$e^- + BeH^+$
$e^- + BeH$
$e^- + Be_nH_m$

$e^-$-impact processes of plasma impurities: Be, BeH$^+$ and various berillium hydrides

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March 20-22, 2013
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Published in

- R Celiberto, R K Janev and D Reiter
  State-to-state electron impact cross sections for $BeH^+$
molecular ions in ITER-like fusion edge plasmas with $Be$ walls,
Published in

- R Celiberto, R K Janev and D Reiter
  State-to-state electron impact cross sections for BeH\(^+\) molecular ions in ITER-like fusion edge plasmas with Be walls, Plasma Phys. Control. Fusion 54,035012,(2012)

- R Celiberto, K L Baluja and R K Janev
  Electron-impact State-to-State Resolved Cross Sections and Rate Coefficients for the \(X(\nu) \rightarrow A(\nu')\) Excitation in BeH molecules
  Plasma Sources Science and Technology 22,015008,(2013)

D. Jakimovski  e\(^-\) -impact processes of plasma impurities:  Be, BeH\(^+\) and var
Published in

- R Celiberto, R K Janev and D Reiter
  State-to-state electron impact cross sections for $\text{BeH}^+$
  molecular ions in ITER-like fusion edge plasmas with $\text{Be}$ walls,

- R Celiberto, K L Baluja and R K Janev
  Electron-impact State-to-State Resolved Cross Sections and
  Rate Coefficients for the $X(\nu) \rightarrow A(\nu')$ Excitation in $\text{BeH}$
  molecules
  Plasma Sources Science and Technology 22,015008,(2013)

- T Maihom, I Sukuba, R Janev, K Becker, T Märk, A Kaiser, J
  Limtrakul, J Urban, P Mach and M Probst
  Electron impact ionization cross sections of beryllium and
  beryllium hydrides
State-to-state electron impact cross sections for $BeH^+$ molecular ions in ITER-like fusion edge plasmas with $Be$ walls,

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$e^-$-impact processes of plasma impurities: $Be, BeH^+$ and var
Electron impact cross sections of vibrationally state-selective $v_i \rightarrow v_f$ transitions in $(F^1\Lambda = A^1\Sigma^+, B^1\Pi)$

$$e^-(\epsilon_i) + BeH^+(X^1\Sigma^+, v_i) \rightarrow e^-(\epsilon_f) + BeH^+(F^1\Lambda, v_f), \quad (1)$$

Coulomb-Born approximation (for details see [1]):

- first order perturbation interaction
- Coulomb waves in initial and final state for $e^-$ motion

Rotational degree of freedom NOT considered $J_i = J_f = 0$

\[
\sigma_{v_i \rightarrow v_f}^{X \rightarrow F} (\varepsilon_i) = g \left[ \frac{3}{4\pi^2} \right] \frac{\pi}{k_i^2} |M_{v_i \rightarrow v_f}^{X \rightarrow F}|^2 f_{E1}(\eta, \zeta); \quad F = A, B \tag{2}
\]

\begin{itemize}
  \item \( k_i = \sqrt{2\varepsilon_i}, \quad k_f = \sqrt{2\varepsilon_f}, \quad \zeta = \eta_f - \eta_i, \quad \eta_f = k_f^{-1}, \quad \eta_i = k_i^{-1} \)
  \item \(|v_i > = \xi_{v_i}(R) \quad |v_f > = \xi_{v_f}(R)\): vibrational wave functions
  \item \( g = 1 \ (X \rightarrow A), \ g = 2 \ (X \rightarrow B) \) is a statistical factor
\end{itemize}

\[
\lim_{\varepsilon_i \rightarrow E_{th}} f_{E1}(\eta, \zeta) \rightarrow \frac{32\pi^3}{9\sqrt{3}} \left(1 + 0.218|\zeta|^{-2/3} \ldots \right) \rightarrow \frac{32\pi^3}{9\sqrt{3}}
\]

