New CXS data for boron.

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Collisions studied.

We have considered the following projectiles:

- Ne^{10+}, $Ar^{18+, 17+, 16+}$ (rare gases are added in the plasma edge).
- B^{5+} (can be formed due to the boronization of the first wall).

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Energy range $\approx 1 - 1000$ keV/amu.
We have applied two methods:

1. Semiclassical approach with a molecular basis.
2. Eikonal CTMC

Organization.

1. Description of the methods.
2. Previous results:
   - Ne^{10+} + H(1s) collisions. (J. Phys. B, 37, 4323 (2004))
   - $Ar^{16+,17+,18+}$ + H(1s) collisions. (J. Phys. B, 39, L91 (2006))
3. B^{5+} + H(1s)collisions. (Plasma Phys. Control. Fusion 48, 1585 (2006)) .
4. Collisions with H(2s).
5. Summary

Semiclassical treatment.

- **Impact parameter approximation:**
  - Nuclear rectilinear trajectories $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$
  - Semiclassical equation

$$\left[H - \mathrm{i} \left. \frac{\partial}{\partial t} \right|_{\boldsymbol{r}} \right] \Psi(\boldsymbol{r}, t; v, b) = 0$$

- **Molecular expansion:**

$$\Psi(\boldsymbol{r}, t; v, b) = \exp\left[\mathrm{i}U(\boldsymbol{r}, t)\right] \sum_k a_k(t; v, b) \boldsymbol{\chi_k}(\boldsymbol{r}, R) e^{-\mathrm{i}\int_0^t E_k(t')dt'}$$

  - $\boldsymbol{\chi_k}(\boldsymbol{r}, R)$ are molecular orbitals.
  - $\exp(\mathrm{i}U)$ is a Common Translation Factor.

Semiclassical treatment.

Total cross sections:

$$\sigma_{nlm}^{\mathrm{A,H}}(v) = 2\pi \int |a_{nlm}^{\mathrm{A,H}}(v, b, t \to \infty)|^2 b\mathrm{d}b = 2\pi \int P_{nlm}^{\mathrm{A,H}}(v, b) b\mathrm{d}b$$

Pseudostates can be introduced to evaluate ionization cross sections and to extend the method to high energies

IP-CTMC methods

- Impact parameter approximation: $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$
- Classical distribution function $\rho(\boldsymbol{r}, \boldsymbol{p}, t)$, solution of the Liouville's equation:

$$\frac{\partial \rho}{\partial t} = -[\rho, H]$$

Taking

$$\rho(\boldsymbol{r}, \boldsymbol{p}, t) = \frac{1}{N} \sum_{j=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_j)\delta(\boldsymbol{p} - \boldsymbol{p}_j)$$

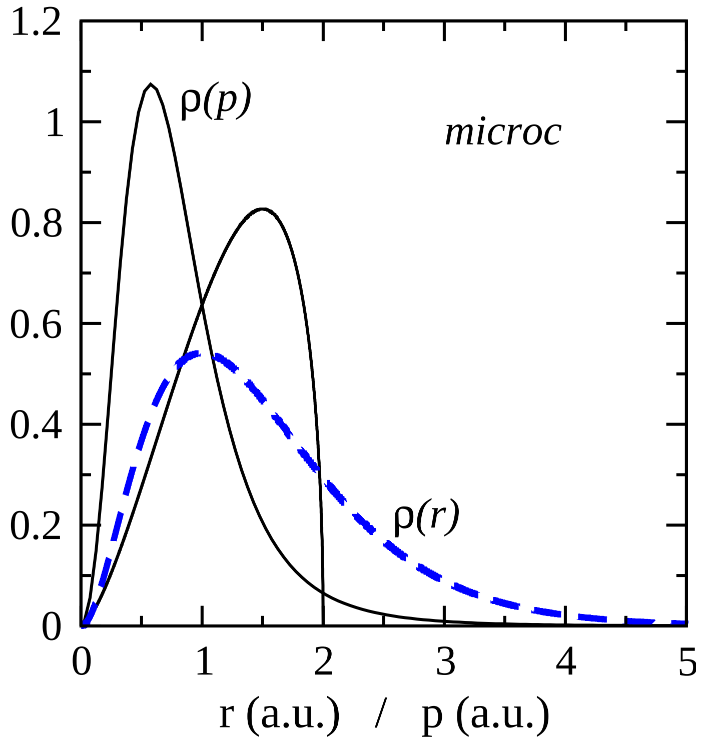
leads to the Hamilton's equations

$$\dot{\boldsymbol{r}}_j = \frac{\partial H}{\partial \boldsymbol{p}_j}; \; \dot{\boldsymbol{p}}_j = -\frac{\partial H}{\partial \boldsymbol{r}_j}$$

Initial distribution.

Initial microcanonical distribution:

$$\rho^m(\boldsymbol{r}, \boldsymbol{p}, E_0) = \frac{(2E_0)^{5/2}}{8\pi^3 Z^3}\,\delta(H - E_0)$$



Initial distribution.

Improved distributions have been proposed (Hardie and Olson J. Phys. B, 27, 36903 (1983)). We have used a hydrogenic distribution, which is a linear combination of 10 microcanonical distributions:

$$\rho(\boldsymbol{r}, \boldsymbol{p}) = \sum_{j=1}^{10} w_j \rho^m(\boldsymbol{r}, \boldsymbol{p}, E_j)$$

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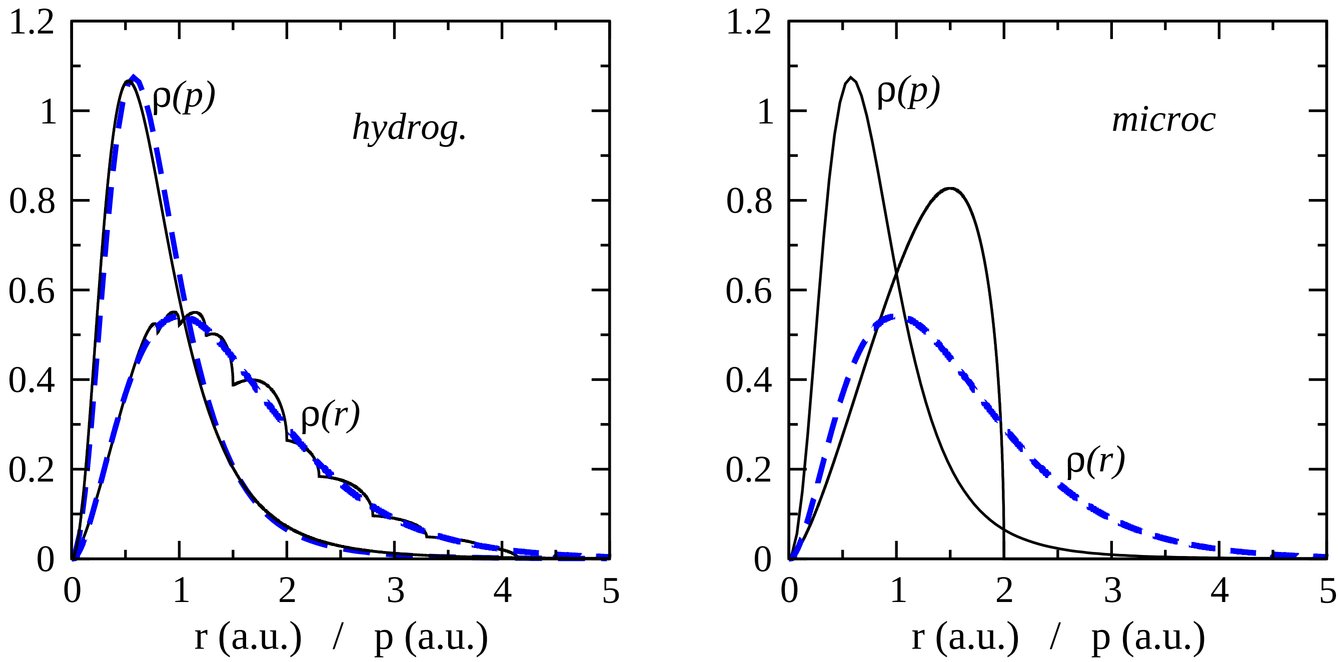


Classical distributions for H(1s) compared to the quantal ones.

