Uncertainties of electron capture cross sections in Be^{4+} + H(1s) collisions.

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Motivation

- Electron capture reactions (Charge exchange) reactions:

$$\mathrm{A^{q+} + H \rightarrow A^{(q-1)+} + H^{+}}$$

- Cross sections required in plasma modelling and diagnostics.
- In this talk collisions with fully stripped ions (one-electron systems).
- Be^{4+} specially relevant.

Previous work

Be^{4+} + H collisions

- No experimental data.
- Need of theoretical data. More than 35 years of calculations.

  Accuracy?

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Table 1
Cross section for reaction (1) calculated with a three-term ($3d\sigma$, $3d\pi$, $4f\sigma$) molecular expansion including the CTF of eq. (4).

Nuclear velocity (atomic units)	E (keV/amu)	Cross section ($cm^2 \times 10^{-16}$)
0.1	0.25	27.42
0.2	1.00	36.94
0.3	2.25	36.27
0.5	6.25	30.54
0.9	20.25	23.36
1.2	36.0	19.89

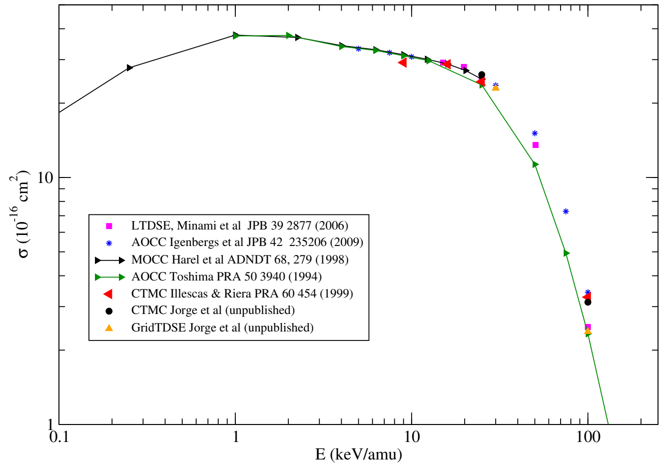
similar to those for C^{4+}–H; like these authors, we incorporate the experimental data for C^{4+}–H collisions [12–14]. Fig. 2 appears crammed with data, so that we also present our results on a separate table, table 1.

different from those obtained using TF. However, this is probably a coincidence, and there is no reason to expect it a priori. It is also significant that the results with TF do not always fall between those without TF for the two choices of origin. This can be explained by the fact that the variation of the calculated cross section with the origin is not monotonous, and it reaches a maximum for an origin between the Be nucleus and the proton. Hence, the difference between the results without TF with the origin on each nucleus cannot be taken as a measure of the uncertainty due to the lack of TF.

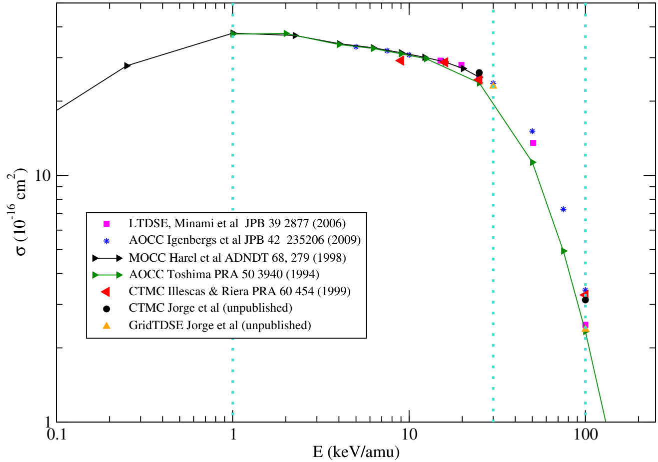
We thank Dr. A. Salin for providing us with his accurate values of the molecular energies and couplings, and Dr. T. Ohyama and Dr. Y. Itikawa for sending us a preprint of their work.

