Calculation of electron capture cross sections in ion collisions with molecules formed in plasma-wall interaction.

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Collisions with BeH(D)

- Be has been selected as the plasma facing component of ITER main chamber because it leads to relatively low impurity concentration and low fuel retention.
- The erosion of the Be wall leads to the release of molecular species, in particular BeD.
- Chemically assisted physical sputtering via BeD significantly contributes to the effective Be sputtering yield [S. Brezinsek et al. Nucl. Fusion 55 063021 (2015)]
- We are interested in the electron capture (EC) reaction

$$H^+ + BeH(X^2\,\Sigma^+) \rightarrow H + BeH^+$$

- No experimental data.

Calculation of ion-molecule collision cross sections

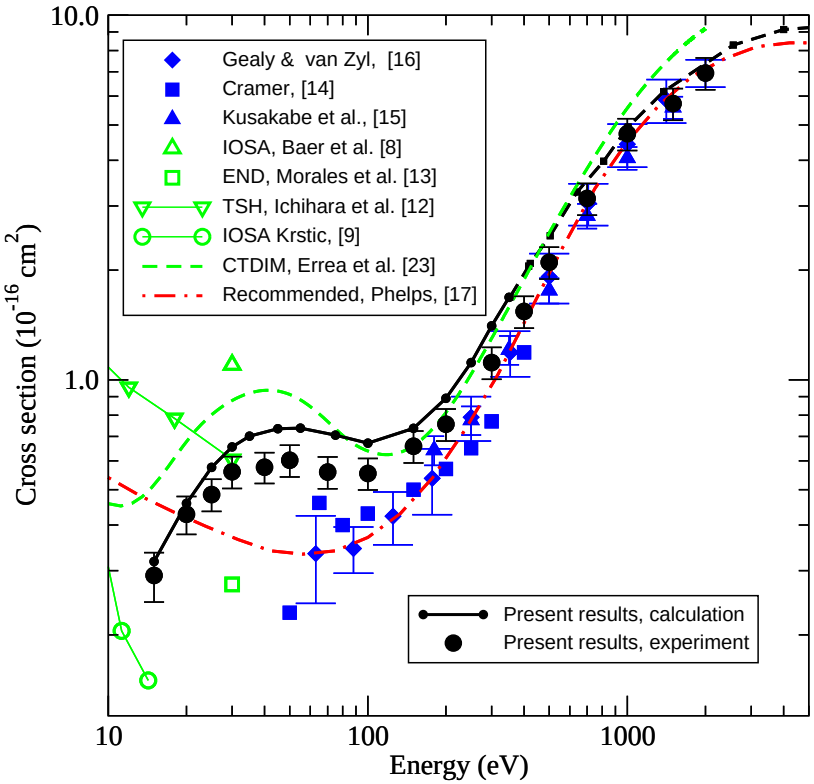
- Is not an extension of ion-atom calculations because of the need to treat the target vibro-rotational motion.
- At high collision energies, the sudden approximations can be employed.

$$\tau_{\mathrm{vib}} \approx 10^{-14}\ \mathrm{s}; \tau_{\mathrm{rot}} \approx 10^{-12}\ \mathrm{s}$$

At $E = 250$ eV/u, $t_{\mathrm{col}} \approx 10^{-16}$ s

- Franck-Condon approximation: The equilibrium geometry is kept frozen during the collision.

Previous calculations on $H^+ + H_2$ collisions.



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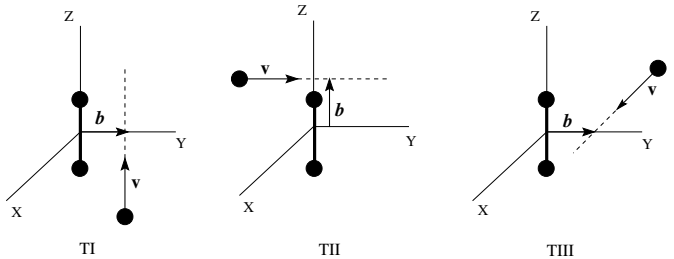
- Sudden vibrational mechanism at high energies.
- Resonant transitions at low energies:

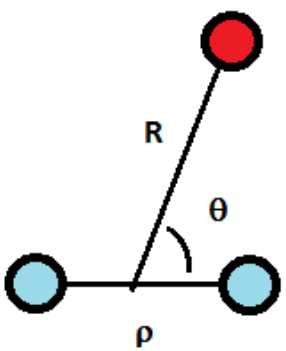
$$H^+ + H_2(\nu = 4) \rightarrow H_2^+(\nu = 0) + H(1s)$$