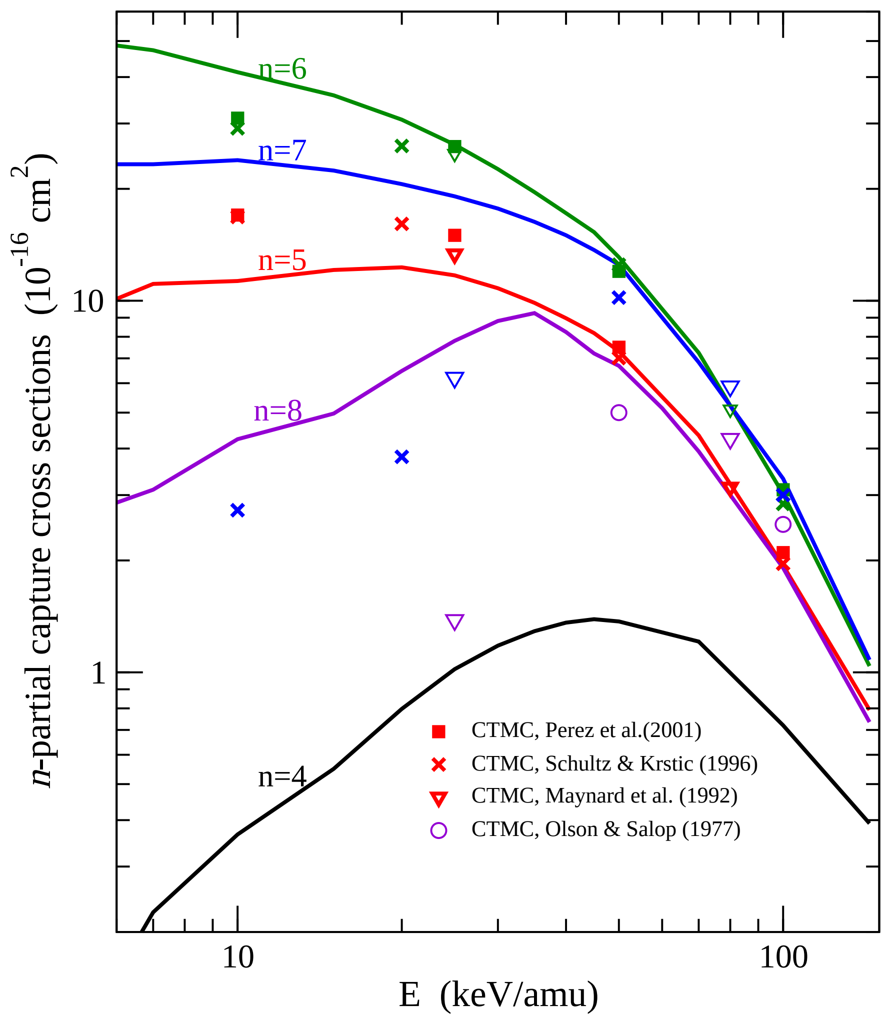
Final states.

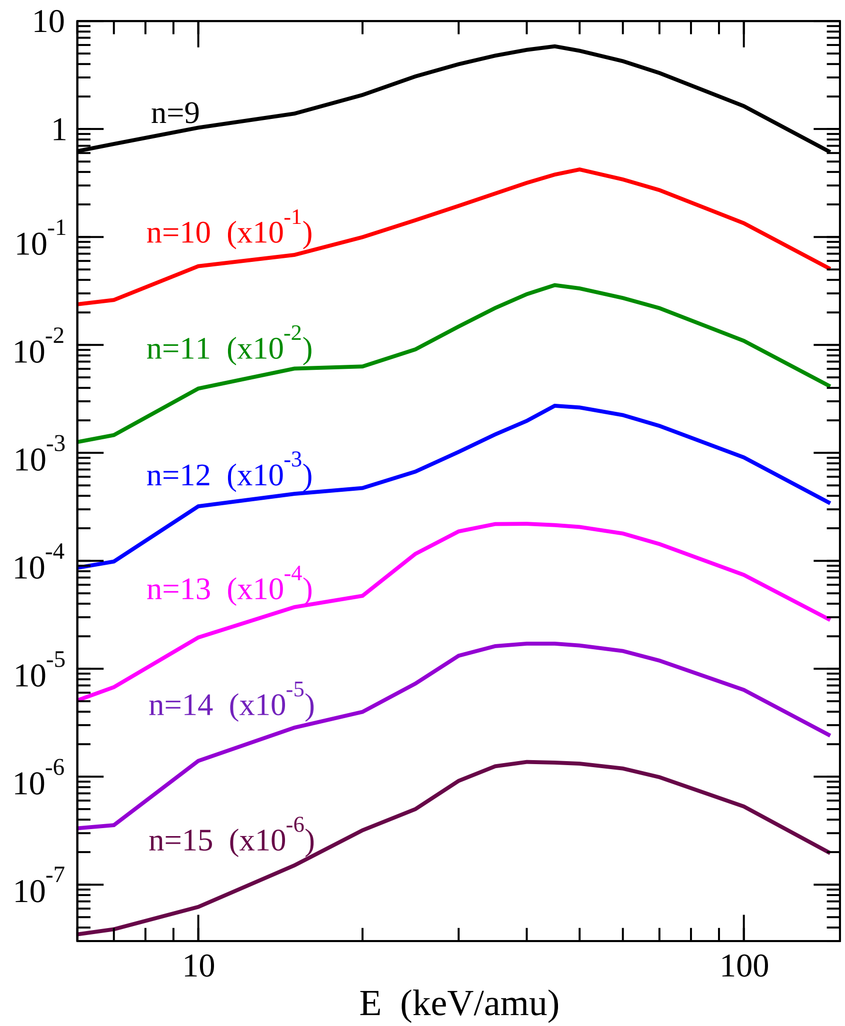
We have employed the binning method of Becker and McKellar (J. Phys. B, 17, 3923 (1984))

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

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

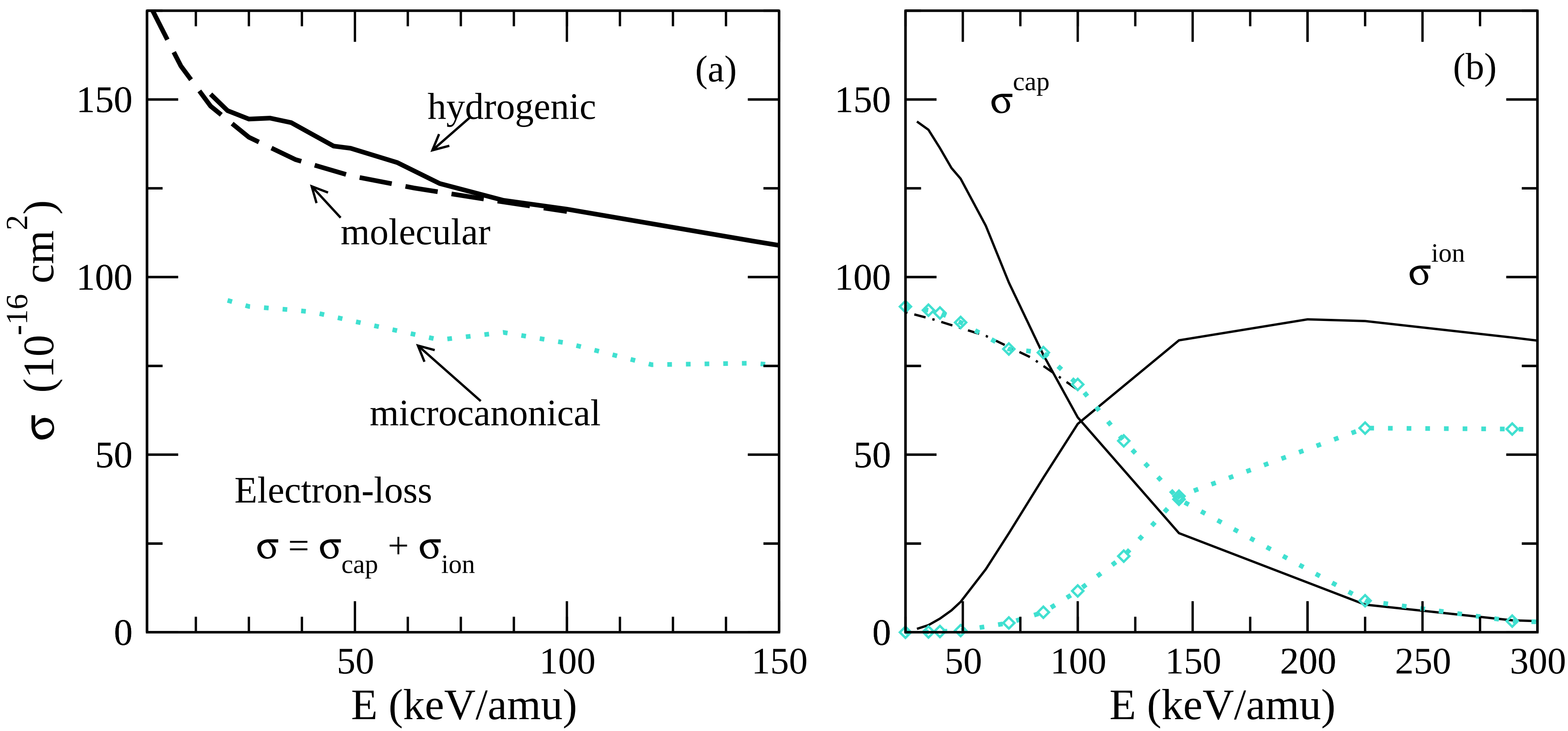
Ne^{10+} + H(1s) collisions.