Using analytic fits of the numerical values for \( V_X(R) \) and \( V_F(R) \), available in [1], the Schrödinger equation had been solved and dipole matrix elements \( M_{v_i \rightarrow v_f}^{X \rightarrow F} \) have been found and, finally the Coulomb-Born cross sections for excitation transitions.

\[ e^- + BeH^+ \\ e^- + BeH \\ e^- + Be_nH_m \]

BeH\(^+\) potential energy curves for relevant states and correlation with corresponding atomic states

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$e^- + BeH^+$
$e^- + BeH$
$e^- + Be_nH_m$

$BeH^+$ dipole moments for the indicated transitions

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$e^-$-impact processes of plasma impurities: Be, BeH$^+$ and var
Analytic fits (3,4) and scaling (5)

\[ \sigma_{0\rightarrow 0}^{X\rightarrow A} = 1.1646 \frac{\ln (0.4181 + 2.3002x)}{0.87915x - 0.39751x^{0.1}} \left( 10^{-16} \text{cm}^2 \right) \]  

(3)

\[ \sigma_{0\rightarrow 0}^{B\rightarrow A} = 0.07746 \sigma_{0\rightarrow 0}^{X\rightarrow A} \]  

(4)

- \( x \) being the reduced energy variable \( x = \frac{\varepsilon_i}{\Delta E_{v_i\rightarrow v_f}} \)
- \( \varepsilon_i \) is incident electron energy
- \( \Delta E_{v_i\rightarrow v_f} \) is the transition energy

All \( v_i \rightarrow v_f \) cross sections for a given \( X \rightarrow F \) transition satisfy the scaling relationship

\[ \sigma_{v_i,v_f} (x\Delta E_{v_i,v_f}) = \frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}} \left( \frac{M_{v_i,v_f}}{M_{0,0}} \right)^2 \sigma_{0,0} (x\Delta E_{00}) \]  

(5)
Analytic expressions (3) and (4) fits data with 2% and 3% accuracy for $X \rightarrow A$ and $X \rightarrow B$.
$e^- + BeH^+$
$e^- + BeH$
$e^- + Be_nH_m$

Full lines: calculated data; dashed lines: results of scaling (5), for $X(v_i) \rightarrow A(v_f)$
$e^- + \text{BeH}^+$
$e^- + \text{BeH}$
$e^- + \text{Be}_n\text{H}_m$

Full lines: calculated data; dashed lines: results of scaling (5), for $X(v_i) \rightarrow B(v_f)$

D. Jakimovski: $e^-$-impact processes of plasma impurities: Be, BeH$^+$ and various berillium hydrides
**Rate coefficients** have been calculated assuming Maxwellian electron energy distribution and fitted with analytic expression

\[
\kappa_{X \rightarrow F} (T) = c_1 \frac{e^{-c_2/T}}{1 + c_3 T^{c_4} + c_5 T^{c_6}} (10^{-9} \text{cm}^3 \text{s}^{-1})
\]

(6)

\(c_i, i = 1 - 6\) optimized for best fit with the calculated data around their maxima

- in region \((10 - 50) \text{eV}\) agreement within 1-3% but
- for \(T \approx 1 \text{eV}\), and for \(T \approx 10^4 \text{eV}\) discrepancies up to 30-40%

For \(v_i, v_f > 0\) one may use **scaling relation**

\[
\kappa_{v_{i,v_{i,v_f}}} \rightarrow F (T) = \left( \frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}} \right)^{1/2} \left( \frac{M_{v_i,v_f}}{M_{0,0}} \right)^2 \kappa_{0 \rightarrow F} \left( T \frac{\Delta E_{0,0}}{\Delta E_{v_i,v_f}} \right)
\]

(7)
\[ e^- + BeH^+ \]
\[ e^- + BeH \]
\[ e^- + Be_nH_m \]

Full lines: calculated data; dashed lines: analytic fits with (6)

