Charge Exchange Cross Section Measurement in Fudan University

Baoren WEI

Fudan University

brwei@fudan.edu.cn

Acknowledgement

Congzhang Gao

Alberto Castro

Chuanlu Yang

Enliang Wang

Yong Gao

Shuncheng Yan

Xinwen Ma

Long Wei

Jie Han

Wandong Yu

Yu Zhang

Baihui Ren

Jun Xiao

Yaming Zou

Baoren Wei

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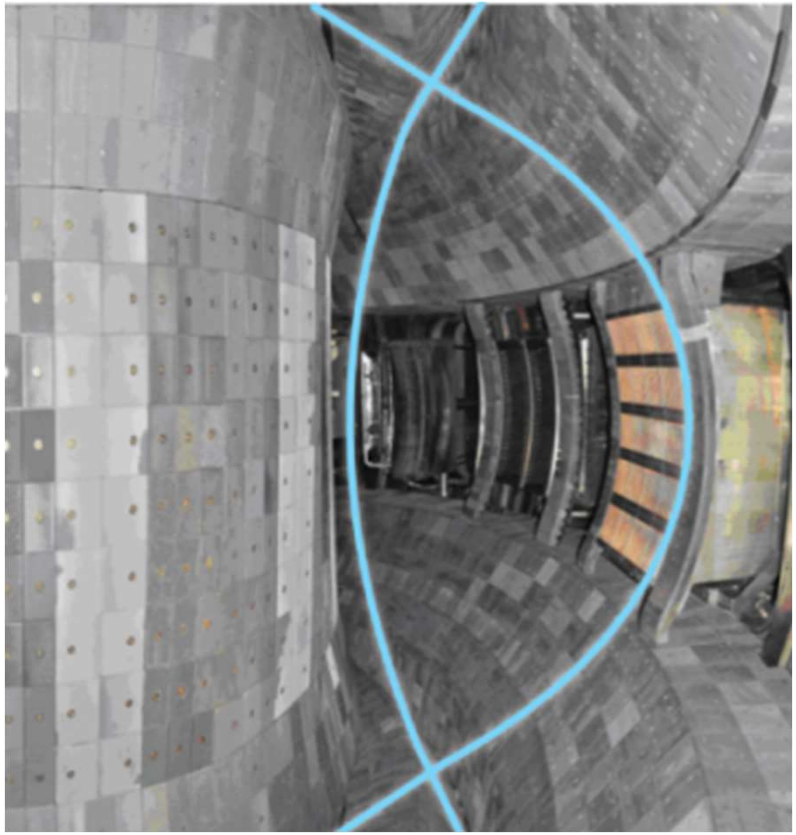
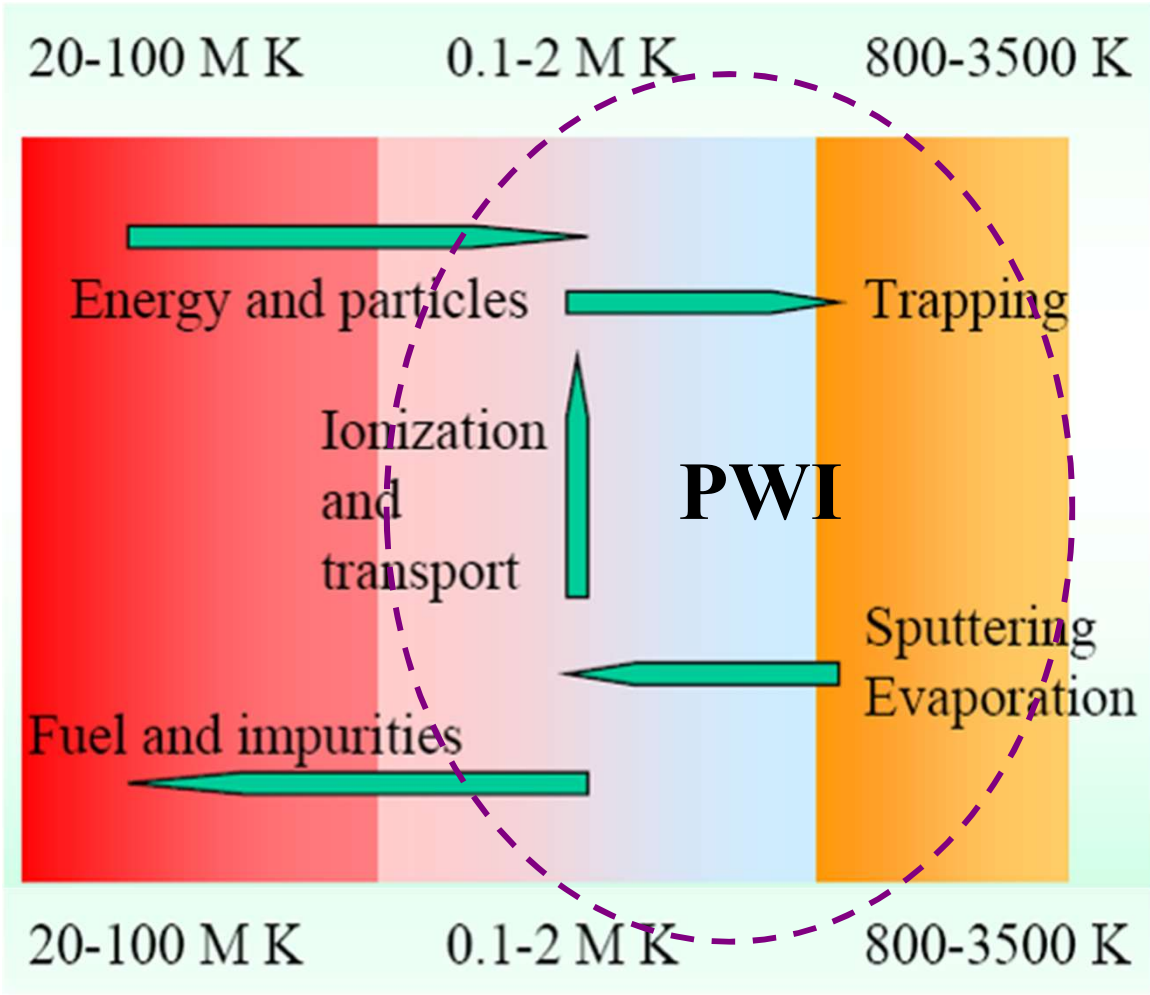
01 Motivation

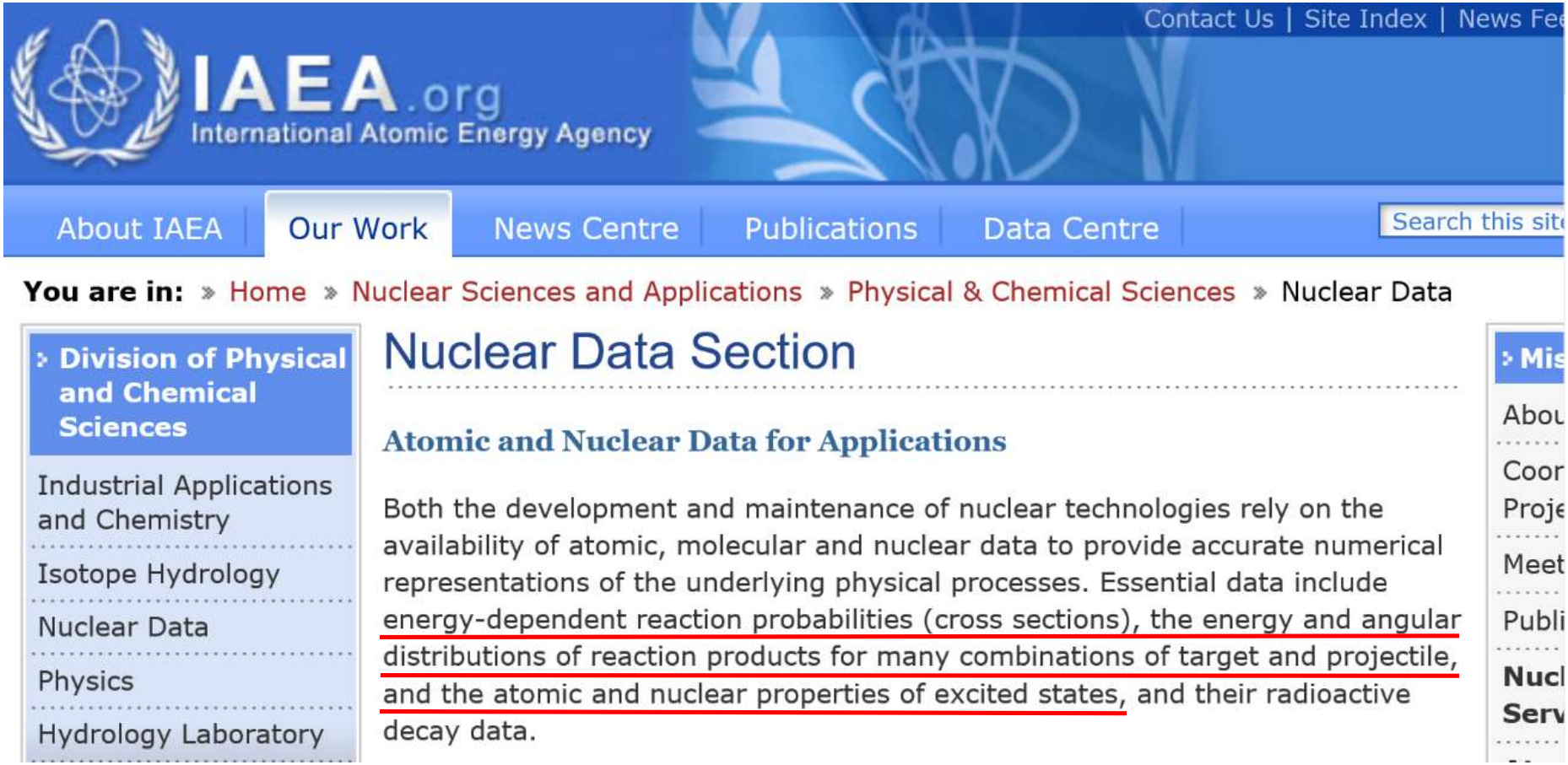
Motivation





Diagnostic and simulation need atomic and molecular data

Motivation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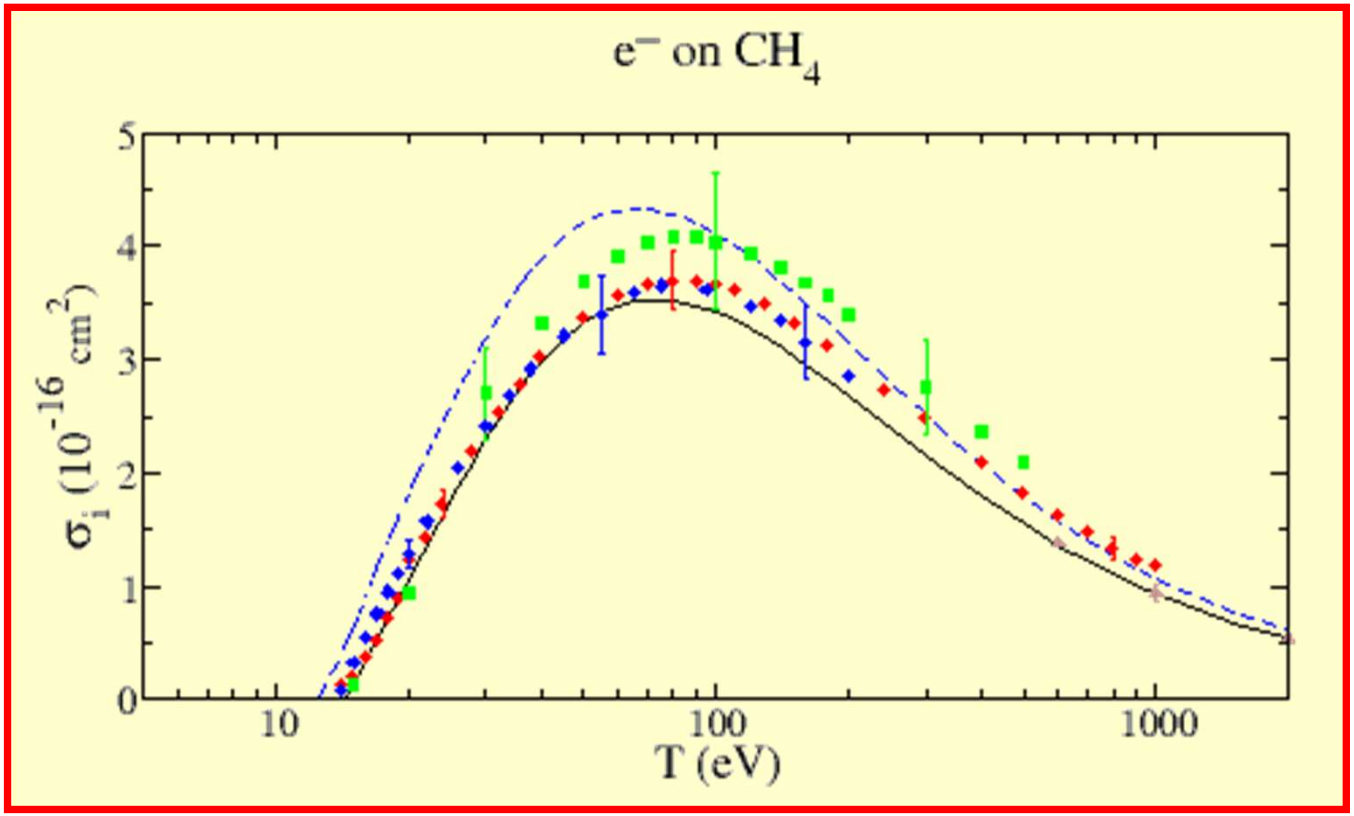
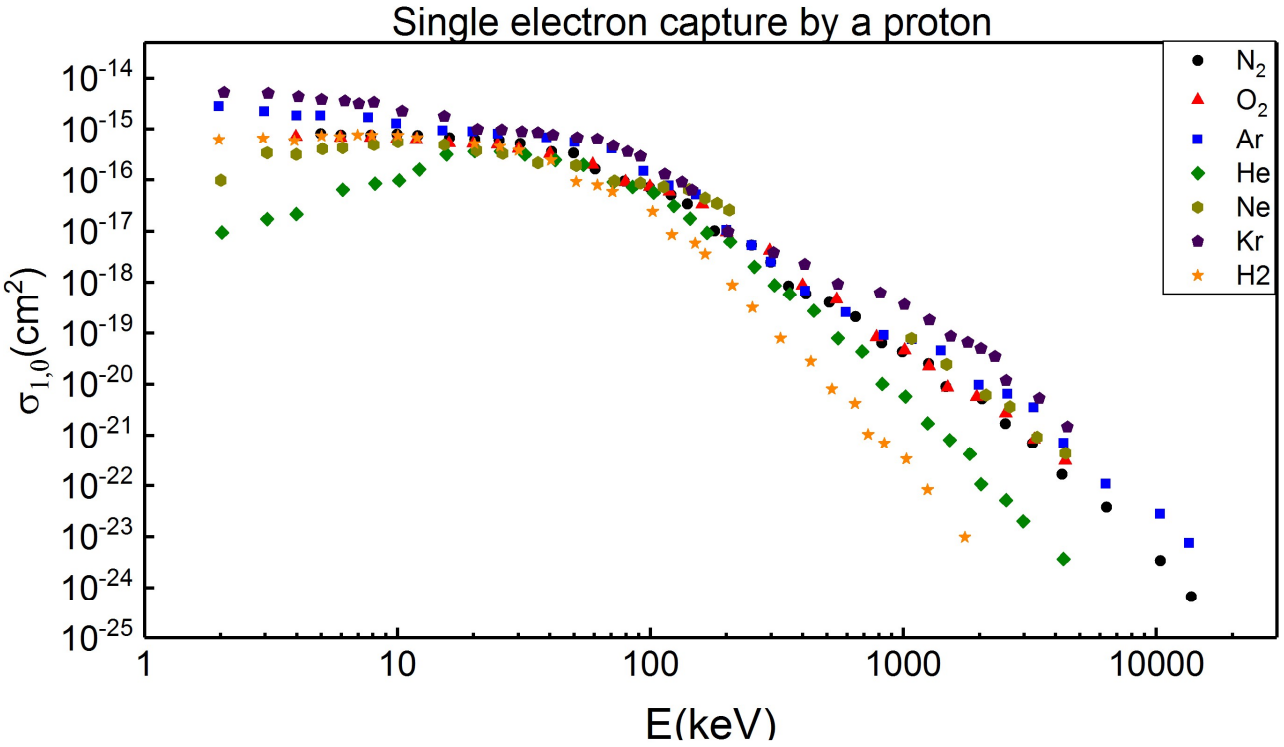
Nuclear Data Section
Atomic and Nuclear Data for Applications
Both the development and maintenance of nuclear technologies rely on the availability of atomic, molecular and nuclear data to provide accurate numerical representations of the underlying physical processes. Essential data include energy-dependent reaction probabilities (cross sections), the energy and angular distributions of reaction products for many combinations of target and projectile, and the atomic and nuclear properties of excited states, and their radioactive decay data.

