Low energy charge exchange of Hydrogen with partially stripped ions.

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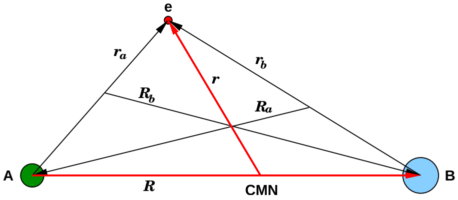
Electron capture

$$X^{q+} + H(1s) \rightarrow X^{(q-1)+} + H^{+}$$

Impact energies $E < 25$ keV/amu

Quantal treatment



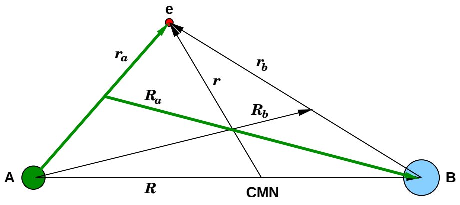
$$\mu = \frac{M_A\, M_B}{M_A + M_B}$$

$$\mu_e = \frac{m_e(M_A + M_B)}{m_e + M_A + M_B}$$

The collision wavefunction is solution of the stationary Schrdinger equation:

$$H\Psi = E\Psi$$

where $H = -\frac{1}{2\mu}\nabla_R^2 - \frac{1}{2\mu_e}\nabla_r^2 + V_{\mathrm{int}}(\mathbf{r}, R) = -\frac{1}{2\mu}\nabla_R^2 + H_{\mathrm{elec}}$



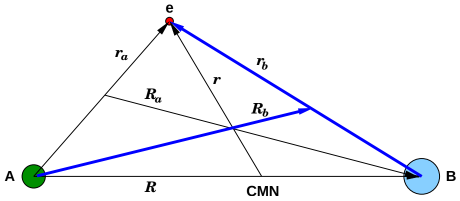
Boundary conditions:

- Elastic and excitation:

$$\Psi \rightarrow \Phi_i^A(\mathbf{r}_a)\mathrm{e}^{\mathrm{i}\mathbf{k}_i\mathbf{R}_a} + \sum_f \Phi_f^A(\mathbf{r}_a) f_{if}(\hat{R}_a)\frac{\mathrm{e}^{\mathrm{i}k_f R_a}}{R_a}$$

- Electron capture:

$$\Psi \rightarrow \sum_f \Phi_f^B(\mathbf{r_b}) f'_{if}(\hat{R}_b)\frac{\mathrm{e}^{\mathrm{i}k'_f R_b}}{R_b}$$



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- Electron capture:

$$\Psi \rightarrow \sum_f \Phi_f^B(\mathbf{r_b}) f'_{if}(\hat{R}_b)\frac{\mathrm{e}^{\mathrm{i}k'_f R_b}}{R_b}$$

Common reaction coordinate.

Thorson y Delos (1978)

$$k_i \left(\frac{\mu}{\mu_a}\right)^{1/2} \xi \sim k_i \, \mathbf{R}_a \text{ (electron bound to nucleus A)}$$

$$k_f \left(\frac{\mu}{\mu_b}\right)^{1/2} \xi \sim k_f \mathbf{R}_b \text{ (electron bound to nucleus B)}$$

Up to $\mathcal{O}(\mu^{-1})$:

$$\xi = \mathbf{R} + \frac{1}{\mu}\mathbf{s}(\mathbf{r},\mathbf{R}) = \mathbf{R} + \frac{1}{\mu}\left[f(\mathbf{r},\mathbf{R})\mathbf{r} - \frac{1}{2}f^2(\mathbf{r},\mathbf{R})\mathbf{R}\right]$$

where f is a switching function

Molecular expansion.

$$\Psi^J(\mathbf{r}, \xi) = \sum_k \chi_k^J(\xi)\phi_k(\mathbf{r}, R = \xi)$$

$\{\phi_k\}$ are eigenfunctions of the clamped-nuclei Born-Oppenheimer electronic Hamiltonian:

$$H_{\mathrm{elec}}(\mathbf{r}, R)\phi_k(\mathbf{r}, R) = \epsilon_k(R)\phi_k(\mathbf{r}, R)$$

Molecular expansion.

$$\Psi^J(\mathbf{r},\boldsymbol{\xi}) = \sum_k \chi_k^J(\boldsymbol{\xi})\phi_k(\mathbf{r}, R = \boldsymbol{\xi})$$

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electronic Hamiltonian:

$$H_{\rm elec}(\mathbf{r}, R)\phi_k(\mathbf{r}, R) = \epsilon_k(R)\phi_k(\mathbf{r}, R)$$

Molecular energies and wavefunctions are required

Molecular expansion.

$$\Psi^J(\mathbf{r}, \boldsymbol{\xi}) = \sum_k \chi_k^J(\boldsymbol{\xi})\phi_k(\mathbf{r}, \xi)$$

Substitution of this expansion into the Schrdinger leads to a set of second order differential equations whose solutions are the nuclear wavefunctions $\chi_k^J(\boldsymbol{\xi})$

Cross sections.

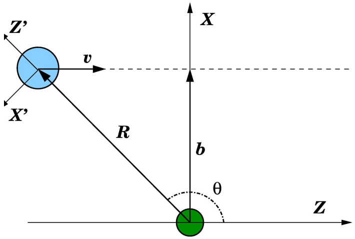
1. Numerical solution of the system of differential equations $\Rightarrow$ $\chi_k^J(\xi)$.
2. Calculation of the S matrix.
3. Total cross section:

$$\sigma_{ij} = \frac{\pi}{k_i^2} \sum_J (2J+1) |S_{ij}^J|^2$$

Semiclassical formalism.

