



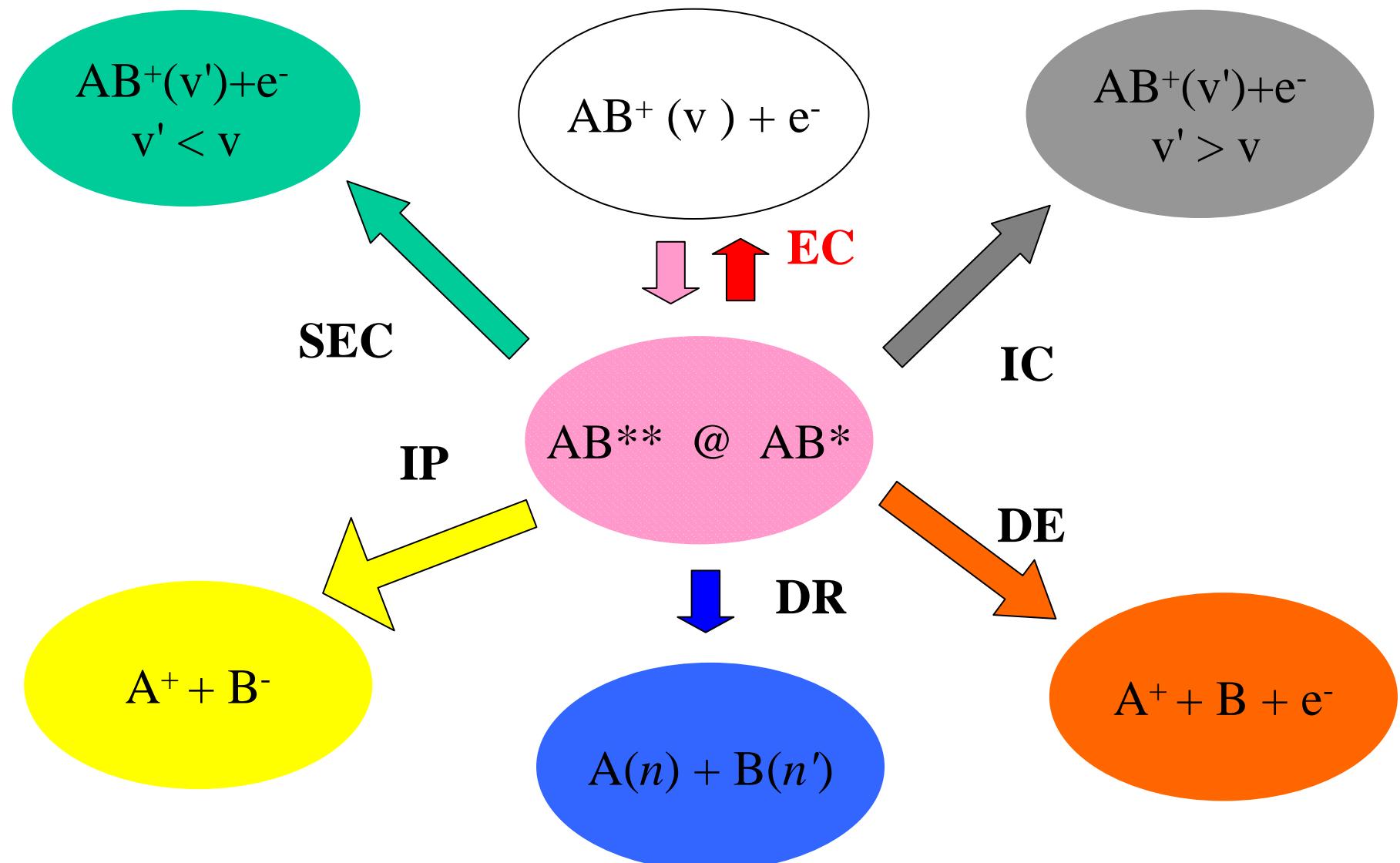
**DISSOCIATIVE RECOMBINATION  
of ELECTRONS with MOLECULAR CATIONS:  
APPLICACTION to  
NO<sup>+</sup>, CO<sup>+</sup>, H<sub>2</sub><sup>+</sup> and ISOTOPES**

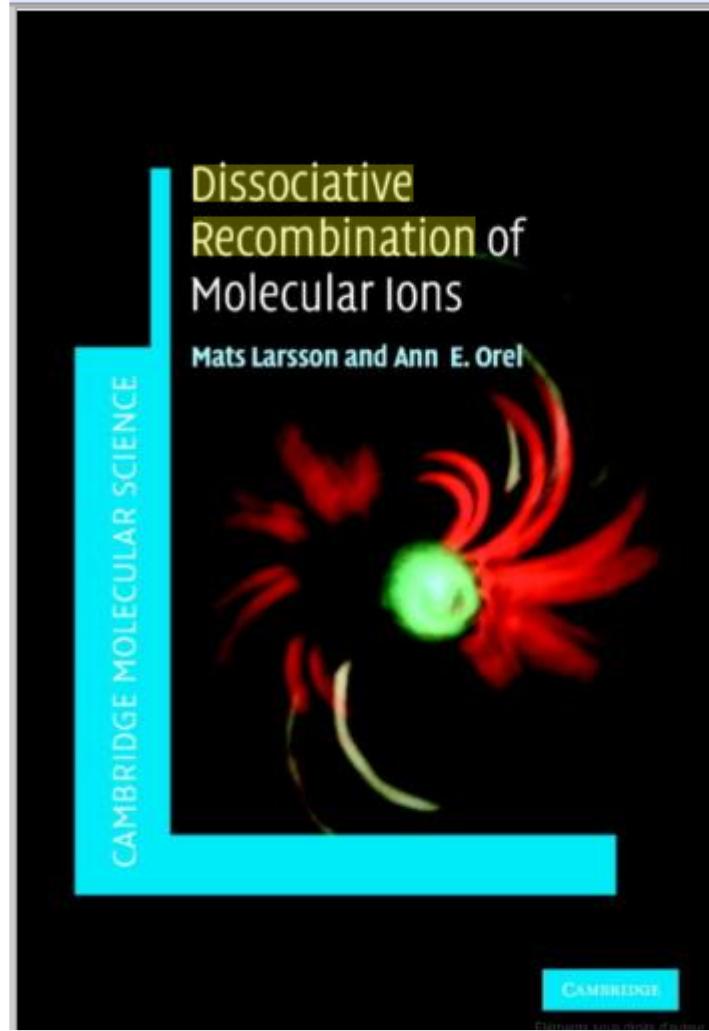
$$e^- + AB^+ \rightarrow A + B, e^- + AB^+, e^- + A^+ + B$$

**Ioan F. SCHNEIDER**

*Equipe “Instabilités, Turbulence, Plasmas”  
Laboratoire Ondes et Milieux Complexes, FRE-3102  
Université du Havre*

## REACTIVE COLLISIONS:





## Previous International Conferences

- 1) Lake Louise, Alberta, Canada (1988),
- 2) Saint Jacut, Brittany, France (1992),
- 3) Ein Gedi, Israel (1995),
- 4) Nässlingen, Stockholm Archipelago, Sweden (1999),
- 5) Chicago, USA (2001),
- 6) Mosbach, Germany (2004),
- 7) Ameland, Netherlands (2007).

## Previous International Conferences

- 8) Kalamazoo, USA (2010)
- 9) Le Havre, France (? 2012)



ELSEVIER

Journal of Nuclear Materials 313–316 (2003) 1202–1205

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journal of  
nuclear  
materials

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[www.elsevier.com/locate/jnucmat](http://www.elsevier.com/locate/jnucmat)

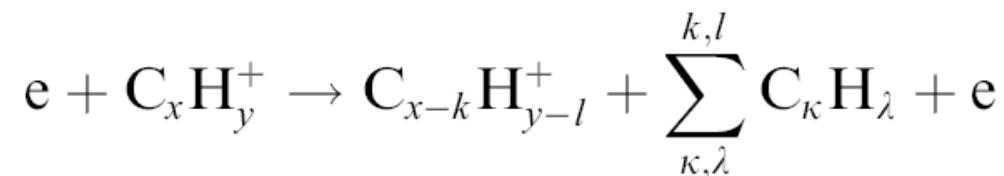
## Unified analytic representation of hydrocarbon impurity collision cross-sections

R.K. Janev <sup>a,b</sup>, D. Reiter <sup>a,\*</sup>

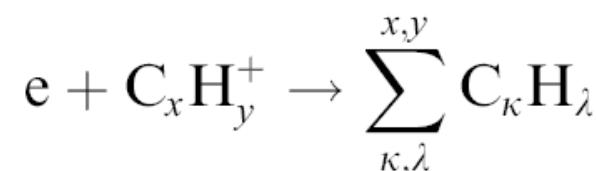
<sup>a</sup> *Institut für Plasmaphysik, Forschungszentrum-Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster,  
D-52425 Jülich, Germany*

<sup>b</sup> *Macedonian Academy of Sciences and Arts, P.O. Box 428, 1000 Skopje, Macedonia*

(3) Dissociative excitation (DE) of  $C_xH_y^+$  ions:



(4) Dissociative recombination (DR):



## Catalytic mechanism of divertor plasma recombination provided by hydrocarbon impurities

R. K. Janev

*National Institute for Fusion Science, 322-6 Oroshi, Toki, Gifu 509-5292, Japan  
and Macedonian Academy of Sciences and Arts, Skopje, Macedonia*

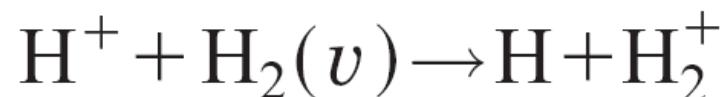
T. Kato

*National Institute for Fusion Science, 322-6 Oroshi, Toki, Gifu 509-5292, Japan*

J. G. Wang

*National Institute for Fusion Science, 322-6 Oroshi, Toki, Gifu 509-5292, Japan  
and Institute for Applied Physics and Computational Mathematics, Beijing, People's Republic of China*

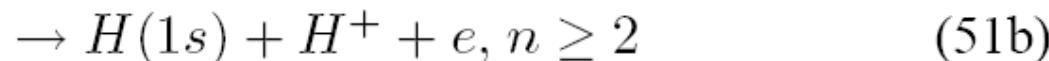
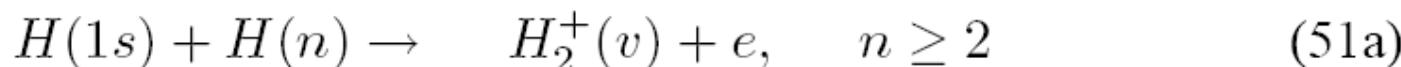
(ii) ion-conversion (IC) recombination mechanism<sup>13,14</sup>



**Report  
4105, Juelich,  
2006**

# **Collision Processes in Low-Temperature Hydrogen Plasmas**

R.K. Janev<sup>1,2</sup>, D. Reiter<sup>1</sup>, U. Samm<sup>1</sup>

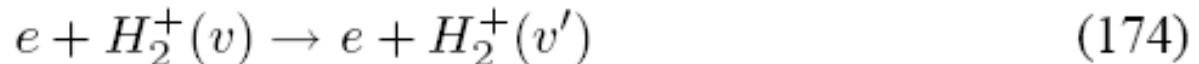


and the associative detachment reaction



## **7.1.1 Vibrational excitation**

Since  $H_2^+(1s\sigma_g)$  ion is a non-polar system, its electron-impact vibrational excitation



# **Atomic Physics in ITER**

## **The Foundation for the Next Step to Fusion Power**

Daren Stotler

*Princeton Plasma Physics Lab*

The 5<sup>th</sup> International Conference on Atomic  
and Molecular Data and Their Applications  
Meudon, France, October 15-19, 2006



# More Complex H<sub>2</sub>, H<sub>2</sub><sup>+</sup> Behavior



- 
- Lower temperatures  $\Rightarrow$  H<sub>2</sub> lifetime extended  $\Rightarrow$  undergo additional processes,
    - Including vibrational excitation & de-excitation,
    - $\Rightarrow$  ion conversion: H<sub>2</sub>(v) + H<sup>+</sup>  $\rightarrow$  H<sub>2</sub><sup>+</sup> + H,
    - Also brings in other species: H<sub>3</sub><sup>+</sup>, H<sup>-</sup>.
  - Initial predictions were for “Molecule Assisted Recombination” [Krasheninnikov 1997],
    - But, ASDEX-U modeling [Fantz 2001], showed instead “Molecule Assisted Dissociation”!
    - Explicitly modeled transport of vibrationally excited molecules!
  - Attempts to fold effects into effective “collisional radiative” rates for H<sub>2</sub>, H<sub>2</sub><sup>+</sup>: [Sawada 1995, Greenland 2001, Pigarov 2002].
  - [Janev 2003] reviews & assesses current data,
    - More data still needed:
      - State-selective processes involving vibrationally excited states,
      - Impact of rotational excitation on plasma kinetics,
      - Isotope specific data.
    - Sawada has more complete model on the way.
    - Still need to be integrated into comprehensive, simplified model for simulations.

# Available cross sections for $\text{H}_2^+$ and OTHER cations, BUT:

- Few or not exhaustive (energy, ro-vibrational excitation of the target)
- Permanent update of input molecular data (PEC's & couplings)
- Need of data for further species/isotopomers
- Need of « new » reactions study:
  - \* inelastic & superelastic collisions
  - \* ion-pair production

