Recombination, excitation and dissociation of hydride molecular cations in low energy electron collisions

J. Zs Mezei[1-4], F. Colboc[1], D. O. Kashinsky[5], D. A. Little[6], M. D. Epée Epée[7], S. Niyonzima[8], N. Pop[9], C. M. Coppola[10], K. Chakrabarti[11], O. Motapon[7], A. Bultel[12], K. Hassouni[2], D. Talbi[13], A. P. Hickman[14], A. Faure[15], J. Tennyson[6] and I. F. Schneider[1,3]

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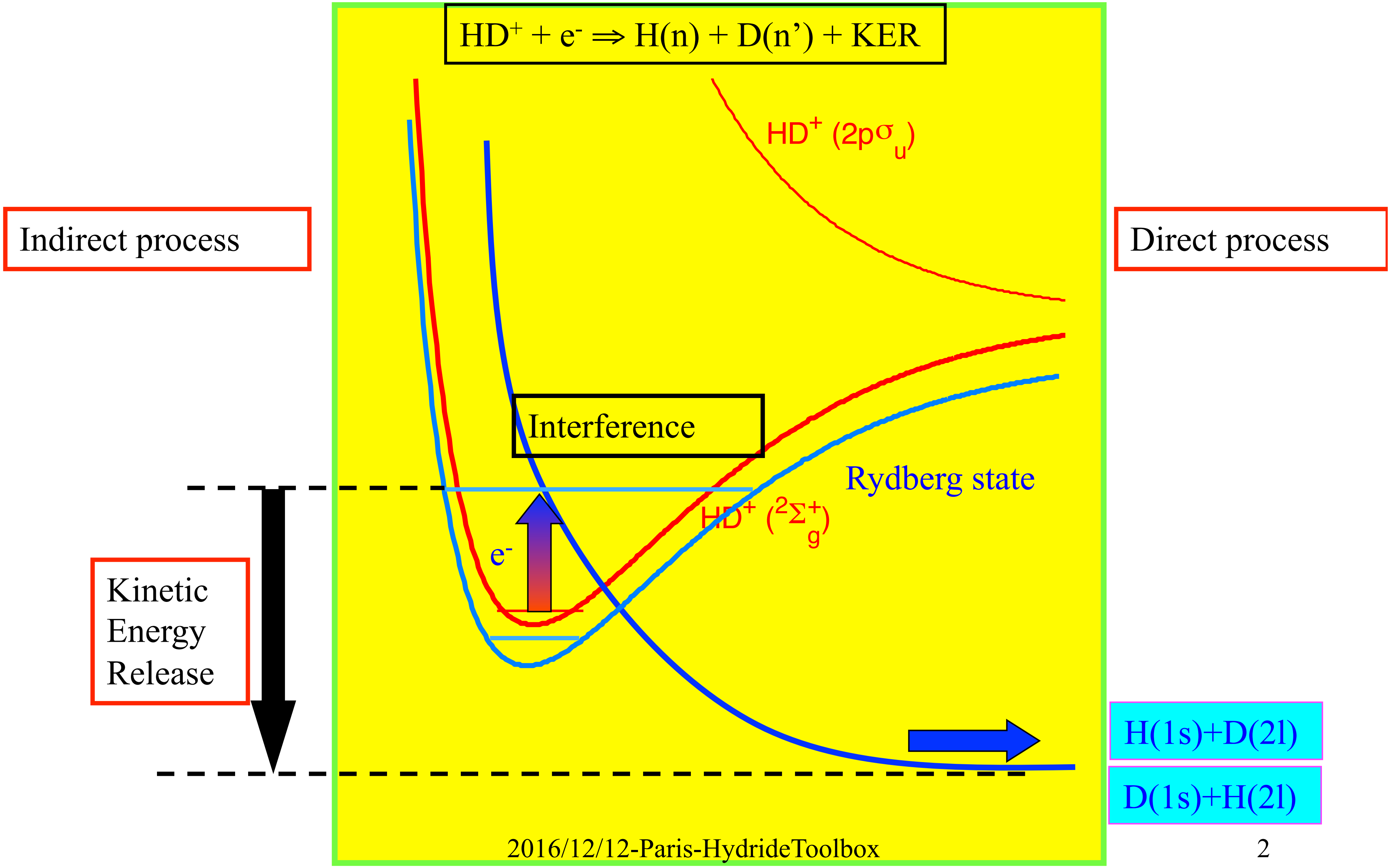
$$AB^+(N_i^+, v_i^+) + e^- \rightarrow A + B$$

$$\rightarrow AB^+(N_f^+, v_f^+) + e^-$$

$$\rightarrow A + B^+ + e^-$$

Electron-cold molecular ion reaction: Dissociative Recombination

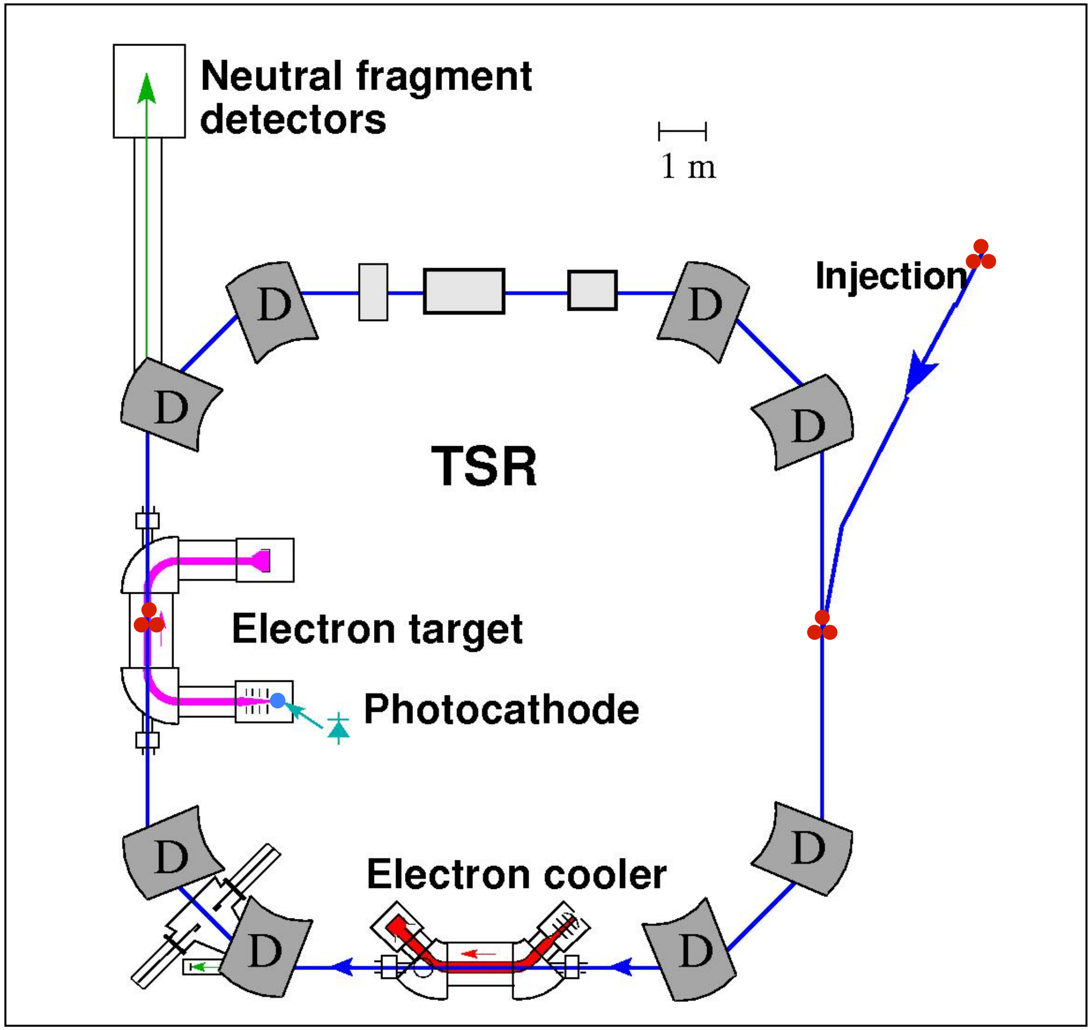


Storage ring measurements: concept

Advantages

- radiative relaxation of internal excitations (rotation, vibration)
- direct measurement
- 100% detection efficiency
- high resolution

- Vibrations cool ✓
- Rotations stay forever ✗



Kreckel et al., PRA A 66, 052509 (2002),
Kreckel et al., New J. Phys. 6, 151 (2004)

Benchmarking:

a NOT-SO-Hydride system,

H_2^+ (or isotopologues) + e^- :

maximum ACCURACY

$HD^+ + e^-$

PHYSICAL REVIEW A **90**, 012706 (2014)

Rotational transitions induced by collisions of HD^+ ions with low-energy electrons

O. Motapon,[1,2] N. Pop,[3] F. Argoubi,[4] J. Zs Mezei,[2,5,6] M. D. Epee Epee,[1] A. Faure,[7] M. Telmini,[4]
J. Tennyson,[8] and I. F. Schneider[2,5]