Motivation



Motivation



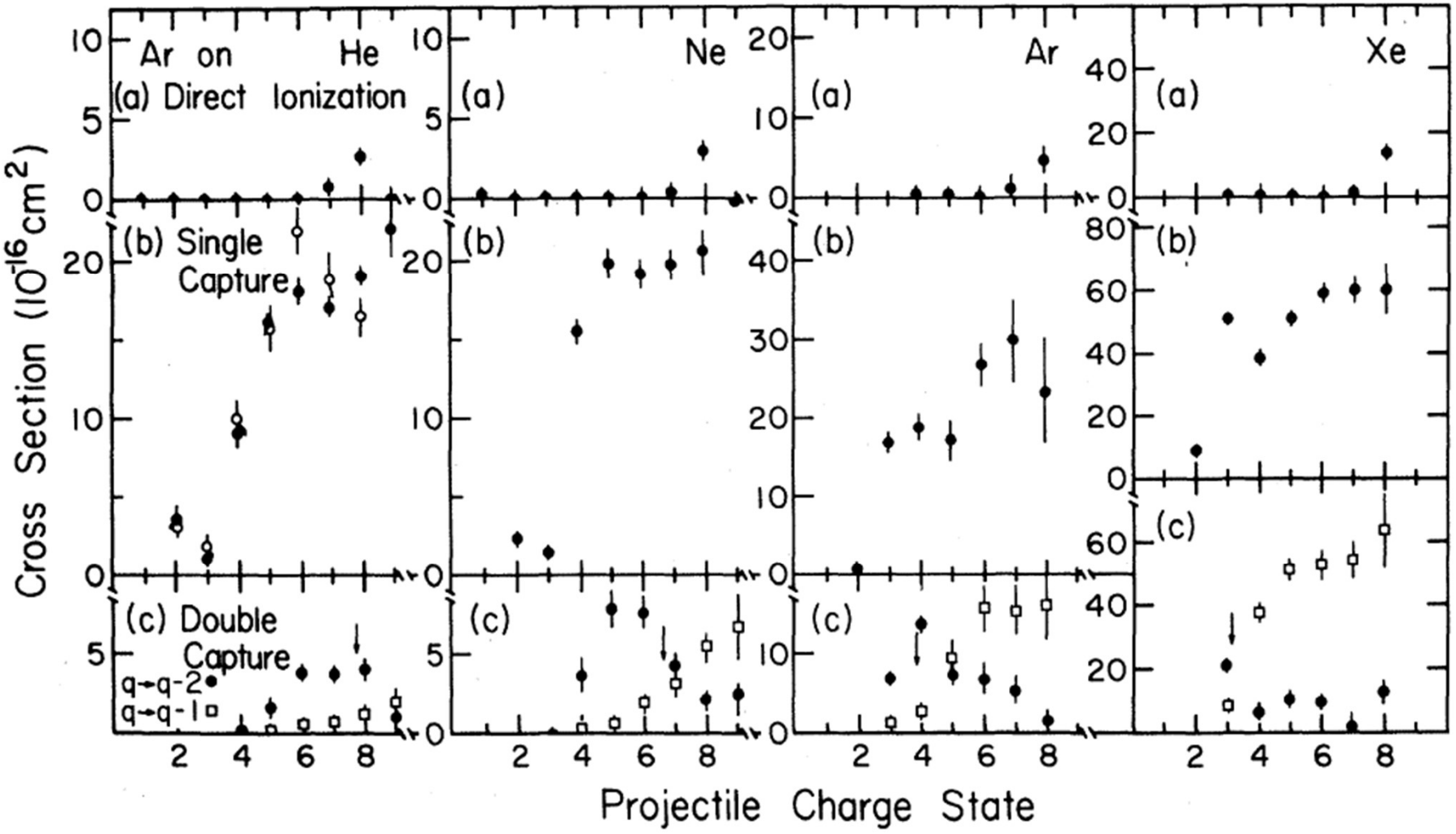
Single electron capture Cross Section

Single electron capture by a proton

Authors	Years	Energy(keV)	Target gases
Stier and Barnett	1956	3-200	H_2,N_2,O_2,He,Ne,Ar
Barnett and Reynolds	1958	250-1000	H_2,N_2,He,Ar
Szostak *et al.*	1961	4000	N_2
Gordeev and Panov	1964	1-40	H_2,N_2,Ar
Hollricher	1965	1.5-30	H_2,D_2
Berkner *et al.*	1965	6450-10000	N2,He,Ar
de Heer *et al.*	1966	10-140	H_2,N_2,O_2,He,Ne,Ar,Xe
Schryber	1967	1000-4400	H_2,N_2,O_2,He,Ne,Ar,Xe
Toburen *et al.*	1968	100-2500	H_2,N_2,O_2,He,Ar,Kr,CO,CO_2,H_2O,CH_4,C_2H_6
Acerbi *et al.*	1969	32500-37700	N_2,O_2,Ar

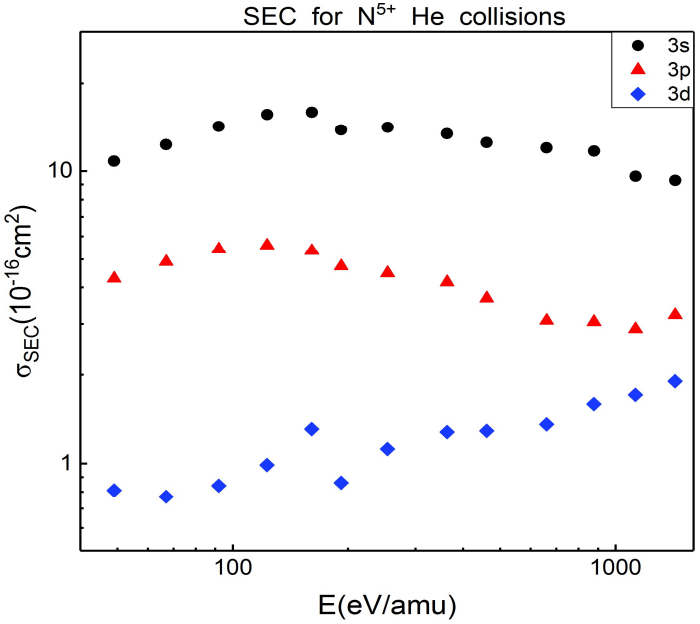
Motivation

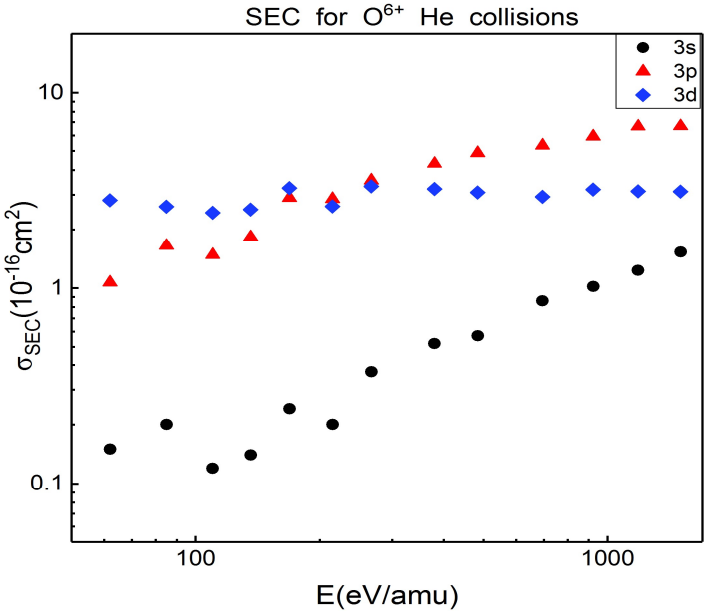
Absolute charge exchange cross sention

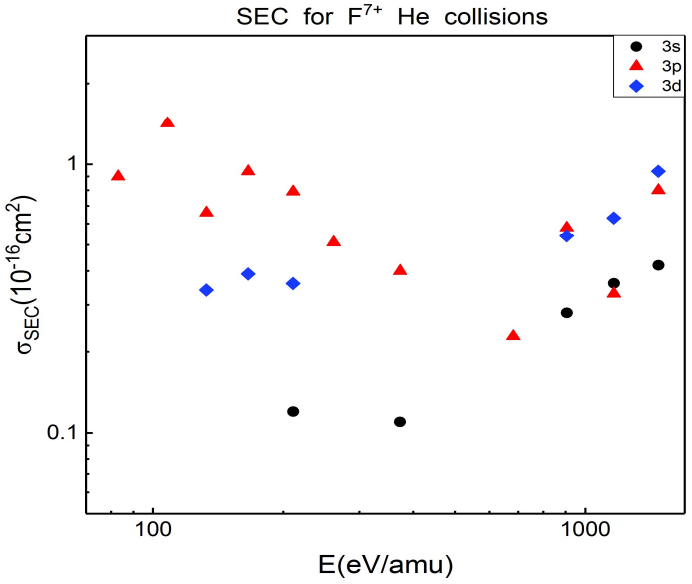


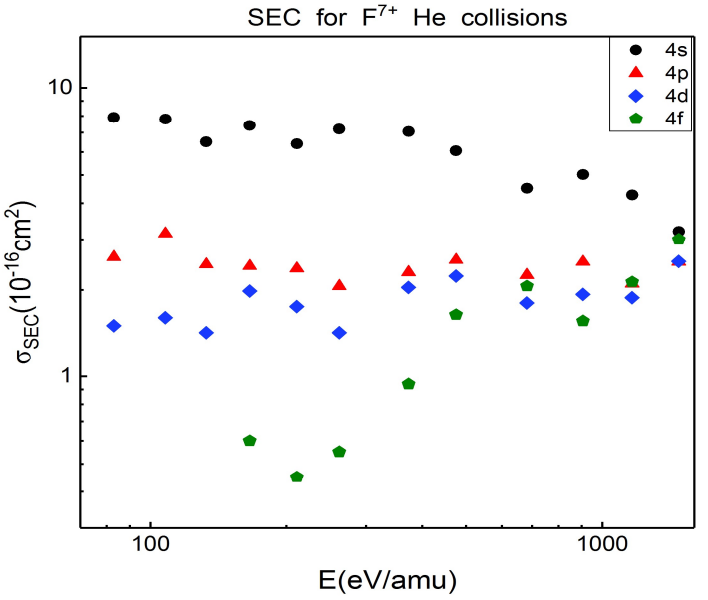
C. L. Cocke et al, PRL 1981, 46, 1671

Motivation









PRA 1994, 49, 363

Motivation

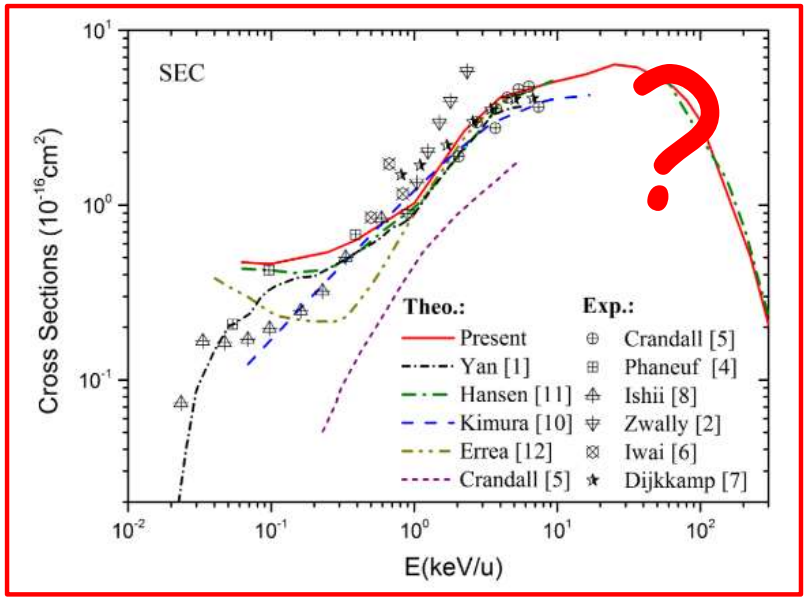
THE ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES, 234:14 (4pp), 2018 January https://doi.org/10.3847/1538-4365/aaa02c

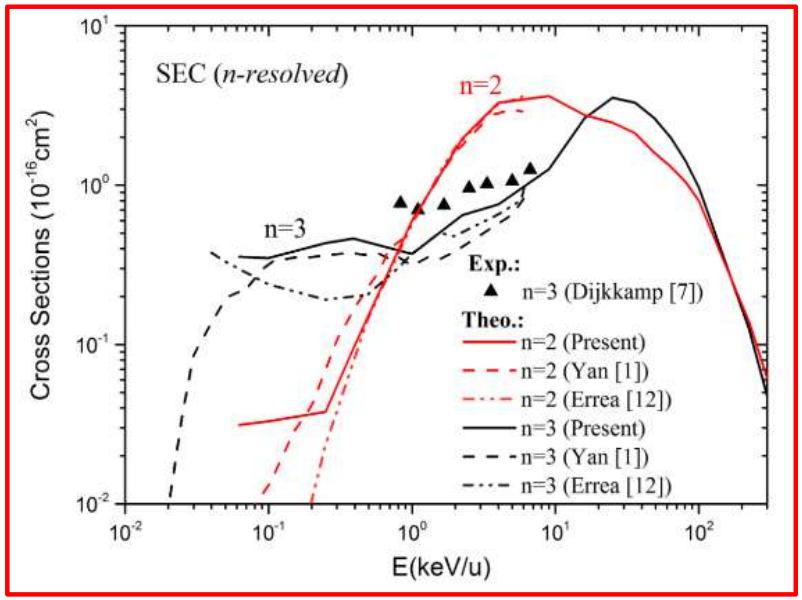
Measurement of Absolute Single and Double Charge Exchange Cross Sections for $Si^{(7-10)+}$ at 0.88–2.50 KeV/u Impacting He and H_2