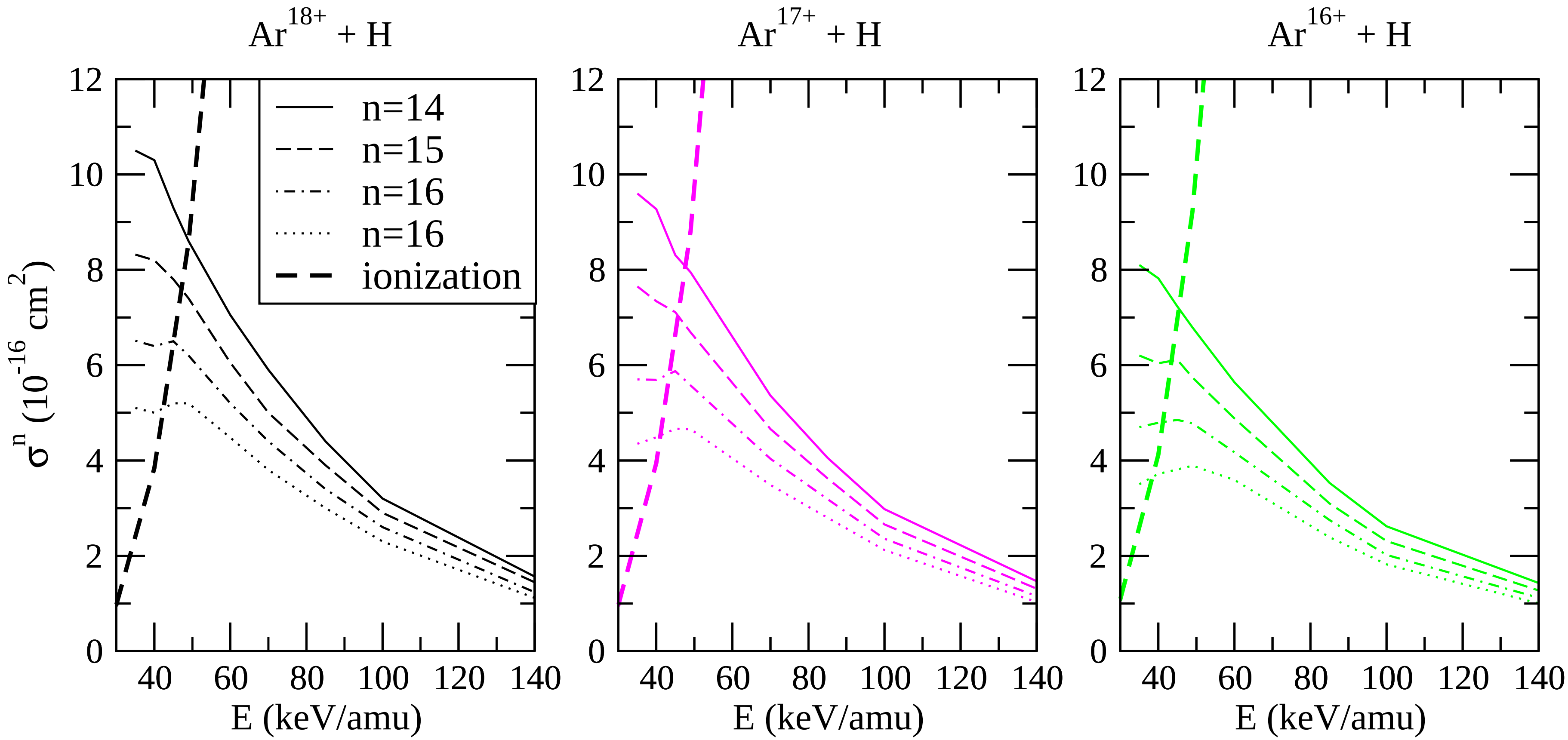


Details in J. Phys. B 37 4323 (2004)

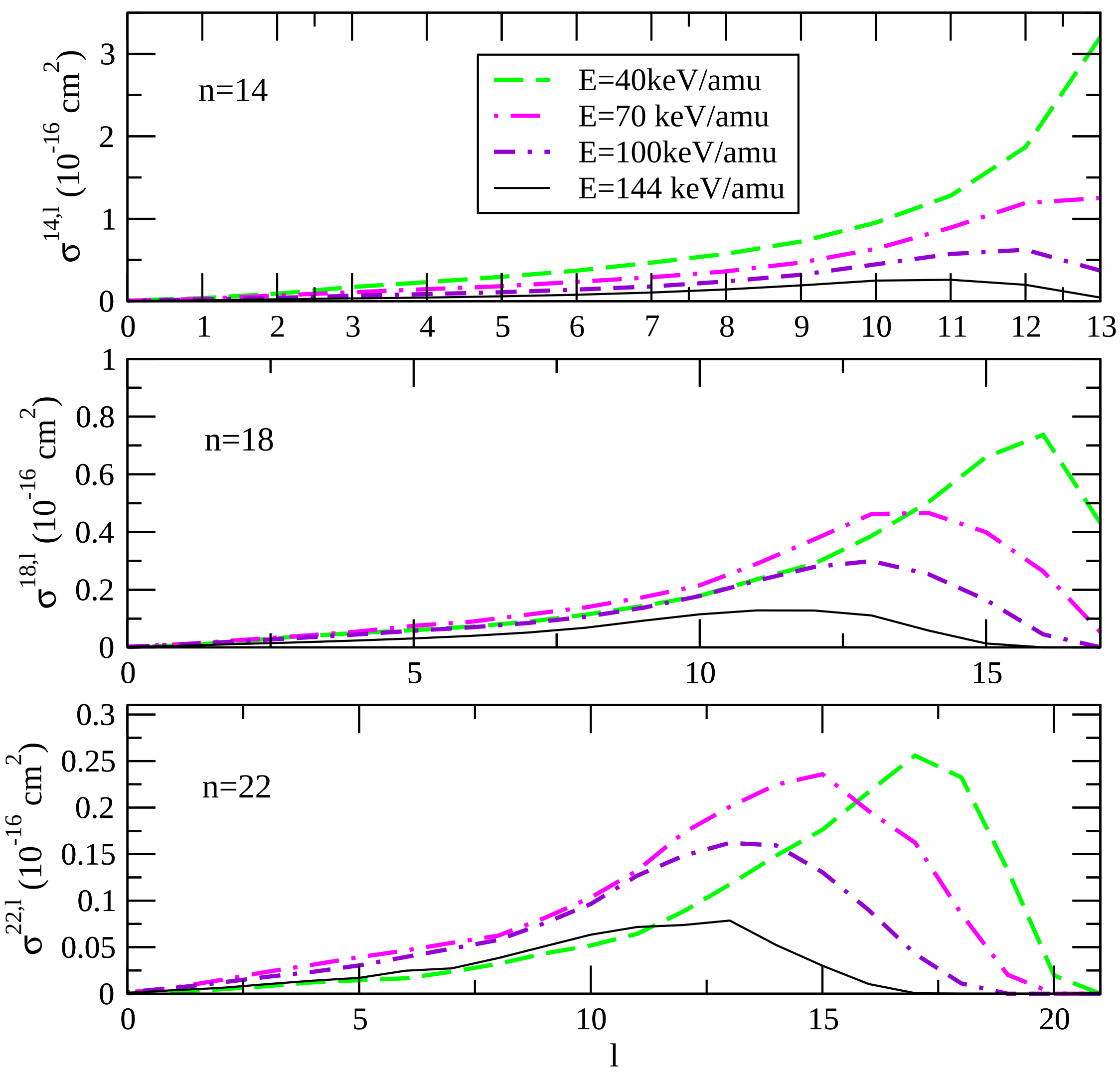
Ar^{18+} + H(1s) collisions.



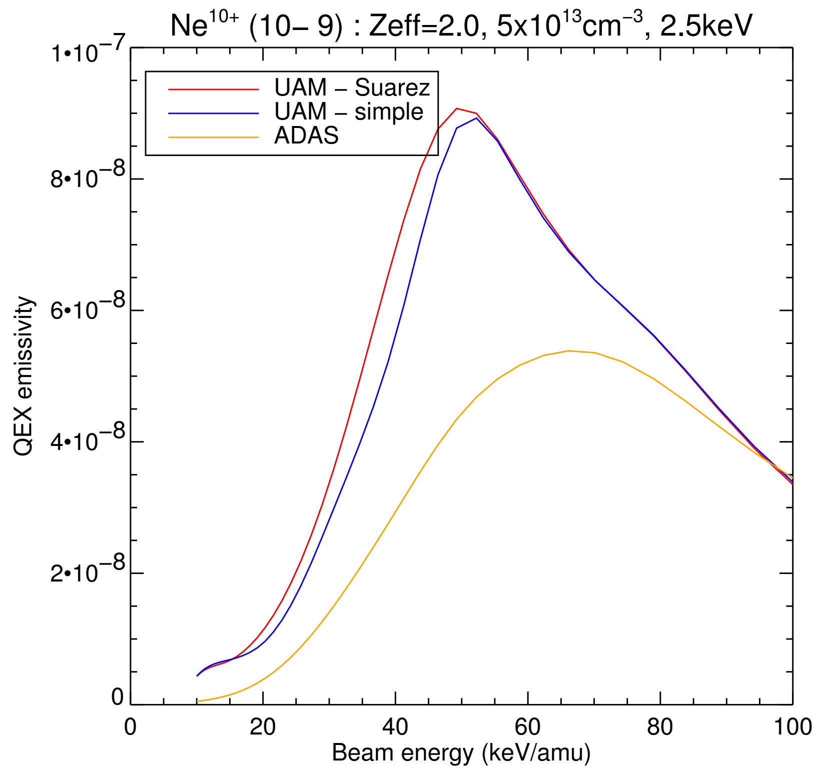
Ar^{q+} + H(1s) collisions.

