Experiments on Electron-Ion Collisions for Fusion

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Principal Collaborators

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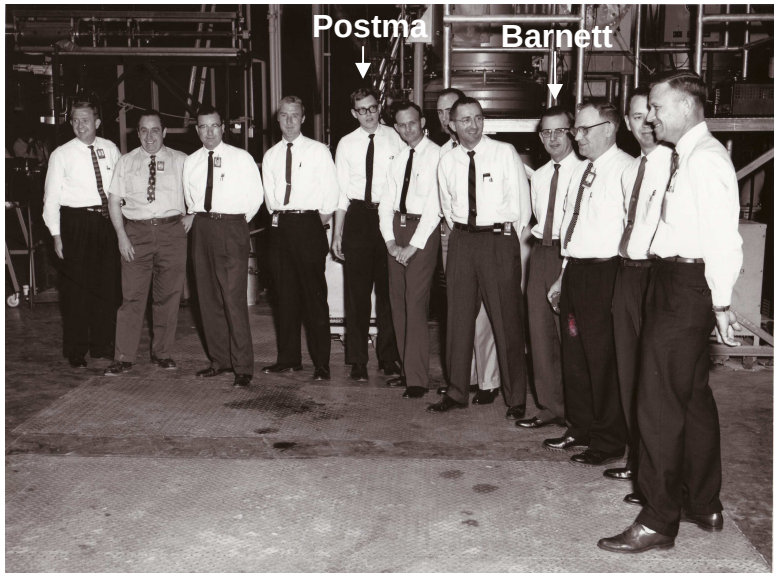
- Stockholm Univ. – Mats Larsson, Rich Thomas
- Univ. Giessen – Alfred Müller, Stefan Schippers
- Auburn Univ. – Mike Fogle (expt), Mitch Pindzola, Stuart Loch, Connor Balance (theory)
- Univ. College London – Tony Smith

History of AMO Group and CFADC

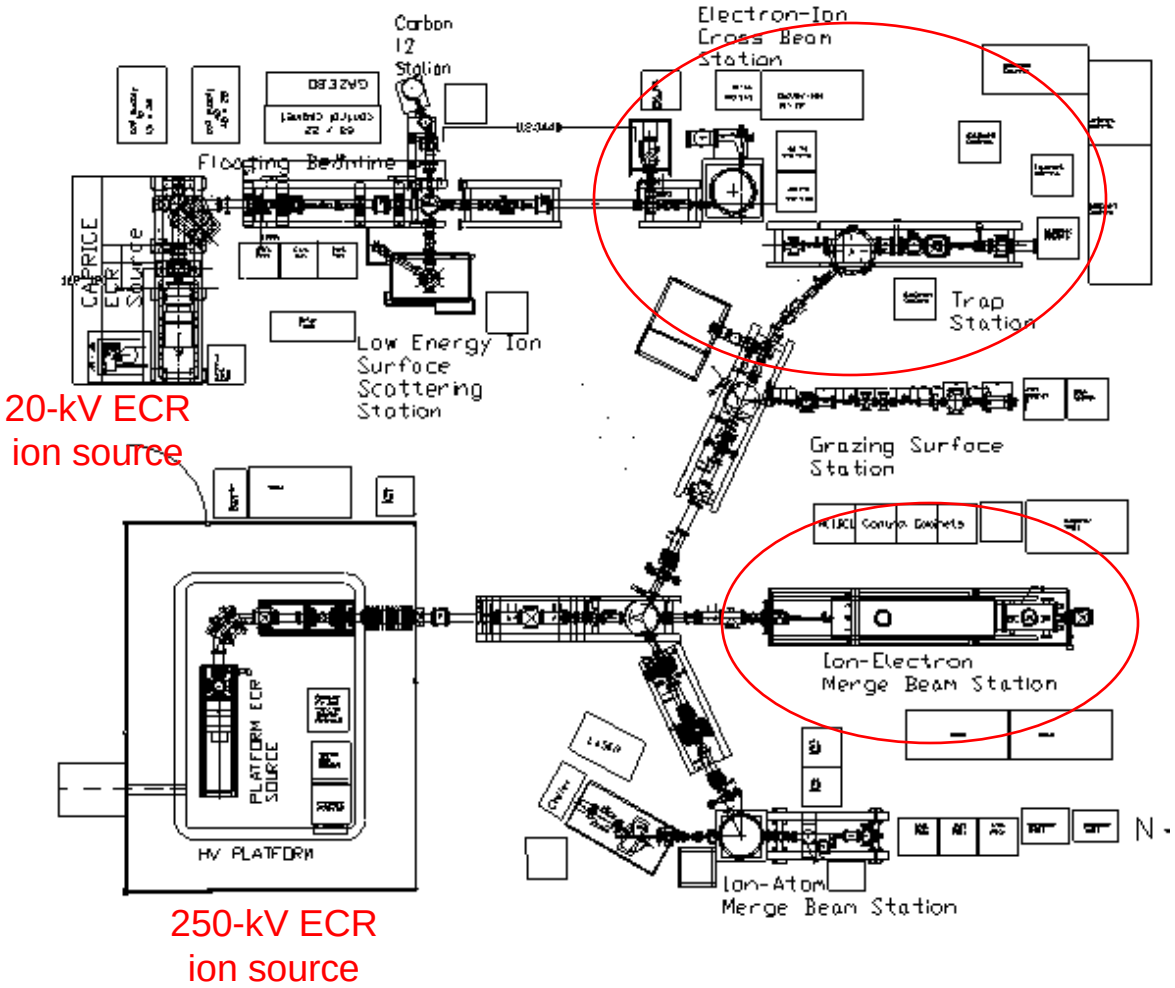


Barnett & Group, FED 1961

MIRF (Bldg 6000B), 2011

- Atomic data center for fusion started by Clarence Barnett in 1959
- Barnett's atomic physics group joined the Physics Division in 1975
- Current composition of the AMO group:
  - Multicharged Ion Research Facility (MIRF)
  - Controlled Fusion Atomic Data Center (CFADC)
  - Fusion Theory Program

Multicharged Ion Research Facility (MIRF)



- ECR ion sources on 20-kV and 250-kV platforms
- Merged electron-ion experiment (MEIBEL)
- Crossed electron-ion experiment (XBEAM)
- ICCE ion trap
- Merged ion-atom experiment (CEX)
- Floating surface experiment (PMI)
- Grazing surface experiment

Motivation

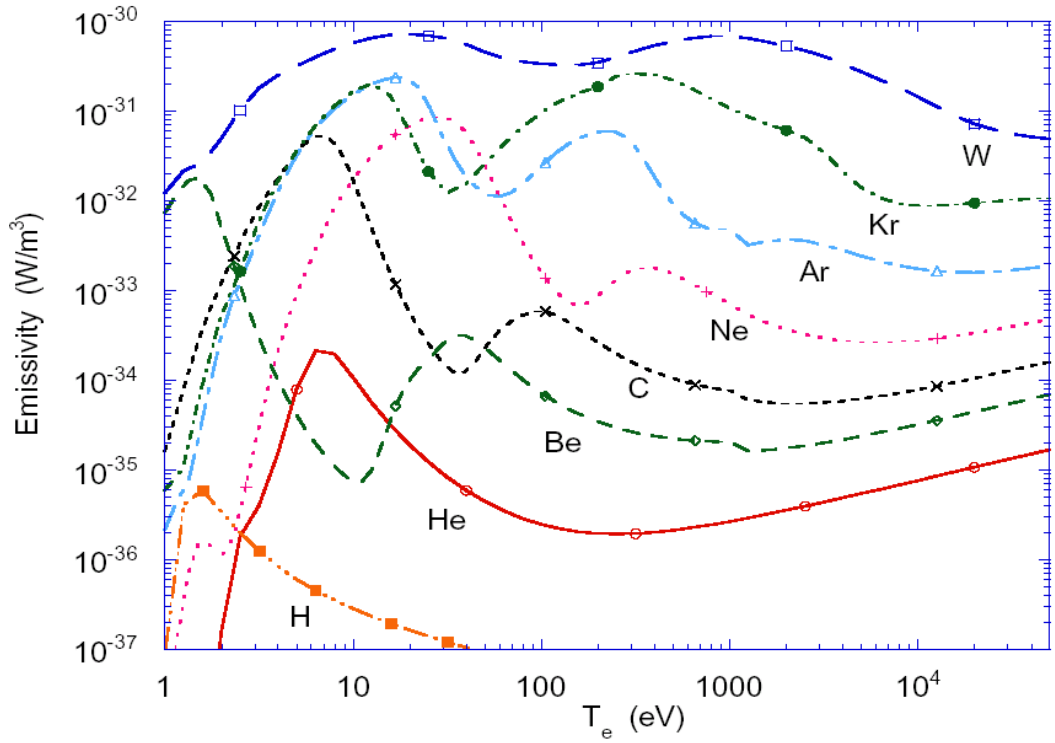
- Produce experimental data for inelastic collisions of electrons with atomic and molecular ions needed for diagnosing and modeling fusion and other plasmas

- Provide accurate, reliable benchmarks for theoretical techniques that produce the bulk of atomic data for fusion and stimulate theoretical efforts in electron-impact processes, especially for molecular dissociation where theory is almost non-existent

Motivation: Atomic Physics for ITER

"Impurity radiation losses are the principal means of reducing the power to the divertor target. These losses depend on the radiation rate coefficients and the charge state distributions of the impurities, which are determined by the balance of ionization, recombination and transport processes for each impurity charge state."

"In general, line radiation from electron impact excitation accounts for about 90% or more of the radiation losses from impurities with three or more bound electrons."



ITER Physics Basics, Ch. 4, Nucl. Fusion 39, 2137 (1999).

Collisions with Atomic Ions

- Ionization $e + A^{q+} \rightarrow e + A^{(q+1)+} + e$
  - Contributions of metastable ions
  - Importance of Excitation-Autoionization

  ORNL: First measurement for multicharged ions (MCI)

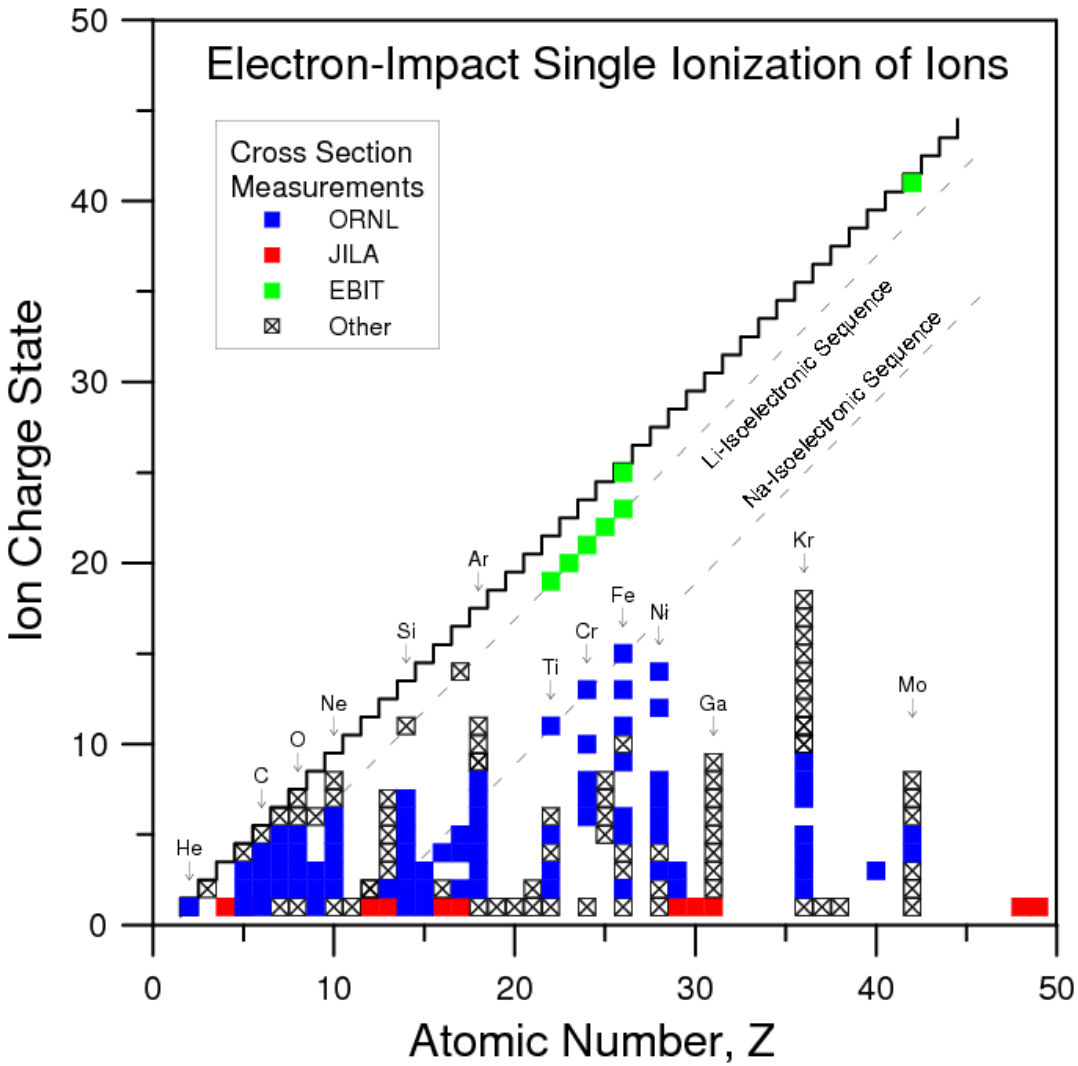
- Excitation $e + A^{q+}(i) \rightarrow e + A^{q+}(f)$
  - Improved resolution of MEIBEL technique
  - Dielectronic resonances

  ORNL: First measurement for MCI

- Dielectronic Recombination $e + A^{q+} \rightarrow A^{(q-1)+**} \rightarrow A^{(q-1)+} + h\nu$

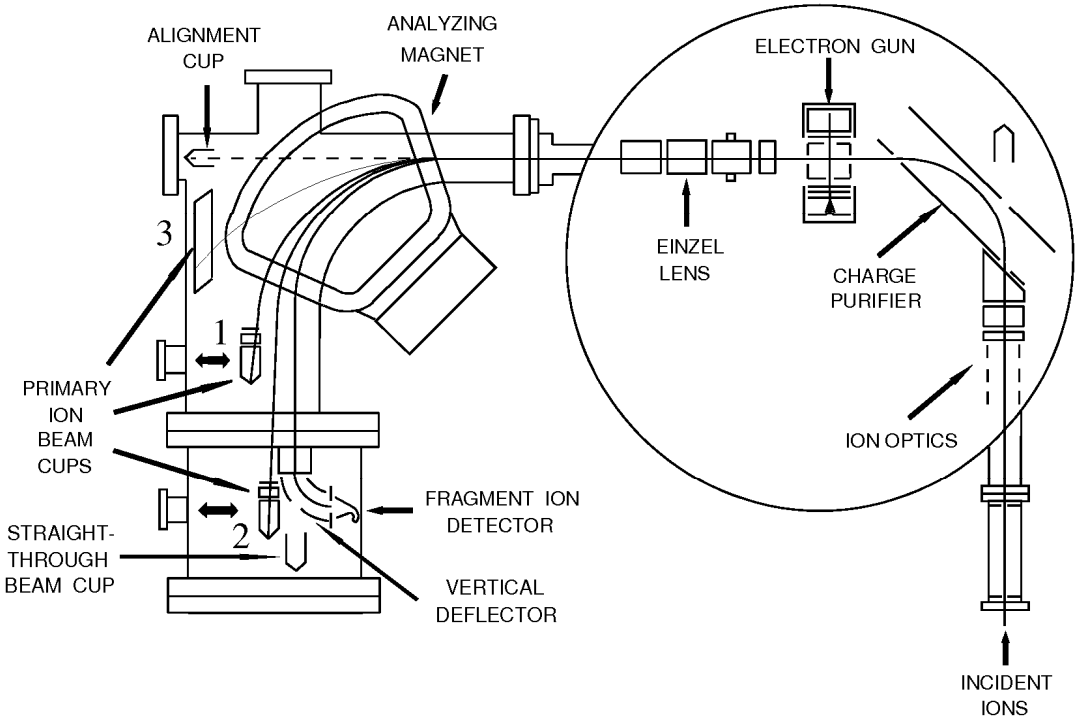
  ORNL: First measurement for MCI

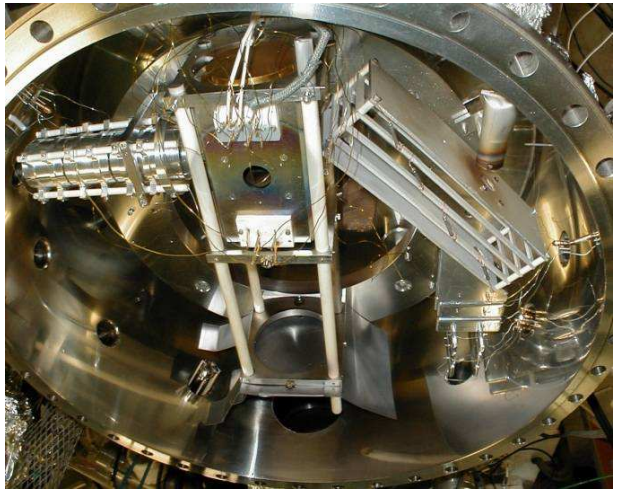
Electron-Impact Single Ionization Measurements



Absolute cross sections for single-ionization have been measured for **94** atomic ion charge states at ORNL

Electron-Ion Crossed Beams Experiment (XBEAM)



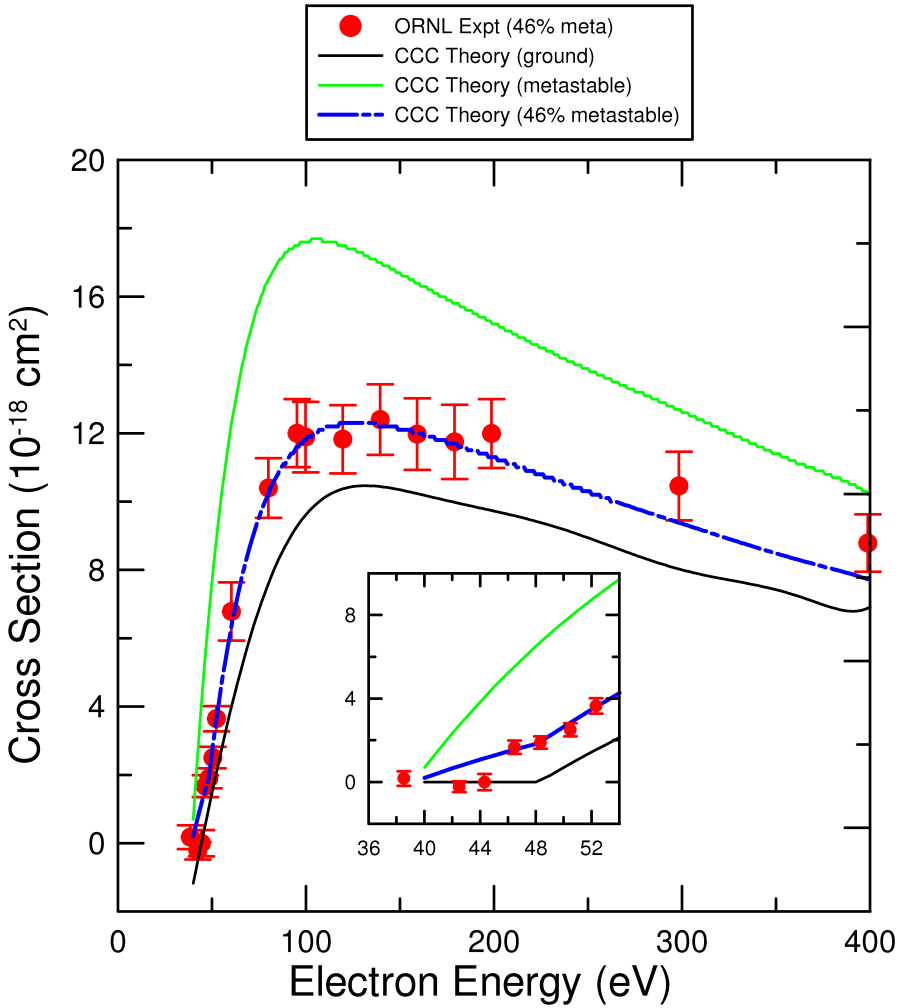


Absolute Cross Section:

$$\sigma(E) = \frac{R}{I_e I_i} \frac{q e^2 v_e v_i}{\sqrt{v_e^2 + v_i^2}} \frac{F}{\varepsilon}$$