(Errea et al. Phys. Lett. A 92, 232)

Total cross section



Total cross section



In this talk:

- $1 < E < 100$ keV/u. Semiclassical calculations.
- Uncertainties of *n*-partial CX cross sections in CC calculations.
- Accuracy and uncertainties of CTMC results.
- Some results of the numerical integration of the TDSE.

Impact parameter method

In general valid for $E > 250$ eV/u

- Rectilinear nuclear trajectories $\mathbf{R} = \mathbf{b} + \mathbf{v}t$
- The electron wavefunction is a solution of:

$$\left[H_{\mathrm{el}} - \mathrm{i}\frac{\partial}{\partial t} \right] \Psi = 0$$

with

$$H_{\mathrm{el}} = -\frac{1}{2}\nabla_r^2 + V_{\mathrm{P}} + V_{\mathrm{T}}$$

Molecular expansion

MOCC

$$\Psi(\mathbf{r},t;b,v) = D(\mathbf{r},t)\sum_k a_k(t;b,v)\phi_k(\mathbf{r};R)\exp\left(-\mathrm{i}\int \epsilon_k(R)\mathrm{d}t\right)$$

where ϕ_k are molecular orbitals that fullfil:

$$H_{\mathrm{el}}\phi_k = \epsilon_k\phi_k$$

and $D(\mathbf{r},t)$ is a common translation factor.

Atomic expansion

AOCC

$$\Psi(\mathbf{r}, t; b, v) = \sum_k a_k(t; b, v)\phi_k^{\mathrm{P}}(\mathbf{r}; R) \exp\left(-\mathrm{i}\epsilon_k^{\mathrm{P}}\right) D^{\mathrm{P}} + \sum_l a_l(t; b, v)\phi_l^{\mathrm{T}}(\mathbf{r}; R) \exp\left(-\mathrm{i}\epsilon_l^{\mathrm{T}}\right) D^{\mathrm{T}}$$

where ϕ_k^{P}, ϕ_l^{T} are atomic orbitals that fulfill:

$$\left[-\frac{1}{2}\nabla_r^2 + V_{\mathrm{P}}\right]\phi_k^{\mathrm{P}} = \epsilon_k^{\mathrm{P}}\phi_k^{\mathrm{P}}; \quad \left[-\frac{1}{2}\nabla_r^2 + V_{\mathrm{T}}\right]\phi_l^{\mathrm{T}} = \epsilon_l^{\mathrm{T}}\phi_l^{\mathrm{T}}$$

and $D^{\mathrm{P,T}}$ are plane-wave translation factors

CC methods

Computational procedure

- Calculation of couplings $M_{kl} =< \psi_k D^k | H_{\mathrm{el}} - \mathrm{i}\partial/\partial t | \psi_l D^l >$.
- Integration of the system of differential equations for a_k.

$$\mathrm{i}\dot{\mathbf{a}} = \mathbf{S}^{-1}\mathbf{M}\mathbf{a}$$

- Integration of transition probabilities.

$$\sigma_k = 2\pi \int_0^{b_{\max}} bP(b)\mathrm{d}b = 2\pi \int_0^{b_{\max}} b|a_k(t_{\max})|^2 \mathrm{d}b$$

Eikonal CTMC Method

- The projectile follows **straight-line trajectories**: $\mathbf{R} = \mathbf{b} + \mathbf{v}t$
- Electronic motion is described by a **classical distribution function** $\rho(\mathbf{r}, \mathbf{p}, t)$[a]

[a] Abrines & Percival, Proc. Phys. Soc. **88**, 861

Eikonal CTMC Method

In practice

- Hamilton's equations are solved for each electron trajectory ($N \approx 10^5$):

$$\dot{\mathbf{r}}_j = \frac{\partial H\mathrm{el}}{\partial \mathbf{p}_j};\ \dot{\mathbf{p}}_j = -\frac{\partial H\mathrm{el}}{\partial \mathbf{r}_j}$$

with:

$$H_{\mathrm{el}} = \frac{p^2}{2} - \frac{Z_T}{r_T} - \frac{Z_P}{r_P}$$

- Energy criterion is applied at $t_{\mathrm{fin}} = \frac{500}{v}$ to select
  - **Ionization** ($E_T > 0,\ E_P > 0$)
  - **Capture** ($E_T > 0,\ E_P < 0$)

