



# Nuclear spin restrictions in gas phase collisions: more experiments are needed

*Dieter Gerlich*

## Introduction

Experiments and models

## Experimental

Ions in cryogenic traps

## Probing $\text{H}_3^+(\text{J},\text{G})$ with He

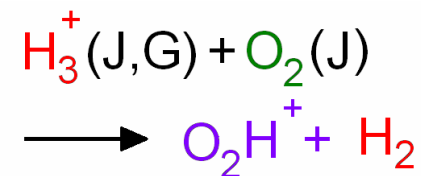
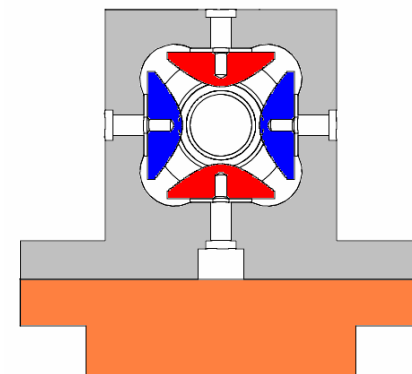
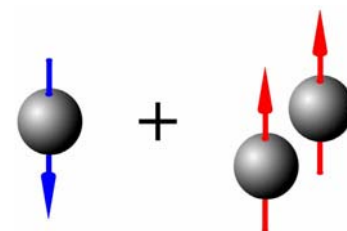
Ortho-para transitions in the trap

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

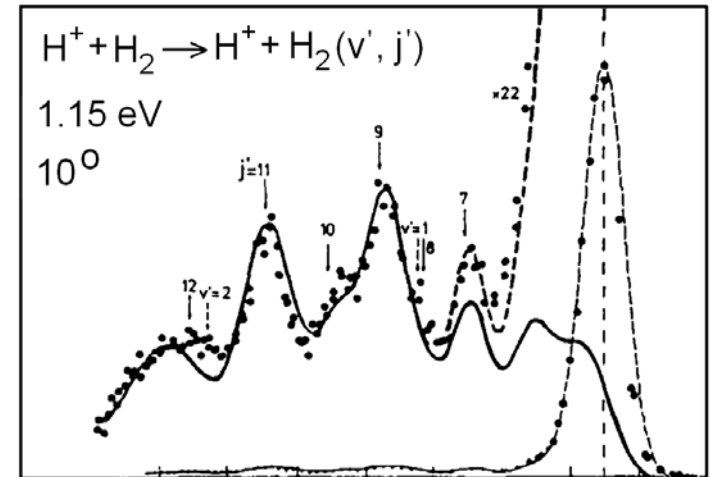
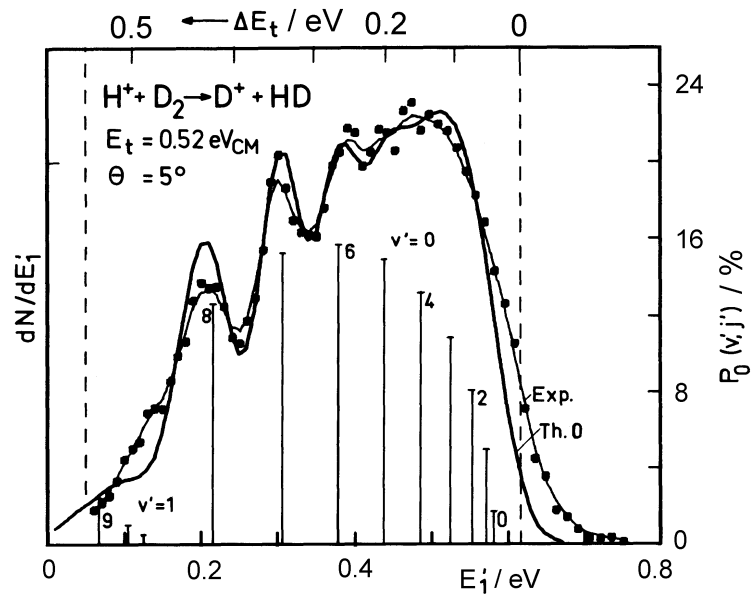
In situ ortho-para conversion?

## Outlook

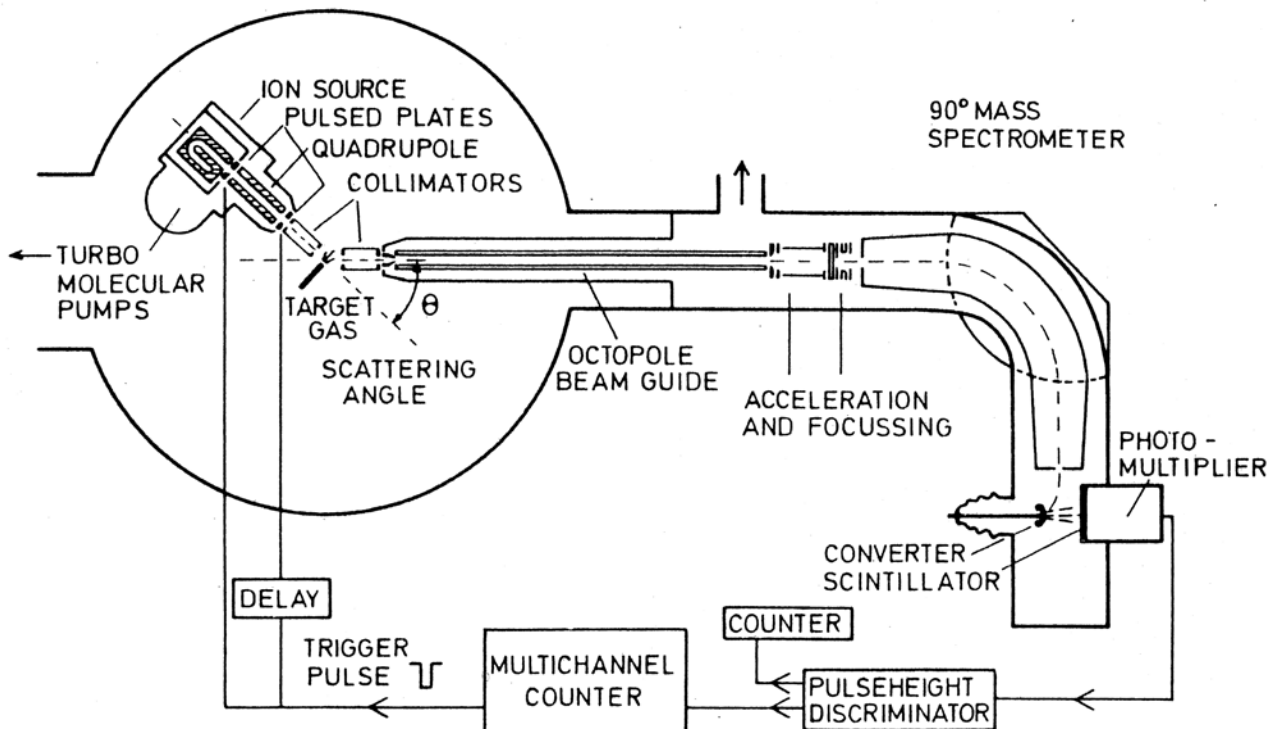
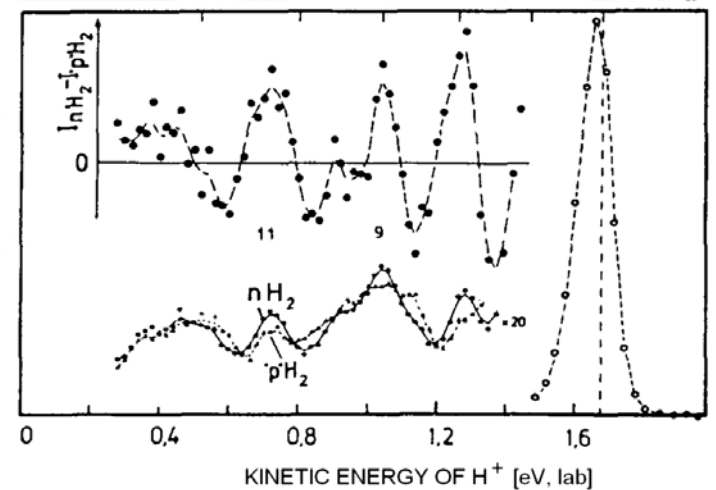
More experimental activities!



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



INTENSITY [arb.U]



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

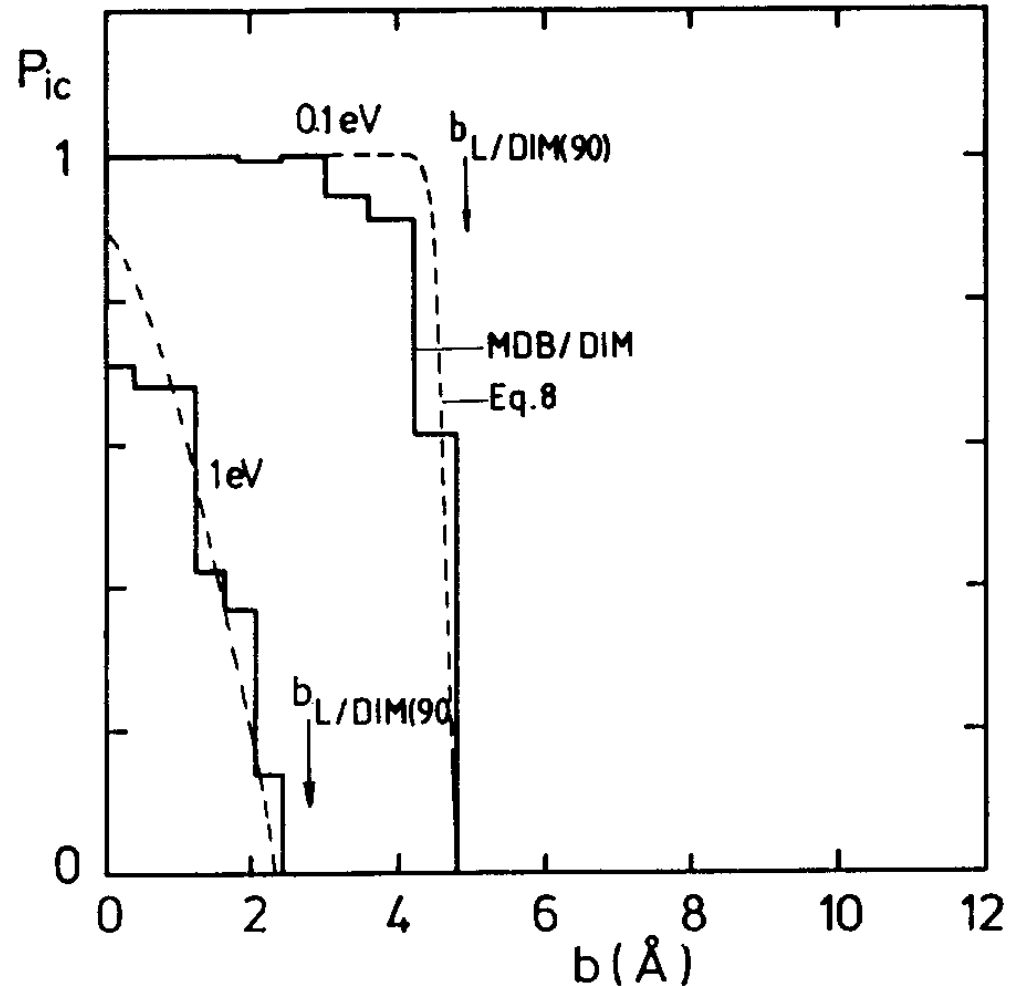
$$\sigma_{jv \rightarrow j'v'}^E = \frac{\pi}{k^2(2j+1)} \sum_{J=0}^1 \sum_{J_m=0}^{J_m} \frac{2J+1}{N^{JEII}} \sum_{l=|J-j|}^{J+j} P_{lv}^{JEII} \times \sum_{l'=|J-j'|}^{J+j'} P_{l'v'}^{JEII} g_{jj'}$$

$$N^{JEII} = \sum_{v=0}^{v_m} \sum_{j=0}^{j_m} \sum_{l=|J-j|}^{J+j} P_{lv}^{JEII} g_{jj'}$$

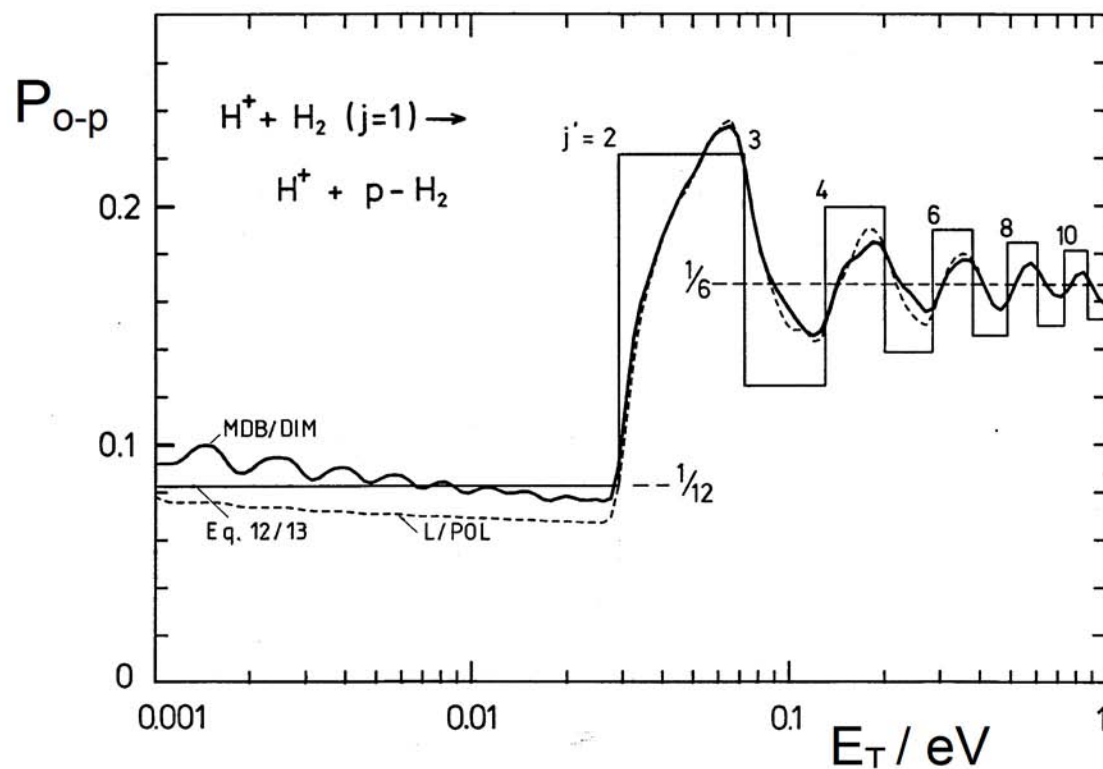
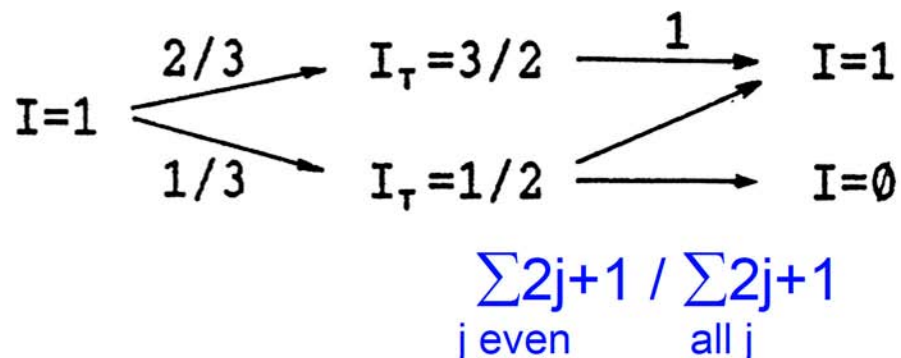
$$P_{ic} = A(E, E_T, \mu) \cdot f(l, E_T, \mu)$$

$$\text{CNS: } g_{jj'} = \begin{cases} 3 & \text{if } j' \text{ odd} \\ 1 & \text{if } j' \text{ even} \end{cases}$$