- Straight-line nuclear trajectories:

$$\mathbf{R} = \mathbf{b} + \mathbf{v}t$$



Semiclassical formalism.

- Straight-line nuclear trajectories:

$$\mathbf{R} = \mathbf{b} + \mathbf{v}t$$

- Eikonal equation:

$$\left[H_{\mathrm{elec}} - \mathrm{i} \frac{\partial}{\partial t} \bigg|_r \right] \Psi(\mathbf{r}, t) = 0$$

- Molecular expansion:

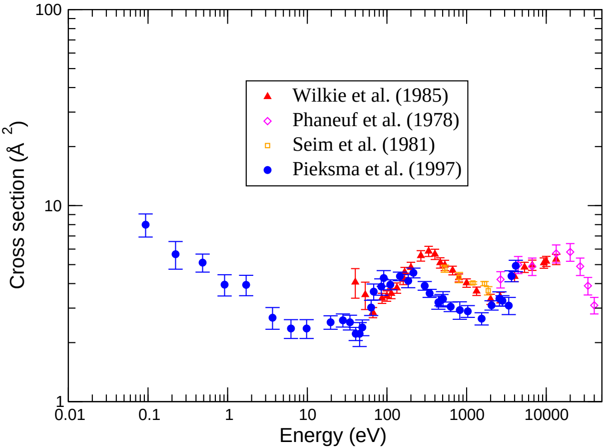
$$\Psi(\mathbf{r}, t) = \exp\left[\mathrm{i} U(\mathbf{r}, t)\right] \sum_j a_j(t) \phi_j(\mathbf{r}, R) \exp\left(-\mathrm{i} \int_0^t \epsilon_j \mathrm{d}t' \right)$$

Cross sections.

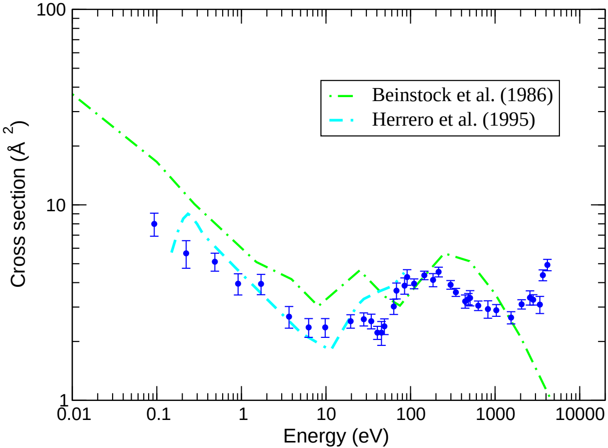
$$\sigma_{ij}(v) = 2\pi \int_0^{\infty} b\, P_{ij}(b, v) \mathrm{d}b$$

$$P_{ij}(b, v) = \lim_{t \to \infty} \left| \left\langle \phi_j(r) D^j(r, t) | \Psi \right\rangle \right|^2 = \lim_{t \to \infty} |a_j(t;\ b, v)|^2$$

Cross section. $N^{2+}(2s^22p\ \ ^2P^\circ) + H(1s) \rightarrow N^+ + H^+$



Cross section. $N^{2+}(2s^2 2p\ \ ^2P^\circ) + H(1s) \rightarrow N^+ + H^+$



Processes studied.

$$N^{2+}(2s^2 2p\ \ {}^2P^\circ) + H(1s) \rightarrow N^+ + H^+$$

$$N^{2+}(2s2p^2\ \ {}^4P) + H(1s) \rightarrow N^+ + H^+$$

$$N^{2+}(2s^2 2p\ \ ^2P^\circ) + H(1s) \rightarrow N^+ + H^+$$

Molecular states:

- singlets
- triplets

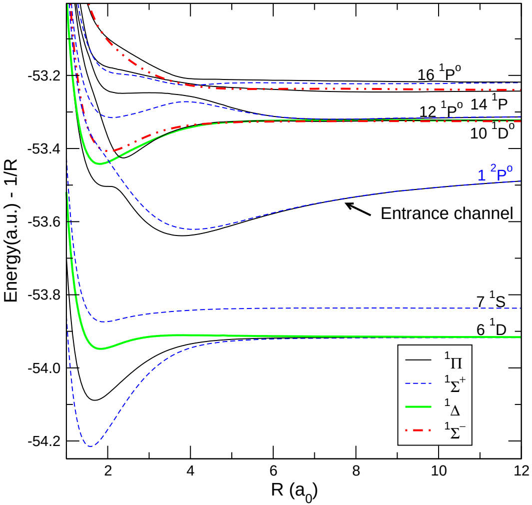
$$N^{2+}(2s^2 2p\ \ {}^2P^\circ) + H(1s) \rightarrow N^+ + H^+$$