Transition probabilities and cross sections

- Transition probabilities:

$$P^{i,c}(v,b) = \int d\mathbf{r} \int d\mathbf{p}\, \rho^{i,c}(\mathbf{r},\mathbf{p},v,b,t_{\mathrm{fin}})$$

- Total cross sections:

$$\sigma^{i,c}(v) = 2\pi \int_0^\infty db\, b\, P^{i,c}(v,b)$$

Calculation of partial cross sections

Classical phase space of captured electrons is partitioned into exclusive subspaces[a]:

$$[(n-1)\,(n-\frac{1}{2})\,n]^{1/3} < \mathbf{n_c} \leq [n\,(n+\frac{1}{2})\,(n+1)]^{1/3}$$

$$l < \frac{n}{n_c}\,\mathbf{l_c} \leq l+1$$

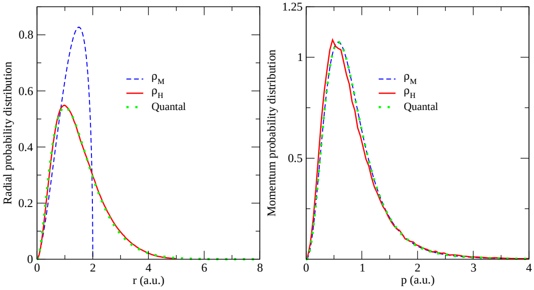
with $\mathbf{n_c} = Z_P/\sqrt{-2E_P}$ and $\mathbf{l_c} = |(\mathbf{r}-\mathbf{b}-\mathbf{v}t) \wedge (\mathbf{p}-\mathbf{v})|$.

[a] Becker & MacKellar , JPB **17**, 3923

Initial distribution

Microcanonical (standard)

$$\rho_M(\mathbf{r}, \mathbf{p}, v, b, t \to \infty) = \frac{1}{8\pi^3}\, \delta\left(\frac{p^2}{2} - \frac{1}{r} + \frac{1}{2}\right)$$



Initial distribution

Microcanonical (standard)

$$\rho_M(\mathbf{r},\mathbf{p},v,b,t\to\infty) = \frac{1}{8\pi^3}\,\delta\left(\frac{p^2}{2}-\frac{1}{r}+\frac{1}{2}\right)$$

Hydrogenic

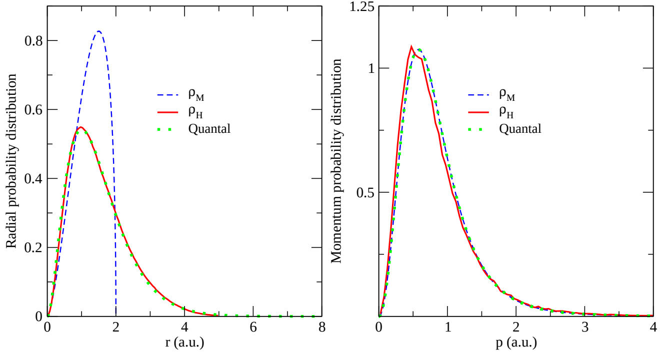
$$\rho_H(\mathbf{r},\mathbf{p},v,b,t\to\infty) = \sum_{k=1}^{\mathcal{N}}\frac{(-2\epsilon_k^{5/2})}{8\pi^3}\,a_k\,\delta\left(\frac{p^2}{2}-\frac{1}{r}-\epsilon_k\right)$$

linear combination of $\mathcal{N}$ microcanonicals [a] with average energy

$< \epsilon > \simeq -\frac{1}{2}$ a.u..

