1.3215E-01 | 1.9275E-17 |
| | | | | 1.3682E-01 | 1.9431E-17 |
| | | | | 1.4165E-01 | 1.9593E-17 |
| | | | | 1.4666E-01 | 1.9761E-17 |
| | | | | 1.5184E-01 | 1.9934E-17 |
| | | | | 1.5720E-01 | 2.0102E-17 |
| | | | | 1.6275E-01 | 2.0221E-17 |
| | | | | 1.6850E-01 | 2.0345E-17 |
| | | | | 1.7446E-01 | 2.0474E-17 |
| | | | | 1.8062E-01 | 2.0559E-17 |
| | | | | 1.8700E-01 | 2.0580E-17 |
| | | | | 1.9360E-01 | 2.0602E-17 |
| | | | | 2.0044E-01 | 2.0625E-17 |
| | | | | 2.0752E-01 | 2.0638E-17 |
| | | | | 2.1485E-01 | 2.0649E-17 |
| | | | | 2.2244E-01 | 2.0660E-17 |
| | | | | 2.3030E-01 | 2.0668E-17 |
| | | | | 2.3843E-01 | 2.0646E-17 |
| | | | | 2.4685E-01 | 2.0622E-17 |
| | | | | 2.5557E-01 | 2.0598E-17 |
| | | | | 2.6460E-01 | 2.0573E-17 |
| | | | | 2.7395E-01 | 2.0547E-17 |
| | | | | 2.8362E-01 | 2.0529E-17 |
| | | | | 2.9364E-01 | 2.0527E-17 |
| | | | | 3.0401E-01 | 2.0525E-17 |
| | | | | 3.1475E-01 | 2.0523E-17 |
| | | | | 3.2587E-01 | 2.0521E-17 |
| | | | | 3.3738E-01 | 2.0493E-17 |
| | | | | 3.4929E-01 | 2.0444E-17 |
| | | | | 3.6163E-01 | 2.0393E-17 |
| | | | | 3.7441E-01 | 2.0341E-17 |
| | | | | 3.8763E-01 | 2.0299E-17 |
| | | | | 4.0132E-01 | 2.0296E-17 |
| | | | | 4.1550E-01 | 2.0293E-17 |
| | | | | 4.3017E-01 | 2.0290E-17 |
| | | | | 4.4537E-01 | 2.0287E-17 |

4.6110E-01 2.0284E-17
4.7739E-01 2.0280E-17
4.9425E-01 2.0222E-17
5.1171E-01 2.0156E-17
5.2978E-01 2.0088E-17
5.4849E-01 2.0017E-17
5.6787E-01 1.9943E-17
5.8792E-01 1.9840E-17
6.0869E-01 1.9668E-17
6.3019E-01 1.9490E-17
6.5245E-01 1.9306E-17
6.7550E-01 1.9115E-17
6.9936E-01 1.8920E-17
7.2406E-01 1.8744E-17
7.4963E-01 1.8562E-17
7.7611E-01 1.8373E-17
8.0353E-01 1.8178E-17
8.3191E-01 1.7980E-17
8.6129E-01 1.7838E-17
8.9172E-01 1.7691E-17
9.2321E-01 1.7538E-17
9.5582E-01 1.7380E-17
9.8958E-01 1.7219E-17
1.0245E+00 1.7073E-17
1.0607E+00 1.6922E-17
1.0982E+00 1.6766E-17
1.1370E+00 1.6604E-17
1.1771E+00 1.6437E-17
1.2187E+00 1.6243E-17
1.2618E+00 1.6036E-17
1.3063E+00 1.5821E-17
1.3525E+00 1.5599E-17
1.4003E+00 1.5337E-17
1.4497E+00 1.5048E-17
1.5009E+00 1.4748E-17
1.5539E+00 1.4463E-17
1.6088E+00 1.4208E-17
1.6656E+00 1.3943E-17
1.7245E+00 1.3670E-17
1.7854E+00 1.3387E-17
1.8485E+00 1.3118E-17
1.9137E+00 1.2842E-17
1.9813E+00 1.2556E-17
2.0513E+00 1.2311E-17
2.1238E+00 1.2084E-17
2.1988E+00 1.1848E-17
2.2765E+00 1.1605E-17
2.3569E+00 1.1330E-17
2.4401E+00 1.1028E-17
2.5263E+00 1.0714E-17
2.6155E+00 1.0390E-17
2.7079E+00 1.0054E-17
2.8036E+00 9.7664E-18
2.9026E+00 9.5083E-18
3.0051E+00 9.2466E-18
3.1113E+00 9.0323E-18
3.2212E+00 8.8104E-18
3.3350E+00 8.5808E-18
3.4528E+00 8.3560E-18
3.5747E+00 8.1292E-18
3.7010E+00 7.8945E-18
3.8317E+00 7.6514E-18
3.9670E+00 7.3642E-18
4.1072E+00 7.0666E-18
4.2522E+00 6.7689E-18
4.4024E+00 6.4820E-18
4.5579E+00 6.1850E-18
4.7189E+00 6.0042E-18
4.8856E+00 5.8180E-18
5.0582E+00 5.6422E-18
5.2369E+00 5.4760E-18
5.4218E+00 5.3039E-18
5.6133E+00 5.1427E-18
5.8116E+00 4.9816E-18
6.0169E+00 4.8147E-18
6.2294E+00 4.6290E-18
6.4495E+00 4.4354E-18
6.6773E+00 4.2702E-18
6.9131E+00 4.2004E-18
7.1573E+00 4.1281E-18
7.4101E+00 4.0533E-18
7.6718E+00 3.9182E-18

7.9428E+00 3.7740E-18
8.2234E+00 3.6247E-18
8.5138E+00 3.5378E-18
8.8146E+00 3.4316E-18
9.1259E+00 3.3217E-18
9.4483E+00 3.2079E-18
9.7820E+00 3.0981E-18
1.0128E+01 2.9848E-18
1.0485E+01 2.8675E-18
1.0856E+01 2.7461E-18
1.1239E+01 2.6562E-18
1.1636E+01 2.5706E-18
1.2047E+01 2.4820E-18
1.2473E+01 2.3980E-18
1.2913E+01 2.3444E-18
1.3369E+01 2.2890E-18
1.3841E+01 2.2315E-18
1.4330E+01 2.1721E-18
1.4837E+01 2.1103E-18
1.5361E+01 2.0435E-18
1.5903E+01 1.9743E-18
1.6465E+01 1.9026E-18
1.7046E+01 1.8389E-18
1.7649E+01 1.7841E-18
1.8272E+01 1.7273E-18
1.8917E+01 1.6686E-18
1.9586E+01 1.6077E-18
2.0277E+01 1.5575E-18
2.0994E+01 1.5160E-18
2.1735E+01 1.4730E-18
2.2503E+01 1.4284E-18
2.3298E+01 1.3822E-18
2.4121E+01 1.3334E-18
2.4973E+01 1.2829E-18
2.5855E+01 1.2306E-18
2.6768E+01 1.1836E-18
2.7713E+01 1.1370E-18
2.8692E+01 1.0888E-18
2.9706E+01 1.0409E-18
3.0755E+01 1.0054E-18
3.1841E+01 9.7106E-19
3.2966E+01 9.3793E-19
3.4130E+01 9.0593E-19
3.5336E+01 8.7502E-19
3.6584E+01 8.4517E-19
3.7876E+01 8.1634E-19
3.9214E+01 7.8849E-19
4.0599E+01 7.6158E-19
4.2033E+01 7.3560E-19
4.3518E+01 7.1051E-19
4.5055E+01 6.8627E-19
4.6647E+01 6.6285E-19
4.8294E+01 6.4024E-19
5.0000E+01 6.1840E-19