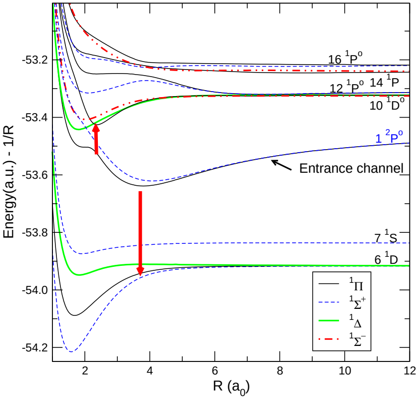
Molecular states:
- singlets
- triplets

$$N^{2+}(2s2p^2\ \ {}^4P) + H(1s) \rightarrow N^+ + H^+$$

Molecular states:
- triplets
- quintets

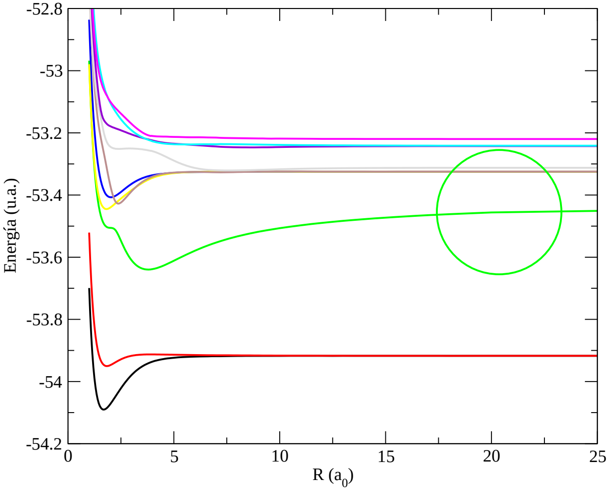
Potential energy curve, singlets

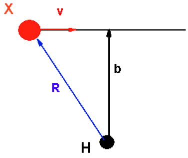




i	Atomic state	Molecular states
1	$N^{2+}(2s^2 2p\ ^2P^\circ)$	$^{1,3}\Sigma^+$, $^{1,3}\Pi$
3	$N^{2+}(2s2p^2\ ^2D)$	$^{1,3}\Sigma^+$, $^{1,3}\Pi$, $^{1,3}\Delta$
4	$N^{2+}(2s2p^2\ ^2S)$	$^{1,3}\Sigma^+$
6	$N^+(2s^2 2p^2\ ^1D)$	$^1\Sigma^+$, $^1\Pi$, $^1\Delta$
7	$N^+(2s^2 2p^2\ ^1S)$	$^1\Sigma^+$
10	$N^+(2s2p^3\ ^1D^\circ)$	$^1\Sigma^-$, $^1\Pi$, $^1\Delta$
12	$N^+(2s^2 2p3s\ ^1P^\circ)$	$^1\Sigma^+$, $^1\Pi$
14	$N^+(2s^2 2p3p\ ^1P)$	$^1\Sigma^-$, $^1\Pi$
16	$N^+(2s2p^3\ ^1P^\circ)$	$^1\Sigma^+$, $^1\Pi$

Collision history (States $^1\Sigma^-$, $^1\Pi_-$, $^1\Delta_-$)





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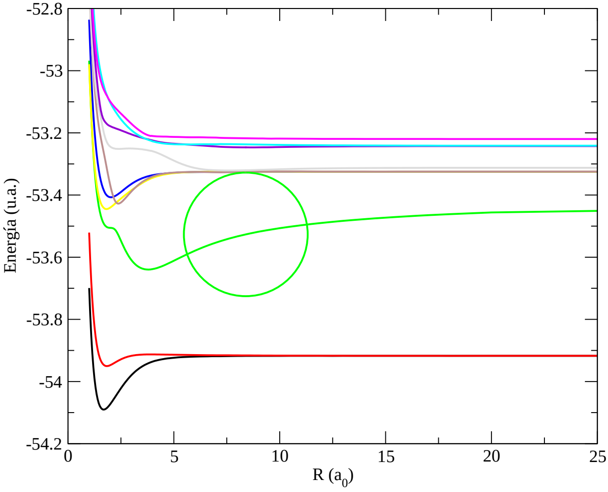

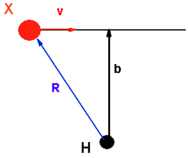

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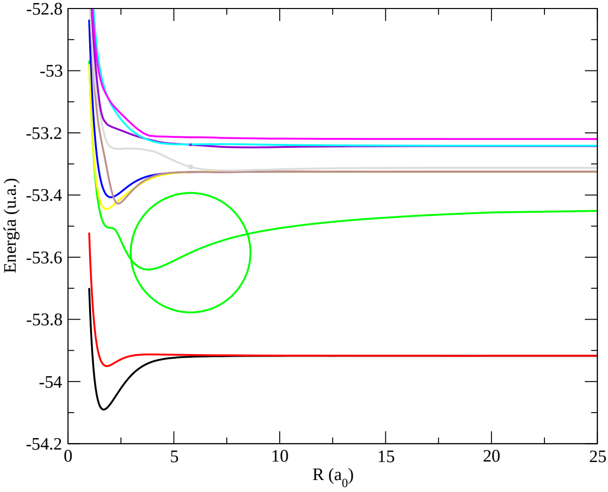
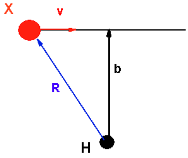
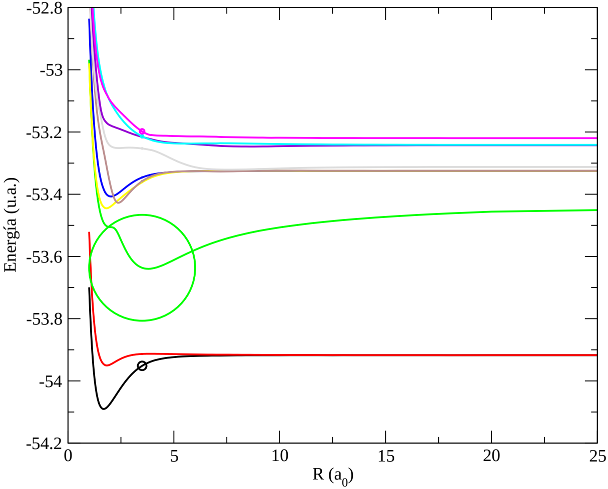
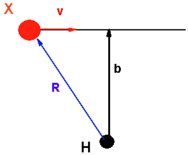