[a] Hardie and Olson, JPB, **16**, 1983

Initial distribution H(1s)



Numerical integration of the TDSE

- Previous calculations of Minami *et al*. (JPB 39, 2877 (2006)) for $Be^{4+} + H(1s)$. (LTDSE)
- New calculations using the program GridTDSE of Suarez *et al*. CPC 180, 2025 (2009).

GridTDSE

$$\left(H_{\rm el}(\mathbf{r},t) - {\rm i}\frac{\partial}{\partial t}\right)\Psi(\mathbf{r},t;b,v) = 0$$

The numerical solution of this equation has the form:

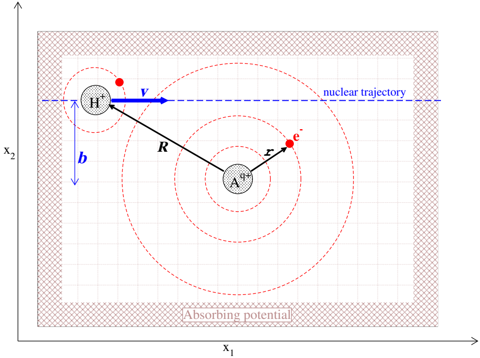
$$\mathbf{\Psi}(t+\Delta) = \mathbf{\Psi}(t-\Delta) - 2{\rm i}\Delta(\mathbf{T}+\mathbf{V})\mathbf{\Psi}(t),$$

where the components of vector $\mathbf{\Psi}$ are the values of the wavefunction in the grid points.

In practice:

$$V_{\rm P}(\mathbf{r}) = -\frac{Z_p}{\sqrt{|\,\mathbf{r}\,|^2+\epsilon_p}}$$

$$V_{\rm T}(\mathbf{r},t) = -\frac{Z_t}{\sqrt{|\mathbf{r}-\vec{R}|^2+\epsilon_t}} \quad , \quad \mathbf{R} = (b, 0, z_{min} + vt)$$



Grids

- G1

  -22 a.u.$\leq x_i \leq$ 22 a.u.

  (221^3 points)

- G2

  -22 a.u.$\leq x_i \leq$ 22 a.u.

  (320^3 points)

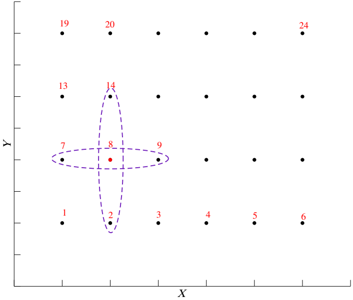
- G3

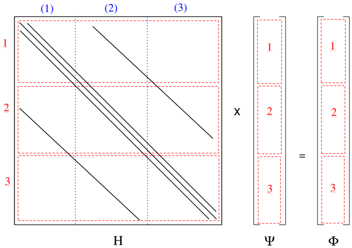
  -30 a.u.$\leq x_i \leq$ 30 a.u.

  (301^3 points)

Mask function

$$M(\vec{r}) = \prod_{i=1,3} \begin{cases} 1 & \text{if} \quad r_i^{L-} < r_i < r_i^{L+} \\ \exp\left\{-\sigma_i (r_i - r_i^{L\pm})^2\right\} & \text{elsewhere} \end{cases}$$


19
20
24
13
14
7
8
9
1
2
3
4
5
6
Y
X


(1)
(2)
(3)
1
2
3
x
=
H
Ψ
Φ

Low energy, $E = 1$ keV/u

Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n{=}3) + H^+$

Calculation	Cross section 10^{-16}cm^2
MOCC-17[a]	34.70
MOCC-88[b]	34.5
MOCC-96[a]	34.42
gridTDSE (G1)	33.20
AOCC-170[c]	34.4