1.0365E-01 1.9304E-17
1.0731E-01 2.2636E-17
1.1110E-01 2.5589E-17
1.1502E-01 2.8449E-17
1.1908E-01 3.0953E-17
1.2329E-01 3.3098E-17
1.2765E-01 3.5255E-17
1.3215E-01 3.7031E-17
1.3682E-01 3.8870E-17
1.4165E-01 4.0774E-17
1.4666E-01 4.2811E-17
1.5184E-01 4.4915E-17
1.5720E-01 4.5553E-17
1.6275E-01 4.6214E-17
1.6850E-01 4.7287E-17
1.7446E-01 4.8499E-17
1.8062E-01 4.9753E-17
1.8700E-01 5.0567E-17
1.9360E-01 5.0997E-17
2.0044E-01 5.1442E-17
2.0752E-01 5.1902E-17
2.1485E-01 5.2379E-17
2.2244E-01 5.2877E-17
2.3030E-01 5.3406E-17
2.3843E-01 5.3954E-17
2.4685E-01 5.4521E-17
2.5557E-01 5.5108E-17
2.6460E-01 5.5195E-17
2.7395E-01 5.5284E-17
2.8362E-01 5.5376E-17
2.9364E-01 5.5471E-17
3.0401E-01 5.5570E-17
3.1475E-01 5.5676E-17
3.2587E-01 5.5785E-17
3.3738E-01 5.5899E-17
3.4929E-01 5.5641E-17
3.6163E-01 5.5370E-17
3.7441E-01 5.5089E-17
3.8763E-01 5.4567E-17
4.0132E-01 5.3773E-17
4.1550E-01 5.2951E-17
4.3017E-01 5.2100E-17
4.4537E-01 5.1266E-17
4.6110E-01 5.0819E-17
4.7739E-01 5.0357E-17
4.9425E-01 4.9879E-17
5.1171E-01 4.9384E-17
5.2978E-01 4.8872E-17
5.4849E-01 4.8342E-17
5.6787E-01 4.7793E-17
5.8792E-01 4.7224E-17
6.0869E-01 4.6636E-17
6.3019E-01 4.6149E-17
6.5245E-01 4.6568E-17
6.7550E-01 4.6013E-17
6.9936E-01 4.5384E-17
7.2406E-01 4.4797E-17
7.4963E-01 4.4342E-17
7.7611E-01 4.3871E-17
8.0353E-01 4.3383E-17
8.3191E-01 4.2877E-17
8.6129E-01 4.2360E-17
8.9172E-01 4.1827E-17
9.2321E-01 4.1276E-17
9.5582E-01 4.0705E-17
9.8958E-01 4.0075E-17
1.0245E+00 3.9408E-17
1.0607E+00 3.8717E-17
1.0982E+00 3.8002E-17
1.1370E+00 3.7261E-17
1.1771E+00 3.6674E-17
1.2187E+00 3.6129E-17
1.2618E+00 3.5563E-17
1.3063E+00 3.4978E-17
1.3525E+00 3.4373E-17
1.4003E+00 3.3746E-17
1.4497E+00 3.3096E-17
1.5009E+00 3.2450E-17
1.5539E+00 3.1848E-17
1.6088E+00 3.1224E-17
1.6656E+00 3.0578E-17
1.7245E+00 2.9909E-17

CROSS SECTION= BF3-VIB 2 (NU 2)
THRESHOLD= 8.6000E-02 eV
CHANGE IN = 0
(>0 = IONIZATION, <0 = LOSS)
NUMBER POINTS= 200
ENERGY (eV), XSECTION (cm**2)

5.0000E-02 0.0000E+00
5.1766E-02 0.0000E+00
5.3595E-02 0.0000E+00
5.5488E-02 0.0000E+00
5.7448E-02 0.0000E+00
5.9477E-02 0.0000E+00
6.1578E-02 0.0000E+00
6.3753E-02 0.0000E+00
6.6004E-02 0.0000E+00
6.8336E-02 0.0000E+00
7.0750E-02 0.0000E+00
7.3249E-02 0.0000E+00
7.5836E-02 0.0000E+00
7.8514E-02 0.0000E+00
8.1288E-02 0.0000E+00
8.4159E-02 0.0000E+00
8.7132E-02 1.7033E-19
9.0209E-02 6.3357E-19
9.3396E-02 1.2848E-18
9.6695E-02 4.6116E-18
1.0011E-01 1.4976E-17

1.7854E+00 2.9271E-17
1.8485E+00 2.8795E-17
1.9137E+00 2.8301E-17
1.9813E+00 2.7790E-17
2.0513E+00 2.7261E-17
2.1238E+00 2.6720E-17
2.1988E+00 2.6192E-17
2.2765E+00 2.5645E-17
2.3569E+00 2.5079E-17
2.4401E+00 2.4494E-17
2.5263E+00 2.4045E-17
2.6155E+00 2.3607E-17
2.7079E+00 2.3153E-17
2.8036E+00 2.2683E-17
2.9026E+00 2.2209E-17
3.0051E+00 2.1730E-17
3.1113E+00 2.1234E-17
3.2212E+00 2.0730E-17
3.3350E+00 2.0267E-17
3.4528E+00 1.9788E-17
3.5747E+00 1.9333E-17
3.7010E+00 1.8915E-17
3.8317E+00 1.8483E-17
3.9670E+00 1.8036E-17
4.1072E+00 1.7549E-17
4.2522E+00 1.7042E-17
4.4024E+00 1.6520E-17
4.5579E+00 1.6046E-17
4.7189E+00 1.5555E-17
4.8856E+00 1.5055E-17
5.0582E+00 1.4647E-17
5.2369E+00 1.4225E-17
5.4218E+00 1.3788E-17
5.6133E+00 1.3405E-17
5.8116E+00 1.3034E-17
6.0169E+00 1.2650E-17
6.2294E+00 1.2252E-17
6.4495E+00 1.1981E-17
6.6773E+00 1.1704E-17
6.9131E+00 1.1418E-17
7.1573E+00 1.1122E-17
7.4101E+00 1.0815E-17
7.6718E+00 1.0488E-17
7.9428E+00 1.0146E-17
8.2234E+00 9.7912E-18
8.5138E+00 9.4336E-18
8.8146E+00 9.1159E-18
9.1259E+00 8.7869E-18
9.4483E+00 8.4463E-18
9.7820E+00 8.1917E-18
1.0128E+01 7.9600E-18
1.0485E+01 7.7201E-18
1.0856E+01 7.4718E-18
1.1239E+01 7.1963E-18
1.1636E+01 6.8868E-18
1.2047E+01 6.5665E-18
1.2473E+01 6.3942E-18
1.2913E+01 6.2342E-18
1.3369E+01 6.0687E-18
1.3841E+01 5.8973E-18
1.4330E+01 5.7188E-18
1.4837E+01 5.5289E-18
1.5361E+01 5.3322E-18
1.5903E+01 5.1285E-18
1.6465E+01 4.9177E-18
1.7046E+01 4.7811E-18
1.7649E+01 4.6419E-18
1.8272E+01 4.4978E-18
1.8917E+01 4.3486E-18
1.9586E+01 4.2229E-18
2.0277E+01 4.0943E-18
2.0994E+01 3.9611E-18
2.1735E+01 3.8376E-18
2.2503E+01 3.7163E-18
2.3298E+01 3.5907E-18
2.4121E+01 3.4486E-18
2.4973E+01 3.2882E-18
2.5855E+01 3.1353E-18
2.6768E+01 3.0324E-18
2.7713E+01 2.9258E-18
2.8692E+01 2.8155E-18
2.9706E+01 2.7105E-18

3.0755E+01 2.6032E-18
3.1841E+01 2.5062E-18
3.2966E+01 2.4434E-18
3.4130E+01 2.3784E-18
3.5336E+01 2.3112E-18
3.6584E+01 2.2433E-18
3.7876E+01 2.1753E-18
3.9214E+01 2.1049E-18
4.0599E+01 2.0320E-18
4.2033E+01 1.9602E-18
4.3518E+01 1.8872E-18
4.5055E+01 1.8116E-18
4.6647E+01 1.7507E-18
4.8294E+01 1.7025E-18
5.0000E+01 1.6526E-18

BF3-VIB 3 (NU 3)
THRESHOLD= 1.8000E-01 eV
CHANGE IN $\epsilon = 0$
(>0 = IONIZATION, <0 = LOSS)
NUMBER POINTS= 200
ENERGY (eV), XSECTION (cm**2)

5.0000E-02 0.0000E+00
5.1766E-02 0.0000E+00
5.3595E-02 0.0000E+00
5.5488E-02 0.0000E+00
5.7448E-02 0.0000E+00
5.9477E-02 0.0000E+00
6.1578E-02 0.0000E+00
6.3753E-02 0.0000E+00
6.6004E-02 0.0000E+00
6.8336E-02 0.0000E+00
7.0750E-02 0.0000E+00
7.3249E-02 0.0000E+00
7.5836E-02 0.0000E+00
7.8514E-02 0.0000E+00
8.1288E-02 0.0000E+00
8.4159E-02 0.0000E+00
8.7132E-02 0.0000E+00
9.0209E-02 0.0000E+00
9.3396E-02 0.0000E+00
9.6695E-02 0.0000E+00
1.0011E-01 0.0000E+00
1.0365E-01 0.0000E+00
1.0731E-01 0.0000E+00
1.1110E-01 0.0000E+00
1.1502E-01 0.0000E+00
1.1908E-01 0.0000E+00
1.2329E-01 0.0000E+00
1.2765E-01 0.0000E+00
1.3215E-01 0.0000E+00
1.3682E-01 0.0000E+00
1.4165E-01 0.0000E+00
1.4666E-01 0.0000E+00
1.5184E-01 0.0000E+00
1.5720E-01 0.0000E+00
1.6275E-01 0.0000E+00
1.6850E-01 0.0000E+00
1.7446E-01 0.0000E+00
1.8062E-01 1.2956E-19
1.8700E-01 1.0877E-18
1.9360E-01 1.6568E-17
2.0044E-01 2.4757E-17
2.0752E-01 3.7540E-17
2.1485E-01 5.0180E-17
2.2244E-01 7.5814E-17
2.3030E-01 9.7450E-17
2.3843E-01 1.2793E-16
2.4685E-01 1.6886E-16
2.5557E-01 2.0409E-16
2.6460E-01 2.5102E-16
2.7395E-01 2.8871E-16
2.8362E-01 3.2716E-16
2.9364E-01 3.6841E-16
3.0401E-01 4.0844E-16
3.1475E-01 4.4672E-16
3.2587E-01 4.7905E-16
3.3738E-01 5.0918E-16
3.4929E-01 5.2785E-16
3.6163E-01 5.4718E-16
3.7441E-01 5.6169E-16
3.8763E-01 5.6514E-16