Collision history (States $^1\Sigma^-$, $^1\Pi_-$, $^1\Delta_-$))





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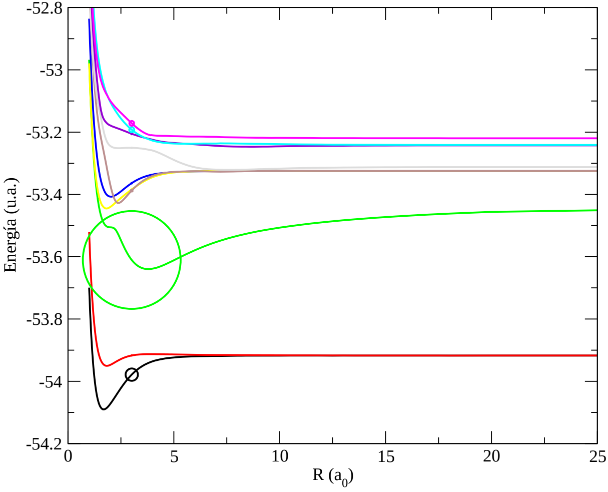

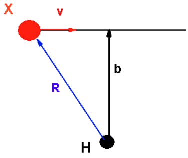

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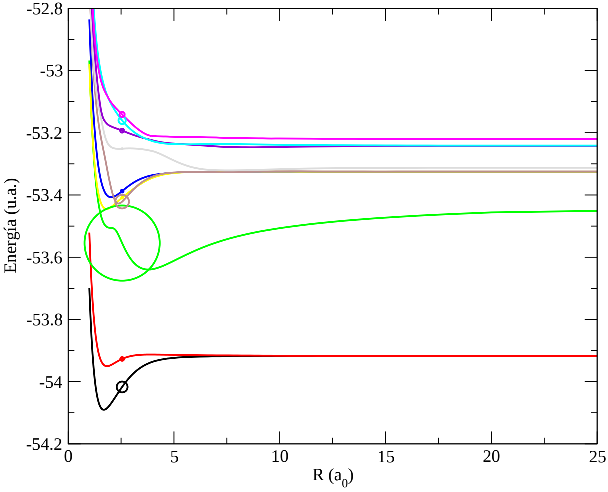

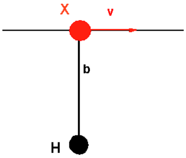

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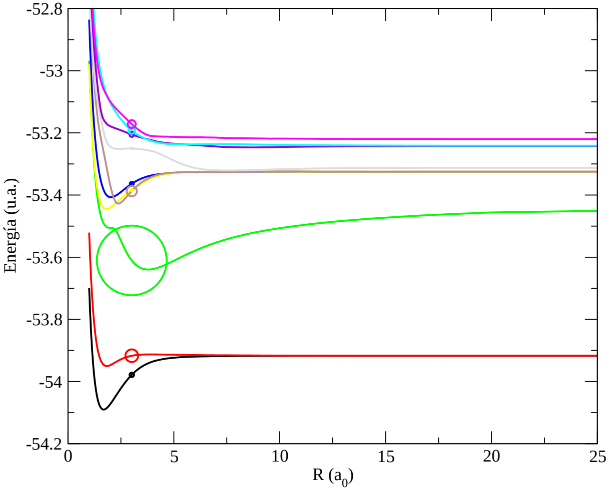

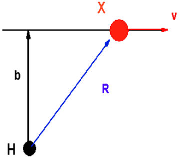

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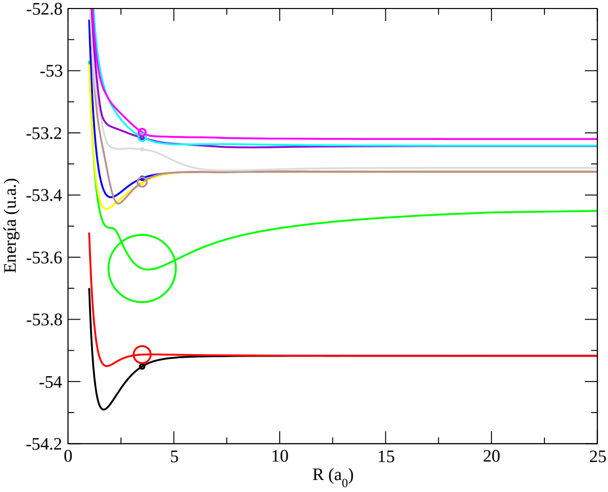

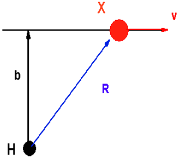

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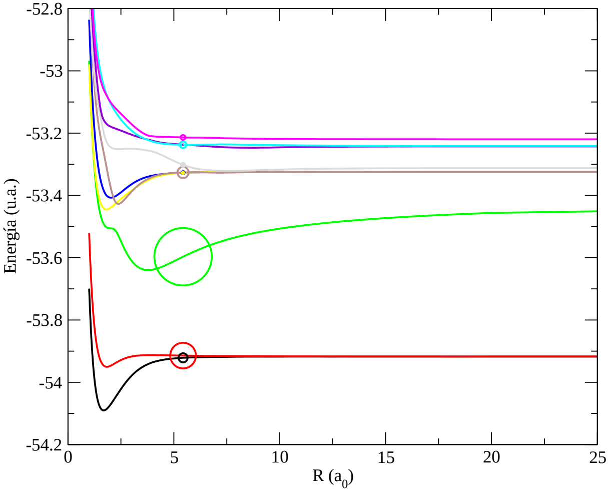