[a] Errea et al. JPB 31, 3527

[b] Harel et al. ADNDT 68, 279

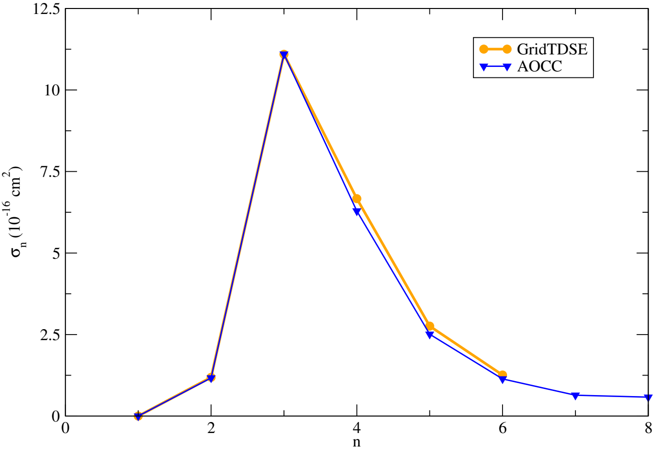
[c] Igenbergs et al. JPB 42 35206

Low energy, $E = 1$ keV/u

Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n{=}4) + H^+$ at $E = 1$ keV/u.

Calculation	Cross section $10^{-16}cm^2$
MOCC-17[a]	2.45
MOCC-88[b]	3.17
MOCC-96[a]	3.11
gridTDSE (G1)	3.27
AOCC-170[c]	3.10

Intermediate energy, $E = 30$ keV/u



Intermediate energy, $E = 30$ keV/u

Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n=3) + H^{+}$

Calculation	Cross section $10^{-16}\mathrm{cm}^2$
gridTDSE (G3)	11.09
AOCC-170[a]	11.1 [b]

[a] Igenbergs et al. JPB 42 35206

[b] $\pm 0.4 \times 10^{-16}$ cm^2, based on the convergence study of Igenbergs et al.

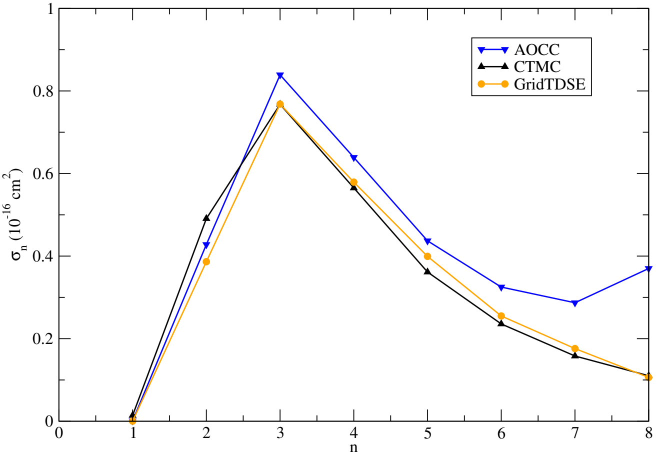
$E = 30$ keV/u

Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n{=}4) + H^{+}$

Calculation	Cross section $10^{-16} cm^2$
gridTDSE (G3)	6.67
AOCC-170[a]	6.29

[a] Igenbergs et al. JPB 42 35206

High energy, $E = 100$ keV/u



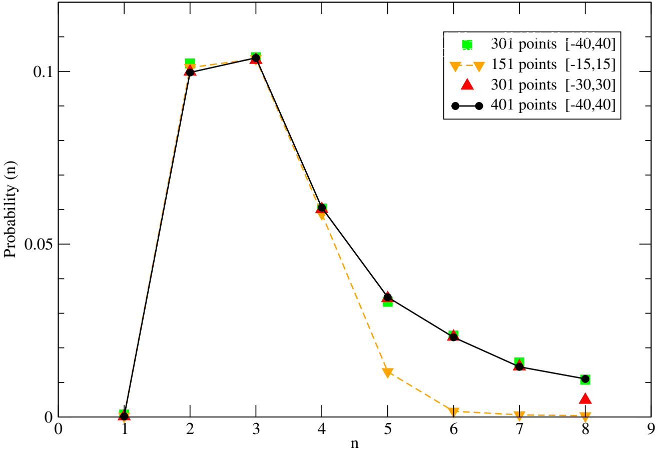
$E = 100$ keV/u

Convergence of the CTMC calculation. Partial cross sections (10^{-16}cm^2)

n	1×10^5 traj.	5×10^5 traj.
1	0.0141	0.0141
2	0.491	0.494
3	0.768	0.768
4	0.565	0.560
5	0.361	0.363
6	0.236	0.238
7	0.158	0.161
8	0.110	0.113
..	.....	.....
15	0.0169	0.0194