# My colleagues



**O. Motapon, Douala,**



**F. O. Waffeu Tamo\*, Le Havre & Douala**



**D. R. Backodissa-Kiminou,**

*Le Havre*



**F. Lique, Le Havre**

2009/10/05, ADAS meeting



**C. Laville,**

*Le Havre & Montréal*

## COLLABORATIONS

### Theory

**A. Suzor-Weiner, Ch. Junge, O. Dulieu, Paris-South University**

**L. Tchang-Brillet, Paris VI University & Obs. de Paris @ Meudon**

**A. E. Orel, University of California @ Davis**

**L. Pichl, International Christian University, Tokyo**

**J. Tennyson, University College London,**

**D. Tudorache, Ecole Centrale de Paris**

### Experiment

**A. Wolf, D. Zajfman, D. Schwalm & team, MPIK & Weizmann Inst.**

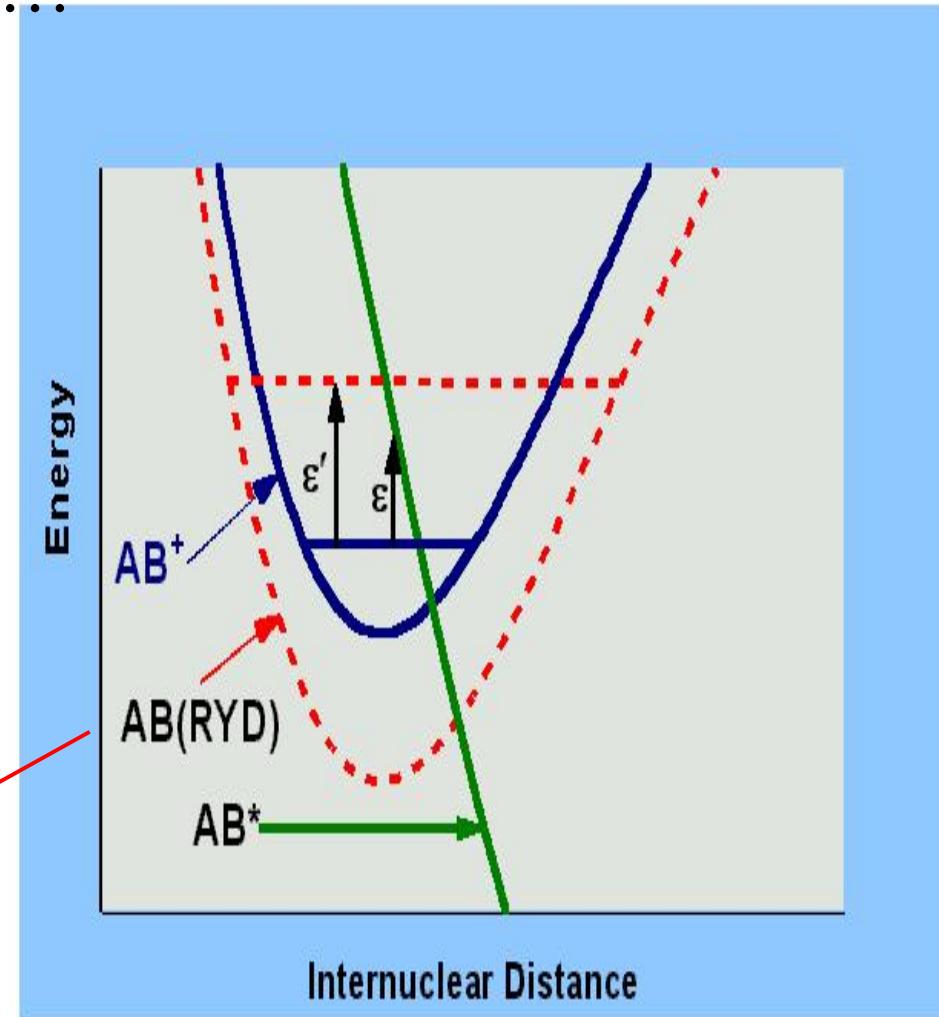
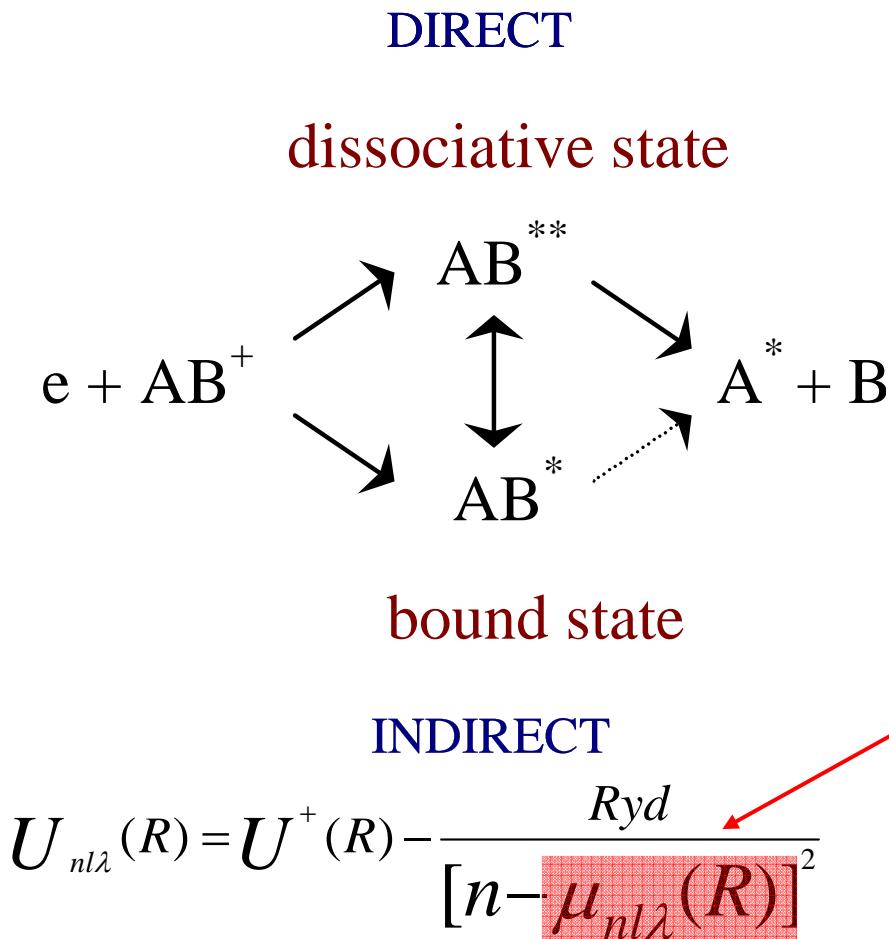
**X. Urbain, Louvain la Neuve Catholic University**

**M. Larsson & team, Stockholm University**

### Kinetics

**A. Bultel, P. Vervisch, B. Chéron, CORIA, Rouen University**

# Multichannel Quantum Defect Theory: Seaton, Fano, Jungen, Green, Suzor-Weiner, ...

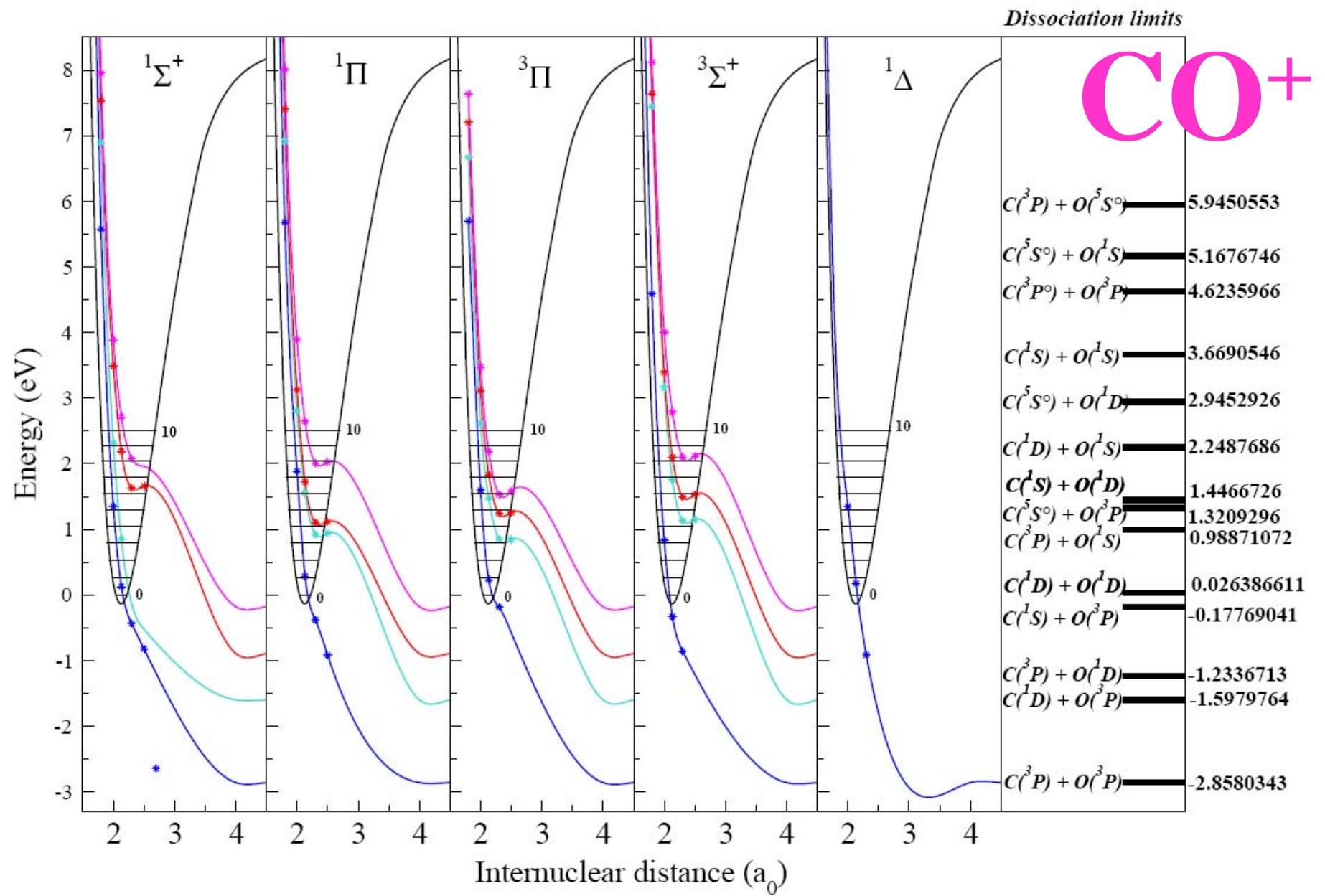


If  $n \geq n_0$ ,  $\mu_{nl\lambda} \approx \mu_{l\lambda}$  (energy independent) **ALMOST...!?**

2009/10/05, ADAS meeting

# **TARGET in its GROUND STATE**

2009/10/05, ADAS meeting



CO<sup>+</sup>

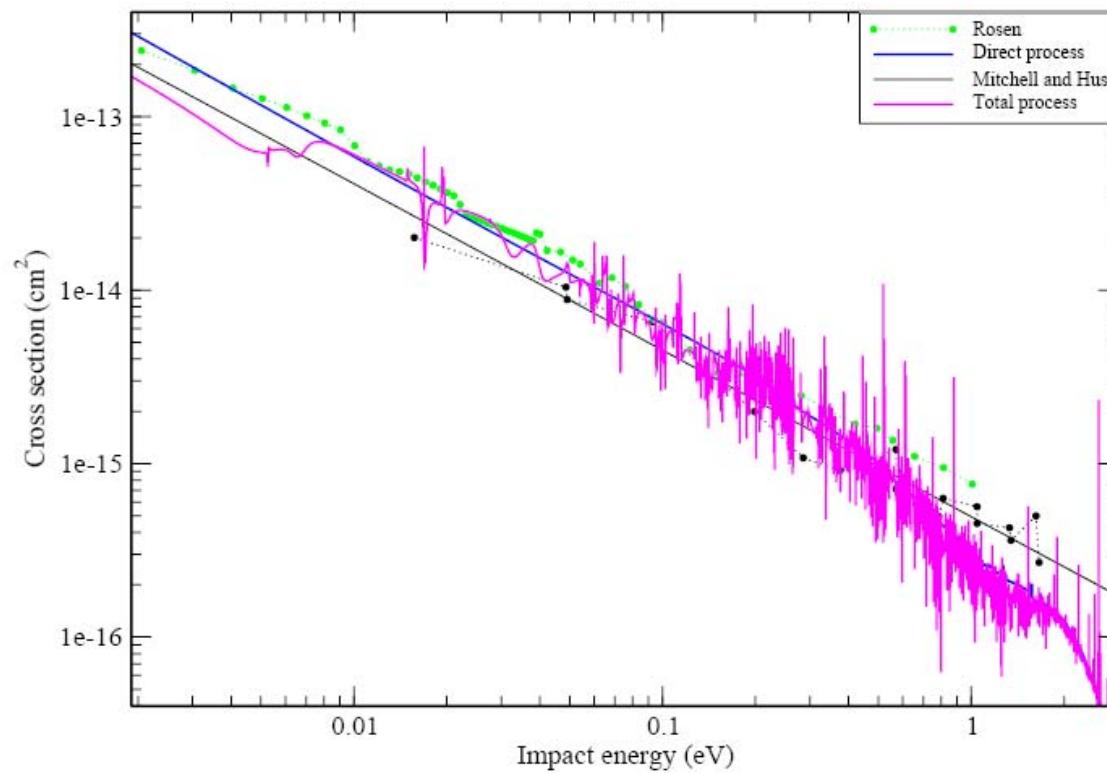


Figure 5: CO<sup>+</sup> DR cross sections: Direct process in blue and, total process in magenta in which we can see the manifestation of Rydberg series as resonances. In black and green, the experiment results of Mitchell and Rosen respectively.

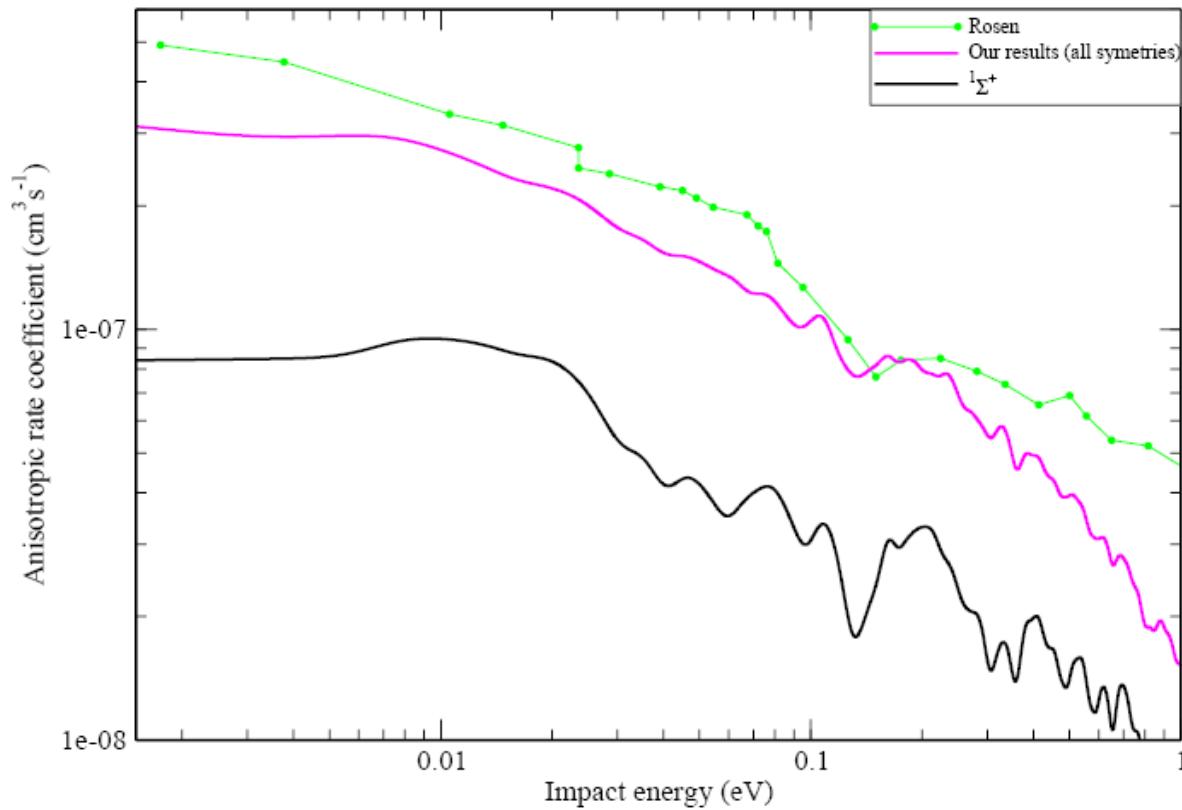


Figure 7: Anisotropic rate coefficients. Rosen experiment results are in green. Our theoretical results are in magenta for all symmetries and in black for the  ${}^1\Sigma^+$  CO symmetrie which represents very well the shape of expériment results.