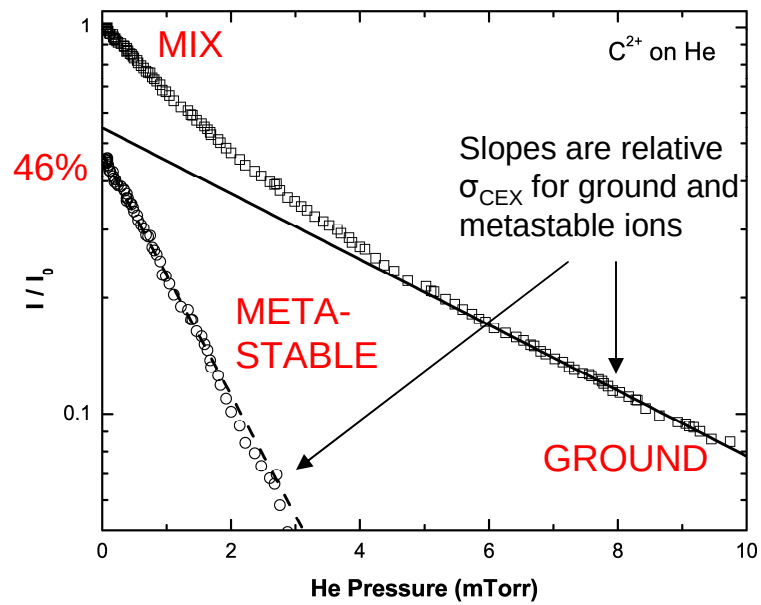
- Electron energies 2-2000 eV
- Product/parent ions magnetically separated – single ionization 1+ up to 16+ ions; product ion rates up to 10^6/s measured
- Ions produced in ECR or colutron (hot-filament) ion sources
- Apparatus can also be used for dissociation measurements – heavy ion fragments ($M_{fragment} \geq 1/3\ M_{parent}$)
- Total absolute uncertainties typically ~10%

Ionization of Be-like C^{2+}



Fogle et al., Ap. J. Suppl. Ser. ***175****, 543 (2008)*

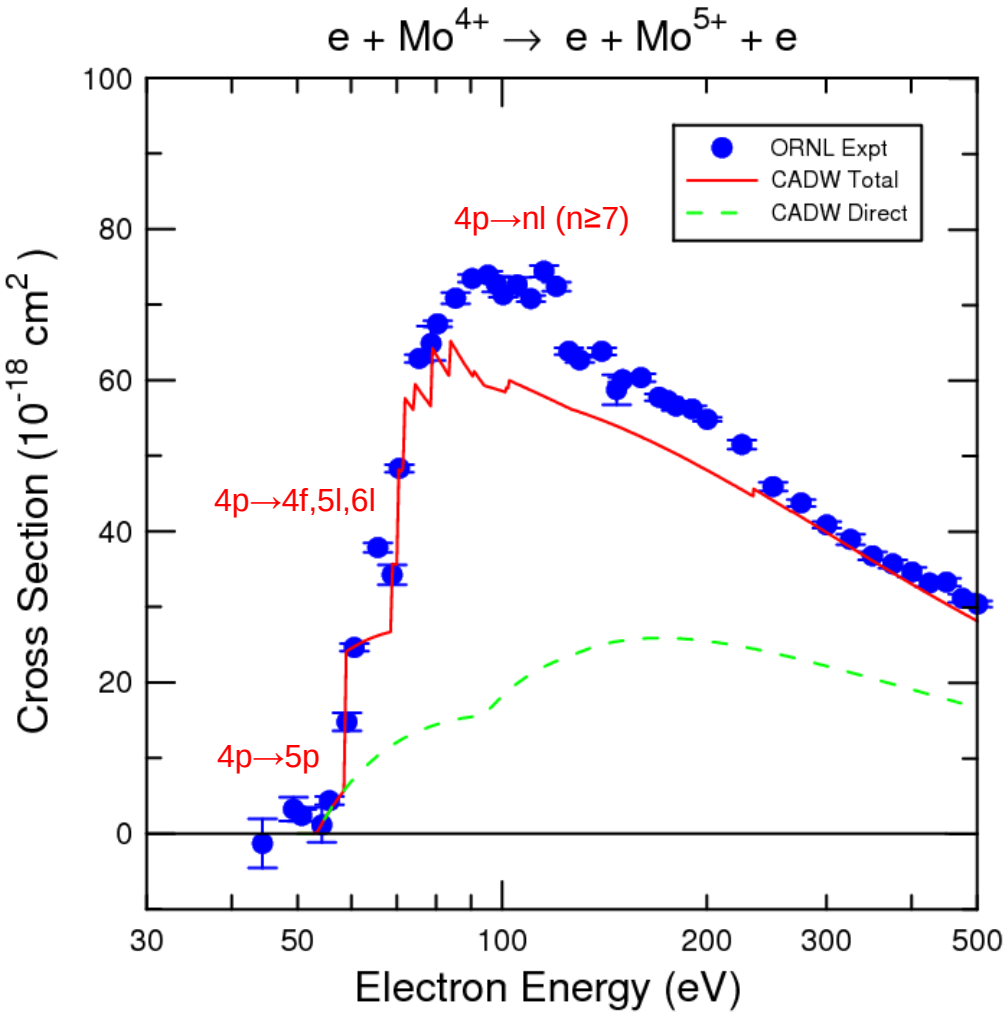
- Target ion beams from ECR source are mix of $2s^2\ ^1S$ ground state ions and $2s2p\ ^3P$ metastables
- Metastable fraction determined to be 46% by gas attenuation technique



Importance of Excitation-Autoionization

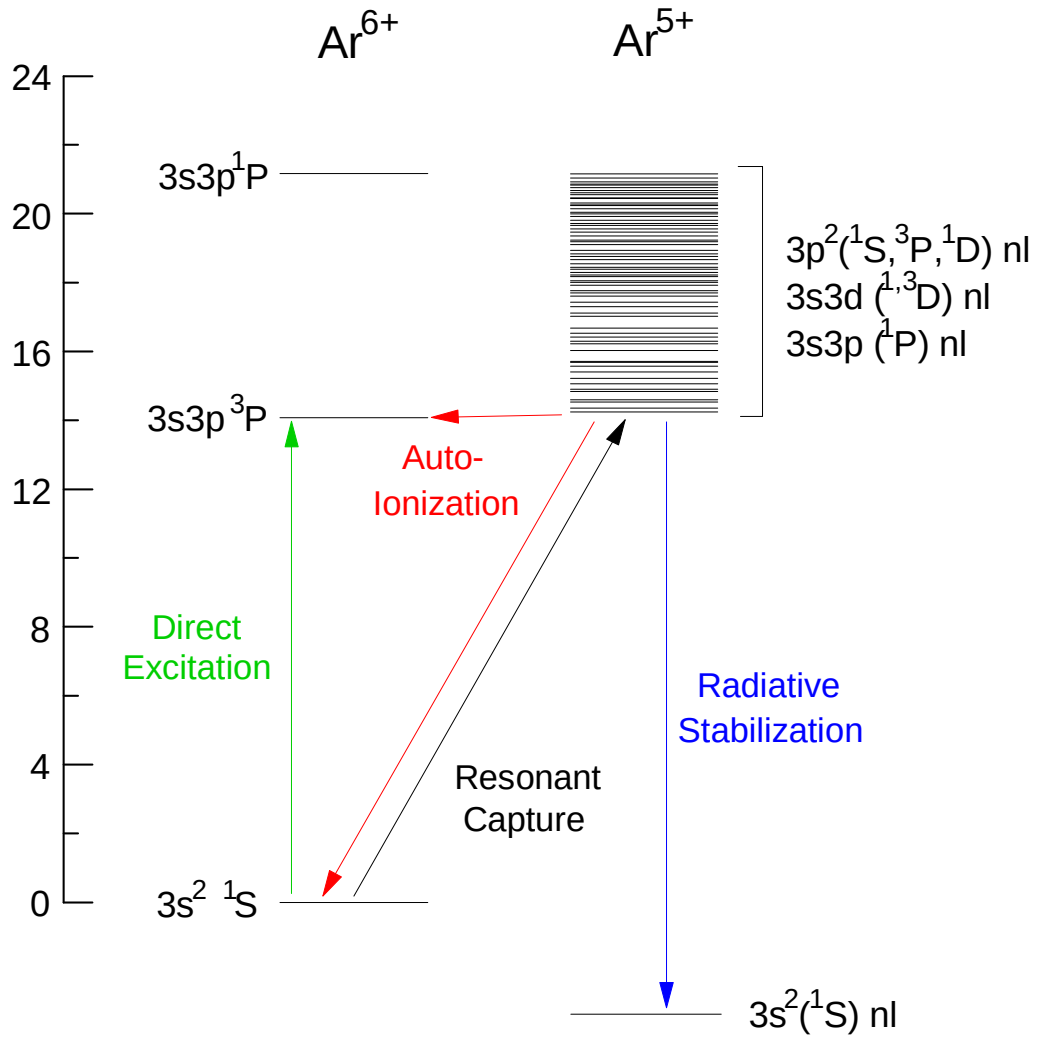
- For Mo^{4+} ($4p^6 4d^2$), Excitation-Autoionization (EA) contributes about 75% of the cross section below 100 eV

- Good agreement with theory for included excitations, but higher transitions need to be included (4p→nl, n≥7)



Bannister et al., Phys. Rev. A ***52****, 413 (1995)*

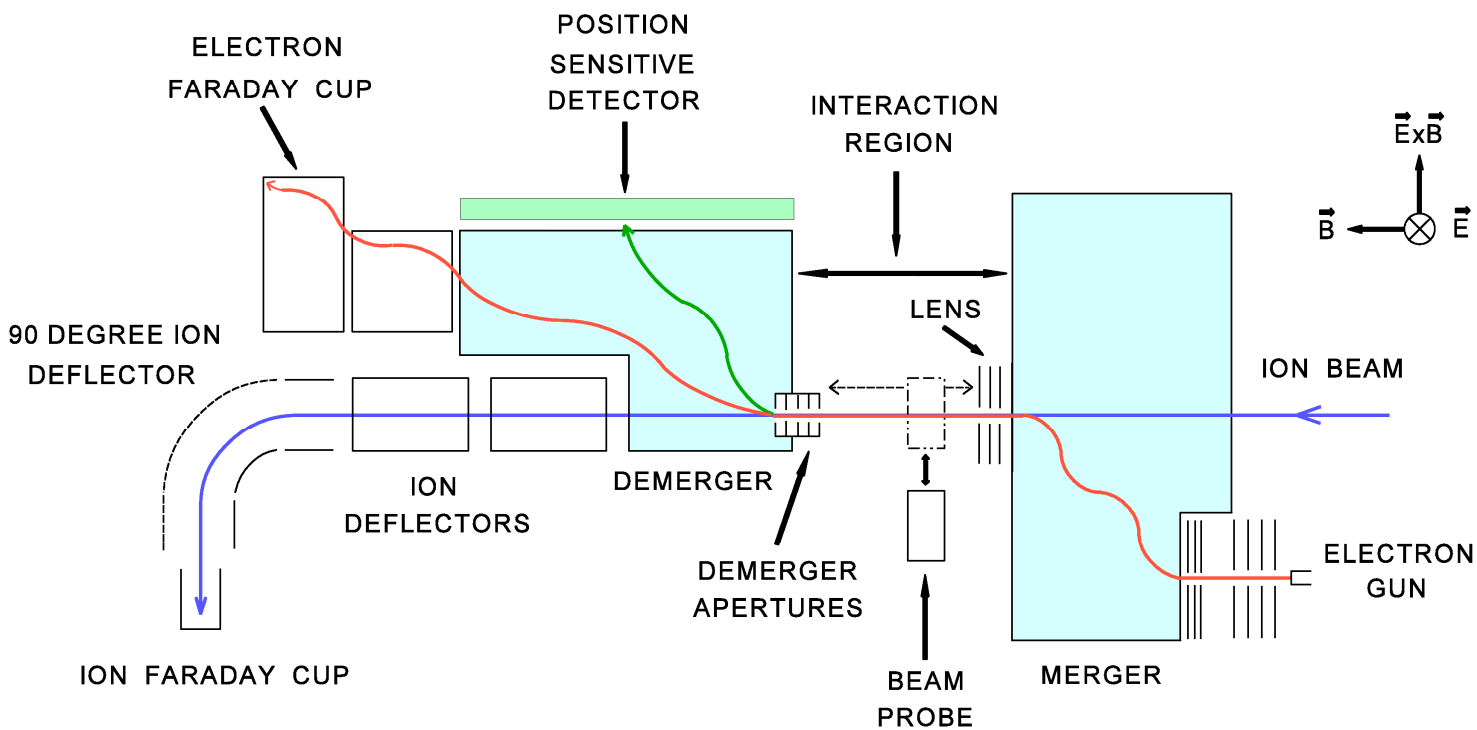
Electron-Impact Excitation



Resonant capture of an electron can result in:

- Dielectronic resonance in excitation (excited state)
- Elastic resonance (ground state)
- Dielectronic recombination (lower charge state)

Merged Electron-Ion Beams Energy-Loss (MEIBEL) Experiment

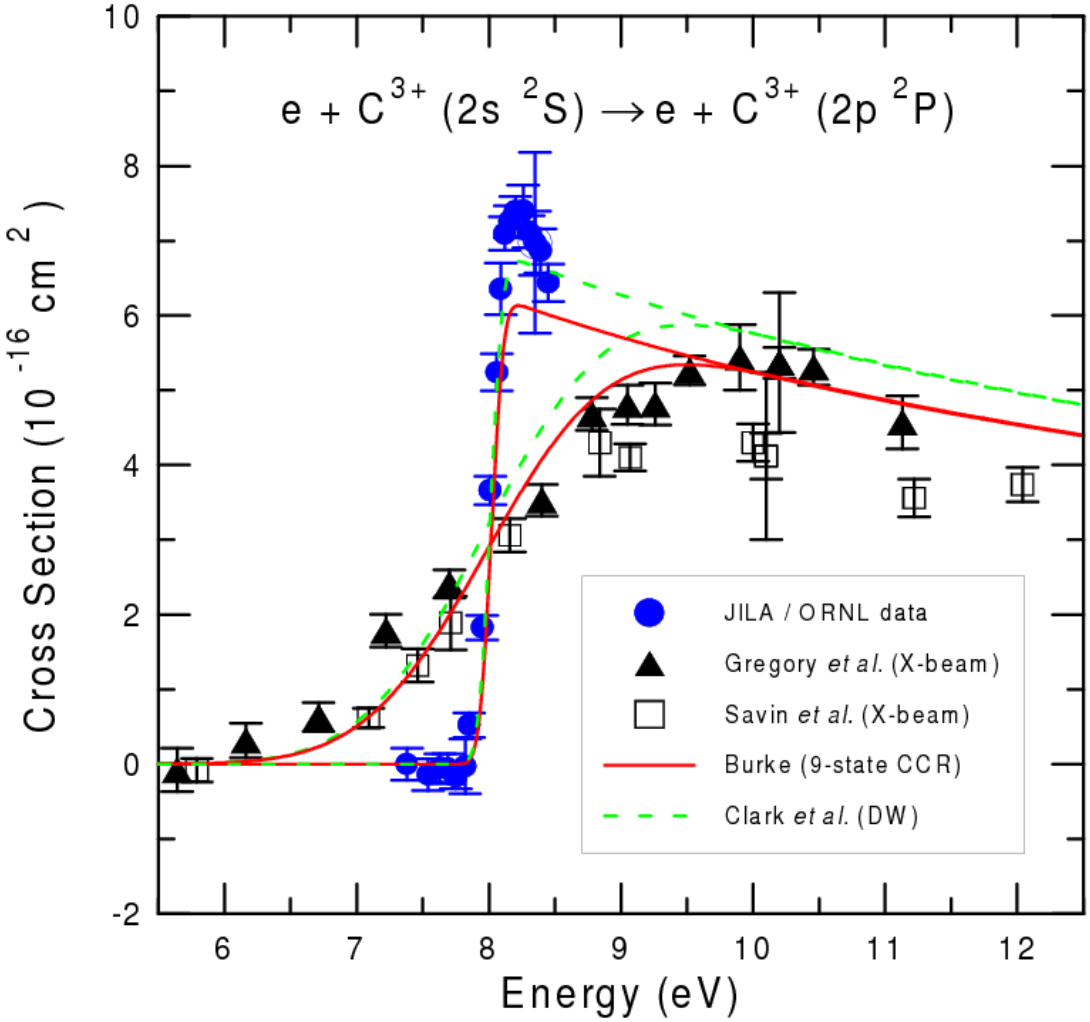


Advantages of MEIBEL technique:

- ► Higher energy resolution (merged beams)
- ► Measurement of forbidden transitions (energy loss)
- ► Higher collection/detection efficiency for electrons than photons