$E = 100$ keV/u

CX probability, $b = 1$, GridTDSE calculation



$E = 100$ keV/u

Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n{=}3) + H^{+}$

Calculation	Cross section $10^{-16}cm^2$
gridTDSE (G3)	0.768
CTMC	0.768

$E = 100$ keV/u

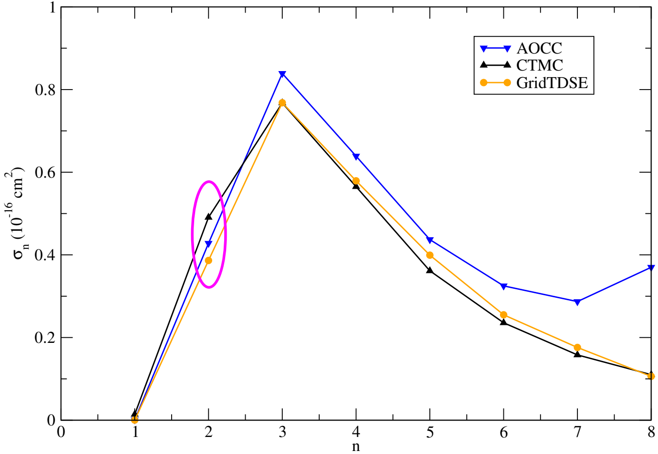
Total cross sections for Be^{4+} + H(1s) → $Be^{3+}(n=4)$ + H^+

Calculation	Cross section 10^{-16}cm^2
gridTDSE (G3)	0.579
CTMC	0.560

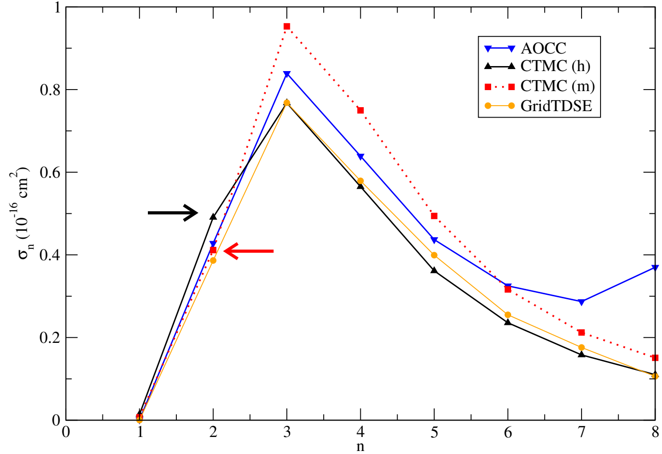
Total cross sections for Be^{4+} + H(1s) → $Be^{3+}(n=5)$ + H^+

Calculation	Cross section 10^{-16}cm^2
gridTDSE (G3)	0.398
CTMC	0.363

$E = 100$ keV/u



$E = 100$ keV/u

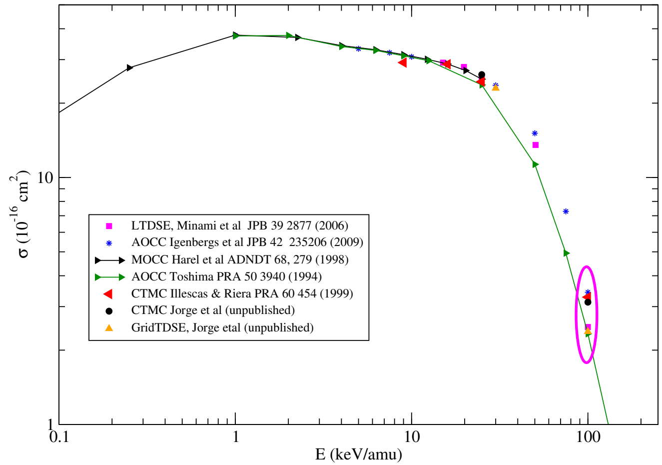

AOCC
CTMC (h)
CTMC (m)
GridTDSE
σ_n (10^{-16} cm^2)
n
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4
5
6
7
8