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# HD<sup>+</sup>

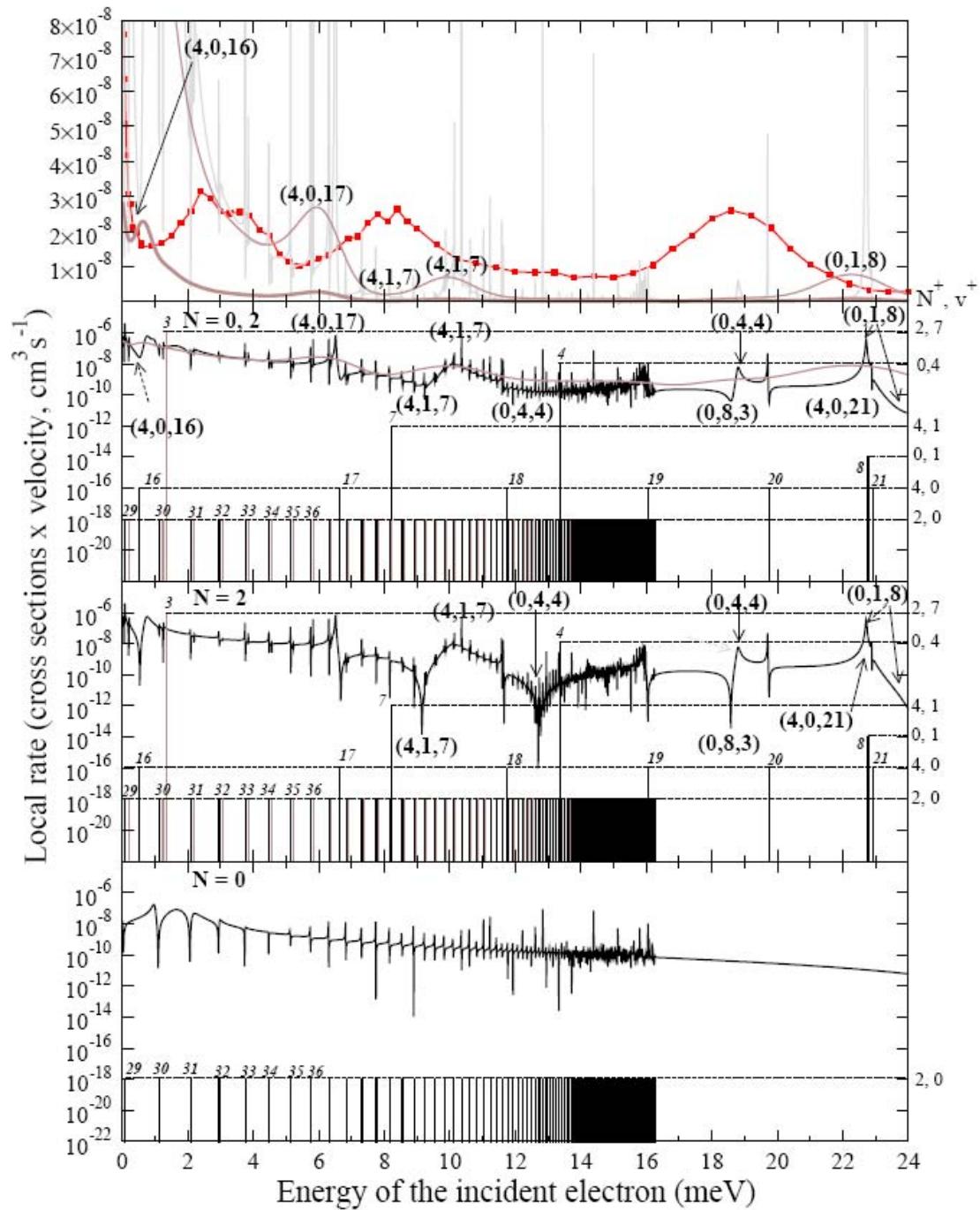
*Waffeu Tamo, Buhr  
et al 2004-2008*

N<sub>i</sub><sup>+</sup>=0, v<sub>i</sub><sup>+</sup>=0

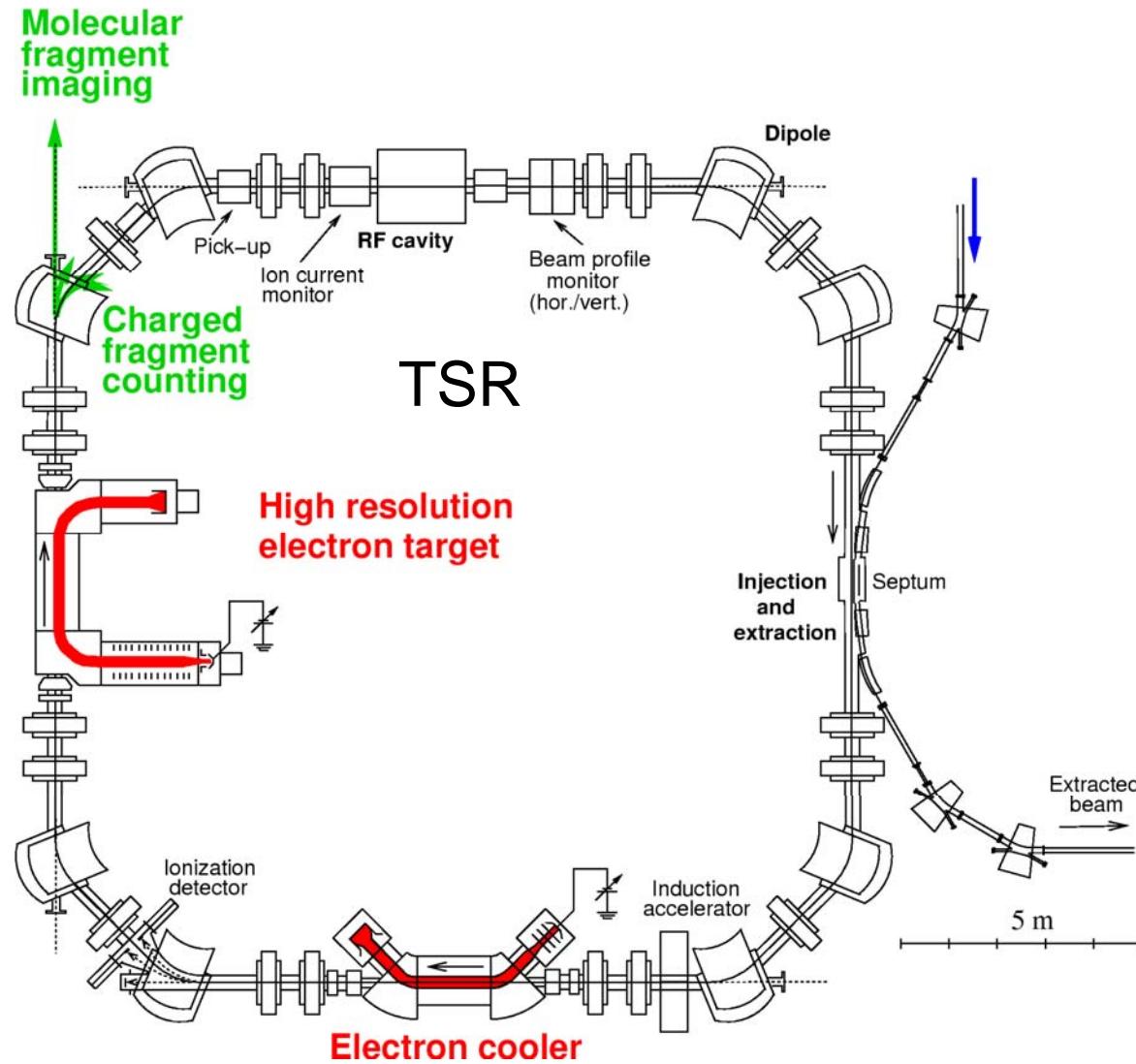
Hyperfine Interact (2006) 172:111-124  
DOI 10.1007/s10751-007-9575-7

Progress in stored ion beam experiments on atomic  
and molecular processes

Andreas Wolf · Henrik Buhr · Manfred Grieser ·  
Robert von Hahn · Michael Lestinsky · Eva Lindroth ·  
Dmitry A. Orlov · Stefan Schippers · Ioan F. Schneider



# Collision experiments at TSR



2009/10/05, ADAS meeting

**CROSS SECTION  
DEPENDENCIE** on  
**ROTATIONAL  
EXCITATION**

**of the TARGET**

2009/10/05, ADAS meeting

# $\text{HD}^+$ DR, vibrationally relaxed

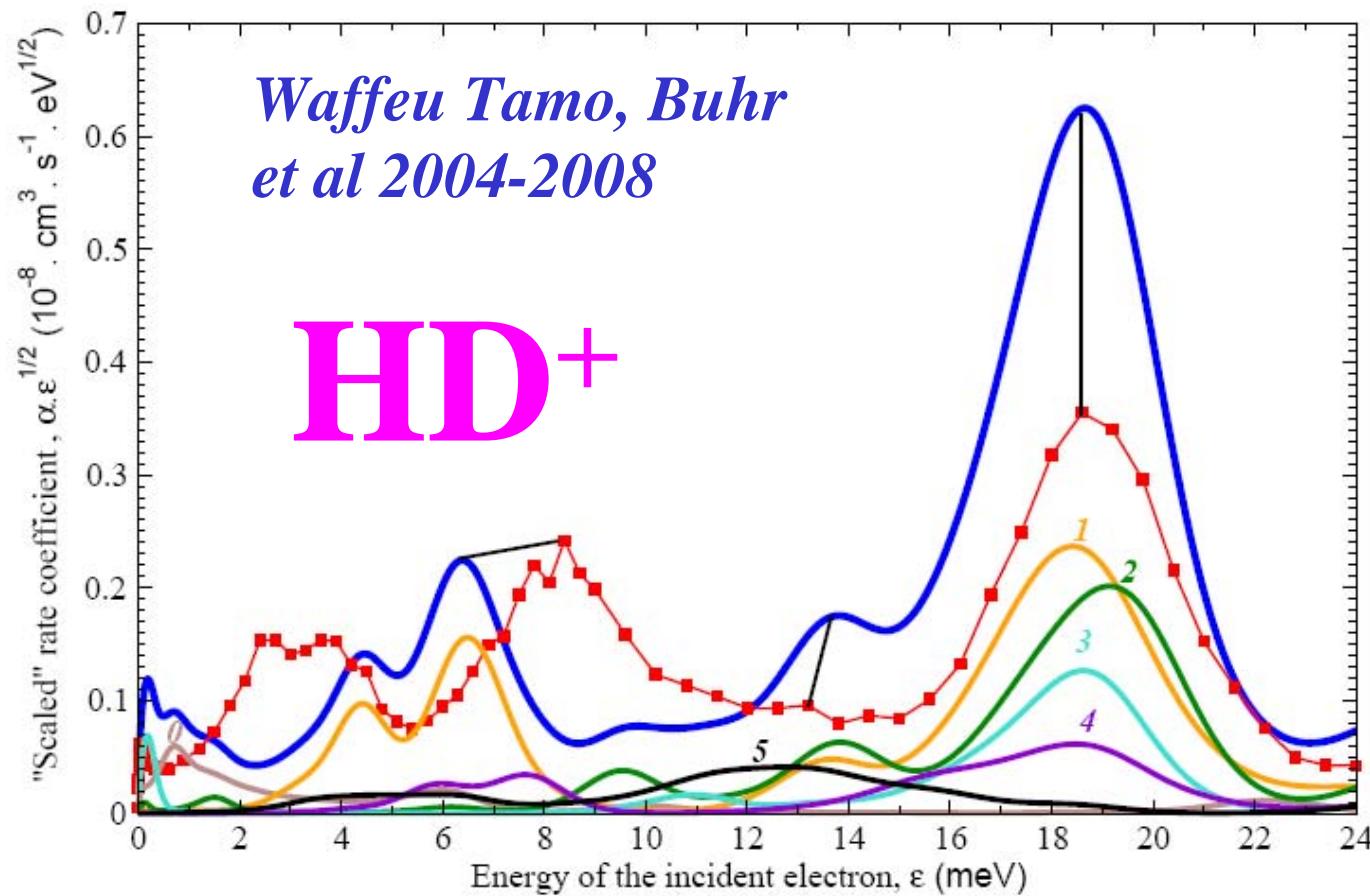


FIG. 5.3: Contribution des états rotationnels  $N_i^+ = 0, 1, 2, 3, 4, 5$  (brun, orange, vert, turquoise, violet, noir, respectivement) au taux de recombinaison dissociative des ions  $\text{HD}^+$  (calculs MQDT (bleu) et expérience(rouge)).

## Rotational Cooling of HD<sup>+</sup> Molecular Ions by Superelastic Collisions with Electrons

D. Shafir,<sup>1</sup> S. Novotny,<sup>2</sup> H. Buhr,<sup>2</sup> S. Altevogt,<sup>2</sup> A. Faure,<sup>3</sup> M. Grieser,<sup>2</sup> A. G. Harvey,<sup>4</sup> O. Heber,<sup>1</sup> J. Hoffmann,<sup>2</sup> H. Kreckel,<sup>2</sup> L. Lammich,<sup>2</sup> I. Nevo,<sup>1</sup> H.B. Pedersen,<sup>2</sup> H. Rubinstein,<sup>1</sup> I.F. Schneider,<sup>5</sup> D. Schwalm,<sup>1,2</sup> J. Tennyson,<sup>4</sup> A. Wolf,<sup>2</sup> and D. Zajfman<sup>1</sup>

<sup>1</sup>Department of Particle Physics, Weizmann Institute of Science, 76100 Rehovot, Israel

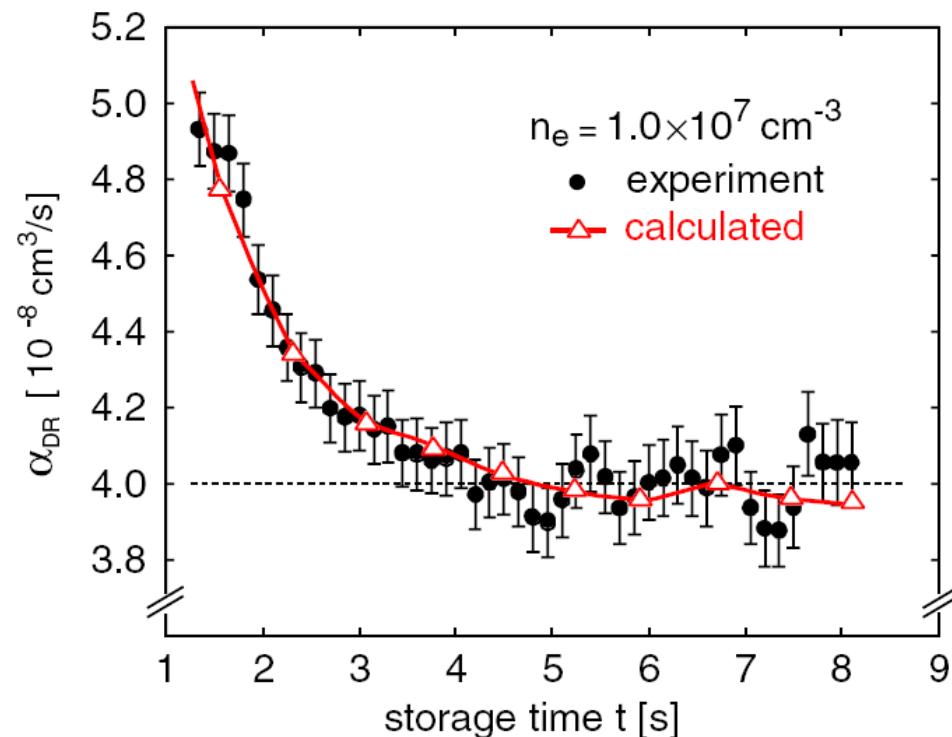
<sup>2</sup>Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

<sup>3</sup>Laboratoire d'Astrophysique de Grenoble, Université Joseph Fourier, UMR 5571 CNRS, Grenoble, France

<sup>4</sup>Department of Physics and Astronomy, University College London, London WC1E6BT, United Kingdom

<sup>5</sup>Laboratory of Waves and Complex Media, FRE-CNRS-3102, University of Le Havre, France

HD<sup>+</sup>



$$\tilde{\alpha}_0 = 3.8 \pm 0.1, \quad \tilde{\alpha}_3 = 4.0 \pm 0.2, \quad \text{and} \quad \tilde{\alpha}_6 = 9.0 \pm 1.3$$

in units of  $10^{-8}$  cm<sup>3</sup>/s. The total DR rate coefficients

Fig. 2. Note that this result constitutes another example for the  $J$  dependence of the DR cross section of molecular hydrogen ions [5], and that these values compare favorably, in particular, when taking the error of the absolute DR scale of 20% into account, to the corresponding averaged values of 5.3, 4.0, and  $10.3 \times 10^{-8}$  cm<sup>3</sup>/s, respectively, derived within the MQDT approach [16].