PHYSICAL REVIEW A **96**, 052703 (2017)

Single- and double-electron transfer in low- and intermediate-energy C^{4+} + He collisions

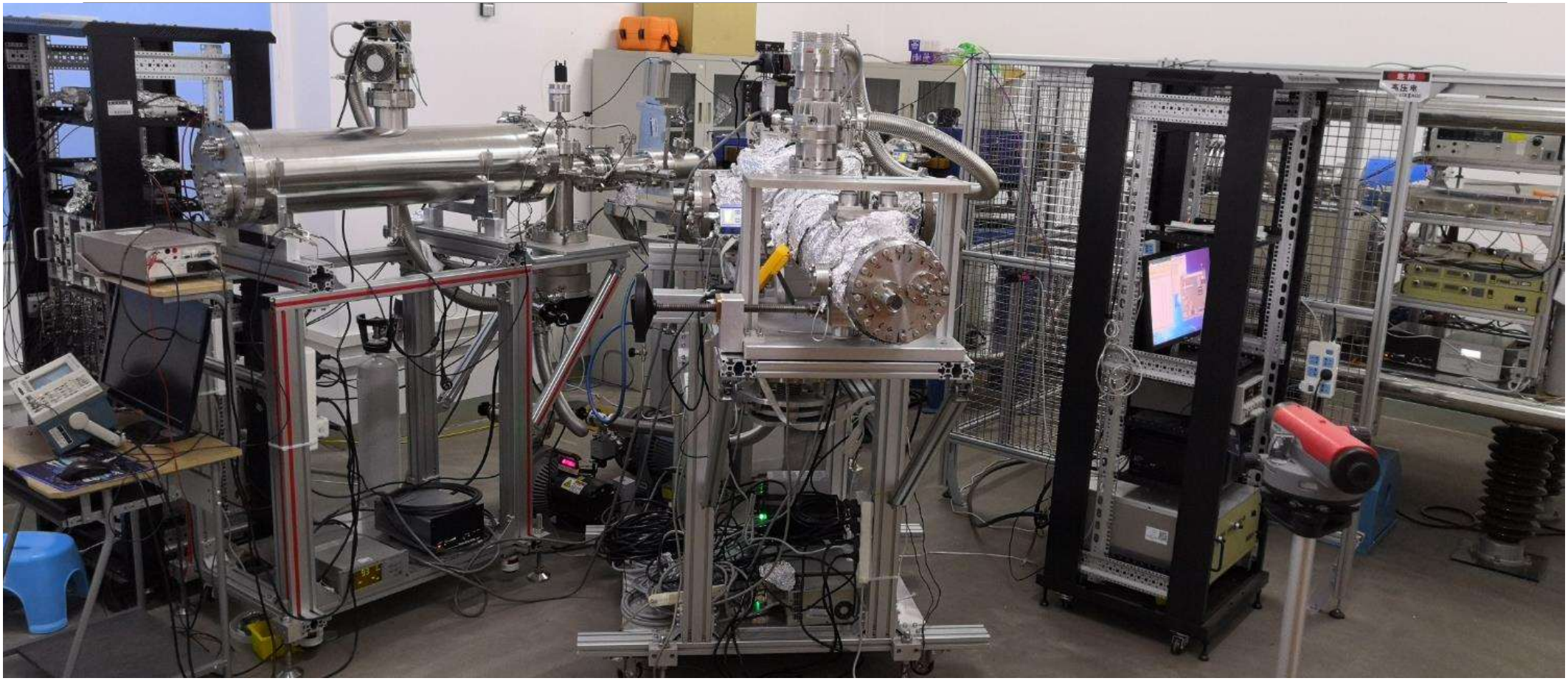
J. W. Gao,[1,2,*] Y. Wu,[1] N. Sisourat,[2] J. G. Wang,[1] and A. Dubois[2]