3D beam overlaps measured with translating video probe → Absolute cross sections

MEIBEL: Improved Resolution

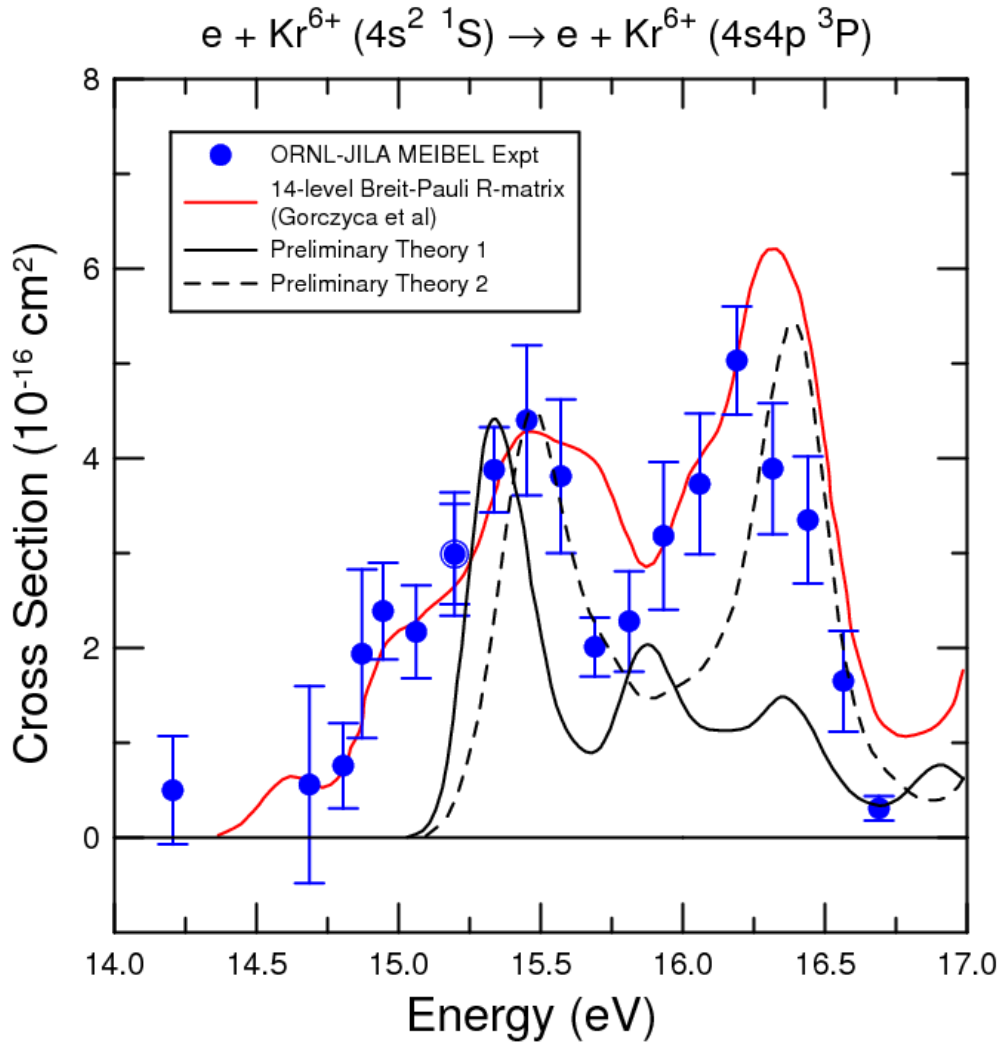


- XBEAM measurements of fluorescence (photons)
  $\Delta E \approx 1.5\text{-}2.0$ eV
- MEIBEL measurements of electron energy loss
  $\Delta E \approx 0.2$ eV

Bannister et al., Phys. Rev. A ***57****, 278 (1998)*

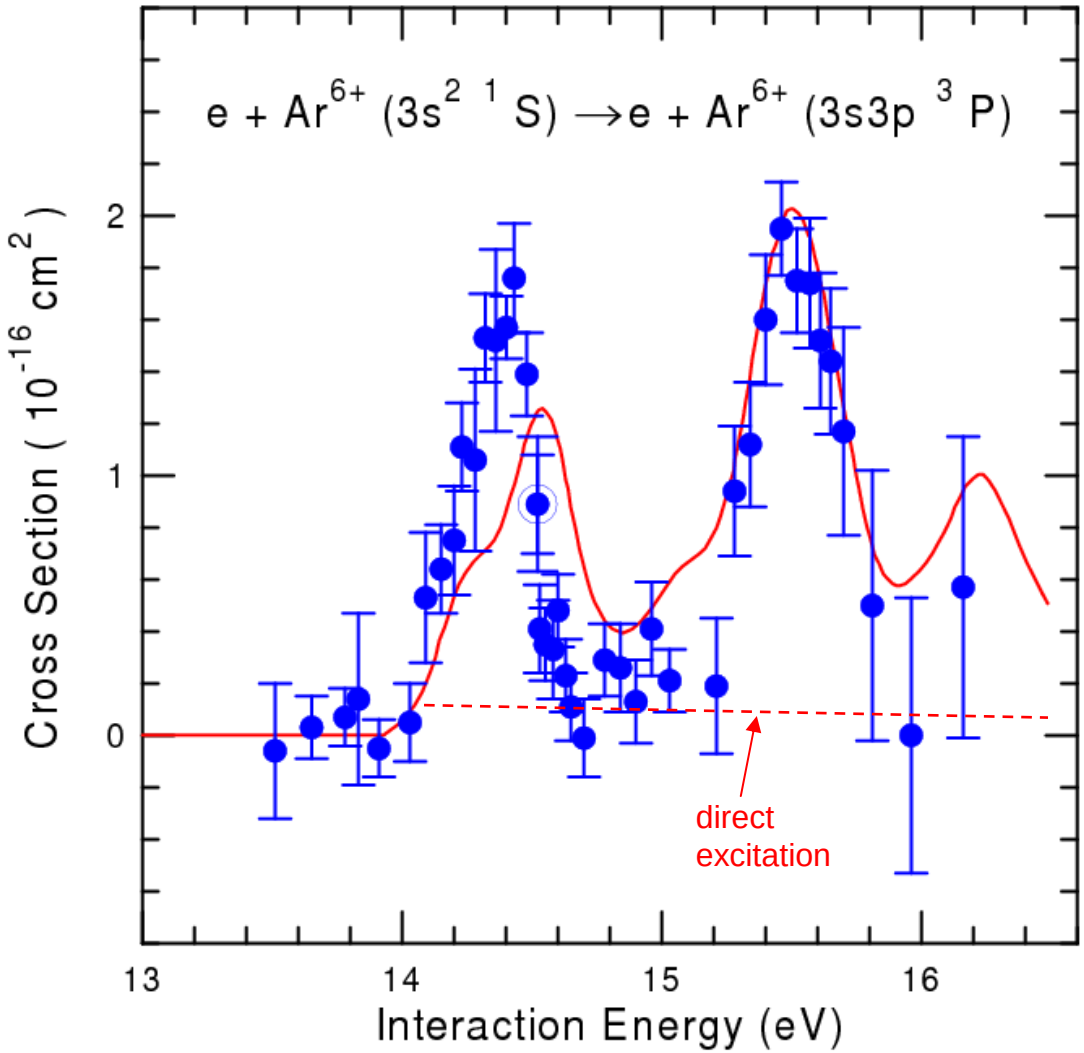
Dielectronic Resonances in Kr^{6+}

- First measurements of dielectronic resonances in electron-impact excitation
- First measurements of a forbidden transition
- Theoretical results took one year longer to produce!



Bannister et al., Phys. Rev. Lett. ***72****, 3336 (1994)*

Dielectronic Resonances in Ar^{6+}

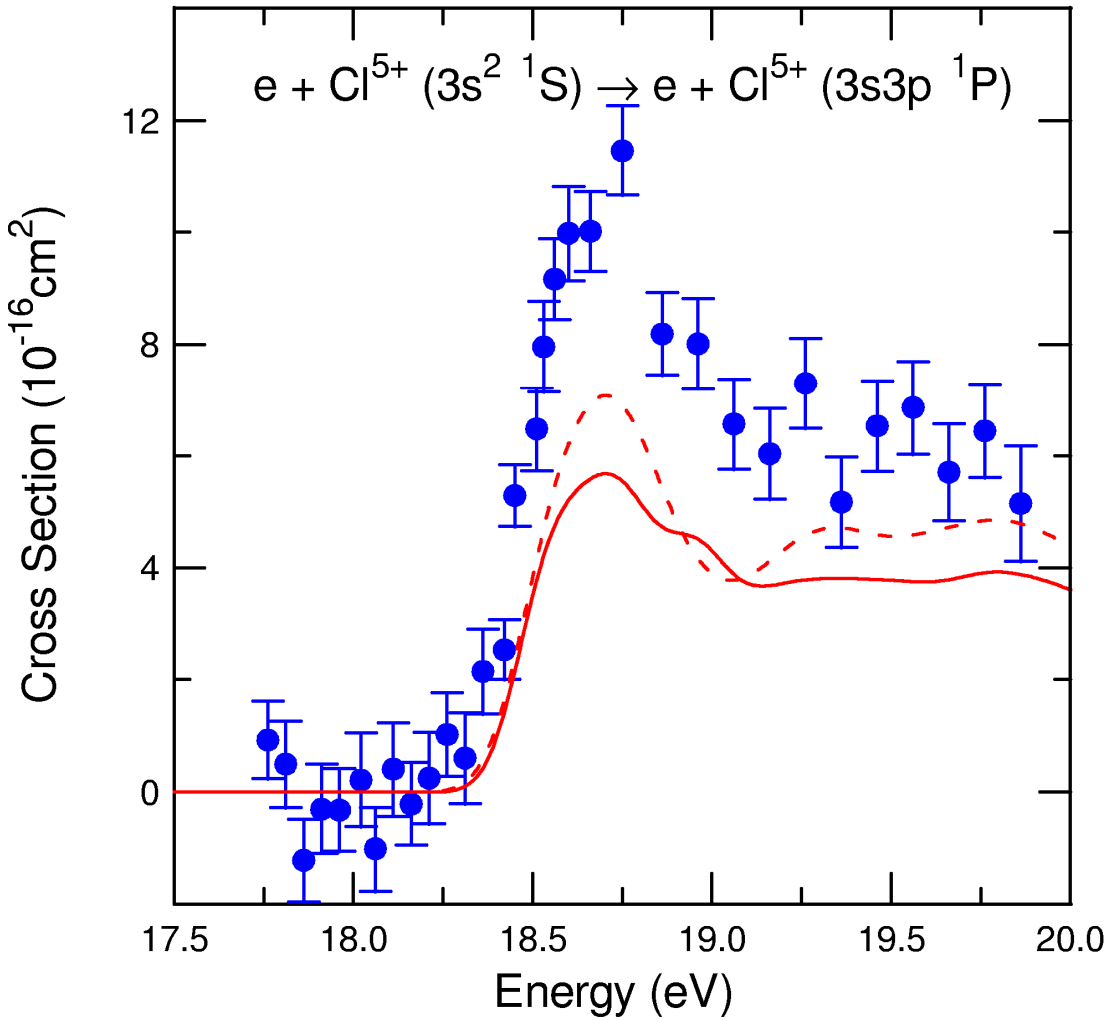


- Close-coupling R-matrix theory predicts second resonance feature accurately, but not the first
- Theoretical predictions of DR resonances in excitations are "hit or miss" – need experimental benchmarks for refinement

*Chung et al., Phys. Rev. A **55**, 2044 (1997)*

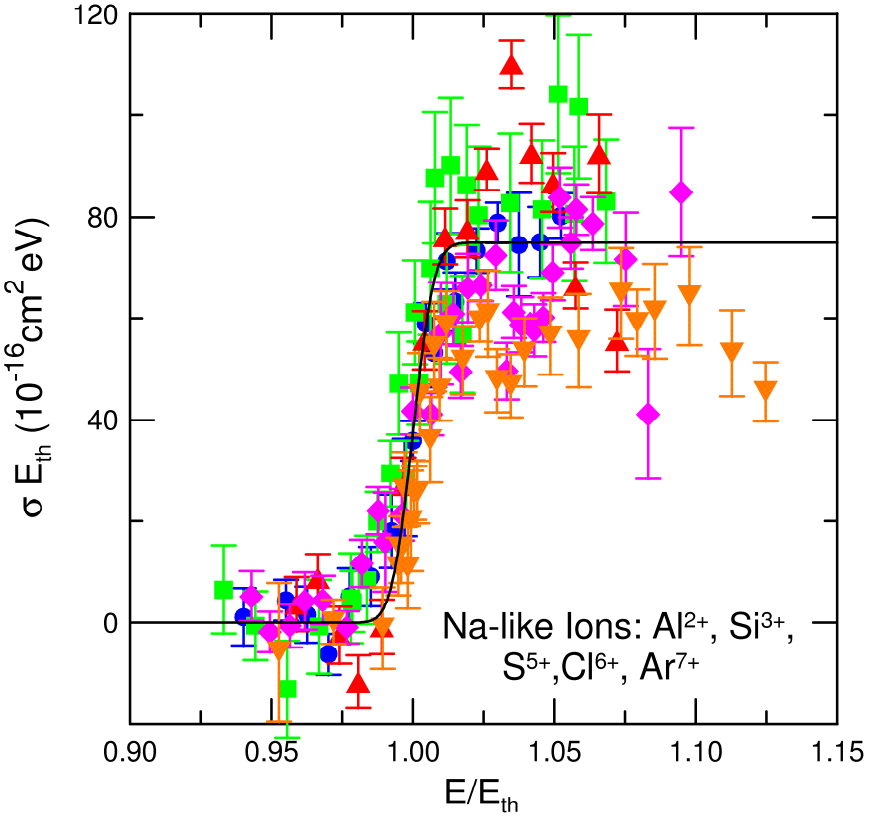
Resonance Contributions for Cl^{5+}

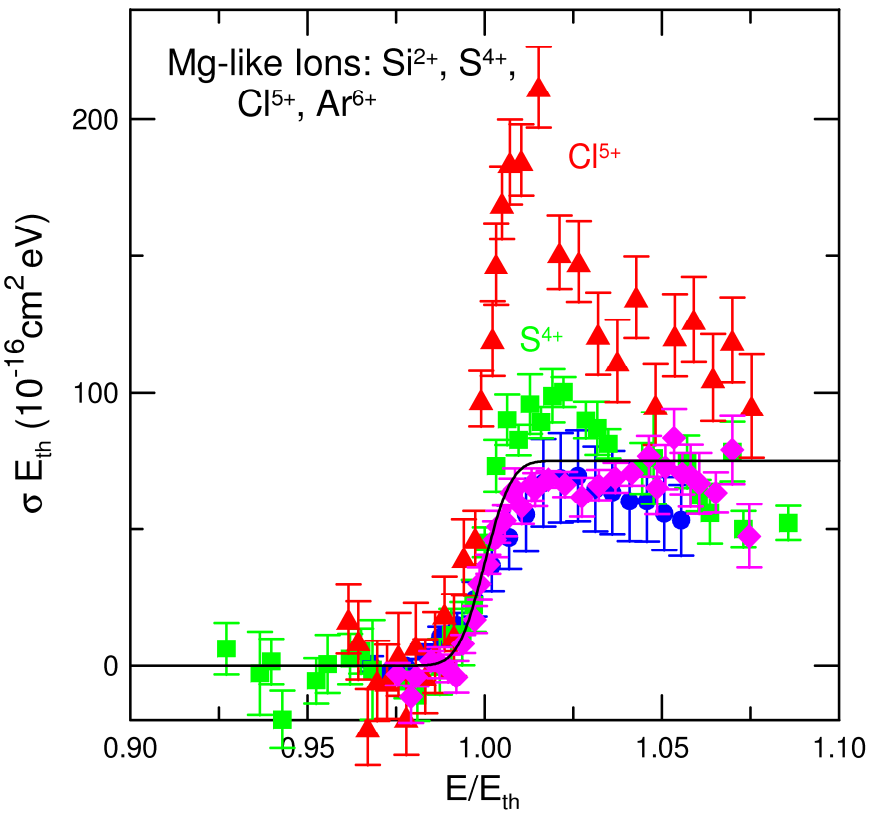
- Resonance contributions to an allowed transition have also been measured
- Theory underestimates resonance contribution!



*Djurić et al., Phys. Rev. A **65**, 052711 (2002)*

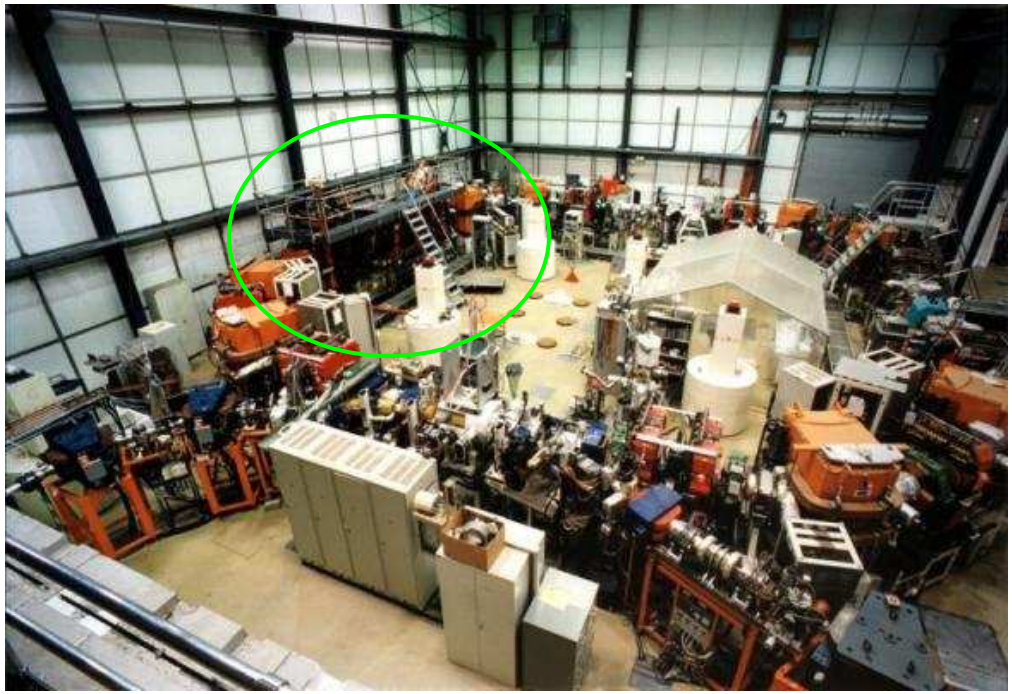
Scaling for Allowed Excitations of Na-like and Mg-like Ions

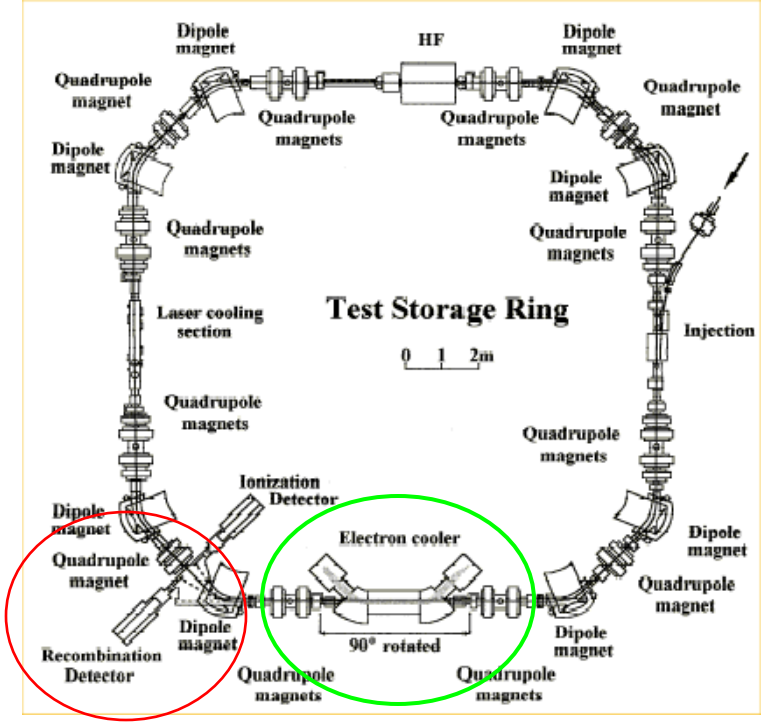




- Bethe scaling of allowed transitions from ground state of Na-like and Mg-like ions works well except for Cl^{5+} (near-threshold resonance)