**HD<sup>+</sup>**



PHYSICAL REVIEW A 77, 052711 (2008)

**Decisive role of rotational couplings in the dissociative recombination and superelastic collisions  
of  $\text{H}_2^+$  with low-energy electrons**

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*ICTP, Strada Costiera 11, 34014 Trieste, Italy*

*and Department of Physics, Faculty of Science, University of Douala, P.O. Box 24157, Douala, Cameroon*

Francois Olivier Waffeu Tamo

*Centre for Atomic Molecular Physics and Quantum Optics (CEPAMOQ), Faculty of Science, University of Douala,  
P.O. Box 8580, Douala, Cameroon*

*and Laboratoire de Mécanique, Physique et Géosciences, UFR Sciences et Techniques,  
Université du Havre, 25, rue Philippe Lebon, Boîte Postale 540, 76058, Le Havre, France*

Xavier Urbain

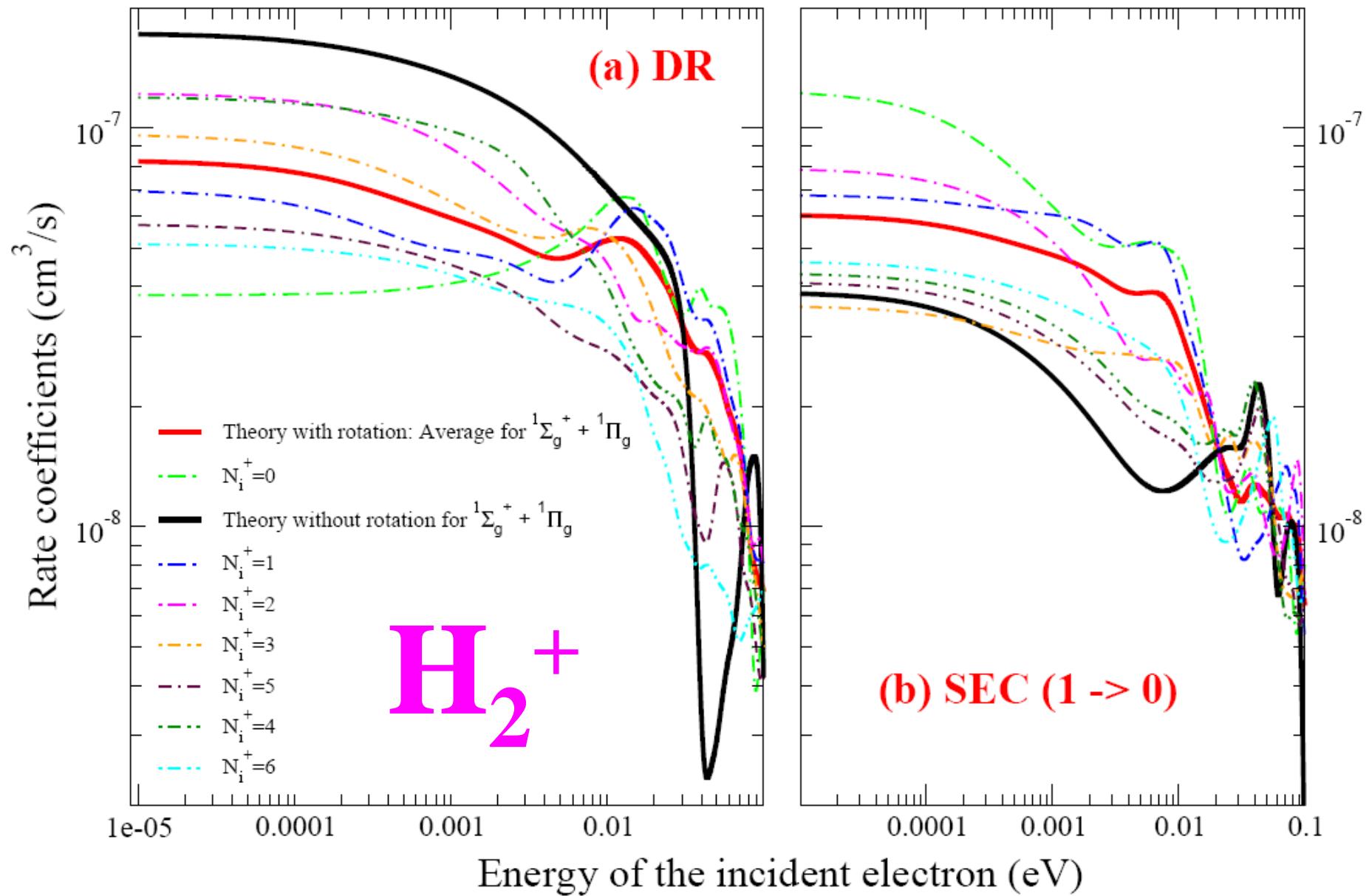
*Laboratoire PAMO, Université Catholique de Louvain, chemin du cyclotron 2, 1348, Louvain-La-Neuve, Belgium*

Ioan F. Schneider

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Boîte Postale 540, 76058, Le Havre, France*

(Received 28 December 2007; published 20 May 2008)

# Partial and average rate coefficients for $v_i^+ = 1$



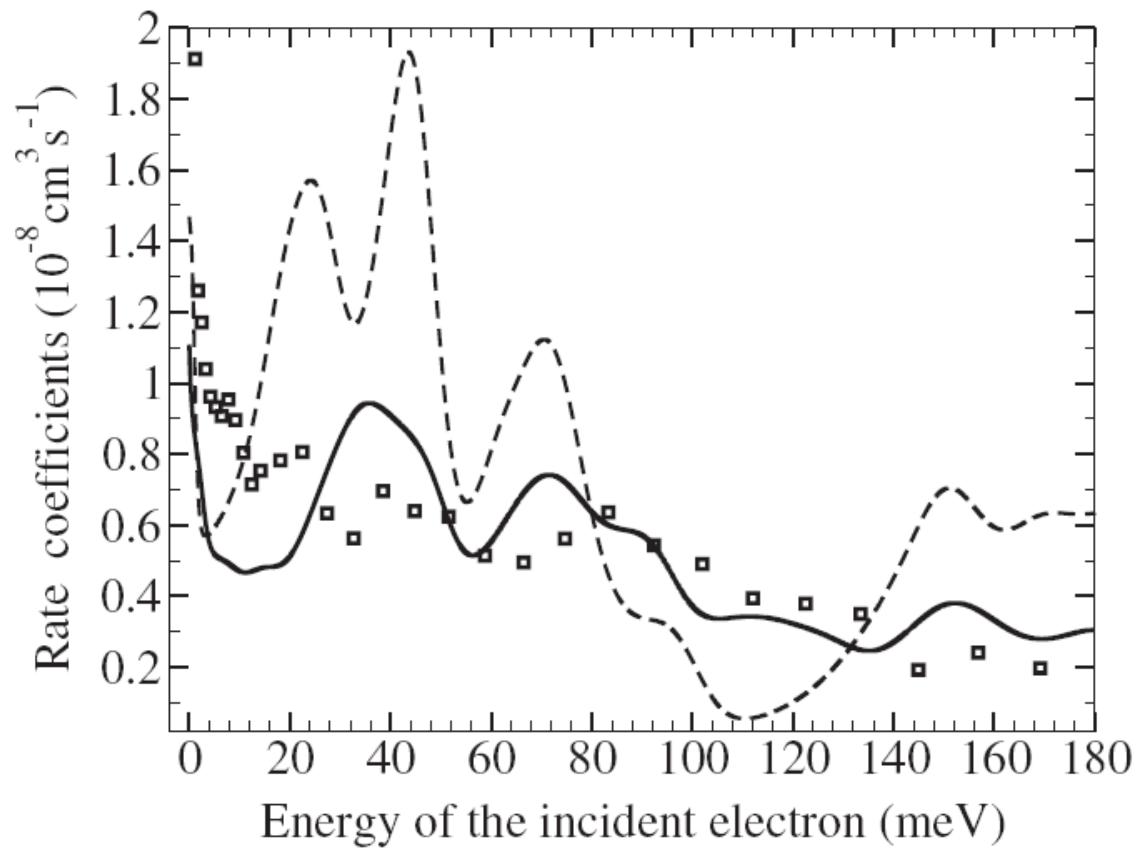


FIG. 1. Rate coefficients for dissociative recombination from  $v_i^+ = 0$ . Dashed line, theory without rotation [22]; full line, theory with rotation; squares, experiment [24]. Better agreement with experiment is found in the rotational case. Also a sensitivity with respect to the quantum defect is observed.

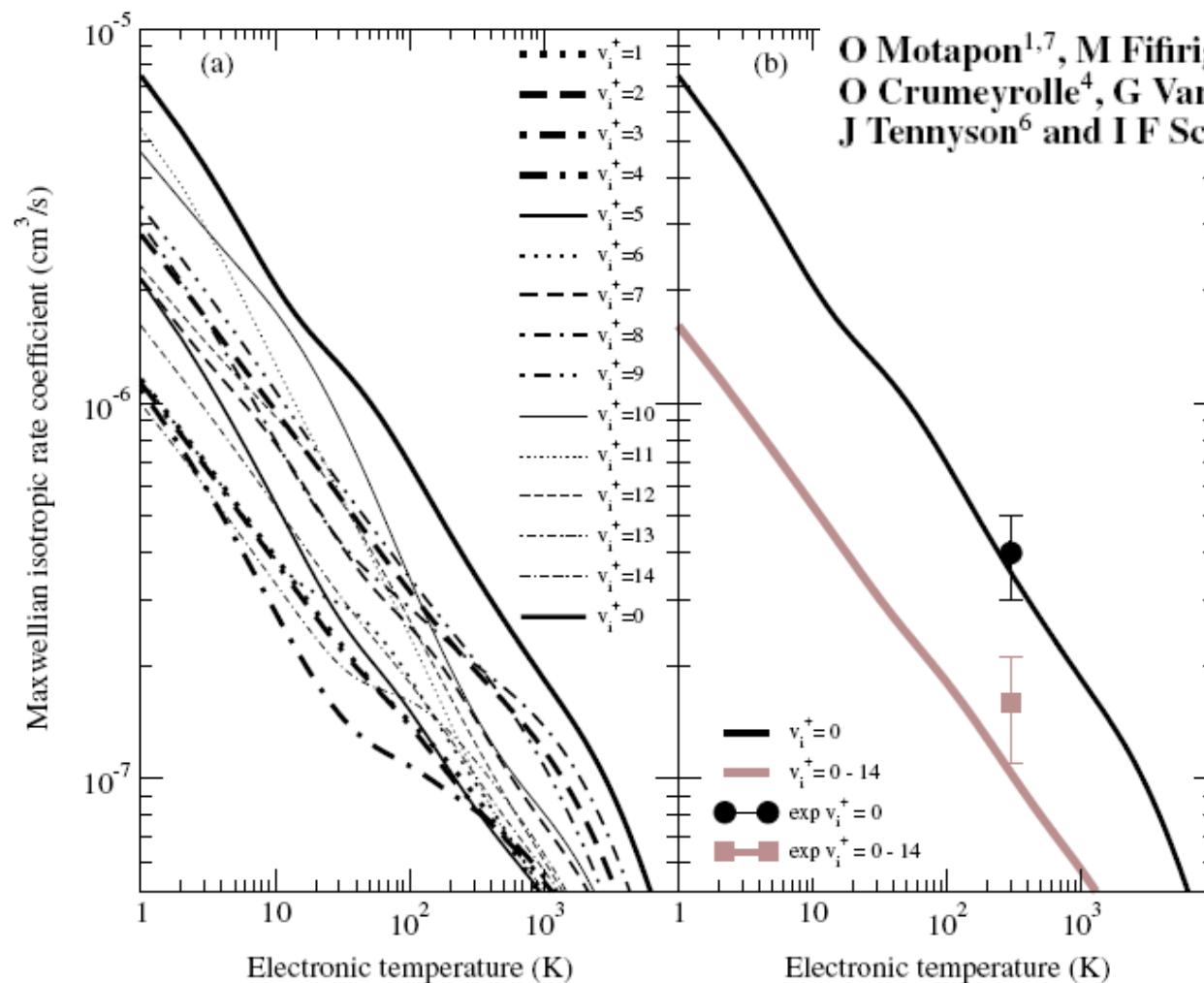
**CROSS SECTION  
DEPENDENCIE** on

**VIBRATIONAL  
EXCITATION**

**of the TARGET**

2009/10/05, ADAS meeting

# Reactive collisions between electrons and $\text{NO}^+$ ions: rate coefficient computations and relevance for the air plasma kinetics



O Motapon<sup>1,7</sup>, M Fifirig<sup>2</sup>, A Florescu<sup>3,8</sup>, F O Waffeu Tamo<sup>1,4</sup>,  
O Crumeyrolle<sup>4</sup>, G Varin-Bréant<sup>4</sup>, A Bultel<sup>5</sup>, P Vervisch<sup>5</sup>,  
J Tennyson<sup>6</sup> and I F Schneider<sup>4</sup>

NO<sup>+</sup>

# $\text{H}_2^+$

TABLE I. Rate coefficients for dissociative recombination of  $\text{H}_2^+$  with electrons of near-zero kinetic energy.

$v_i^+$	Theory [22] ( $10^{-8}$ cm $^3$ /s)	Theory (this work) ( $10^{-8}$ cm $^3$ /s)	Experiment [24] ( $10^{-8}$ cm $^3$ /s)
0	1.47	1.12	$1.87 \pm 0.15$
1	17.16	8.31	$18.7 \pm 11.2$
2	5.16	5.37	$15.3 \pm 9.5$
3	9.61	16.46	$18.0 \pm 11.5$
4	9.17	14.90	$9.9 \pm 6.3$

# H<sub>2</sub><sup>+</sup>

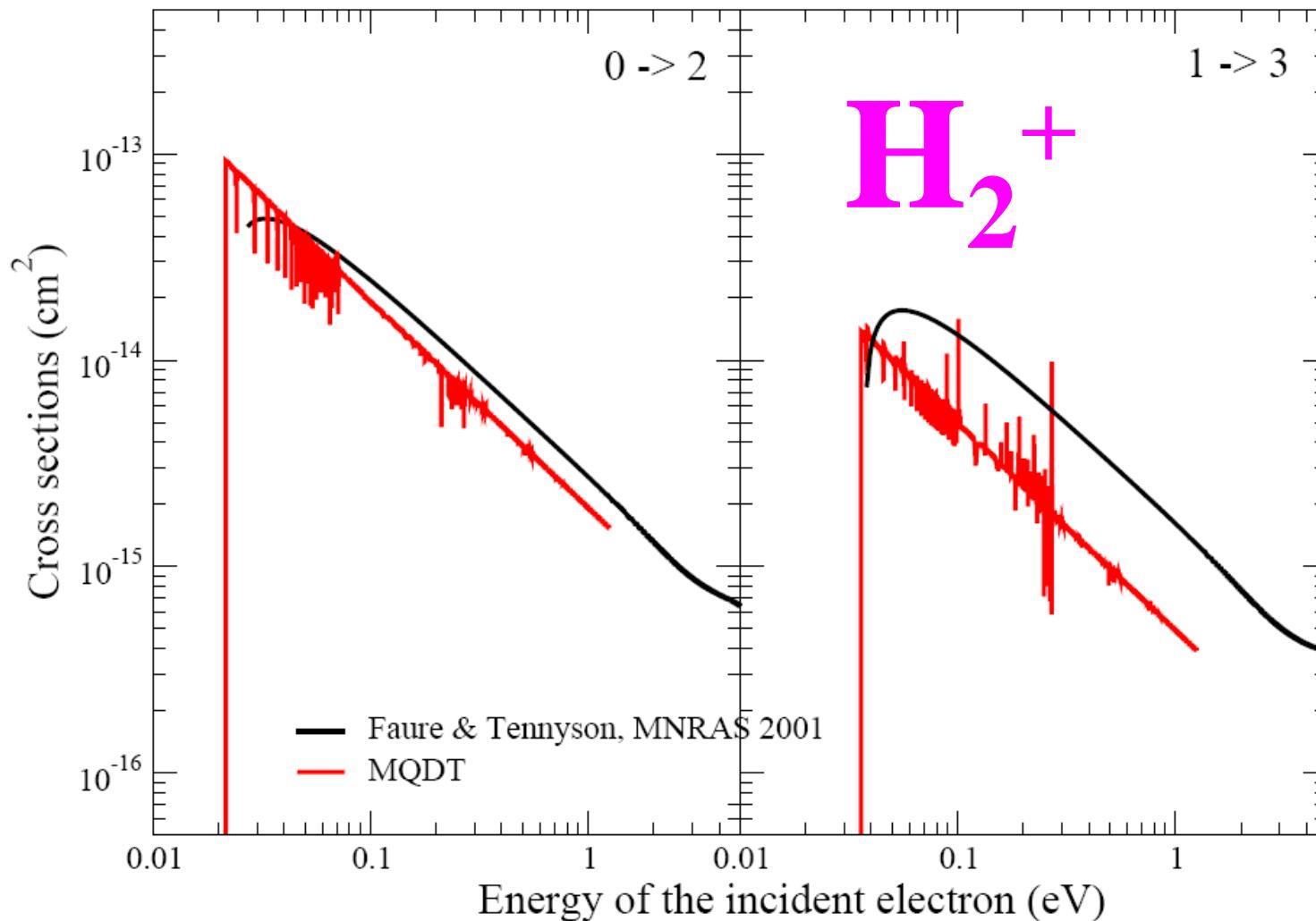
TABLE II. Rate coefficients for superelastic collisions of H<sub>2</sub><sup>+</sup> with electrons of near-zero kinetic energy.