$HD^+ + e^- \rightarrow$

$\rightarrow HD^* \rightarrow$

$\rightarrow H + D$

+

Average on ROTATIONAL distribution, T_{rot} …+…

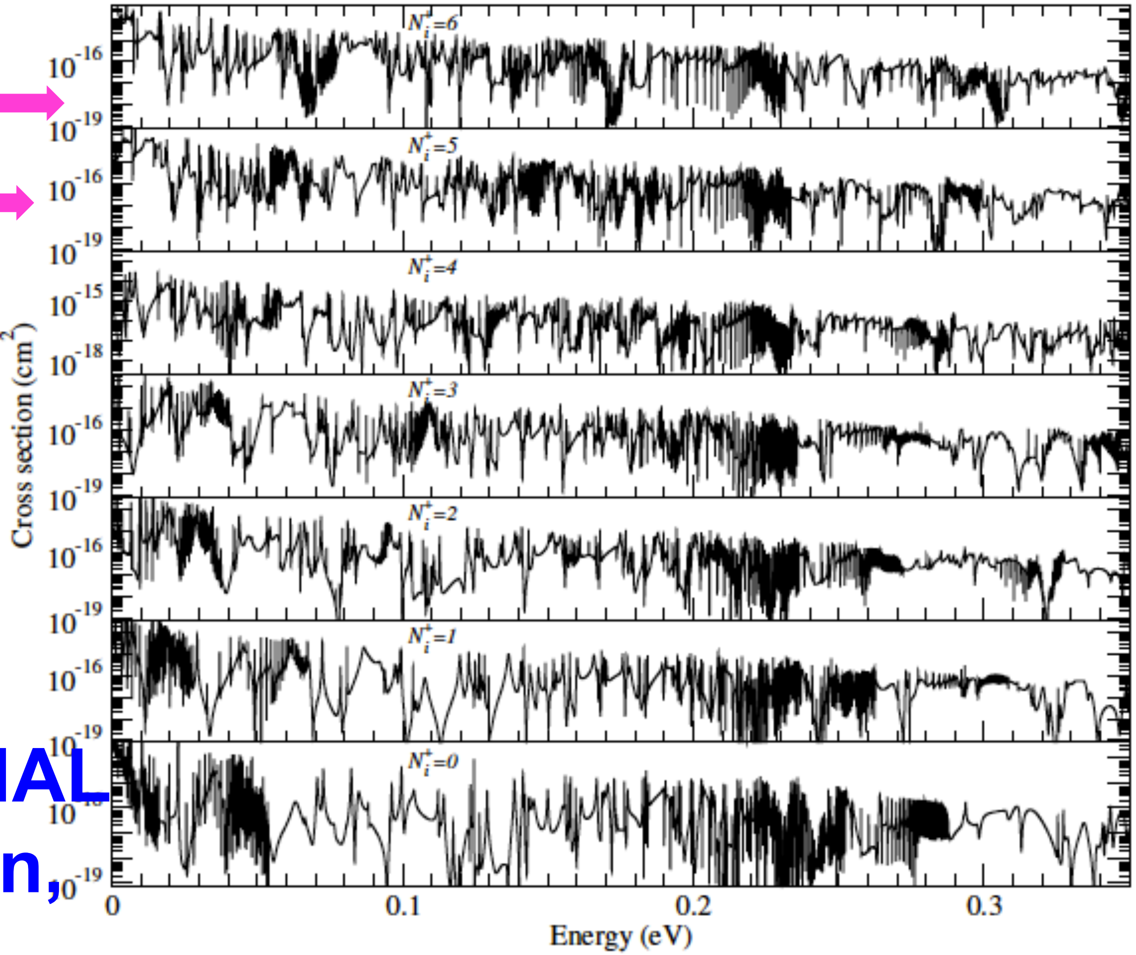
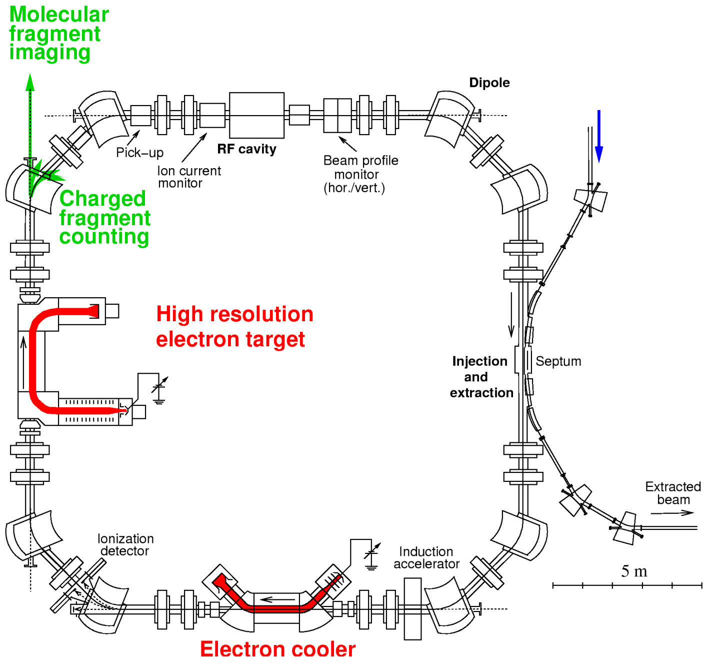


Figure 3. DR cross sections of HD^+ initially in one of its lowest rotational level N_i^+ (vibrational ground state).



...+ Convolution with ANISOTROPIC Maxwell Distribution:

$$\alpha = < v\sigma > = \int\int\int \sigma(v) v f(v_d, \mathbf{v}) d\mathbf{v} \qquad (1)$$

$$f(v_d, \mathbf{v}) = \frac{m}{2\pi k T_{e\perp}} exp(-\frac{m v_\perp^2}{2kT_{e\perp}}) \sqrt{\frac{m}{2\pi k T_{e\parallel}}} exp(-\frac{m(v_\parallel - v_d)^2}{2kT_{e\parallel}}) \qquad (2)$$

Best parameters:

T_{long} = 20 μeV= 0,23 K=0,16 cm^{-1}

T_{trans} = 500 μeV= 5,80 K=4,03 cm^{-1}

PHYSICAL REVIEW A **90**, 012706 (2014)

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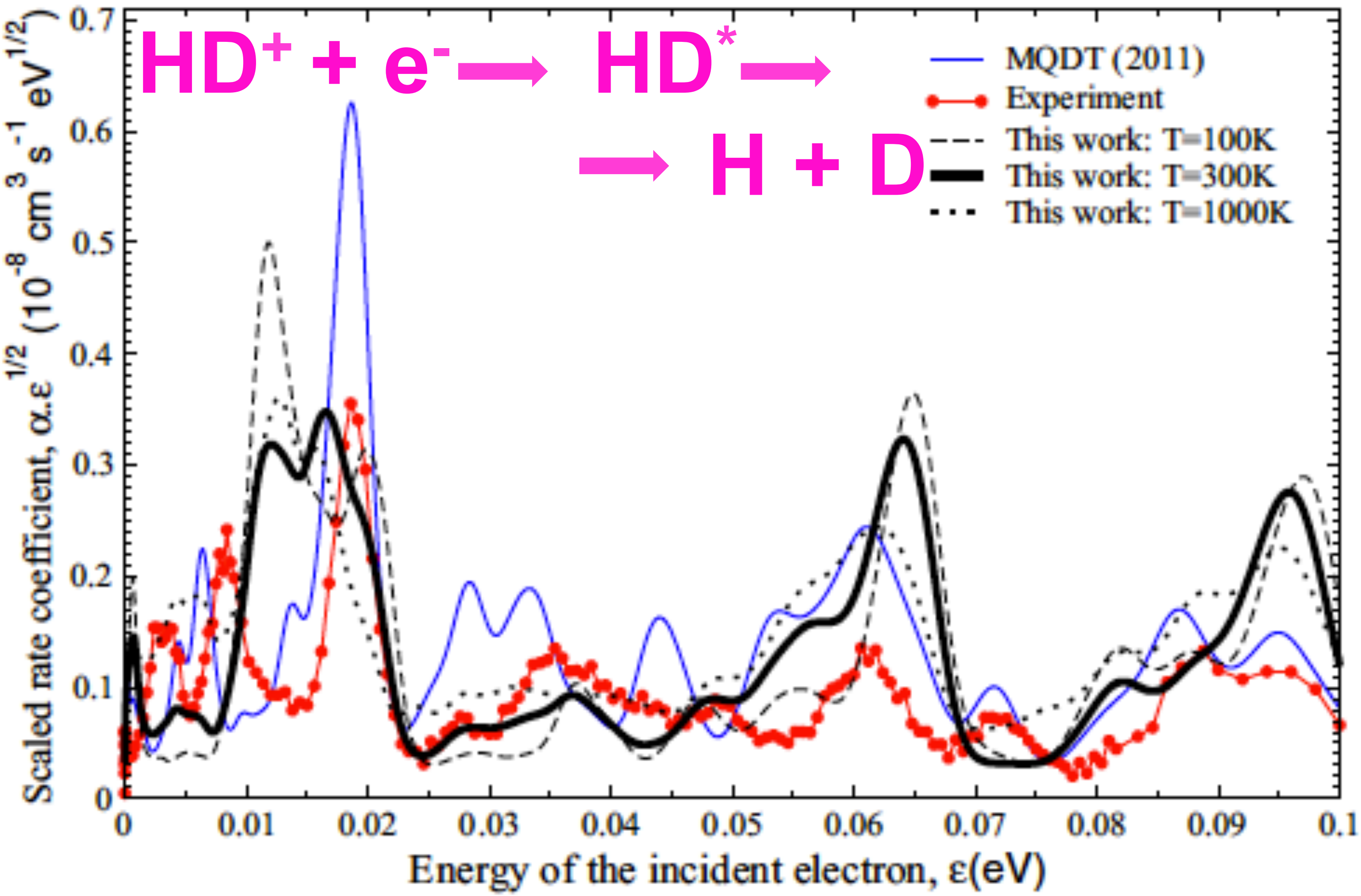