DR Measurements at Heidelberg
Test Storage Ring (TSR)

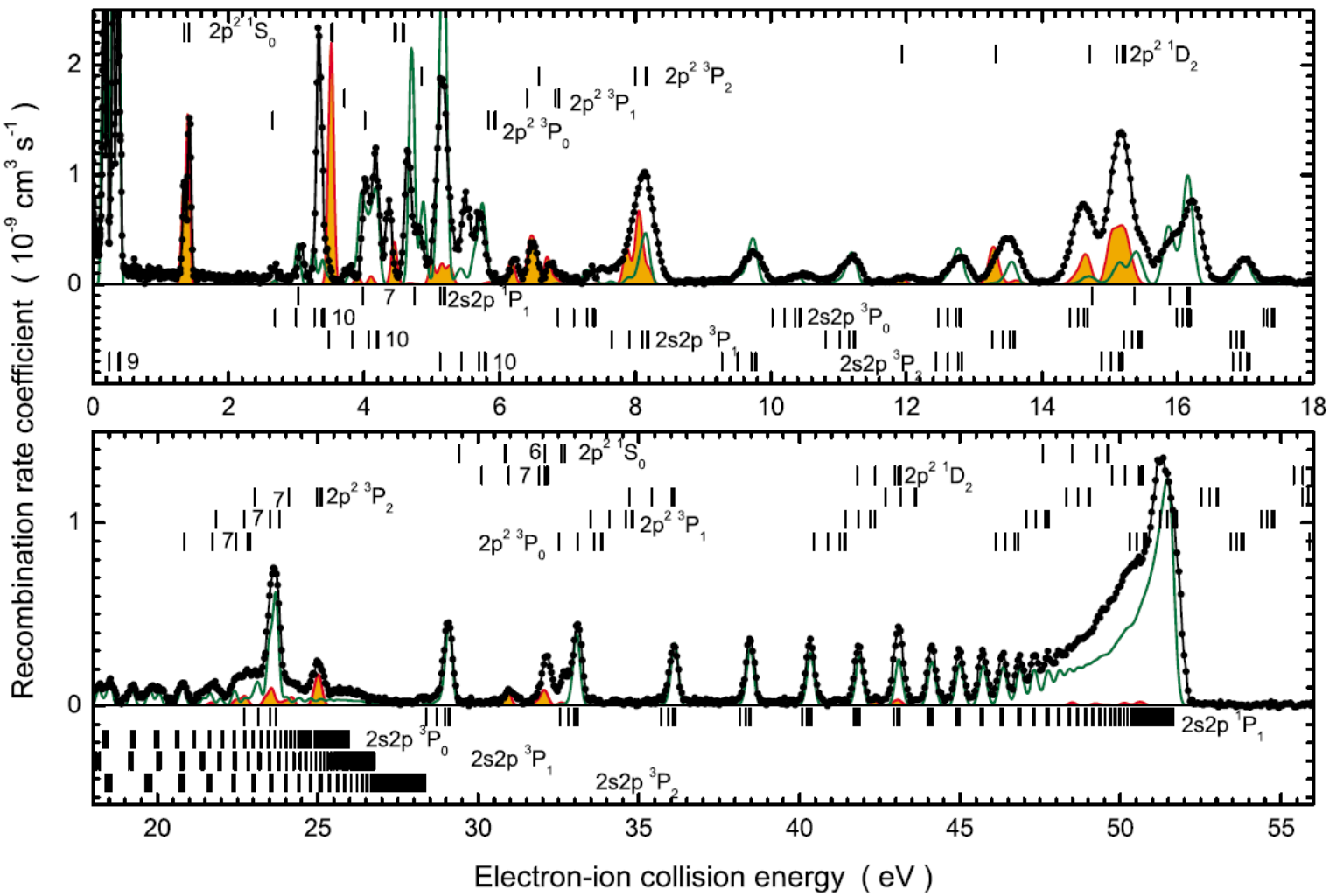




Electron cooler also serves as target for electron-ion recombination experiments

Dielectronic Recombination of Cl^{13+}

First measurements of TRI-ELECTRONIC recombination (TR) [yellow peaks]

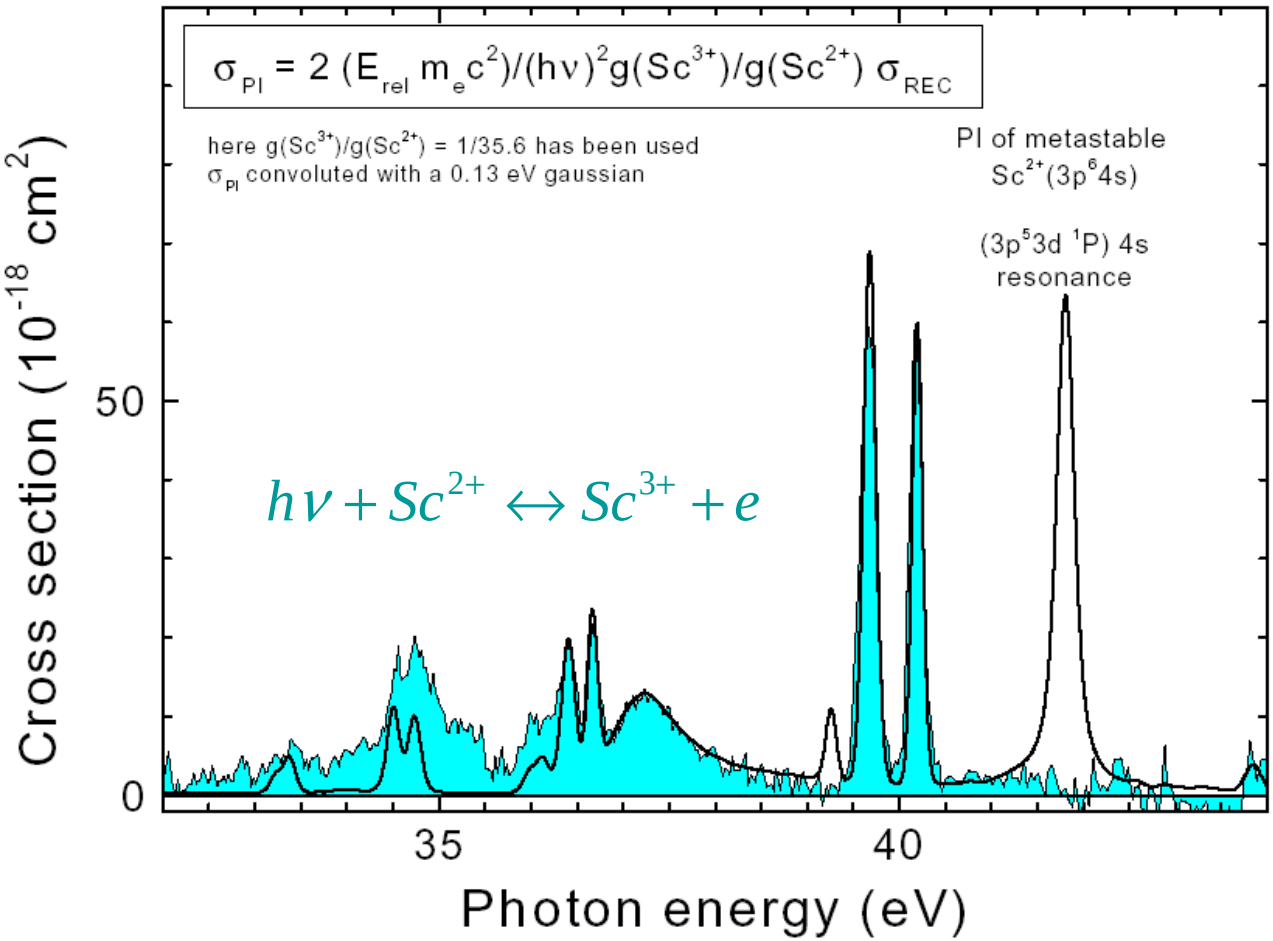


Schnell et al., Phys. Rev. Lett. ***91****, 043001 (2003)*

Dielectronic Recombination of Sc^{3+}

compared with Photoionization of Sc^{2+}

Schippers et al., Phys. Rev. Lett. ***89****, 193002 (2002)*



- DR measurements performed at TSR (Heidelberg) and PI measurements at ALS (Berkeley)
- Asymmetric feature observed near 37 eV due to interference connected to $3p^5 3d^2$ ^2F states of Sc^{2+} and predicted by theory
- Results demonstrate micro-reversibility of DR and PI (detailed balance)

Research was NATO Collaboration with groups of R. Phaneuf, A. Müller, S. Ricz, C. Cisneros, A. Wolf

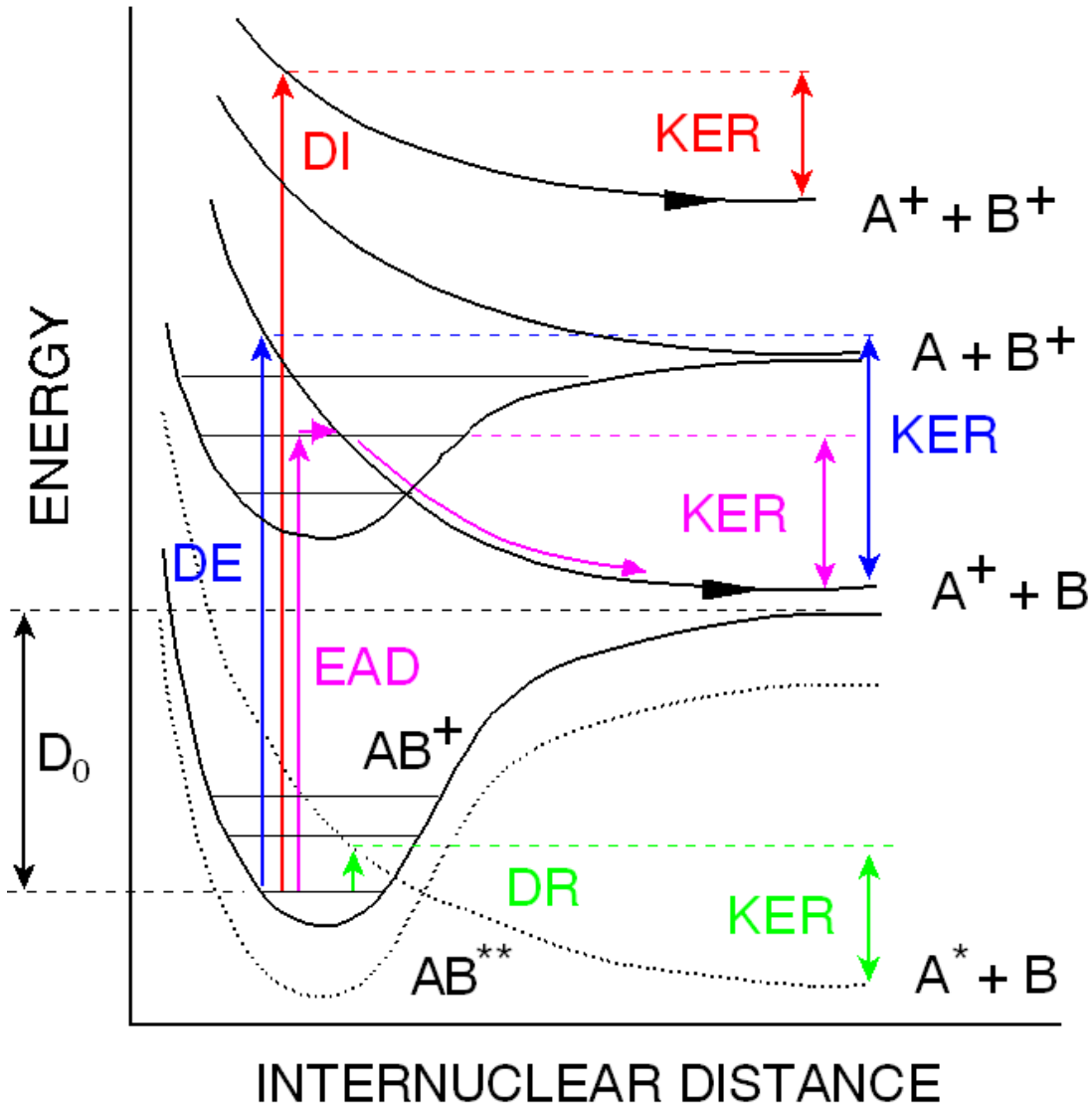
Collisions with Molecular Ions

Important in high-density, low-temperature edge and divertor plasmas: impurity transport, energy balance, detachment (MAR) …

- Dissociative Recombination (DR) $e + AB^+ \rightarrow A + B$
  - Measurements of cross sections / rate coefficients and chemical branching fractions (ie, percent of chemically-active products)
  - DR dynamics probed with fragment imaging

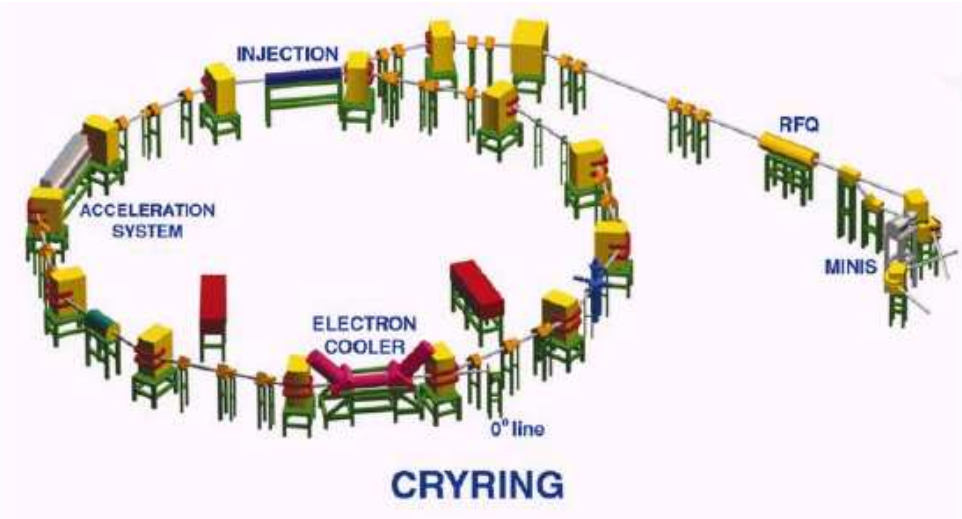
- Dissociative Excitation (DE) and Dissociative Ionization (DI) $e + AB^+ \rightarrow A^+ + B + e$
  - DE competes with DR around 10 eV and dominates at higher E
  - DE can be enhanced at low energies (below DI threshold) by Excitation-Autodissociation (EAD) process

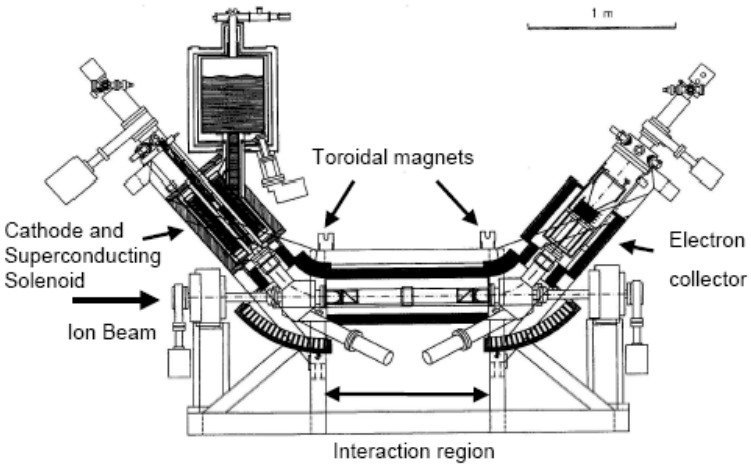
Dissociation Mechanisms



- Transition from bound state to dissociative state always yields excess energy carried off by the fragments – Kinetic Energy of Release (KER)
- Dissociative recombination (DR) can occur at E ~ 0 eV, but dissociative excitation (DE) has a threshold equal to the dissociation energy D_0 of the molecular ion, that is the energy difference between the ground state of the AB^+ ion and the asymptotic energy of the separated fragments $A^+ + B$

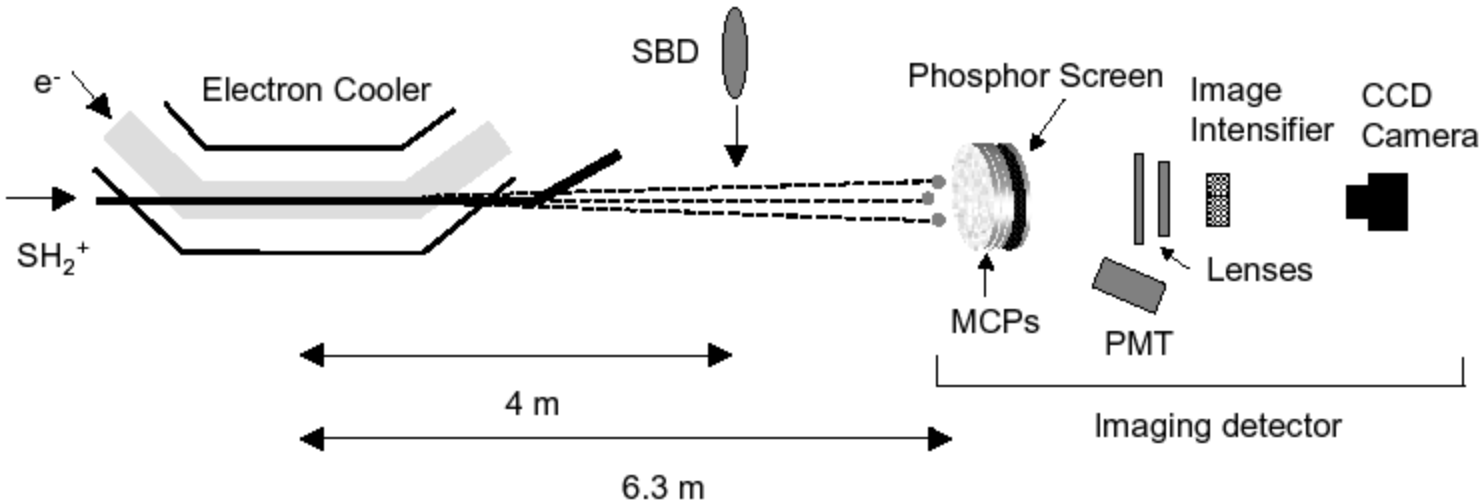
Dissociative Recombination Measurements at CRYRING (Stockholm)