$v \rightarrow v'$	Experiment [23] (10 <sup>-8</sup> cm <sup>3</sup> /s)	Theory [22] (10 <sup>-8</sup> cm <sup>3</sup> /s)	Theory (this work) (10 <sup>-8</sup> cm <sup>3</sup> /s)	Experiment [24] (10 <sup>-8</sup> cm <sup>3</sup> /s)
1 → 0	60	4.47	18.82	39 ± 8
2 → 1	120	16.95	38.48	76 ± 16
2 → 0		3.15	3.48	
3 → 2	220	9.61	52.16	121 ± 26
3 → 1		6.73	11.42	
3 → 0		1.70	1.67	
4 → 3	240	27.20	94.03	146 ± 30
4 → 2		2.61	16.31	
4 → 1		3.78	5.26	
4 → 0		1.07	1.18	

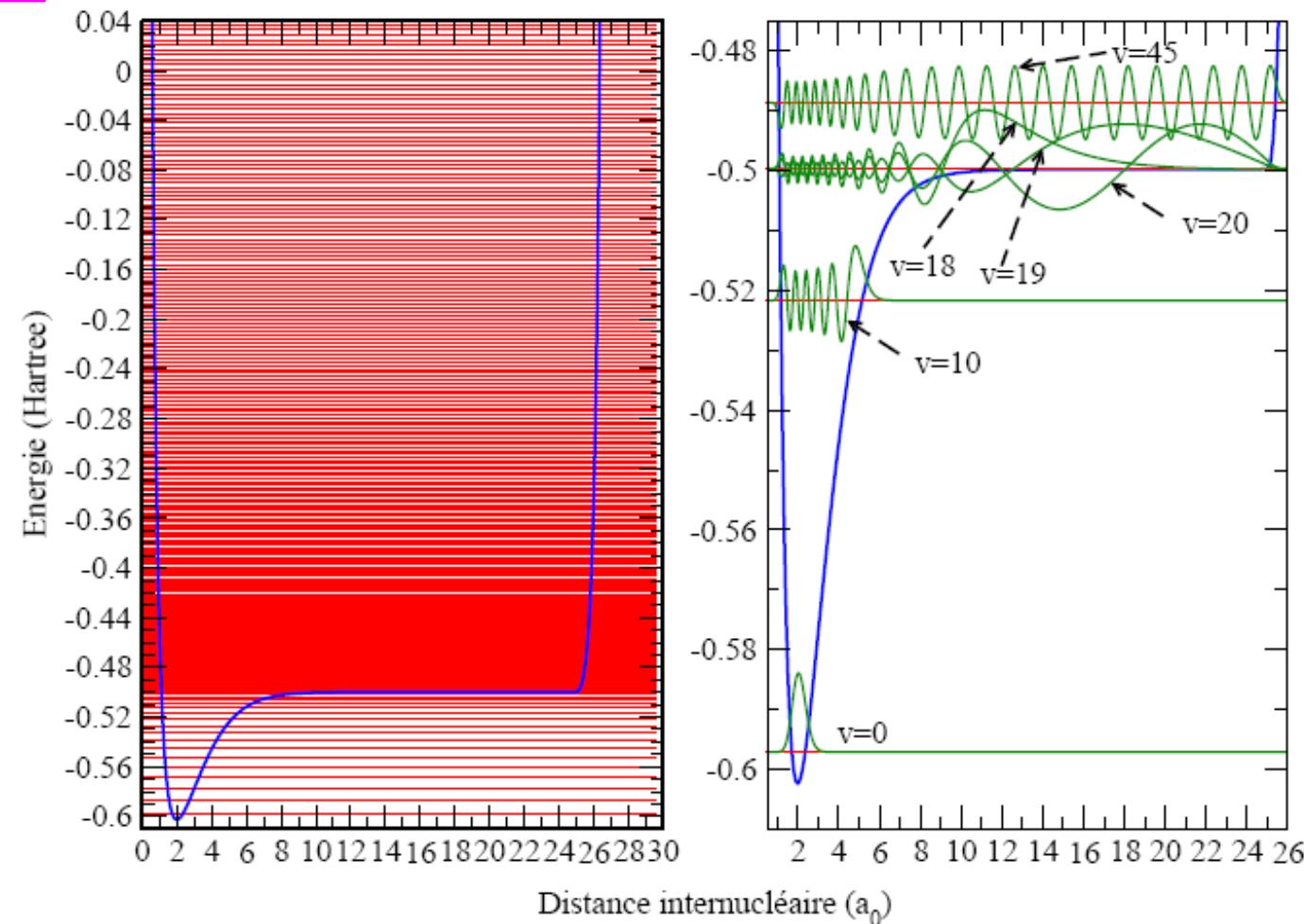
# **Work in PROGRESS**

**(since ADAS/2008 @ Juelich)**

# Rotational (DE-)EXCITATION



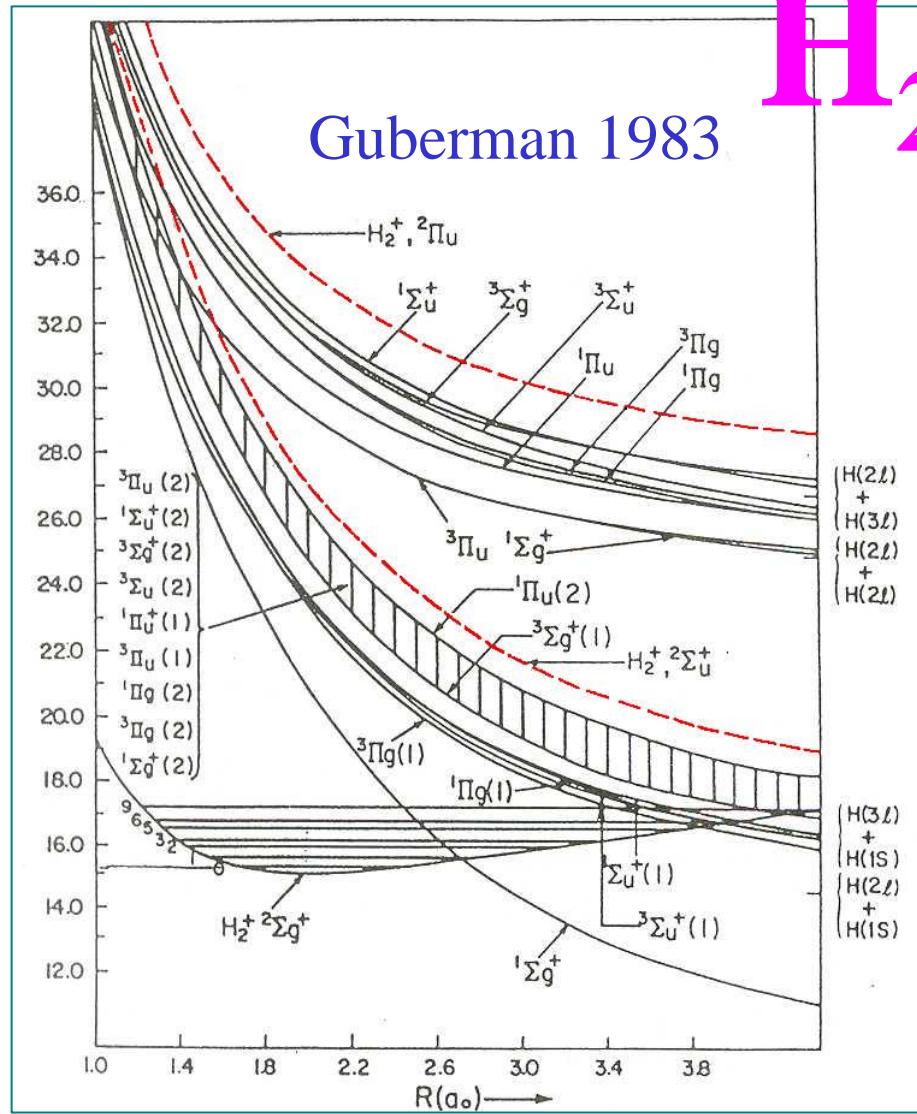
# $\text{H}_2^+$ Dissociative Excitation



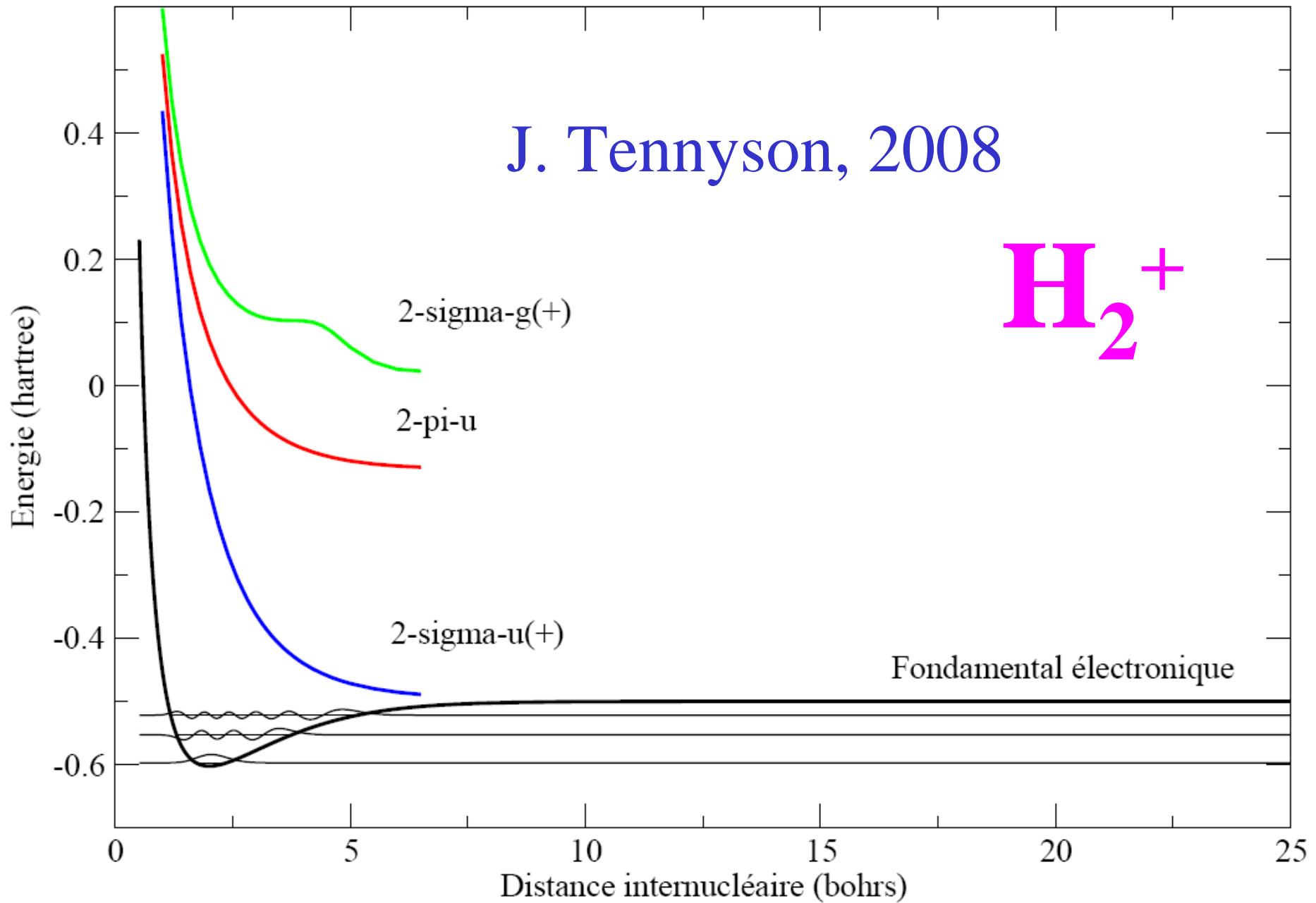
2009/10/05, ADAS meeting

**D. BACKODISSA (2008)**

# $\text{H}_2^+ / \text{H}_2$

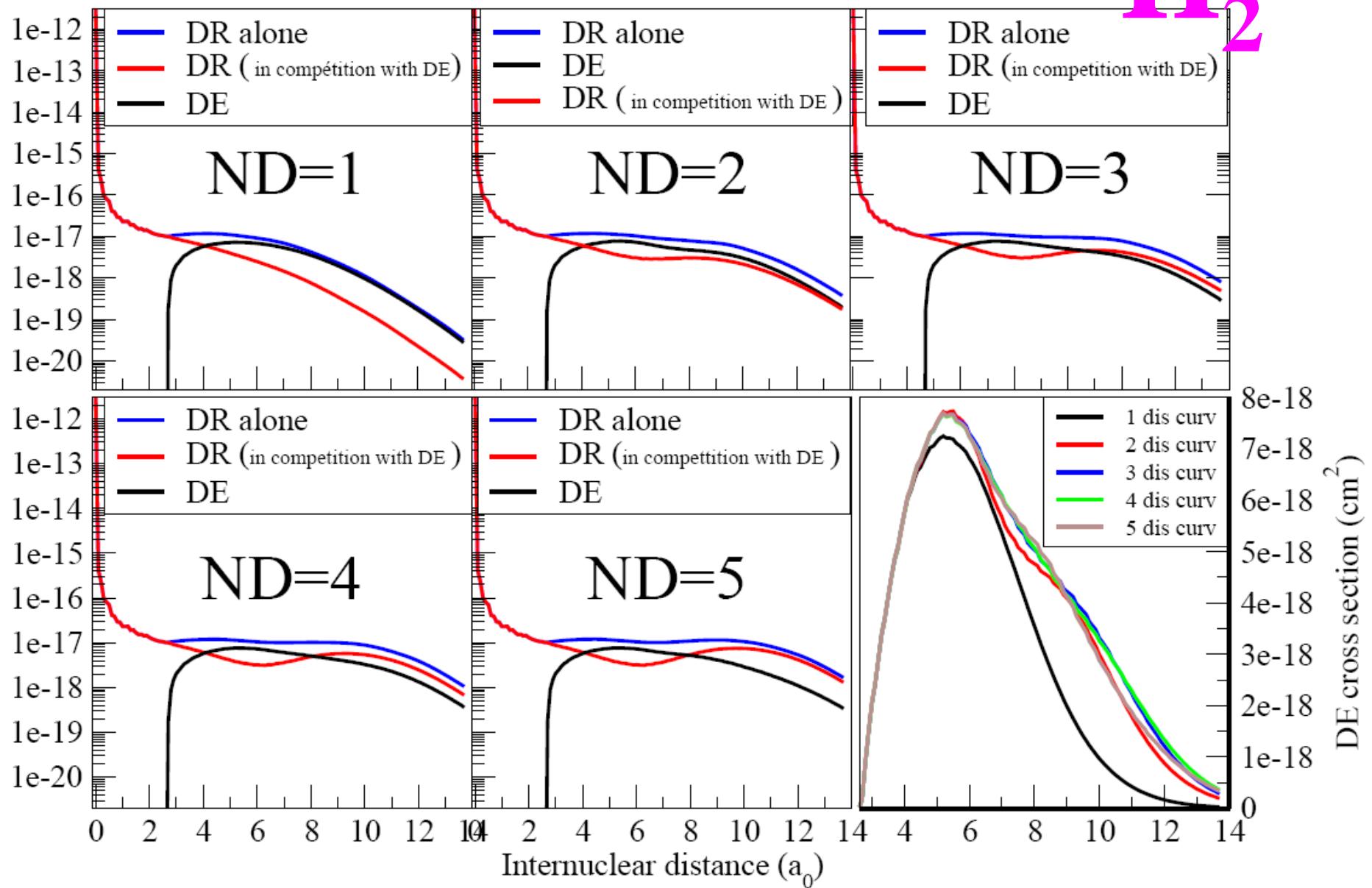


2009/10/05, ADAS meeting



# DR and DE cross sections ( $\text{cm}^2$ )

(In the last panel, DE cross sections are presented in linear scale)



# Anisotropic fragmentation in low-energy dissociative recombination

S. Novotny<sup>1</sup>, H. Rubinstein<sup>2</sup>, H. Buhr<sup>1,2</sup>, O. Novotný<sup>1</sup>, J. Hoffmann<sup>1</sup>,  
M.B. Mendes<sup>1</sup>, D.A. Orlov<sup>1</sup>, M.H. Berg<sup>1</sup>, M. Froese<sup>1</sup>,  
A.S. Jaroshevich<sup>1,3</sup>, B. Jordon-Thaden<sup>1</sup>, C. Krantz<sup>1</sup>, M. Lange<sup>1</sup>,  
M. Lestinsky<sup>1</sup>, A. Petrignani<sup>1</sup>, I.F. Schneider<sup>4</sup>, D. Shafir<sup>2</sup>,  
F.O. Waffeu Tamo<sup>4</sup>, D. Zajfman<sup>2</sup>, D. Schwalm<sup>1,2</sup> and A. Wolf<sup>1</sup>

<sup>1</sup>Max-Planck-Institut für Kernphysik, D-69117 Heidelberg, Germany

<sup>2</sup>Weizmann Institute of Science, Rehovot 76100, Israel

<sup>3</sup>Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

<sup>4</sup>University of Le Havre, 76058 Le Havre, France

In press, 2009

**HD<sup>+</sup>**

2009/10/05, ADAS meeting

# HD<sup>+</sup> @ LOW energy: theory vs experiment

## ANGULAR distribution of the dissociation products

*Guberman 2004: CI simple model*

**HD<sup>+</sup>**

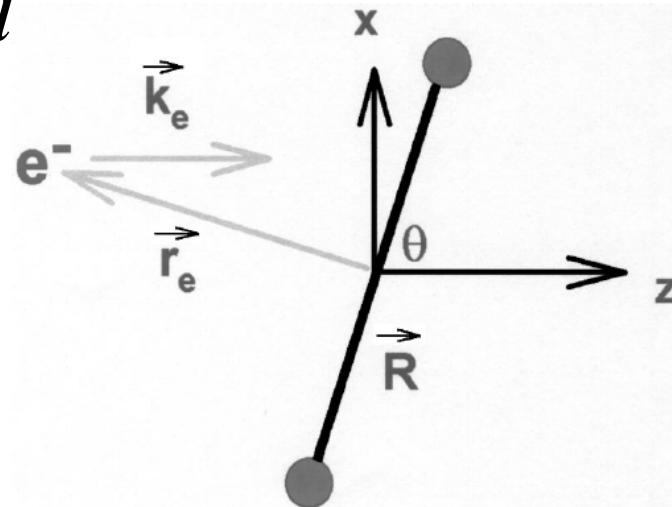


FIG. 1. Coordinates for electron ( $e^-$ ) capture by a diatomic ion. The inter-nuclear axis,  $\vec{R}$ , is oriented at an angle  $\vartheta$  from the  $z$  axis and lies in the  $xz$  plane. The incoming electron at position  $\vec{r}_e$ , relative to the center of charge of the ion, has wave vector  $\vec{k}_e$  and is moving parallel to the  $z$  axis.