02 Charge Exchange of HCI

150 kV HCI platform



Molecular fragmentation

Collision cross section

Surface interaction

COLTRIMS

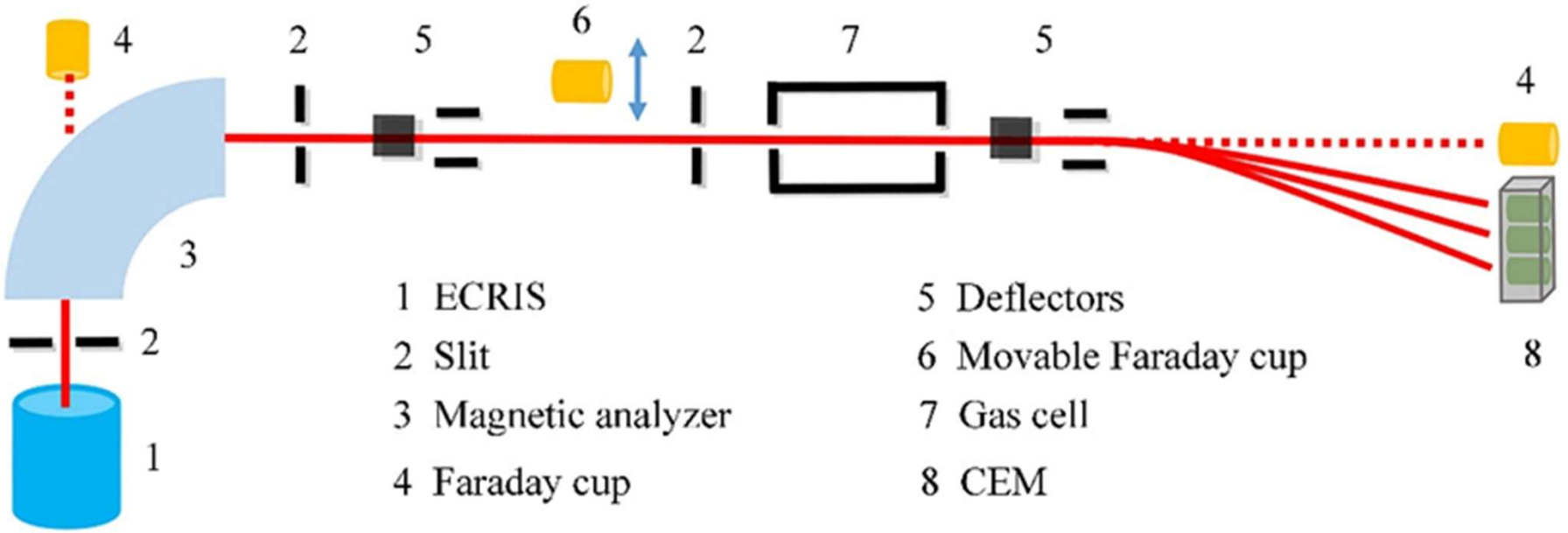
CS measurement device

……

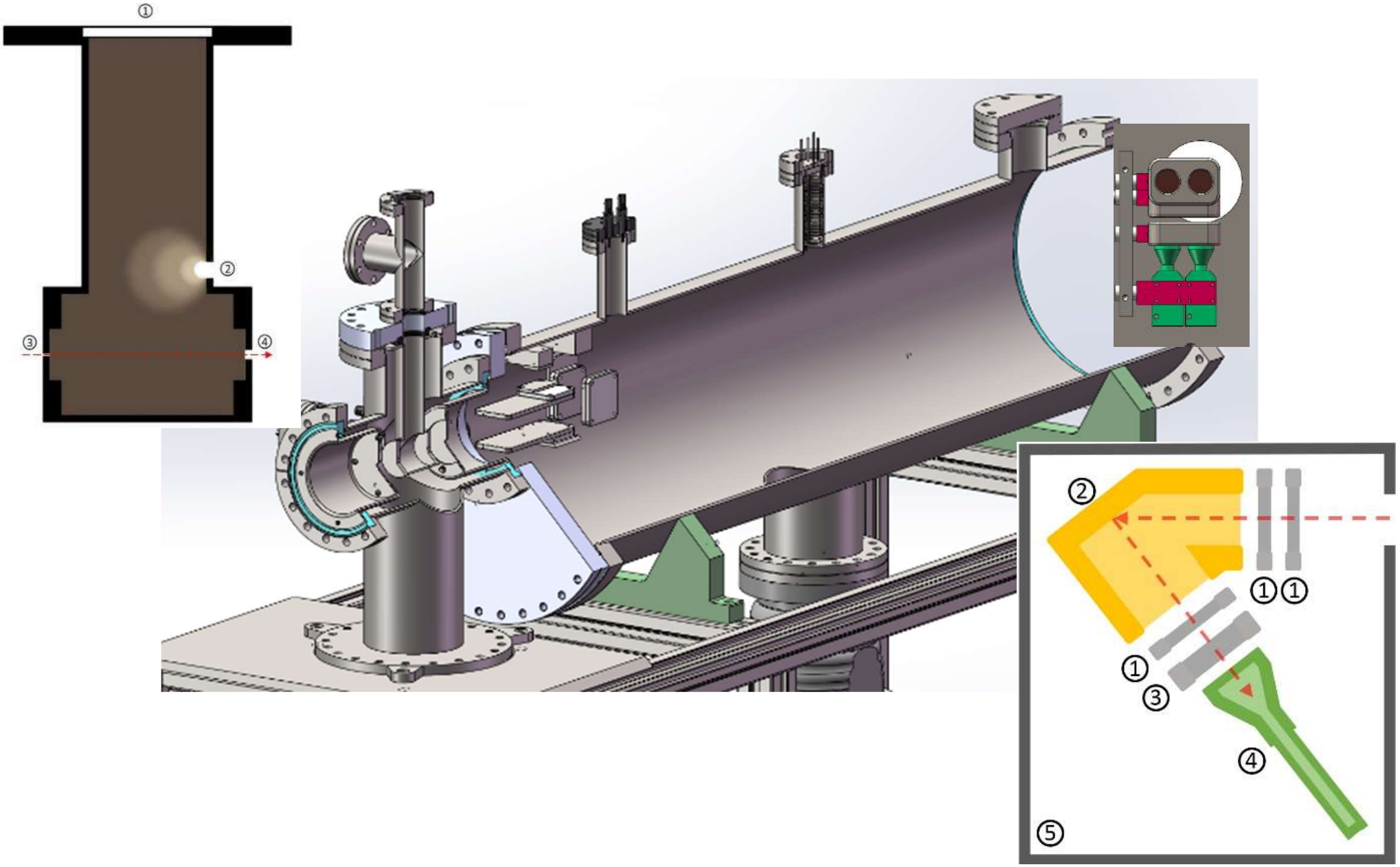
Absolute Cross Section

- Absolute single and double electron capture cross section

$$\sigma_{q,q-j} = \frac{kT}{PL}\frac{qI_{q-j}}{(q-j)I_q}$$

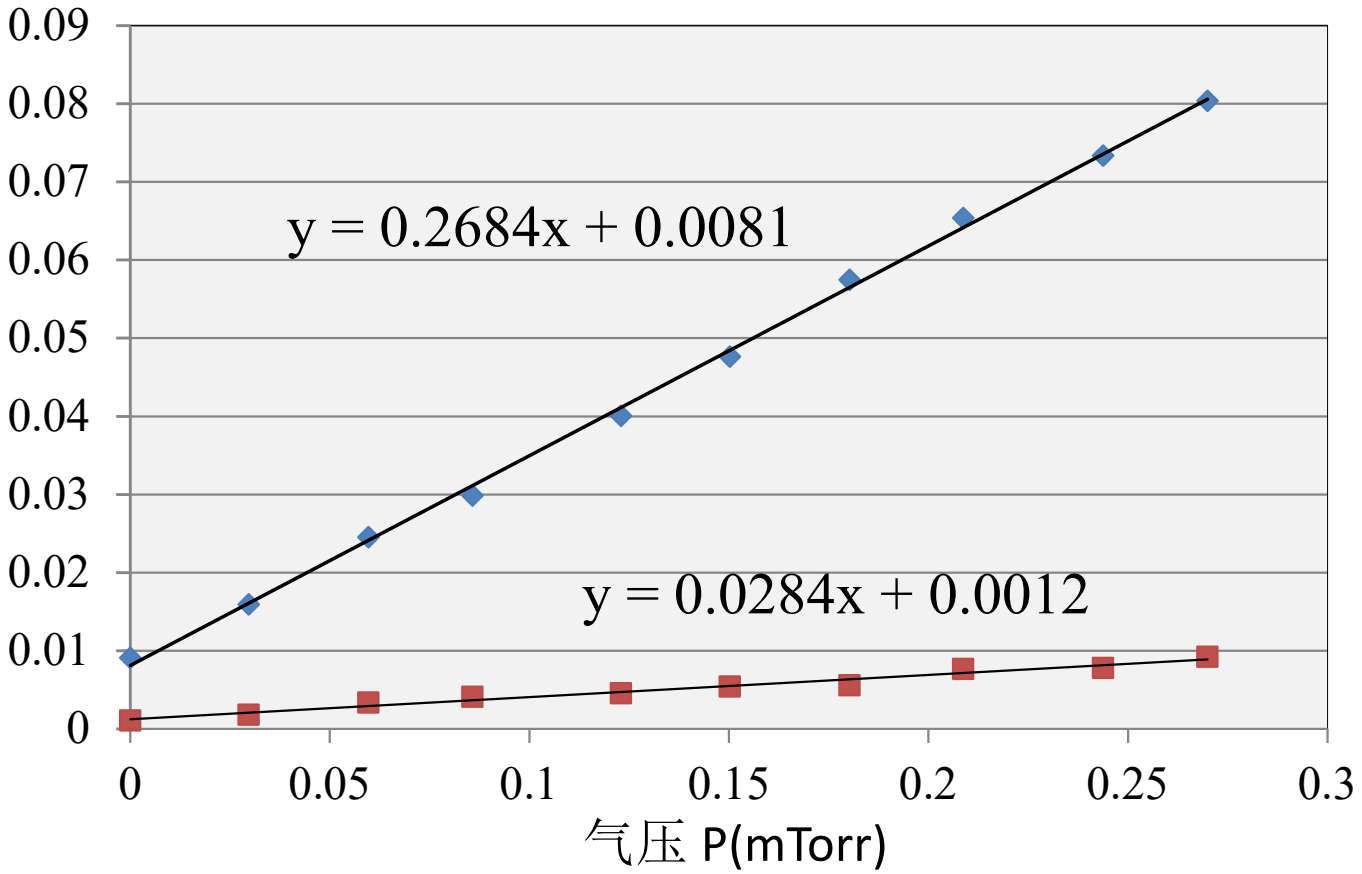


Absolute Cross Section



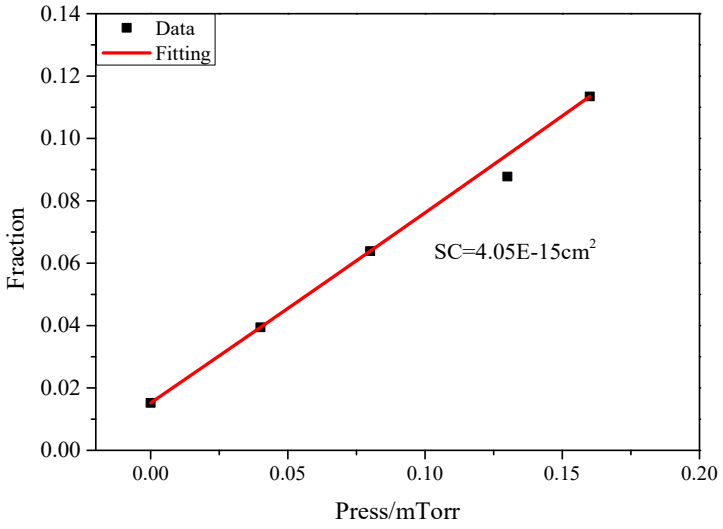
Absolute Cross Section

$$\sigma_{q,q-j} = \frac{kT}{PL}\frac{qI_{q-j}}{(q-j)I_q}$$

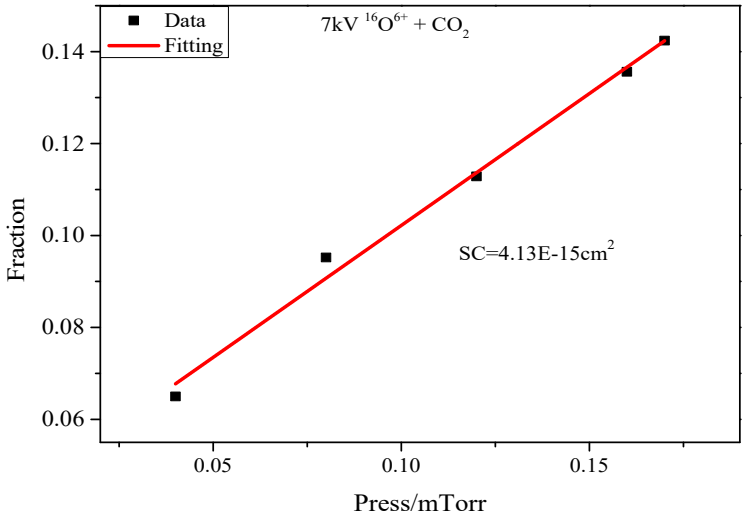


Absolute Cross Section

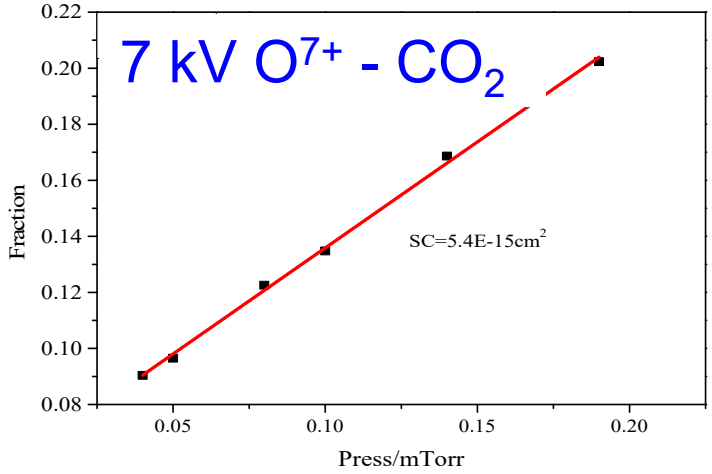
7 kV O^{5+} - CO_2

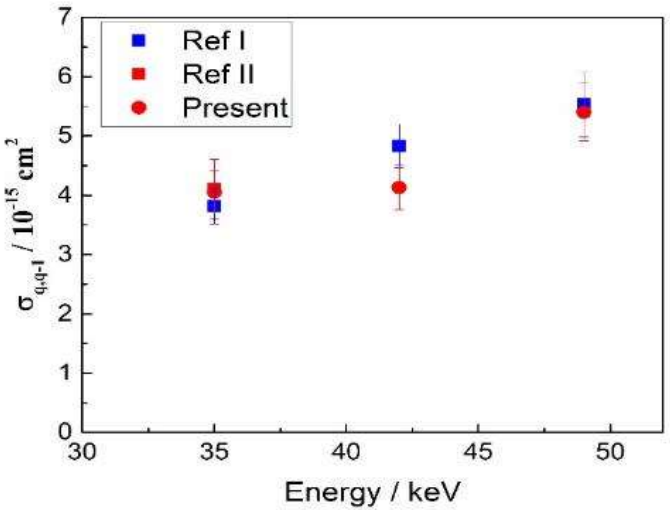


7 kV O^{6+} - CO_2



7 kV O^{7+} - CO_2

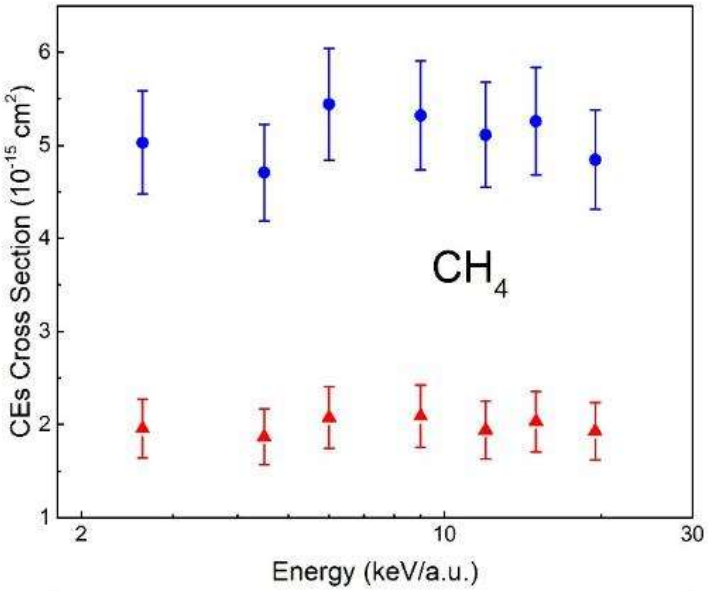


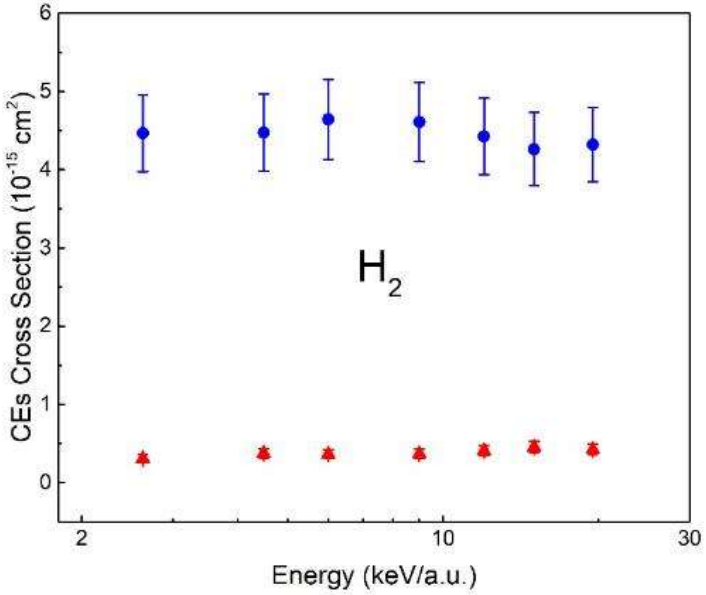


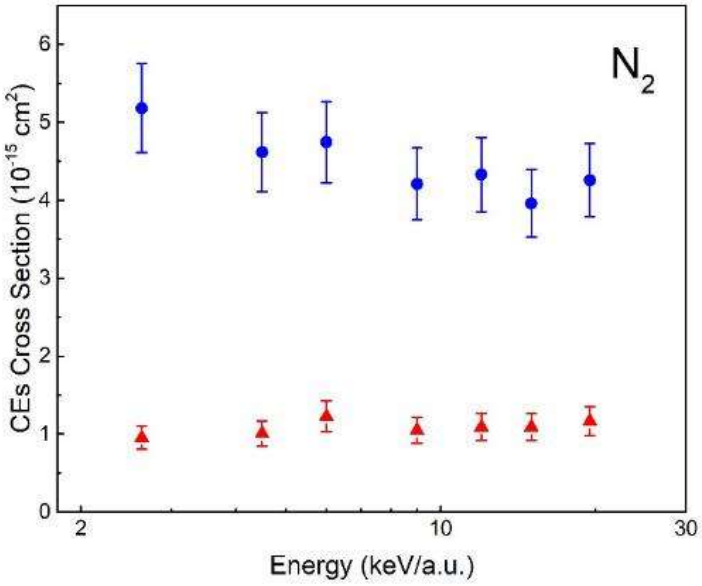
Ref I, PRA-75-032704, Ref II, PRA-63-062707

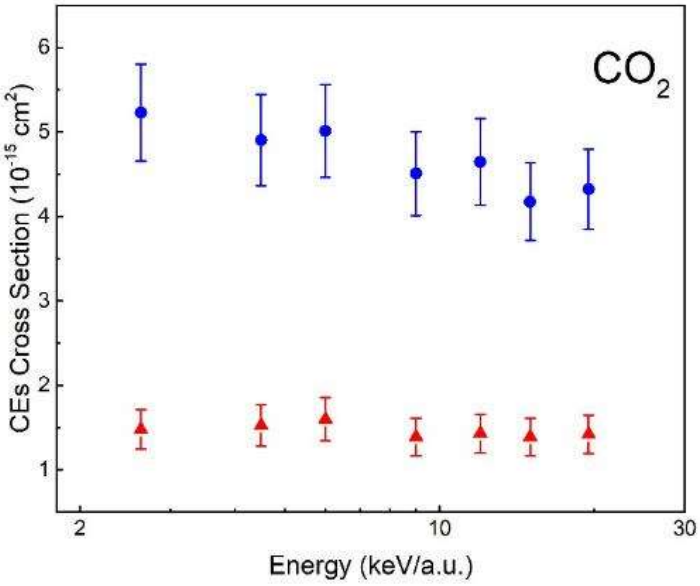
Absolute Cross Section

Single and Double EC Cross Section for O^{6+}.









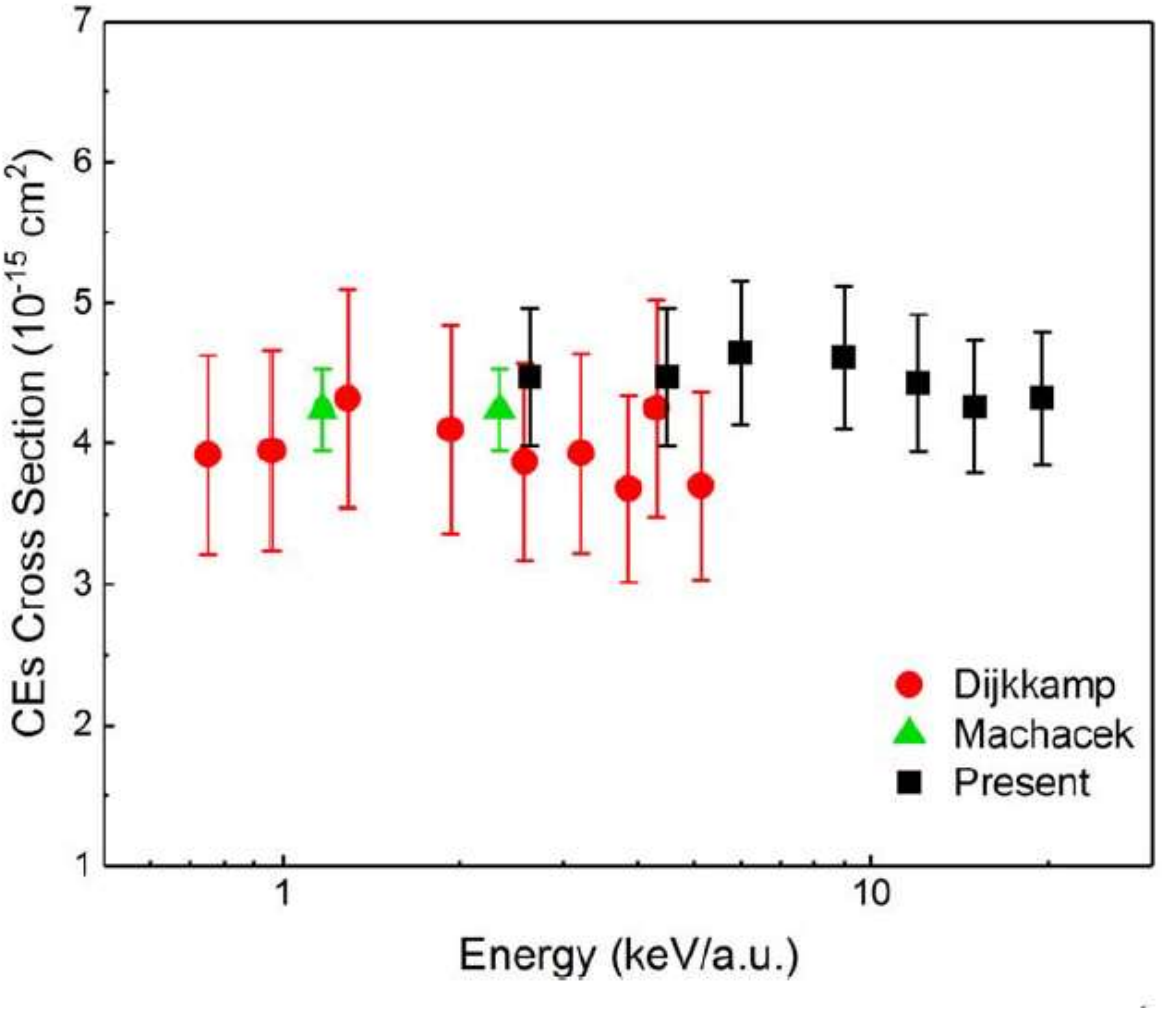
Absolute Cross Section

Single and Double EC Cross Section for O^{6+}.