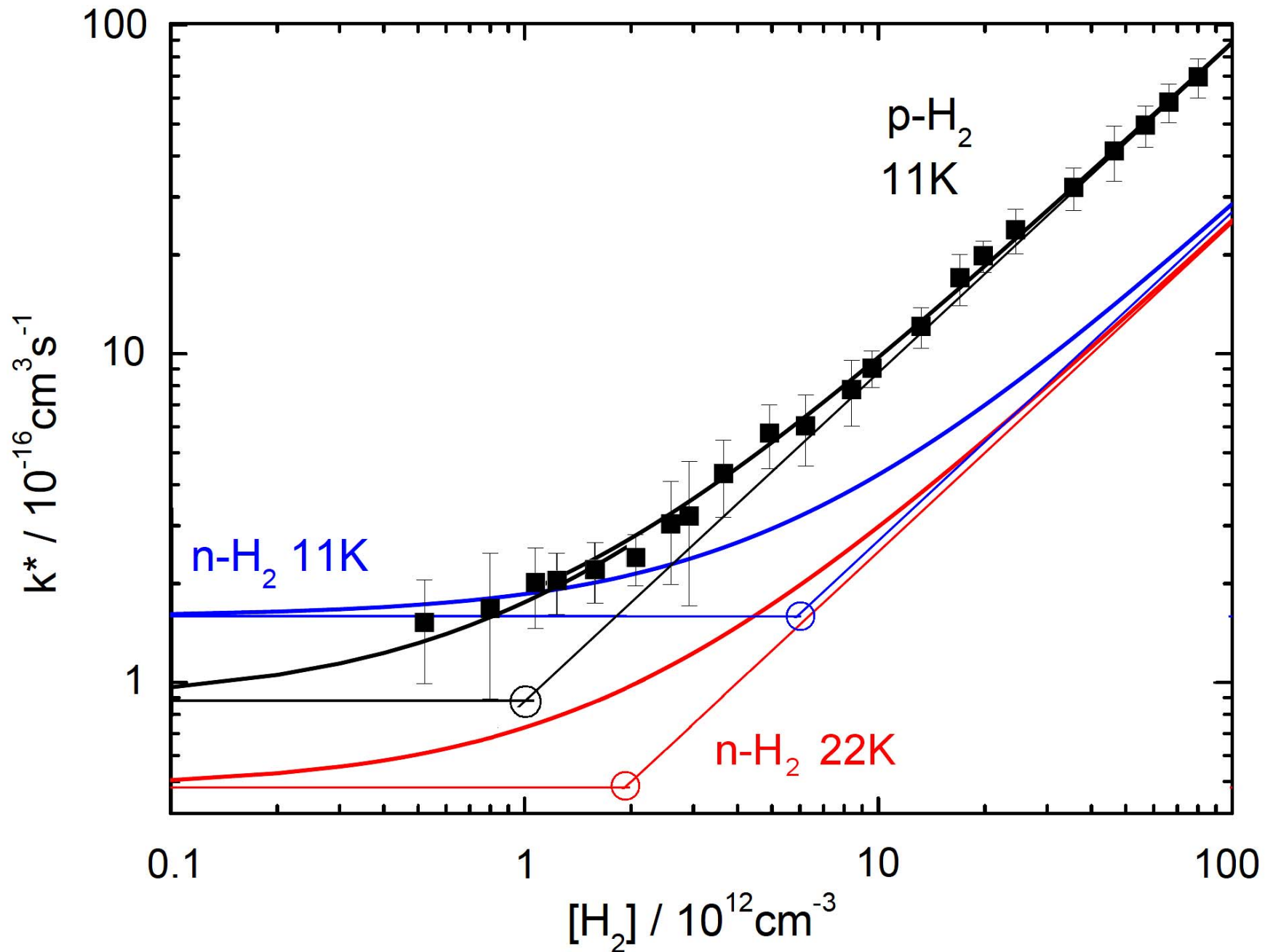
$$\text{FNS: } g_{jj'} = \begin{cases} 5 & \text{if } j \text{ and } j' \text{ are odd} \\ 1 & \text{else} \end{cases}$$



# Ortho para transitions in reactive $\text{H}^+ + \text{H}_2(j)$ collisions

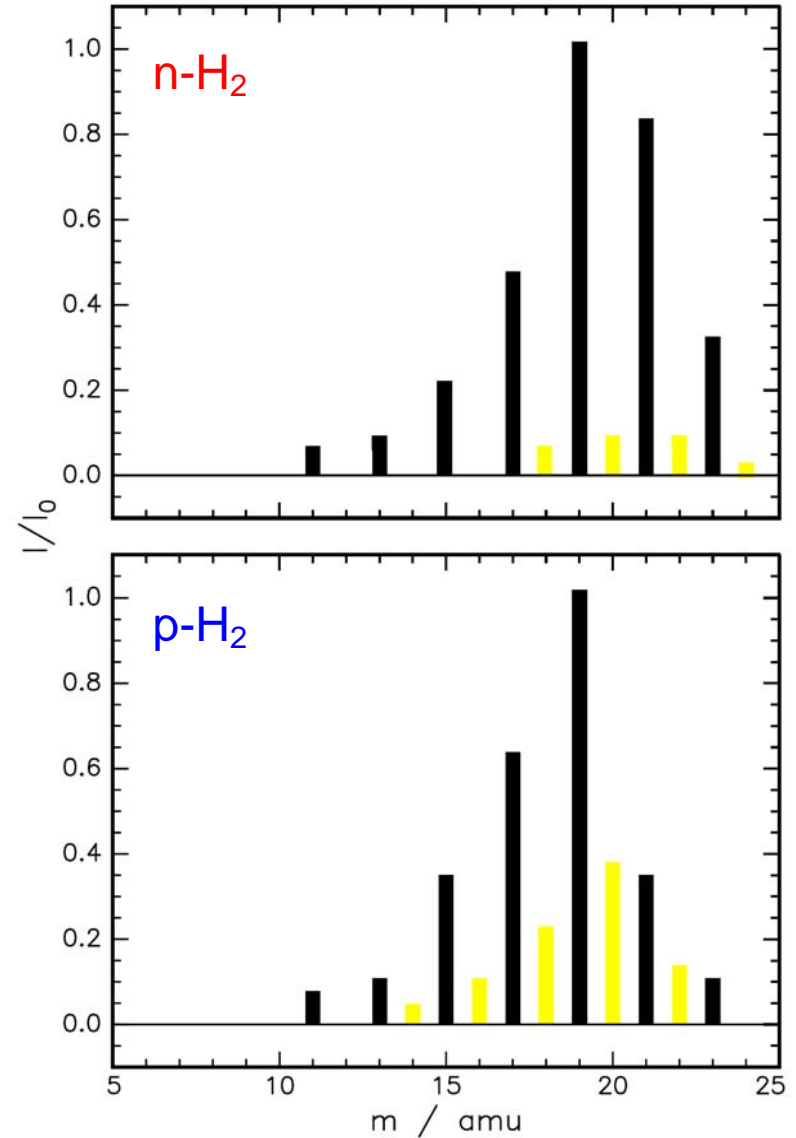
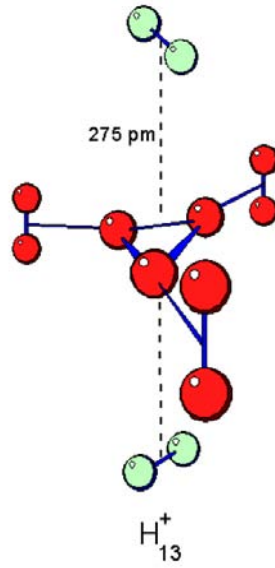
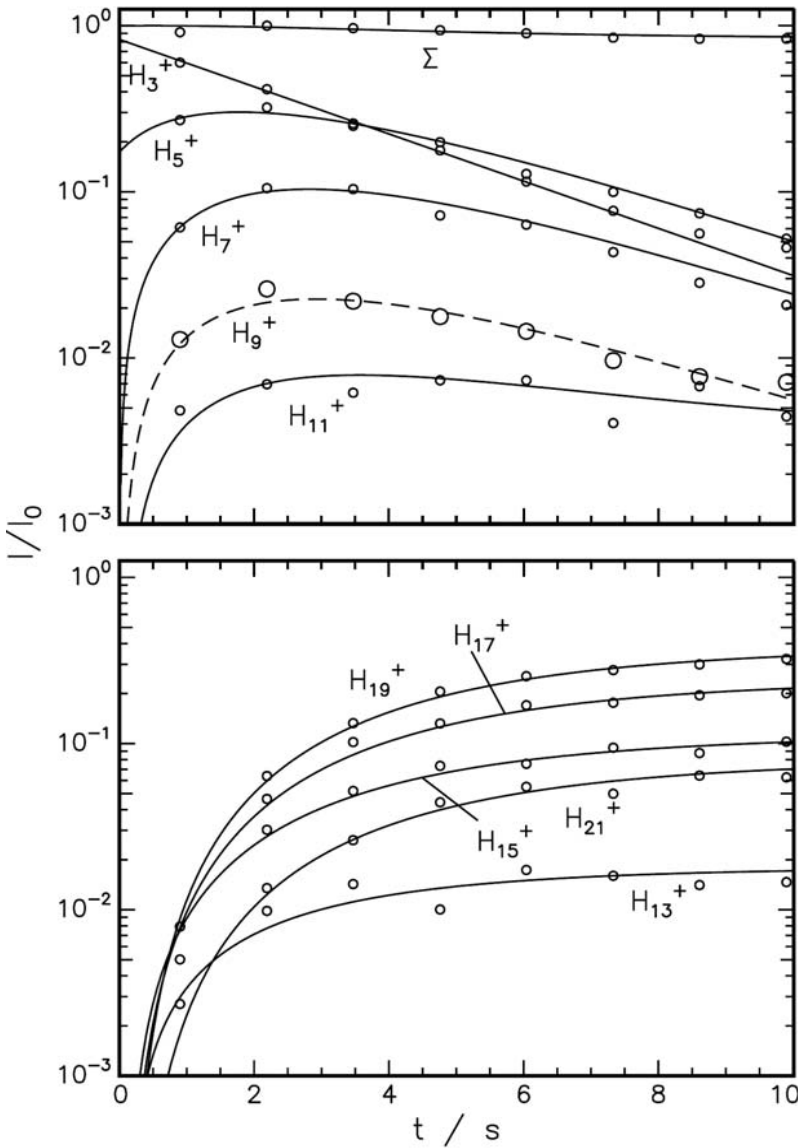


# H<sup>+</sup> + H<sub>2</sub>: Radiative association



# $H_n^+$ cluster growth stationary equilibrium: $n = 19$

$T = 10$  K,  $[H_2] = 10^{14}$  cm $^{-3}$ , storage time 10 s





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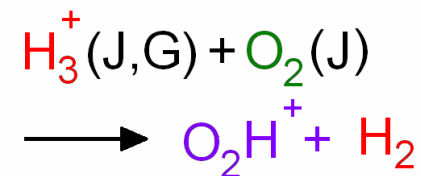
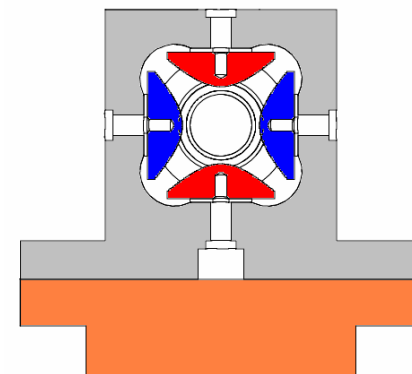
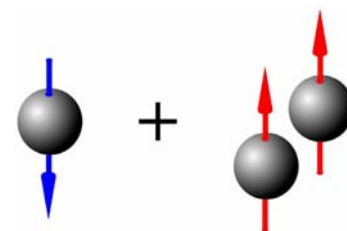
Ortho-para transitions in the trap

## $FeO^+ + H_2$

In situ ortho-para conversion?

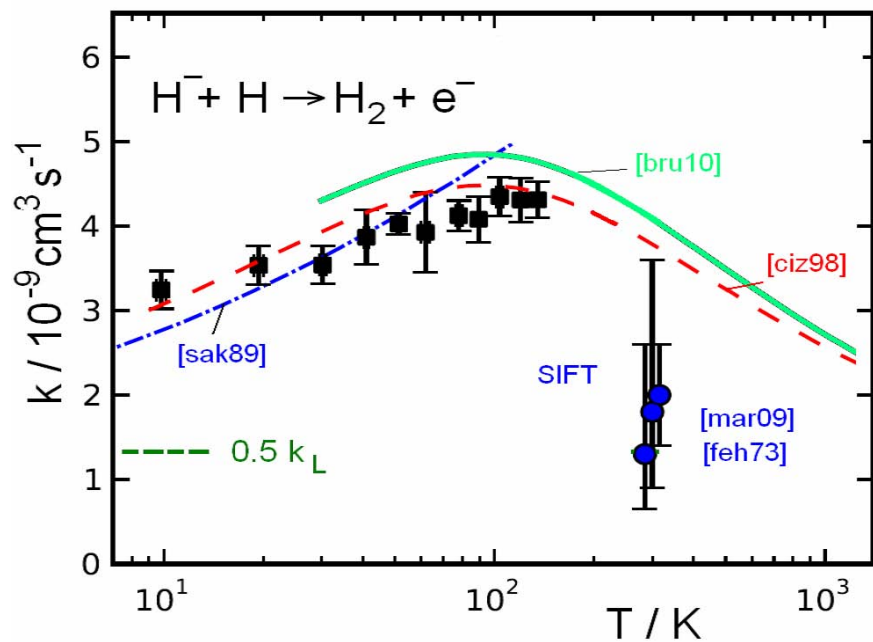
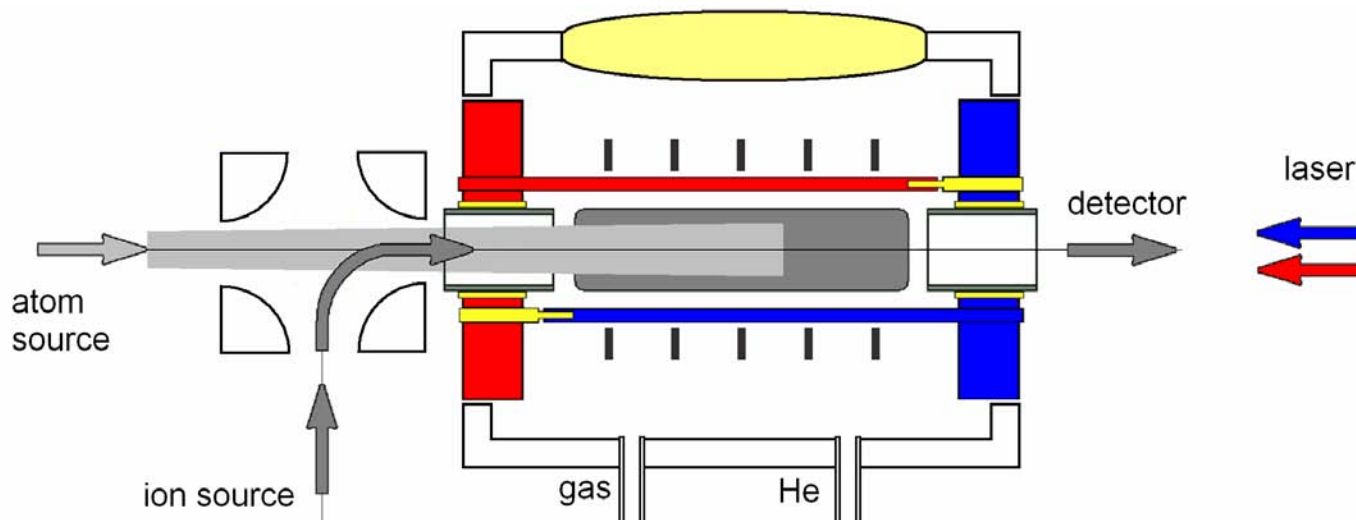
## Outlook

More experimental activities!