*Novotny et al 2006: TSR, imaging*

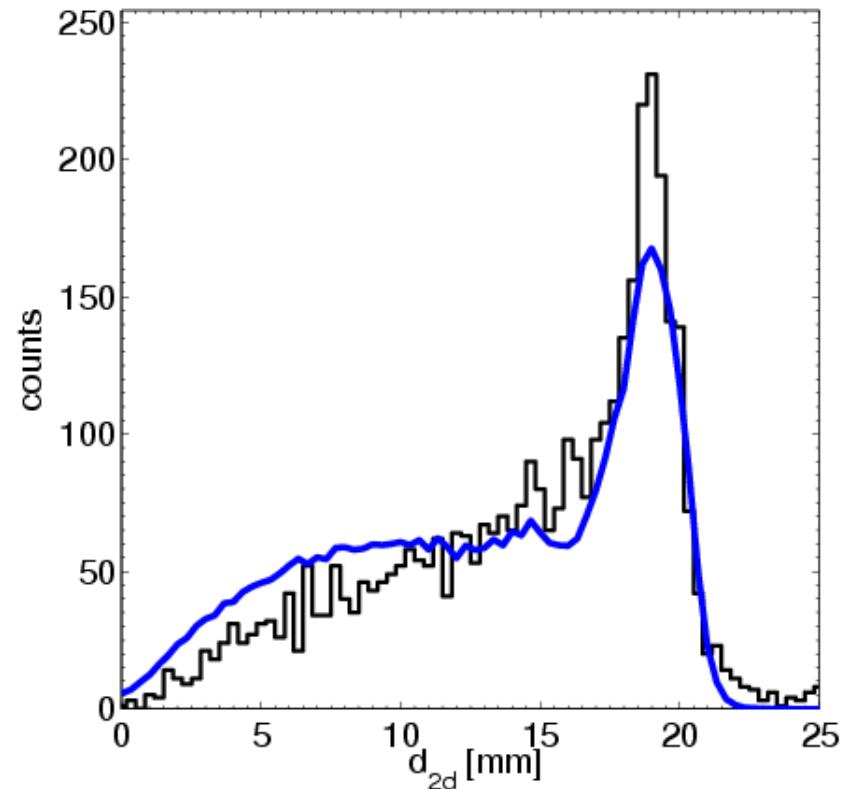
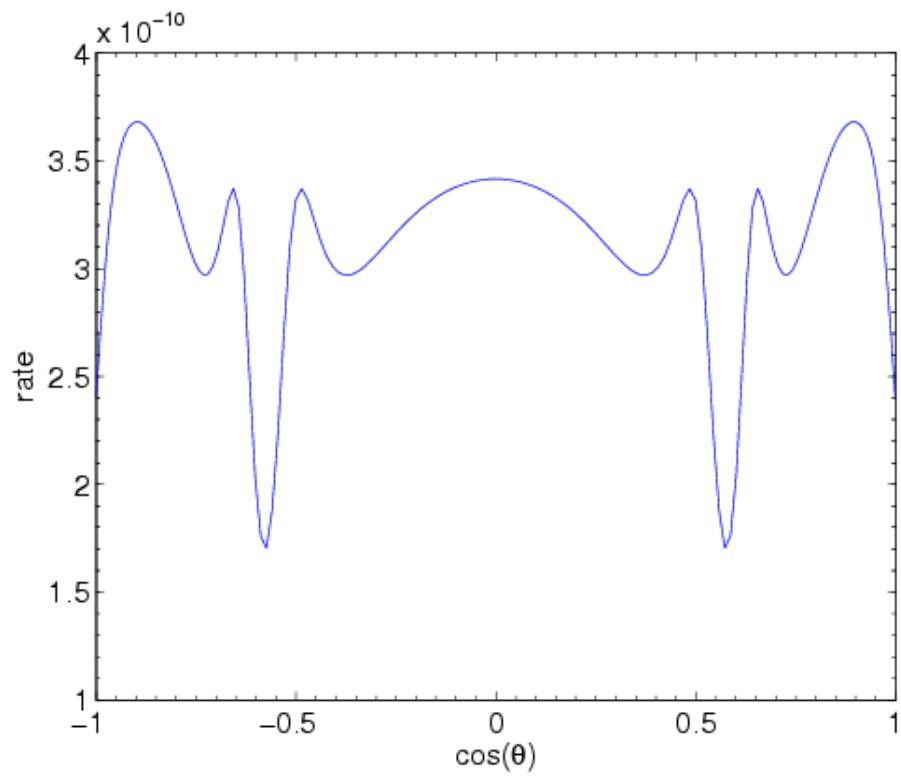
*Waffeu Tamo & Schneider 2006-2007: MQDT modelling →*

$$V_{\text{el}}^m(k_e, \vec{R}) = \sum_{\ell=|m|}^{\infty} V_{\ell|m|}(k_e, R) Y_{\ell m}(\hat{R}), \quad (11)$$

Compare latest MQDT results on angular distribution with 2D data  
(July 2006)

$E_e = 75.10$  meV;  $T_{\text{rot}} = 360$  K

HD<sup>+</sup>



— data  
— with MQDT calculation

2009/10/05, ADAS meeting

# Dissociative recombination of $\text{CF}^+$ : experiment and theory

O Novotný<sup>1</sup>, O Motapon<sup>2</sup>, M H Berg<sup>1</sup>, D Bing<sup>1</sup>, H Buhr<sup>1,3</sup>, H Fadil<sup>1</sup>,  
J Hoffmann<sup>1</sup>, A S Jaroshevich<sup>4</sup>, B Jordon-Thaden<sup>1</sup>, C Krantz<sup>1</sup>,  
M Lange<sup>1</sup>, M Lestinsky<sup>1</sup>, M Mendes<sup>1</sup>, S Novotny<sup>1</sup>, A Petrignani<sup>1</sup>,  
D A Orlov<sup>1</sup>, I F Schneider<sup>5</sup>, A E Orel<sup>6</sup> and A Wolf<sup>1</sup>

<sup>1</sup> Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, D-69117 Heidelberg, Germany

<sup>2</sup> Department of Physics, Faculty of Science, University of Douala, P.O. Box 24157 Douala, Cameroon

<sup>3</sup> Department of Particle Physics, Weizmann Institute of Science, Rehovot 76100, Israel

<sup>4</sup> Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

<sup>5</sup> Laboratoire de Mécanique, Physique et Géosciences, Université du Havre, 25, rue Philippe Lebon, P.O. Box 540, 76058 Le Havre Cedex, France

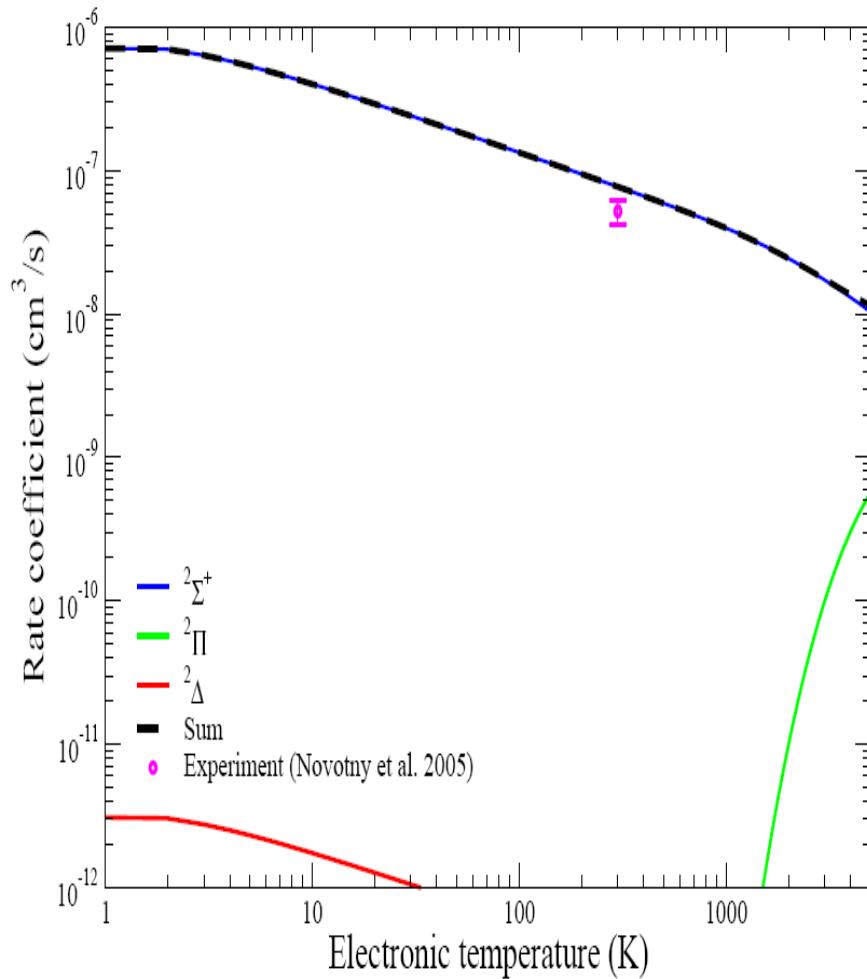
<sup>6</sup> Department of Applied Science, University of California at Davis, Davis CA 95616 USA

In press, 2009

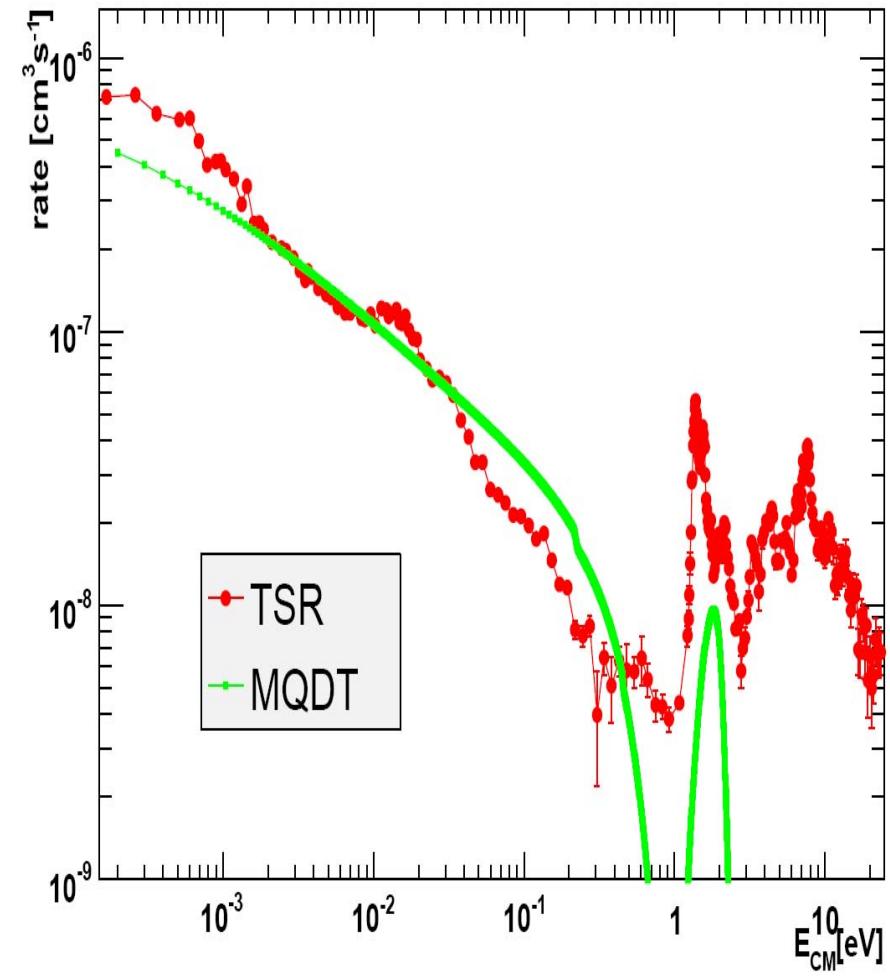
$\text{CF}^+$



## RESULTS vs EXPERIMENTS



Maxwell ISOTROPIC rate coefficients



Maxwell ANISOTROPIC rate coefficients

# The « H<sub>2</sub><sup>+</sup> DR project»

**Collaboration with Ch. Jungen, C. H. Greene, J. Tennyson**

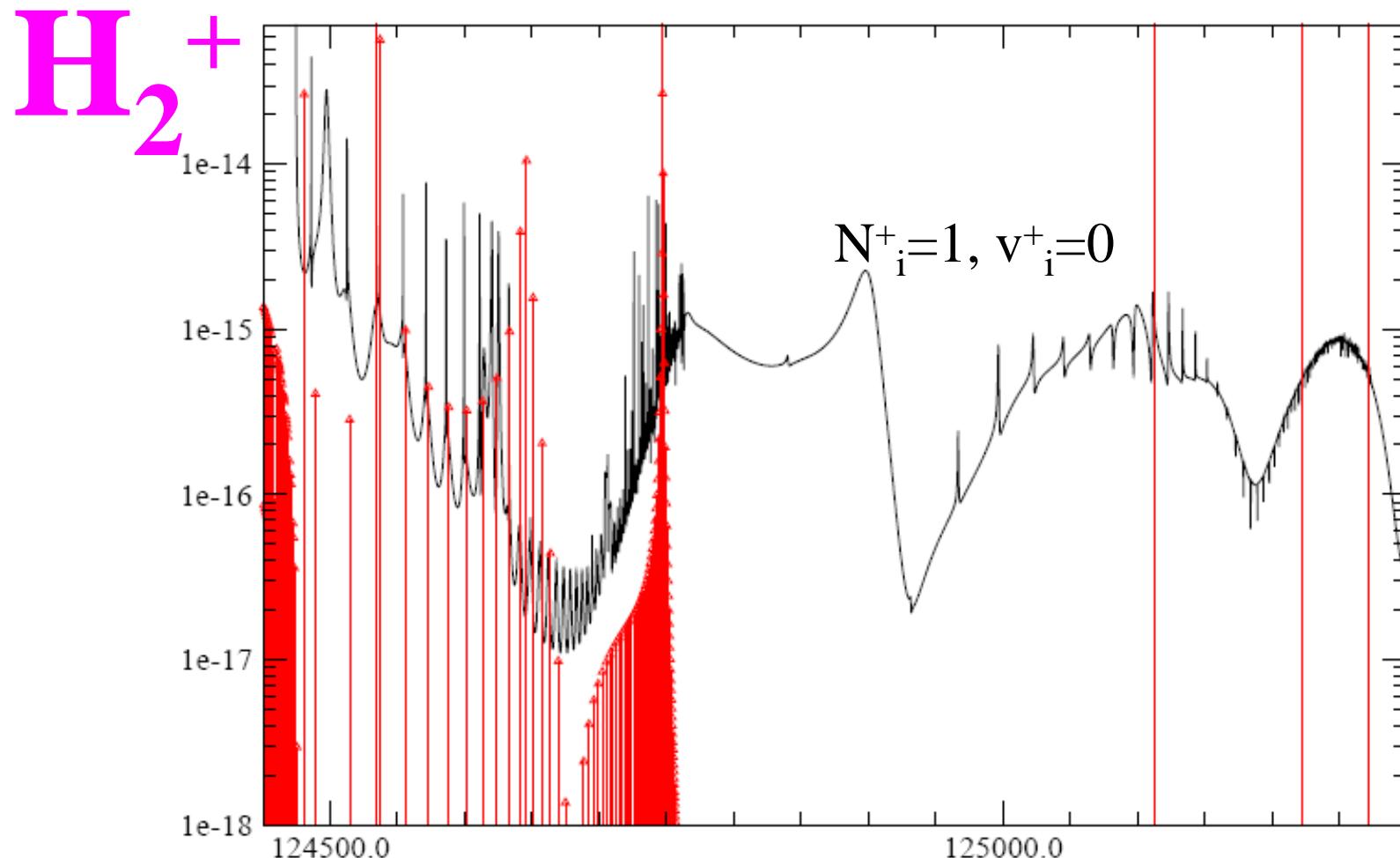
- MQDT « global » treatment
  - States and couplings from self-consistent computations
  - Energy dependence of couplings and quantum defects
- « Total » rotational treatment (including SPIN)
- Angular distribution