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\( e^- \) -impact processes of plasma impurities: \( Be, BeH^+ \) and various berillium hydrides
\[ e^- + BeH^+ \]
\[ e^- + BeH \]
\[ e^- + Be_nH_m \]

Full lines: calculated data; dashed lines: with scaling (7)

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\( e^- \)-impact processes of plasma impurities: Be, BeH\(^+\) and various berillium hydrides
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\(-\) -impact processes of plasma impurities: Be, BeH\(^+\) and various berillium hydrides

Full lines: calculated data; dashed lines: with scaling (7)
Electron-impact State-to-State Resolved Cross Sections and Rate Coefficients for the $X(\nu) \rightarrow A(\nu')$ Excitation in $BeH$ molecules

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\[ e^- (\varepsilon_i) + \text{BeH} (X^2\Sigma, \nu) \rightarrow e^- (\varepsilon_f) + \text{BeH} (A^2\Pi, \nu') \]  

(8)

has been calculated with **R-matrix** method, for \( \varepsilon_i < 15 \text{eV} \)

For higher energies, **threshold modified Mott-Massey approximation (TM MM)** expression has been used:

\[
\sigma_{v,v'} (\varepsilon_i)_{\text{TM MM}} = \frac{4\pi}{3\varepsilon_i} g |M_{v,v'} (R)|^2 \ln \frac{\sqrt{\Delta E_{v,v'}}}{|\sqrt{\varepsilon_i} - \sqrt{\varepsilon_i - \Delta E_{v,v'}}|} 
\]

(9)

in units \((a_0^2)\)

- \(M_{v,v'} = \langle v'|D_{X\rightarrow A} (R)|v \rangle\) is the matrix element
- \(D_{X\rightarrow A} (R)\) is the transition dipole moment (TDM)
- \(g = 2\) is a degeneracy factor

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\(e^-\)-impact processes of plasma impurities: Be, BeH\(^+\) and var.
Threshold modified Mott-Massey approximation

From Born cross section for optically (dipole) allowed molecular transitions \((k_i = \sqrt{2\varepsilon_i}, k_f = \sqrt{2(\varepsilon_i - \Delta E_{v',v'})})\) are the momenta)

\[
\sigma_{v,v'}(\varepsilon_i) = \frac{8\pi}{3k_i^2} g|M_{v,v'}|^2 \int \frac{|k_i + k_f|}{|k_i - k_f|} dK = \frac{8\pi}{3k_i^2} g|M_{v,v'}|^2 \ln \frac{k_i + k_f}{|k_i - k_f|} \quad (a_0^2)
\]

The Mott and Massey approximation is obtained by replacing the upper limit with constant constant \(K_0 = \sqrt{2\Delta E_{v',v'}}\). With,

\(|k_i - k_f| = |k_i^2 - k_f^2|/(k_i + k_f) \approx \Delta E_{v',v'}/k_i\) one may proceed to integration. . . But from the result of this integration, at the threshold: \(\sigma(\varepsilon_i \rightarrow \Delta E_{v',v'}) \rightarrow \sim \ln 2 \neq 0\). To avoid the divergence it is sufficient: \(|k_i - k_f| = |\sqrt{2\varepsilon_i} - \sqrt{2(\varepsilon_i - \Delta E_{v',v'})}| \Rightarrow (9)

... TM MM
Potential energies and dipole moment (right scale); note almost parallel run of the two curves
\[ e^- + \text{BeH}^+ \]
\[ e^- + \text{BeH} \]
\[ e^- + \text{Be}_n\text{H}_m \]

\[ X(0) \rightarrow A(0) \]

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\[ e^- \] -impact processes of plasma impurities: \( \text{Be, BeH}^+ \) and var.
\[ e^- + BeH^+ \]
\[ e^- + BeH \]
\[ e^- + Be_nH_m \]

\[ X(0) \rightarrow A(0) \]