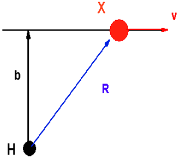

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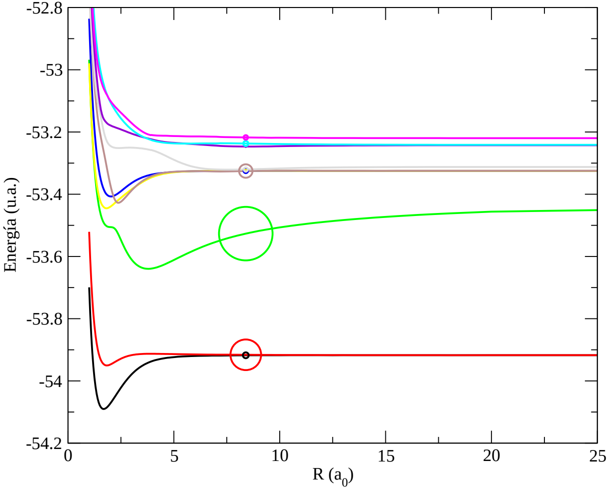

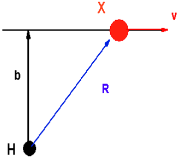

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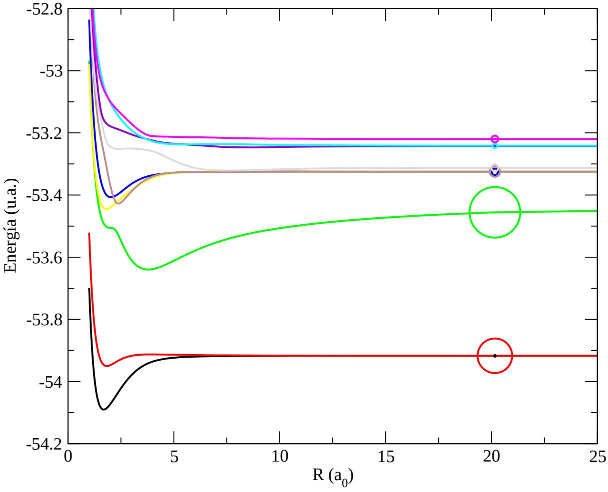

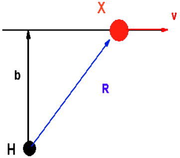

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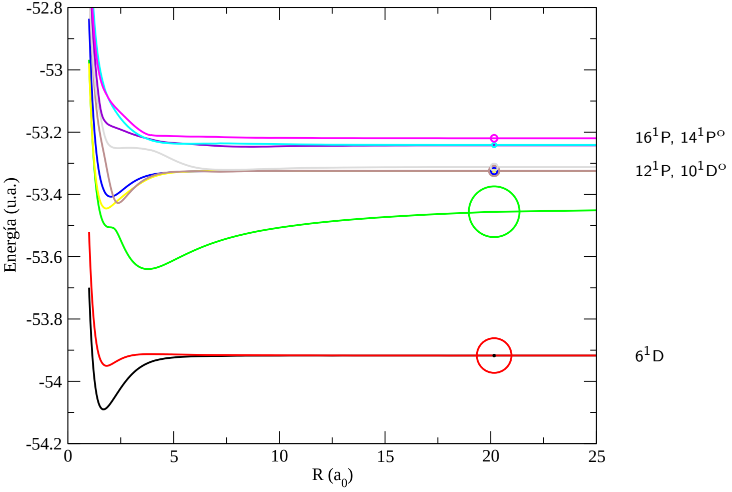
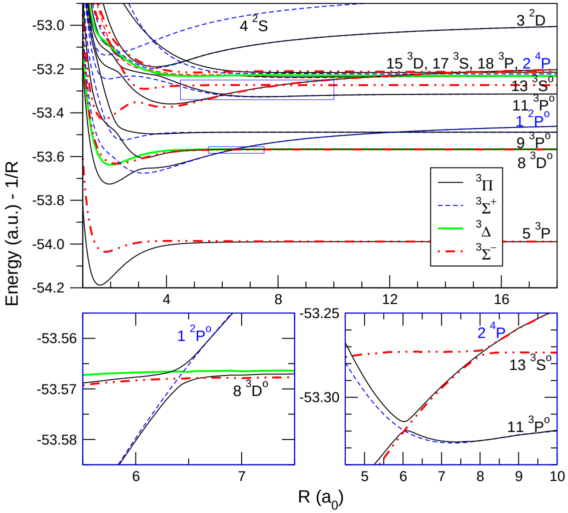


Potential energy curves, Triplets



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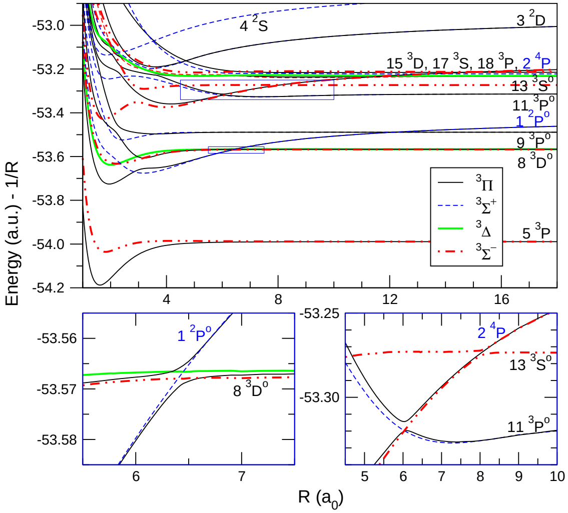
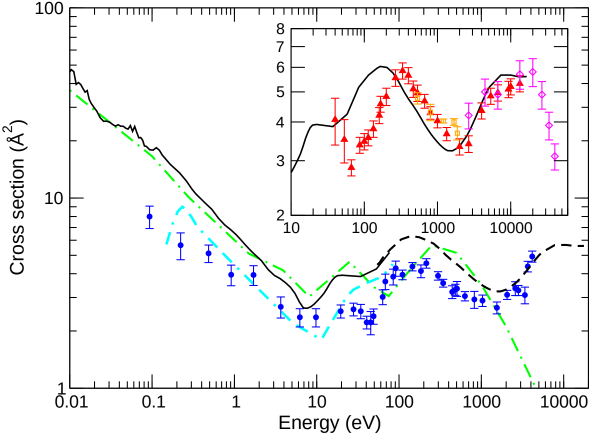