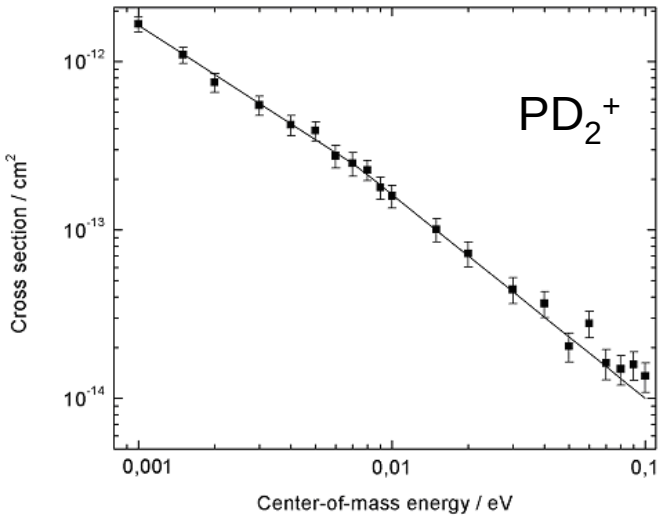
- CRYRING is a 51.6-m circumference heavy-ion storage ring
- Ring can store ions with energies up to a maximum of 96 x $(q/M)^2$ MeV/amu
- Cooler uses 7.9 eV – 8.1 keV electrons in 40-mm diameter beam in interaction region with expansion factor of 100; longitudinal and transverse relative energy spreads as low as 0.05 meV and 1.0 meV

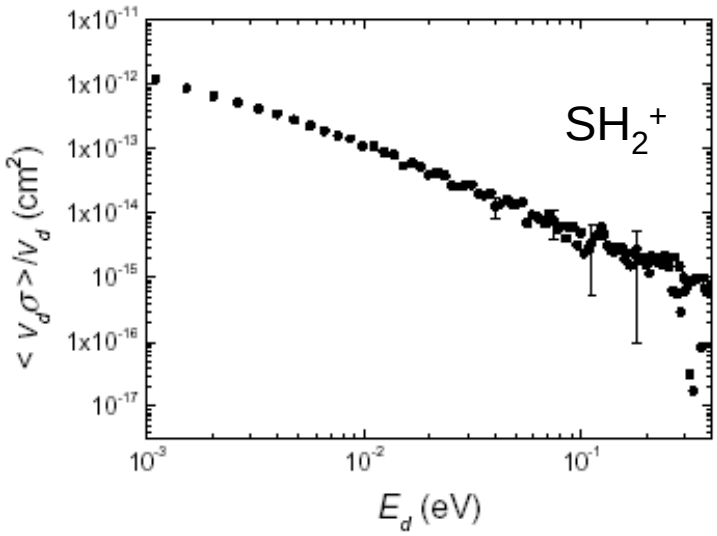
CRYRING Experiments

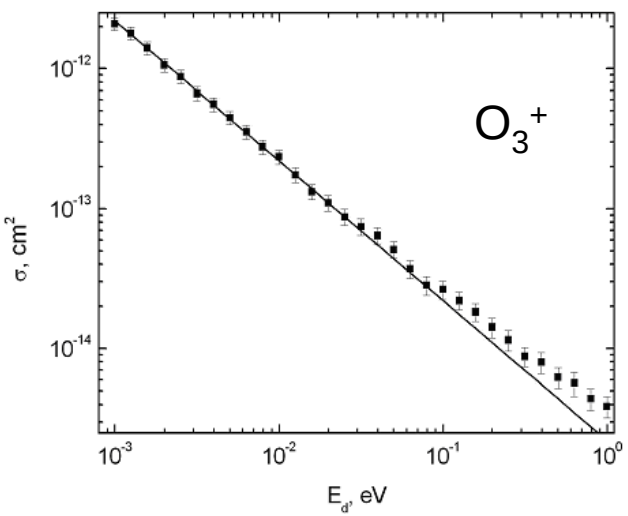


- Neutrals produced by DR in electron cooler escape ring at first dipole magnet – “zero degree arm”
- Cross sections and CBFs measured using solid-state surface-barrier detector
- Dynamics measured with fragment imaging detector

DR: Cross Sections



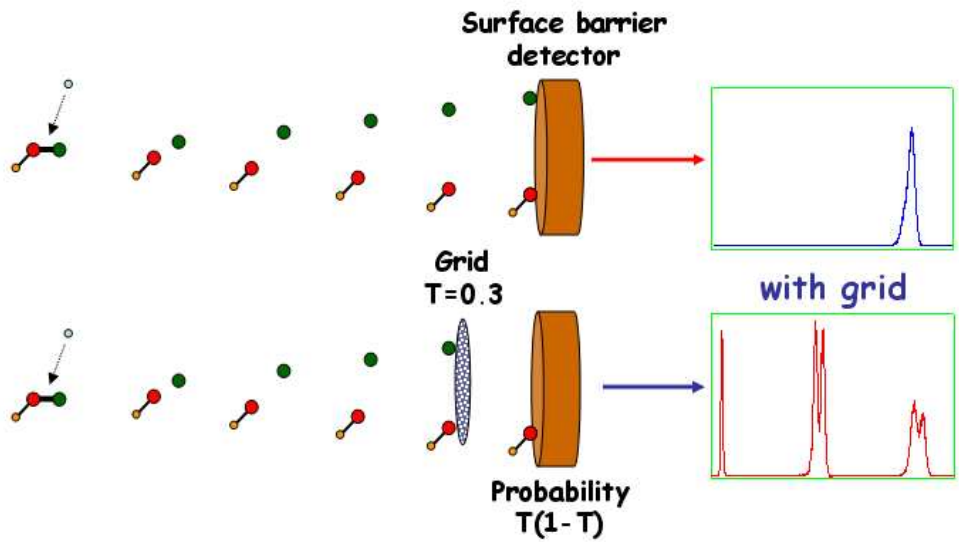


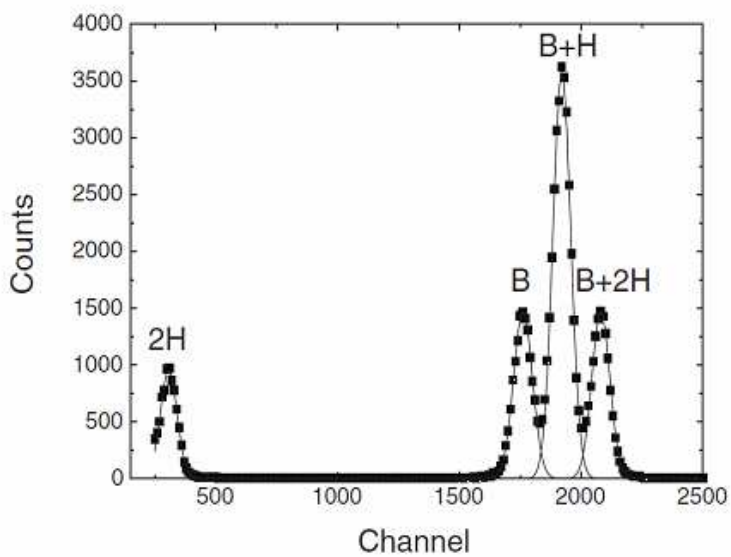


- At low energies (< 100 meV), DR cross sections fall off as E^{-1}

*Zhaunerchyk et al., Mol. Phys.**103**, 2735 (2005)*
*Hellberg et al., J. Chem. Phys. **122**, 224314 (2005)*
*Zhaunerchyk et al., Phys. Rev. A **77**, 022704 (2008)*

DR: Chemical Branching Fractions

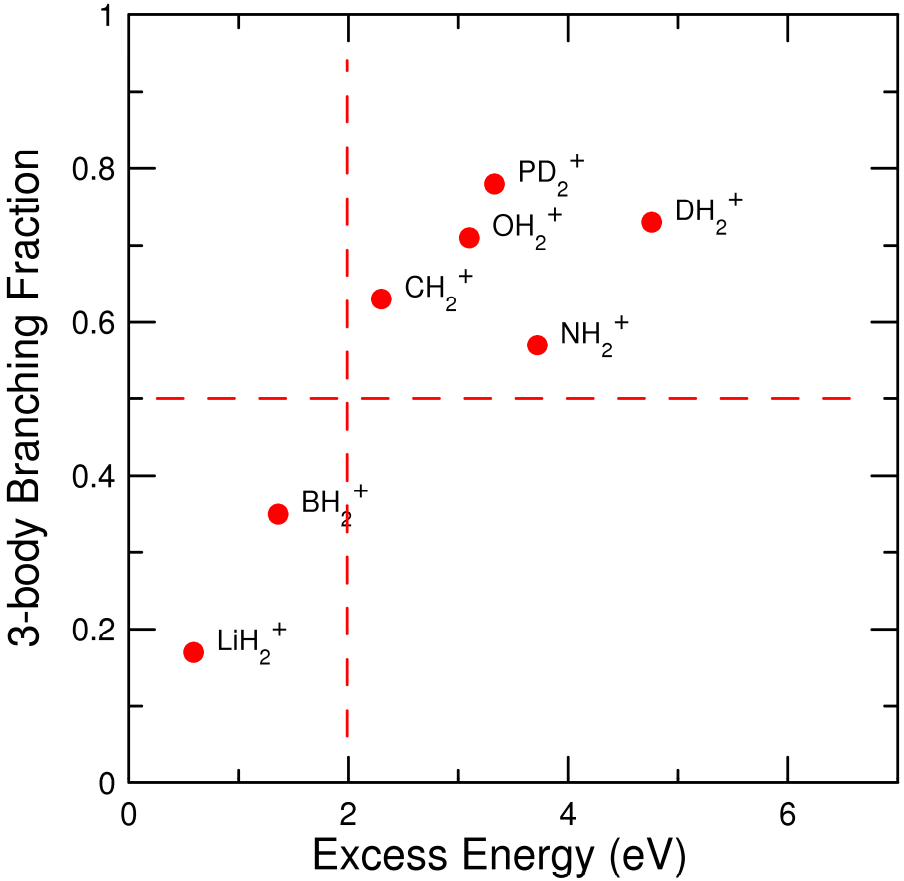




- Without grid, all events lead to full energy signal on SBD
- With grid, the energy spectrum is dependent on the CBF and the grid transmission T
- Measured CBF for BH_2^+ at 0 eV:
  - B+ H_2 0.09 ± 0.02
  - BH + H 0.56 ± 0.03
  - B + H + H 0.35 ± 0.05

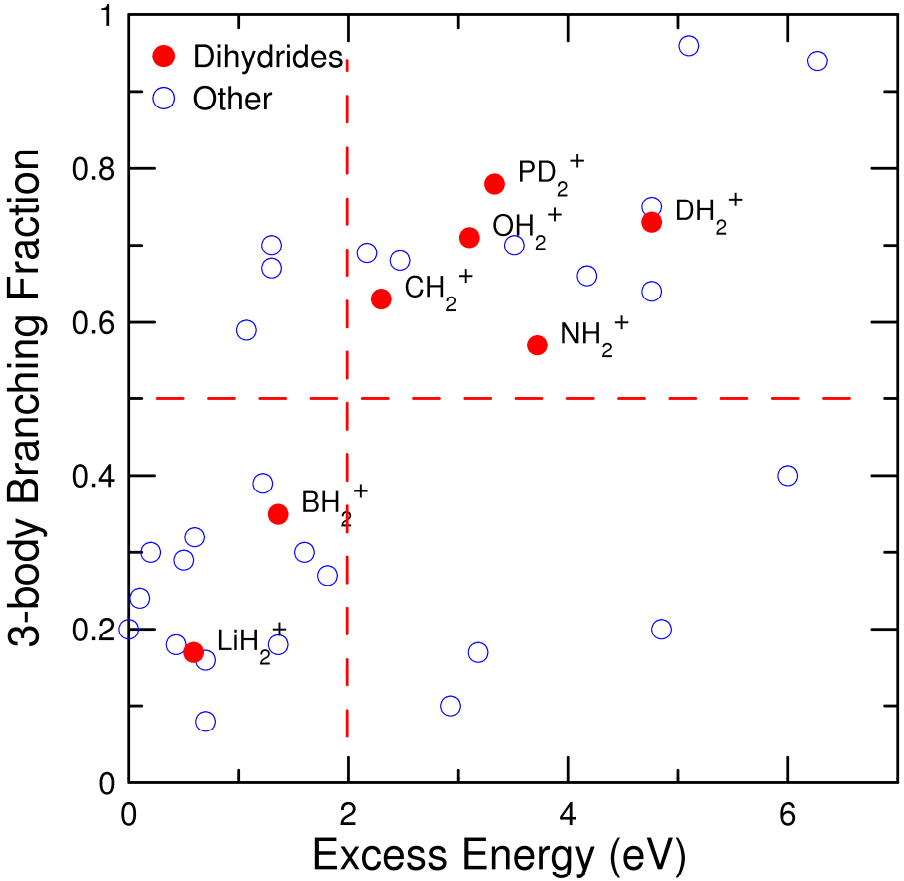
*Zhaunerchyk et al., Phys. Rev. A **78**, 024701 (2008)*

DR: Chemical Branching Fractions



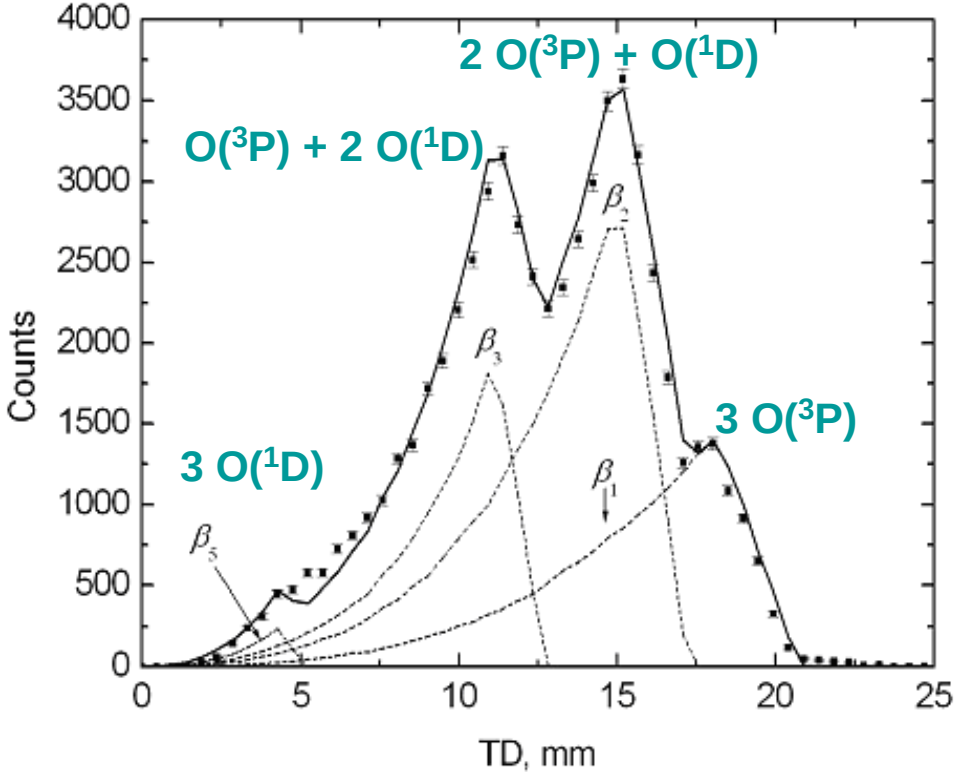
- For XH_2^+ di-hydrides, CBF favors X+H+H three-body channel when excess energy exceeds 2 eV

DR: Chemical Branching Fractions



- For XH_2^+ di-hydrides, CBF favors three-body X+H+H channel when excess energy exceeds 2 eV
- Trend does not hold for all systems with 3-body channels

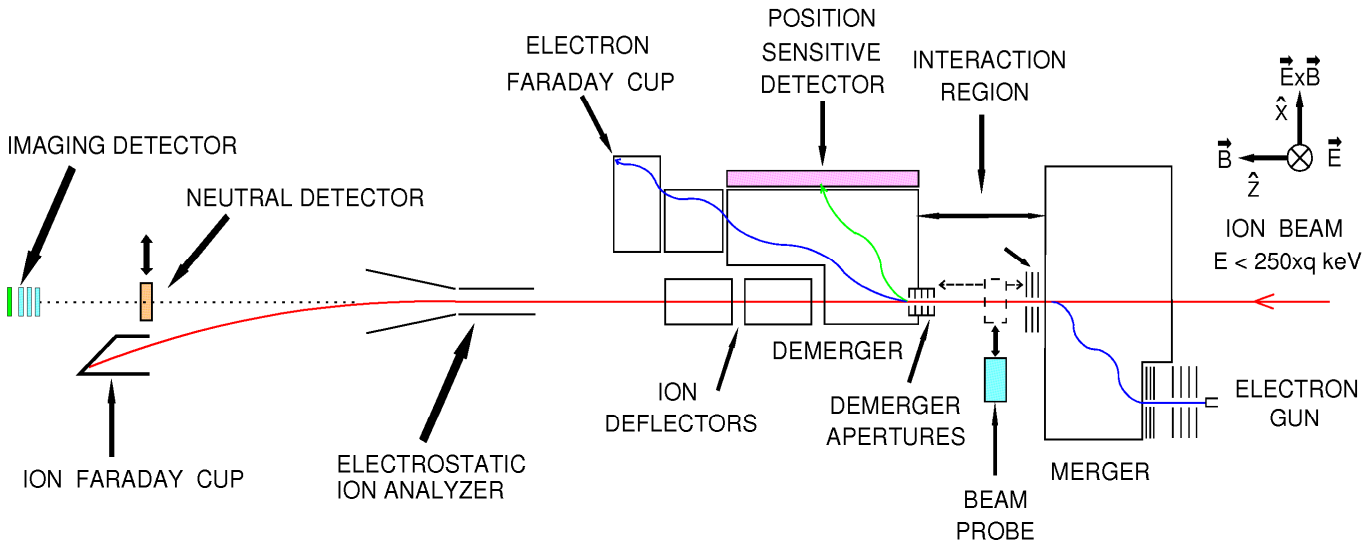
DR: Fragment Imaging of O_3^+



- Events discriminated to select 3-body dissociation parallel to detector, all within narrow time window
- Plot of total displacement (TD) of O + O + O atoms from CM
- Monte Carlo simulations fit to data yield the branching ratios for energetically-accessible states of O (in order of decreasing KER):
  - 3 $O(^3P)$ 0.30
  - 2 $O(^3P)$ + $O(^1D)$ 0.46
  - $O(^3P)$ + 2 $O(^1D)$ 0.23
  - 3 $O(^1D)$ 0.01