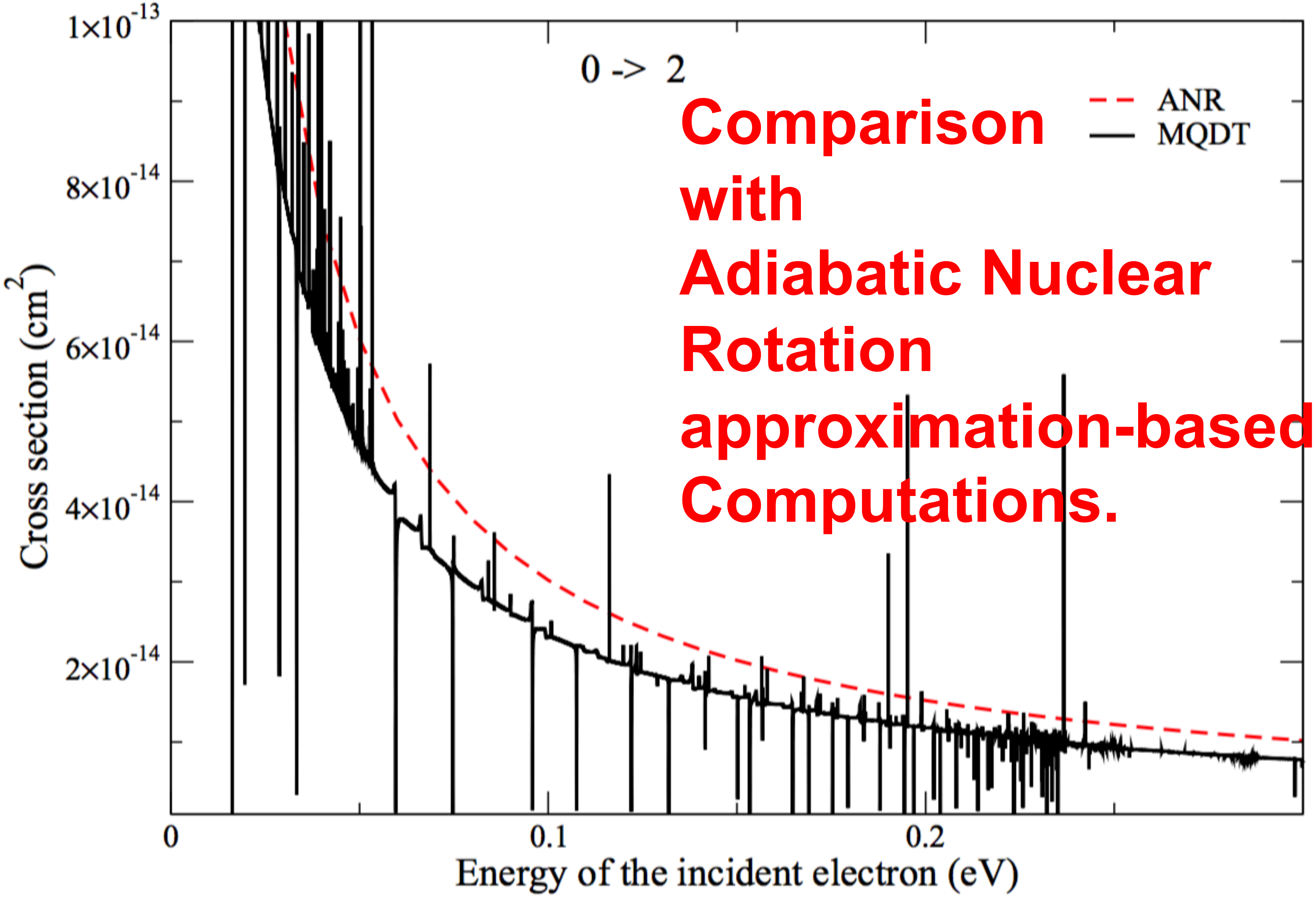

FIG. 2. (Color online) Zoom in the linear scale of the cross section for the transition $0 \rightarrow 2$, in the ground vibrational state of $HD^+(X\,^2\Sigma_g^+)$. Black solid curve: MQDT computations; red dashed curve: ANR approximation-based computations.

For the modelers:

Maxwell rate-coefficients

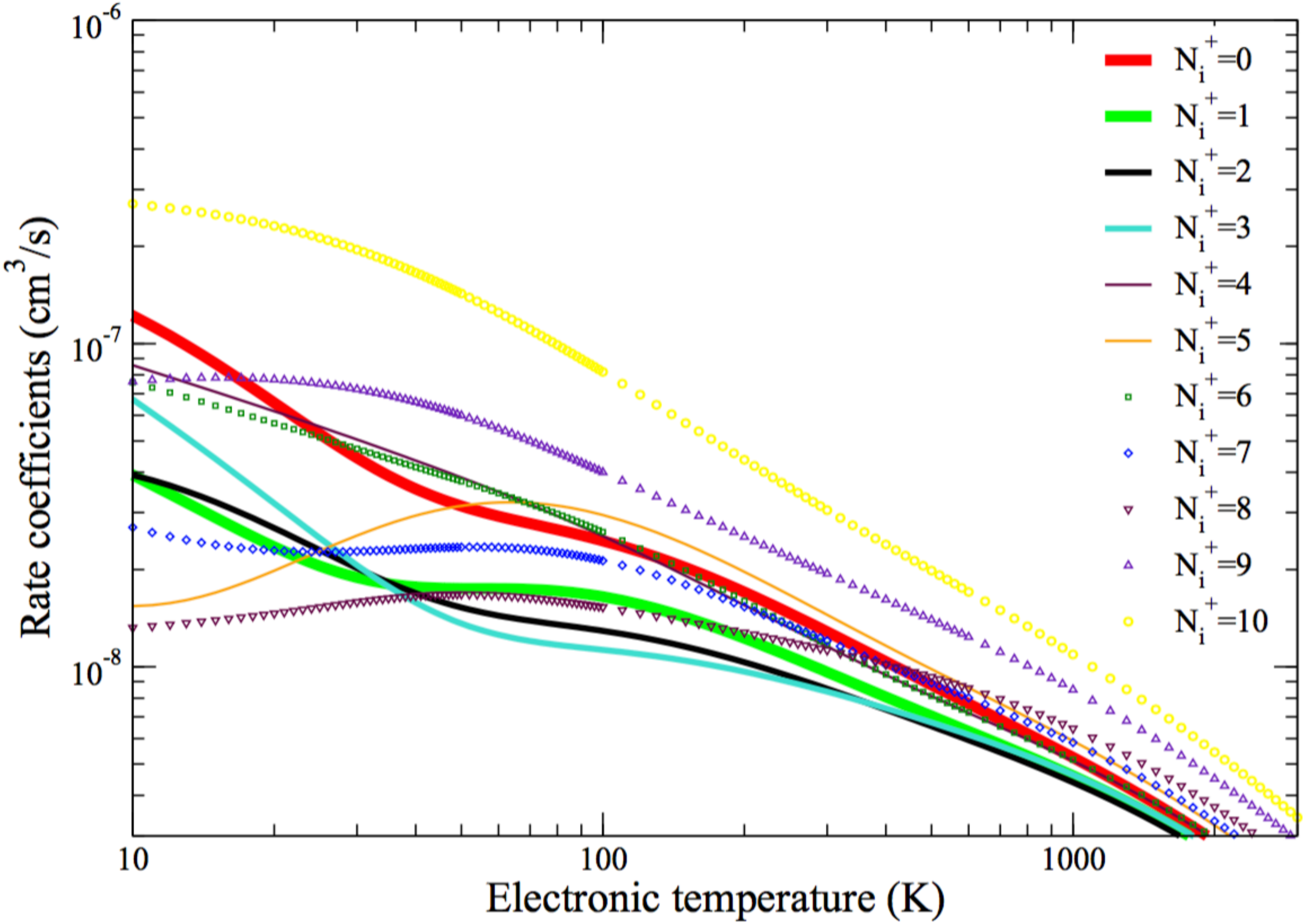

FIG. 9. (Color online) Maxwell isotropic rate coefficients for the dissociative recombination $HD^+(X\,^2\Sigma_g^+)$ with $v_i^+ = 0$ as a function of initial rotational level, $N_i^+ = 0$ to 10 .

EPJ Web of Conferences **84**, 01001 (2015)
DOI: 10.1051/epjconf/20158401001

A. Wolf[1,a], O. Novotný[2], H. Buhr[2], C. Krantz[2],
I.F. Schneider[3], O. Motapon[4] and J.Zs. Mezei[3,5]

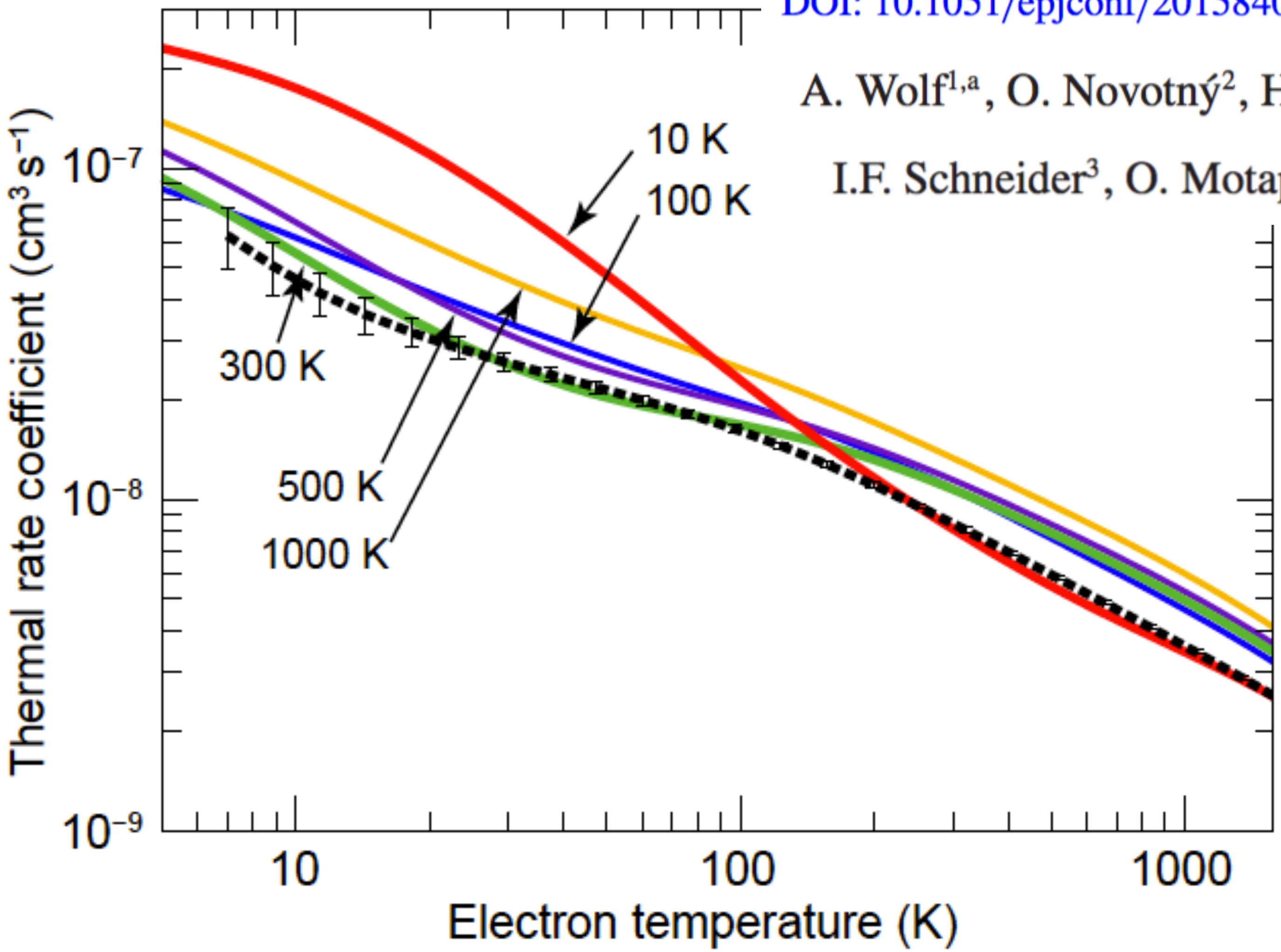

Fig. 2. Thermal rate coefficient for HD^+ DR as a function of the electron temperature. Experiment is given by a the thick dashed line; 1σ estimated experimental errors due to uncertainties in the electron beam temperatures are also indicated. Theory is obtained for the given rotational temperatures.