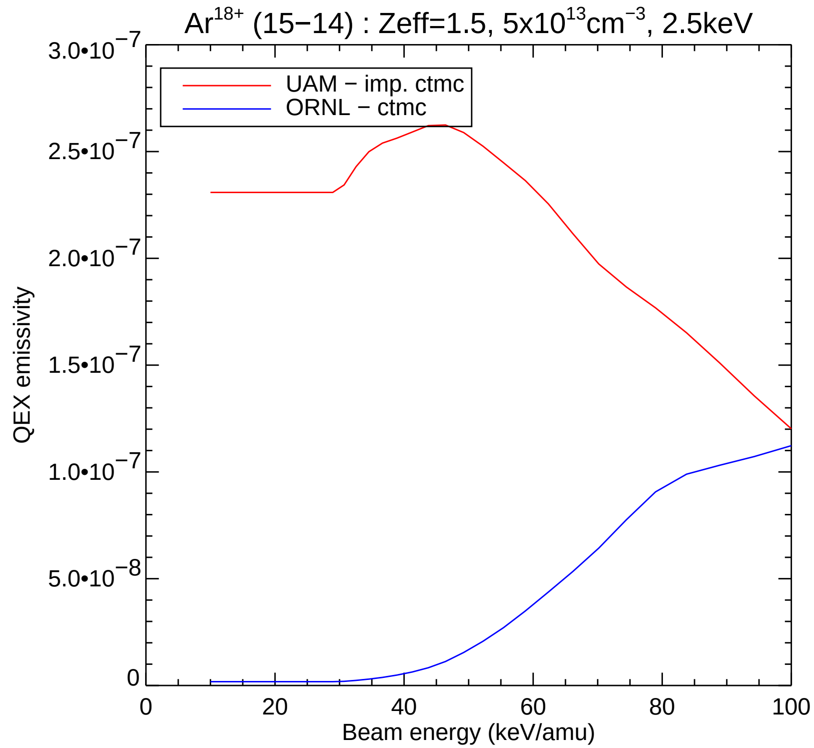


Ar^{18+} + H(1s) collisions.



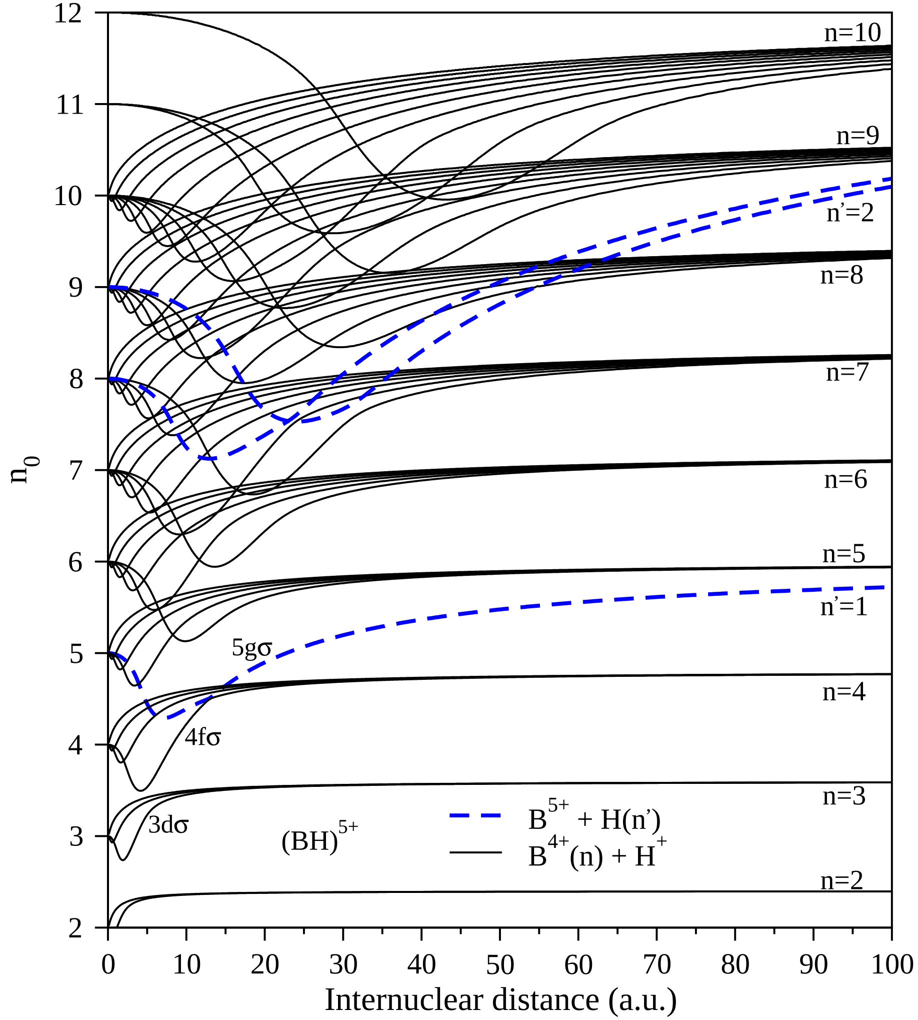
Effective emission coefficients.





O'Mullane (2006)

B^{5+} + H collisions.

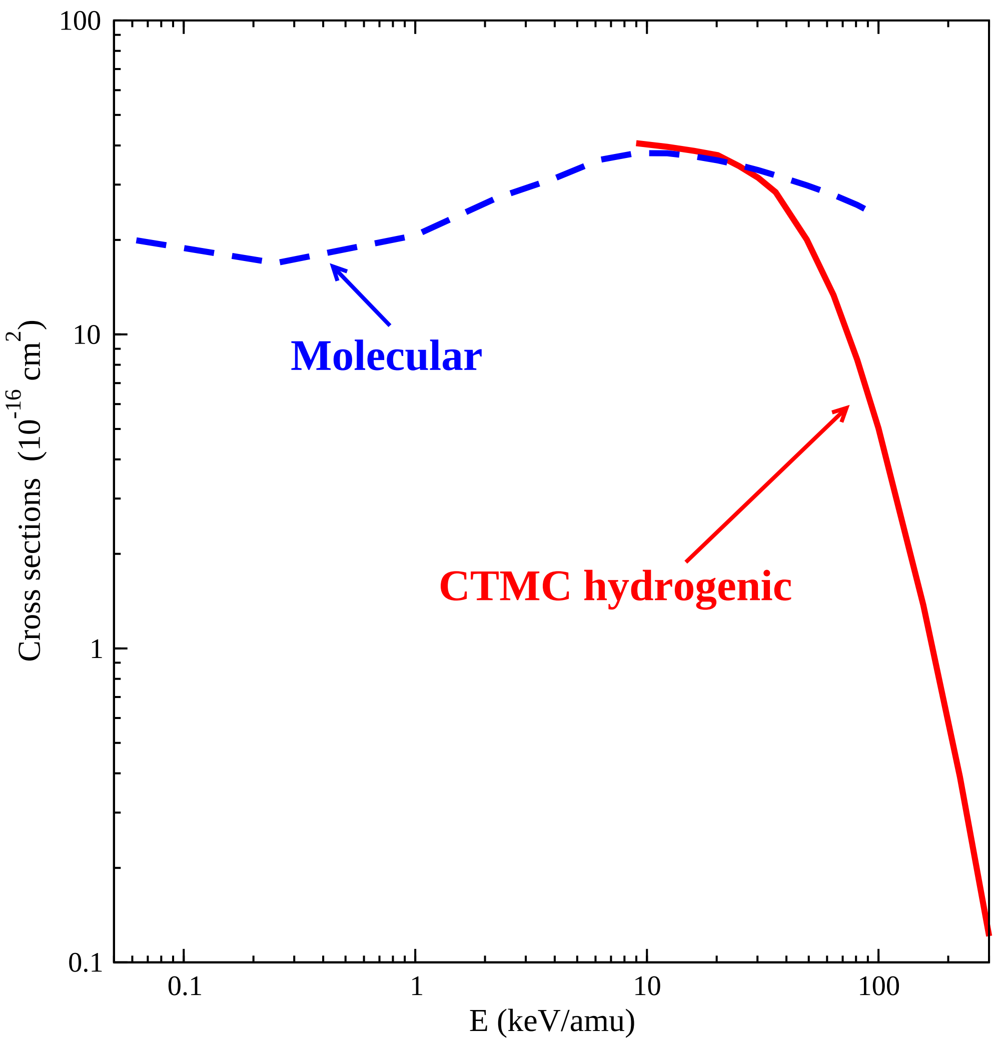


310 OEDMs.

Main exit channels:

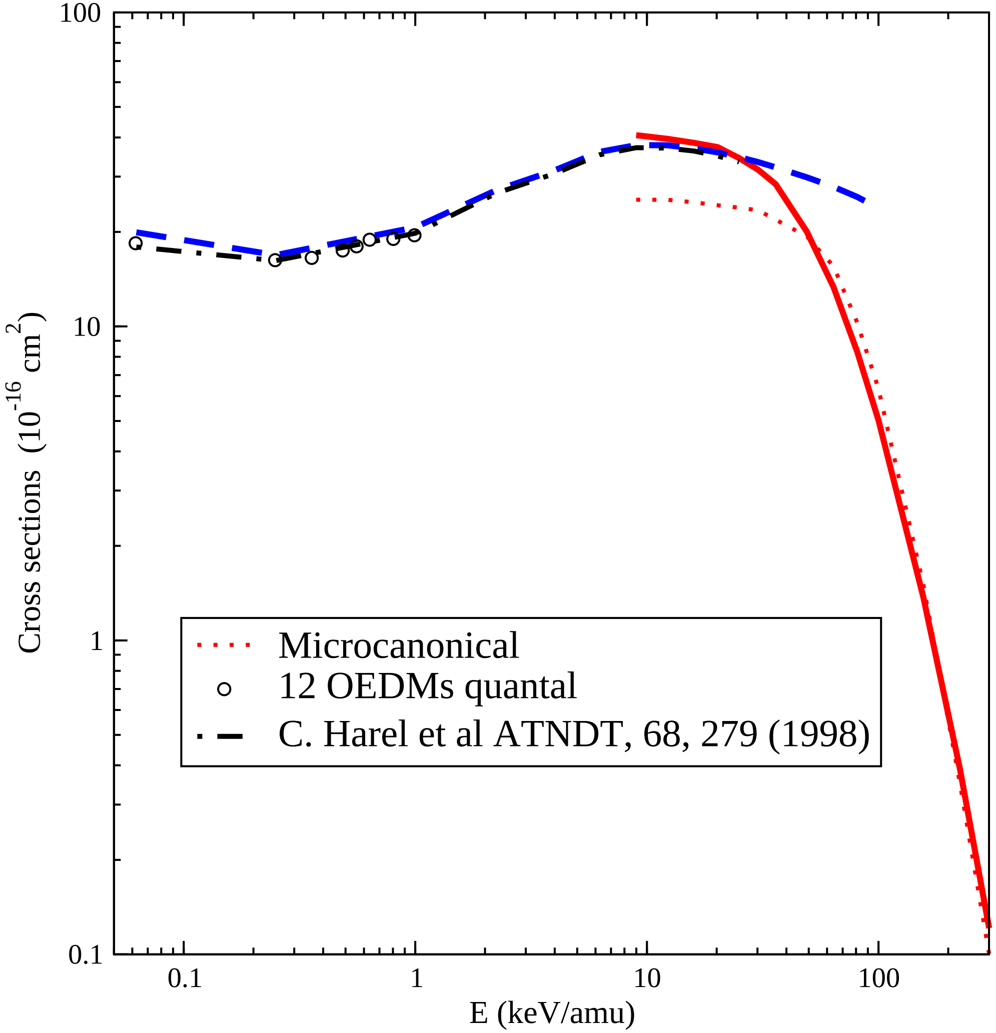
- n=4 for EC from H(1s).
- n=7 for EC from H(2s).

B^{5+} + H(1s) collisions.



Present results.

B^{5+} + H(1s) collisions.



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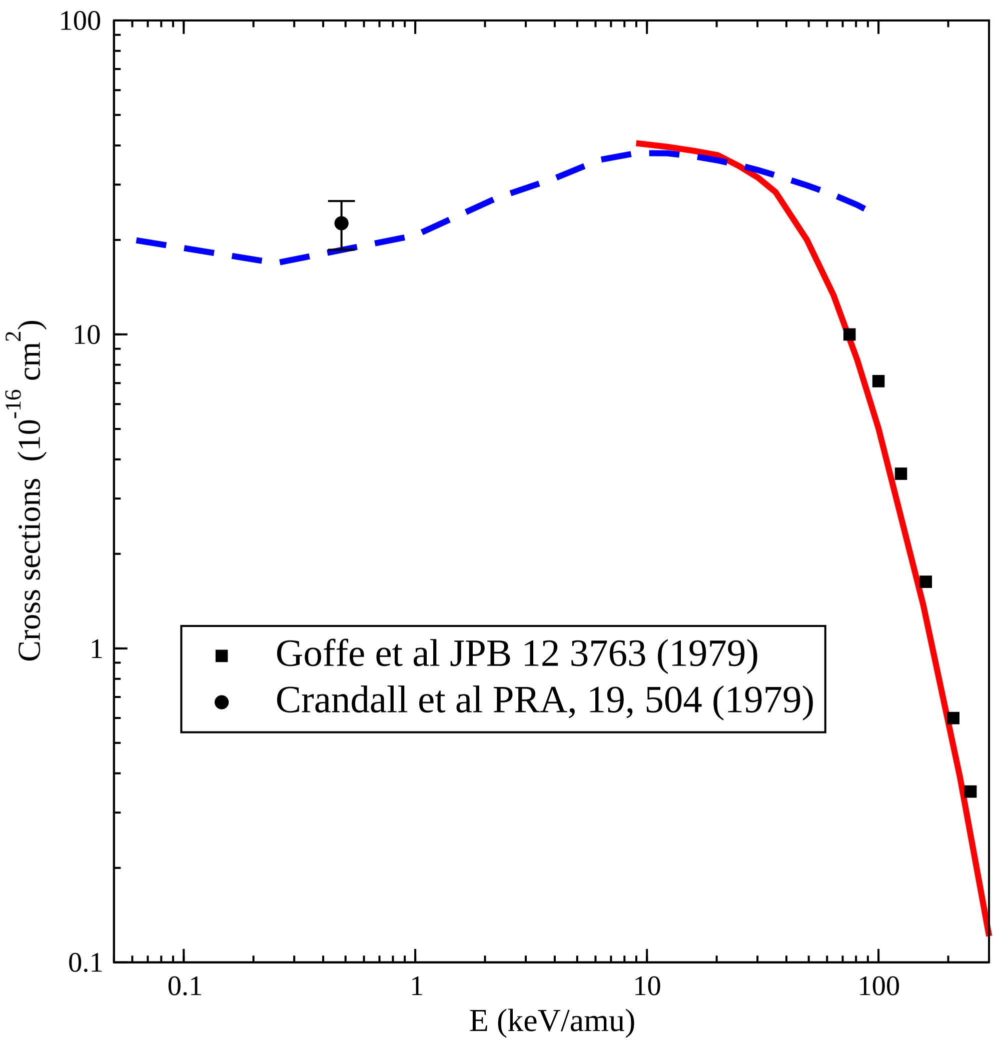
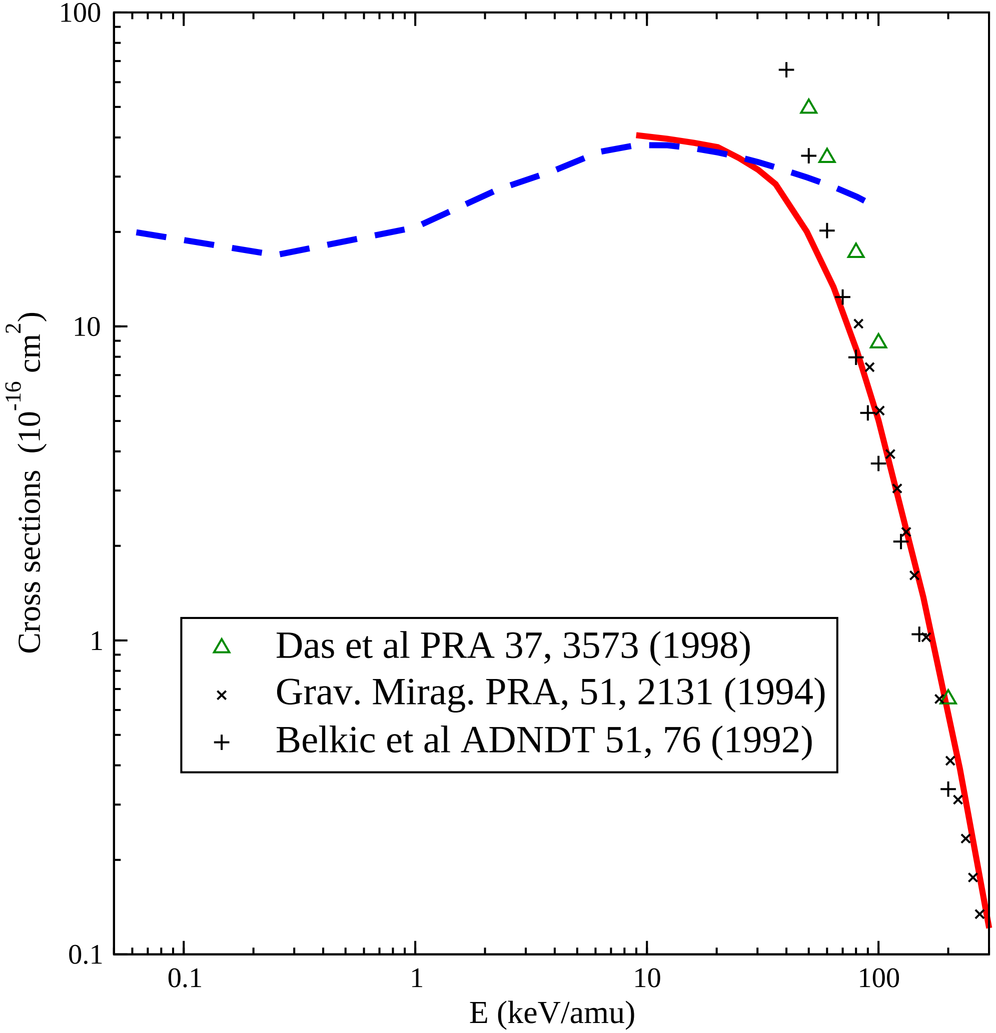