Main exit channels:

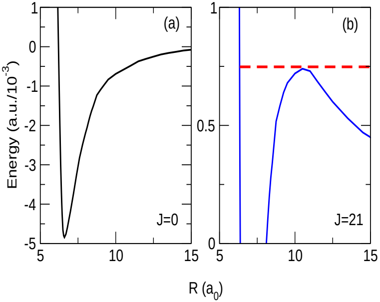
- $N^+(2s2p^3\ ^3D^\circ)$ + H^+ (8)
- $N^+(2s^22p3s\ ^3P^\circ)$ + H^+ (11)

Cross section. $N^{2+}(2s^22p\ \ ^2P^{\circ}) + H(1s) \rightarrow N^{+} + H^{+}$



(Phys. Rev. A 70, 022707)

Langevin model.



- Semiclassical treatment
- $P = 1$ para $b < b_{\max}$

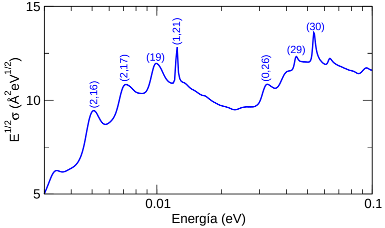
$$\sigma = 2\pi \int_0^{b_{\max}} bP(b)\mathrm{d}b \simeq \pi b_{\max}^2$$

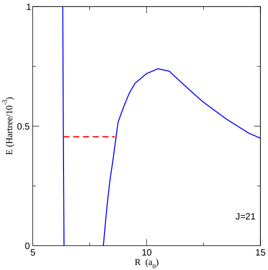
- Ion-induced dipole interaction

$$b_{\max} = (2\alpha q^2/E)^{1/4}$$

$$\sigma \sim \mathbf{cte} \times \mathbf{E}^{-1/2}$$

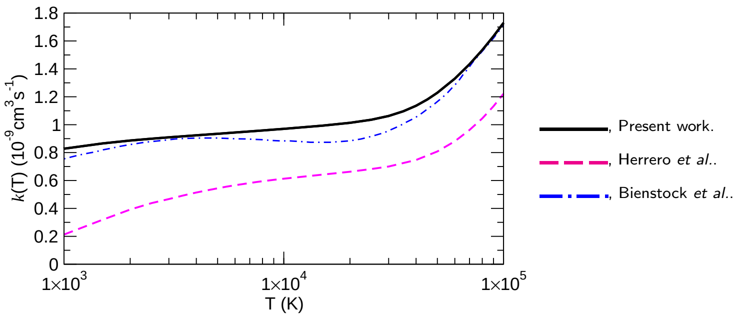
Cross section. $N^{2+}(2s^2 2p\ \ ^2P^\circ) + H(1s) \rightarrow N^+ + H^+$





(Phys. Rev. A, 74, 225202)

Rate coefficients.



$$k(T) = \left(\frac{\mu}{2\pi K_B T}\right)^{3/2} 4\pi \int_0^\infty v_r^3 \sigma_{if}(v_r) \exp\left(\frac{-\mu v_r^2}{2K_B T}\right) \mathrm{d}v_r$$

Reactions studied.

- $$O^{2+}(2s^2 2p^2\ {}^3P) + H(1s) \rightarrow O^+ + H^+$$
- $$O^{2+}(2s^2 2p^2\ {}^1D) + H(1s) \rightarrow O^+ + H^+$$
- $$O^{2+}(2s^2 2p^2\ {}^1S) + H(1s) \rightarrow O^+ + H^+$$

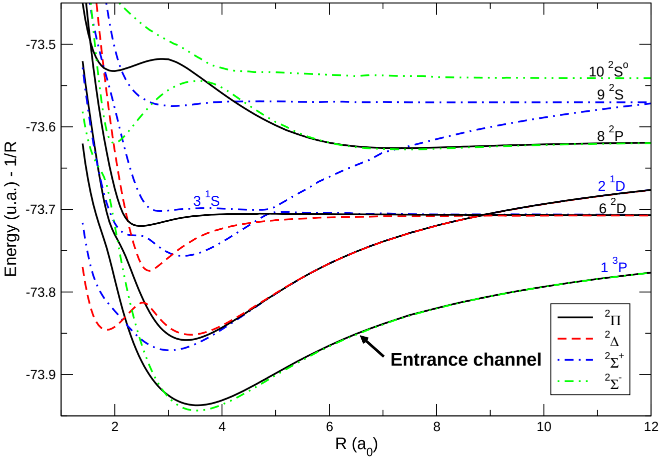
Previous calculations of Cabello *et al.* (2003)