$H_2^+ + e^-$

$H_2^+ + e^-$

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MNRAS **455**, 276–281 (2015) doi:10.1093/mnras/stv2329

Reactive collisions of very low-energy electrons with H_2^+: rotational transitions and dissociative recombination

M. D. Epée Epée,[1] J. Zs Mezei,[2,3,4] O. Motapon,[1,5★] N. Pop[6] and I. F. Schneider[2,3★]

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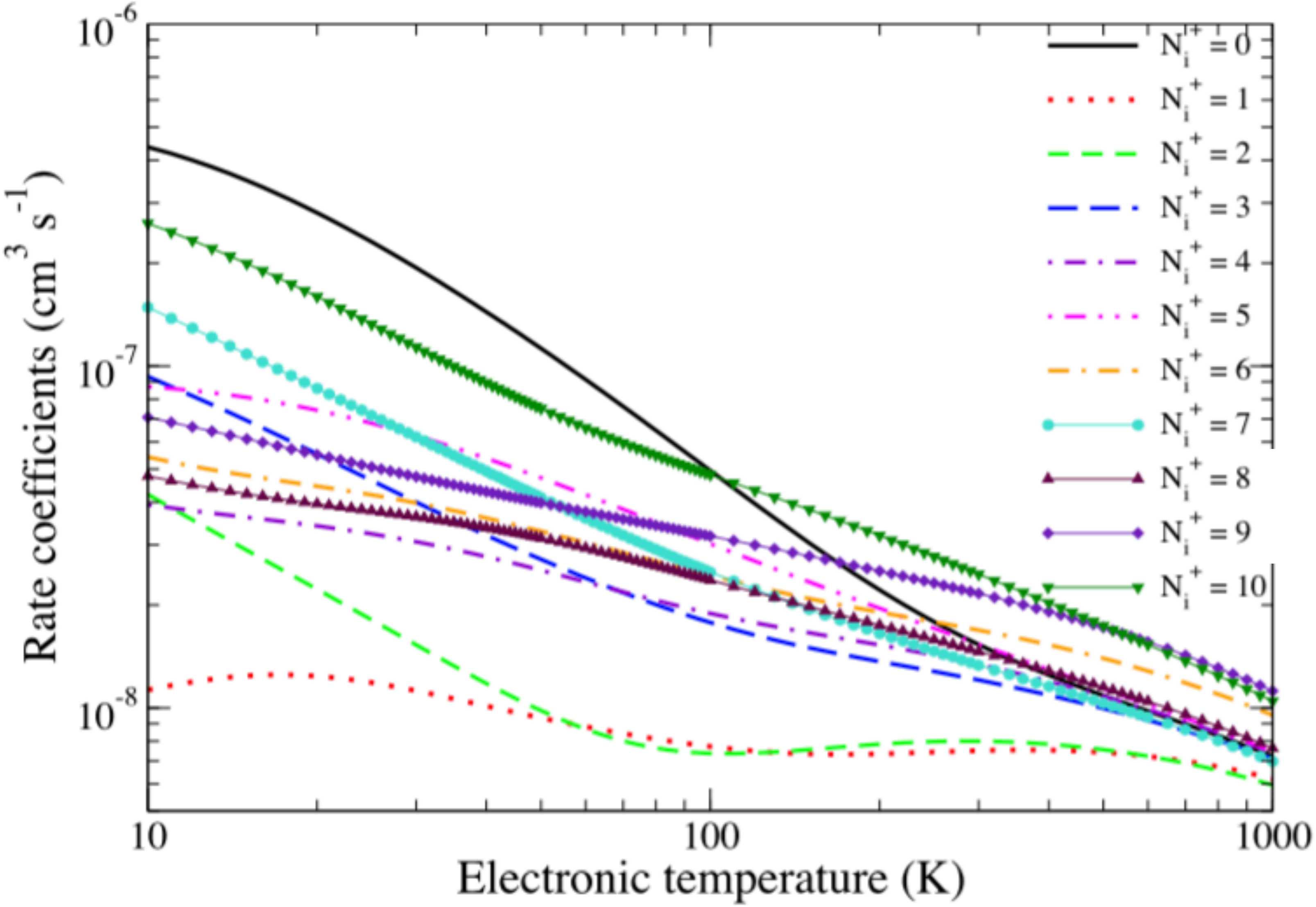


Figure 4. Maxwell rate coefficients for the DR of $H_2^+(X^2\Sigma_g^+)$ on its ground vibrational level $v_i^+ = 0$, as a function of its initial rotational level, $N_i^+ = 0$ to 10.

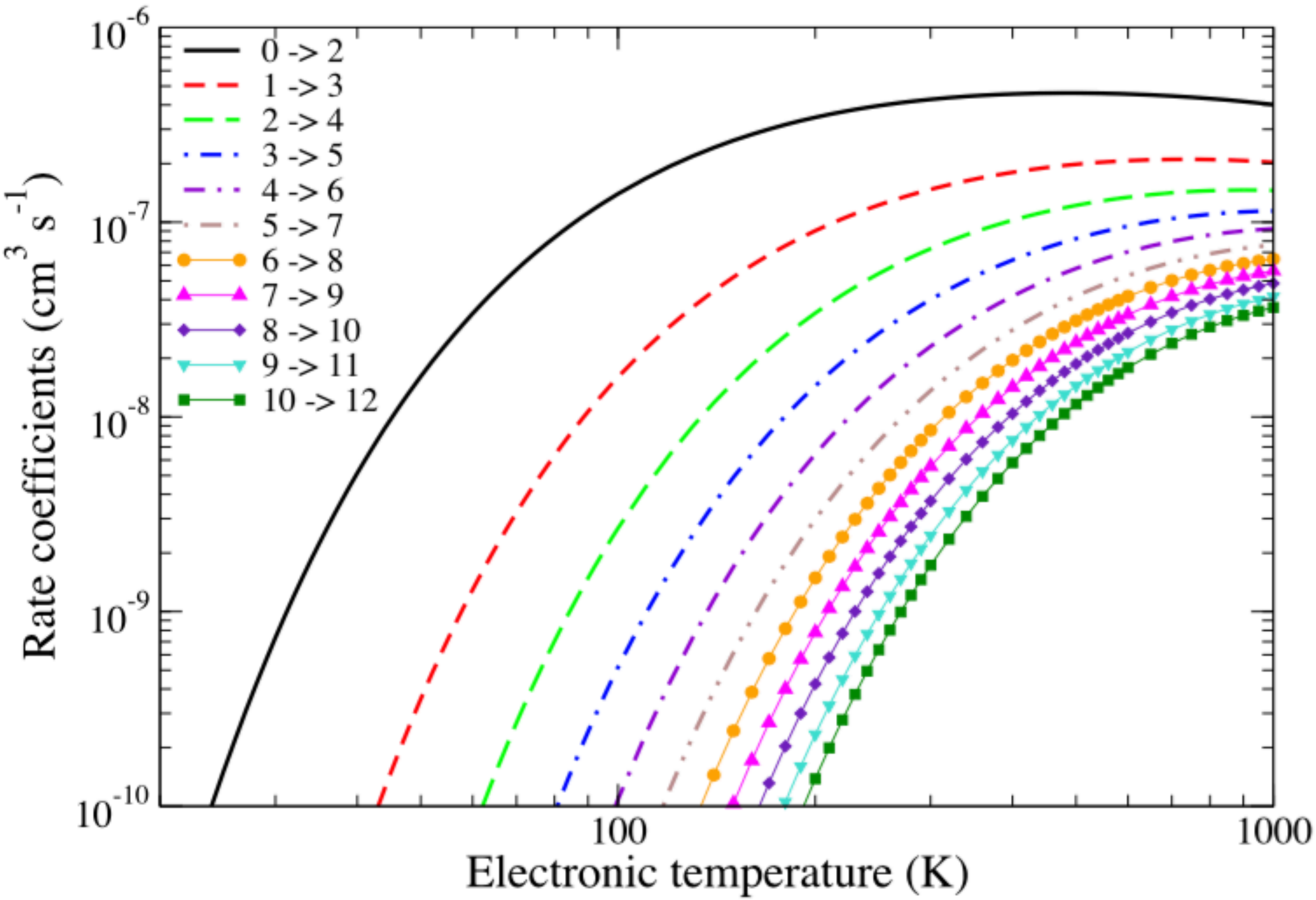
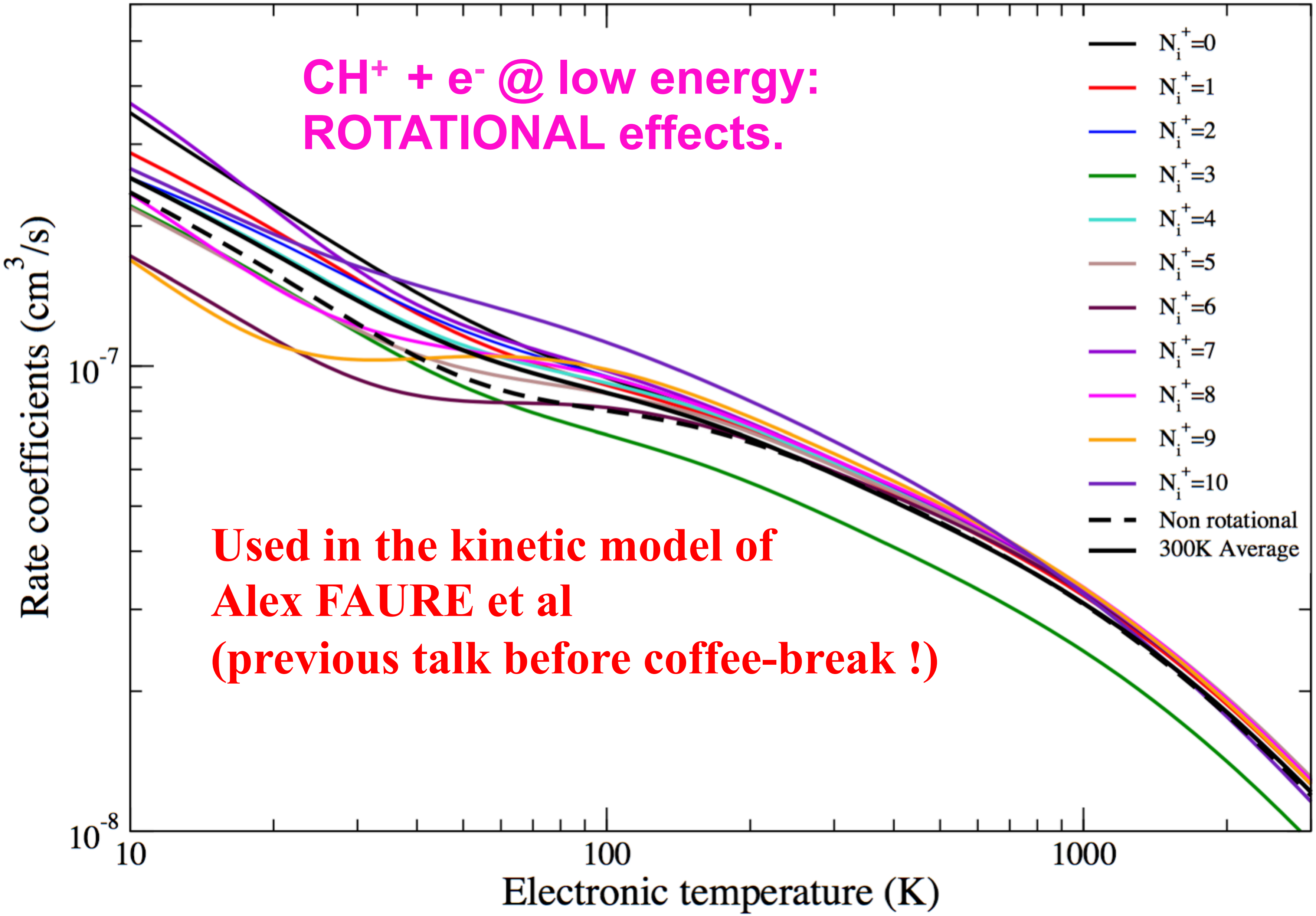
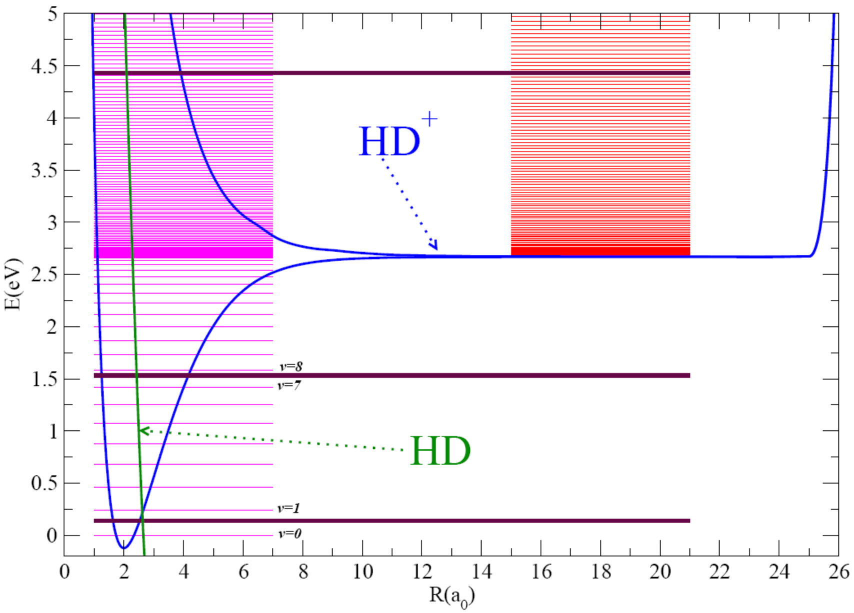