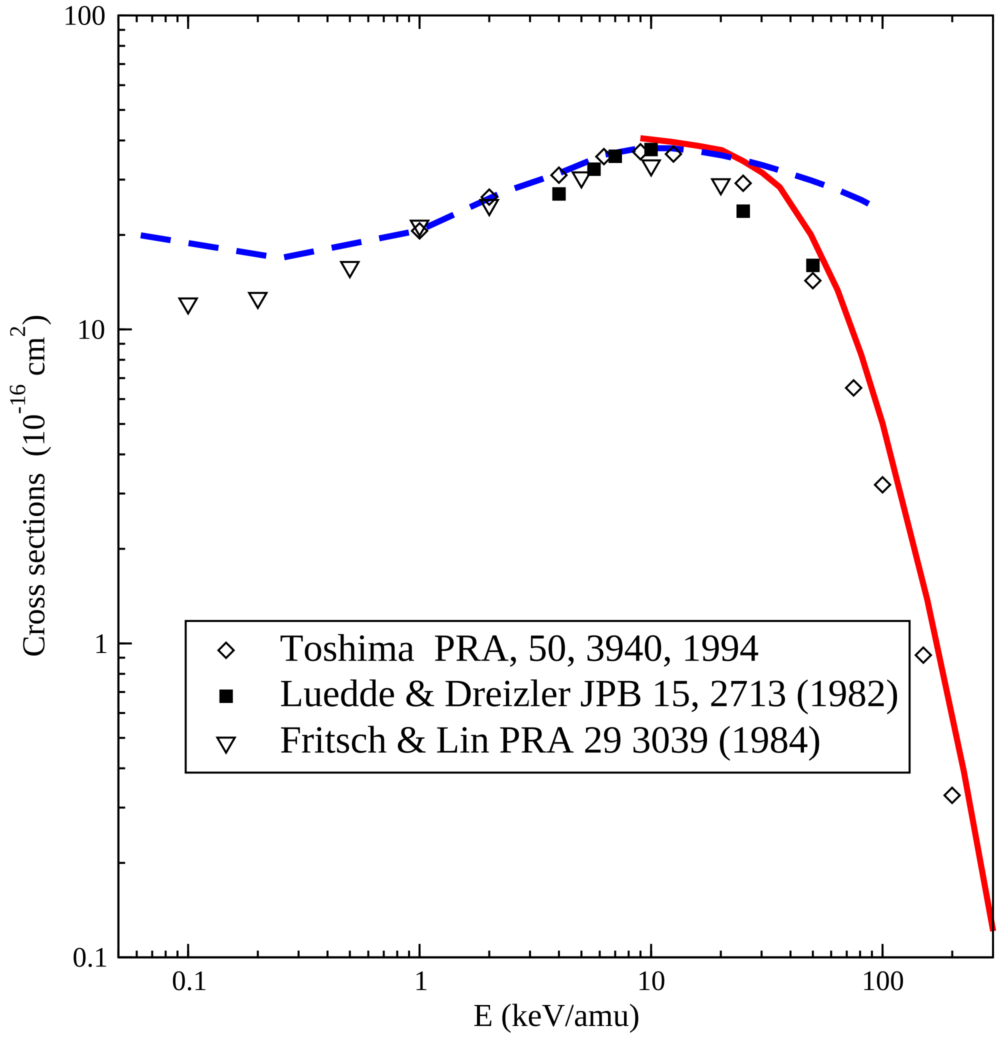
Comparison with experiments.

B^{5+} + H(1s) collisions.



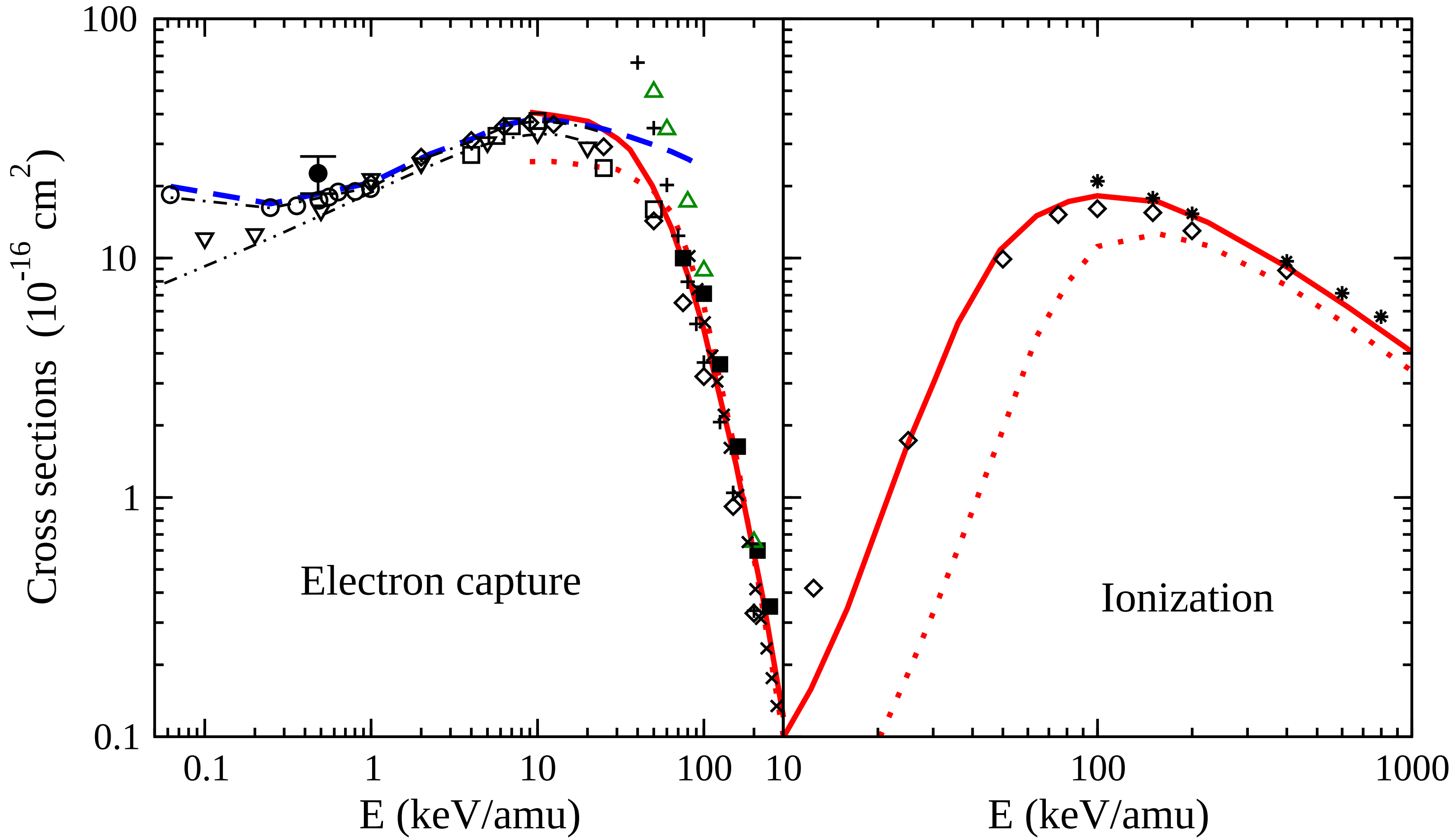
Previous calculations. High energy.

B^{5+} + H(1s) collisions.