keV/u	process	Target			
		CO_2	CH_4	H_2	N_2
2.63	$\sigma_{q,q-1}$	5.23 ± 0.58	5.03 ± 0.55	4.47 ± 0.49	5.18 ± 0.57
	$\sigma_{q,q-2}$	1.48 ± 0.24	1.96 ± 0.31	0.31 ± 0.05	0.95 ± 0.15
4.50	$\sigma_{q,q-1}$	4.90 ± 0.54	4.71 ± 0.52	4.47 ± 0.49	4.62 ± 0.51
	$\sigma_{q,q-2}$	1.53 ± 0.24	1.87 ± 0.30	0.38 ± 0.06	1.01 ± 0.16
6.00	$\sigma_{q,q-1}$	5.01 ± 0.55	5.44 ± 0.60	4.64 ± 0.51	4.74 ± 0.52
	$\sigma_{q,q-2}$	1.60 ± 0.26	2.07 ± 0.33	0.36 ± 0.06	1.23 ± 0.20
9.00	$\sigma_{q,q-1}$	4.51 ± 0.50	5.32 ± 0.59	4.61 ± 0.51	4.21 ± 0.46
	$\sigma_{q,q-2}$	1.39 ± 0.22	2.09 ± 0.33	0.37 ± 0.06	1.05 ± 0.17
12.0	$\sigma_{q,q-1}$	4.65 ± 0.51	5.11 ± 0.56	4.43 ± 0.49	4.33 ± 0.48
	$\sigma_{q,q-2}$	1.43 ± 0.23	1.94 ± 0.31	0.41 ± 0.07	1.09 ± 0.17
15.0	$\sigma_{q,q-1}$	4.18 ± 0.46	5.26 ± 0.58	4.26 ± 0.47	3.96 ± 0.44
	$\sigma_{q,q-2}$	1.39 ± 0.22	2.03 ± 0.33	0.45 ± 0.07	1.09 ± 0.17
19.5	$\sigma_{q,q-1}$	4.32 ± 0.48	4.84 ± 0.53	4.32 ± 0.48	4.26 ± 0.47
	$\sigma_{q,q-2}$	1.42 ± 0.23	1.93 ± 0.31	0.42 ± 0.07	1.17 ± 0.19

Absolute Cross Section

Single Electron Capture Cross Section of O^{6+} - H_2



Astrophys. J. Supp. Series (2021) 253:6

Absolute Cross Section

Table 1. Individual and total experimental uncertainties

Source of error	**Error at the 1σ confidence level (%)**
Error in Temperature	
Temperature difference between air chamber and pressure gauge	1
Temperature fluctuation	0.1
Error in Pressure	
Accuracy of pressure gauge	0.25
Pressure fluctuation	3
Error in collision cell length	6.6
Error in count of CEM	
Uncertainty of detection efficiency	8
Effect of background vacuum	2
Data statistics	2
Total error	11.2

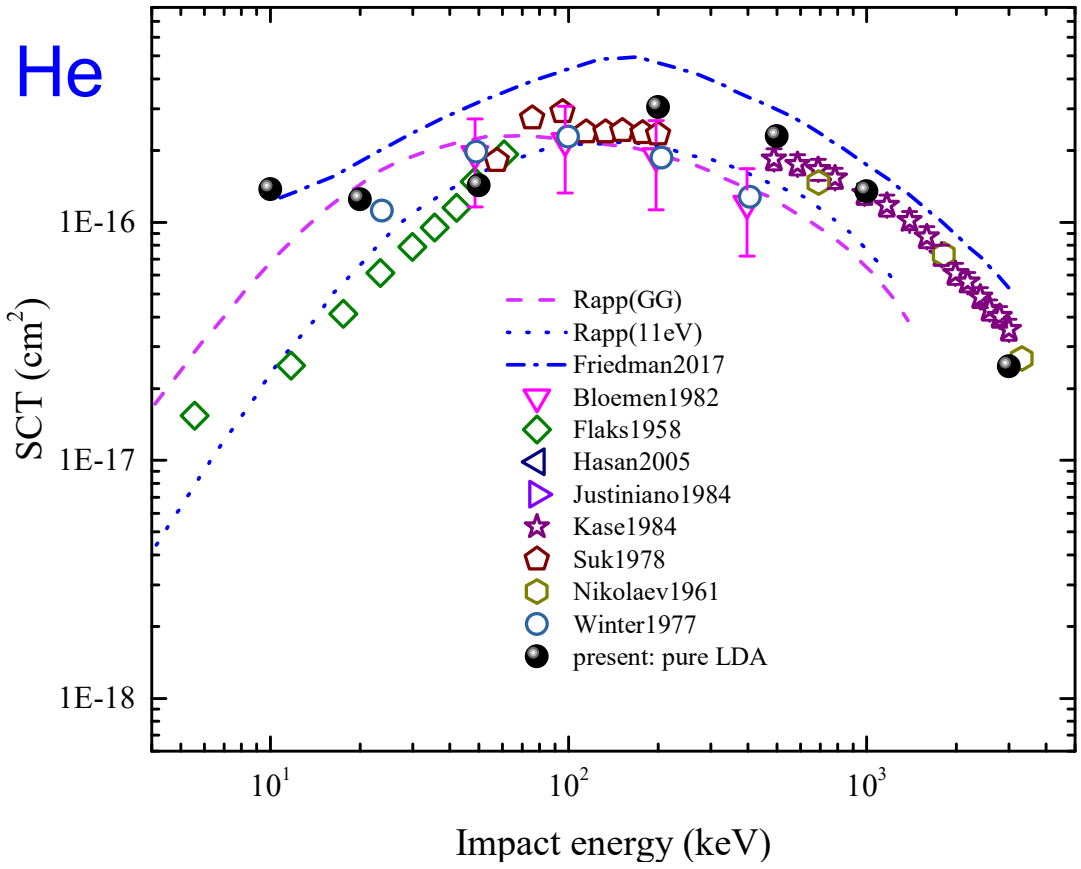
Astrophys. J. Supp. Series (2021) 253:6

Absolute Cross Section

Simulation: time-dependent DFT coupling with MD

Many-electron systems with large spacial scale

Ne^{2+} - He



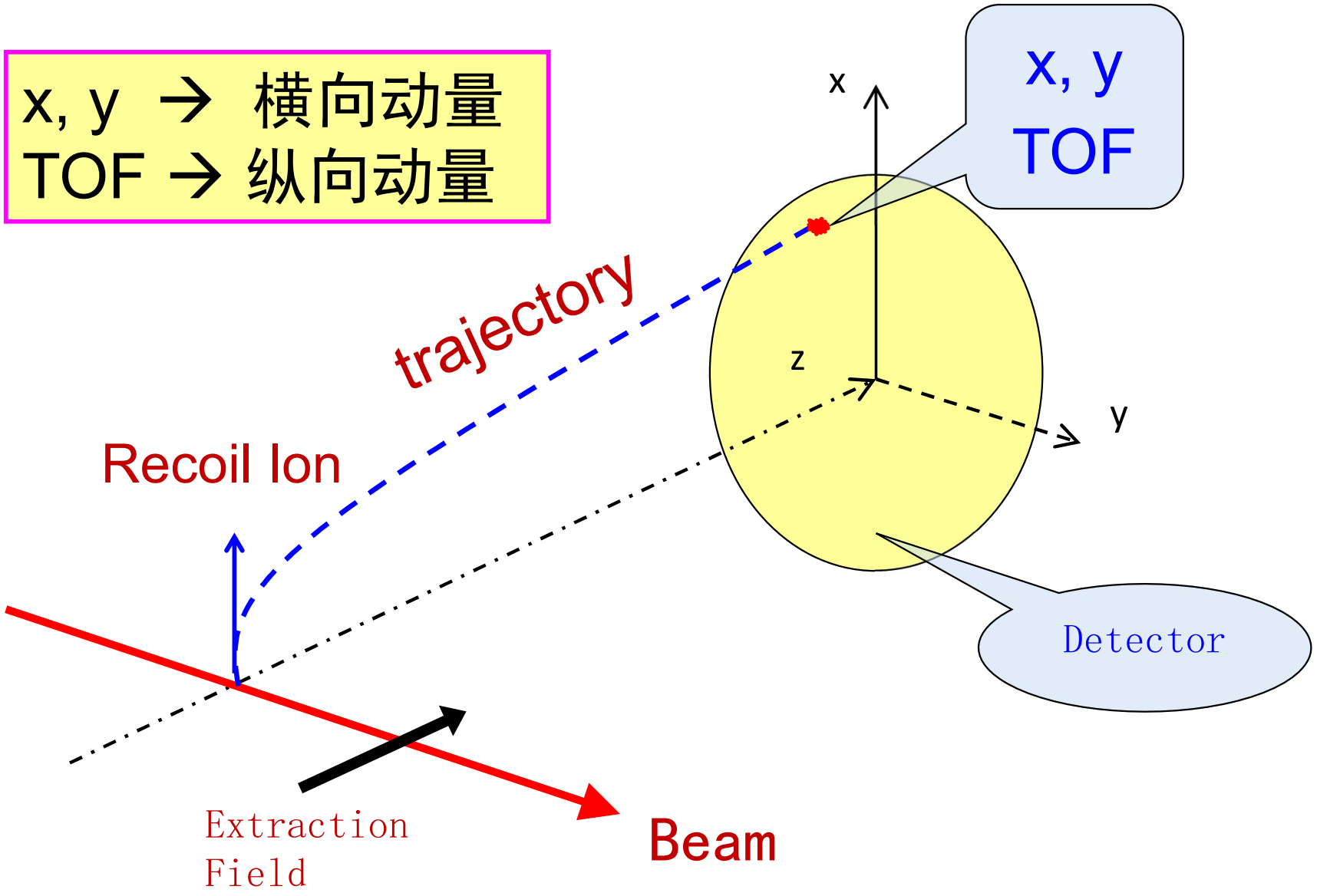
Phys. Rev. A **97**, 032706 (2018)

Phys. Rev. A **103** 032816 (2021)

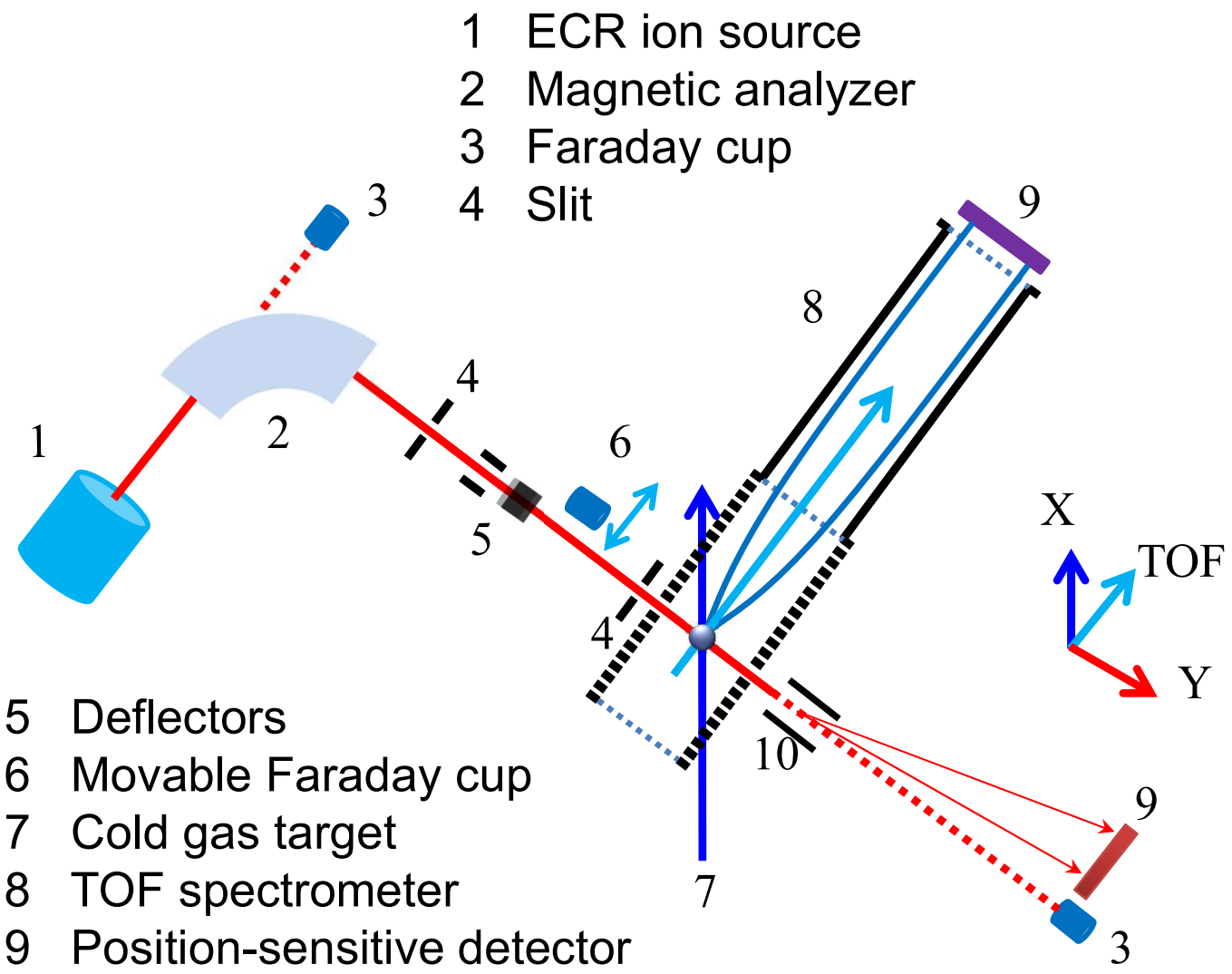
03 Experiment on COLTRIMS

COLTRIMS

x, y → 横向动量
TOF → 纵向动量



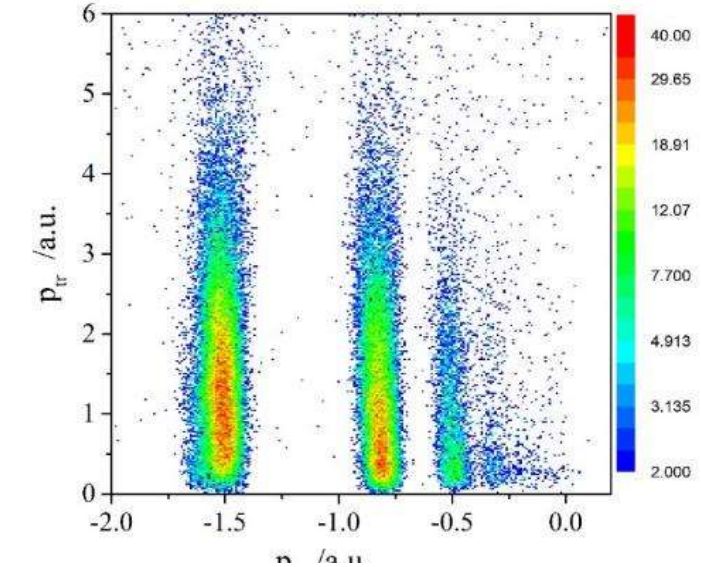
COLTRIMS

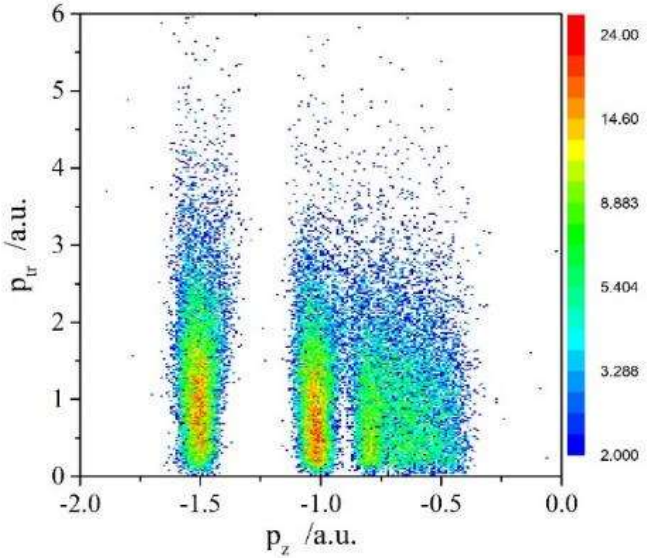


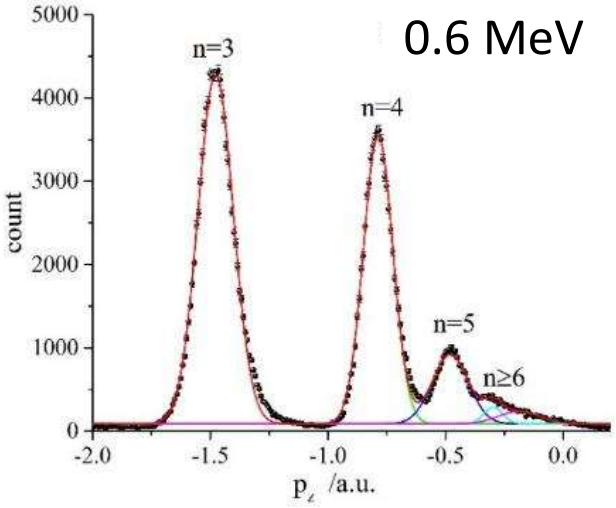
Y. Zhang *et al*, PRA (2018)