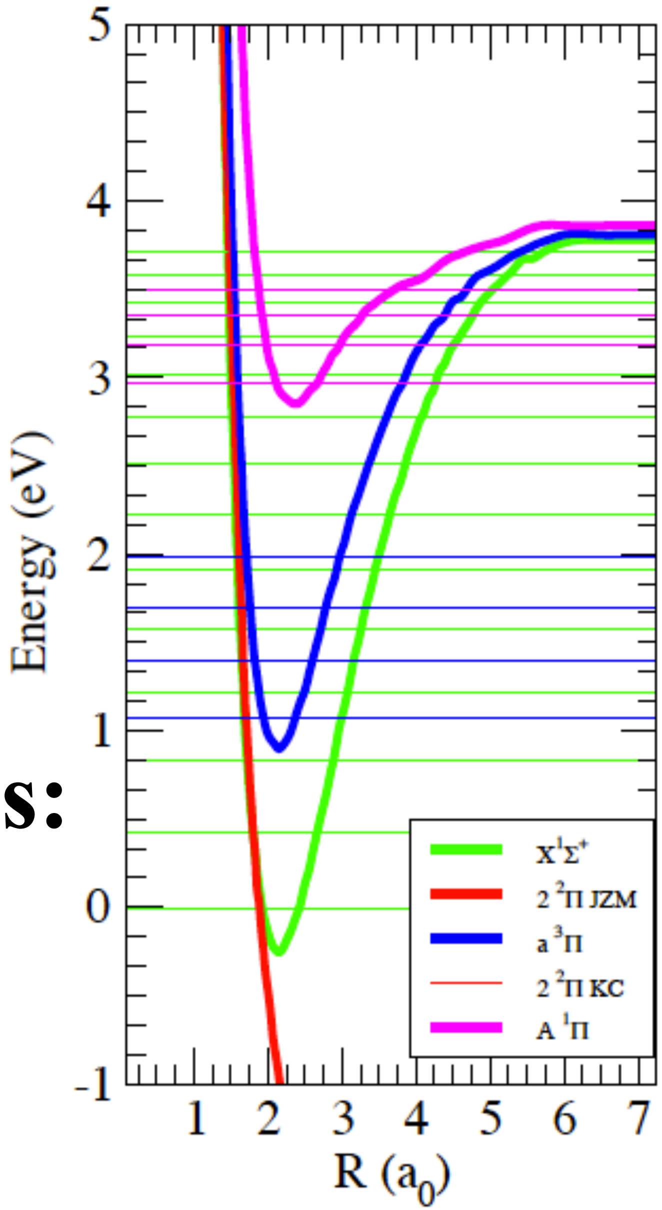
Figure 3. Maxwell rate coefficients for rotational excitation $N_i^+ \to N_i^+ + 2$, with $N_i^+ = 0$ to 10 of $H_2^+(X^2\Sigma_g^+)$ on its ground vibrational level $v_i^+ = 0$.

$CH^+ + e^-$


CH+ + e- @ low energy:
ROTATIONAL effects.
Used in the kinetic model of
Alex FAURE et al
(previous talk before coffee-break !)
Rate coefficients (cm3/s)
10-7
10-8
10
100
1000
Electronic temperature (K)
Ni+=0
Ni+=1
Ni+=2
Ni+=3
Ni+=4
Ni+=5
Ni+=6
Ni+=7
Ni+=8
Ni+=9
Ni+=10
Non rotational
300K Average

$CH^+ + e^-$ @ high energy





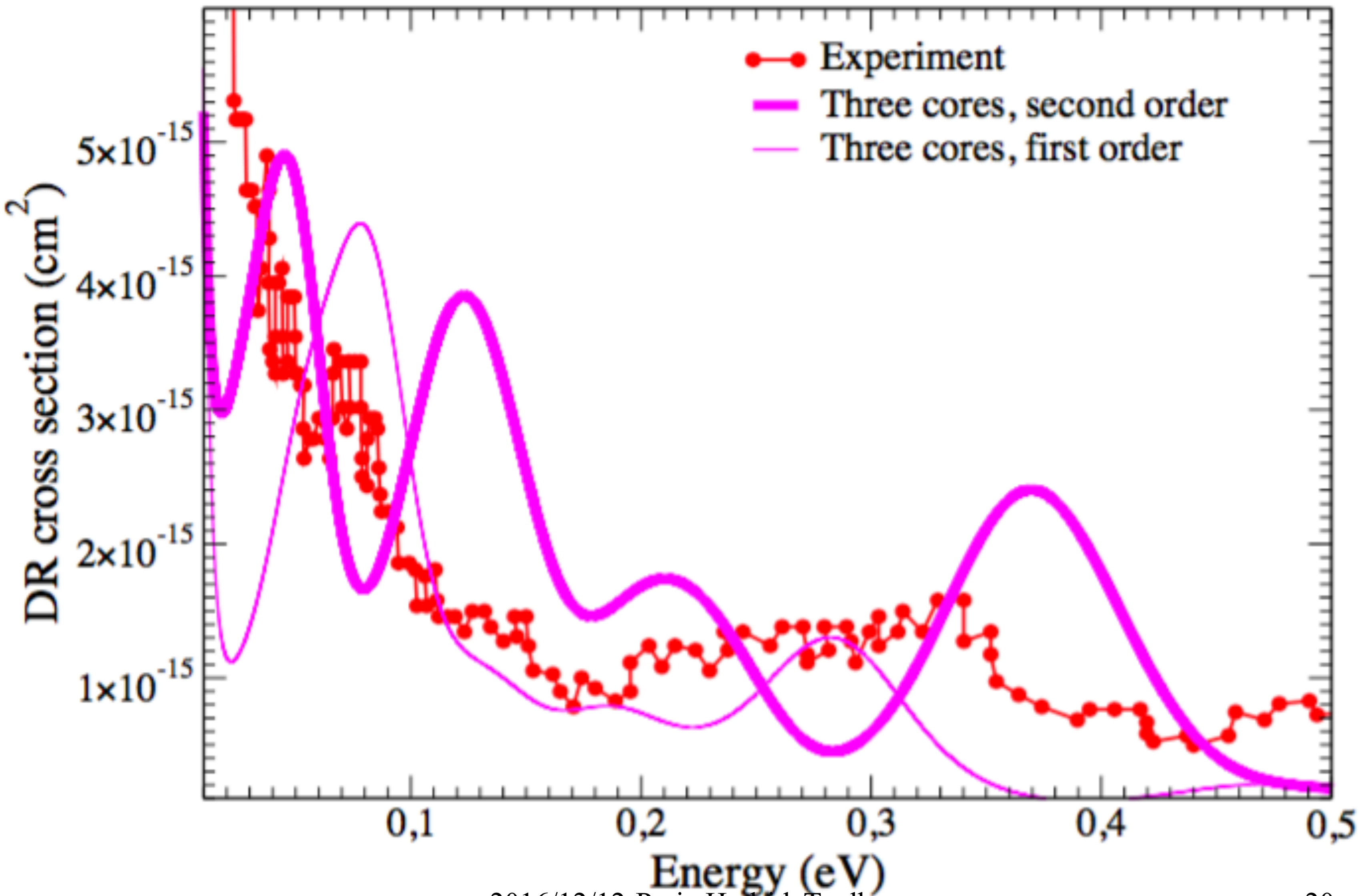
CH^+: BOUND ionic cores:

c1, c2, c3

+

electron

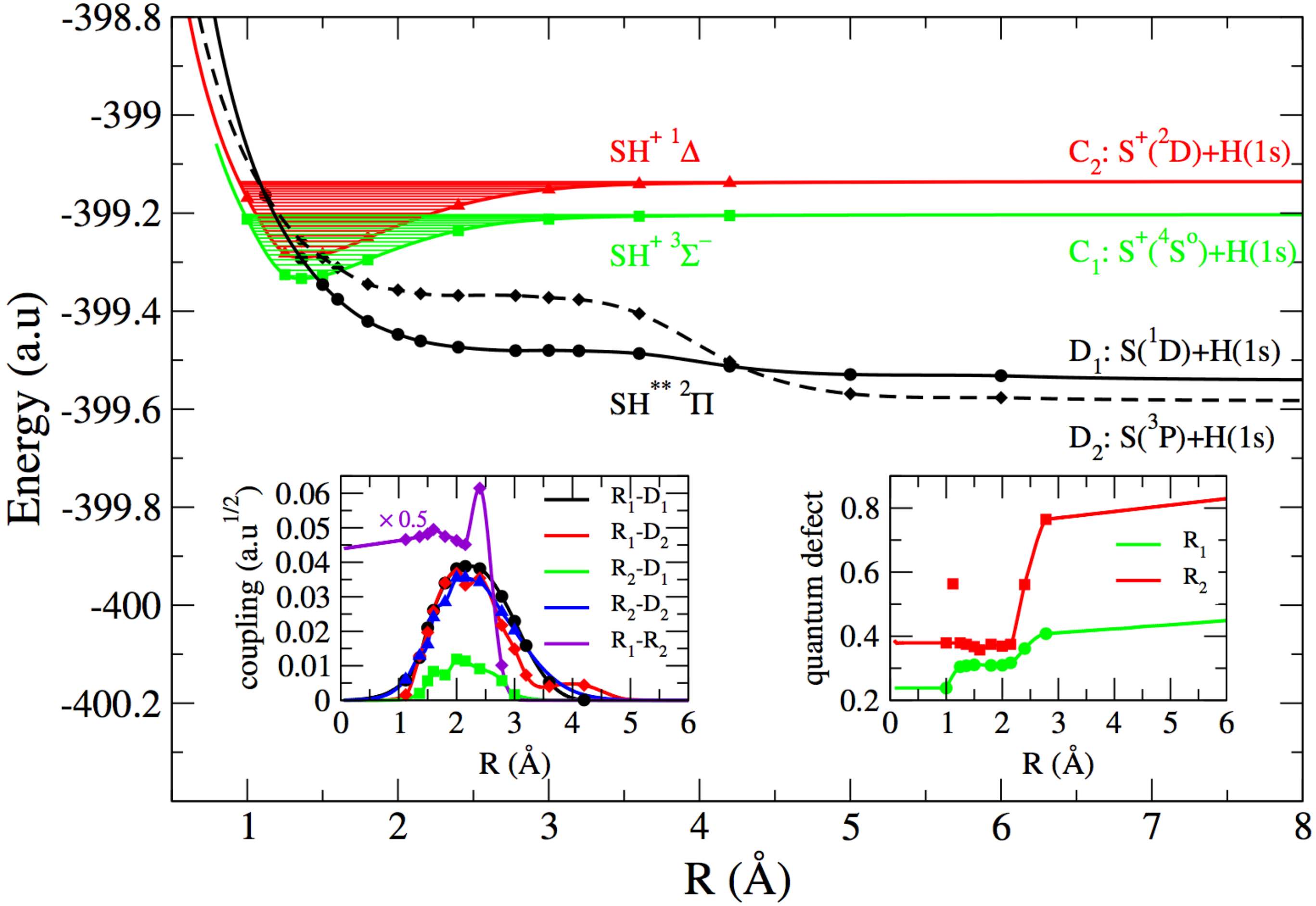
CH^+ + e^- @ high energy: rotational efects neglected, but account of the core-excited Rydberg states:



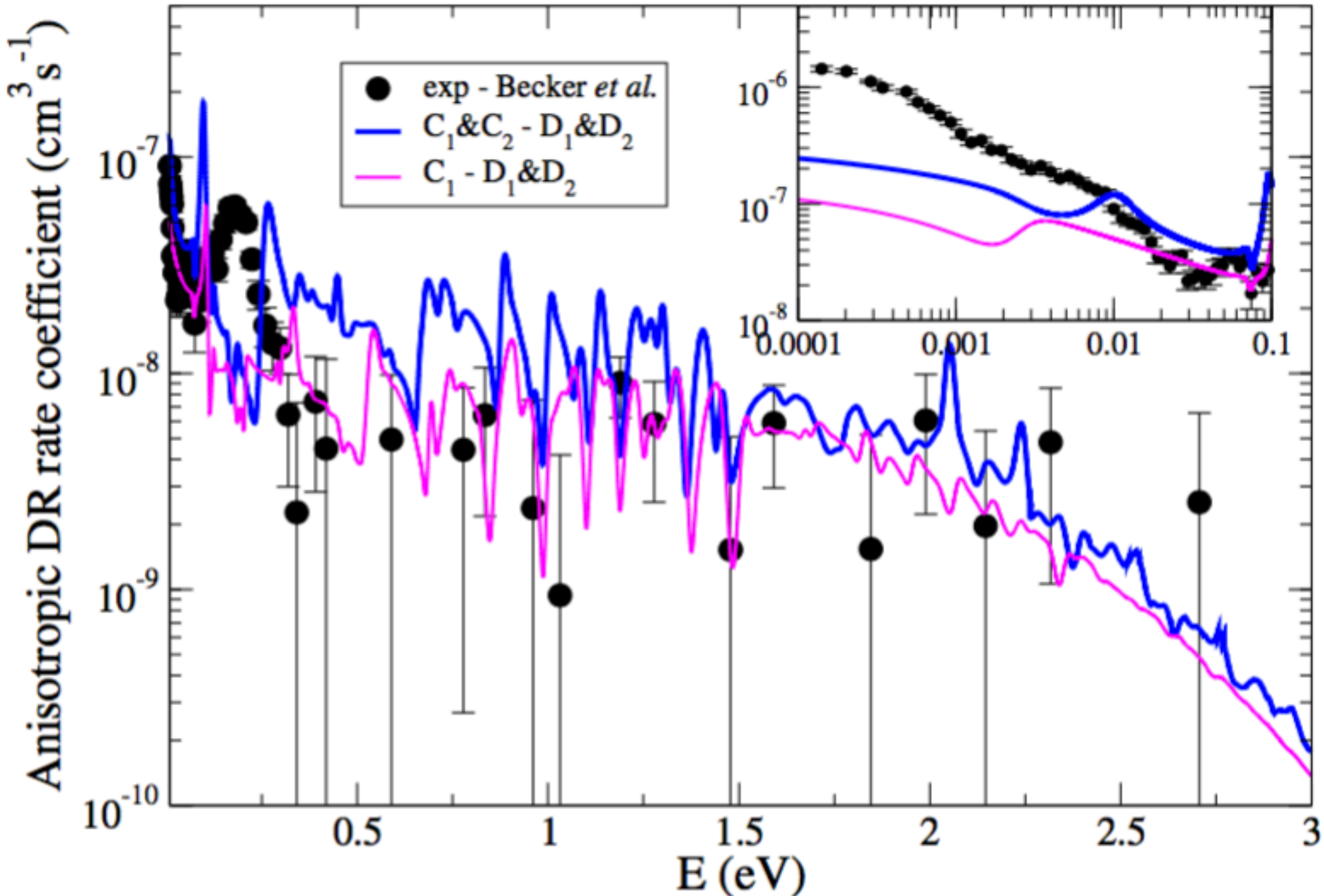
$SH^+ + e^-$

$SH^+ + e^-$: rotational efects neglected, account of the core-excited Rydberg states:

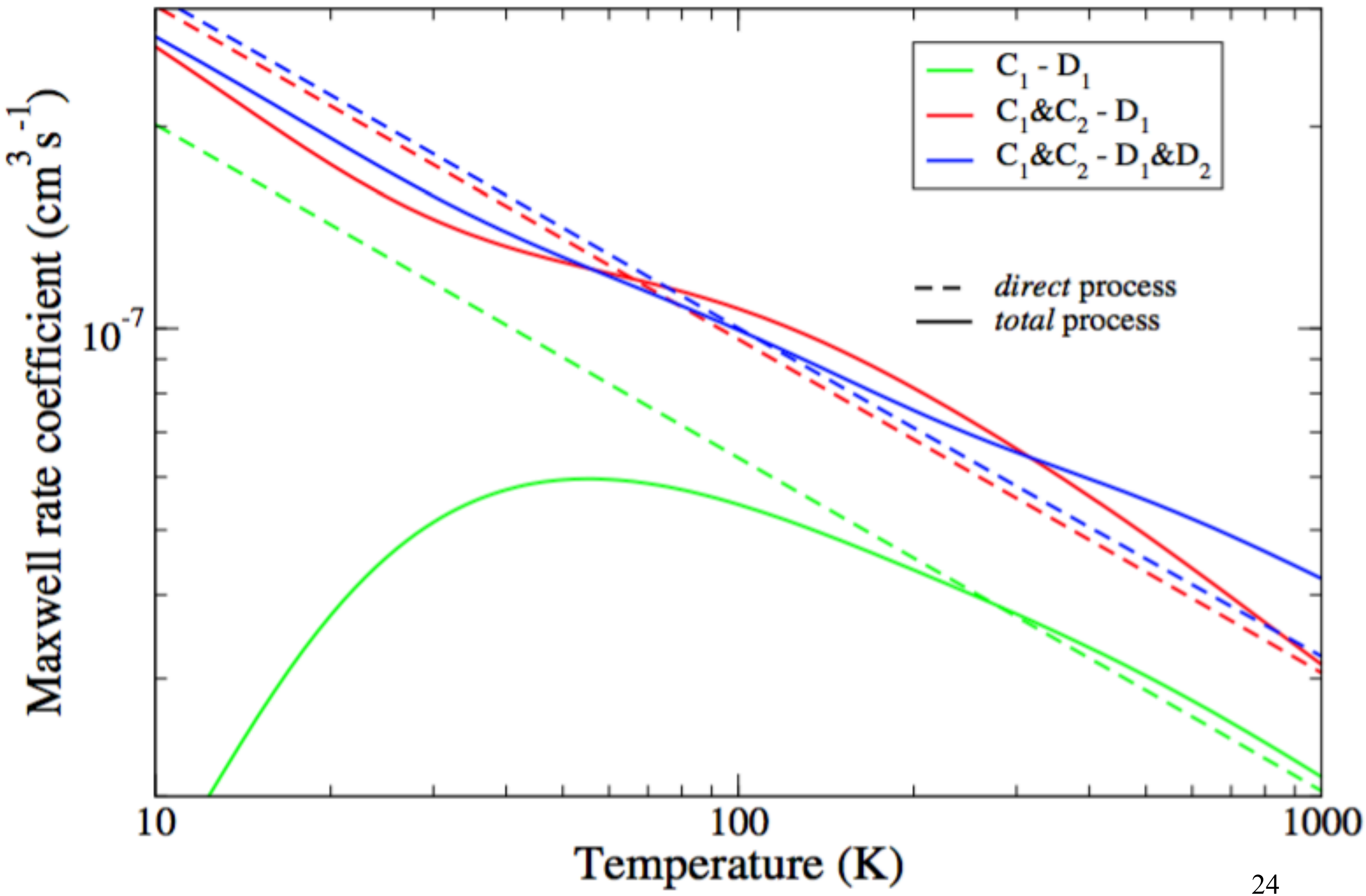
Bock-diagonalization method, Talbi et al 2015:



$SH^+ + e^-$: rotational efects neglected, account of the core-excited Rydberg states:



$SH^+ + e^-$



C1 - D1
C1&C2 - D1
C1&C2 - D1&D2
direct process
total process
10-7
Maxwell rate coefficient (cm3 s-1)
10
100
1000
Temperature (K)

$$BeH^{+} + e^{-}$$

Journal of Molecular Spectroscopy

Volume 311, May 2015, Pages 76–83

Theory and Spectroscopy

Beryllium monohydride (BeH): Where we are now, after 86 years of spectroscopy

Nikesh S. Dattani

Due to its simplicity, BeH is expected to be present in astronomical contexts such as exoplanetary atmospheres, cool stars, and the interstellar medium [27], but in the context of astronomy, has only been found on our Sun, in the two studies described in [28, 29].

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Mon. Not. R. Astron. Soc. **425,** 34–43 (2012) doi:10.1111/j.1365-2966.2012.21367.x

ExoMol line lists – I. The rovibrational spectrum of BeH, MgH and CaH in the $X\,^2\Sigma^+$ state

Benjamin Yadin, Thomas Veness, Pierandrea Conti, Christian Hill,
Sergei N. Yurchenko and Jonathan Tennyson★

Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London

BeH is one of the simplest heteronuclear diatomic molecules, and hence it is a strong contender for being observed in contexts such as exoplanetary atmospheres, cool stars and the interstellar medium. However, there are only very few astrophysical records of BeH, for example, a detection of $A\,^2\Sigma^+ \rightarrow X\,^2\Sigma^+$ emission lines of BeH in the sunspot umbra spectra by Wöhl (1971) and Shanmugavel et al. (2008).

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Atomic Data and Nuclear Data Tables ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Low-energy collisions between electrons and BeH^+: Cross sections and rate coefficients for all the vibrational states of the ion

S. Niyonzima [a,b], S. Ilie [a,c], N. Pop [a,c], J. Zs. Mezei [a,d,e,f], K. Chakrabarti [g], V. Morel [h], B. Peres [h], D.A. Little [i], K. Hassouni [d], Å. Larson [j], A.E. Orel [k], D. Benredjem [e], A. Bultel [h], J. Tennyson [i], D. Reiter [l], I.F. Schneider [a,e,*]

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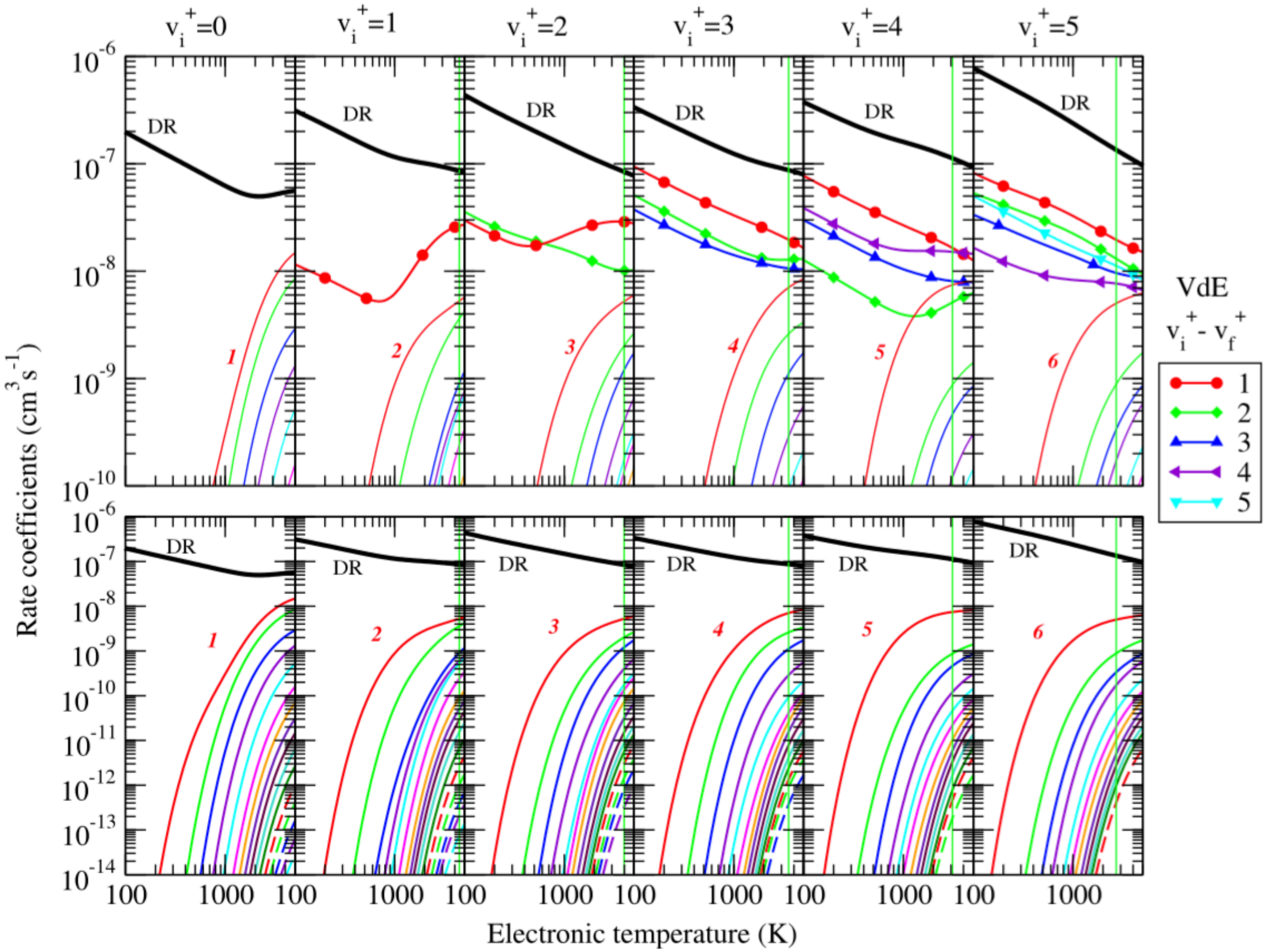
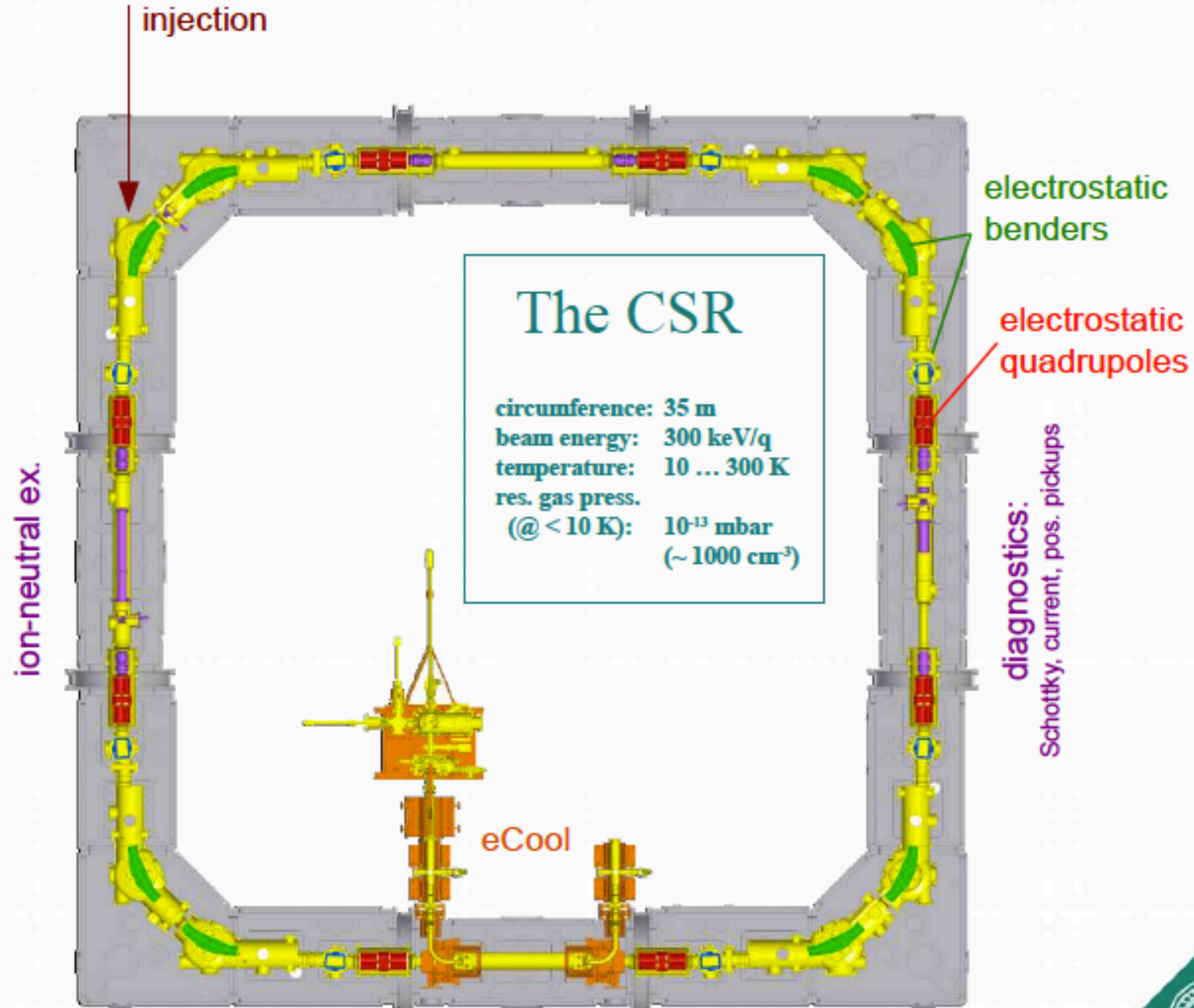