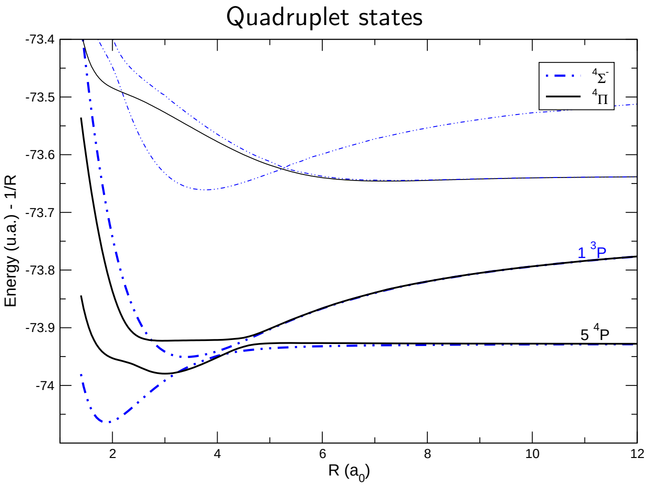
$$O^{2+}(2s^2 2p^2\,{}^3P) + H(1s) \rightarrow O^{+} + H^{+}$$

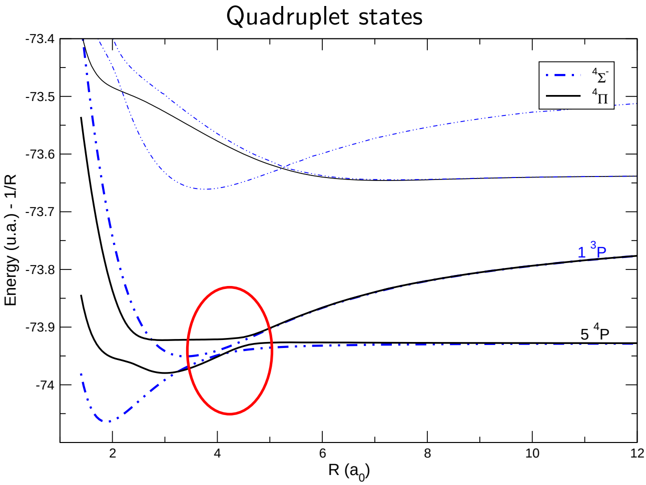
Molecular states:

- doublets
- quadruplets

Doublet states

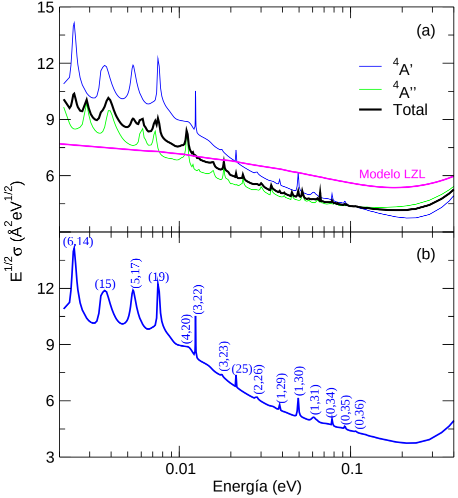



Quadruplet states
-73.4
-73.5
-73.6
-73.7
-73.8
-73.9
-74
Energy (u.a.) - 1/R
2
4
6
8
10
12
R (a0)
4Σ-
4Π
1 3P
5 4P

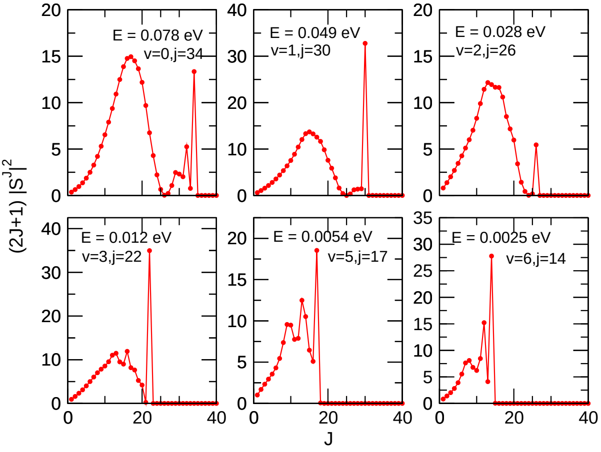


Main product: $O^{+}(2s2p^{4}\ ^{4}P) + H^{+}$

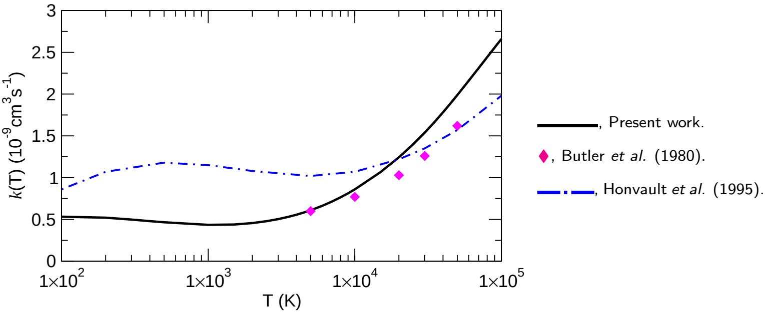
Cross section. $O^{2+}(2s^2 2p^2\ ^3P) + H(1s) \rightarrow O^+ + H^+$



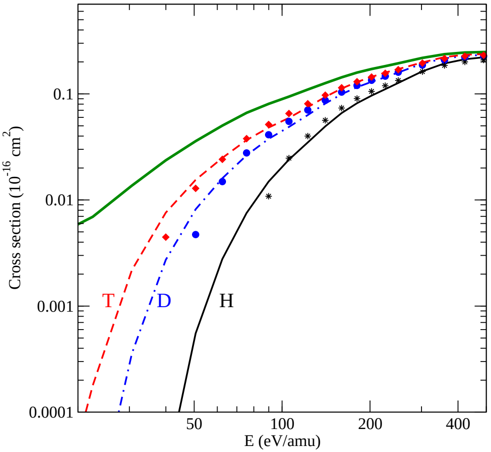
S matrix


E = 0.078 eV
v=0,j=34
E = 0.049 eV
v=1,j=30
E = 0.028 eV
v=2,j=26
E = 0.012 eV
v=3,j=22
E = 0.0054 eV
v=5,j=17
E = 0.0025 eV
v=6,j=14
(2J+1) |S^J|^2
J

Rate coefficients.