Previous calculations on $H^+ + H_2$ collisions. Orientation average

Trajectory average



θ-average



Int. J. Mol. Sci. **2002**, *3* 152

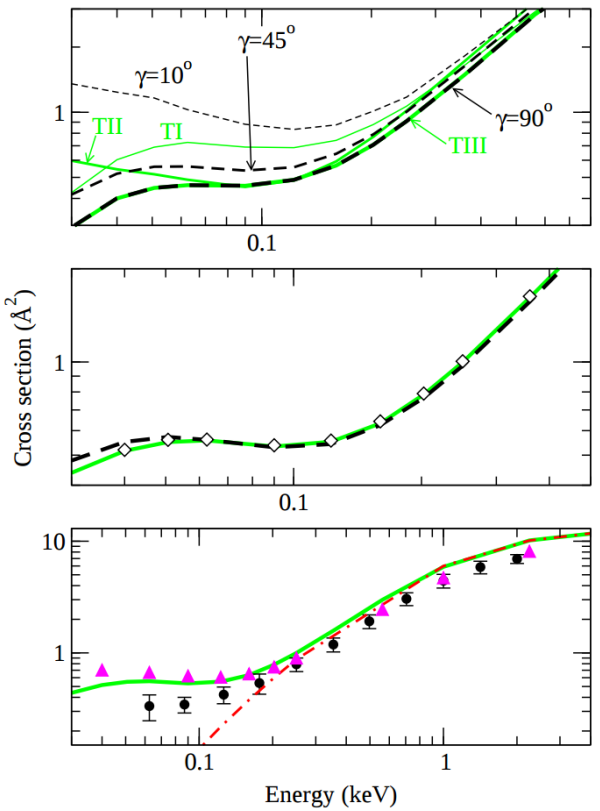
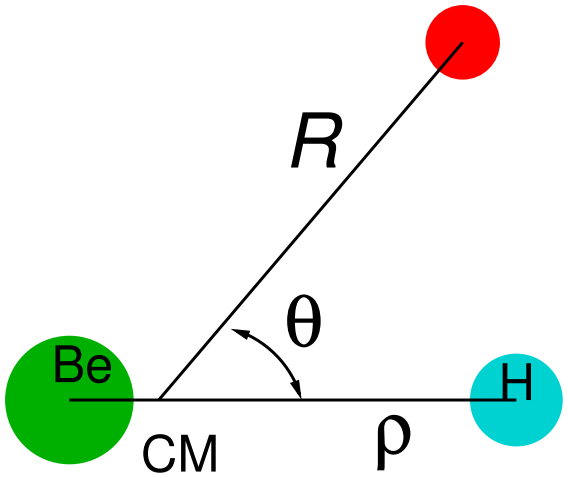


Figure 3: Charge transfer cross sections calculated using different approximations. Top panel: comparison between cross sections obtained for three characteristic trajectories (grey lines, $\sigma_{\mathrm{I}}^{\mathrm{ct}}$, $\sigma_{\mathrm{II}}^{\mathrm{ct}}$ and $\sigma_{\mathrm{III}}^{\mathrm{ct}}$) with those obtained with the isotropic approximation at three angles (dashed lines,

Basic equations



- Non-relativistic Hamiltonian

$$H = T_R + H_{\text{int}}$$

$$H_{\text{int}}(\boldsymbol{r}, \boldsymbol{R}, \boldsymbol{\rho}) = T_\rho + H_{\text{el}}(\boldsymbol{r}, \boldsymbol{R}, \boldsymbol{\rho})$$

Eikonal approximation

- Classical nuclear motion $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}\,t$
- Semiclassical equation for the electronic motion

$$H_{\text{int}}\,\Psi^{\text{EIK}} - \mathrm{i}\,\left.\frac{\partial \Psi^{\text{EIK}}}{\partial t}\right|_{\boldsymbol{r},\boldsymbol{\rho}} = 0$$

Sudden approximation

Sudden-vibrational (SV) approximation

The vibro-rotational motion is slow compared to the relative motion

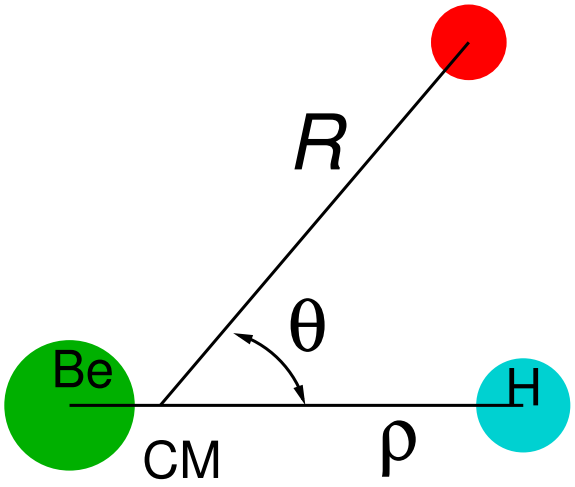
$$\Psi_{0jm}^{\mathrm{SV}} = \rho^{-1} Y_{jm}(\hat{\boldsymbol{\rho}}) \chi_0(\rho) D(\boldsymbol{r}, t) \sum_k a_k(t; b, v, \boldsymbol{\rho}) \times \phi_k(\boldsymbol{r}; R, \rho, \theta) \exp\left[-\mathrm{i} \int_0^t \epsilon_k \mathrm{d}t'\right]$$

where $\phi_k(\boldsymbol{r}; R, \rho, \theta)$ are three-center electronic functions, eigenfunctions of the clamped-nuclei electronic Hamiltonian H_{el}.