LABORATOIRE ONDES  
et MILIEUX COMPLEXES

2009/10/05, ADAS meeting

## Comparaison with the photo-dissociation calculations of Christian JUNGEN



2009/10/05, ADAS meeting

**« Ultimate » aim:  
to provide MORE & BETTER data than this:...**

# Reactive collisions between electrons and molecular hydrogen cation isotopomers: Cross-sections and rate coefficients for HD<sup>+</sup> and DT<sup>+</sup>

M.C. Stroe<sup>1, 2</sup>, M. Fifirig<sup>2</sup>, F.O. Waffeu Tamo<sup>1, 3</sup>, O. Motapon<sup>3</sup>, O. Crumeyrolle<sup>1</sup>,  
G. Varin-Breant<sup>1</sup>, A. Bultel<sup>4</sup>, P. Vervisch<sup>4</sup>, A. Suzor-Weiner<sup>5</sup>, I.F. Schneider<sup>1</sup>

<sup>1</sup> Laboratoire de Mécanique, Physique et Géosciences, Université du Havre, F-76058 Le Havre, France

<sup>2</sup> Department of Physics, Faculty of Chemistry, University of Bucharest, RO-70346 Bucharest, Romania

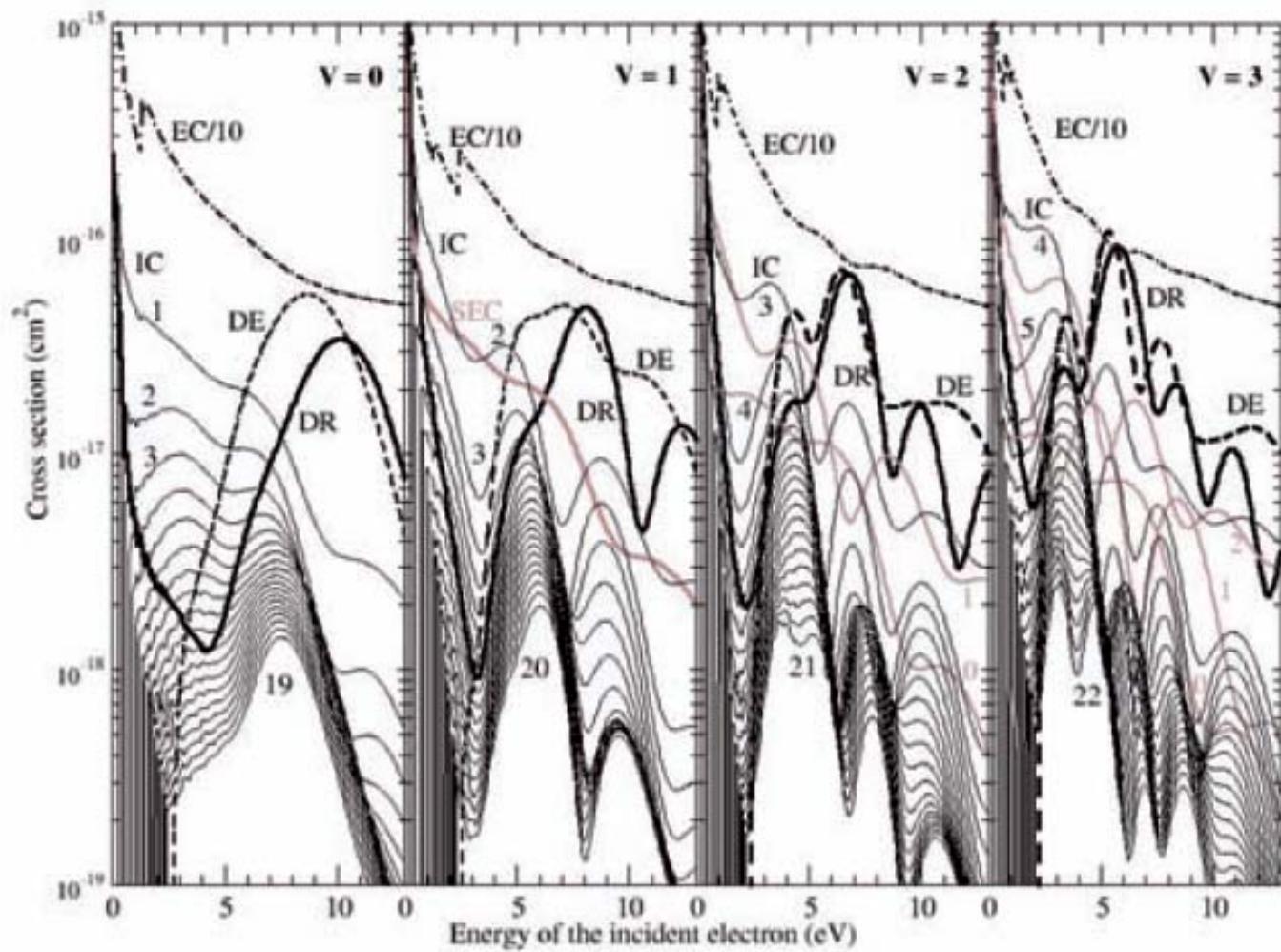
<sup>3</sup> Center for Atomic, Molecular Physics and Quantum Optics, University of Douala, 00237 Douala, Cameroon

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**Figure 6.** Reactive collisions of DT<sup>+</sup> molecular ion in a given vibrational state  $v$  with electrons (cross-sections): bold line — DR, broken line — DE, dashed dotted line — elastic collisions (EC), grey line — superelastic collisions (SEC) and thin line — inelastic collisions (IC). The numbers attached to the IC and SEC curves stand for the final vibrational states.



Thanks  
for  
your attention !

ADAS meeting

## Experiments: MULTIPLE pass/MERGED beams-STORAGE RINGS

# Why storage rings ?

$$T_{\text{long}} = 20 \mu\text{eV} = 0,23 \text{ K} = 0,16 \text{ cm}^{-1}$$

$$T_{\text{trans}} = 500 \mu\text{eV} = 5,80 \text{ K} = 4,03 \text{ cm}^{-1}$$

- 1) high luminosity, 2) high resolution, 3) variable relative energy, 4) low background
- ..... 5) quenching of vibrationally excited states for molecular ions.

### Neutral-particle emission in collisions of electrons with biomolecular ions in an electrostatic storage ring

T Tanabe,<sup>1</sup> K Noda,<sup>2</sup> M Saito,<sup>3</sup> H Takagi,<sup>4</sup> E B Starikov<sup>5</sup> and M Tateno<sup>6,7</sup>

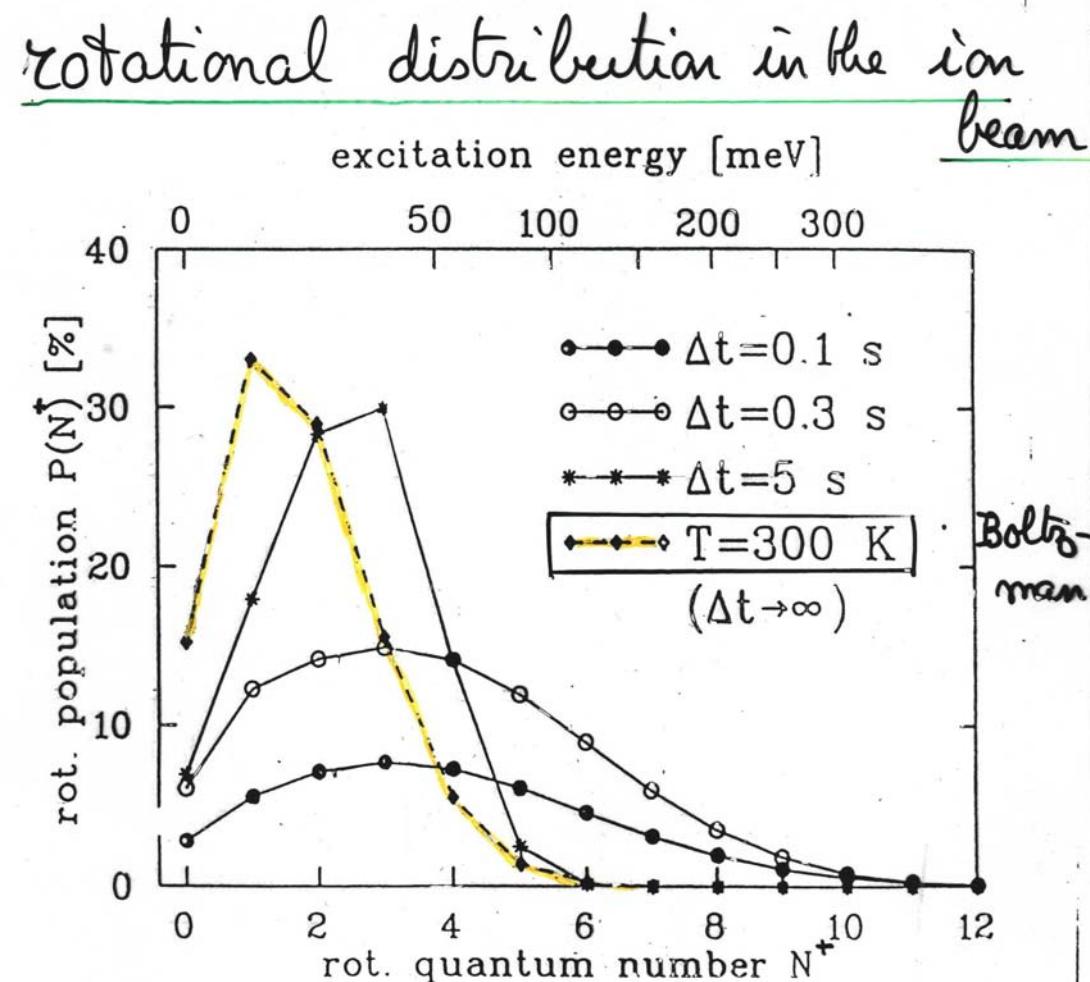
## Experiments: MULTIPLE pass/MERGED beams-STORAGE RINGS

### The ANISOTROPIC Maxwell distribution function

$$\alpha = \langle v\sigma \rangle = \iiint \sigma(v) v f(v_d, v) d\mathbf{v} \quad (1)$$

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

## Experiments: MULTIPLE pass/MERGED beams-STORAGE RINGS



P. Förck (thesis), 1994, Heidelberg

# Experiments: MULTIPLE pass/MERGED beams-STORAGE RINGS

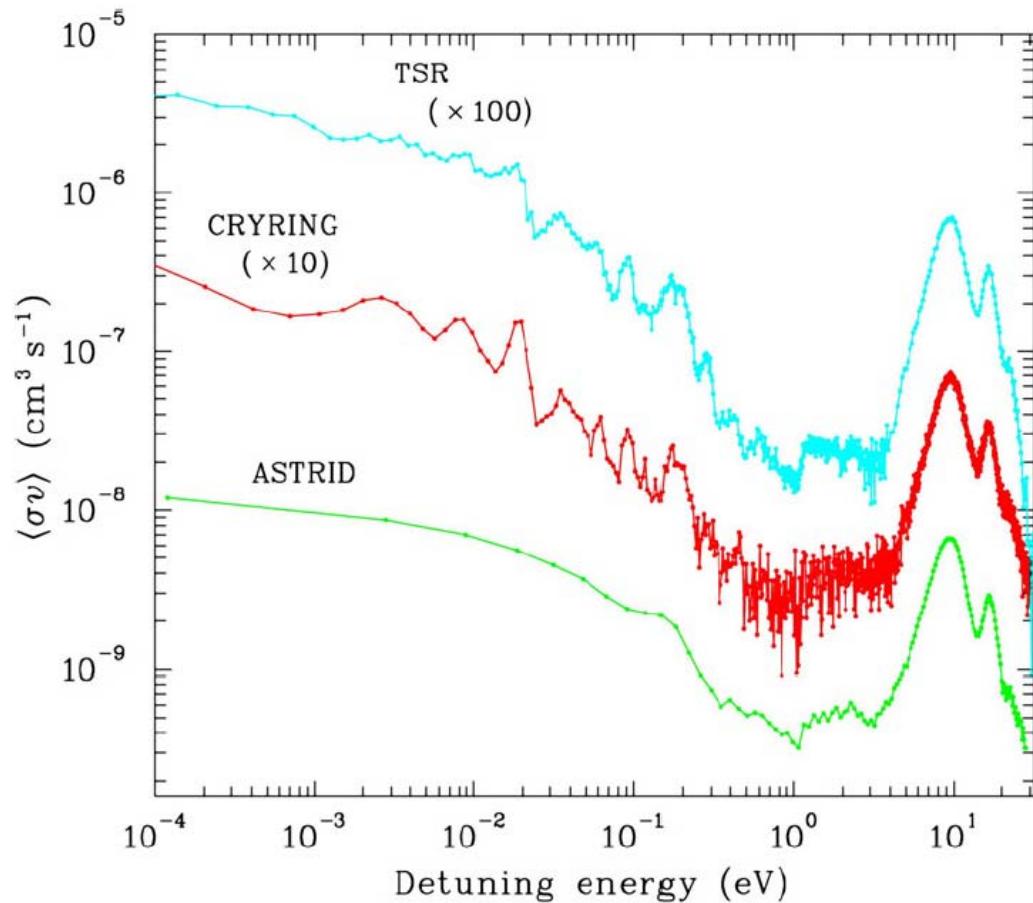
## Ion Storage Rings



ESR  
TARN (TOKYO) ----->

2009/10/05, ADAS meeting

## Experiments: MULTIPLE pass/MERGED beams-STORAGE RINGS



Dissociative recombination rate coefficient for  $\text{HD}^+$  ( $v = 0$ ) ions measured at the three storage ring facilities ASTRID, CRYRING and TSR. The electron coolers used have different transverse electron temperatures amounting to 20 meV (ASTRID), 4.5 meV (TSR) and 2 meV (CRYRING).