4.0132E-01 5.6870E-16
4.1550E-01 5.7040E-16
4.3017E-01 5.7091E-16
4.4537E-01 5.7144E-16
4.6110E-01 5.7198E-16
4.7739E-01 5.6850E-16
4.9425E-01 5.5946E-16
5.1171E-01 5.5010E-16
5.2978E-01 5.4259E-16
5.4849E-01 5.4255E-16
5.6787E-01 5.4251E-16
5.8792E-01 5.4246E-16
6.0869E-01 5.4242E-16
6.3019E-01 5.3598E-16
6.5245E-01 5.2507E-16
6.7550E-01 5.1561E-16
6.9936E-01 5.0966E-16
7.2406E-01 5.0350E-16
7.4963E-01 4.9713E-16
7.7611E-01 4.9053E-16
8.0353E-01 4.8374E-16
8.3191E-01 4.7725E-16
8.6129E-01 4.7053E-16
8.9172E-01 4.6356E-16
9.2321E-01 4.5636E-16
9.5582E-01 4.4890E-16
9.8958E-01 4.4117E-16
1.0245E+00 4.3362E-16
1.0607E+00 4.2609E-16
1.0982E+00 4.1830E-16
1.1370E+00 4.1023E-16
1.1771E+00 4.0188E-16
1.2187E+00 3.9341E-16
1.2618E+00 3.8726E-16
1.3063E+00 3.8089E-16
1.3525E+00 3.7429E-16
1.4003E+00 3.6746E-16
1.4497E+00 3.6039E-16
1.5009E+00 3.5307E-16
1.5539E+00 3.4584E-16
1.6088E+00 3.3958E-16
1.6656E+00 3.3310E-16
1.7245E+00 3.2640E-16
1.7854E+00 3.2008E-16
1.8485E+00 3.1397E-16
1.9137E+00 3.0765E-16
1.9813E+00 3.0110E-16
2.0513E+00 2.9595E-16
2.1238E+00 2.9133E-16
2.1988E+00 2.8654E-16
2.2765E+00 2.8159E-16
2.3569E+00 2.7646E-16
2.4401E+00 2.7105E-16
2.5263E+00 2.6541E-16
2.6155E+00 2.5956E-16
2.7079E+00 2.5351E-16
2.8036E+00 2.4724E-16
2.9026E+00 2.4194E-16
3.0051E+00 2.3754E-16
3.1113E+00 2.3298E-16
3.2212E+00 2.2826E-16
3.3350E+00 2.2337E-16
3.4528E+00 2.1915E-16
3.5747E+00 2.1486E-16
3.7010E+00 2.1042E-16
3.8317E+00 2.0583E-16
3.9670E+00 2.0107E-16
4.1072E+00 1.9614E-16
4.2522E+00 1.9138E-16
4.4024E+00 1.8794E-16
4.5579E+00 1.8439E-16
4.7189E+00 1.8071E-16
4.8856E+00 1.7690E-16
5.0582E+00 1.7317E-16
5.2369E+00 1.6948E-16
5.4218E+00 1.6565E-16
5.6133E+00 1.6211E-16
5.8116E+00 1.5890E-16
6.0169E+00 1.5558E-16
6.2294E+00 1.5215E-16
6.4495E+00 1.4859E-16
6.6773E+00 1.4502E-16