Substitution into the semiclassical equation leads to a set of differential equations for the coefficients a_k. The transition probabilities are then obtained from:

$$P_{i0jm}^{f\nu j'm'}(b, v) = \lim_{t\to\infty} \left| \langle \Psi_{f\nu j'm'} | \Psi_{0jm}^{\mathrm{SV}} \rangle \right|^2$$

Orientation average

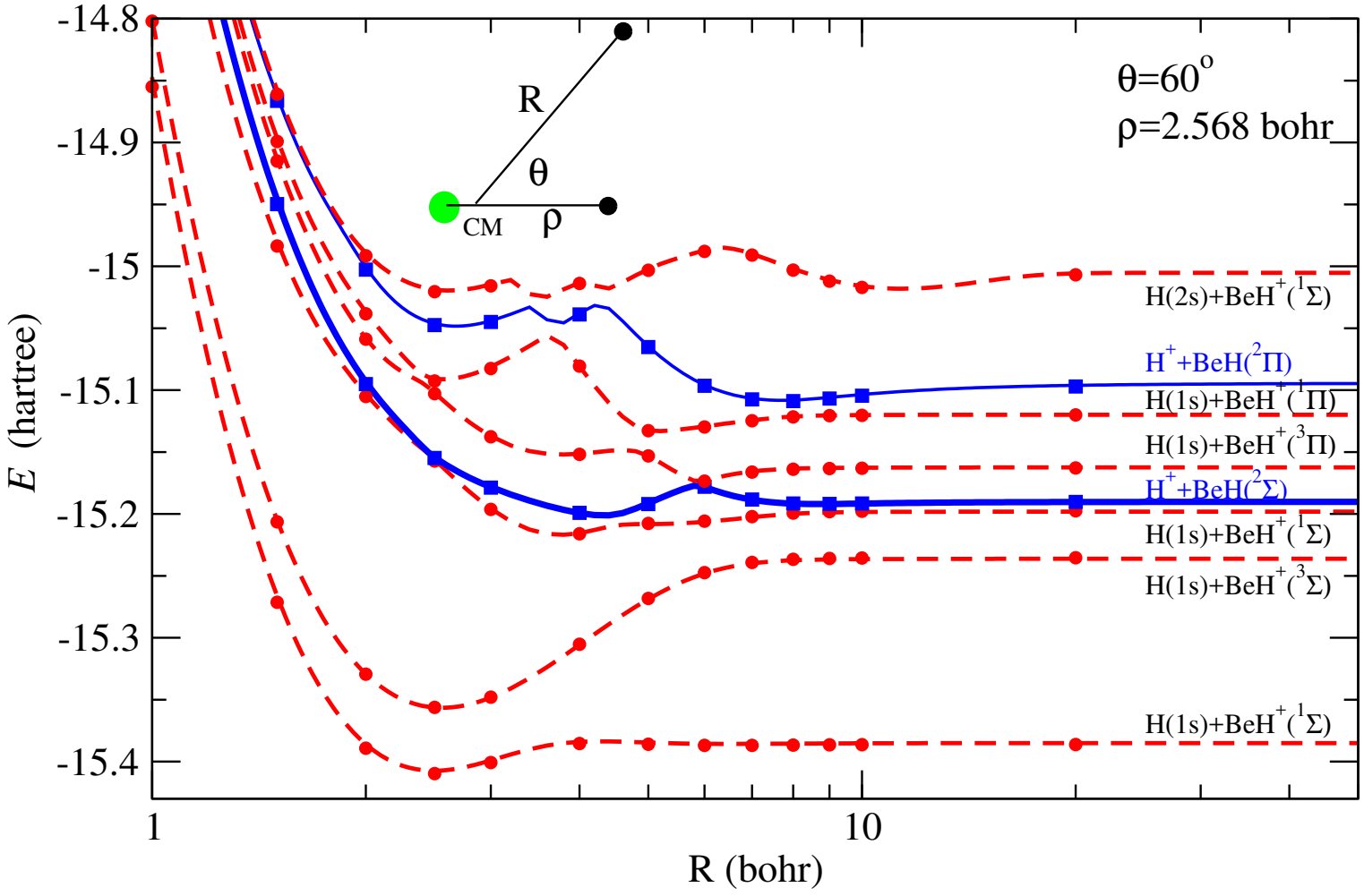


Isotropic approximation: Calculations for collision with fixed values of θ.