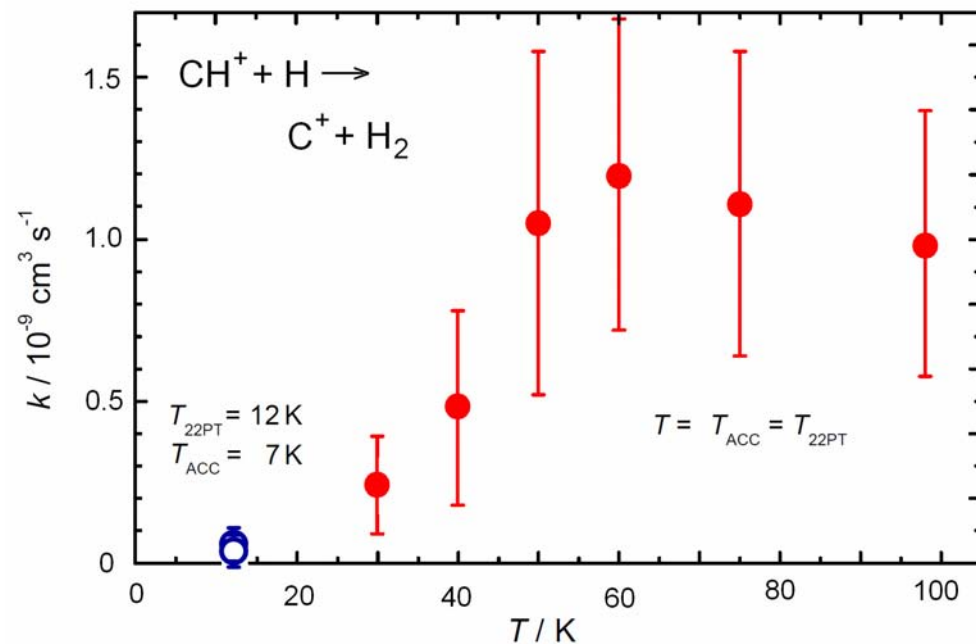




# AB 22PT Chemnitz, since 2010 Prague



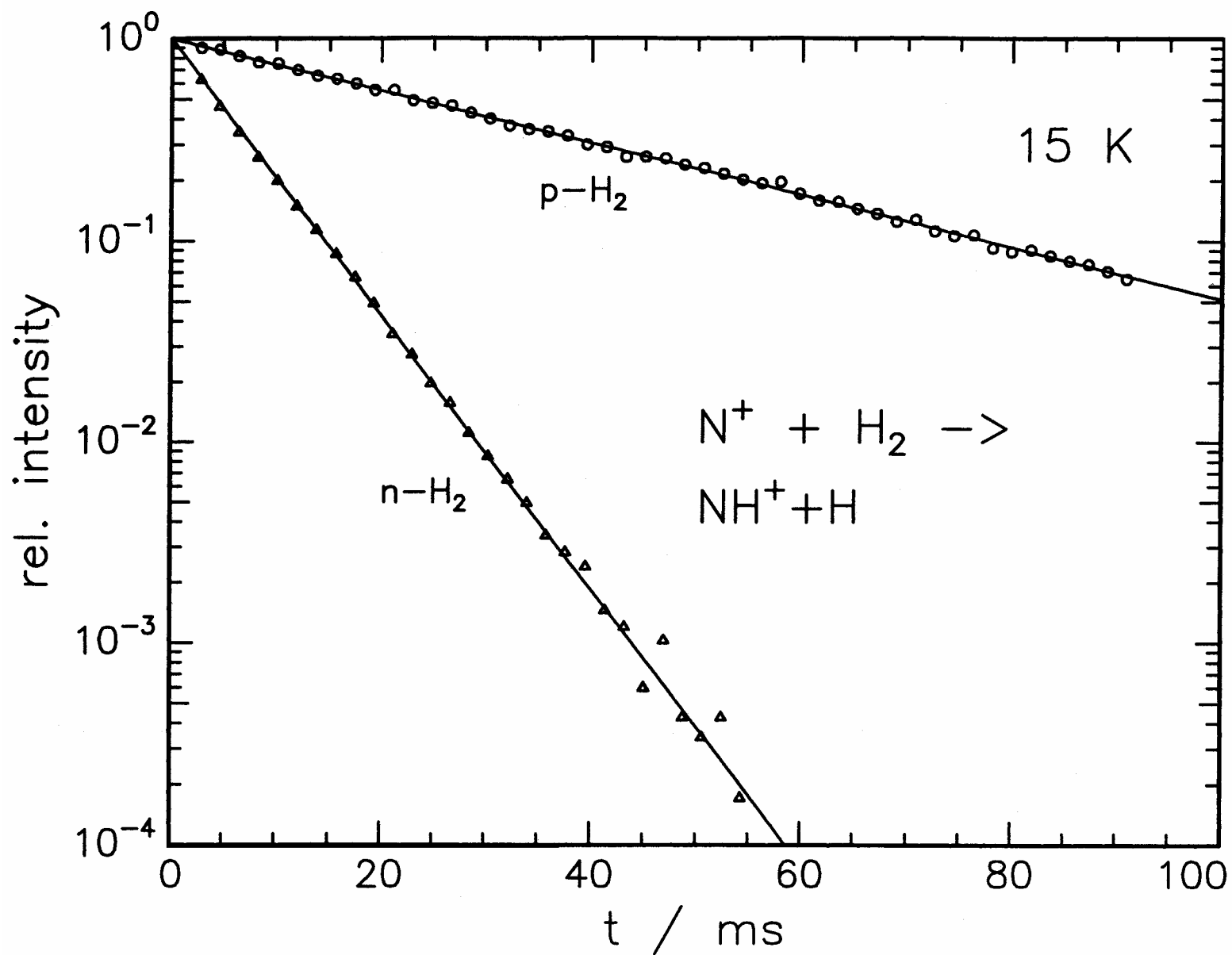
$\text{H}^- + \text{D} / \text{D}^- + \text{H}$