Graph 4. Dissociative recombination (DR, thick line), vibrational excitation (VE, thin lines) and vibrational de-excitation (VdE, symbols and thick lines) Maxwell rate coefficients of ground ($v_i^+ = 0$) and excited ($v_i^+ = 1, \ldots, 5$) BeH^+ in its electronic ground state (total mechanism). For VE, since the rate coefficients decrease monotonically with the excitation, the lowest final vibrational quantum number of the target is indicated only, and the lower panels extend the range down to 10^{-14} cm^3/s.

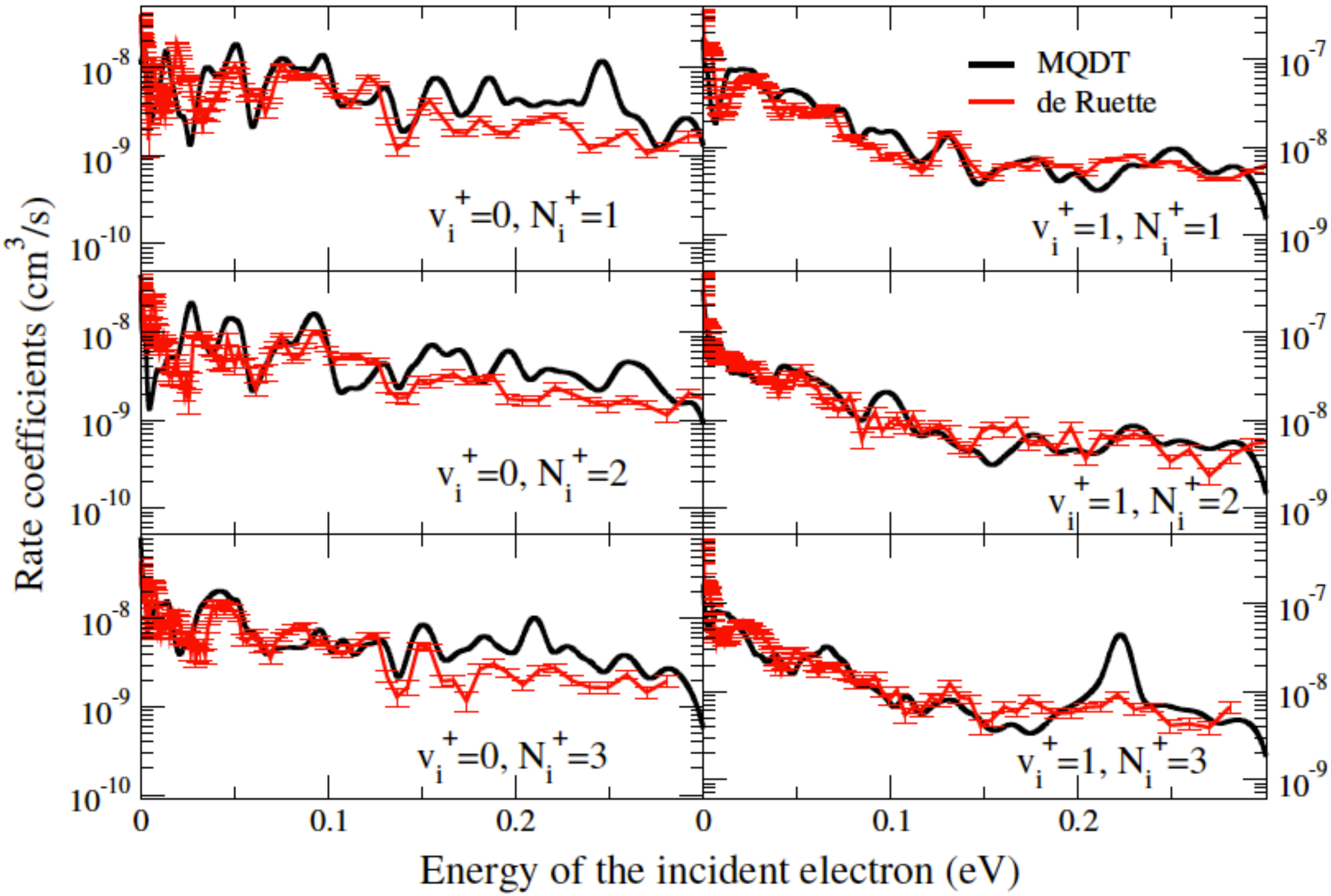
And …
the FUTURE


injection
electrostatic benders
electrostatic quadrupoles
diagnostics:
Schottky, current, pos. pickups
ion-neutral ex.
eCool
The CSR
circumference: 35 m
beam energy: 300 keV/q
temperature: 10 … 300 K
res. gas press.
(@ < 10 K): 10^-13 mbar
(~ 1000 cm^-3)

Are we prepared ?

$H_2^+(N_i^+, v_i^+) + e^- \longrightarrow H + H$

1st state-to-state comparison experiment/theory ever !



Perspectives:

$OH^+ + e^-$

$HCl^+ + e^-$

$ArH^+ + e^-$

$\text{Polyatomic}^+ + e^-$

...

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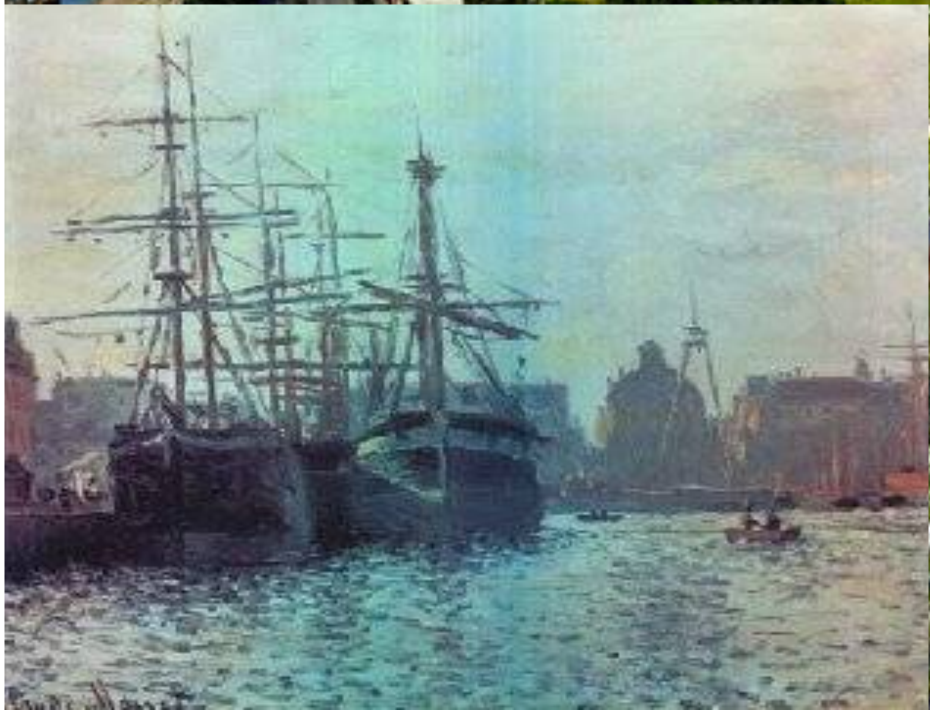
$$AB^+(N_i^+, v_i^+) + e^- \longrightarrow A + B$$
$$\longrightarrow AB^+(N_f^+, v_f^+) + e^-$$
$$\longrightarrow A + B^+ + e^-$$


1 16:30




Thank you for
your attention !