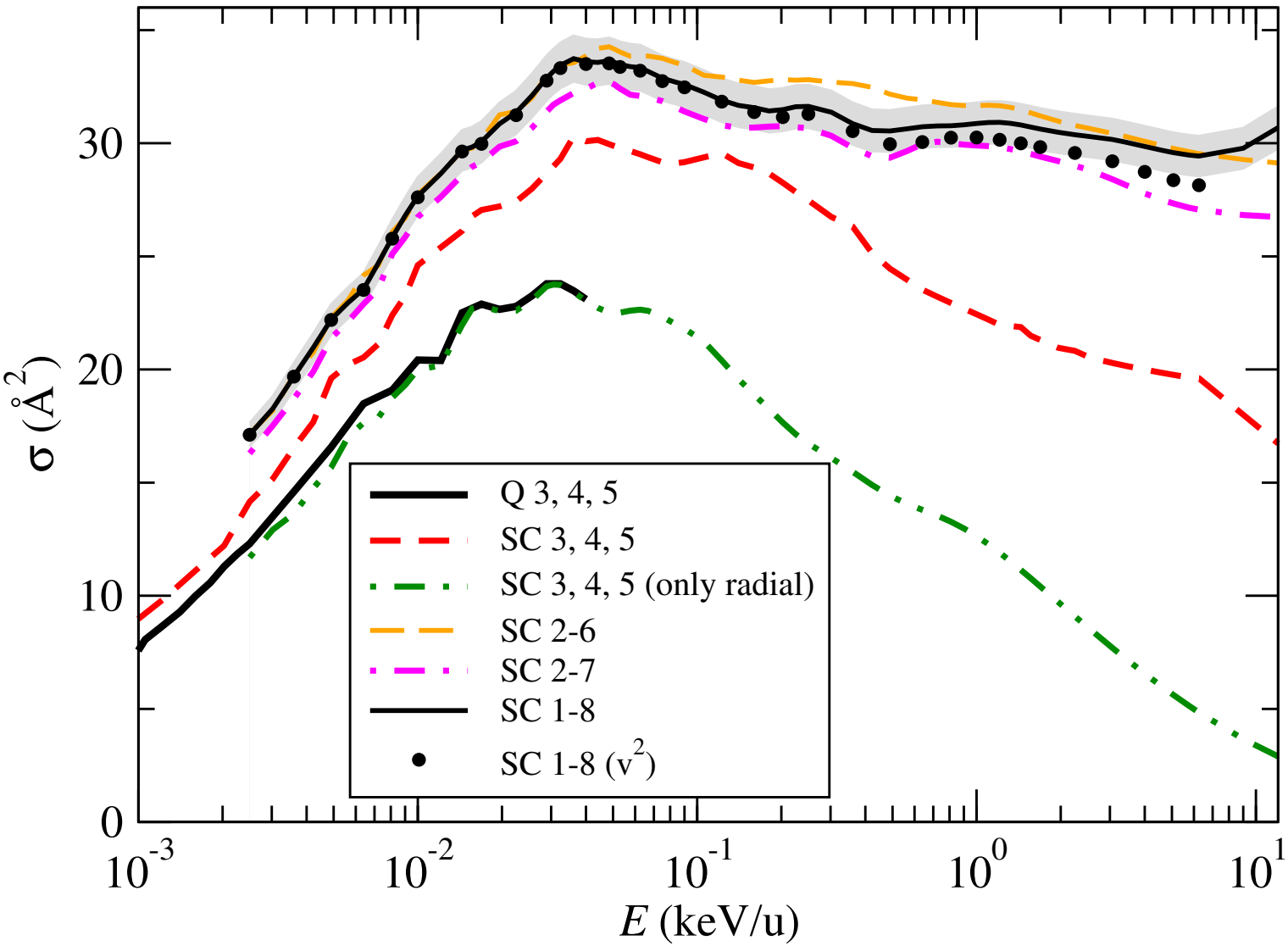
$$\overline{\sigma}_f^{\mathrm{SV}}(E) \approx \overline{\sigma}_f^{\mathrm{iso}}(E) = \frac{1}{2}\int_{-1}^{1} \mathrm{d}(\cos\theta)\sigma_f^{\mathrm{iso}}(E,\theta)$$

$$= \pi \int_{-1}^{1} \mathrm{d}(\cos\theta) \int_0^{\infty} \mathrm{d}\rho\chi_0^2(\rho) \int_0^{\infty} \mathrm{d}b\, b\, P_f^{\mathrm{iso}}(b,E,\rho,\theta)$$