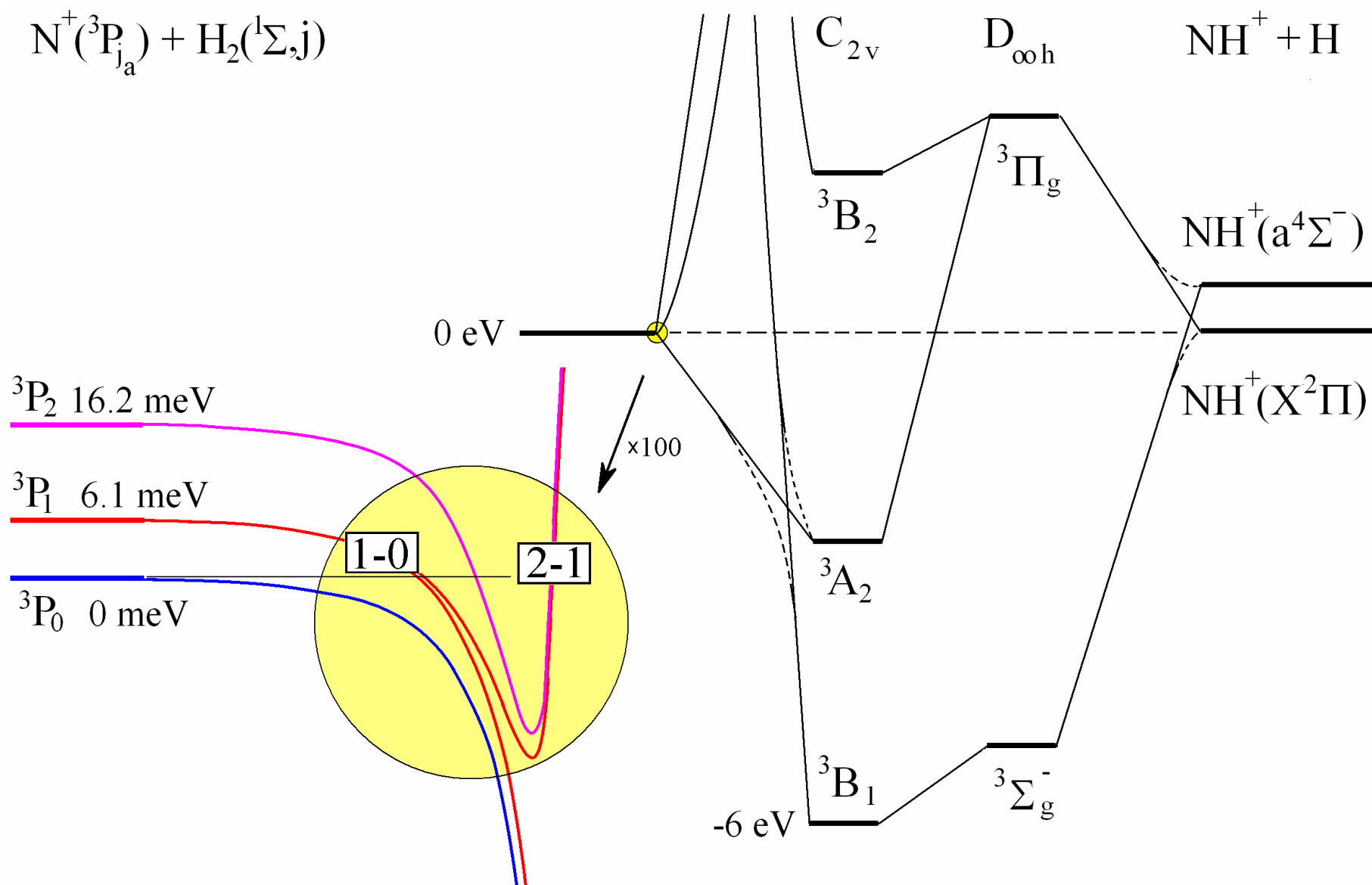
$\text{CH}^+ + \text{H}$



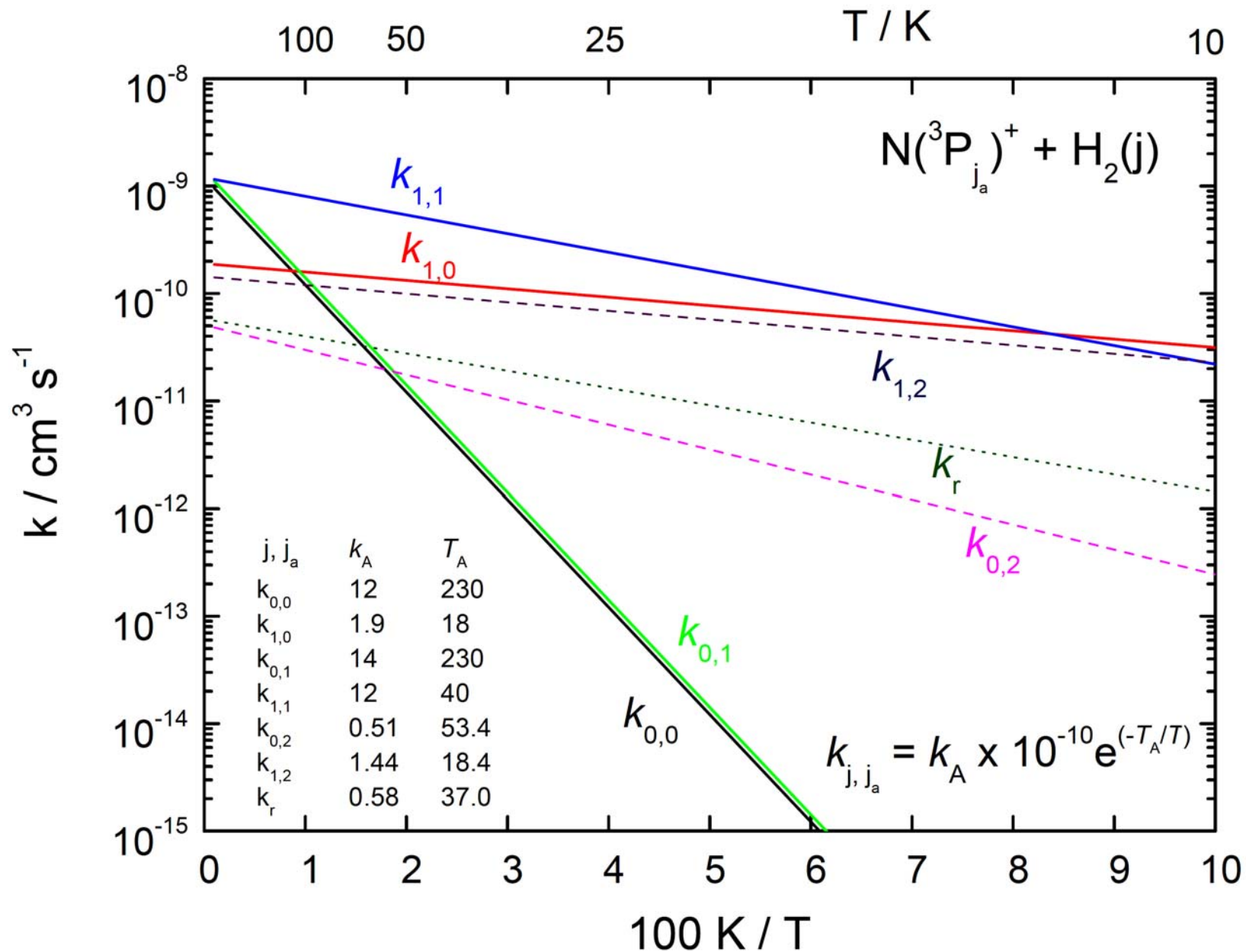
# $N^+ + p/n\text{-H}_2$ at 15K



# Correlation diagram

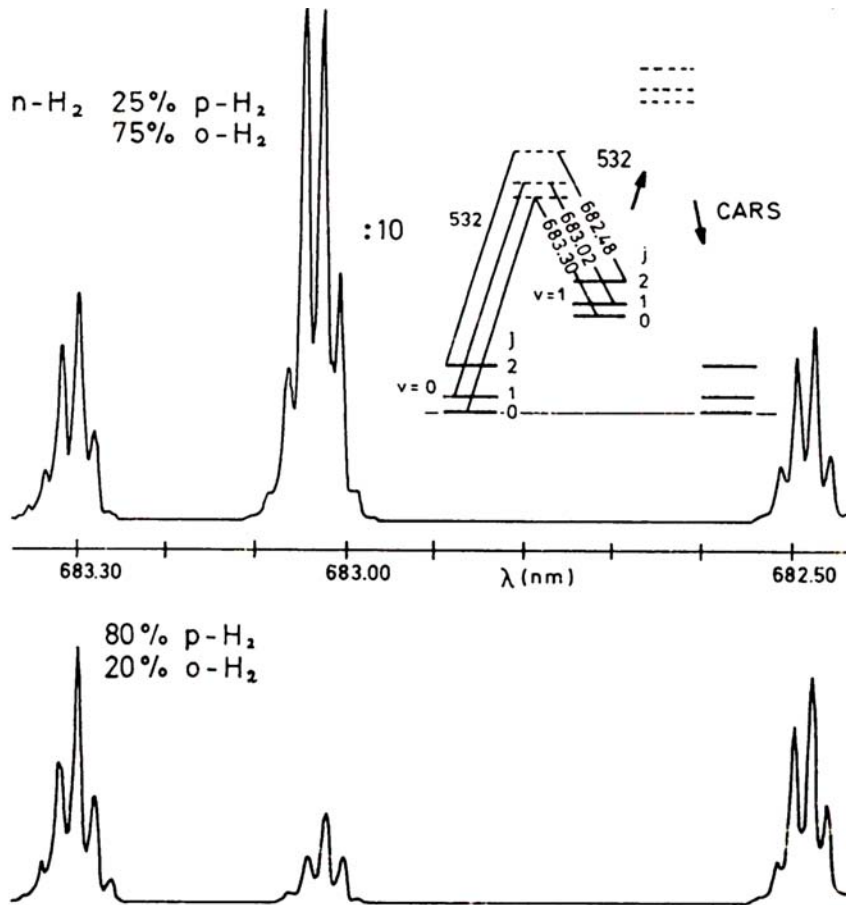


# $N^+ + H_2$ state specific rate coefficients $k(j, j_a)$

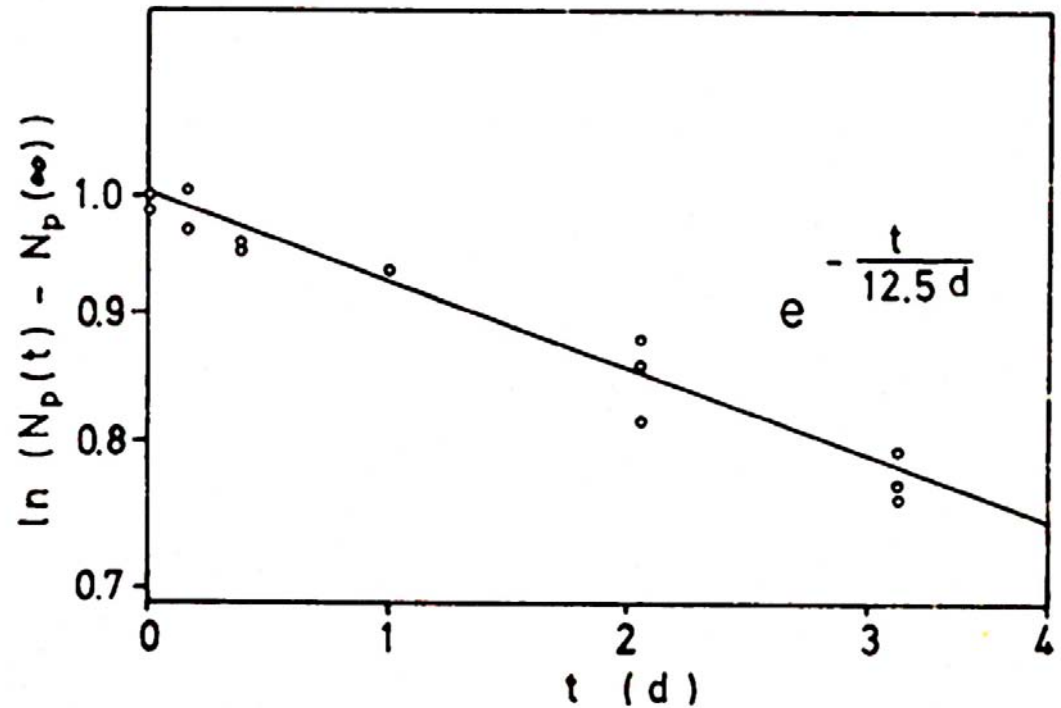


# para-ortho conversion: gas inlet system

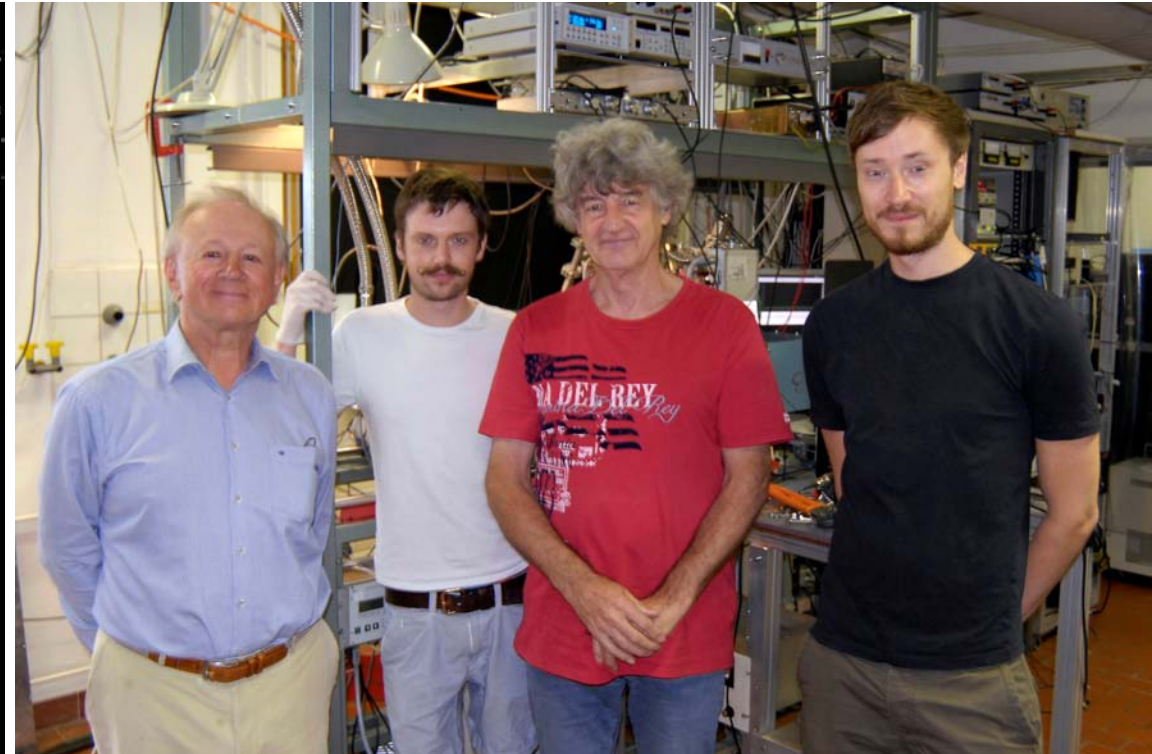
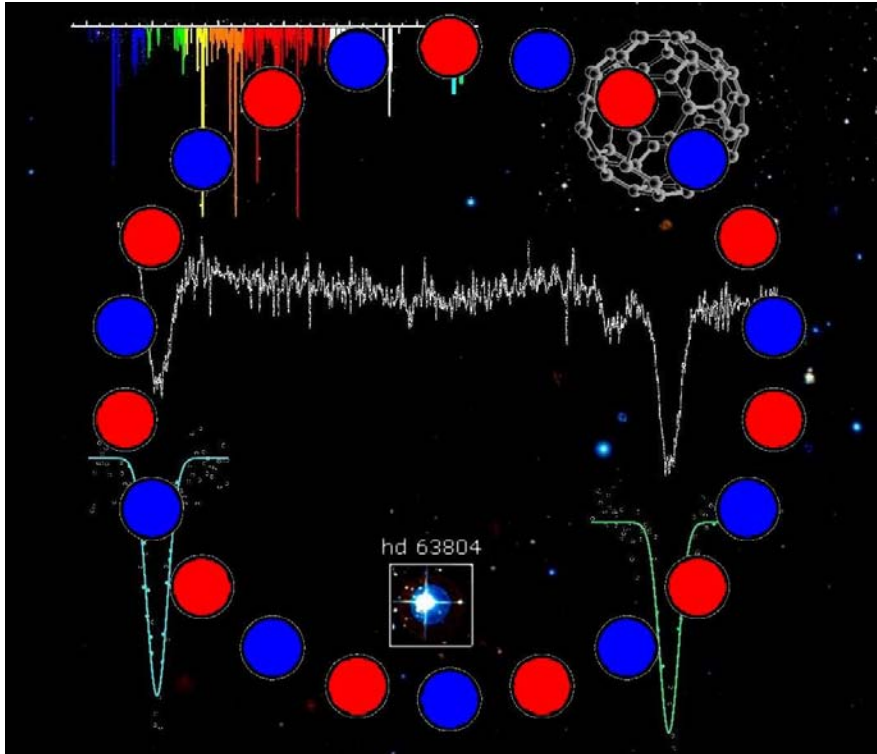
CARS spectrum of n-H<sub>2</sub>  
and enriched p-H<sub>2</sub>



reconversion in a stainless steel  
gas inlet system:  $\tau = 12.5$  d

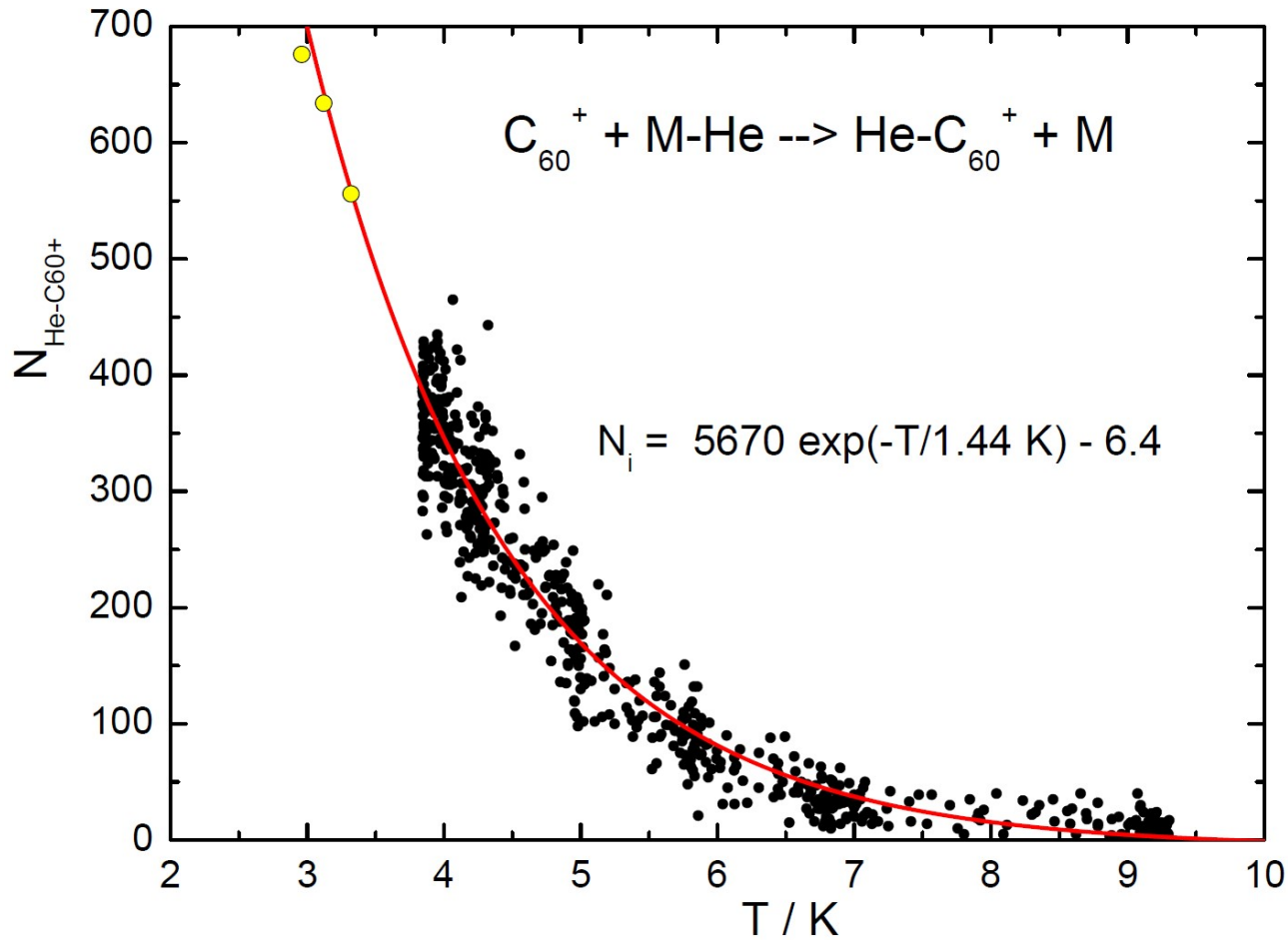


# DIBs in 22-pole



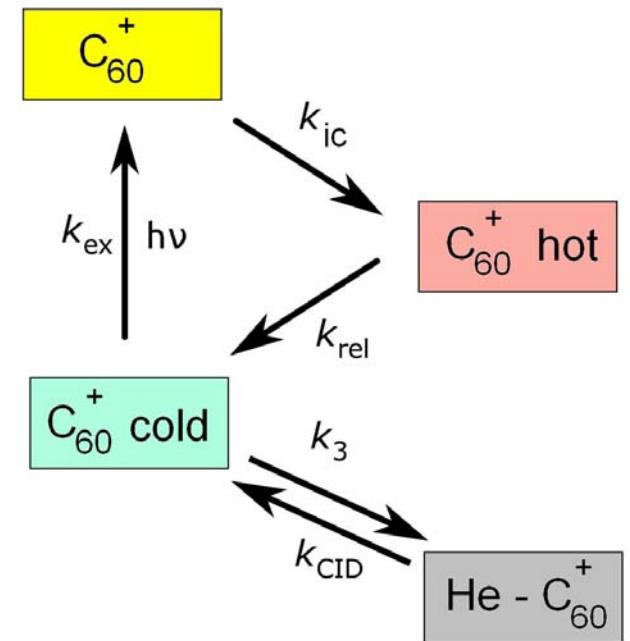
**E. K. Campbell, M. Holz, D. Gerlich & J. P. Maier**  
***Nature* 523 (2015) 322**