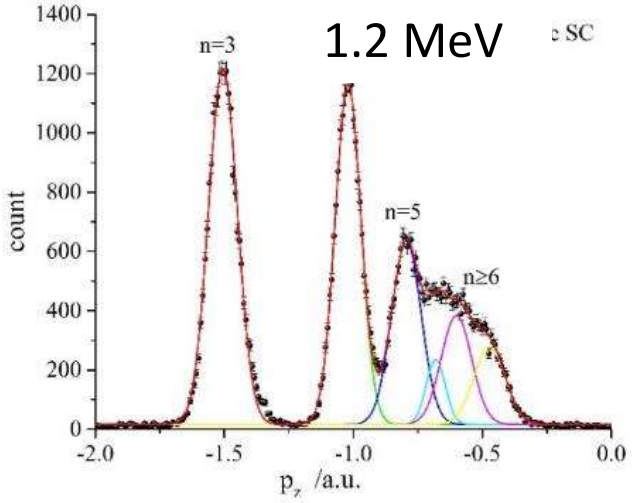
State-resolved measurements

$O^{6+}(1s^2)+He \rightarrow O^{5+}(1s^2\,nl)+He^{+}(1s)$



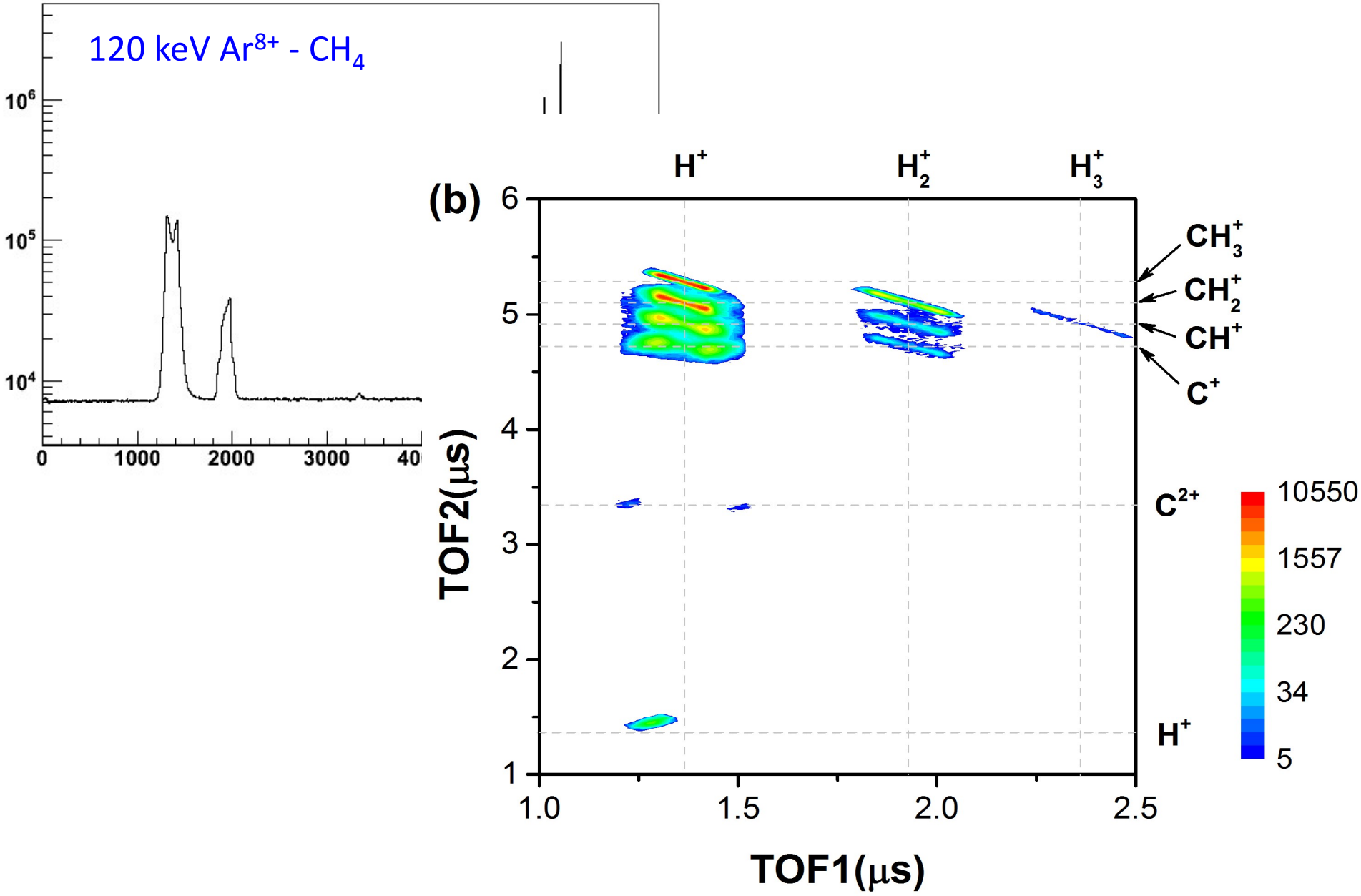






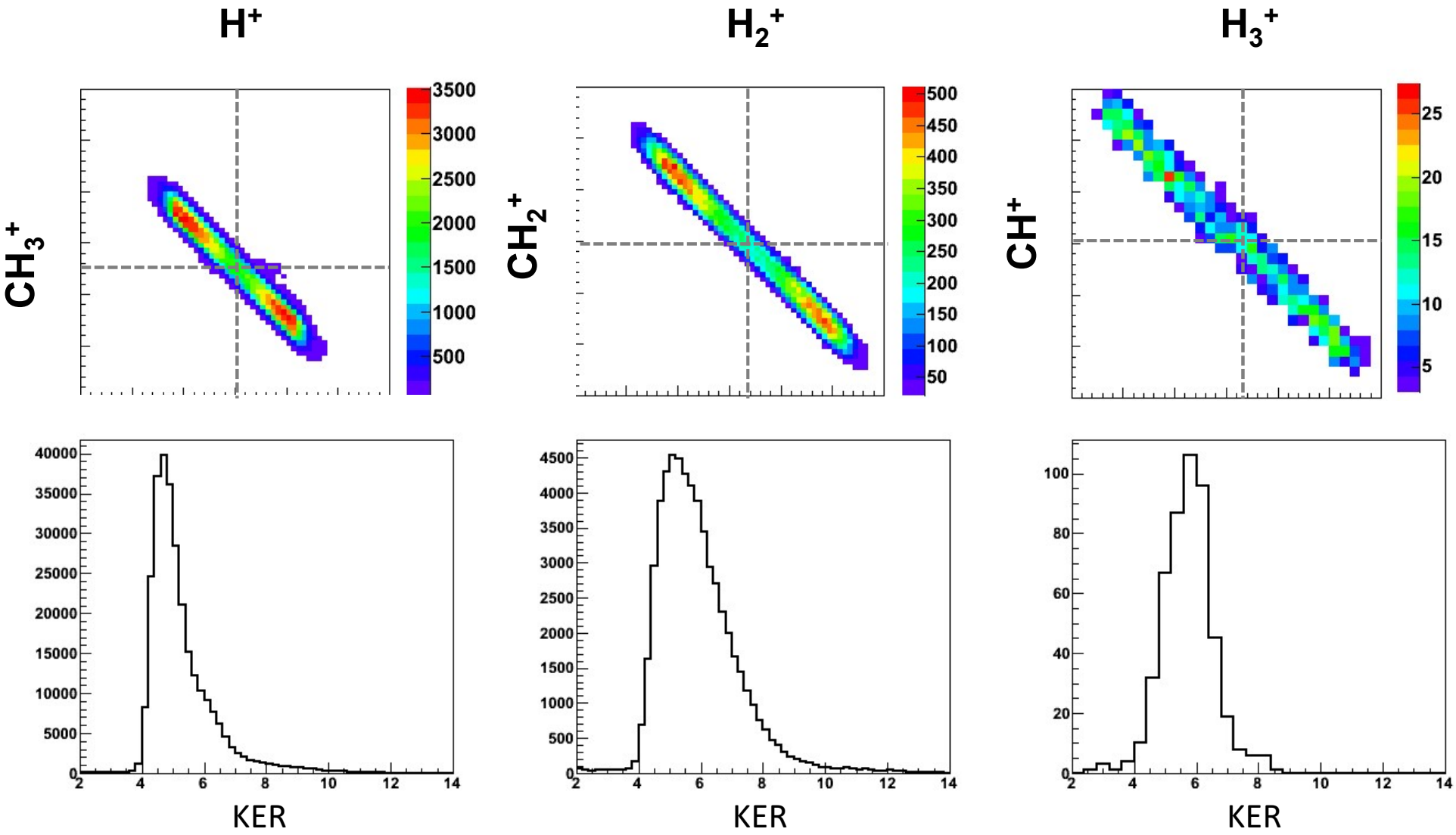
From Dr. Yong Gao and Dr. Shuncheng Yan

Coincidence TOF map



KER spectra

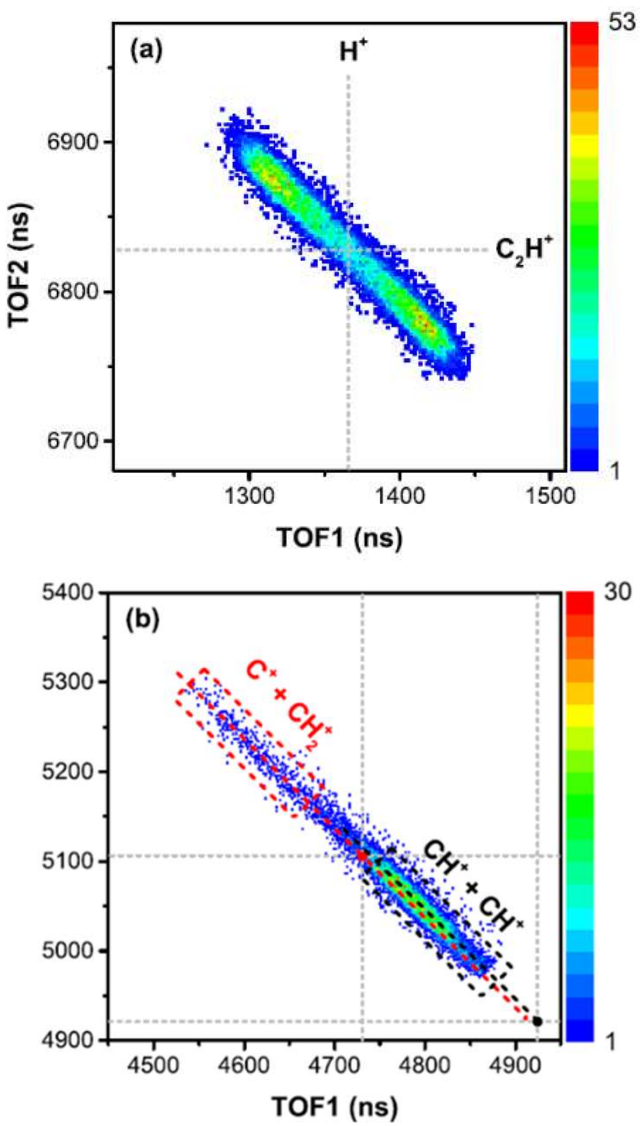
120 keV Ar^{8+} - CH_4

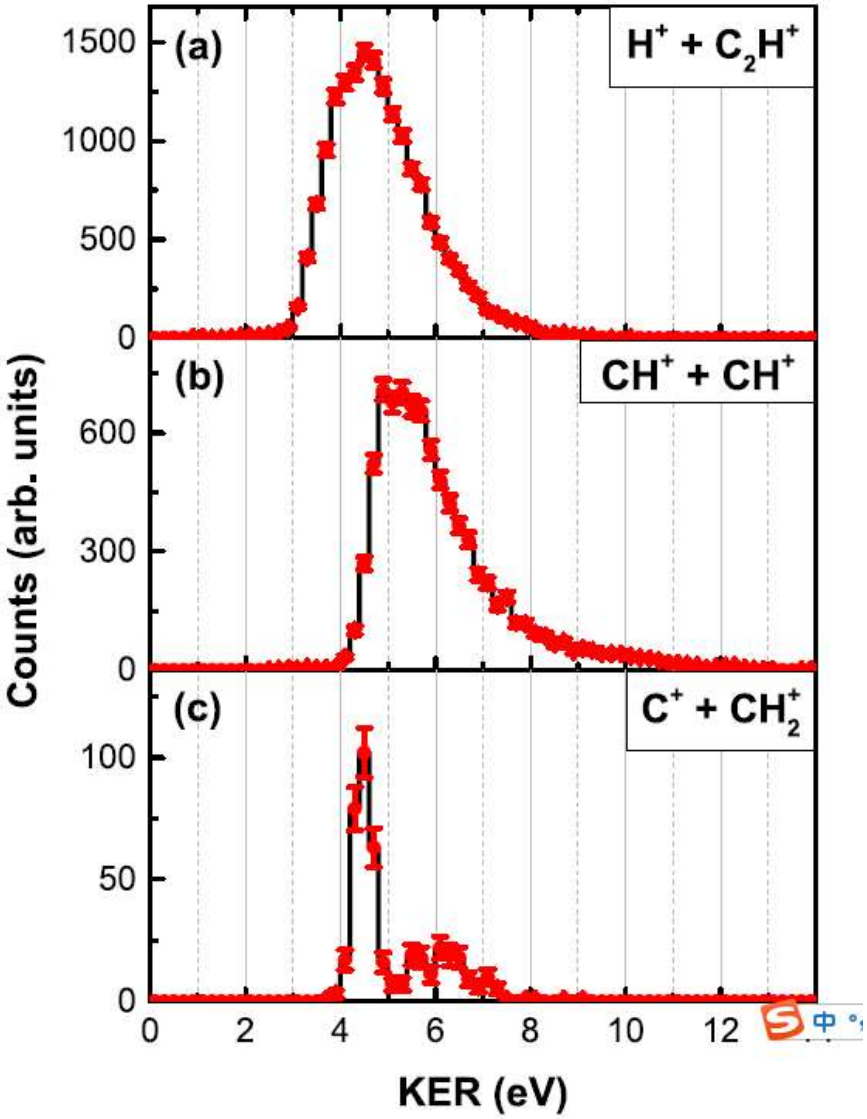


Y. Zhang *et al*, JCP **150**, 204303 (2019)

KER spectra

120 keV Ar^{8+} - CH_4

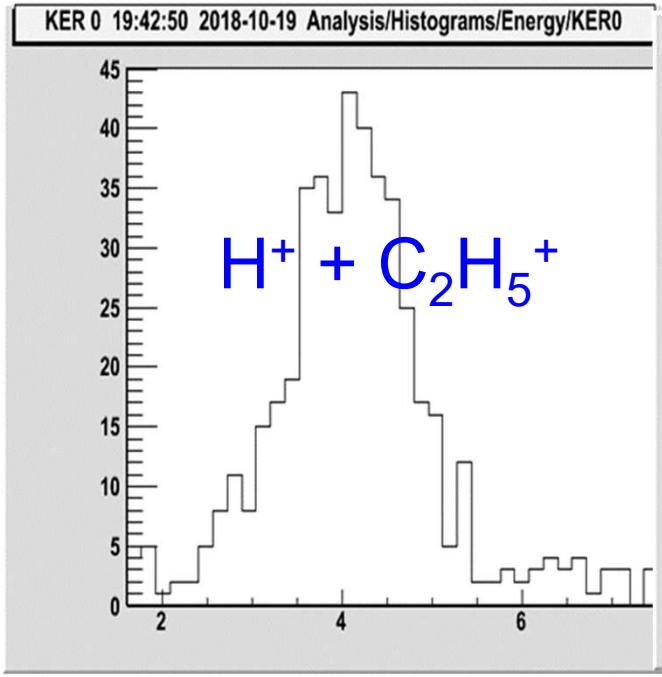


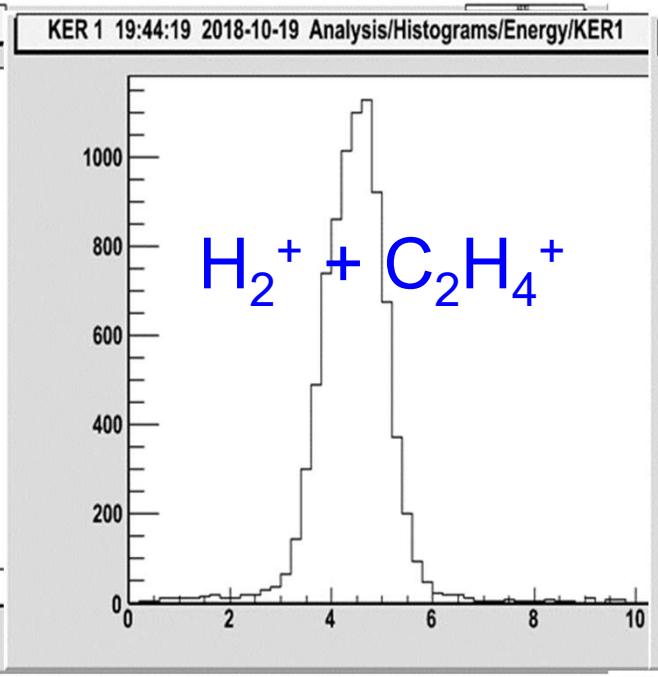


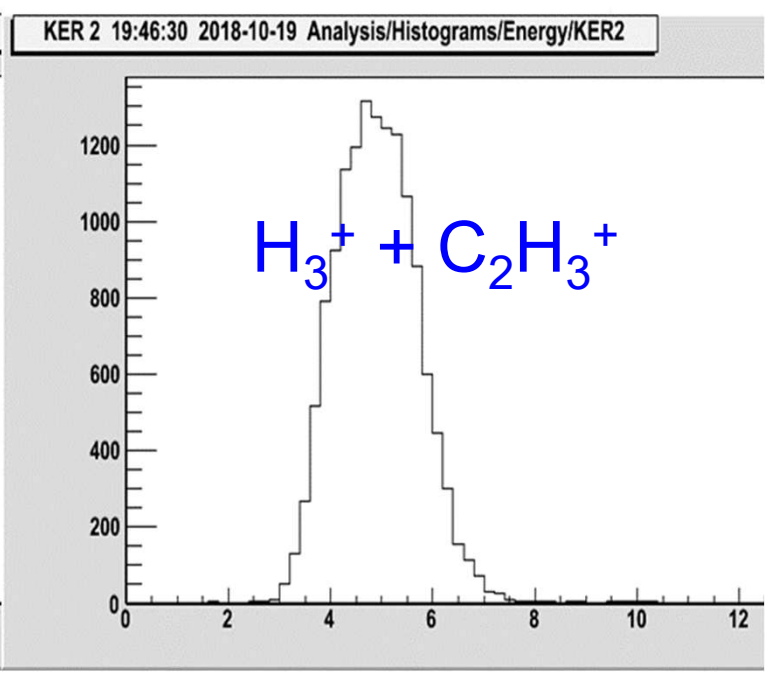
Y. Zhang *et al*, JCP **150**, 204303 (2019)

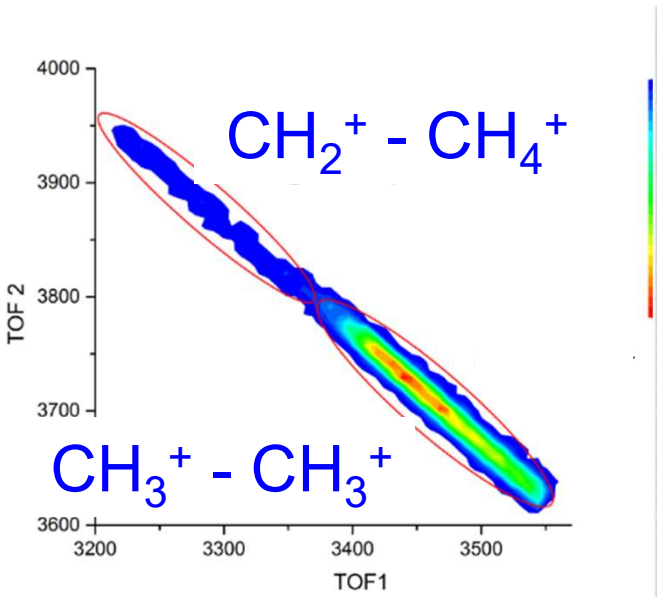
KER spectra