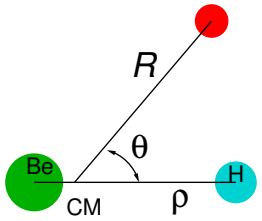
Electronic energies

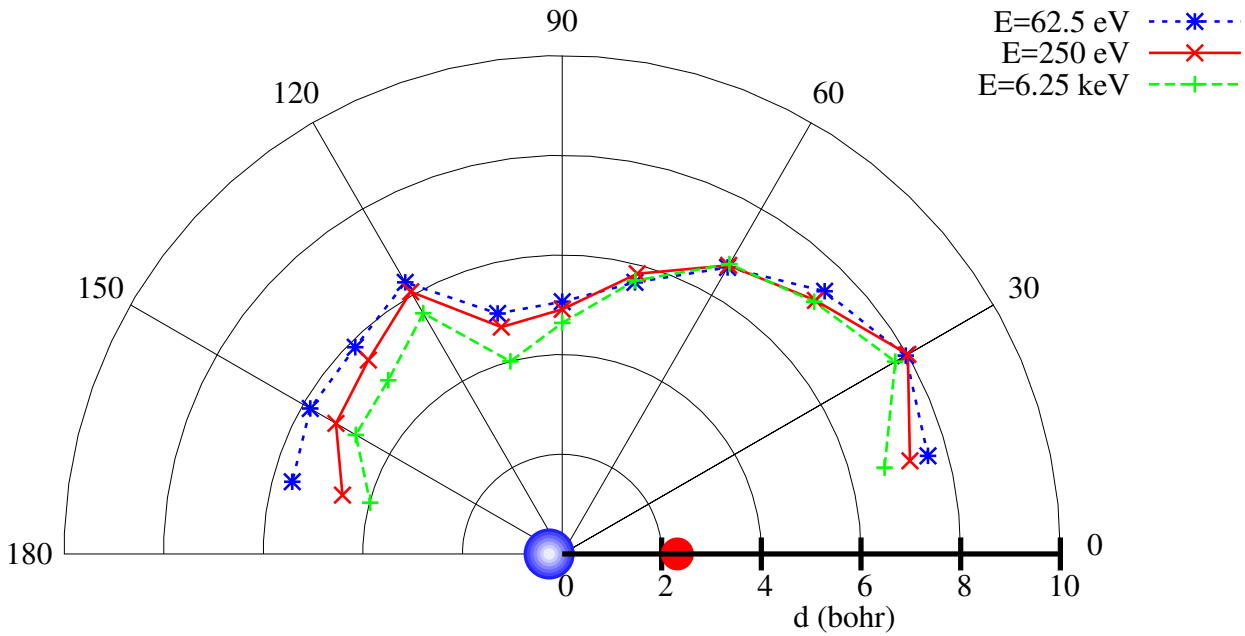


Total cross section, FC, orientation averaged



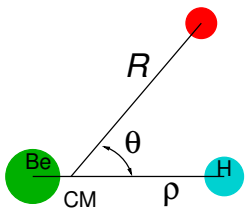
Total cross section, FC, orientation dependent