# Cooling $C_{60}^+$ , attaching He



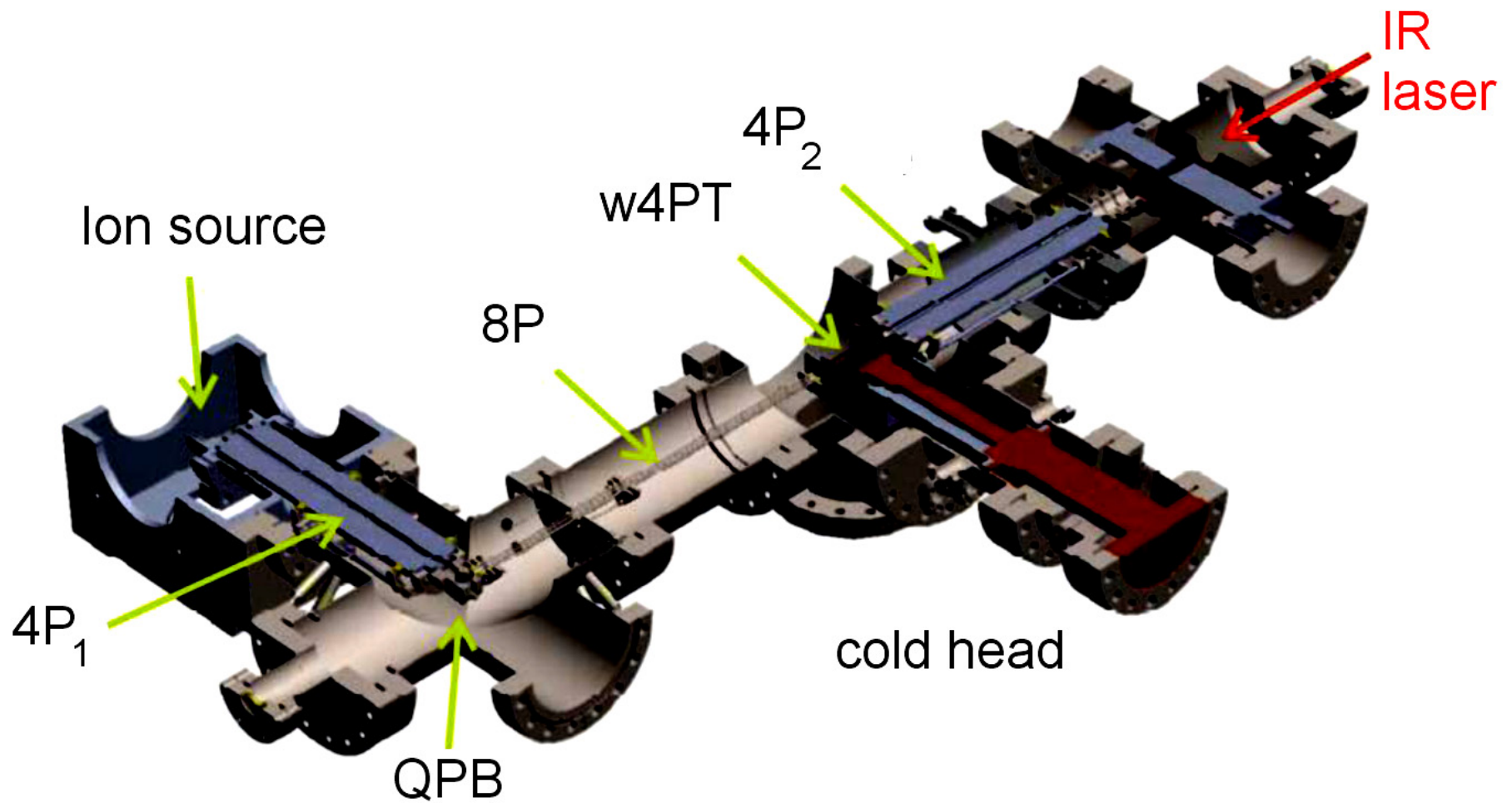
First synthesis of  $He-C_{60}^+$

ISORI  
02.09.2014



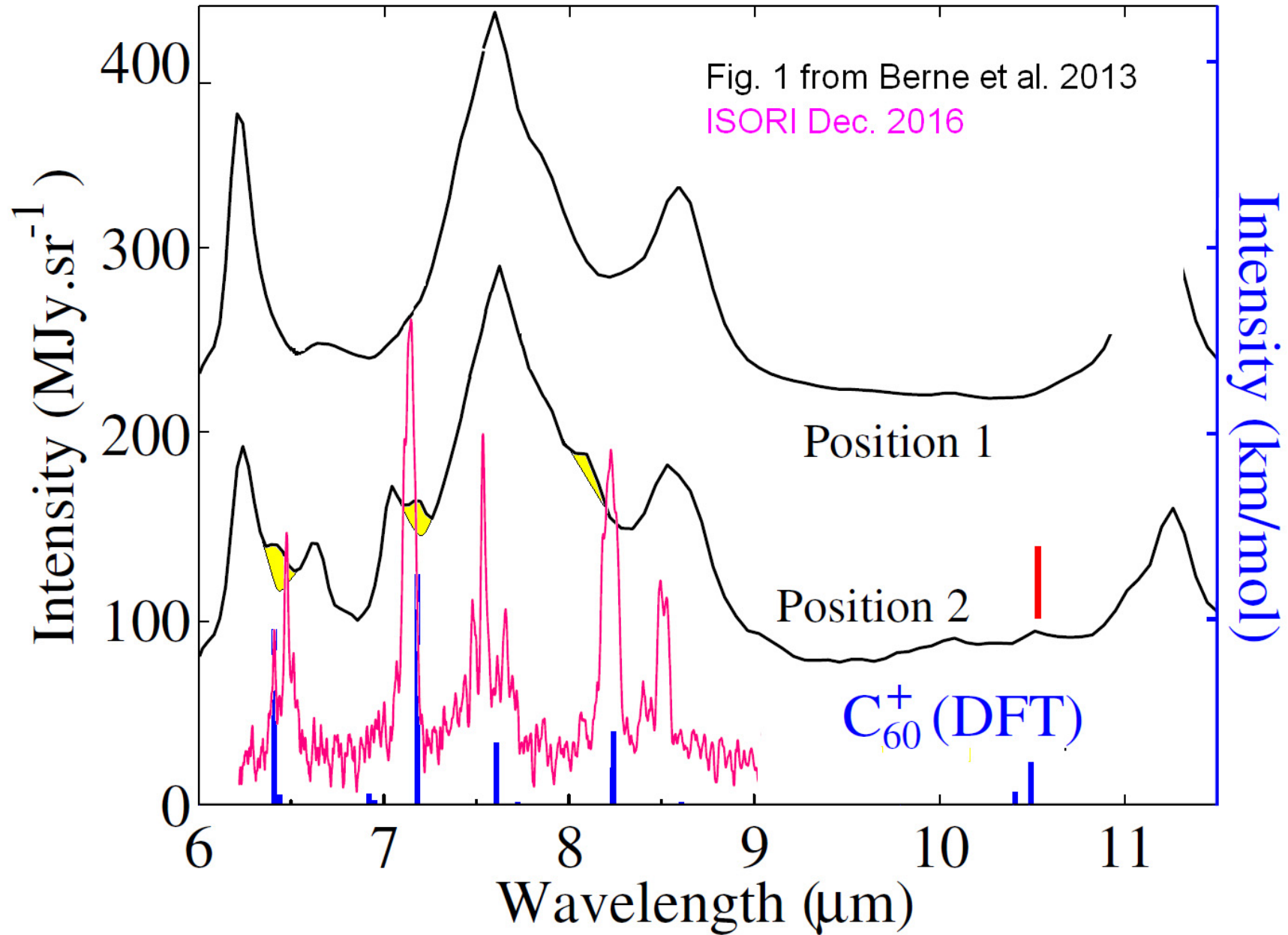


# The ISORI instrument





# First gas phase IR spectra of He-C<sub>60</sub><sup>+</sup>





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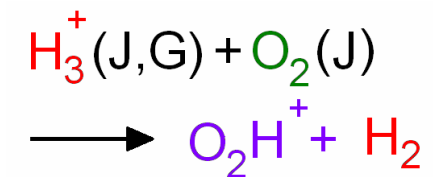
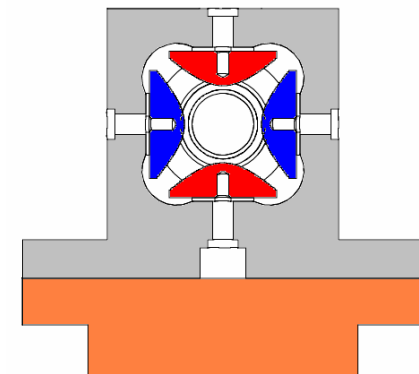
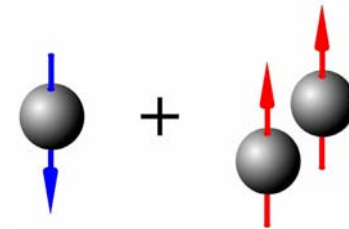
Ortho-para transitions in the trap

## $FeO^+ + H_2$

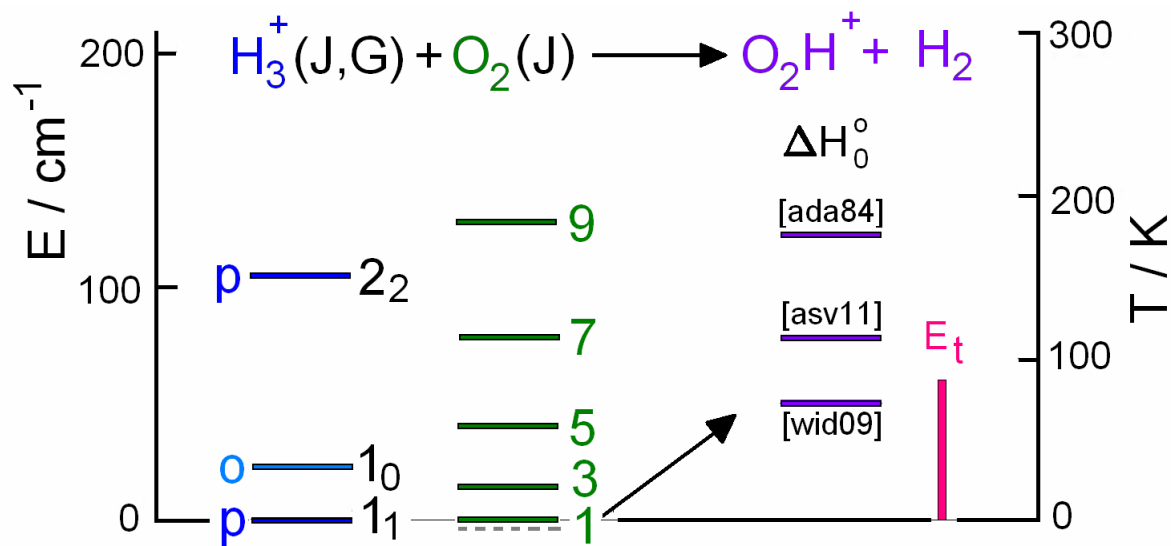
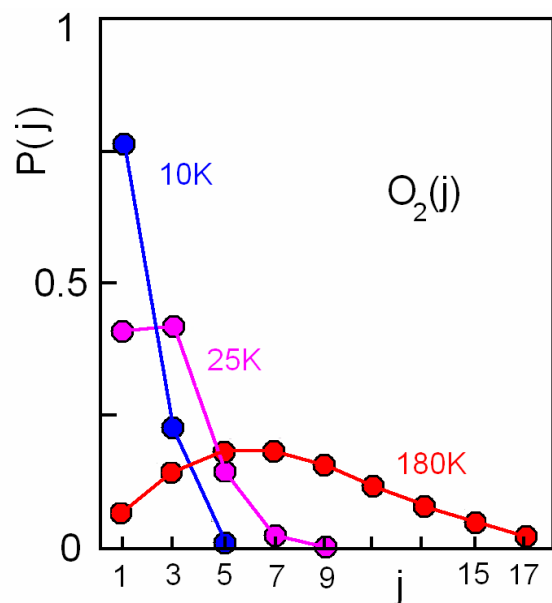
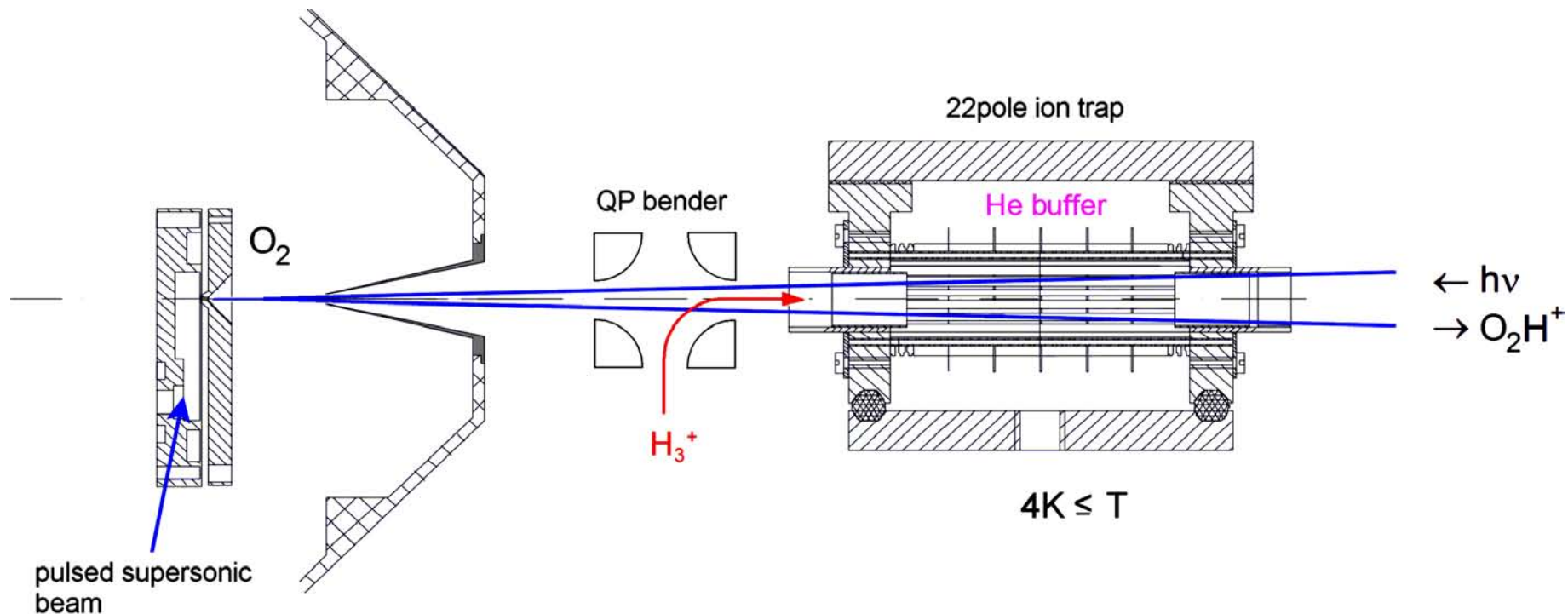
In situ ortho-para conversion?

## Outlook

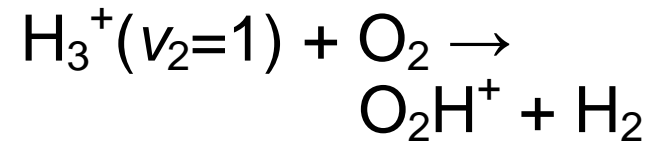
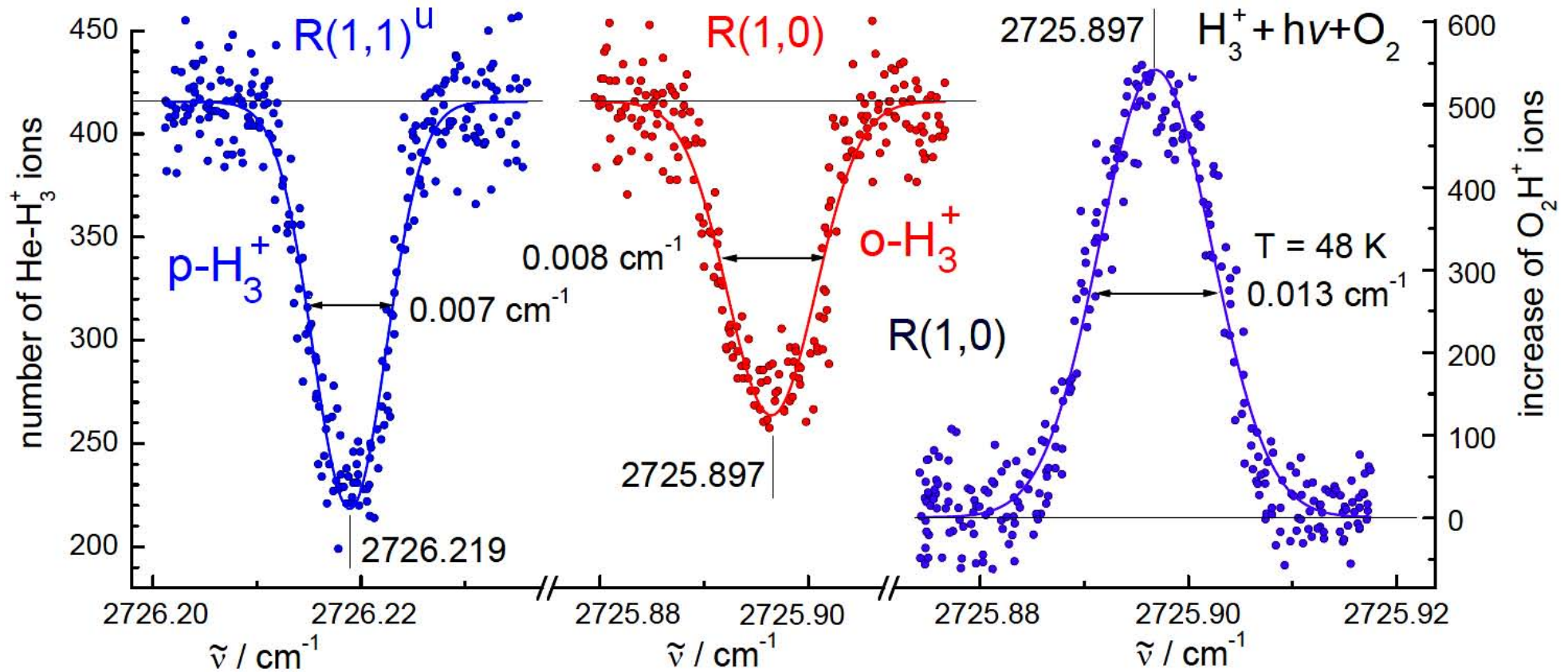
More experimental activities!



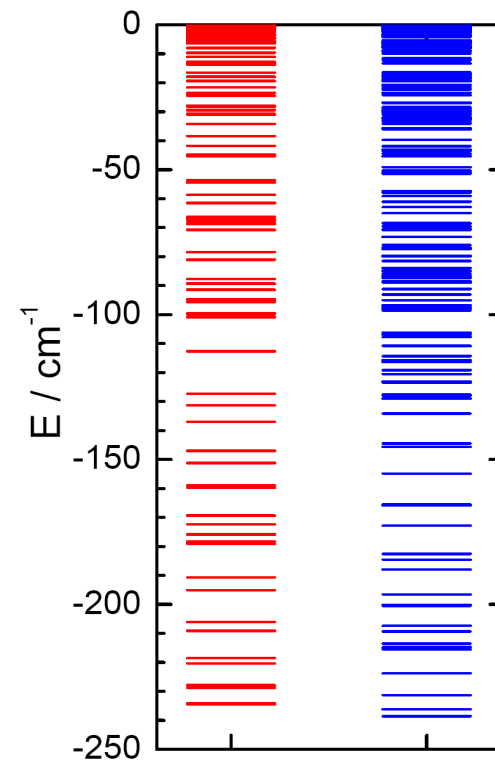
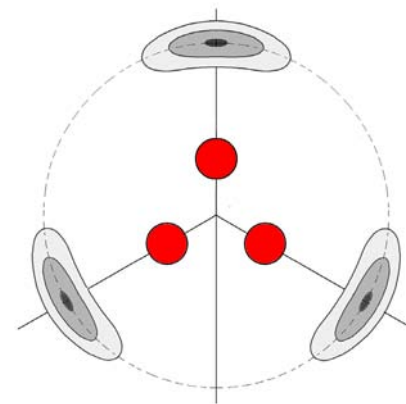
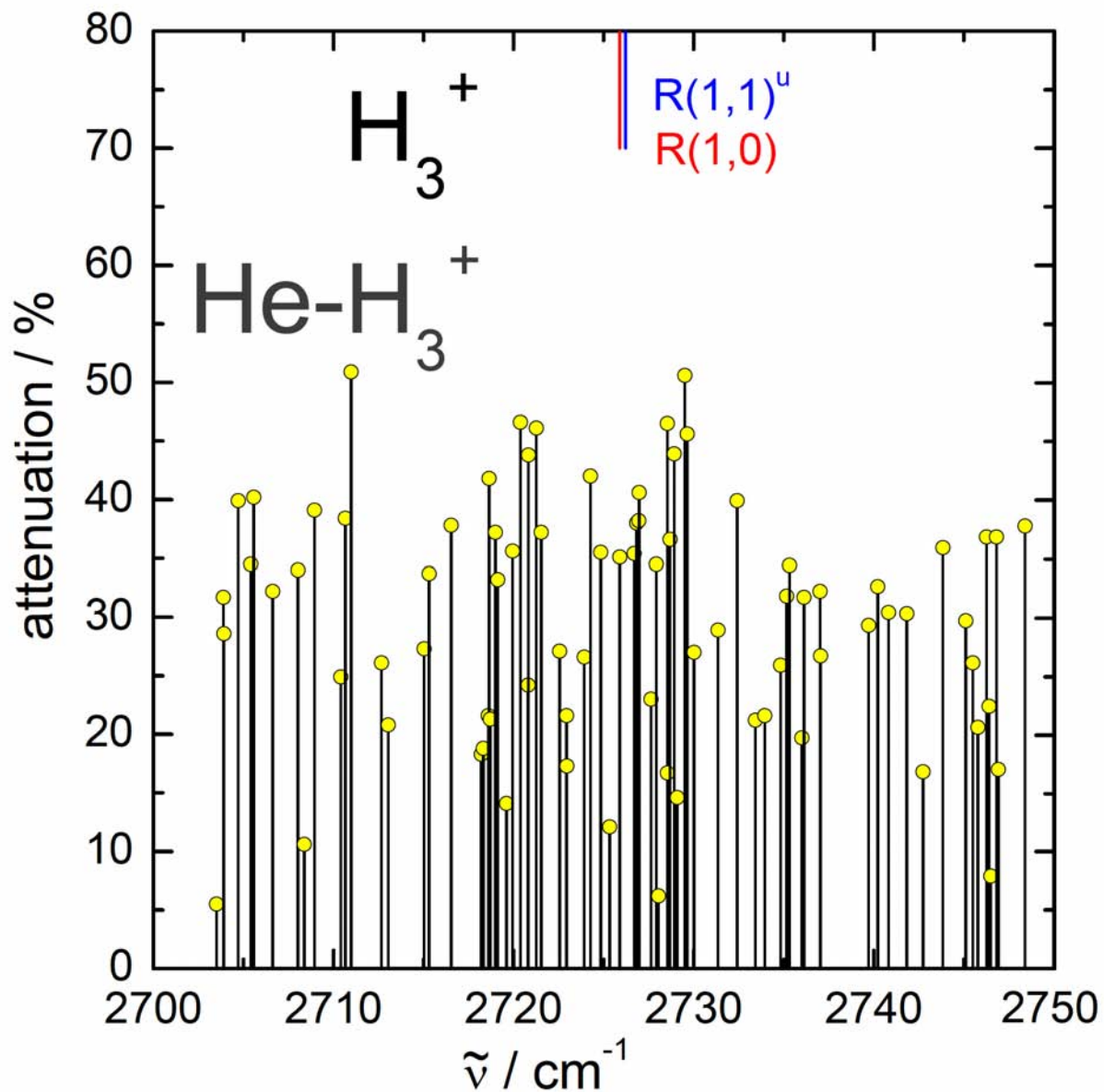
# H<sub>3</sub><sup>+</sup>(J,G): probing with O<sub>2</sub>