| | | | | | |
|------------|------------|------------|------------|------------|------------|
| 6.9131E+00 | 1.4171E-16 | 9.0209E-02 | 0.0000E+00 | 1.5539E+00 | 0.0000E+00 |
| 7.1573E+00 | 1.3828E-16 | 9.3396E-02 | 0.0000E+00 | 1.6088E+00 | 0.0000E+00 |
| 7.4101E+00 | 1.3472E-16 | 9.6695E-02 | 0.0000E+00 | 1.6656E+00 | 0.0000E+00 |
| 7.6718E+00 | 1.3126E-16 | 1.0011E-01 | 0.0000E+00 | 1.7245E+00 | 0.0000E+00 |
| 7.9428E+00 | 1.2842E-16 | 1.0365E-01 | 0.0000E+00 | 1.7854E+00 | 0.0000E+00 |
| 8.2234E+00 | 1.2548E-16 | 1.0731E-01 | 0.0000E+00 | 1.8485E+00 | 0.0000E+00 |
| 8.5138E+00 | 1.2243E-16 | 1.1110E-01 | 0.0000E+00 | 1.9137E+00 | 0.0000E+00 |
| 8.8146E+00 | 1.1928E-16 | 1.1502E-01 | 0.0000E+00 | 1.9813E+00 | 0.0000E+00 |
| 9.1259E+00 | 1.1622E-16 | 1.1908E-01 | 0.0000E+00 | 2.0513E+00 | 0.0000E+00 |
| 9.4483E+00 | 1.1372E-16 | 1.2329E-01 | 0.0000E+00 | 2.1238E+00 | 0.0000E+00 |
| 9.7820E+00 | 1.1112E-16 | 1.2765E-01 | 0.0000E+00 | 2.1988E+00 | 0.0000E+00 |
| 1.0128E+01 | 1.0844E-16 | 1.3215E-01 | 0.0000E+00 | 2.2765E+00 | 0.0000E+00 |
| 1.0485E+01 | 1.0566E-16 | 1.3682E-01 | 0.0000E+00 | 2.3569E+00 | 0.0000E+00 |
| 1.0856E+01 | 1.0279E-16 | 1.4165E-01 | 0.0000E+00 | 2.4401E+00 | 0.0000E+00 |
| 1.1239E+01 | 1.0002E-16 | 1.4666E-01 | 0.0000E+00 | 2.5263E+00 | 0.0000E+00 |
| 1.1636E+01 | 9.7243E-17 | 1.5184E-01 | 0.0000E+00 | 2.6155E+00 | 0.0000E+00 |
| 1.2047E+01 | 9.4370E-17 | 1.5720E-01 | 0.0000E+00 | 2.7079E+00 | 0.0000E+00 |
| 1.2473E+01 | 9.2060E-17 | 1.6275E-01 | 0.0000E+00 | 2.8036E+00 | 0.0000E+00 |
| 1.2913E+01 | 9.0096E-17 | 1.6850E-01 | 0.0000E+00 | 2.9026E+00 | 0.0000E+00 |
| 1.3369E+01 | 8.8063E-17 | 1.7446E-01 | 0.0000E+00 | 3.0051E+00 | 0.0000E+00 |
| 1.3841E+01 | 8.5958E-17 | 1.8062E-01 | 0.0000E+00 | 3.1113E+00 | 0.0000E+00 |
| 1.4330E+01 | 8.3779E-17 | 1.8700E-01 | 0.0000E+00 | 3.2212E+00 | 0.0000E+00 |
| 1.4837E+01 | 8.1641E-17 | 1.9360E-01 | 0.0000E+00 | 3.3350E+00 | 0.0000E+00 |
| 1.5361E+01 | 7.9702E-17 | 2.0044E-01 | 0.0000E+00 | 3.4528E+00 | 0.0000E+00 |
| 1.5903E+01 | 7.7695E-17 | 2.0752E-01 | 0.0000E+00 | 3.5747E+00 | 0.0000E+00 |
| 1.6465E+01 | 7.5617E-17 | 2.1485E-01 | 0.0000E+00 | 3.7010E+00 | 0.0000E+00 |
| 1.7046E+01 | 7.3466E-17 | 2.2244E-01 | 0.0000E+00 | 3.8317E+00 | 0.0000E+00 |
| 1.7649E+01 | 7.1238E-17 | 2.3030E-01 | 0.0000E+00 | 3.9670E+00 | 0.0000E+00 |
| 1.8272E+01 | 6.9218E-17 | 2.3843E-01 | 0.0000E+00 | 4.1072E+00 | 0.0000E+00 |
| 1.8917E+01 | 6.7258E-17 | 2.4685E-01 | 0.0000E+00 | 4.2522E+00 | 0.0000E+00 |
| 1.9586E+01 | 6.5228E-17 | 2.5557E-01 | 0.0000E+00 | 4.4024E+00 | 0.0000E+00 |
| 2.0277E+01 | 6.3127E-17 | 2.6460E-01 | 0.0000E+00 | 4.5579E+00 | 0.0000E+00 |
| 2.0994E+01 | 6.0951E-17 | 2.7395E-01 | 0.0000E+00 | 4.7189E+00 | 0.0000E+00 |
| 2.1735E+01 | 5.8910E-17 | 2.8362E-01 | 0.0000E+00 | 4.8856E+00 | 0.0000E+00 |
| 2.2503E+01 | 5.6960E-17 | 2.9364E-01 | 0.0000E+00 | 5.0582E+00 | 0.0000E+00 |
| 2.3298E+01 | 5.4941E-17 | 3.0401E-01 | 0.0000E+00 | 5.2369E+00 | 0.0000E+00 |
| 2.4121E+01 | 5.2851E-17 | 3.1475E-01 | 0.0000E+00 | 5.4218E+00 | 0.0000E+00 |
| 2.4973E+01 | 5.0708E-17 | 3.2587E-01 | 0.0000E+00 | 5.6133E+00 | 0.0000E+00 |
| 2.5855E+01 | 4.8828E-17 | 3.3738E-01 | 0.0000E+00 | 5.8116E+00 | 0.0000E+00 |
| 2.6768E+01 | 4.6881E-17 | 3.4929E-01 | 0.0000E+00 | 6.0169E+00 | 0.0000E+00 |
| 2.7713E+01 | 4.4866E-17 | 3.6163E-01 | 0.0000E+00 | 6.2294E+00 | 0.0000E+00 |
| 2.8692E+01 | 4.2779E-17 | 3.7441E-01 | 0.0000E+00 | 6.4495E+00 | 0.0000E+00 |
| 2.9706E+01 | 4.1360E-17 | 3.8763E-01 | 0.0000E+00 | 6.6773E+00 | 0.0000E+00 |
| 3.0755E+01 | 4.0151E-17 | 4.0132E-01 | 0.0000E+00 | 6.9131E+00 | 0.0000E+00 |
| 3.1841E+01 | 3.8900E-17 | 4.1550E-01 | 0.0000E+00 | 7.1573E+00 | 0.0000E+00 |
| 3.2966E+01 | 3.7604E-17 | 4.3017E-01 | 0.0000E+00 | 7.4101E+00 | 0.0000E+00 |
| 3.4130E+01 | 3.6263E-17 | 4.4537E-01 | 0.0000E+00 | 7.6718E+00 | 0.0000E+00 |
| 3.5336E+01 | 3.4874E-17 | 4.6110E-01 | 0.0000E+00 | 7.9428E+00 | 0.0000E+00 |
| 3.6584E+01 | 3.3437E-17 | 4.7739E-01 | 0.0000E+00 | 8.2234E+00 | 0.0000E+00 |
| 3.7876E+01 | 3.2062E-17 | 4.9425E-01 | 0.0000E+00 | 8.5138E+00 | 0.0000E+00 |
| 3.9214E+01 | 3.0935E-17 | 5.1171E-01 | 0.0000E+00 | 8.8146E+00 | 0.0000E+00 |
| 4.0599E+01 | 2.9769E-17 | 5.2978E-01 | 0.0000E+00 | 9.1259E+00 | 0.0000E+00 |
| 4.2033E+01 | 2.8562E-17 | 5.4849E-01 | 0.0000E+00 | 9.4483E+00 | 0.0000E+00 |
| 4.3518E+01 | 2.7346E-17 | 5.6787E-01 | 0.0000E+00 | 9.7820E+00 | 0.0000E+00 |
| 4.5055E+01 | 2.6458E-17 | 5.8792E-01 | 0.0000E+00 | 1.0128E+01 | 1.1208E-18 |
| 4.6647E+01 | 2.5539E-17 | 6.0869E-01 | 0.0000E+00 | 1.0485E+01 | 7.7331E-18 |
| 4.8294E+01 | 2.4587E-17 | 6.3019E-01 | 0.0000E+00 | 1.0856E+01 | 1.6528E-17 |
| 5.0000E+01 | 2.3602E-17 | 6.5245E-01 | 0.0000E+00 | 1.1239E+01 | 2.2993E-17 |
| | | 6.7550E-01 | 0.0000E+00 | 1.1636E+01 | 3.9597E-17 |
| | | 6.9936E-01 | 0.0000E+00 | 1.2047E+01 | 5.6275E-17 |
| | | 7.2406E-01 | 0.0000E+00 | 1.2473E+01 | 6.2869E-17 |
| | | 7.4963E-01 | 0.0000E+00 | 1.2913E+01 | 6.9838E-17 |
| | | 7.7611E-01 | 0.0000E+00 | 1.3369E+01 | 7.7397E-17 |
| | | 8.0353E-01 | 0.0000E+00 | 1.3841E+01 | 8.4951E-17 |
| | | 8.3191E-01 | 0.0000E+00 | 1.4330E+01 | 9.2360E-17 |
| | | 8.6129E-01 | 0.0000E+00 | 1.4837E+01 | 9.9133E-17 |
| | | 8.9172E-01 | 0.0000E+00 | 1.5361E+01 | 1.0572E-16 |
| | | 9.2321E-01 | 0.0000E+00 | 1.5903E+01 | 1.1253E-16 |
| | | 9.5582E-01 | 0.0000E+00 | 1.6465E+01 | 1.1796E-16 |
| | | 9.8958E-01 | 0.0000E+00 | 1.7046E+01 | 1.2314E-16 |
| | | 1.0245E+00 | 0.0000E+00 | 1.7649E+01 | 1.2850E-16 |
| | | 1.0607E+00 | 0.0000E+00 | 1.8272E+01 | 1.3404E-16 |
| | | 1.0982E+00 | 0.0000E+00 | 1.8917E+01 | 1.3964E-16 |
| | | 1.1370E+00 | 0.0000E+00 | 1.9586E+01 | 1.4429E-16 |
| | | 1.1771E+00 | 0.0000E+00 | 2.0277E+01 | 1.4911E-16 |
| | | 1.2187E+00 | 0.0000E+00 | 2.0994E+01 | 1.5410E-16 |
| | | 1.2618E+00 | 0.0000E+00 | 2.1735E+01 | 1.5927E-16 |
| | | 1.3063E+00 | 0.0000E+00 | 2.2503E+01 | 1.6195E-16 |
| | | 1.3525E+00 | 0.0000E+00 | 2.3298E+01 | 1.6471E-16 |
| | | 1.4003E+00 | 0.0000E+00 | 2.4121E+01 | 1.6757E-16 |
| | | 1.4497E+00 | 0.0000E+00 | 2.4973E+01 | 1.7053E-16 |
| | | 1.5009E+00 | 0.0000E+00 | 2.5855E+01 | 1.7360E-16 |

BF3-DISSOC EXCITATION
THRESHOLD= 1.0000E+01 eV
CHANGE IN ϵ = 0
(>0 = IONIZATION, <0 = LOSS)
NUMBER POINTS= 200
ENERGY (eV), XSECTION (cm2)**

| | |
|------------|------------|
| 5.0000E-02 | 0.0000E+00 |
| 5.1766E-02 | 0.0000E+00 |
| 5.3595E-02 | 0.0000E+00 |
| 5.5488E-02 | 0.0000E+00 |
| 5.7448E-02 | 0.0000E+00 |
| 5.9477E-02 | 0.0000E+00 |
| 6.1578E-02 | 0.0000E+00 |
| 6.3753E-02 | 0.0000E+00 |
| 6.6004E-02 | 0.0000E+00 |
| 6.8336E-02 | 0.0000E+00 |
| 7.0750E-02 | 0.0000E+00 |
| 7.3249E-02 | 0.0000E+00 |
| 7.5836E-02 | 0.0000E+00 |
| 7.8514E-02 | 0.0000E+00 |
| 8.1288E-02 | 0.0000E+00 |
| 8.4159E-02 | 0.0000E+00 |
| 8.7132E-02 | 0.0000E+00 |