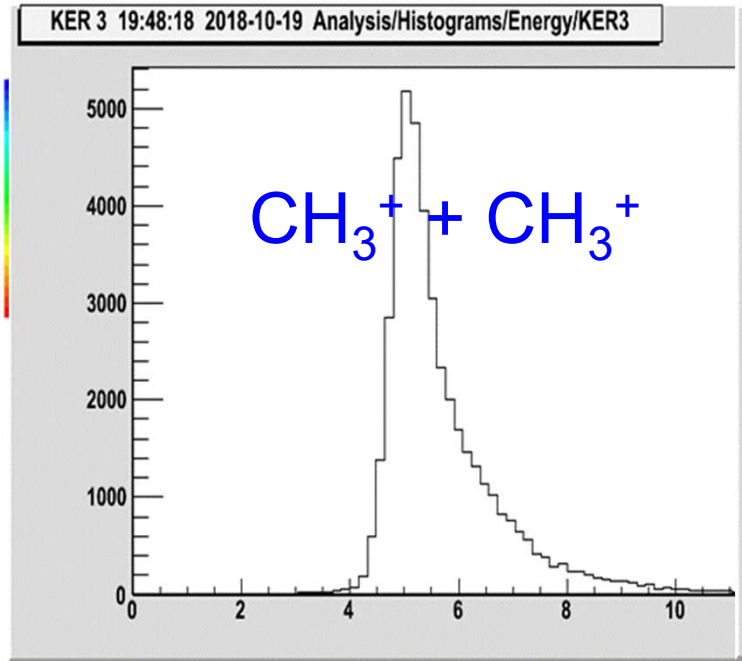
120 keV Ar^{8+} - C_2H_6

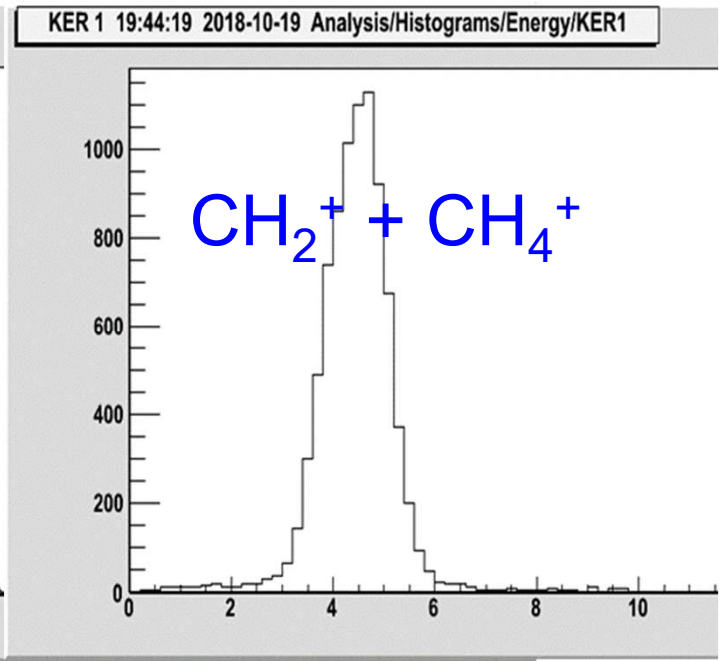




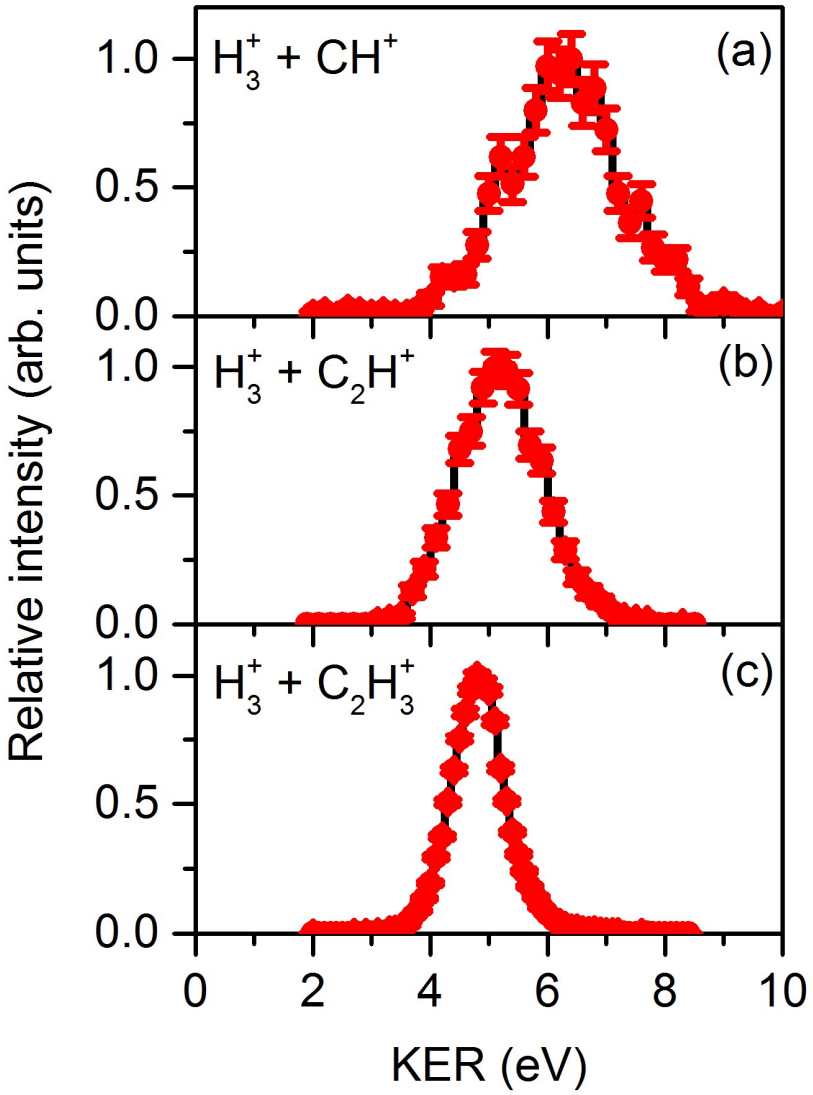








KER spectra



The matching mean KERs in the present collisions tend to be larger than those obtained in intense laser fields.

KER is a good observable or not, when contrasted with field-free theoretical predictions?

Channel	Average KER (eV)		
	300 eV e^-	3 keV/u Ar^{8+}	Intense laser field
$H_3^+ + CH^+$	6.4	6.2	5.4
$H_3^+ + C_2H^+$	5.2	5.1	5.0
$H_3^+ + C_2H_3^+$	4.8	4.9	4.6, 4.0, ~4.3

K. Hoshina *et al*, JCP **134**, 064324 (2011)
R. Kanya *et al*, JCP **136**, 204309 (2012)

Reaction path

- **Gaussian16 program**

✓ density functional theory (DFT)