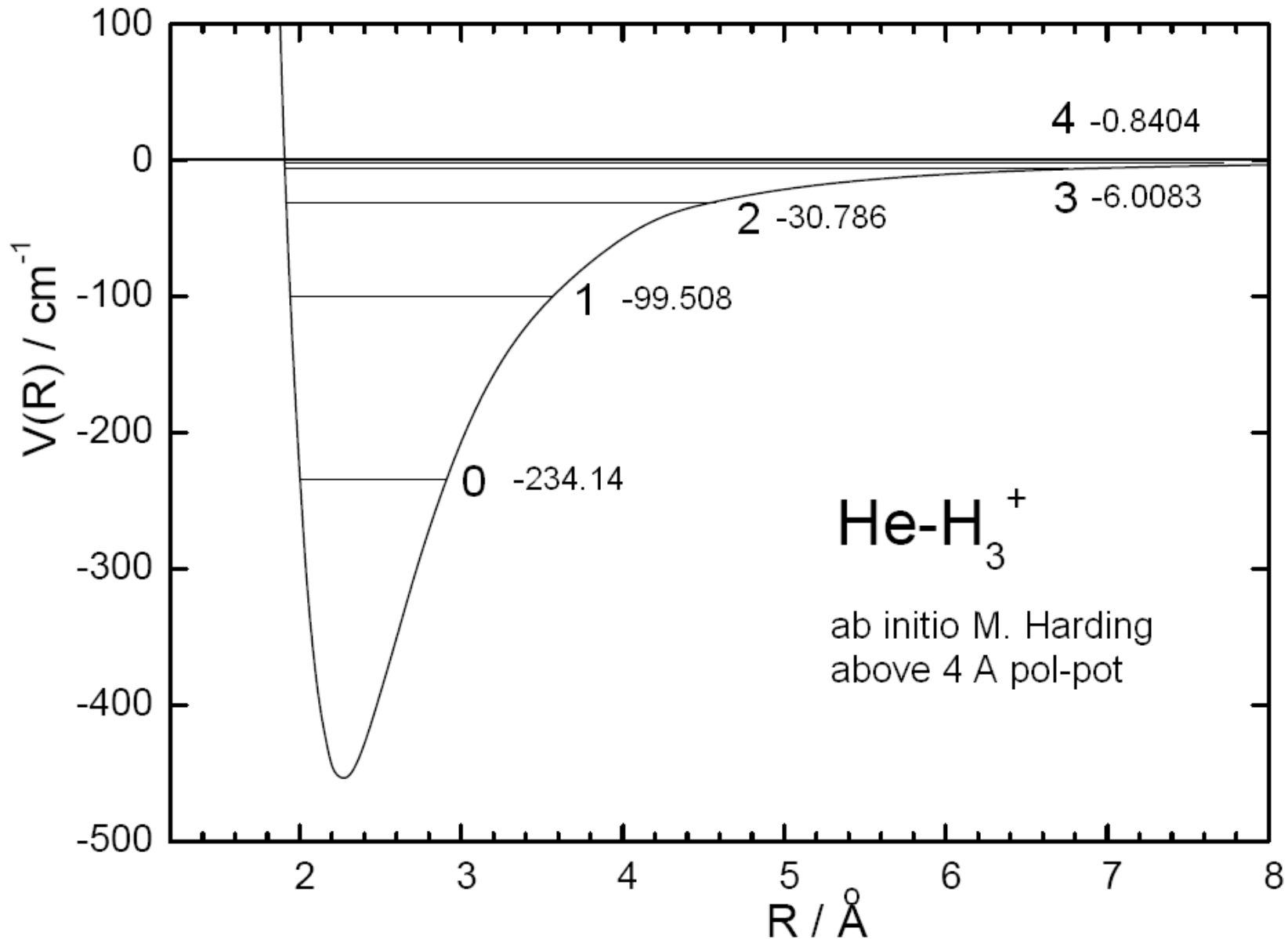
# H<sub>3</sub><sup>+</sup> transitions: LIICG and LICT



# He-H<sub>3</sub><sup>+</sup> system



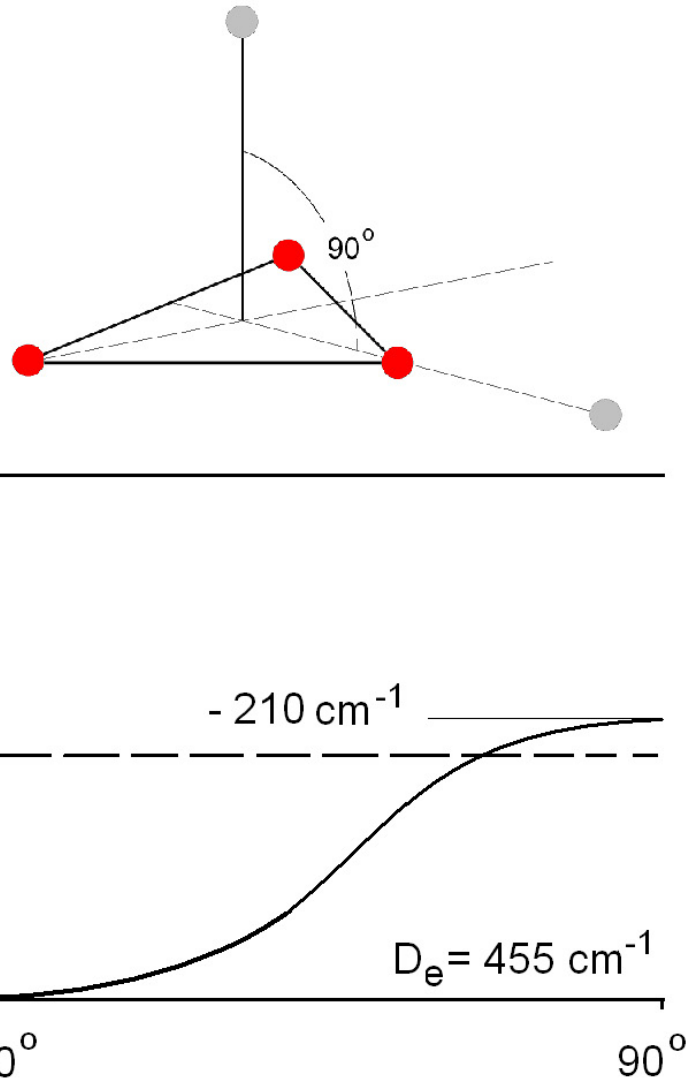
# He-H<sub>3</sub><sup>+</sup> vdW - potential



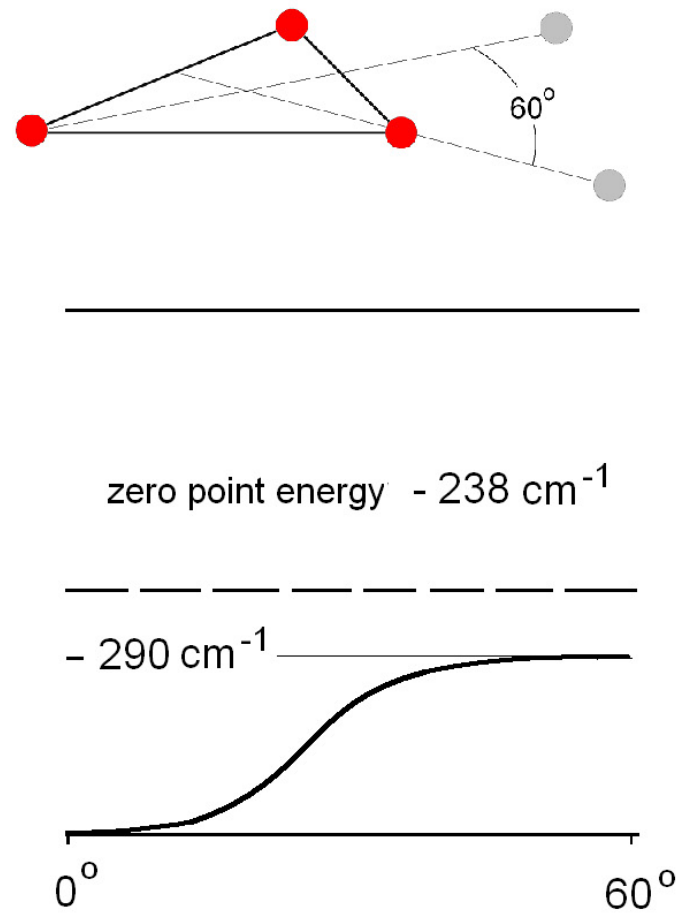


# He-H<sub>3</sub><sup>+</sup> potential

out off plane

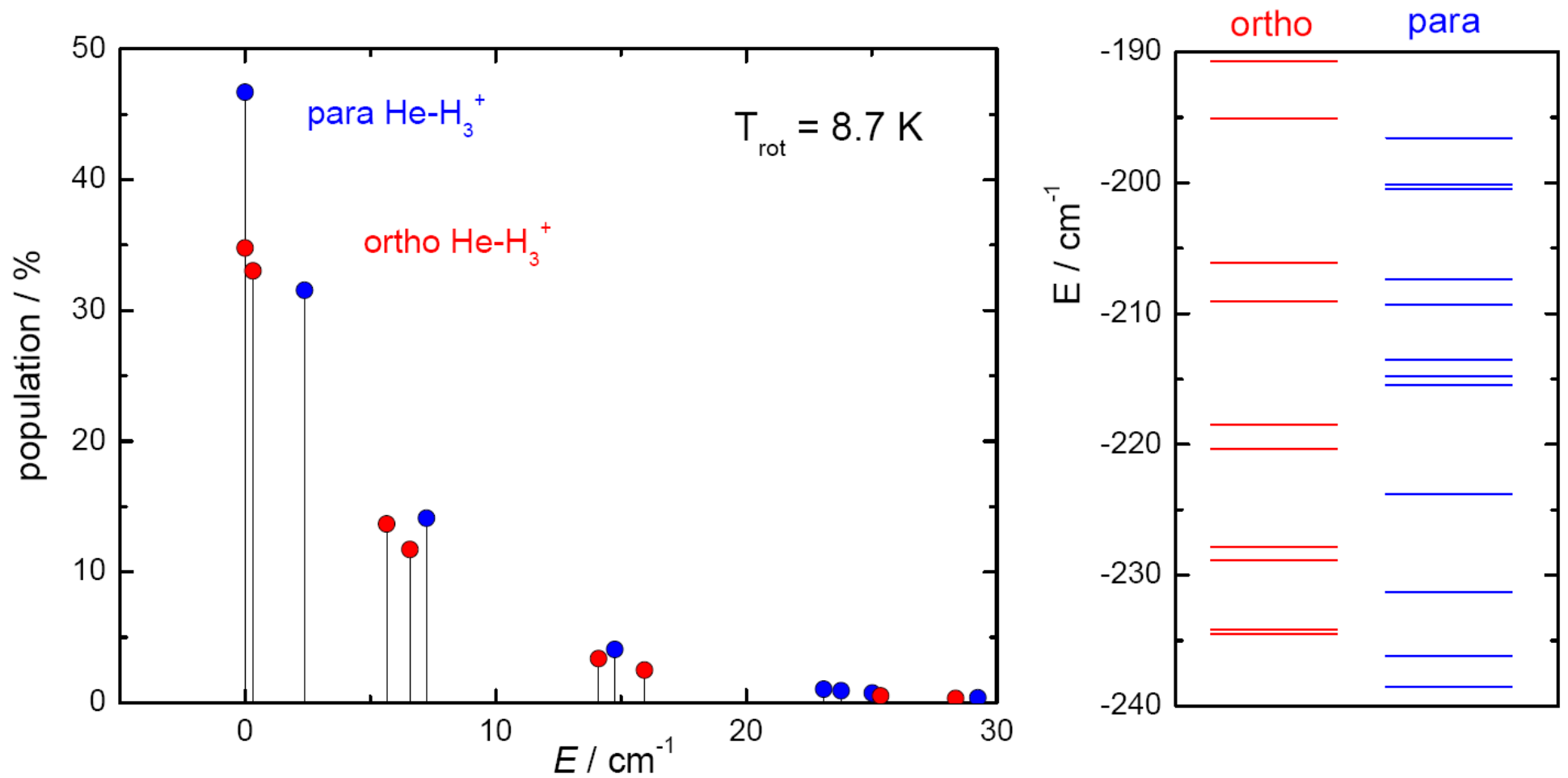


in plane

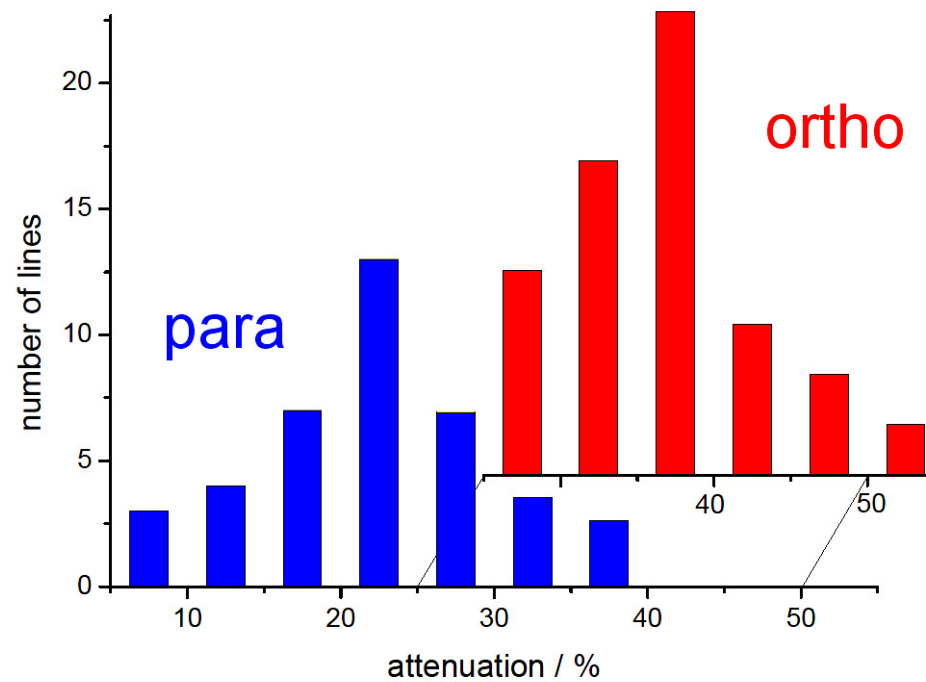
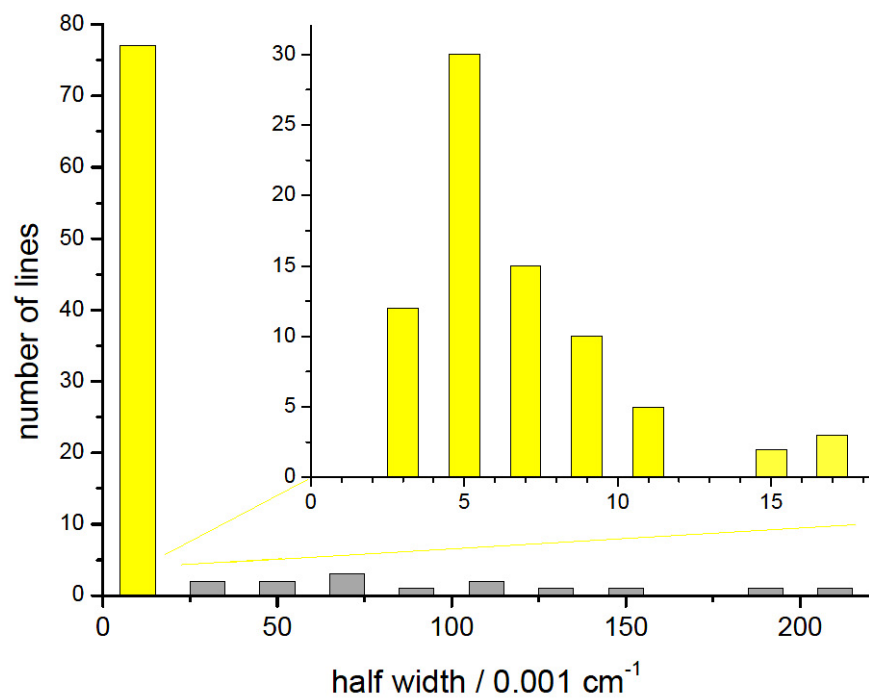