| | | | | | |
|------------|------------|------------|------------|------------|------------|
| 2.6768E+01 | 1.7677E-16 | 3.4929E-01 | 0.0000E+00 | 6.0169E+00 | 0.0000E+00 |
| 2.7713E+01 | 1.7921E-16 | 3.6163E-01 | 0.0000E+00 | 6.2294E+00 | 0.0000E+00 |
| 2.8692E+01 | 1.8011E-16 | 3.7441E-01 | 0.0000E+00 | 6.4495E+00 | 0.0000E+00 |
| 2.9706E+01 | 1.8105E-16 | 3.8763E-01 | 0.0000E+00 | 6.6773E+00 | 0.0000E+00 |
| 3.0755E+01 | 1.8202E-16 | 4.0132E-01 | 0.0000E+00 | 6.9131E+00 | 0.0000E+00 |
| 3.1841E+01 | 1.8302E-16 | 4.1550E-01 | 0.0000E+00 | 7.1573E+00 | 0.0000E+00 |
| 3.2966E+01 | 1.8308E-16 | 4.3017E-01 | 0.0000E+00 | 7.4101E+00 | 0.0000E+00 |
| 3.4130E+01 | 1.8306E-16 | 4.4537E-01 | 0.0000E+00 | 7.6718E+00 | 0.0000E+00 |
| 3.5336E+01 | 1.8303E-16 | 4.6110E-01 | 0.0000E+00 | 7.9428E+00 | 0.0000E+00 |
| 3.6584E+01 | 1.8301E-16 | 4.7739E-01 | 0.0000E+00 | 8.2234E+00 | 0.0000E+00 |
| 3.7876E+01 | 1.8242E-16 | 4.9425E-01 | 0.0000E+00 | 8.5138E+00 | 0.0000E+00 |
| 3.9214E+01 | 1.8151E-16 | 5.1171E-01 | 0.0000E+00 | 8.8146E+00 | 0.0000E+00 |
| 4.0599E+01 | 1.8058E-16 | 5.2978E-01 | 0.0000E+00 | 9.1259E+00 | 0.0000E+00 |
| 4.2033E+01 | 1.7990E-16 | 5.4849E-01 | 0.0000E+00 | 9.4483E+00 | 0.0000E+00 |
| 4.3518E+01 | 1.7932E-16 | 5.6787E-01 | 0.0000E+00 | 9.7820E+00 | 0.0000E+00 |
| 4.5055E+01 | 1.7872E-16 | 5.8792E-01 | 0.0000E+00 | 1.0128E+01 | 0.0000E+00 |
| 4.6647E+01 | 1.7764E-16 | 6.0869E-01 | 0.0000E+00 | 1.0485E+01 | 0.0000E+00 |
| 4.8294E+01 | 1.7557E-16 | 6.3019E-01 | 0.0000E+00 | 1.0856E+01 | 0.0000E+00 |
| 5.0000E+01 | 1.7343E-16 | 6.5245E-01 | 0.0000E+00 | 1.1239E+01 | 0.0000E+00 |
| | | 6.7550E-01 | 0.0000E+00 | 1.1636E+01 | 0.0000E+00 |
| | | 6.9936E-01 | 0.0000E+00 | 1.2047E+01 | 0.0000E+00 |
| | | 7.2406E-01 | 0.0000E+00 | 1.2473E+01 | 0.0000E+00 |
| | | 7.4963E-01 | 0.0000E+00 | 1.2913E+01 | 0.0000E+00 |
| | | 7.7611E-01 | 0.0000E+00 | 1.3369E+01 | 0.0000E+00 |
| | | 8.0353E-01 | 0.0000E+00 | 1.3841E+01 | 0.0000E+00 |
| | | 8.3191E-01 | 0.0000E+00 | 1.4330E+01 | 0.0000E+00 |
| | | 8.6129E-01 | 0.0000E+00 | 1.4837E+01 | 0.0000E+00 |
| | | 8.9172E-01 | 0.0000E+00 | 1.5361E+01 | 0.0000E+00 |
| | | 9.2321E-01 | 0.0000E+00 | 1.5903E+01 | 1.3180E-18 |
| | | 9.5582E-01 | 0.0000E+00 | 1.6465E+01 | 4.2125E-18 |
| | | 9.8958E-01 | 0.0000E+00 | 1.7046E+01 | 6.5851E-18 |
| | | 1.0245E+00 | 0.0000E+00 | 1.7649E+01 | 9.9694E-18 |
| | | 1.0607E+00 | 0.0000E+00 | 1.8272E+01 | 1.3583E-17 |
| | | 1.0982E+00 | 0.0000E+00 | 1.8917E+01 | 2.2588E-17 |
| | | 1.1370E+00 | 0.0000E+00 | 1.9586E+01 | 2.8744E-17 |
| | | 1.1771E+00 | 0.0000E+00 | 2.0277E+01 | 3.6892E-17 |
| | | 1.2187E+00 | 0.0000E+00 | 2.0994E+01 | 4.5533E-17 |
| | | 1.2618E+00 | 0.0000E+00 | 2.1735E+01 | 5.3625E-17 |
| | | 1.3063E+00 | 0.0000E+00 | 2.2503E+01 | 6.1974E-17 |
| | | 1.3525E+00 | 0.0000E+00 | 2.3298E+01 | 7.1662E-17 |
| | | 1.4003E+00 | 0.0000E+00 | 2.4121E+01 | 8.1233E-17 |
| | | 1.4497E+00 | 0.0000E+00 | 2.4973E+01 | 9.1756E-17 |
| | | 1.5009E+00 | 0.0000E+00 | 2.5855E+01 | 1.0364E-16 |
| | | 1.5539E+00 | 0.0000E+00 | 2.6768E+01 | 1.1796E-16 |
| | | 1.6088E+00 | 0.0000E+00 | 2.7713E+01 | 1.3307E-16 |
| | | 1.6656E+00 | 0.0000E+00 | 2.8692E+01 | 1.4878E-16 |
| | | 1.7245E+00 | 0.0000E+00 | 2.9706E+01 | 1.6429E-16 |
| | | 1.7854E+00 | 0.0000E+00 | 3.0755E+01 | 1.7710E-16 |
| | | 1.8485E+00 | 0.0000E+00 | 3.1841E+01 | 1.9037E-16 |
| | | 1.9137E+00 | 0.0000E+00 | 3.2966E+01 | 2.0267E-16 |
| | | 1.9813E+00 | 0.0000E+00 | 3.4130E+01 | 2.1538E-16 |
| | | 2.0513E+00 | 0.0000E+00 | 3.5336E+01 | 2.2924E-16 |
| | | 2.1238E+00 | 0.0000E+00 | 3.6584E+01 | 2.4425E-16 |
| | | 2.1988E+00 | 0.0000E+00 | 3.7876E+01 | 2.5874E-16 |
| | | 2.2765E+00 | 0.0000E+00 | 3.9214E+01 | 2.7137E-16 |
| | | 2.3569E+00 | 0.0000E+00 | 4.0599E+01 | 2.8445E-16 |
| | | 2.4401E+00 | 0.0000E+00 | 4.2033E+01 | 2.9850E-16 |
| | | 2.5263E+00 | 0.0000E+00 | 4.3518E+01 | 3.1426E-16 |
| | | 2.6155E+00 | 0.0000E+00 | 4.5055E+01 | 3.3046E-16 |
| | | 2.7079E+00 | 0.0000E+00 | 4.6647E+01 | 3.4327E-16 |
| | | 2.8036E+00 | 0.0000E+00 | 4.8294E+01 | 3.5653E-16 |
| | | 2.9026E+00 | 0.0000E+00 | 5.0000E+01 | 3.7025E-16 |
| | | 3.0051E+00 | 0.0000E+00 | | |
| | | 3.1113E+00 | 0.0000E+00 | | |
| | | 3.2212E+00 | 0.0000E+00 | | |
| | | 3.3350E+00 | 0.0000E+00 | | |
| | | 3.4528E+00 | 0.0000E+00 | | |
| | | 3.5747E+00 | 0.0000E+00 | | |
| | | 3.7010E+00 | 0.0000E+00 | | |
| | | 3.8317E+00 | 0.0000E+00 | | |
| | | 3.9670E+00 | 0.0000E+00 | | |
| | | 4.1072E+00 | 0.0000E+00 | | |
| | | 4.2522E+00 | 0.0000E+00 | | |
| | | 4.4024E+00 | 0.0000E+00 | | |
| | | 4.5579E+00 | 0.0000E+00 | | |
| | | 4.7189E+00 | 0.0000E+00 | | |
| | | 4.8856E+00 | 0.0000E+00 | | |
| | | 5.0582E+00 | 0.0000E+00 | | |
| | | 5.2369E+00 | 0.0000E+00 | | |
| | | 5.4218E+00 | 0.0000E+00 | | |
| | | 5.6133E+00 | 0.0000E+00 | | |
| | | 5.8116E+00 | 0.0000E+00 | | |