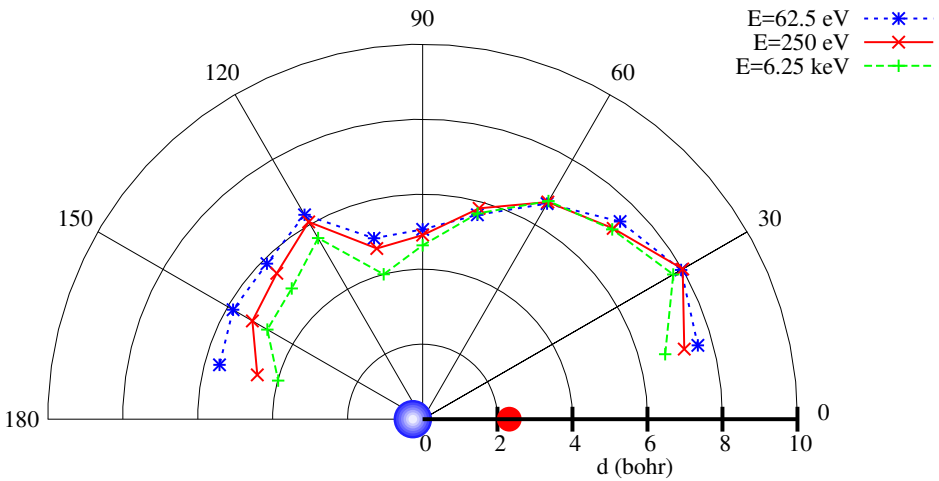


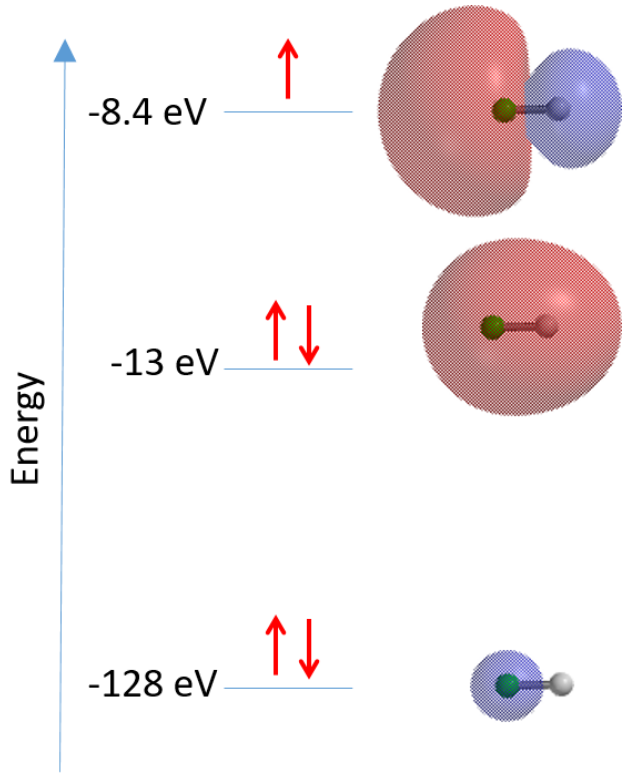


$$d = \sqrt{\frac{1}{\pi} \sum_f \sigma_f^{\mathrm{iso}}(E, \rho_e, \theta)}$$

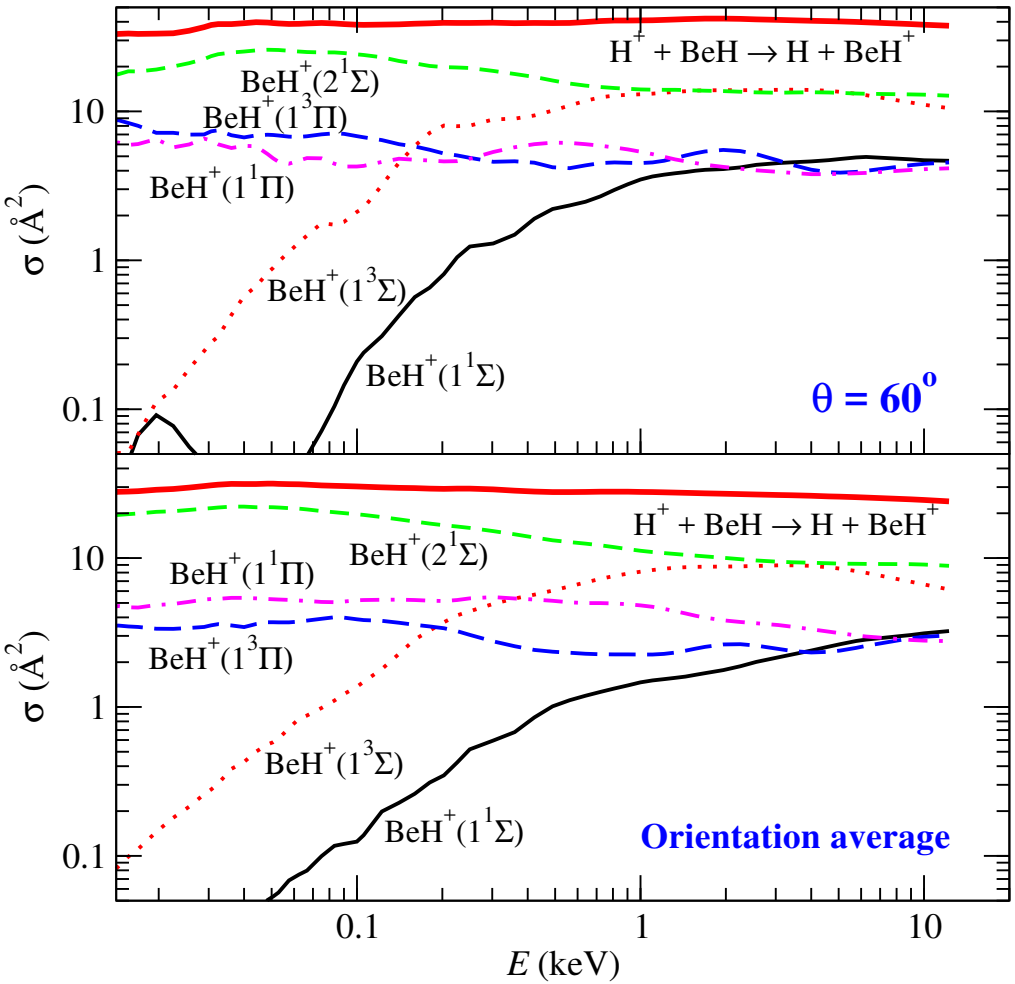
Total cross section, FC, orientation dependent