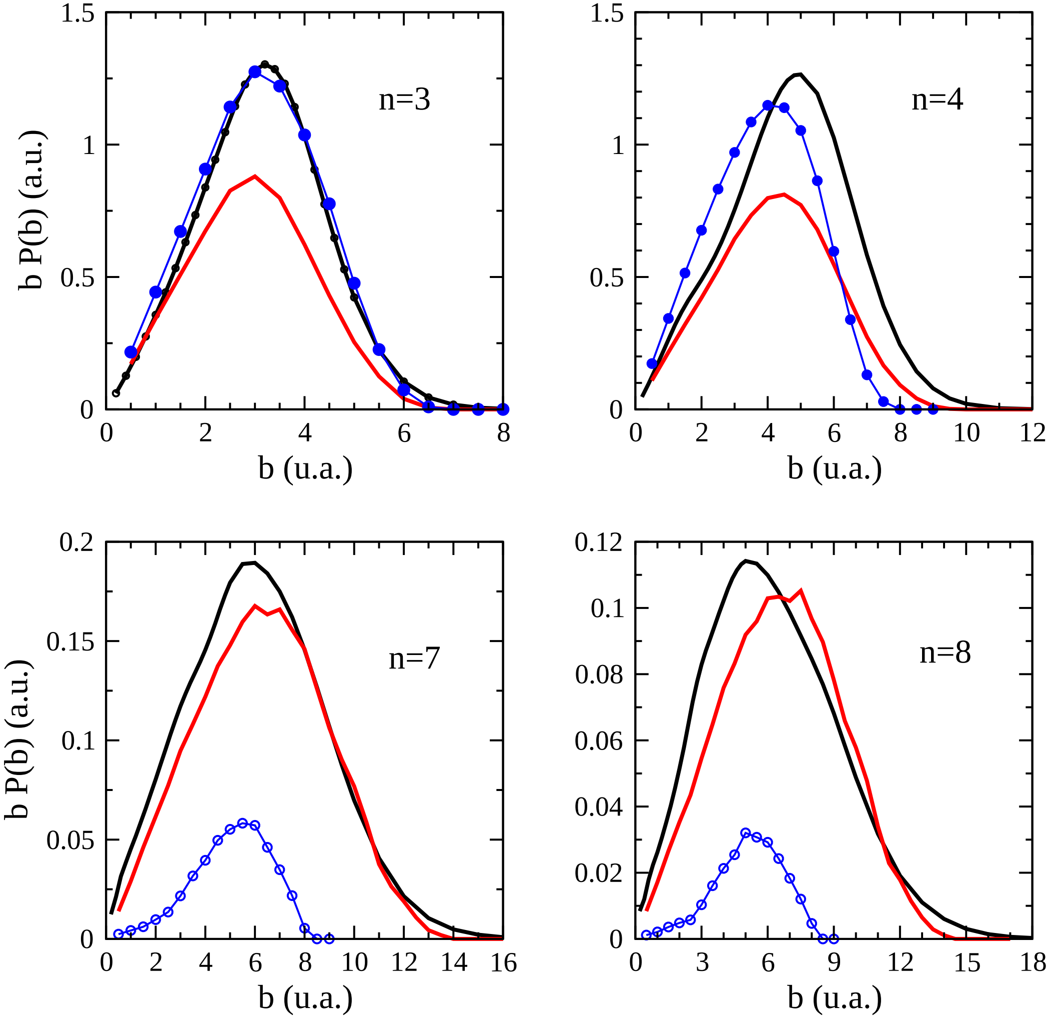
Previous calculations. Intermediate energy.

B^{5+} + H(1s) collisions.



B^{5+} + H(1s) collisions.

$v = 1.2$a.u.



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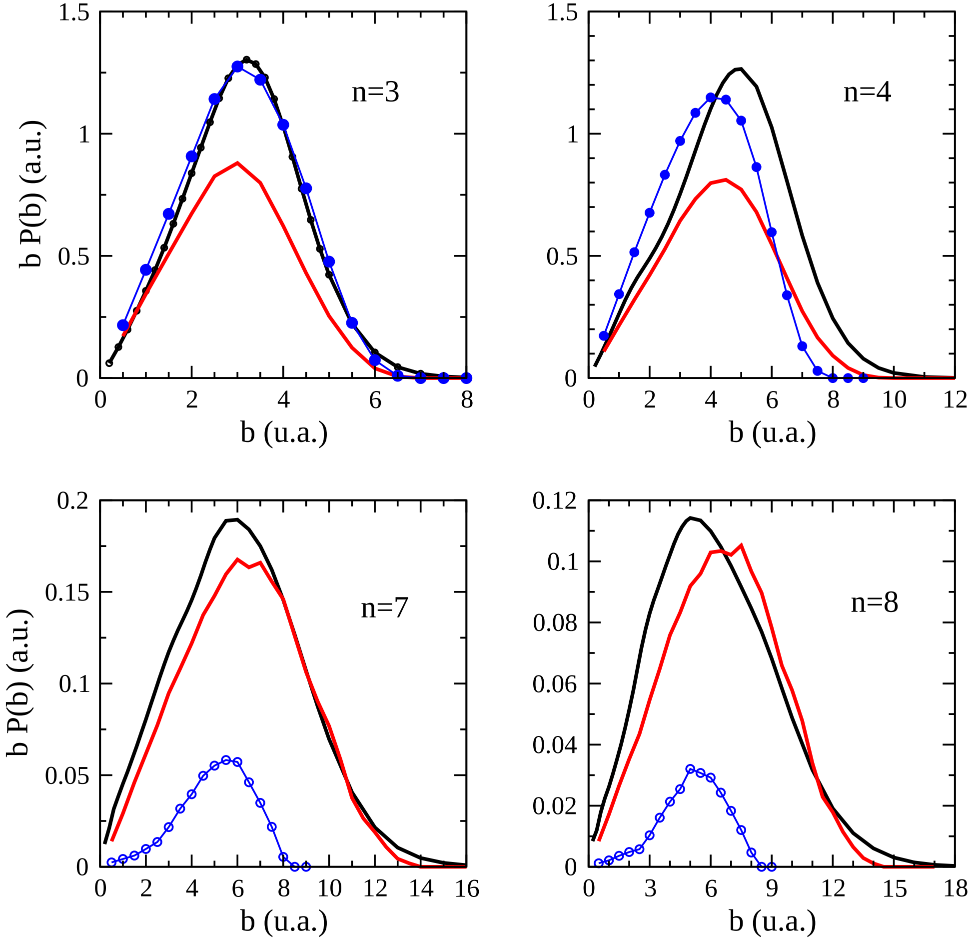
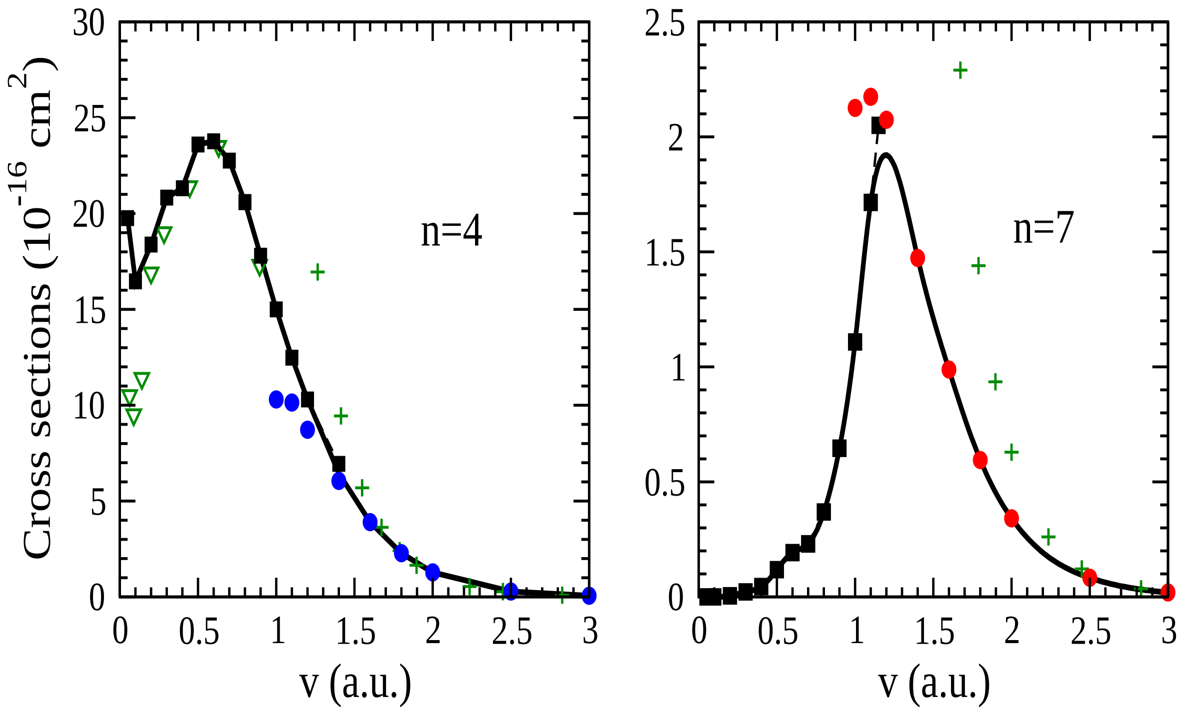


- The microcanonical distribution provides a deficient description of the outer part of the spatial density, involved in long-range inelastic transitions.
- In the hydrogenic distribution, the broadening of the initial molecular energy band enhances the transitions to n=1,2. This implies an underestimation of the probabilities for intermediate levels ($n \sim 3, 4$).