| | | | | | |
|---|------------|--|--|--|--|
| BF3-IONIZATION | | | | | |
| THRESHOLD= 1.5560E+01 eV | | | | | |
| CHANGE IN e=1 | | | | | |
| (>0 = IONIZATION, <0 = LOSS) | | | | | |
| NUMBER POINTS= 200 | | | | | |
| ENERGY (eV), XSECTION (cm**2) | | | | | |
| 5.0000E-02 | 0.0000E+00 | | | | |
| 5.1766E-02 | 0.0000E+00 | | | | |
| 5.3595E-02 | 0.0000E+00 | | | | |
| 5.5488E-02 | 0.0000E+00 | | | | |
| 5.7448E-02 | 0.0000E+00 | | | | |
| 5.9477E-02 | 0.0000E+00 | | | | |
| 6.1578E-02 | 0.0000E+00 | | | | |
| 6.3753E-02 | 0.0000E+00 | | | | |
| 6.6004E-02 | 0.0000E+00 | | | | |
| 6.8336E-02 | 0.0000E+00 | | | | |
| 7.0750E-02 | 0.0000E+00 | | | | |
| 7.3249E-02 | 0.0000E+00 | | | | |
| 7.5836E-02 | 0.0000E+00 | | | | |
| 7.8514E-02 | 0.0000E+00 | | | | |
| 8.1288E-02 | 0.0000E+00 | | | | |
| 8.4159E-02 | 0.0000E+00 | | | | |
| 8.7132E-02 | 0.0000E+00 | | | | |
| 9.0209E-02 | 0.0000E+00 | | | | |
| 9.3396E-02 | 0.0000E+00 | | | | |
| 9.6695E-02 | 0.0000E+00 | | | | |
| 1.0011E-01 | 0.0000E+00 | | | | |
| 1.0365E-01 | 0.0000E+00 | | | | |
| 1.0731E-01 | 0.0000E+00 | | | | |
| 1.1110E-01 | 0.0000E+00 | | | | |
| 1.1502E-01 | 0.0000E+00 | | | | |
| 1.1908E-01 | 0.0000E+00 | | | | |
| 1.2329E-01 | 0.0000E+00 | | | | |
| 1.2765E-01 | 0.0000E+00 | | | | |
| 1.3215E-01 | 0.0000E+00 | | | | |
| 1.3682E-01 | 0.0000E+00 | | | | |
| 1.4165E-01 | 0.0000E+00 | | | | |
| 1.4666E-01 | 0.0000E+00 | | | | |
| 1.5184E-01 | 0.0000E+00 | | | | |
| 1.5720E-01 | 0.0000E+00 | | | | |
| 1.6275E-01 | 0.0000E+00 | | | | |
| 1.6850E-01 | 0.0000E+00 | | | | |
| 1.7446E-01 | 0.0000E+00 | | | | |
| 1.8062E-01 | 0.0000E+00 | | | | |
| 1.8700E-01 | 0.0000E+00 | | | | |
| 1.9360E-01 | 0.0000E+00 | | | | |
| 2.0044E-01 | 0.0000E+00 | | | | |
| 2.0752E-01 | 0.0000E+00 | | | | |
| 2.1485E-01 | 0.0000E+00 | | | | |
| 2.2244E-01 | 0.0000E+00 | | | | |
| 2.3030E-01 | 0.0000E+00 | | | | |
| 2.3843E-01 | 0.0000E+00 | | | | |
| 2.4685E-01 | 0.0000E+00 | | | | |
| 2.5557E-01 | 0.0000E+00 | | | | |
| 2.6460E-01 | 0.0000E+00 | | | | |
| 2.7395E-01 | 0.0000E+00 | | | | |
| 2.8362E-01 | 0.0000E+00 | | | | |
| 2.9364E-01 | 0.0000E+00 | | | | |
| 3.0401E-01 | 0.0000E+00 | | | | |
| 3.1475E-01 | 0.0000E+00 | | | | |
| 3.2587E-01 | 0.0000E+00 | | | | |
| 3.3738E-01 | 0.0000E+00 | | | | |

| | | | | | |
|---|------------|--|--|--|--|
| ***** | | | | | |
| REDO DISSOCIATIVE ATTACHMENT | | | | | |
| TO RESOLVE RESONANCE | | | | | |
| BF3-DIS ATTACHMENT | | | | | |
| THRESHOLD= 1.0700E+01 eV | | | | | |
| CHANGE IN e= -1 | | | | | |
| (>0 = IONIZATION, <0 = LOSS) | | | | | |
| NUMBER POINTS= 60 | | | | | |
| ENERGY (eV), XSECTION (cm**2) | | | | | |
| 1.0000E+01 | 0.0000E+00 | | | | |
| 1.0051E+01 | 0.0000E+00 | | | | |
| 1.0102E+01 | 0.0000E+00 | | | | |
| 1.0153E+01 | 0.0000E+00 | | | | |
| 1.0203E+01 | 0.0000E+00 | | | | |
| 1.0254E+01 | 0.0000E+00 | | | | |
| 1.0305E+01 | 0.0000E+00 | | | | |
| 1.0356E+01 | 0.0000E+00 | | | | |
| 1.0407E+01 | 0.0000E+00 | | | | |
| 1.0458E+01 | 0.0000E+00 | | | | |

1.0508E+01 0.0000E+00
 1.0559E+01 0.0000E+00
 1.0610E+01 0.0000E+00
 1.0661E+01 0.0000E+00
 1.0712E+01 1.0589E-19
 1.0763E+01 5.5970E-19
 1.0814E+01 1.0135E-18
 1.0864E+01 1.2284E-18
 1.0915E+01 1.4003E-18
 1.0966E+01 1.5312E-18
 1.1017E+01 1.6704E-18
 1.1068E+01 1.7959E-18
 1.1119E+01 1.9034E-18
 1.1169E+01 1.9941E-18
 1.1220E+01 2.0690E-18
 1.1271E+01 2.1302E-18
 1.1322E+01 2.1792E-18
 1.1373E+01 2.2109E-18
 1.1424E+01 2.2365E-18
 1.1475E+01 2.2509E-18
 1.1525E+01 2.2511E-18
 1.1576E+01 2.2379E-18
 1.1627E+01 2.2043E-18
 1.1678E+01 2.1468E-18
 1.1729E+01 2.0817E-18
 1.1780E+01 1.9748E-18
 1.1831E+01 1.8470E-18
 1.1881E+01 1.7048E-18
 1.1932E+01 1.5191E-18
 1.1983E+01 1.3490E-18
 1.2034E+01 9.8327E-19
 1.2085E+01 2.2692E-19
 1.2136E+01 0.0000E+00
 1.2186E+01 0.0000E+00
 1.2237E+01 0.0000E+00
 1.2288E+01 0.0000E+00
 1.2339E+01 0.0000E+00
 1.2390E+01 0.0000E+00
 1.2441E+01 0.0000E+00
 1.2492E+01 0.0000E+00
 1.2542E+01 0.0000E+00
 1.2593E+01 0.0000E+00
 1.2644E+01 0.0000E+00
 1.2695E+01 0.0000E+00
 1.2746E+01 0.0000E+00
 1.2797E+01 0.0000E+00
 1.2847E+01 0.0000E+00
 1.2898E+01 0.0000E+00
 1.2949E+01 0.0000E+00
 1.3000E+01 0.0000E+00

3.0000e+01 2.2500e+00
 3.1000e+01 2.3100e+00
 3.2000e+01 2.3800e+00
 3.3000e+01 2.4400e+00
 3.4000e+01 2.4900e+00
 3.5000e+01 2.5400e+00
 3.6000e+01 2.5900e+00
 3.7000e+01 2.6300e+00
 3.8000e+01 2.6800e+00
 3.9000e+01 2.7200e+00
 4.0000e+01 2.7500e+00
 4.1000e+01 2.7900e+00
 4.2000e+01 2.8200e+00
 4.3000e+01 2.8500e+00
 4.4000e+01 2.8800e+00
 4.5000e+01 2.9000e+00
 4.6000e+01 2.9300e+00
 4.7000e+01 2.9500e+00
 4.8000e+01 2.9700e+00
 4.9000e+01 3.0000e+00
 5.0000e+01 3.0200e+00
 5.1000e+01 3.0300e+00
 5.2000e+01 3.0500e+00
 5.3000e+01 3.0700e+00
 5.4000e+01 3.0800e+00
 5.5000e+01 3.1000e+00
 5.6000e+01 3.1100e+00
 5.7000e+01 3.1200e+00
 5.8000e+01 3.1400e+00
 5.9000e+01 3.1500e+00
 6.0000e+01 3.1600e+00
 6.5000e+01 3.1900e+00
 7.0000e+01 3.2200e+00
 7.5000e+01 3.2300e+00
 8.0000e+01 3.2300e+00
 8.5000e+01 3.2300e+00
 9.0000e+01 3.2200e+00
 9.5000e+01 3.2000e+00
 1.0000e+02 3.1800e+00
 1.0500e+02 3.1600e+00
 1.1000e+02 3.1400e+00
 1.1500e+02 3.1100e+00
 1.2000e+02 3.0900e+00
 1.2500e+02 3.0600e+00
 1.3000e+02 3.0300e+00
 1.3500e+02 3.0000e+00
 1.4000e+02 2.9700e+00
 1.4500e+02 2.9400e+00
 1.5000e+02 2.9100e+00
 1.5500e+02 2.8900e+00
 1.6000e+02 2.8600e+00
 1.6500e+02 2.8300e+00
 1.7000e+02 2.8000e+00
 1.7500e+02 2.7700e+00
 1.8000e+02 2.7400e+00
 1.9000e+02 2.6900e+00
 2.0000e+02 2.6300e+00
 2.2500e+02 2.5000e+00
 2.5000e+02 2.3900e+00
 2.7500e+02 2.2800e+00
 3.0000e+02 2.1800e+00
 3.5000e+02 2.0100e+00
 4.0000e+02 1.8600e+00
 4.5000e+02 1.7300e+00
 5.0000e+02 1.6200e+00
 5.5000e+02 1.5300e+00
 6.0000e+02 1.4400e+00
 6.5000e+02 1.3700e+00
 7.0000e+02 1.3000e+00
 7.5000e+02 1.2400e+00
 8.0000e+02 1.1800e+00
 8.5000e+02 1.1300e+00
 9.0000e+02 1.0900e+00
 9.5000e+02 1.0500e+00
 1.0000e+03 1.0100e+00
 1.2500e+03 8.5200e-01
 1.5000e+03 7.4100e-01
 1.7500e+03 6.5700e-01
 2.0000e+03 5.9100e-01
 2.5000e+03 4.9400e-01
 3.0000e+03 4.2500e-01
 4.0000e+03 3.3500e-01