# He-H<sub>3</sub><sup>+</sup> thermal population at 8.7 K



# How to assign the states: statistics





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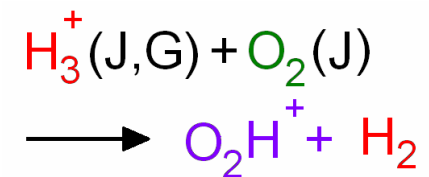
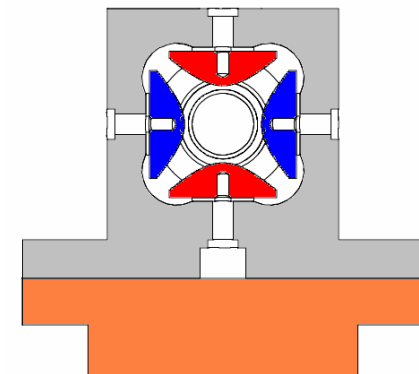
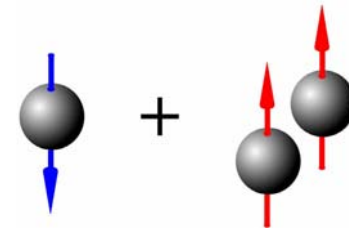
Ortho-para transitions in the trap

## $FeO^+ + H_2$

In situ ortho-para conversion?

## Outlook

More experimental activities!



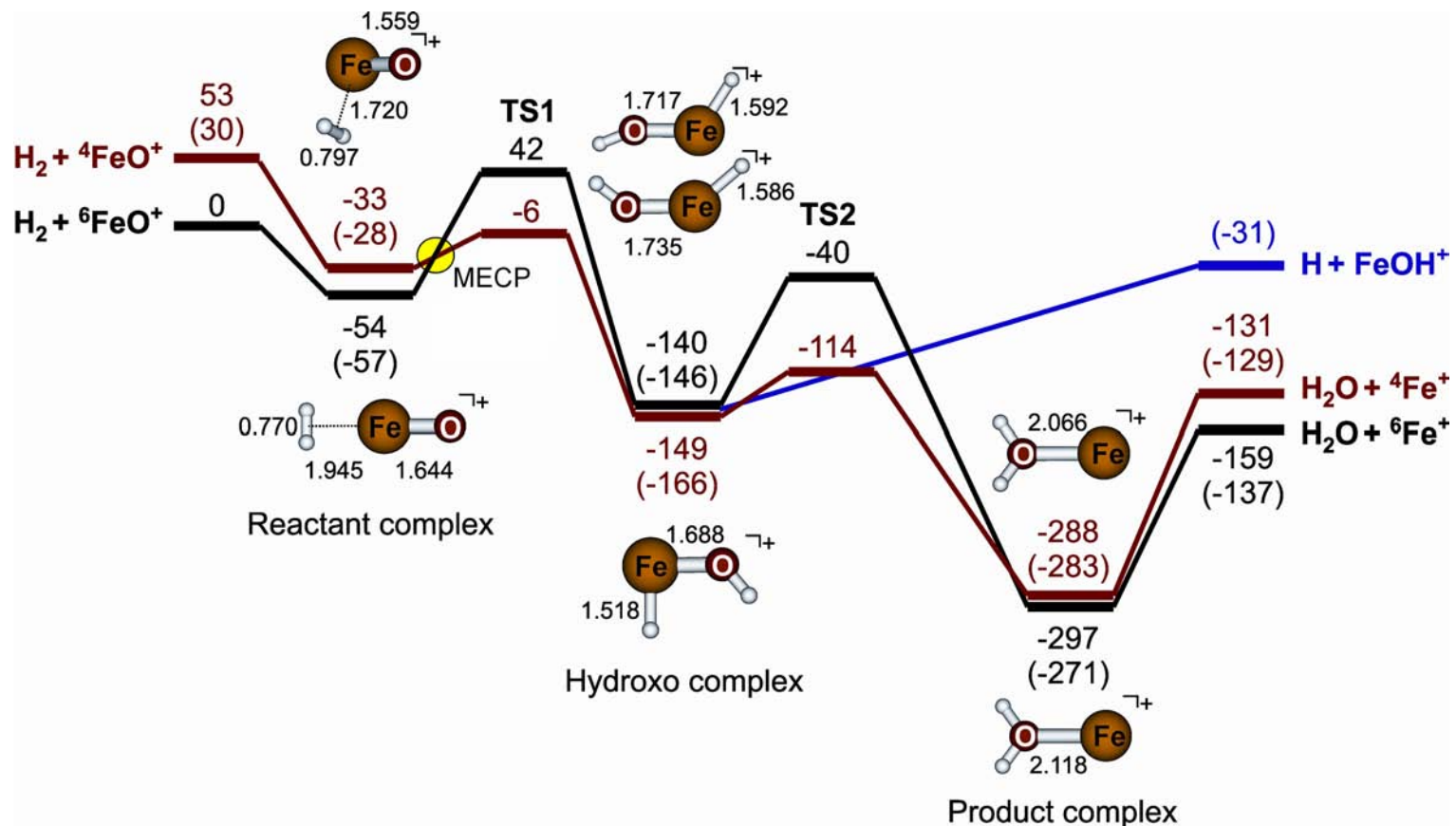


20 years: ICR, SIFT, GIB, TV SIFT, spin forbidden  $k(300 \text{ K}) = 10^{-11} \text{ cm}^3/\text{s}$

S. G. Ard *et al.* J. Phys. Chem. A **118** (2014) 6789

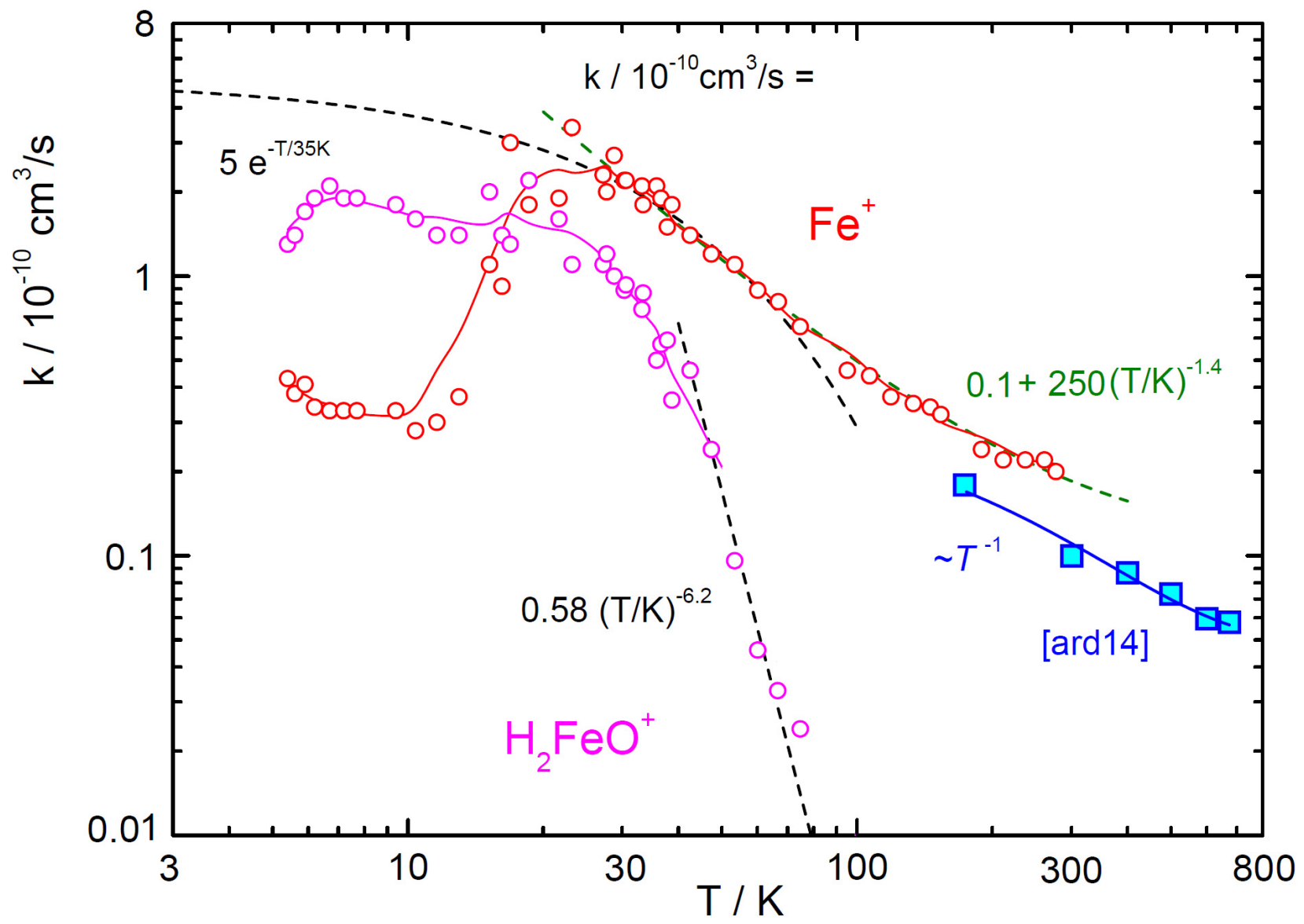
J.N. Harvey, D.P. Tew, Int. J. Mass Spectrom. **354** (2013) 263