Partial cross sections



Line, recommended data.

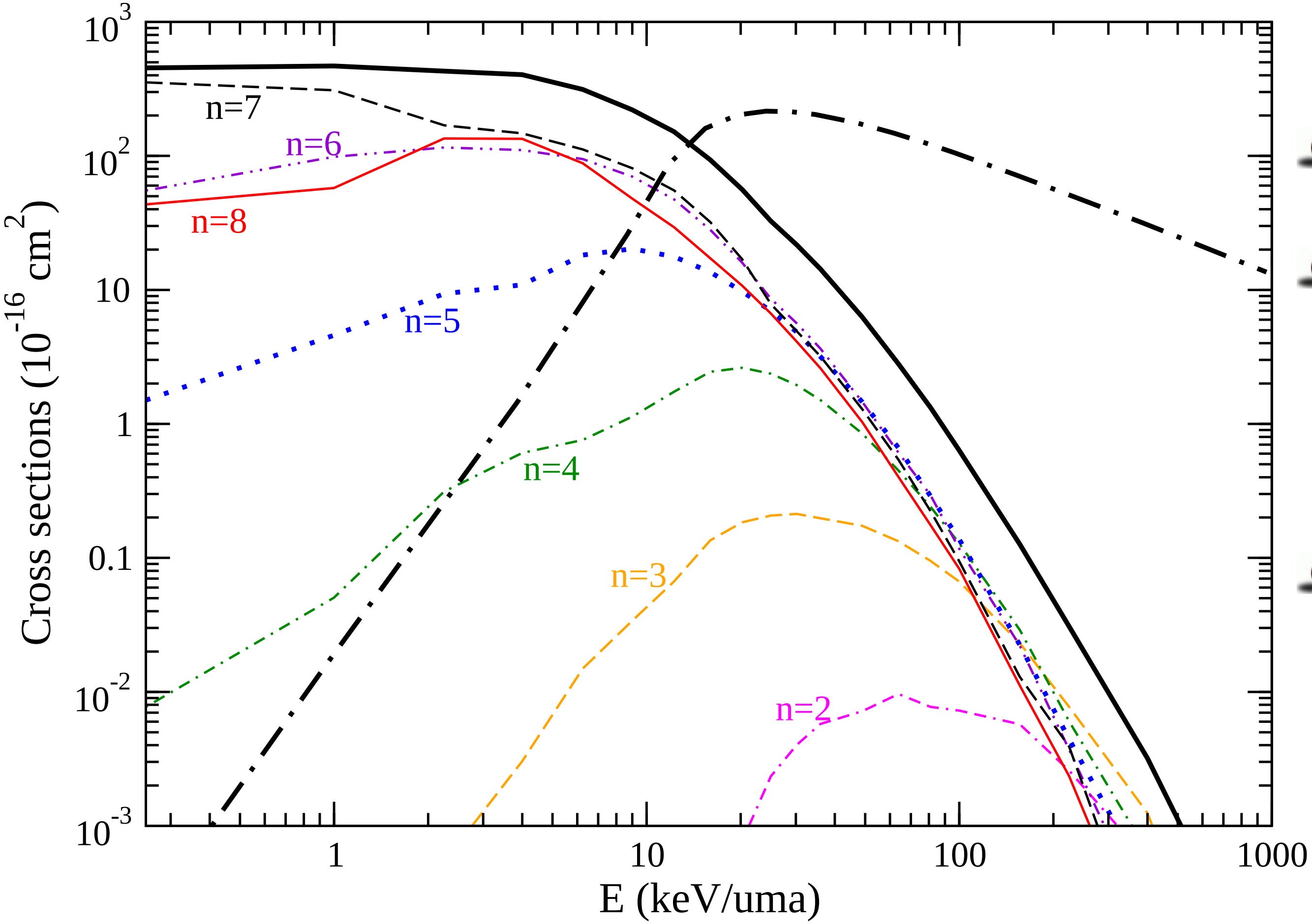
■, semiclassical calculation

●, ●, CTMC calculations

+, Belkič $et\ al$,*At. Data Nucl. Data Tables* **51** 76 (1992)

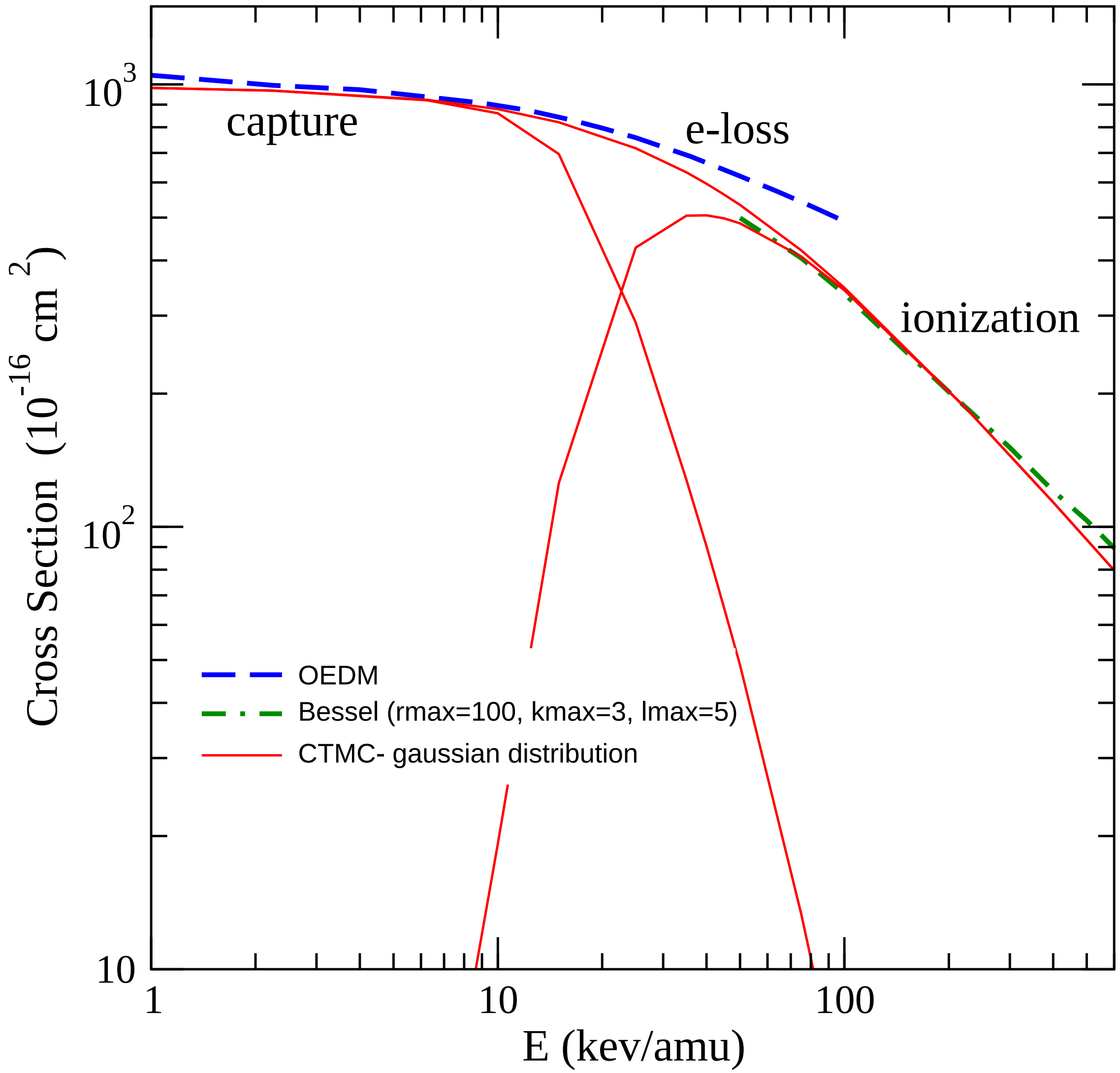
▽,Fritsch and Lin, *Phys. Rev. A* **29** 3039 (1982)

B^{5+} + H(2s) collisions.



- 223 MOs
- Gaussian initial distribution
- $0 < \bar{l}_c < 1$

Ne^{10+} + H(2s) collisions.



Summary.

- Use of complementary methods to cover a large energy range.
- Study of the overlap region:
  - Convergence of the molecular expansion.
  - Influence of the initial distribution in CTMC calculations.
- New recommended data for CX in B^{5+} + H(1s).