5.0000e+03 2.7800e-01
 6.0000e+03 2.3800e-01
 7.0000e+03 2.0800e-01
 8.0000e+03 1.8600e-01
 9.0000e+03 1.6800e-01
 1.0000e+04 1.5300e-01

**CROSS SECTION= BF2-Ionization
ENERGY (eV), XSECTION (cm**2)**

9.4000e+00 1.0700e-07
 1.0000e+01 4.4900e-02
 1.1000e+01 1.2300e-01
 1.2000e+01 2.0100e-01
 1.3000e+01 2.7500e-01
 1.4000e+01 3.4500e-01
 1.5000e+01 4.0800e-01
 1.6000e+01 4.6800e-01
 1.7000e+01 5.5600e-01
 1.8000e+01 6.5600e-01
 1.9000e+01 7.8200e-01
 2.0000e+01 9.0700e-01
 2.1000e+01 1.0300e+00
 2.2000e+01 1.1600e+00
 2.3000e+01 1.2800e+00
 2.4000e+01 1.4100e+00
 2.5000e+01 1.5400e+00
 2.6000e+01 1.6600e+00
 2.7000e+01 1.7700e+00
 2.8000e+01 1.8800e+00
 2.9000e+01 1.9800e+00
 3.0000e+01 2.0800e+00
 3.1000e+01 2.1800e+00
 3.2000e+01 2.2600e+00
 3.3000e+01 2.3500e+00
 3.4000e+01 2.4300e+00
 3.5000e+01 2.5100e+00
 3.6000e+01 2.5800e+00
 3.7000e+01 2.6500e+00
 3.8000e+01 2.7100e+00
 3.9000e+01 2.7800e+00
 4.0000e+01 2.8400e+00
 4.1000e+01 2.8900e+00
 4.2000e+01 2.9400e+00
 4.3000e+01 2.9900e+00
 4.4000e+01 3.0400e+00
 4.5000e+01 3.0900e+00
 4.6000e+01 3.1400e+00
 4.7000e+01 3.1800e+00
 4.8000e+01 3.2200e+00
 4.9000e+01 3.2600e+00
 5.0000e+01 3.3000e+00
 5.1000e+01 3.3400e+00
 5.2000e+01 3.3800e+00
 5.3000e+01 3.4100e+00
 5.4000e+01 3.4400e+00
 5.5000e+01 3.4700e+00
 5.6000e+01 3.5000e+00
 5.7000e+01 3.5300e+00
 5.8000e+01 3.5600e+00
 5.9000e+01 3.5800e+00
 6.0000e+01 3.6100e+00
 6.5000e+01 3.7100e+00
 7.0000e+01 3.7900e+00
 7.5000e+01 3.8500e+00
 8.0000e+01 3.9000e+00
 8.5000e+01 3.9300e+00
 9.0000e+01 3.9600e+00
 9.5000e+01 3.9700e+00
 1.0000e+02 3.9800e+00
 1.0500e+02 3.9800e+00
 1.1000e+02 3.9700e+00
 1.1500e+02 3.9600e+00
 1.2000e+02 3.9500e+00
 1.2500e+02 3.9400e+00
 1.3000e+02 3.9200e+00
 1.3500e+02 3.9000e+00
 1.4000e+02 3.8800e+00
 1.4500e+02 3.8500e+00
 1.5000e+02 3.8300e+00
 1.5500e+02 3.8000e+00
 1.6000e+02 3.7800e+00
 1.6500e+02 3.7500e+00

B.2 Meyappan Data

**CROSS SECTION= BF3-Ionization
ENERGY (eV), XSECTION (cm**2)**

9.4000e+00 0
 9.8500e+00 4.9700e-04
 1.0000e+01 2.2200e-02
 1.1000e+01 1.7500e-01
 1.2000e+01 3.3100e-01
 1.3000e+01 4.8100e-01
 1.4000e+01 6.2300e-01
 1.5000e+01 7.5400e-01
 1.6000e+01 8.7400e-01
 1.7000e+01 9.8400e-01
 1.8000e+01 1.0800e+00
 1.9000e+01 1.1900e+00
 2.0000e+01 1.3100e+00
 2.1000e+01 1.4200e+00
 2.2000e+01 1.5300e+00
 2.3000e+01 1.6400e+00
 2.4000e+01 1.7400e+00
 2.5000e+01 1.8400e+00
 2.6000e+01 1.9300e+00
 2.7000e+01 2.0200e+00
 2.8000e+01 2.1000e+00
 2.9000e+01 2.1800e+00

| | | | |
|------------|------------|------------|------------|
| 1.7000e+02 | 3.7200e+00 | 5.0000e+01 | 3.3400e+00 |
| 1.7500e+02 | 3.6900e+00 | 5.1000e+01 | 3.3900e+00 |
| 1.8000e+02 | 3.6700e+00 | 5.2000e+01 | 3.4400e+00 |
| 1.9000e+02 | 3.6100e+00 | 5.3000e+01 | 3.4900e+00 |
| 2.0000e+02 | 3.5500e+00 | 5.4000e+01 | 3.5400e+00 |
| 2.2500e+02 | 3.4100e+00 | 5.5000e+01 | 3.5900e+00 |
| 2.5000e+02 | 3.2800e+00 | 5.6000e+01 | 3.6300e+00 |
| 2.7500e+02 | 3.1500e+00 | 5.7000e+01 | 3.6800e+00 |
| 3.0000e+02 | 3.0300e+00 | 5.8000e+01 | 3.7200e+00 |
| 3.5000e+02 | 2.8200e+00 | 5.9000e+01 | 3.7600e+00 |
| 4.0000e+02 | 2.6300e+00 | 6.0000e+01 | 3.7900e+00 |
| 4.5000e+02 | 2.4600e+00 | 6.5000e+01 | 3.9600e+00 |
| 5.0000e+02 | 2.3200e+00 | 7.0000e+01 | 4.1000e+00 |
| 5.5000e+02 | 2.1900e+00 | 7.5000e+01 | 4.2100e+00 |
| 6.0000e+02 | 2.0700e+00 | 8.0000e+01 | 4.3000e+00 |
| 6.5000e+02 | 1.9700e+00 | 8.5000e+01 | 4.3700e+00 |
| 7.0000e+02 | 1.8800e+00 | 9.0000e+01 | 4.4300e+00 |
| 7.5000e+02 | 1.7900e+00 | 9.5000e+01 | 4.4700e+00 |
| 8.0000e+02 | 1.7200e+00 | 1.0000e+02 | 4.5100e+00 |
| 8.5000e+02 | 1.6500e+00 | 1.0500e+02 | 4.5300e+00 |
| 9.0000e+02 | 1.5800e+00 | 1.1000e+02 | 4.5500e+00 |
| 9.5000e+02 | 1.5200e+00 | 1.1500e+02 | 4.5600e+00 |
| 1.0000e+03 | 1.4700e+00 | 1.2000e+02 | 4.5600e+00 |
| 1.2500e+03 | 1.2500e+00 | 1.2500e+02 | 4.5600e+00 |
| 1.5000e+03 | 1.0900e+00 | 1.3000e+02 | 4.5600e+00 |
| 1.7500e+03 | 9.6900e-01 | 1.3500e+02 | 4.5500e+00 |
| 2.0000e+03 | 8.7300e-01 | 1.4000e+02 | 4.5300e+00 |
| 2.5000e+03 | 7.3100e-01 | 1.4500e+02 | 4.5200e+00 |
| 3.0000e+03 | 6.3100e-01 | 1.5000e+02 | 4.5000e+00 |
| 4.0000e+03 | 4.9800e-01 | 1.5500e+02 | 4.4800e+00 |
| 5.0000e+03 | 4.1300e-01 | 1.6000e+02 | 4.4600e+00 |
| 6.0000e+03 | 3.5400e-01 | 1.6500e+02 | 4.4400e+00 |
| 7.0000e+03 | 3.1100e-01 | 1.7000e+02 | 4.4200e+00 |
| 8.0000e+03 | 2.7700e-01 | 1.7500e+02 | 4.3900e+00 |
| 9.0000e+03 | 2.5100e-01 | 1.8000e+02 | 4.3700e+00 |
| 1.0000e+04 | 2.2900e-01 | 1.9000e+02 | 4.3100e+00 |
| | | 2.0000e+02 | 4.2600e+00 |
| | | 2.2500e+02 | 4.1200e+00 |
| | | 2.5000e+02 | 3.9800e+00 |
| | | 2.7500e+02 | 3.8400e+00 |
| | | 3.0000e+02 | 3.7100e+00 |
| | | 3.5000e+02 | 3.4700e+00 |
| | | 4.0000e+02 | 3.2500e+00 |
| | | 4.5000e+02 | 3.0500e+00 |
| | | 5.0000e+02 | 2.8800e+00 |
| | | 5.5000e+02 | 2.7300e+00 |
| | | 6.0000e+02 | 2.5900e+00 |
| | | 6.5000e+02 | 2.4700e+00 |
| | | 7.0000e+02 | 2.3500e+00 |
| | | 7.5000e+02 | 2.2500e+00 |
| | | 8.0000e+02 | 2.1600e+00 |
| | | 8.5000e+02 | 2.0700e+00 |
| | | 9.0000e+02 | 1.9900e+00 |
| | | 9.5000e+02 | 1.9200e+00 |
| | | 1.0000e+03 | 1.8500e+00 |
| | | 1.2500e+03 | 1.5800e+00 |
| | | 1.5000e+03 | 1.3800e+00 |
| | | 1.7500e+03 | 1.2300e+00 |
| | | 2.0000e+03 | 1.1100e+00 |
| | | 2.5000e+03 | 9.3100e-01 |
| | | 3.0000e+03 | 8.0400e-01 |
| | | 4.0000e+03 | 6.3600e-01 |
| | | 5.0000e+03 | 5.2800e-01 |
| | | 6.0000e+03 | 4.5300e-01 |
| | | 7.0000e+03 | 3.9800e-01 |
| | | 8.0000e+03 | 3.5500e-01 |
| | | 9.0000e+03 | 3.2100e-01 |
| | | 1.0000e+04 | 2.9300e-01 |