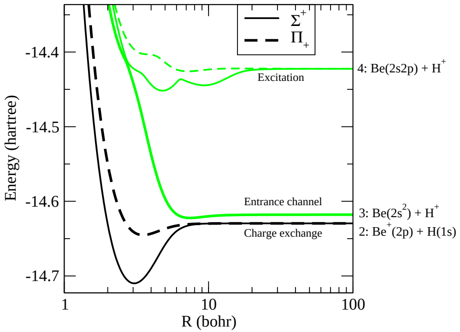


$Li^+ + H(1s) \rightarrow Li + H^+$

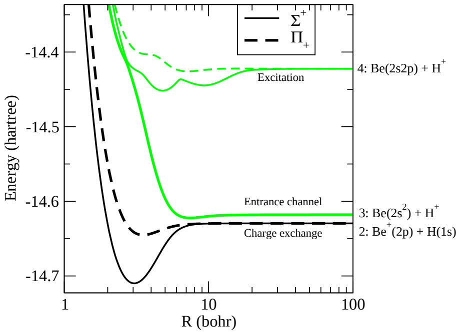


(Phys. Rev. A, 77, 012706)

Potential energy curves BeH^+



Potential energy curves BeH^+

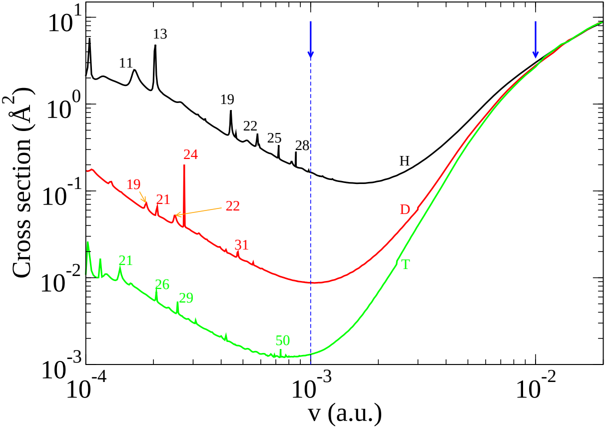


$$H_{11} = -0.0102$$

$$H_{22} = 72.6\, e^{-1.35R} - \frac{36.1644}{2R^4}$$

$$H_{12} = -0.804\, e^{-0.82R}$$

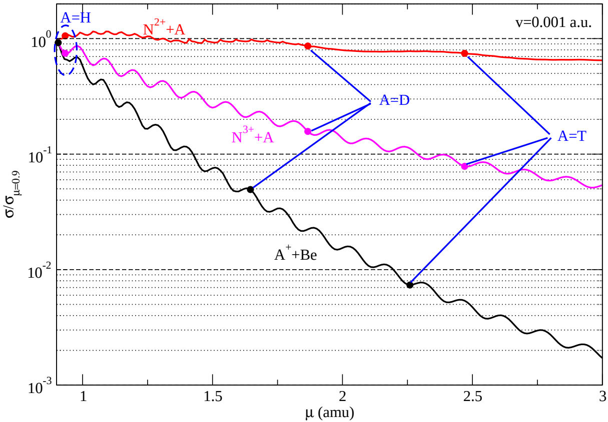
Cross section $Be(2s^2\ ^1S) + H^+ \rightarrow Be^+ + H$



($v = 10^{-3}$a.u. corresponds to $E \approx$ 2.5meV/amu)

(J. Phys. B, 41, 225202)

Isotopic effect

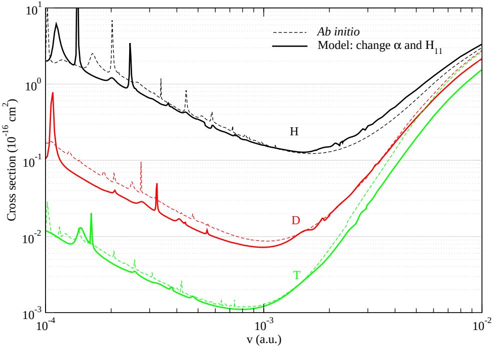


Isotopic effect

The polarizability α of beryllium is changed instead of the reduced mass of the system, in order to keep the relation:

$$\frac{\alpha}{\mu_H} = \frac{\alpha'}{\mu_D} = \frac{\alpha''}{\mu_T}$$

Minimum energy gap (depends on H_{11}) has been changed to keep the same value for the three systems.



Isotopic effect

- 2-state semiclassical model: Transition probability $P \sim \exp(-A/v_R)$.
- The strong isotopic effect is essentially due to the change with μ of the radial velocity v_R in the transition region:

$$v_R = v\sqrt{1 - \frac{2V_1(R)}{\mu v^2} - \frac{b^2}{R^2}}$$

- The isotopic dependence appears explicitly in the fraction

$$\frac{2V_1(R)}{\mu v^2} = -\frac{q^2\alpha}{\mu v^2 R^4}$$

- The isotopic dependence of the CX cross section is a function of the target polarizability and the ion charge.

Summary

- Large-scale quantal and semiclassical calculations.
- Partial cross sections and rate coefficients.
- Resonances
- Isotopic effect.

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