$E = 100$ keV/u

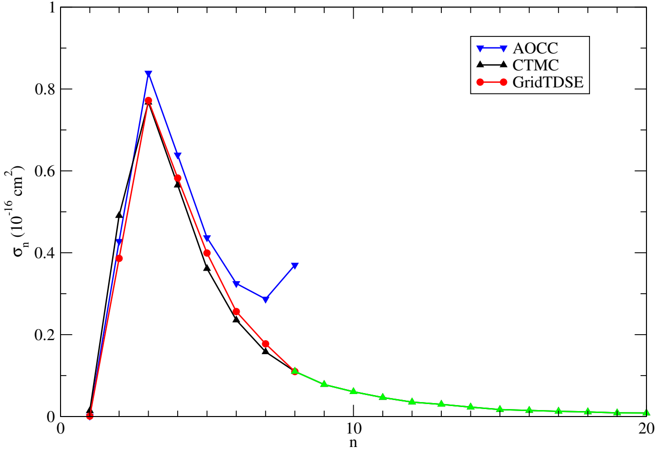
Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n{=}2) + H^{+}$

Calculation	Cross section 10^{-16}cm^2
gridTDSE (G3)	0.398
CTMC (m, 1×10^5 traj.)	0.411
CTMC (m, 5×10^5 traj.)	0.410

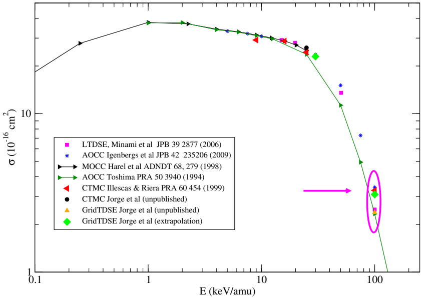
Total cross section



Total cross section, $E = 100$ keV/u



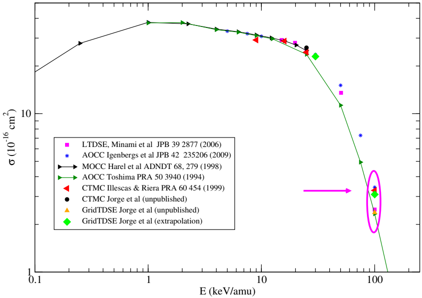
Total cross section



Calculation	σ, Å^2
CTMC (h, 1×10^5 traj.)	3.13
CTMC (h, 5×10^5 traj.)	3.14
GridTDSE (extrap.)	3.09

Uncertainties of the CTMC calculation, Å^2	Statistics	$n<3$	Total
	1.5×10^{-2}	8×10^{-2}	$\approx 1\times10^{-1}$

Total cross section



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Uncertainties of the CTMC calculation, Å^2	Statistics	$n < 3$	Total
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Summary

- MOCC partial cross sections. $|\epsilon| < 3 \times 10^{-1} \AA^2$ at $E = 1$ keV/u.
- AOCC Convergence studies of partial cross sections not available. $|\epsilon| \approx 4 \times 10^{-1} \AA^2$ for total cross section at $E = 30$ keV/u.
- CTMC calculation. Small uncertainties from the statistics. Difficulties for CX into low-n levels.
- Preliminary results of GridTDSE. Precision is a function of the grid density.

Outlook

- Low energies ($E \lesssim 100$ eV): Quantal treatment. Partial-wave expansion.
- Many-electron systems: Precision of the basis functions.

Coworkers

- TCAM group : Luis Errea, Clara Illescas, Ismanuel Rabadán, Jaime Suárez, Alba Jorge.
- Bernard Pons (CELIA, Bordeaux, France)