D. Schröder *et al.* Int. J. Mass Spectrom. Ion Proc. **161** (1997) 175

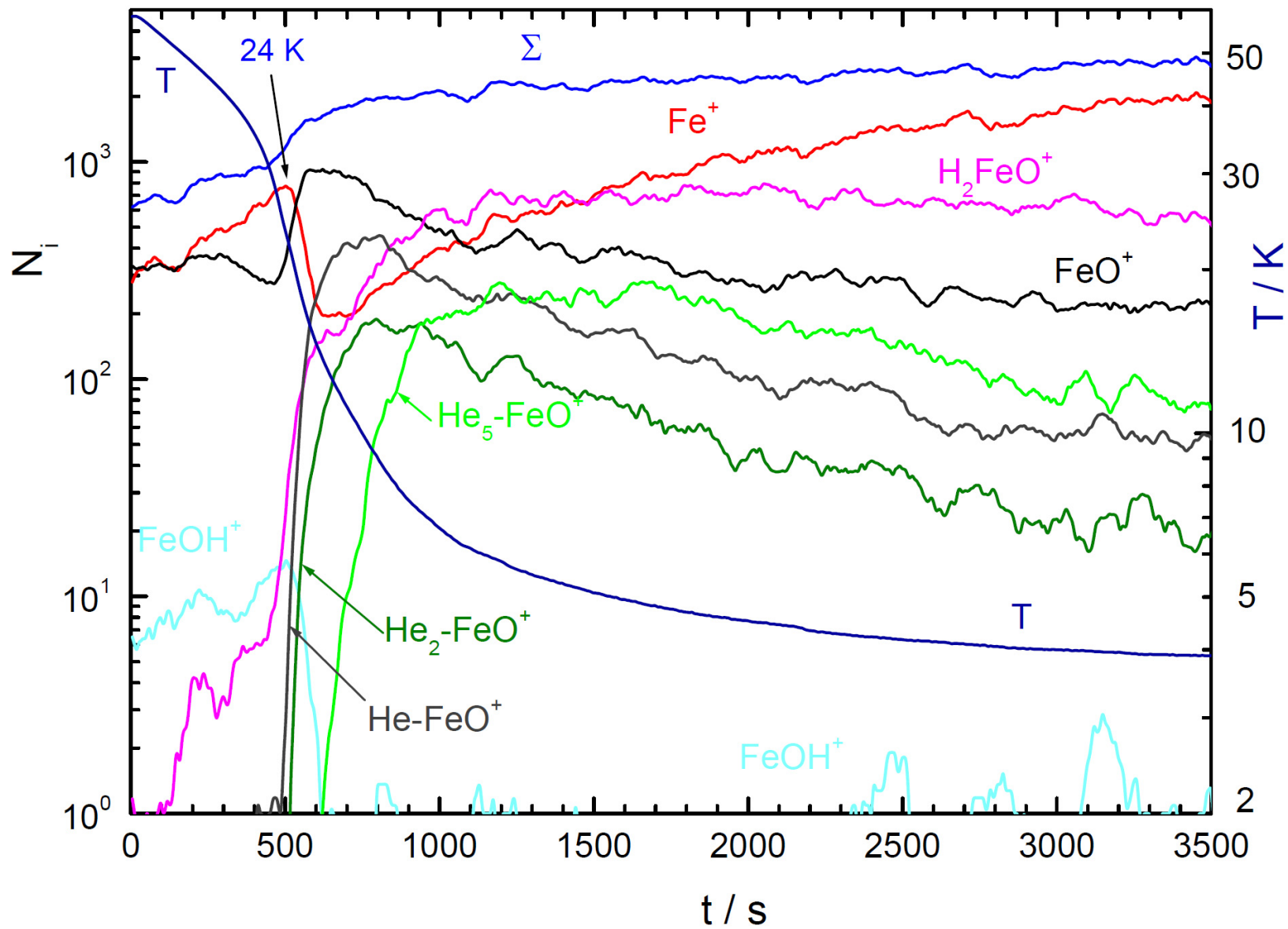


D. Gerlich, J. Jašík, E. Andris, R. Navrátil, J. Roithová, ChemPhysChem **17** (2016) 3723

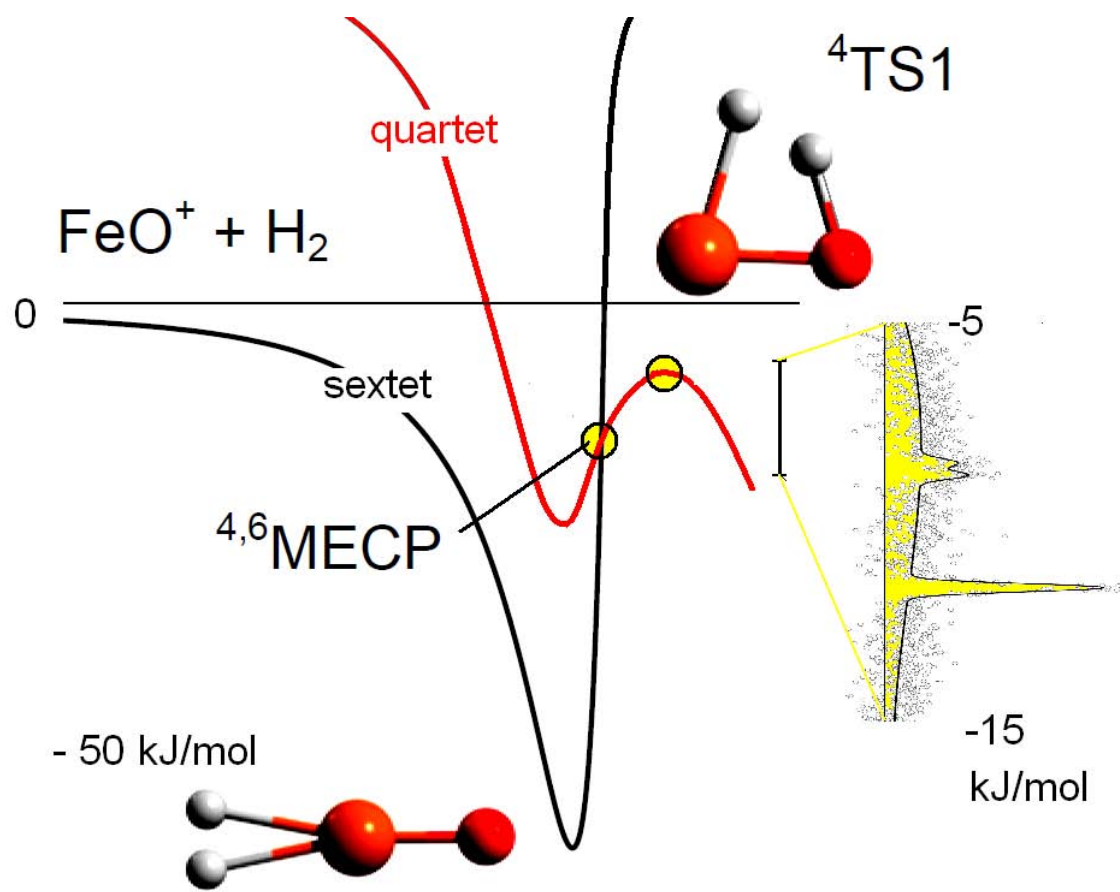
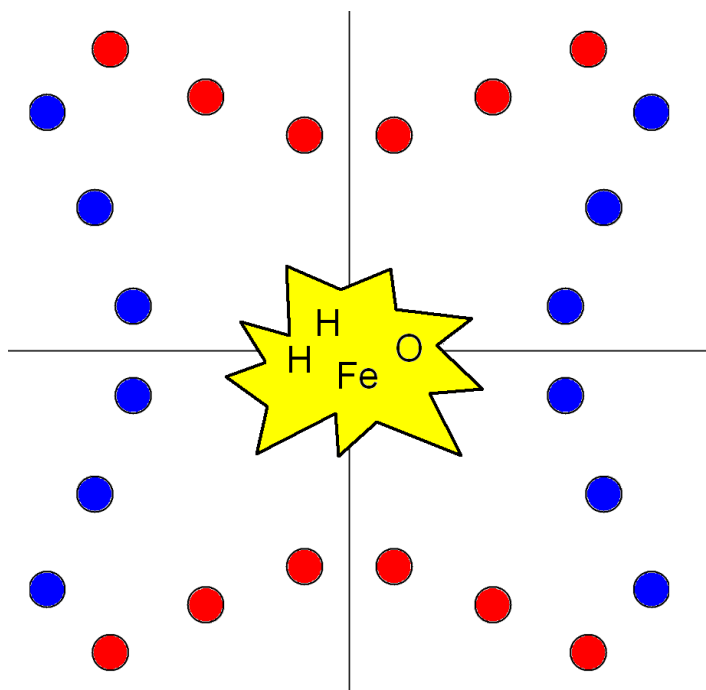
# FeO<sup>+</sup> + H<sub>2</sub> + He



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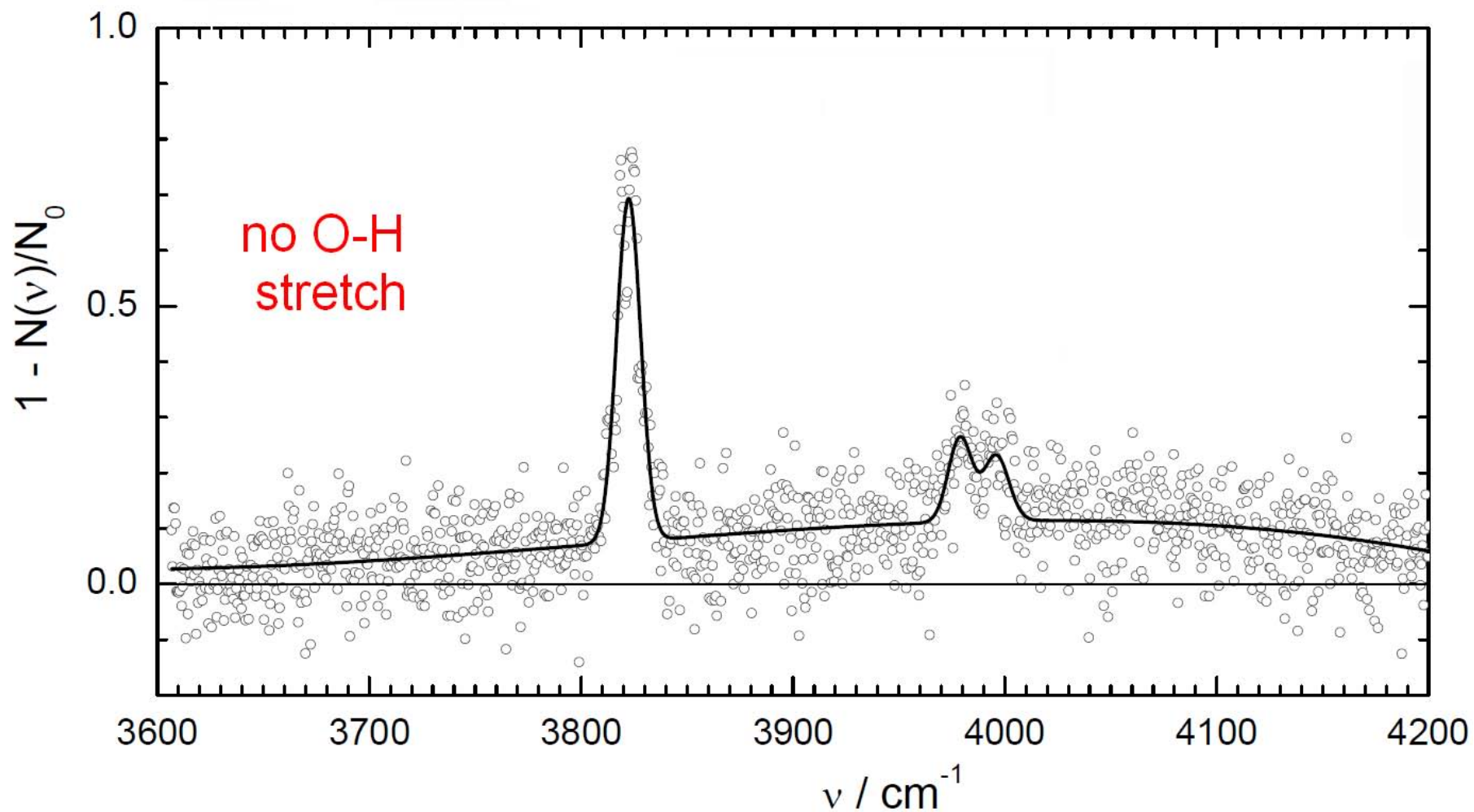
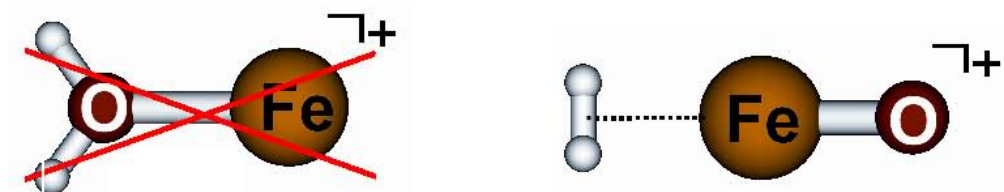


# $[(\text{H}_2)\text{FeO}]^+$ intermediates in the trap





# IR spectrum of the reaction intermediate $[(\text{H}_2)\text{FeO}]^+$





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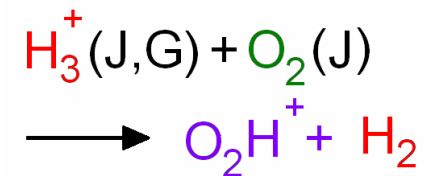
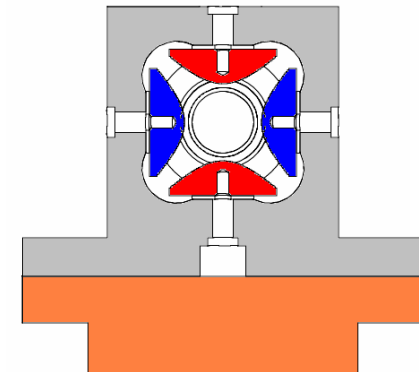
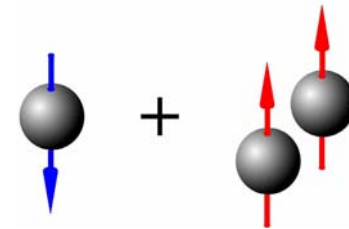
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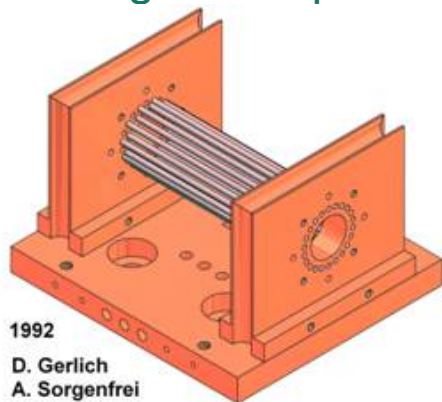
## Outlook

More experimental activities!



# RF multipoles: 22- or 4-pole?

Original 22-pole



## Selection criteria

Cooling:  $T_{\text{coll}} = m_1 T_2 + m_2 T_1 / (m_1 + m_2)$

High order multipole: wide nearly field free region

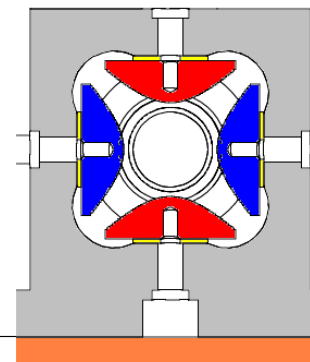
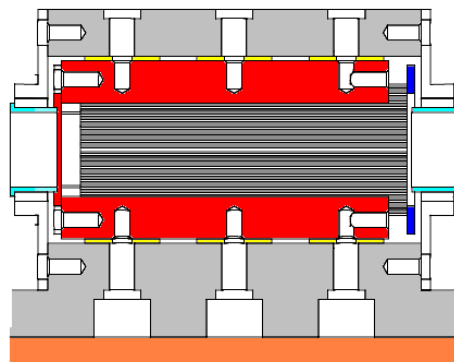
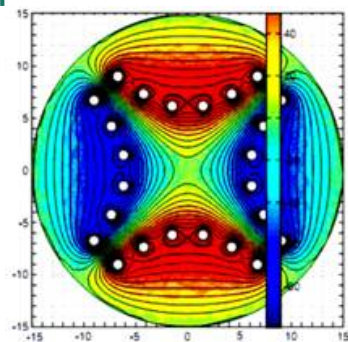
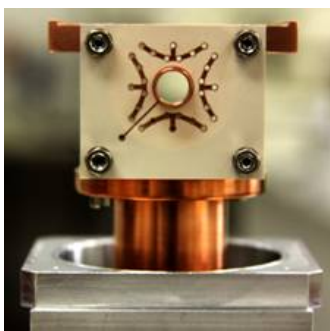
Linear w4PT: harmonic potential

Squeezing ion cloud into the laser beam

Mass selective resonant excitation

Isomer specific gas friction

Wire quadrupole, printed board



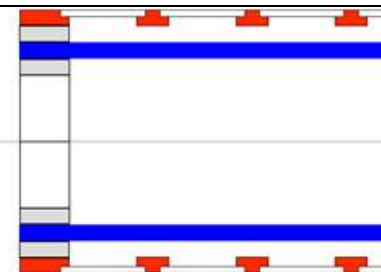
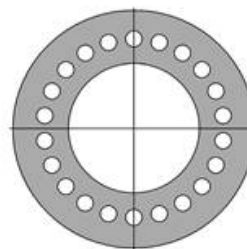
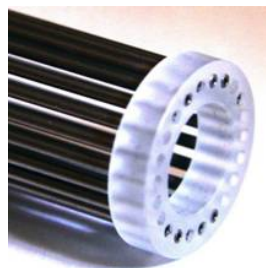
Next generation 22 pole

Sapphire holders

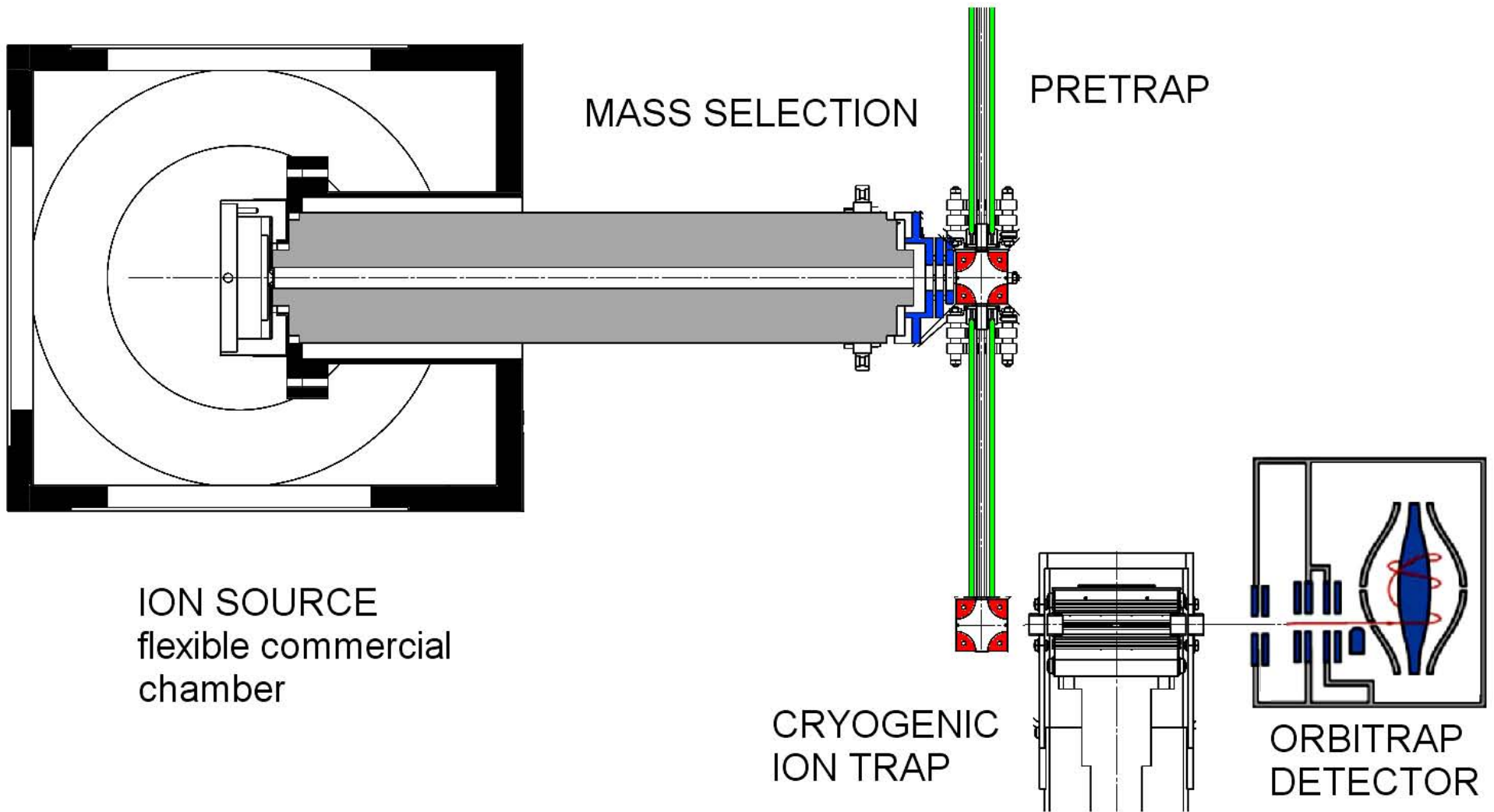
Minimal volume

Integrated correction electrodes

42 pole with 0.5 mm rods



# Cryogenic trap for astrochemistry





Universität Freiburg (C. Schlier)

1969 - 1994

Ionenphysik TU Chemnitz

1994 - 2009

## Cooperations and hospitality

M. Smith, Tucson

2004 - 2010

J. Glosik, Prague

2009 - 2014

J. Maier, E. Campbell, Basel

2002 - 2016

S. Schlemmer, I. Savic, Köln

2010 -

J. Roitova, J. Jasik, Prague

2011 -