**CROSS SECTION= BF-Ionization
ENERGY (eV), XSECTION (cm**2)**

| | |
|------------|------------|
| 9.4000e+00 | 0 |
| 9.8500e+00 | 0 |
| 1.0000e+01 | 0 |
| 1.1000e+01 | 0 |
| 1.2000e+01 | 0 |
| 1.3000e+01 | 0 |
| 1.4000e+01 | 0 |
| 1.5000e+01 | 0 |
| 1.5950e+01 | 1.0500e-07 |
| 1.6000e+01 | 2.1900e-03 |
| 1.7000e+01 | 5.9100e-02 |
| 1.8000e+01 | 1.4400e-01 |
| 1.9000e+01 | 2.5100e-01 |
| 2.0000e+01 | 3.7600e-01 |
| 2.1000e+01 | 5.0000e-01 |
| 2.2000e+01 | 6.2300e-01 |
| 2.3000e+01 | 7.6100e-01 |
| 2.4000e+01 | 9.0600e-01 |
| 2.5000e+01 | 1.0500e+00 |
| 2.6000e+01 | 1.1900e+00 |
| 2.7000e+01 | 1.3300e+00 |
| 2.8000e+01 | 1.4600e+00 |
| 2.9000e+01 | 1.5900e+00 |
| 3.0000e+01 | 1.7100e+00 |
| 3.1000e+01 | 1.8300e+00 |
| 3.2000e+01 | 1.9400e+00 |
| 3.3000e+01 | 2.0500e+00 |
| 3.4000e+01 | 2.1500e+00 |
| 3.5000e+01 | 2.2500e+00 |
| 3.6000e+01 | 2.3500e+00 |
| 3.7000e+01 | 2.4400e+00 |
| 3.8000e+01 | 2.5200e+00 |
| 3.9000e+01 | 2.6100e+00 |
| 4.0000e+01 | 2.6900e+00 |
| 4.1000e+01 | 2.7600e+00 |
| 4.2000e+01 | 2.8400e+00 |
| 4.3000e+01 | 2.9000e+00 |
| 4.4000e+01 | 2.9700e+00 |
| 4.5000e+01 | 3.0400e+00 |
| 4.6000e+01 | 3.1000e+00 |
| 4.7000e+01 | 3.1600e+00 |
| 4.8000e+01 | 3.2200e+00 |
| 4.9000e+01 | 3.2800e+00 |

Appendix C

1.0 RateCalc.m

```
% This function calculates excitation rate coefficients as a function
% of electron temperature in the range 1.5eV < Te < 6eV. It uses the
% model developed in "Collisional Excitation Rates of Complex Atomic
% Ions by Electron Impact" - Clark, Magee, Mann, Merts (The Astrophysical
% Journal, 254:412-418, 1982 March 1. Please refer to the paper for
% coefficients.
% L = ground state orbital quantum number
% S = ground state spin angular quantum number
% Z = atomic charge
% NF = normalization factor (Rates are computed in units of cm^3 / s)
% outfile = File to write results to.

function RateCalc(a0, a1, a2, a3, a4, b1, b2, c0, c1, c2, c3, c4, ...
    d1, d2, L, S, Z, NF, outfile)

% Define range of t
t = 1.5:.1:6;

% Please see above referenced paper.
F1 = (Z + b1 + d1 / Z)^(-2);
F2 = (Z + b2 + d2 / Z)^(-2);
Et = a0 + a1*Z + a2*(Z^2) + a3*(Z^3) + a4*(Z^4);
y = Et ./ t;
Ce = ((8.01e-8).*y) ./ (((2*L + 1)*(2*S + 1)) .* (t .^ (.5)));

E1 = expint(y)';

% Exponential Integral of order 2
% E_(n+1){z} = 1/n [e^(-z) - zE_n{z}]
E2 = (exp(-y) - y.*E1);

T1 = c0.*exp(-y)./y + c1.*E1 + c2.*E2;
T2 = c3.*E1./y + c4.*exp(-y)./y;

R = F1.*Ce.*T1 + F2.*Ce.*T2;

% Normalize rates
R = R .* NF;

% Create and save matrix of Rates vs. Te
d = [t' R'];
eval(['save ''' outfile ''' d -ascii']);
```

2.0 Boron.m

```
% The following script uses RateCalc to compute the excitation rate
% coefficients for Boron. Note that the rate coefficients for each
% transition given in the above paper is first calculated, and the
% resulting sum of reaction rates is used as the overall rate of
% reaction for Boron.
% It is convenient to use the script FitData.m (see Appendix A)
% to fit the calculated data to the Arrhenius form.
```

```

% Calculate rate coefficients for the first transition
boron(-1.1341e1, 3.7007, -5.6339e-2, 2.0624e-3, 0, -2.5357, 2.2823e-1, ...
      2.3051e2, 3.0526e2, -1.1423e2, 1.42e2, -7.9871e1, 1.6273e1, -1.2860e1, ...
      1, 0.5, 5, 1e-6, 'first')

% Calculate rate coefficients for the second transition
boron(-1.3042e1, 4.2204, -9.7416e-3, 3.4929e-4, 0, 1.2389, 2.2454, ...
      1.1548e2, 1.7294e2, -7.4270e1, 6.9007e1, -3.7716e1, -1.6709, -2.5053e1, ...
      1, 0.5, 5, 1e-6, 'second')

% Calculate rate coefficients for the third transition
boron(-1.4969e1, 5.279, -1.0270e-1, 3.4006e-3, 0, -5.5294, -2.1885, ...
      2.4309e2, 3.5044e2, -1.0487e2, 1.9704e2, -5.3362e1, 3.8336e1, -2.2321, ...
      1, 0.5, 5, 1e-6, 'third')

% Calculate rate coefficients for the fourth transition
boron(1.7830e1, -1.2243e1, 1.9563, -1.7541e-3, 1.8977e-5, -5.2852, -7.1461, ...
      -1.5911, 5.1577, -8.1767e-1, 2.9391, -1.1354, 6.2157, 1.7524e1, ...
      1, 0.5, 5, 1e-6, 'fourth')

% Calculate rate coefficients for the fifth transition
boron(7.1403, -9.5604, 1.8991, -6.6362e-4, 3.0004e-5, -2.6613, -2.6047, ...
      -1.9081e3, 1.2813e2, -1.4259e1, 1.2072e2, 1.8988e3, 6.1030, 6.1124, ...
      1, 0.5, 5, 1e-6, 'fifth')

load first;
load second;
load third;
load fourth;
load fifth;

% sum reaction rates for each transition
total_k = first(:,2) + second(:,2) + third(:,2) + fourth(:,2) + fifth(:,2);
total_t = first(:,1);

% create matrix with first column of temperatures and second
% column of reaction rates
total = [total_t total_k];

save total.dat total -ascii;

```


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