State-selected cross sections



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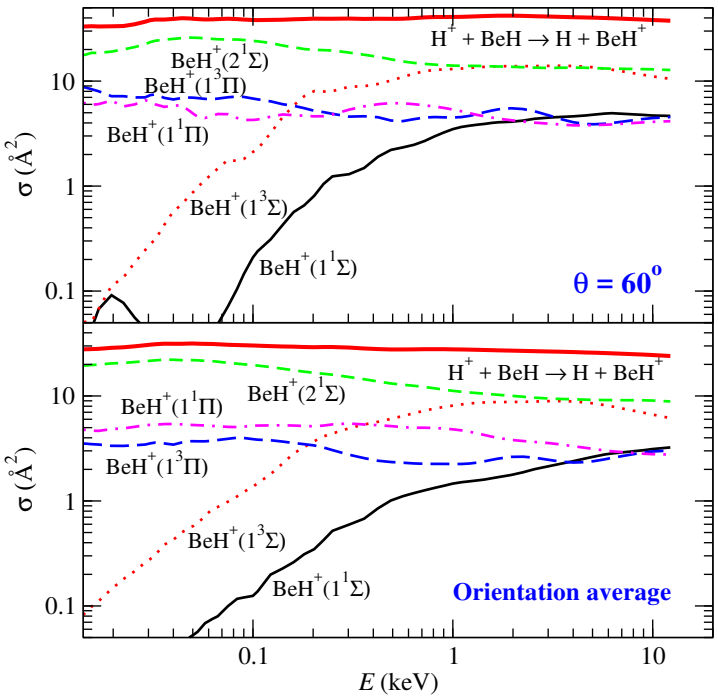
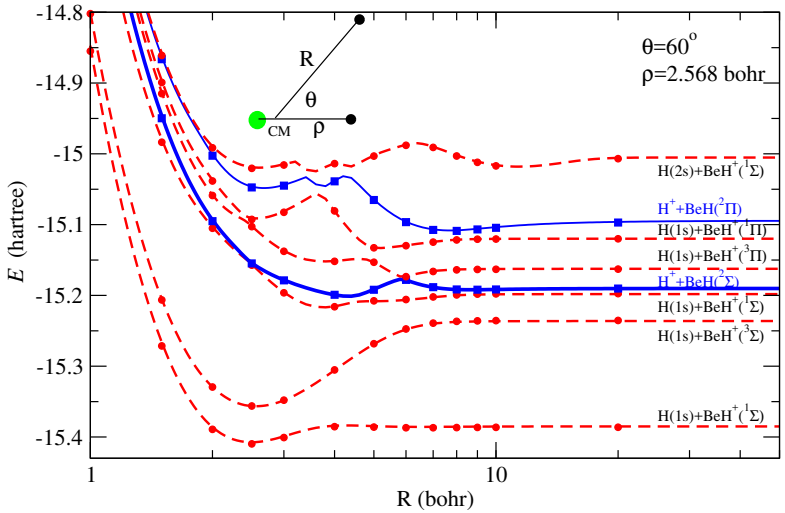
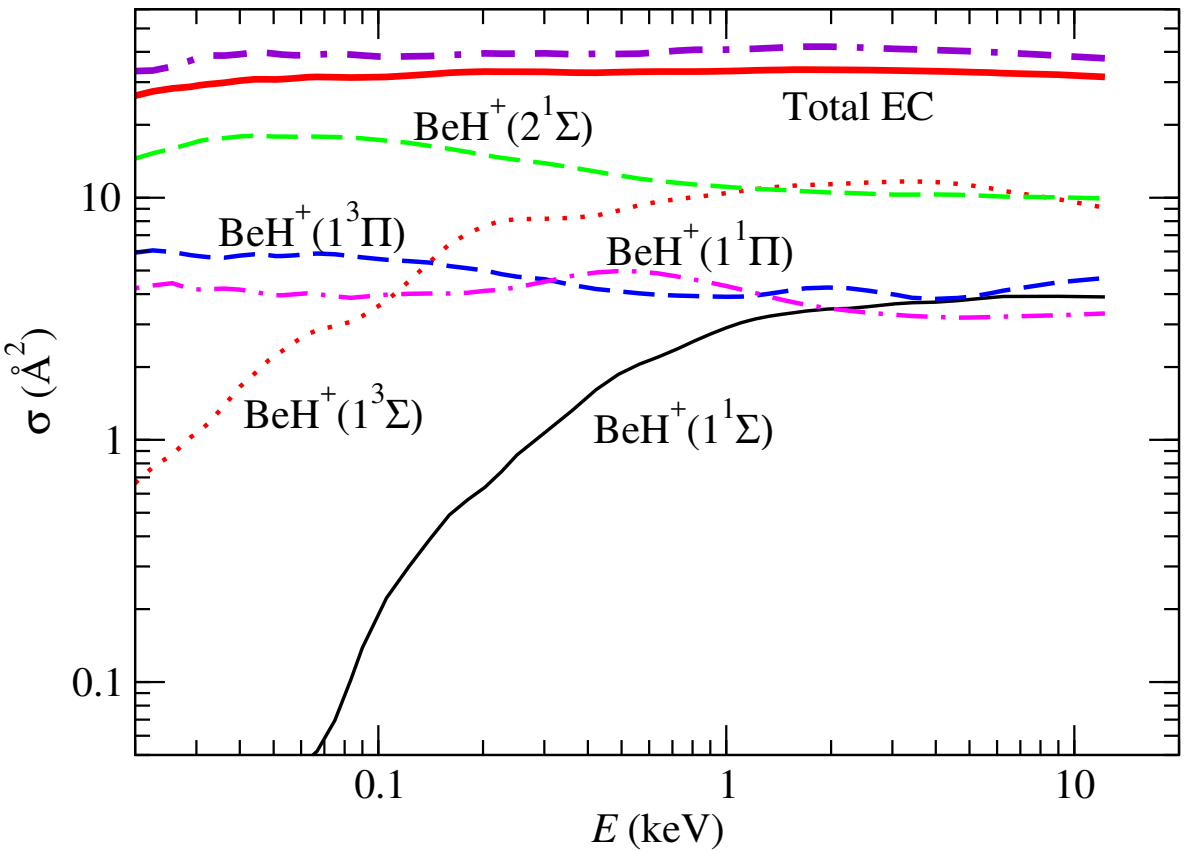
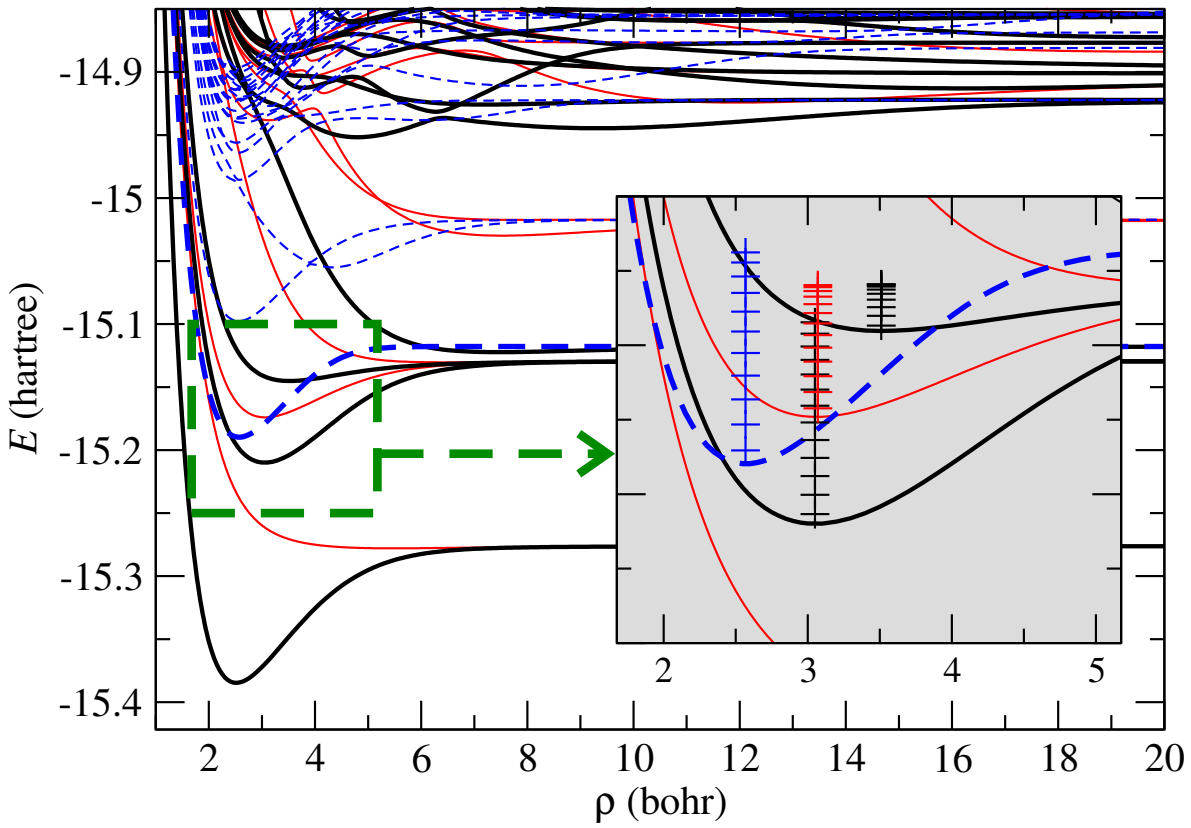




Sudden vibrational approximation



Extension to low energies. Vibronic transitions



Summary

- Total and partial EC cross sections calculated for 25eV $< E <$ 1keV.
- Sizeable values of the EC cross section.
- Significant anisotropy and importance of Coriolis couplings.
- Extensions:
  - Improved trajectory-orientation average.
  - Low energy collisions. Vibronic resonant transitions.

Coworkers

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