✓ B3LYP/aug-cc-pVTZ basis set

- **Reverse activation barrier**

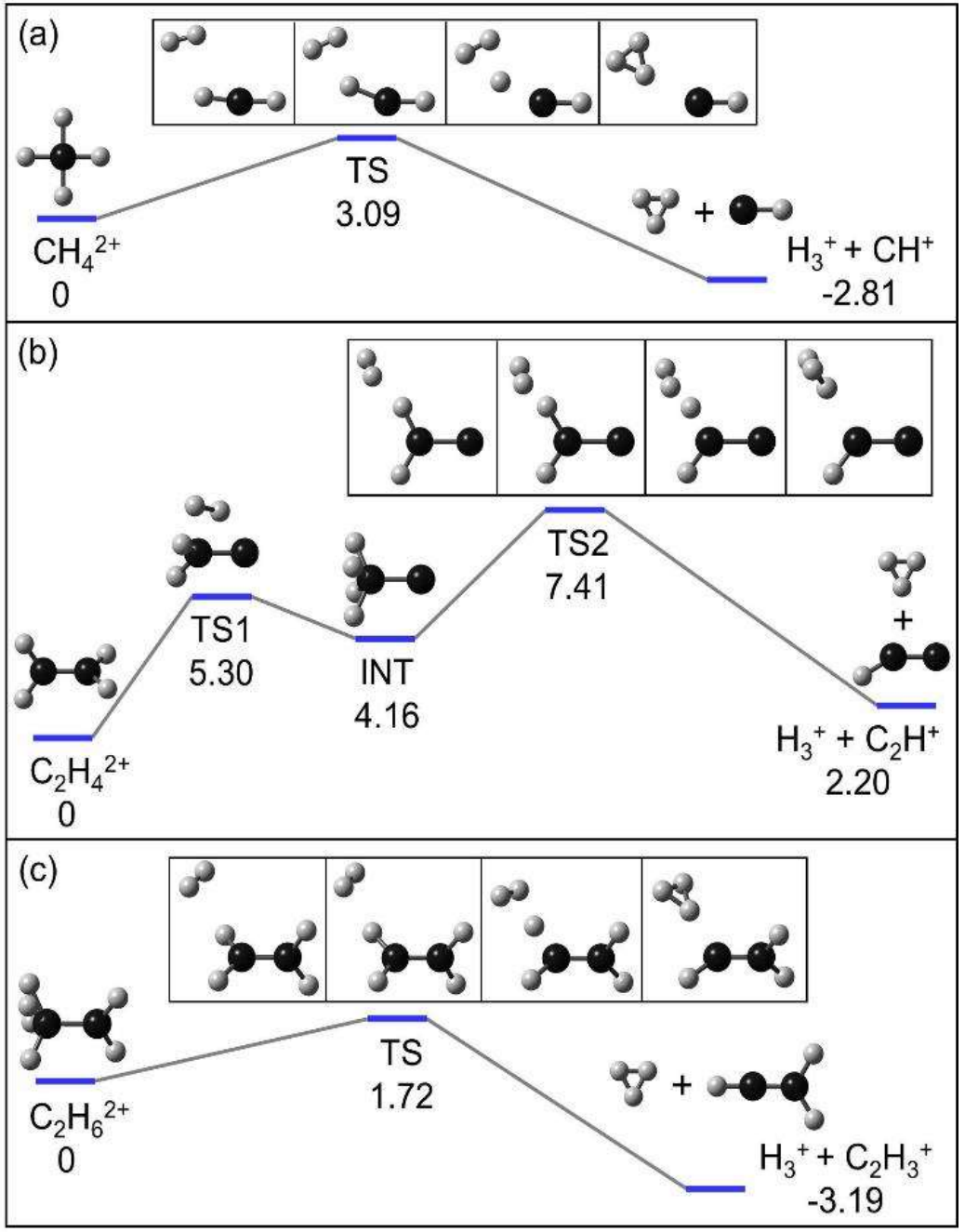
✓ Substantial structural rearrangement

- **Loosely bound transition state**

✓ $[C_xH_{y-2}]^{2+}...H_2$

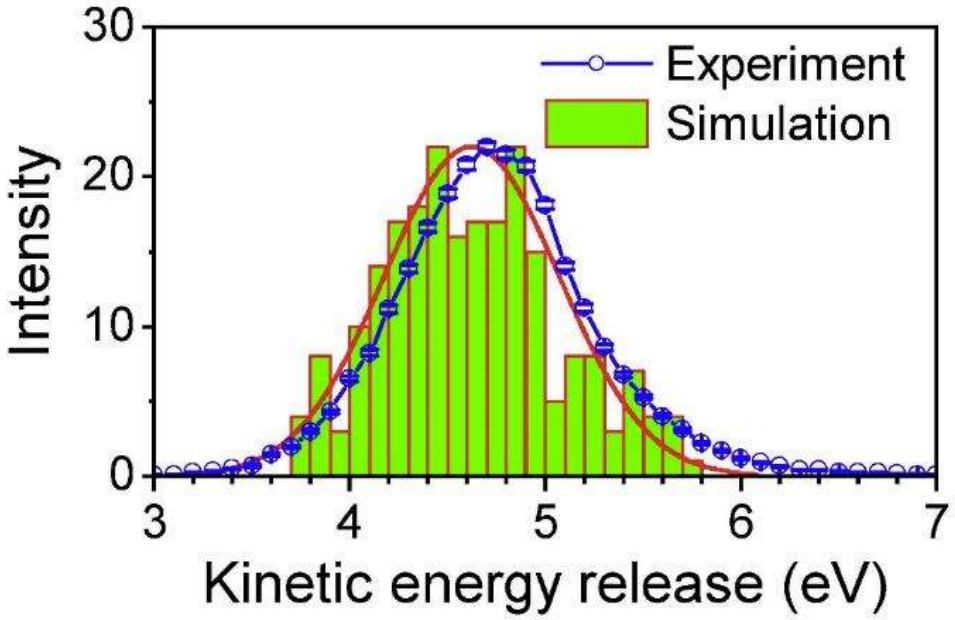
Channel	H_2 moiety	
	Charge	Bond length
$H_3^+ + CH^+$	+0.39 e	0.84 Å
$H_3^+ + C_2H^+$	+0.34 e	0.79 Å
$H_3^+ + C_2H_3^+$	+0.19 e	0.78 Å

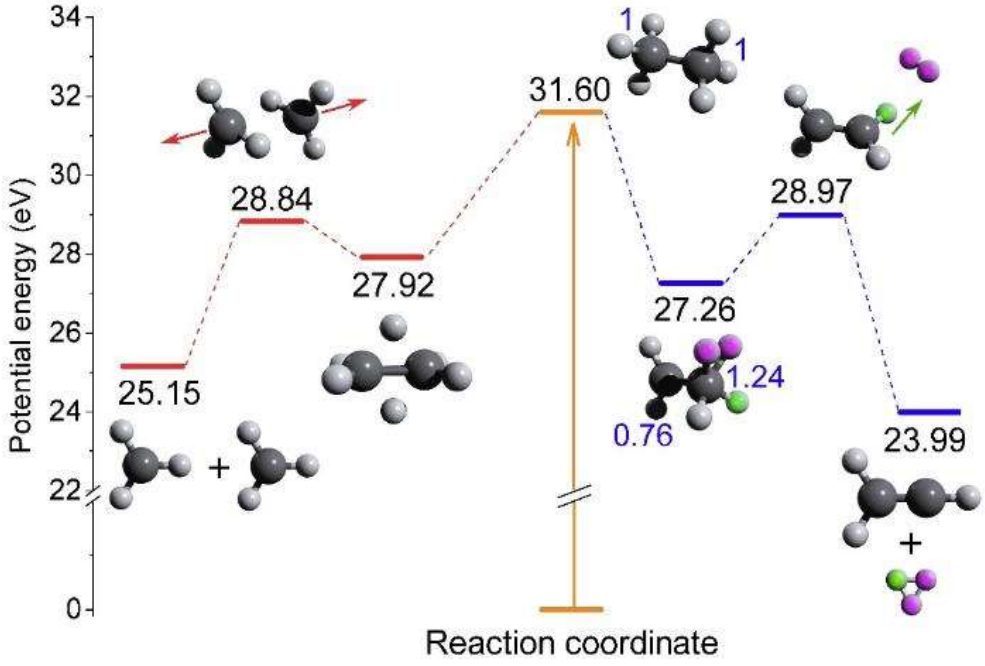
PRA 100, 052706 (2019)



Reaction path

1. Initial conditions: Zero point vibration
2. Simulation: Ab initio molecular dynamics (AIMD), using the Atom-Centered Density Matrix Propagation (ADMP) method B3LYP/cc-pvdz





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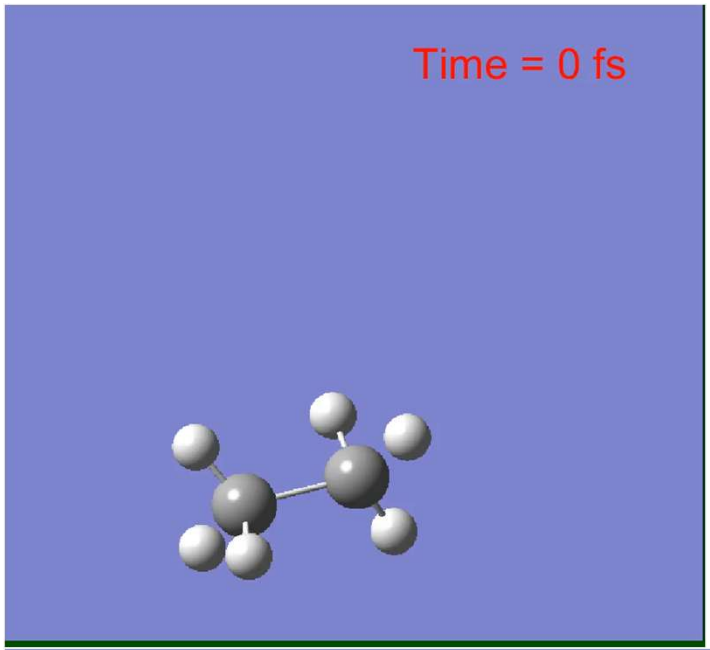
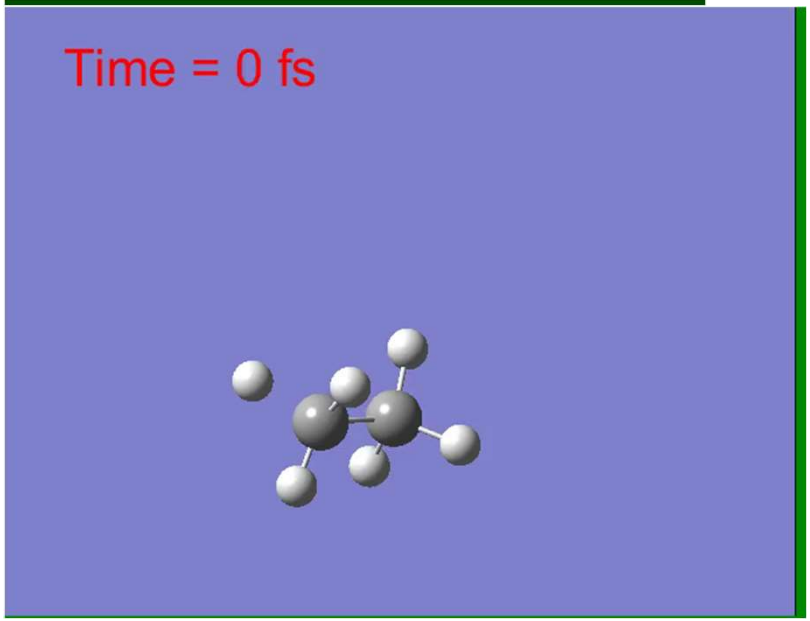
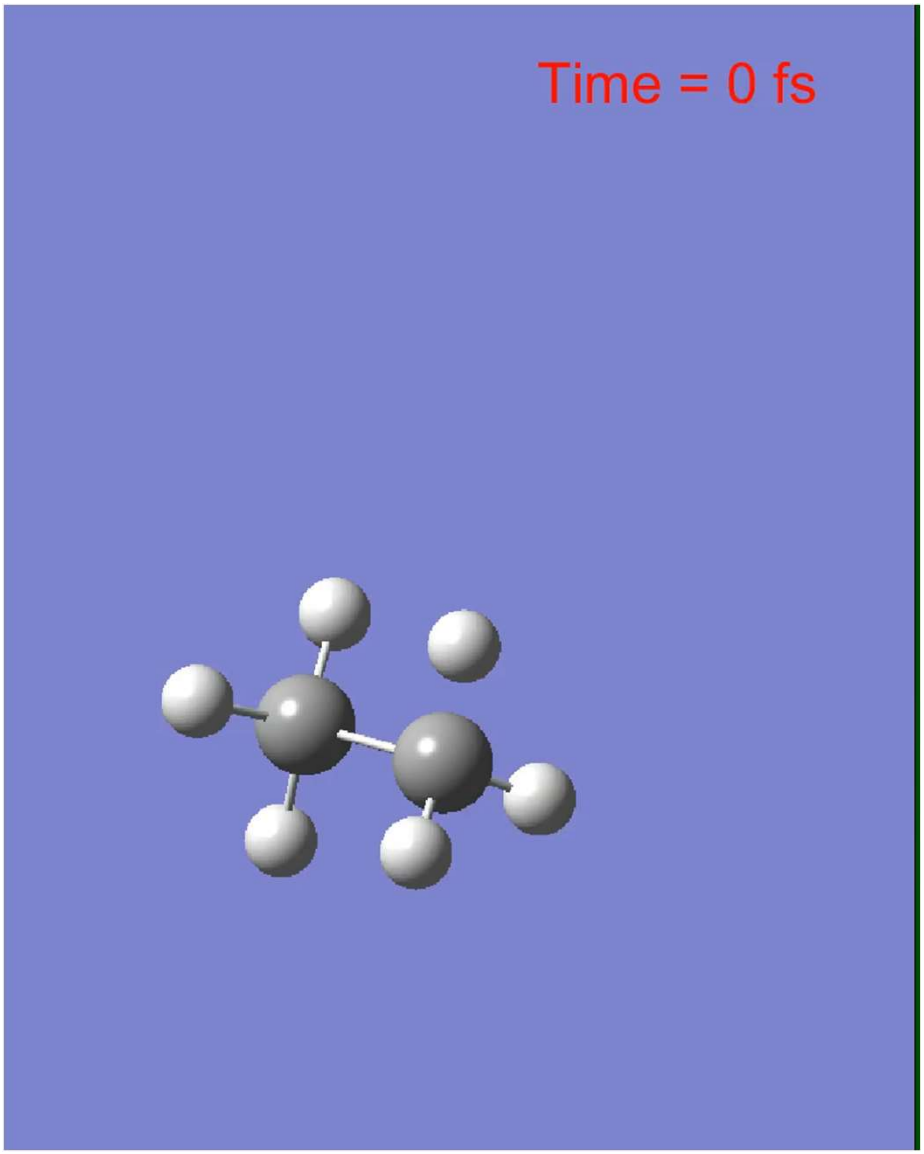
Reaction path







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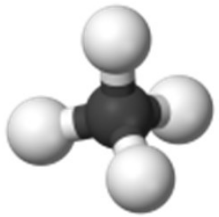
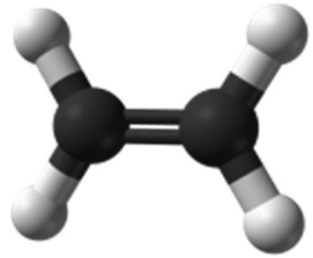
Proton migration channels



$H_3^+ + CH^+$

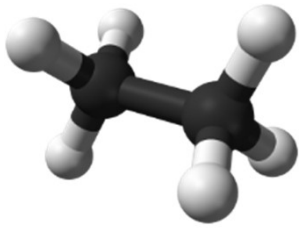
$C^+ + CH_2^+$

Y. Zhang *et al*, JCP (2019)



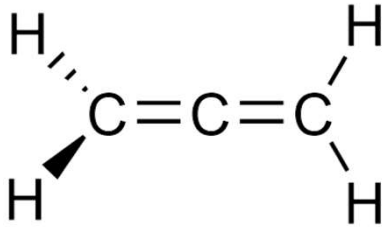
$H_3^+ + C_2H^+$

$CH^+ + CH_3^+$



$H_3^+ + C_2H_3^+$

$CH_2^+ + CH_4^+$



$H_3^+ + C_3H^+$

$CH^+ + C_2H_3^+$

$CH_3^+ + C_2H^+$

04 Summary

Summary

- The absolute EC cross section for O^{6+} interaction with atom and molecule has been measured.
- The charge-transfer cross sections for the Ne^{2+} - He collision has been calculated by the molecular dynamics with time-dependent density-functional theory.
- We have studied the fragmentation of Hydrocarbon molecule induced by HCI and electrons.