- dashed line: R-matrix-normalized TMMM

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\[ e^- \] -impact processes of plasma impurities: Be, BeH\(^+\) and various berillium hydrides
$e^- + \text{BeH}^+$
$e^- + \text{BeH}$
$e^- + \text{Be}_n\text{H}_m$
electron-CH collision cross sections: full lines - TMM; dotted lines - R-matrix

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e$^-$ - impact processes of plasma impurities: Be, BeH$^+$ and various berillium hydrides
R-matrix normalized TM MM

Transition dipole moments (TDMs) $D_{X \rightarrow A}(R)$ used in the TM MM calculations, via squared matrix elements,

$$M_{\nu,\nu'} = \langle \nu' | D_{X \rightarrow A}(R) | \nu \rangle$$

are different from those provided by the R-matrix method and can contribute to the discrepancy observed in the corresponding cross sections. . .

To offset for this effect one includes in (9) a multiplicative factor:

$$\left( \frac{\text{TDM calculated with RM method}}{M_{0,0} \text{ calculated with TDMs from ref.}[1]} \right) = \left( \frac{0.7348}{0.8337} \right)^2 = 0.7768$$

$e^- + BeH^+$
$e^- + BeH$
$e^- + Be_nH_m$

$X(0) \rightarrow A(0)$
Range of incident electron energies enlarged up to 1000 eV;
TMM (eq 9) and Born sections are reduced by the same TDM ratio of 0.7768.

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$e^-$-impact processes of plasma impurities:  Be, BeH$^+$ and var
TM MM cross sections have been fitted by the expression

$$
\sigma_{0,0}(x) = \frac{c_0}{x} \frac{M_{0,0}^2(a.u.)}{\Delta E_{0,0}(eV)} \left[1 - \frac{1}{x}\right]^{c_1} \left[\ln x + c_2 + \frac{c_3}{x}\right]
$$

(10)

in units \(10^{-16} \text{cm}^2\)

- \(x = \Delta E_{0,0}/\varepsilon_i\) is the reduced energy
- \(c_i, i = 1 - 4\) are fit coefficients

with substitution \(0,0 \rightarrow \nu, \nu'\) one gets \(\sigma_{\nu,\nu'}(x)\) as good fitting for other diagonal and nondiagonal transitions \(\nu \rightarrow \nu'\)
$e^{-} + BeH^+$
$e^{-} + BeH$
$e^{-} + Be_nH_m$

Full lines: calculated data; dashed lines: fitted (10)

D. Jakimovski e$^{-}$ -impact processes of plasma impurities: Be, BeH$^+$ and var
Vibrational excitation rate coefficients

convolution of the

- calculated cross sections

- Maxwellean electron energy distribution function

For \( 0 \rightarrow 0 \) the rate coefficient is fitted by

\[
\kappa_{0,0}(T) = \frac{146.39 T^{-0.205}}{1 + 0.00005 T^{1.5}} e^{-2.53/T} \left(10^{-9} \text{cm}^3\text{s}^{-1}\right)
\]

where \( T \) is the temperature in eV.

For other transitions, \( \nu \rightarrow \nu' \) one may reach to a scaling law

\[
\kappa_{\nu,\nu'}(T) = \left[ \frac{\Delta E_{0,0}}{\Delta E_{\nu,\nu'}} \right]^{1/2} \left[ \frac{M_{\nu,\nu'}}{M_{0,0}} \right]^2 \kappa_{0,0} \left[ \frac{\Delta E_{0,0}}{\Delta E_{\nu,\nu'} T} \right] \left(10^{-9} \text{cm}^3\text{s}^{-1}\right)
\]
The reaction equations are:

\[ e^- + BeH^+ \]
\[ e^- + BeH \]
\[ e^- + Be_nH_m \]

Full lines: calculated data; dashed lines: analytically reproduced rate coefficients (12)

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\( e^- \)-impact processes of plasma impurities: Be, BeH\(^+\) and various berillium hydrides
Electron impact ionization cross sections of beryllium and beryllium hydrides

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$e^- + BeH^+$  
$e^- + BeH$  
$e^- + Be_nH_m$  
e$^-$-impact processes of plasma impurities: Be, BeH$^+$ and var.
Methods of calculations:

- Binary-encounter-Bethe (BEB) model
  Y K Kim, M A Ali, M E Rudd, J. Res. NIST 102, 693 (1997)

- Deutsch-Märk (DM) model
Binary-encounter-Bethe (BEB) model

- binary-encounter-dipole (BED) model, with simplification of the term \( df/dE \) for the continuum dipole oscillator strengths
- asymptotic form of the Bethe theory for electron-impact ionization

\[
\sigma_{BEB}(t) = \frac{S}{t + u + 1} \left[ \frac{\ln(t)}{2} \left( 1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} - \frac{\ln(t)}{t + 1} \right]
\]

where \( t = T/B, \ u = U/B, \ S = 4\pi a_0^2 NR^2/B^2, \)

- \( a_0 = 0.5292\text{Å} \) Bohr radius, \( R = 13.6057\text{eV} \) Rydberg energy
- \( T, N \) incident electron energy, electron occupation number
- \( B \) binding energy (ionization potential) and \( U \) average kinetic energy of the orbital, derived from Hartree-Fock calculations with aug-cc-pVTZ basis set [1]

Deutsch-Märk (DM) model

Total single electron-impact ionization cross section $\sigma$ of an atom is expressed as:

$$\sigma(u) = \sum_{n,l} g_{nl} r_{nl}^2 n_{nl} b_{nl}^{(q)}(u) \left[ \frac{\ln(c_{nl}u)}{u} \right], \quad b_{nl}^{(q)}(u) = \frac{A_1 - A_2}{1 + (u/A_3)^p} + A_2$$

- $r_{nl}$ radius of maximum radial density of the atomic subshell $n, l$
- $\xi_{nl}$ number of electrons in that sub-shell
- $g_{nl}$ weighting factors, originally determined form a fitting procedure on reliable experimental section data
- $u = E/N_{nl}$ “reduced energy”, $E$ incident energy of the electrons and $E_{nl}$ is the ionization energy in the $(n, l)$ subshell.
- $A_1, A_2, A_3, p$ and $c_{nl}$ constants, determined from reliable measured cross sections

At $E \to \infty$, $b_{nl}^{(q)} \to A_2 = \text{const.}$; behaviour of $\sigma(u)$ follows the Born-Bethe approximation
Electron impact ionization cross sections of Be
Minimum-energy structures of (a) BeH and (b) BeH$_2$ from QCISD/aug-cc-p VTZ calculations

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Electron impact ionization cross sections of BeH and BeH$_2$ from the DM and BEB methods

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$e^- + BeH^+$
$e^- + BeH$
$e^- + Be_nH_m$
Minimum-energy structures of (a) Be$_2$H$_2$ and (b) Be$_2$H$_4$ from QCISD/aug-cc-p VTZ calculations

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$e^-$-impact processes of plasma impurities: Be, BeH$^+$ and var...
Electron impact ionization cross sections of $\text{Be}_2\text{H}_2$ and $\text{Be}_2\text{H}_4$ from the DM and BEB methods
How well one can fit these sections with a formula?

\[
\sigma (E) = \frac{a_1}{E} \left[ 1 - \frac{E_t}{E} \right]^{a_2} \left[ \ln \frac{E}{E_t} + a_3 + a_4 \frac{E_t}{E} \right]
\]

(13)

where

- \( \sigma \) is expressed in \( 10^{-16} \text{cm}^2 \) and \( E \) in eV
- \( E_t \) is threshold energy, in eV
- \( a_i, i = 1 \cdots 4 \) are fitting parameters

answer?

Very well, indeed!
Cross sections (solid lines) obtained from fitting the DM values to equation (13)
Cross sections (solid lines) obtained from fitting the BEB values to equation (13)

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\[ e^- + BeH^+ \\
\[ e^- + BeH \\
\[ e^- + Be_nH_m \\

Conclusions

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Conclusions

Thank You