*Zhaunerchyk et al., Phys. Rev. A **77**, 022704 (2008)*

DR Measurements using the MEIBEL Apparatus



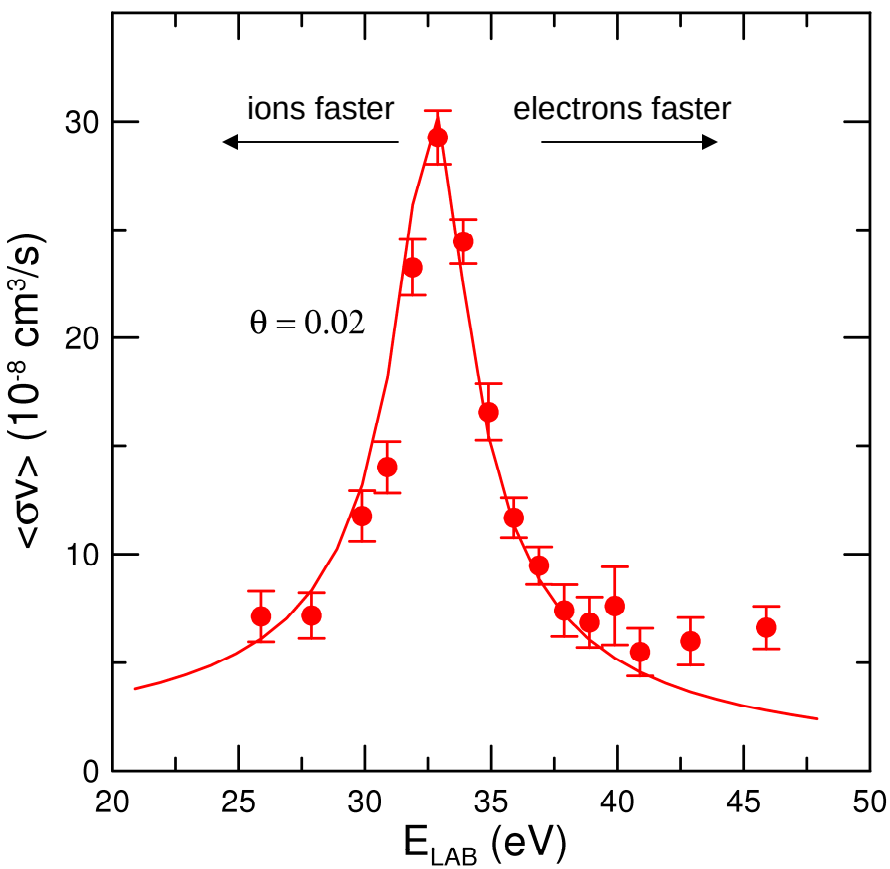
- **ECR ion source on 250-kV platform enables detection of neutral fragments from DR**
- **Capability for DR is needed with reduced availability of CRYRING and TSR rings**

- Surface barrier detector enables measurement of both DR and DE rate coefficients
- Fragment imaging detector provides information on dynamics of dissociation including initial and final state distributions
- Electron energy-loss measurements can be used to probe excitation

DR on MEIBEL: Rate Coefficients

DR of 120 keV H_2^+ ions by E_{cm} = 0 – 1.0 eV electrons

$$e^- + H_2^+ (v) \rightarrow H(1s) + H(2l) + KER(2,v)$$

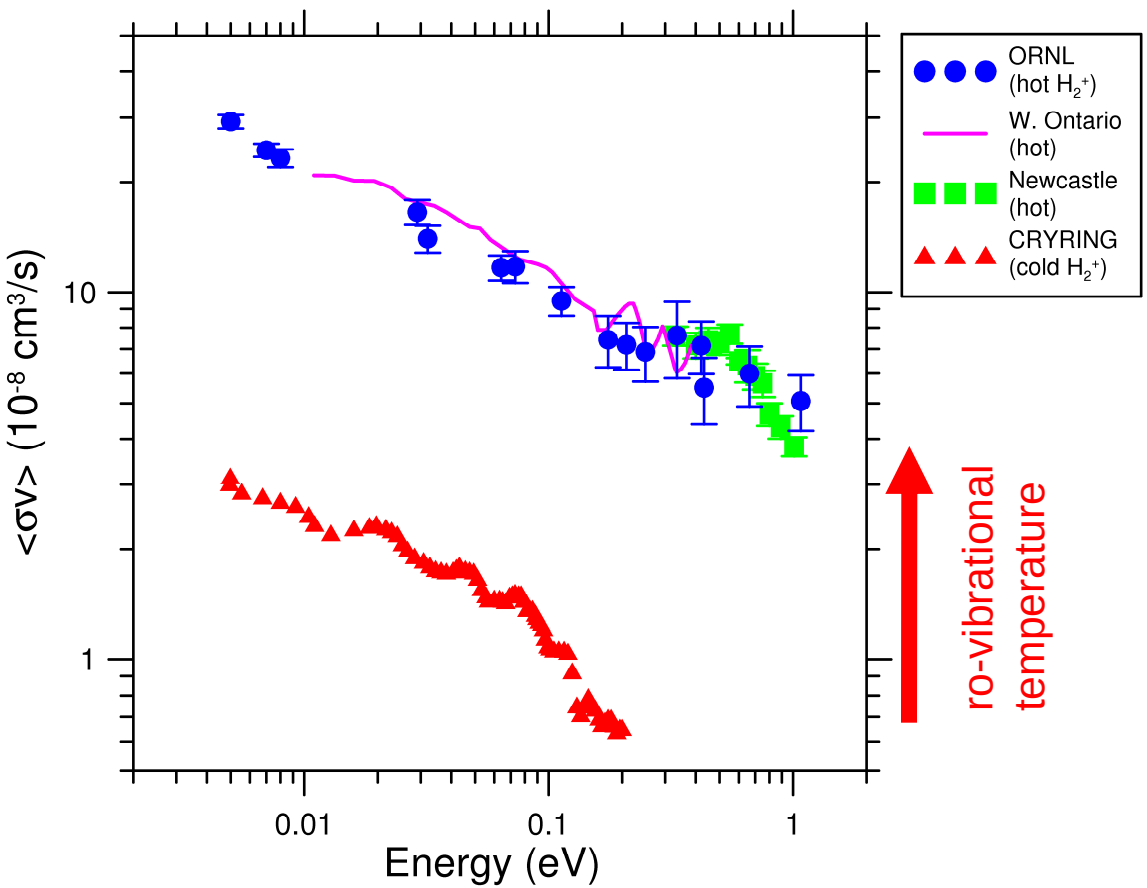


- Plot of DR rate vs. E_{LAB} shows clear peak corresponding to $E_{CM} \approx 0$
- Solid curve assumes that $\sigma_{DR} \sim E_{CM}^{-1}$ but with a finite mean angle θ between the ion and electron beams

DR on MEIBEL: Rate Coefficients

DR of 120 keV H_2^+ ions by E_{cm} = 0 – 1.0 eV electrons

$$e^- + H_2^+ (v) \rightarrow H(1s) + H(nl) + KER(n,v)$$



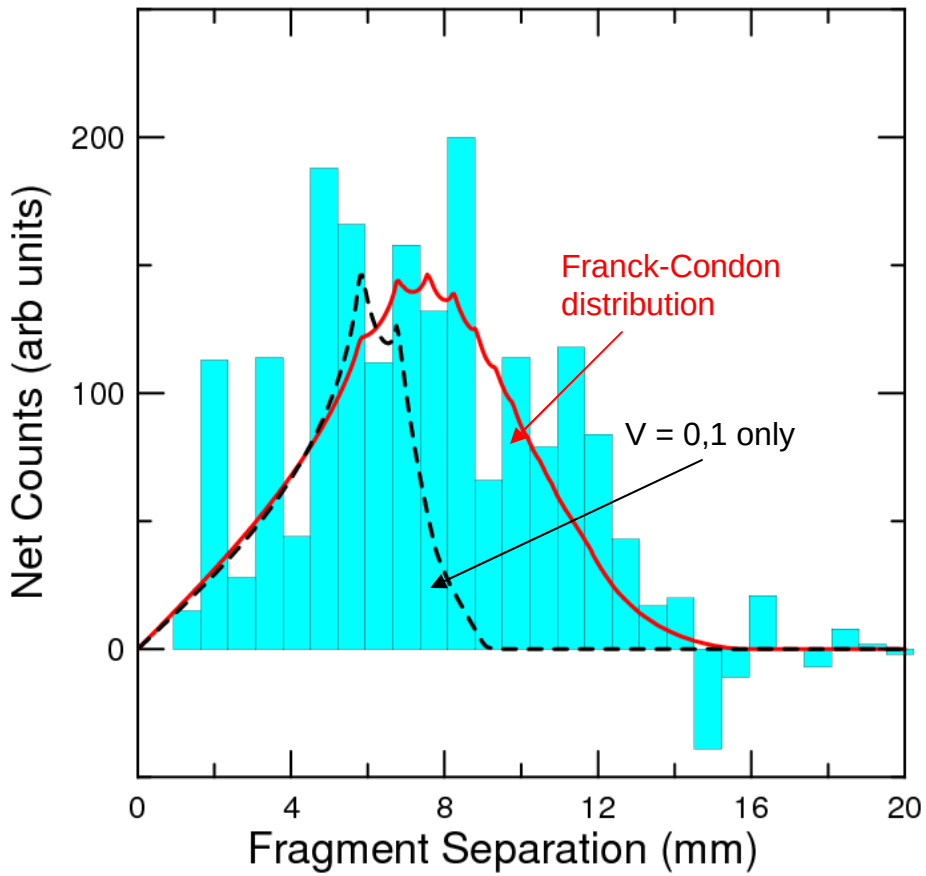
Measured absolute rate coefficients are in excellent agreement with other results for hot H_2^+ ions (single-pass experiments)

DR rate for H_2^+ is strongly dependent on ro-vibrational distribution

DR on MEIBEL: Fragment Imaging

DR of 120 keV H_2^+ ions by E_{cm} = 0 eV electrons

$$e^- + H_2^+ (v) \rightarrow H(1s) + H(2l) + KER(2,v)$$

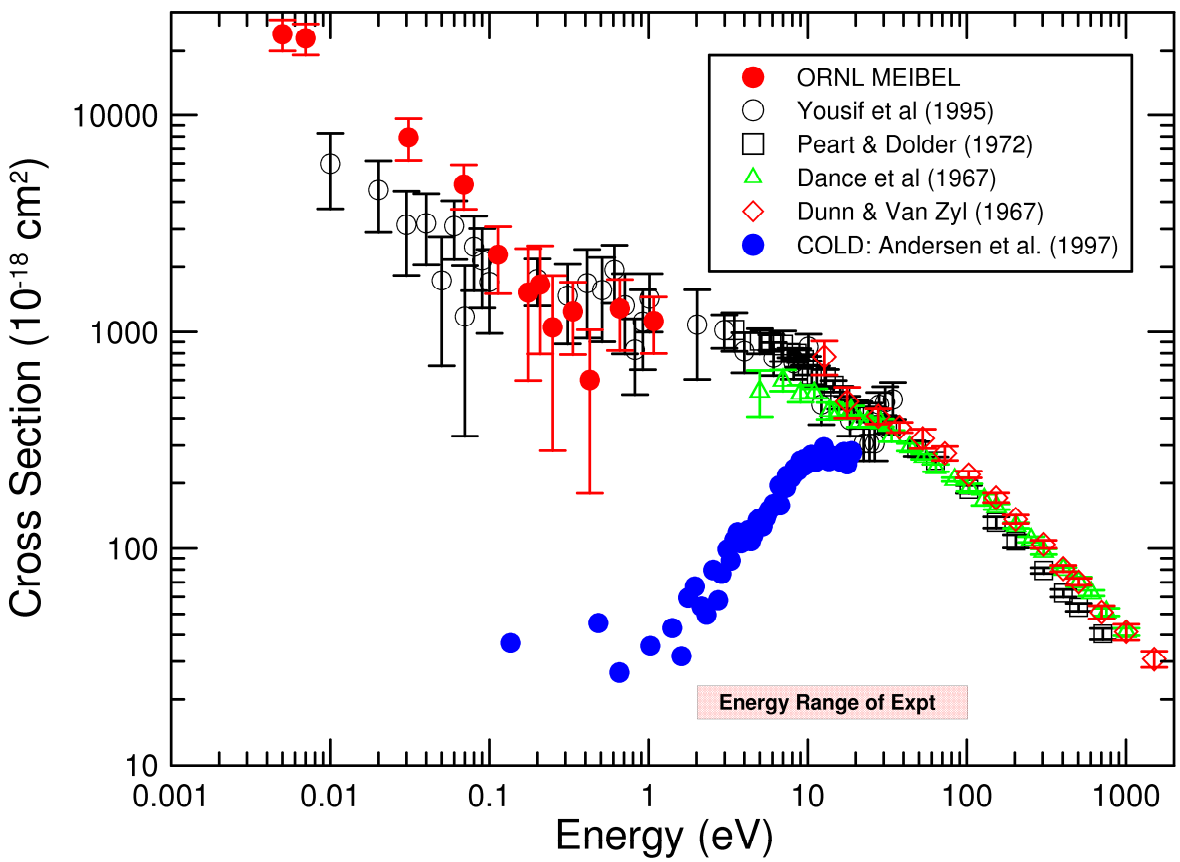


- **Fragment separation distributions measured with 320 nA of electrons (E_{cm}=0) and without electrons (dissociation on residual gas at $1x10^{-10}$ Torr)**
- **Simulated distributions assumes isotropic distribution of DR fragments and uses analytical form given by Saito *et al.* [Phys Rev A 61, 062707 (2000)].**
- **Measurements are consistent with Franck-Condon vibrational distribution ("hot")**

DE on MEIBEL: Rate Coefficients

DE of 120 keV H_2^+ ions by E_{cm} = 0 – 1.0 eV electrons

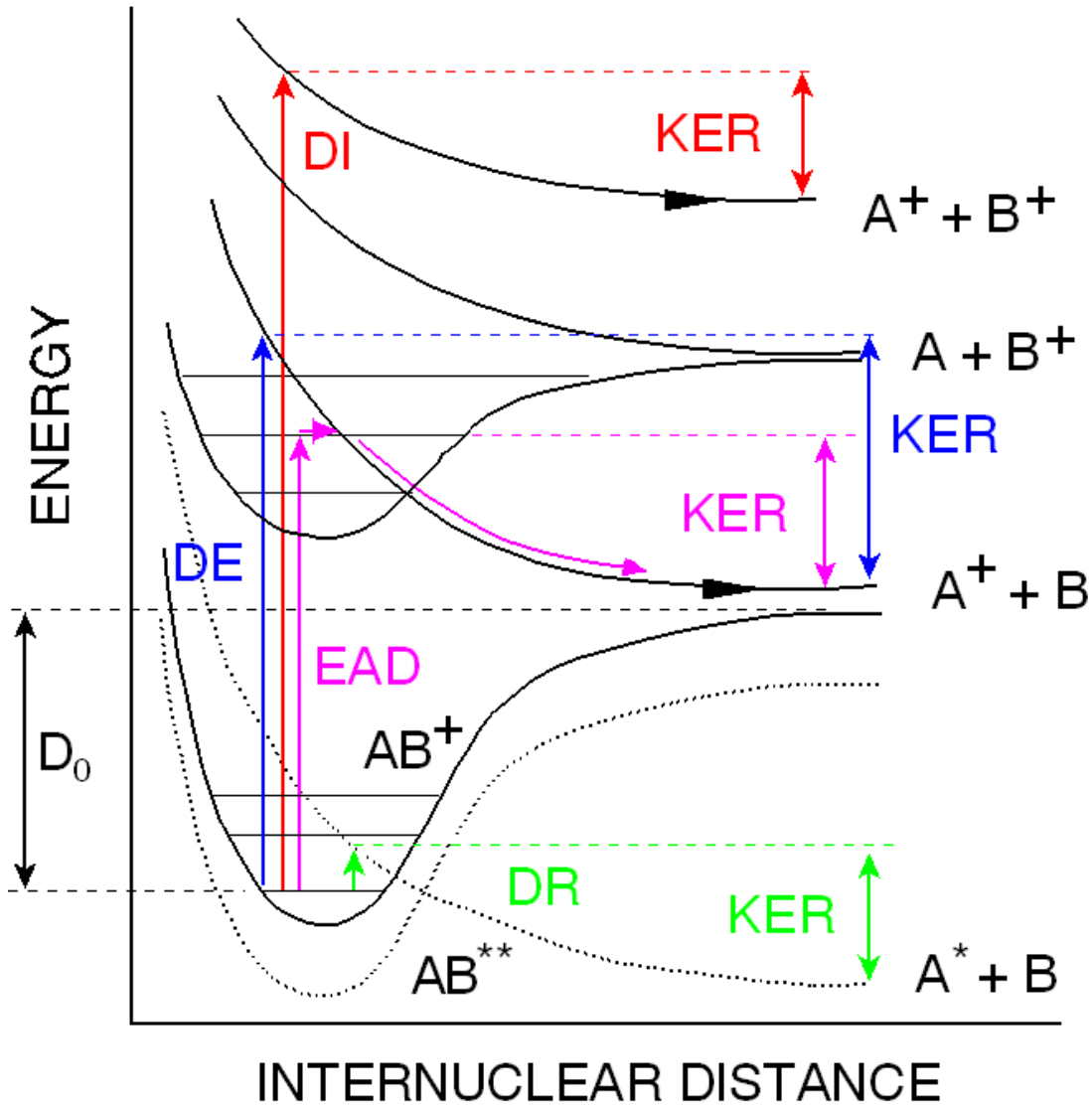
$e + H_2^+ \rightarrow H^+ +$ products



Above 0.1 eV, our measured absolute cross sections for DE are in fair agreement with Yousif's results for hot H_2^+ ions (single-pass experiment)

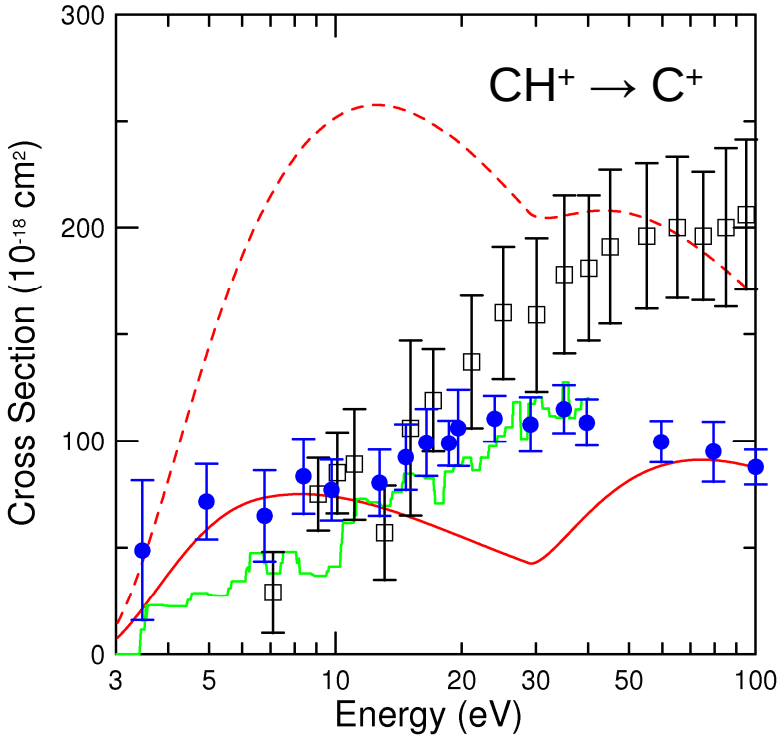
DE cross sections also very dependent on ro-vibrational distribution