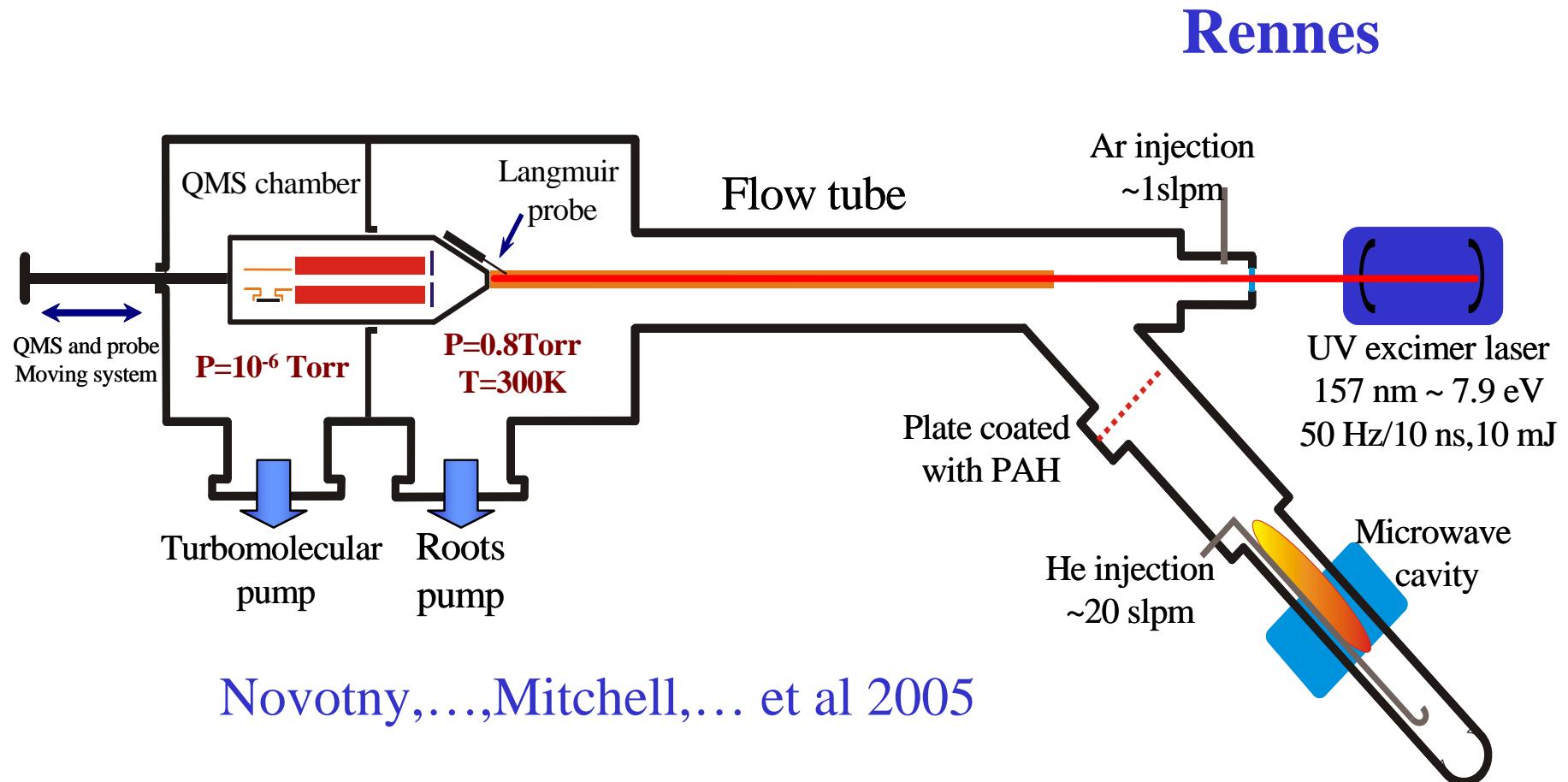
### Molecular ion recombination in merged beams: experimental results on small systems and future perspectives

M Larsson

Institute of Physics Publishing  
doi:10.1088/1742-6596/4/1/007

Journal of Physics: Conference Series 4 (2005) 50–57  
Sixth International Conference on Dissociative Recombination  
2009/10/05, ADAS meeting

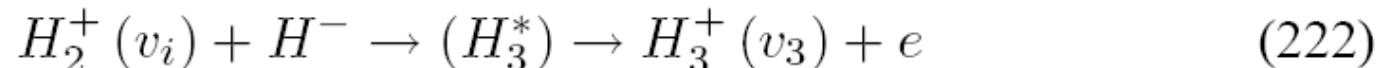
# Experiments: FALP



Novotny,..., Mitchell,... et al 2005

## 7.4.2 Associative and non-associative detachment

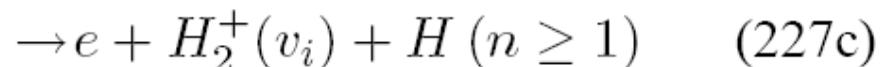
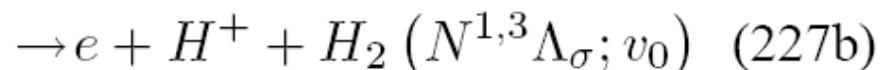
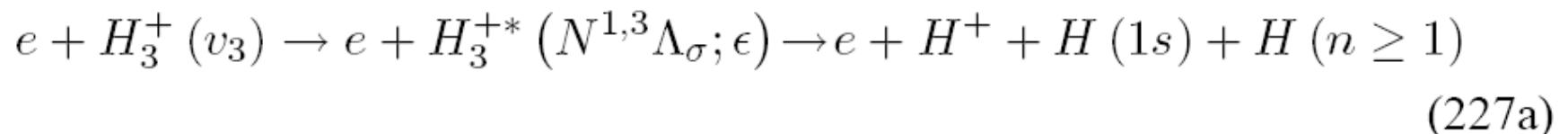
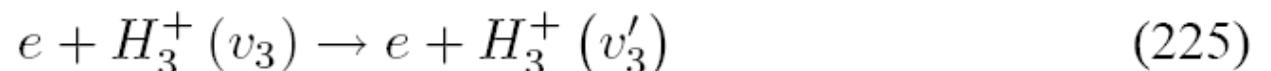
The associative detachment (AD) reaction

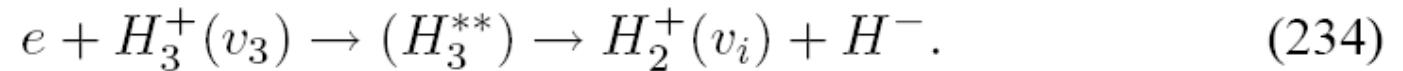
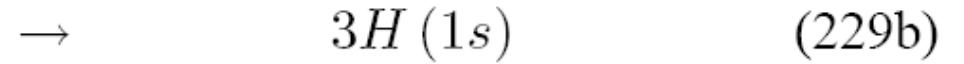
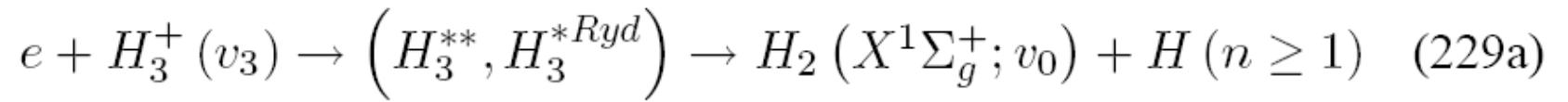


## 8.1 Collision processes of $H_3^+$ with electrons

### 8.1.1 Vibrational excitation

The electron impact vibrational excitation of  $H_3^+(v_3)$





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# Nuclear Fusion Research

Understanding Plasma-Surface Interactions

With 210 Figures

Example of data needs  
For  $\text{H}_2^+$  & isotopomers:

• • •



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## Janev, Fantz, Reiter 2005

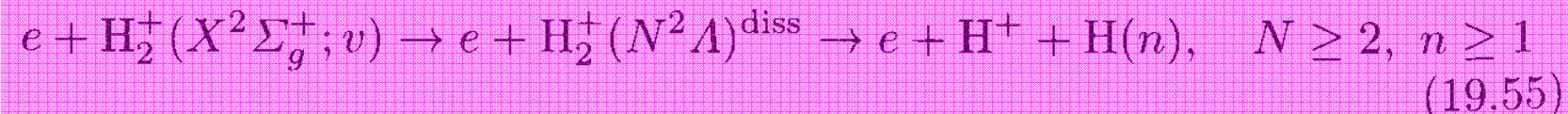
The chain of reactions, which played the key role in these arguments, was, firstly, a vibrational excitation of molecules by electron impact (through resonant  $\text{H}_2^-$  levels), then, secondly, an ion conversion:  $p + \text{H}_2(v) \rightarrow \text{H} + \text{H}_2^+$ , followed by, thirdly, an immediate dissociative recombination:  $e + \text{H}_2^+ \rightarrow \text{H} + \text{H}^*$ . The excited atom decays by spontaneous emission. At the end of

The dominant electron-impact process at low collision energies is the dissociative recombination



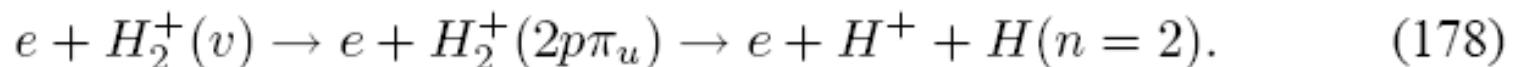
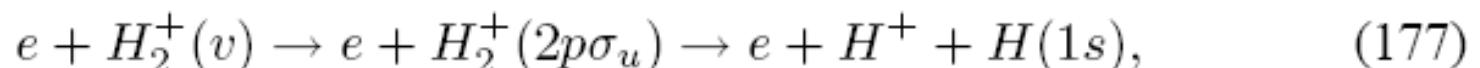
which has been subject to many experimental [78] and theoretical [79, 80] studies. The most detailed cross-section calculations of reactions (19.52) have been performed in [80] by using the multi-channel quantum defect theory (MQDT). The  $n$ -distribution of excited products from reaction (19.52) obtained in MQDT calculations support the earlier semi-empirical assessment [14], at least for the lower  $v$ -states.

At higher collision energies, the most important electron-impact processes of  $\text{H}_2^+(X; v)$  are



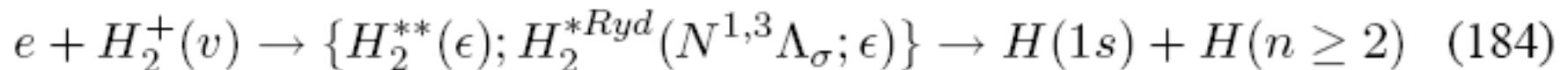
### 7.1.2 Dissociative excitation

The simplest mechanism of dissociative excitation (DE) of  $H_2^+(X^2\Sigma_g^+; v)$  ion by electron impact is its excitation to the two lowest dissociative excited states,  $(2p\sigma_u; ^2\Sigma_u^+)$  and  $(2p\pi_u; ^2\Pi_u)$ ,



### 7.1.3 Dissociative recombination

In view of its importance for the recombination of low-temperature plasmas, dissociative recombination (DR) process



CO<sup>+</sup>

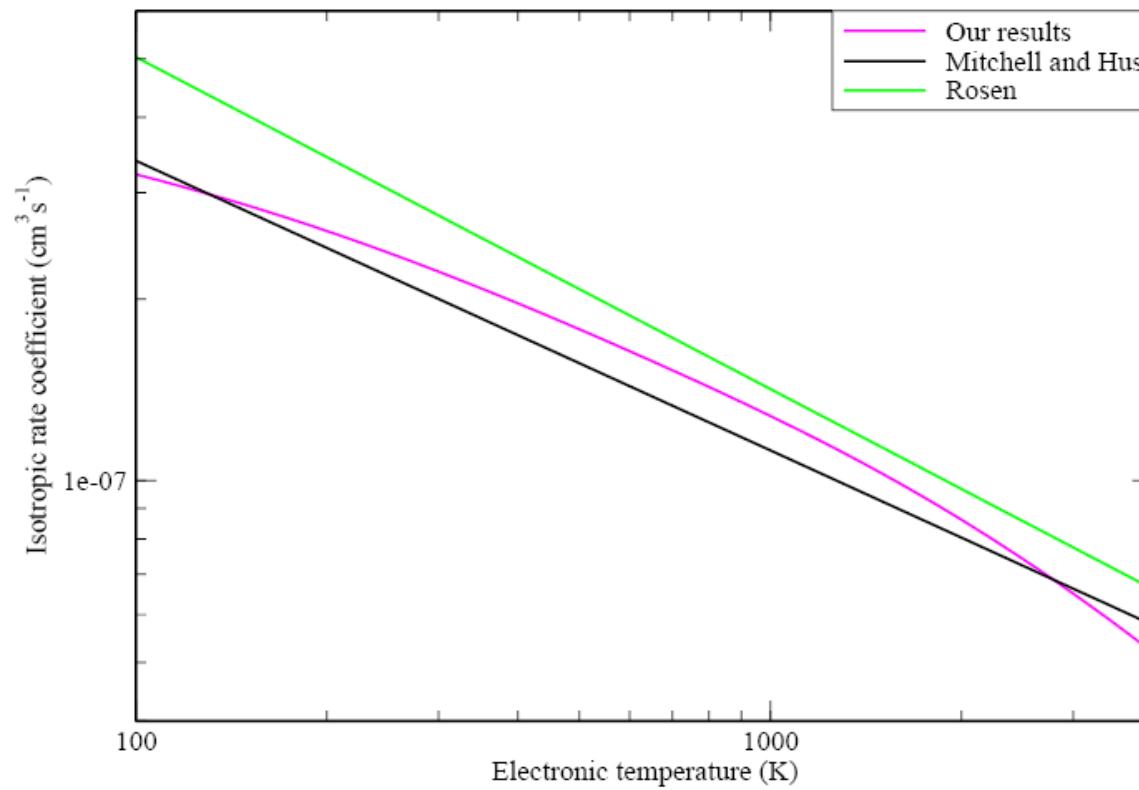


Figure 6: *Isotropic rate coefficients. Our theoretical results are represented in magenta. In black and green, the experiment results of Mitchell and Rosen respectively.*

$\text{H}_2^+$

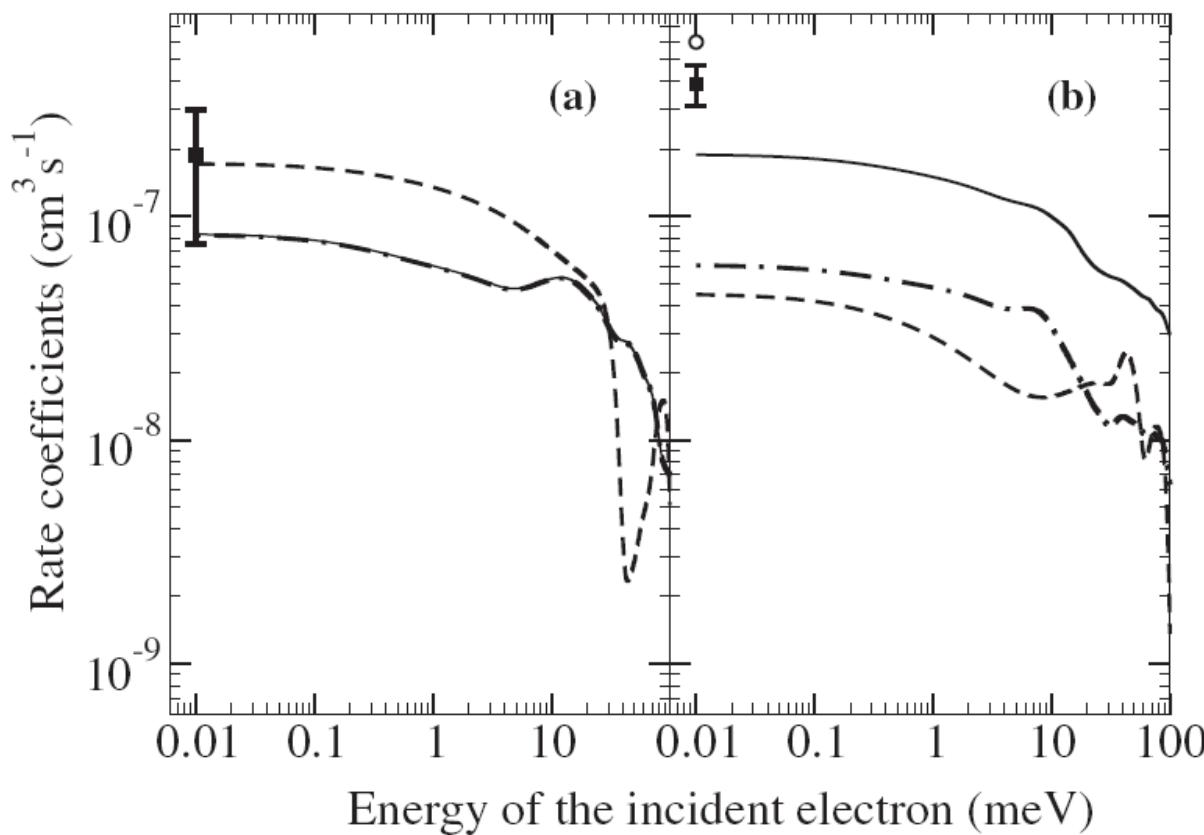


FIG. 2. Rate coefficients for (a) dissociative recombination and (b) superelastic collisions from  $v_i^+ = 1$ . Dashed lines, theory without rotation [22]; dash-dotted lines, theory with rotation for  ${}^1\Sigma_g^+ + {}^1\Pi_g$ ; full black lines, theory with rotation for all symmetries; squares, experiment [24]; circle, experiment [23].