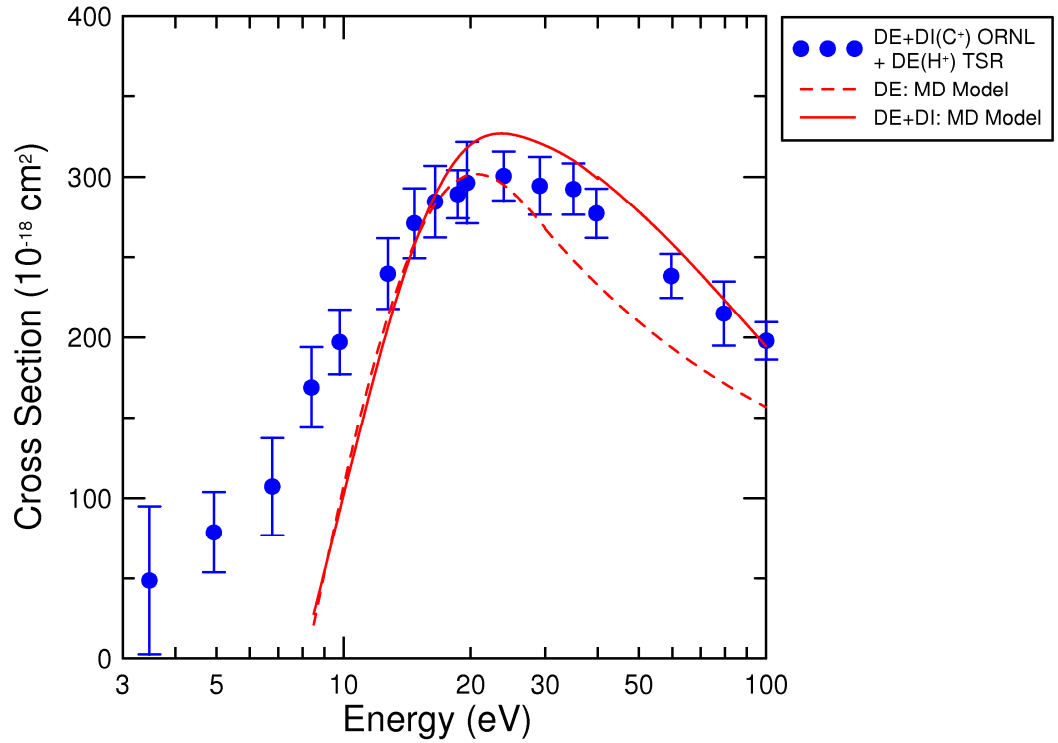
Dissociation Mechanisms (DE +DI)



- At E ~ 0 eV, DR is the dominant dissociation mechanism
- Typically DE becomes more important when E > 10 eV

DE/DI Measurements using XBEAM: CH^+





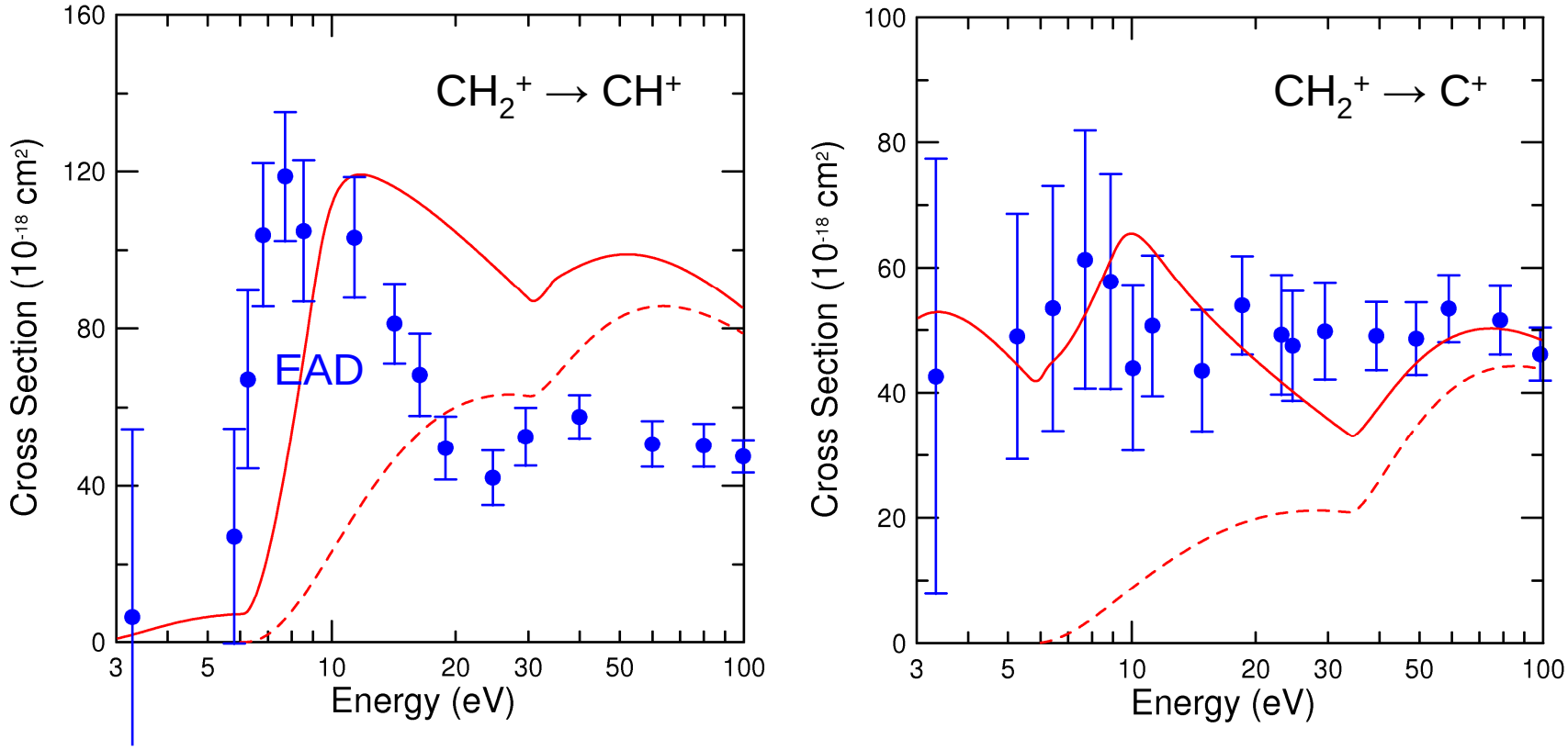
- For E < 30 eV, all experiments in reasonable agreement
- HYDKIN database (solid curve) is ok on magnitude, but shape is not correct
- Previous data from Janev & Reiter (dashed curve, Jülich-3966) grossly overestimates DE contribution

- **These refinements in the HYDKIN database result in improvements in the B2-EIRENE modeling code**

- Monte-Carlo energy-deposition model by D. R. Schultz for total DE and DE+DI in very good agreement for E > 10 eV
- No other theory exists for these systems!

*Bannister et al., Phys. Rev. A **68**, 042714 (2003)*

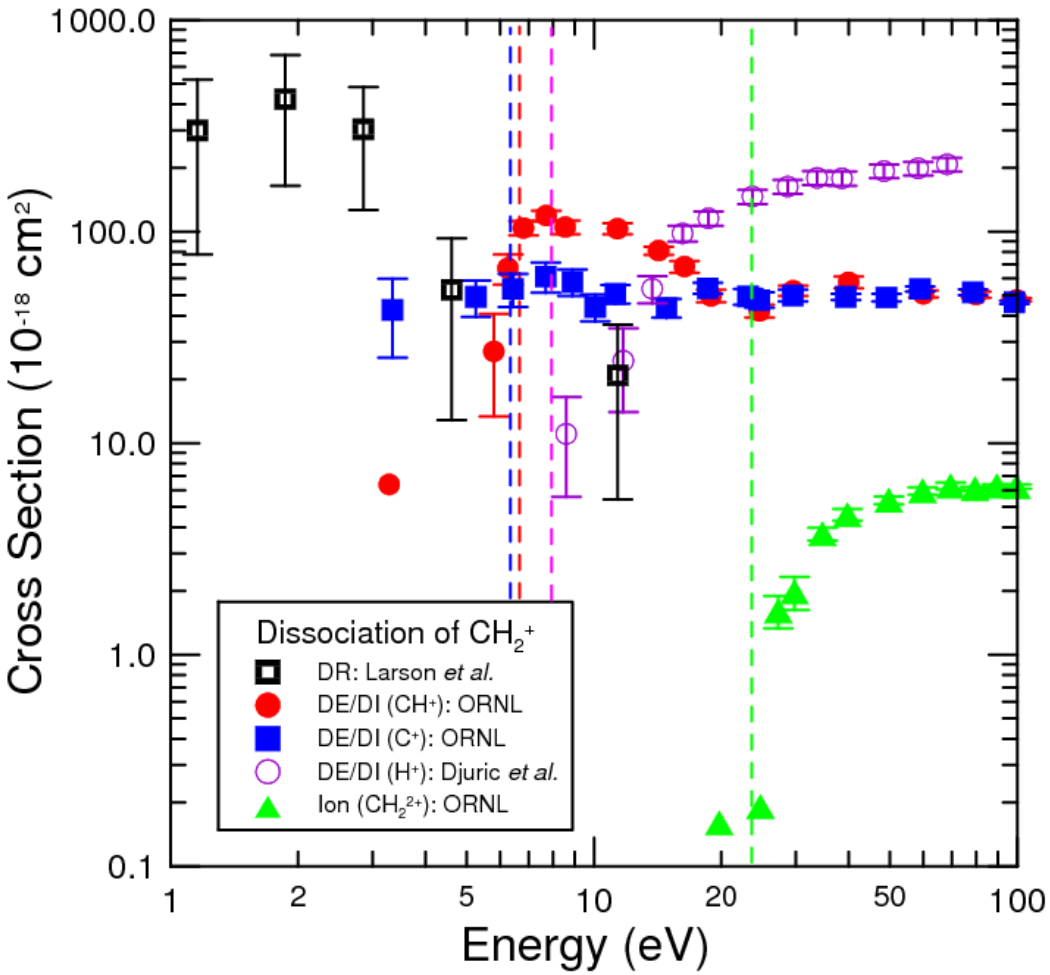
DE/DI Measurements using XBEAM: CH_2^+



- Overall agreement between semi-empirical data of Janev & Reiter is improving (from Jülich-3966 to HYDKIN), but energy dependences not quite right – more refinements to model functions needed!

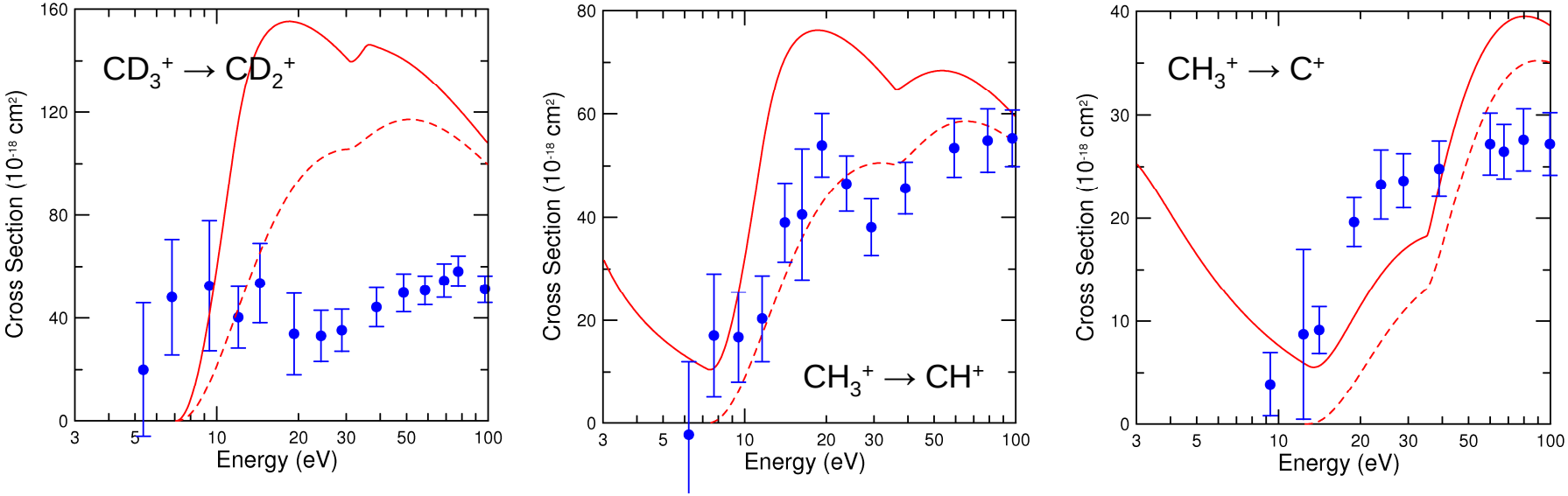
*Vane et al., Phys. Rev. A **75**, 052715 (2007)*

Complete Picture for CH_2^+ Dissociation



- DR dominates at low E
- In the 5-15 eV, all the dissociation processes are comparable
- DE/DI yielding H^+ fragments is dominant at highest E

DE/DI Measurements using XBEAM: CH_3^+



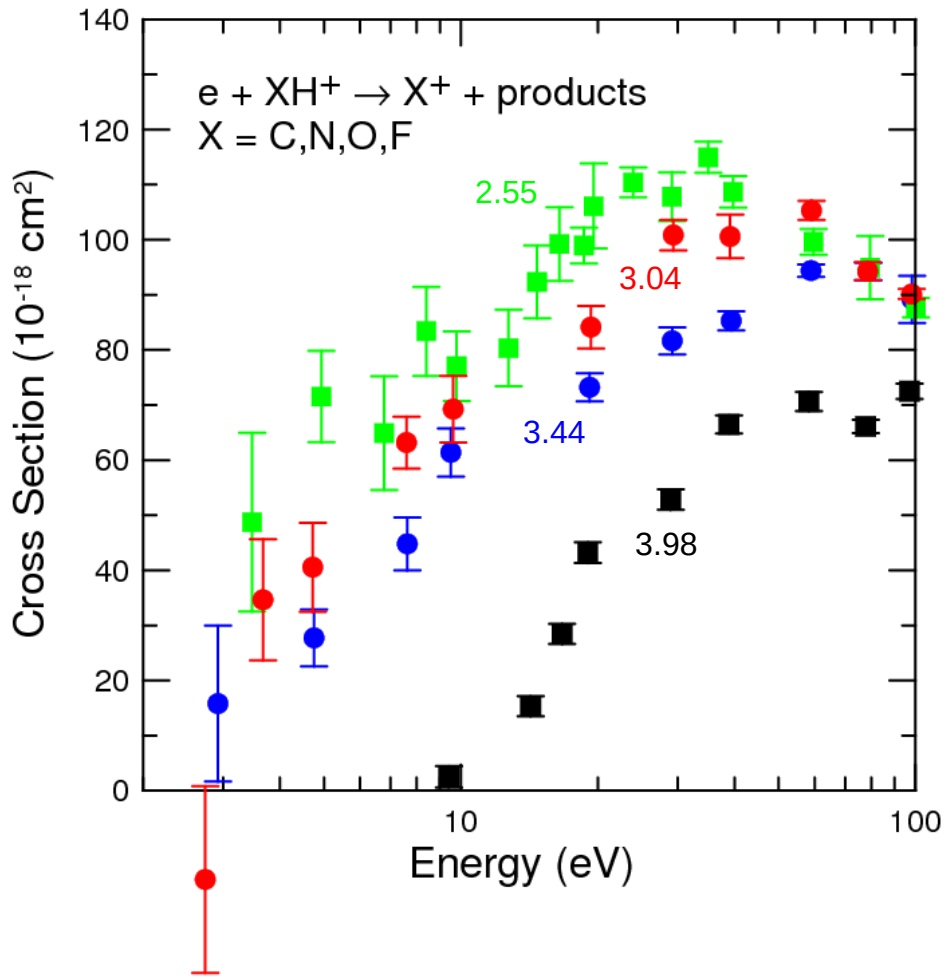
- For CH_3^+/CD_3^+, the predictions of Janev & Reiter are very "hit or miss"

*Bahati et al., Phys. Rev. A **79**, 052703 (2009)*

Summary of Hydrocarbon Data

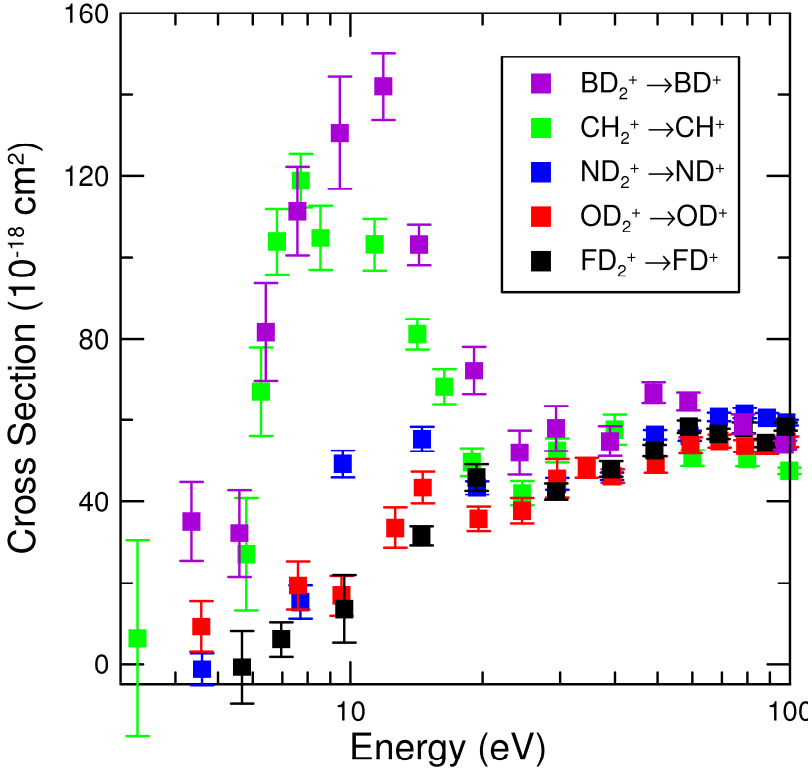
Process	σ (10^{-18} cm^2) 10 eV (DE only)		σ (10^{-18} cm^2) 60 eV (DE + DI)	
	HYDKIN	Experiment	HYDKIN	Experiment
$CH^+ \rightarrow C^+$	74	77	81	100
$CH_2^+ \rightarrow CH^+$	112	105	98	51
$CH_2^+ \rightarrow C^+$	65	44	49	53
$CH_3^+ \rightarrow CH_2^+$	60	53	133	51
$CH_3^+ \rightarrow CH^+$	32	17	68	53
$CH_3^+ \rightarrow C^+$	8	4	37	27

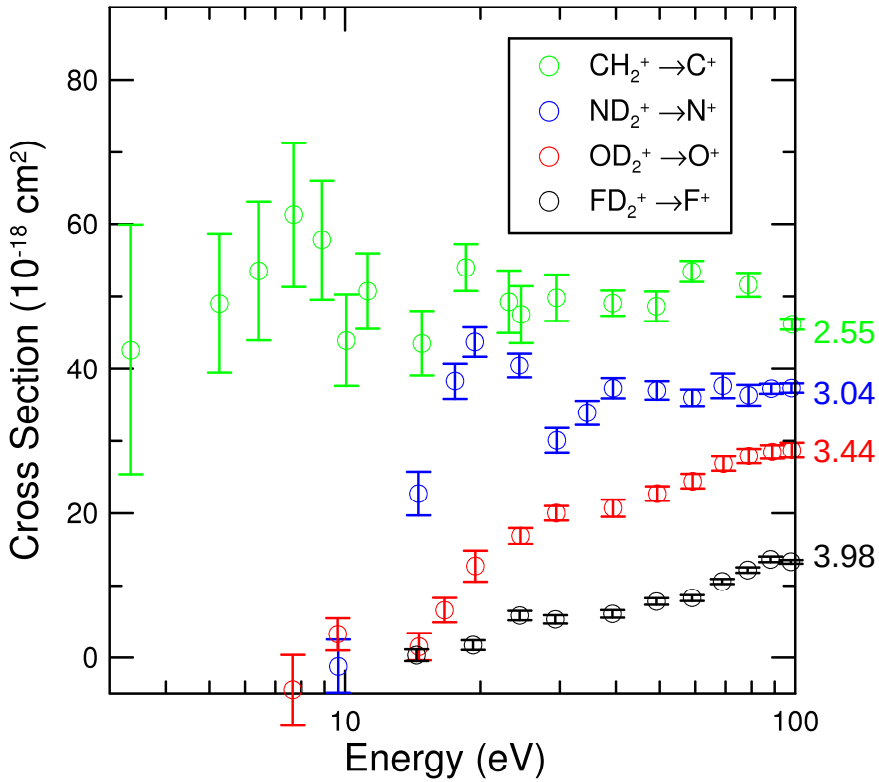
DE/DI of Hydrides



- Systematic study of XH^+ hydrides (X=C,N,O,F) shows decreasing cross section for X^+ production with increasing electronegativity of X partner
- This is also reflected in the increasing threshold for the X^+ fragment channel

DE/DI of Di-Hydrides

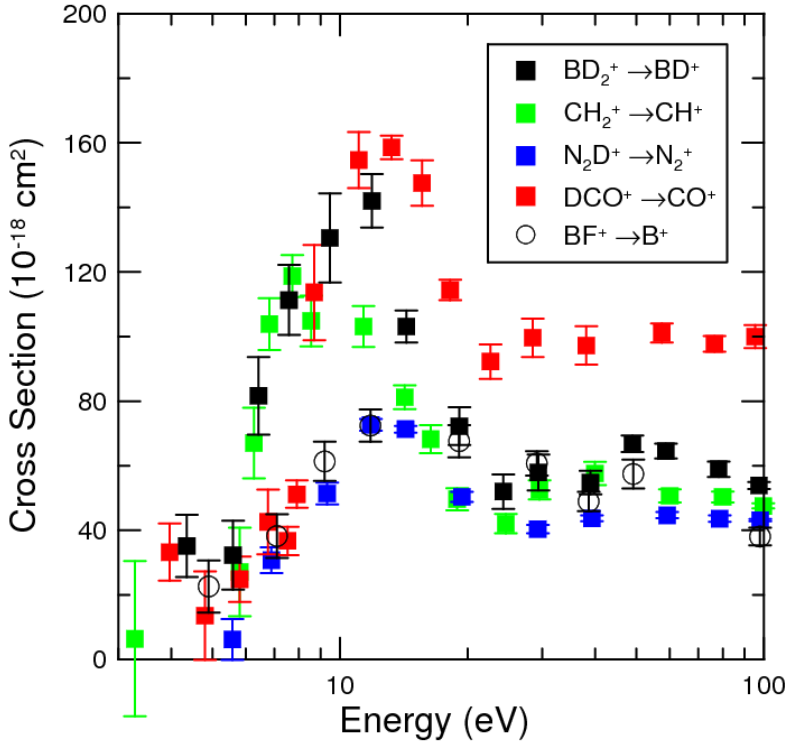


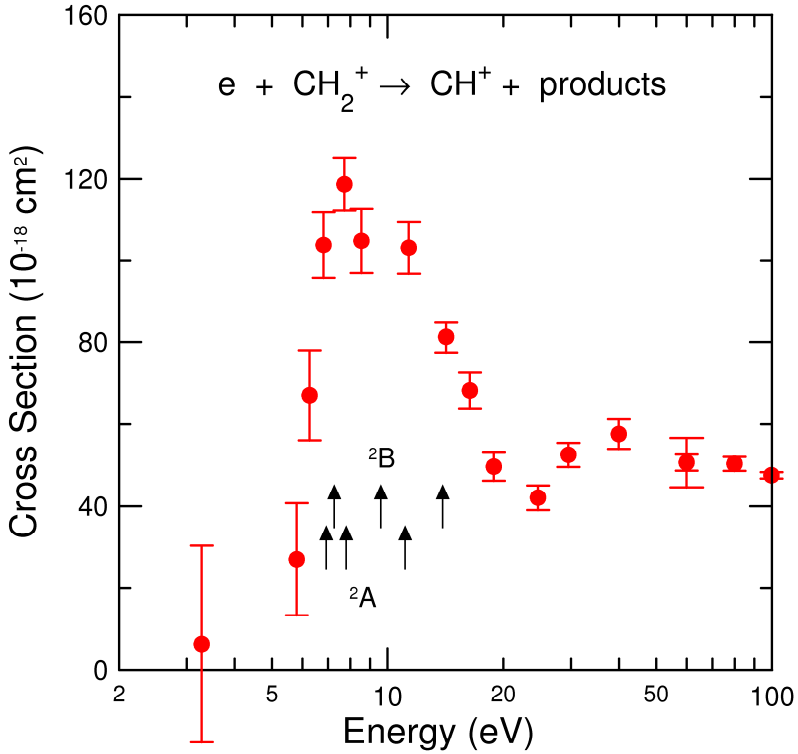


- For E > 30 eV, there is "universal" cross section for XH^+ production
- At lower energies, DE of BD_2^+ and CH_2^+ shows significant enhancement due to EAD; OD_2^+ and FD_2^+ show none
- DE results for X^+ fragment channel show same trend as for XH^+ hydrides

*Fogle et al., Phys. Rev. A **82**, 042720 (2010)*

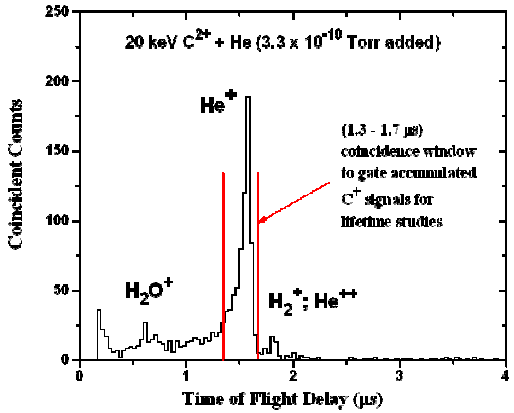
Excitation-Autodissociation (EAD)



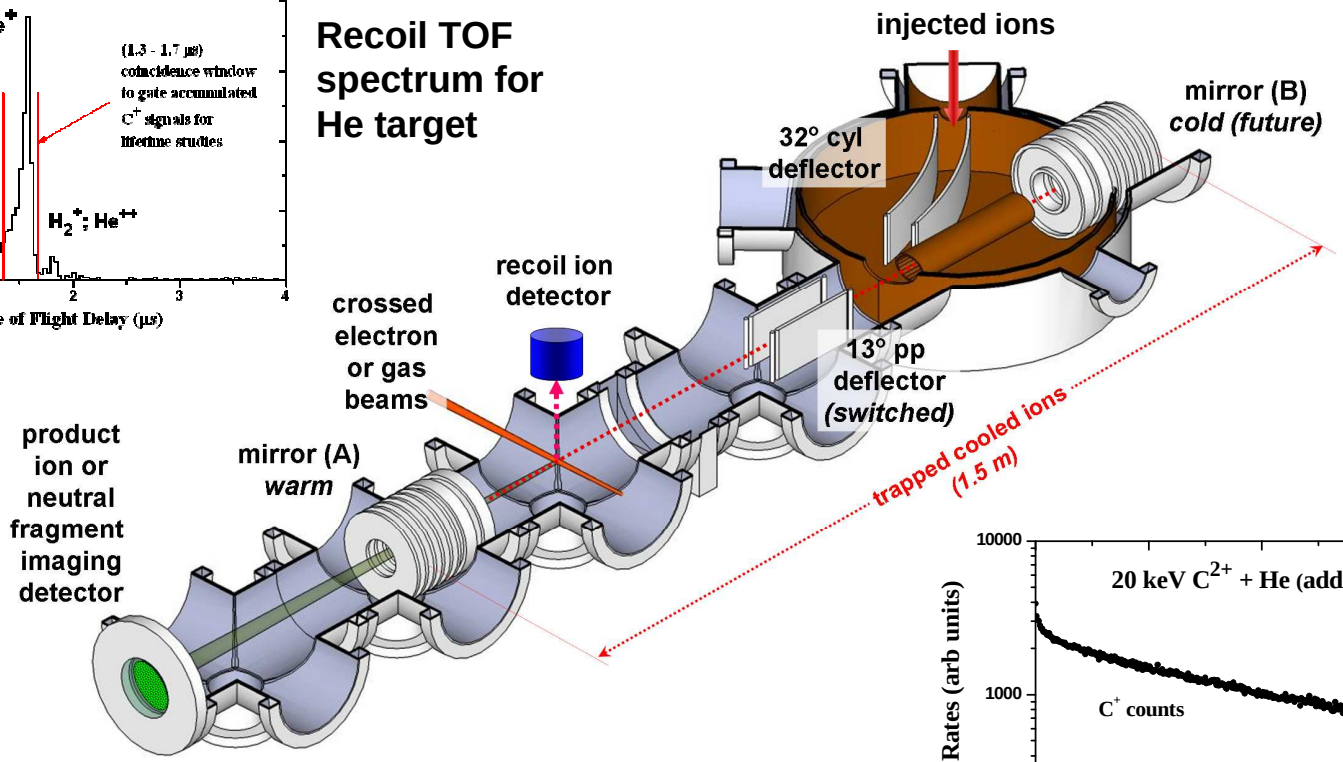


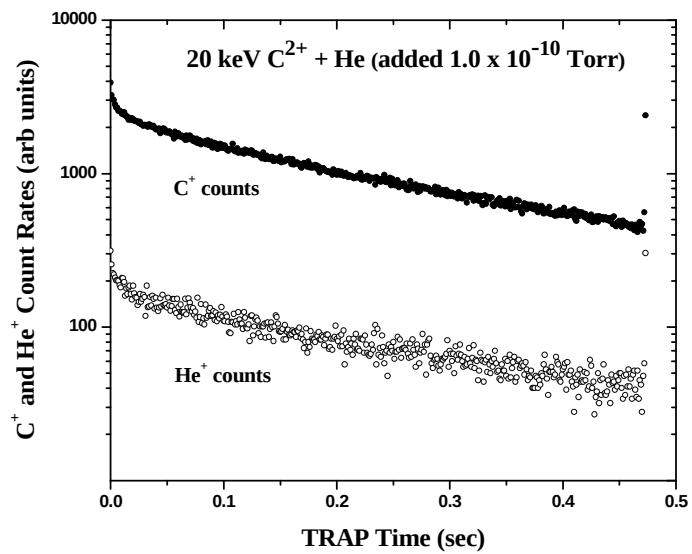
- EAD contributions to DE have been measured in at least 5 systems; peak usually occurs at energies around 2-3 times threshold and ends with opening of DI channels
- EAD peak clearly lines up with bound excited states lying above the dissociation limit for CH_2^+
- Future energy-loss measurements (with higher resolution) using MEIBEL should yield additional insights into EAD process by measuring cross sections for excitation to the bound excited states

Ion Cooling & Characterization Endstation (ICCE) Electrostatic Trap



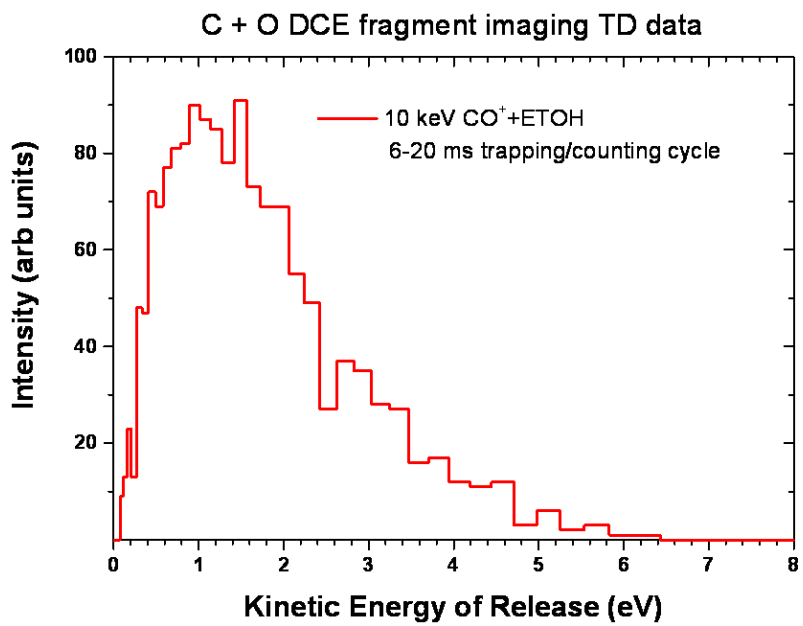
Recoil TOF spectrum for He target

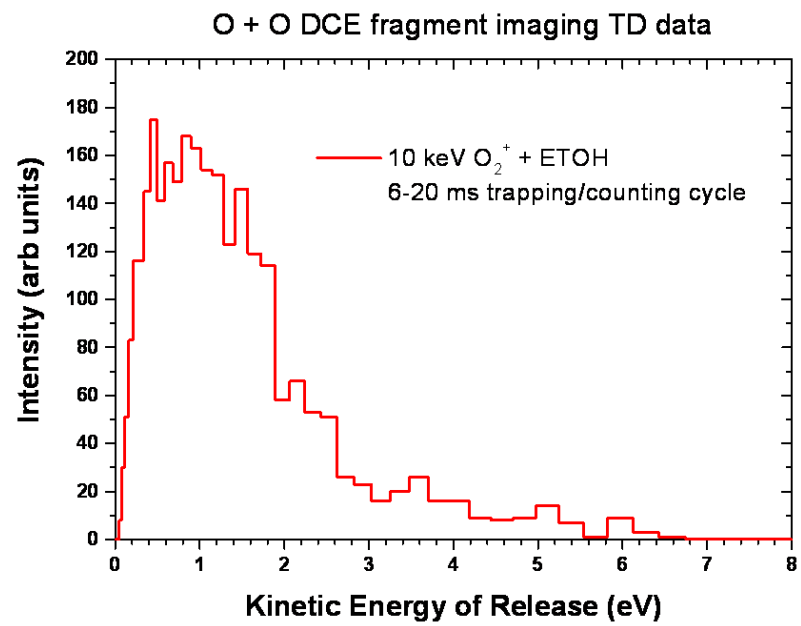




Lifetime curves for detected C^+ ions and He^+ recoil ions for 20 keV C^{2+} ions stored in trap. Analysis yields 50% 2s2p ^3P metastable ions.

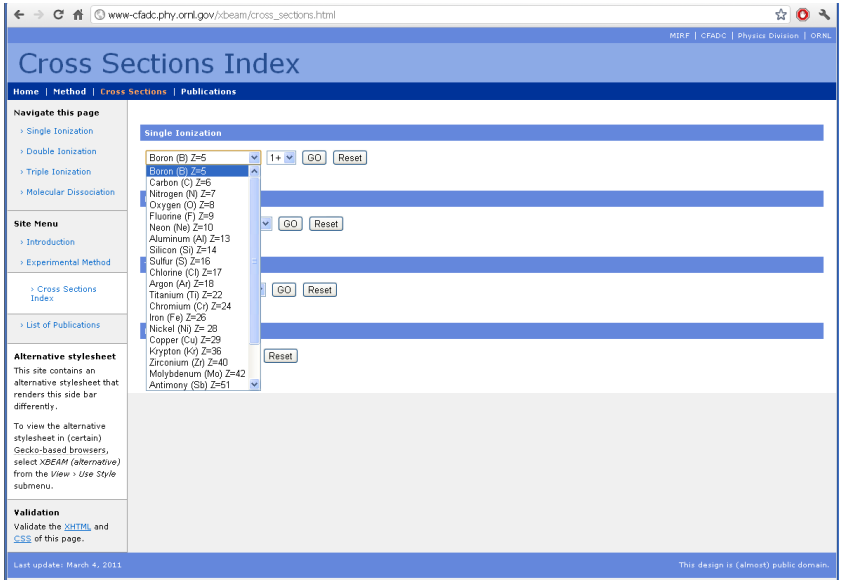
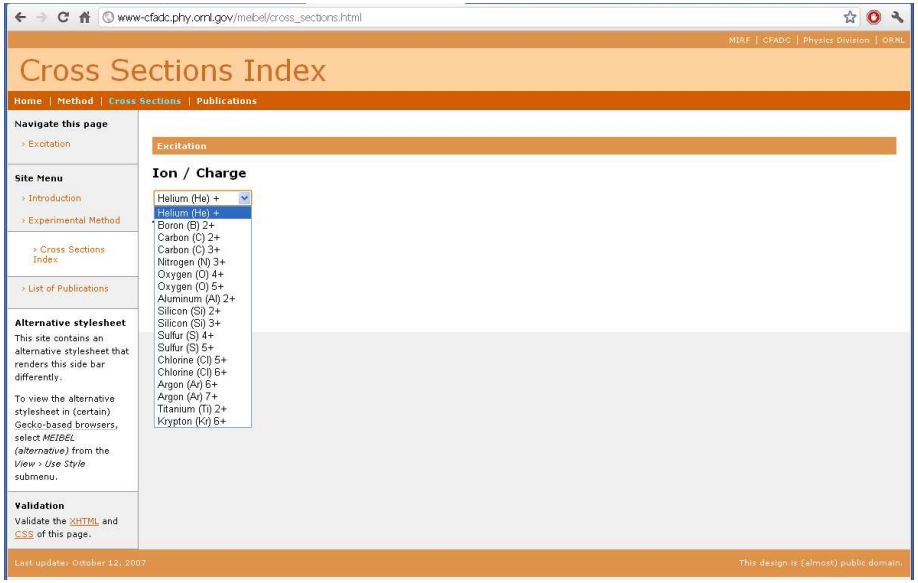
ICCE Trap Fragment Imaging





- Measured fragment KER distributions for CO^+ (left) and O_2^+ (right) ions undergoing dissociative charge exchange with CH_3CH_2OH without dissociating the target ethyl alcohol molecule -- coincidence between C+O or O+O atoms on imaging detector and $CH_3CH_2OH^+$ ions on recoil detector

- Future: study KER distributions as a function of the storage time in the trap, i.e., as a function of the vibrational distribution

CFADC Website

- http://www-cfadc.phy.ornl.gov – theoretical/experimental data, Redbooks, bibliography
- XBEAM: http://www-cfadc.phy.ornl.gov/xbeam/ All published ionization and dissociation data available online. [102 ionization, 20 dissociation cross sections]
- MEIBEL: http://www-cfadc.phy.ornl.gov/meibel/ All published excitation data available online. [25 excitation cross sections]