Investigation of electron capture in swift C^{4+} (1s2s ^3S) ion collisions with gas targets using a zero-degree Auger projectile spectroscopy apparatus built within the L45 beam line at the "Demokritos" 5.5 MV tandem accelerator

Ph.D. Thesis Defense
by

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NCSR "Demokritos", Institute of Nuclear and Particle Physics

Advisory Committee: **T. J. M. Zouros (Professor, University of Crete)**
E. P. Benis (Assistant Professor, University of Ioannina)
S. Harissopulos (Director of Research, INPP Demokritos)

Investigation of Single Electron Capture (SEC) in fast (MeV/u) ion – atom collision systems

$$C^{4+}(1s2s\ ^3S) + He \xrightarrow{SEC} C^{3+}(1s2s2p\ ^4P,\ ^2P_{\pm}) + He^{+}$$

$$R_m = \frac{\sigma_m(^4P)}{\sigma_m(^2P_+) + \sigma_m(^2P_-)}$$

- Spin statistics validation – Applications in Plasma Physics
- Difficulties in direct spectra interpretation
- Most recent interpretations unclear with conflicting results

Presentation Outline

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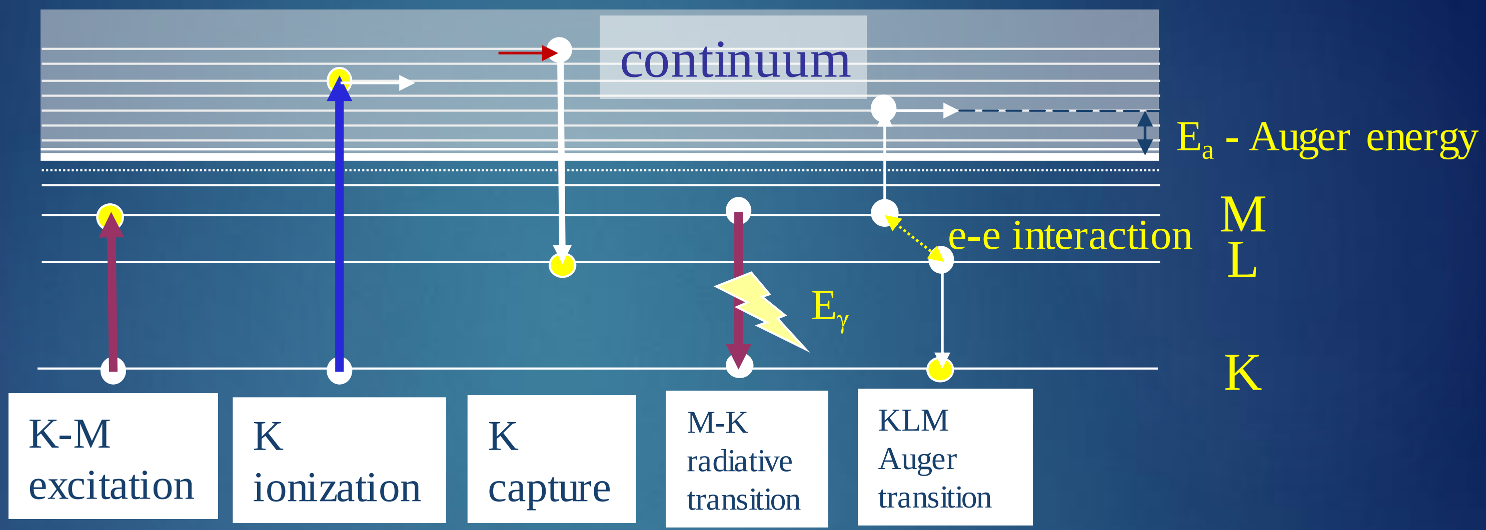
ΔΗΜΟΚΡΙΤΟΣ

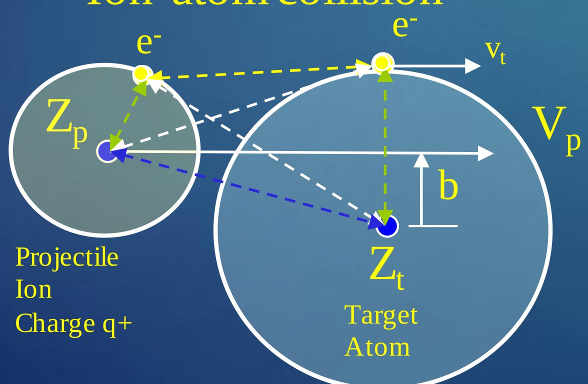
Introduction to Ion-Atom collisions and Auger projectile spectroscopy

Fundamental Processes

Atomic Energy levels



Ion-atom collision

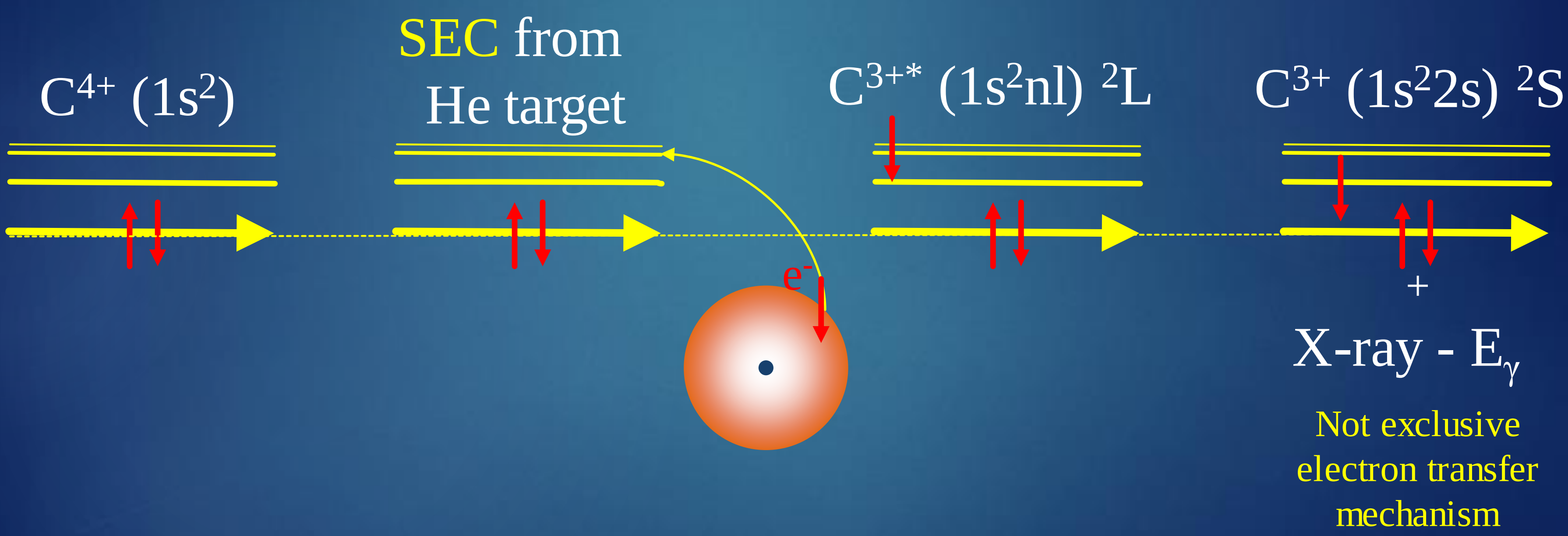


Atomic Structure: q, Z_p, Z_t, E_x, E_a…
Collision Dynamics: b, V_p, v_t …

Projectile spectroscopy: Few-electrons - simpler environment for testing theories

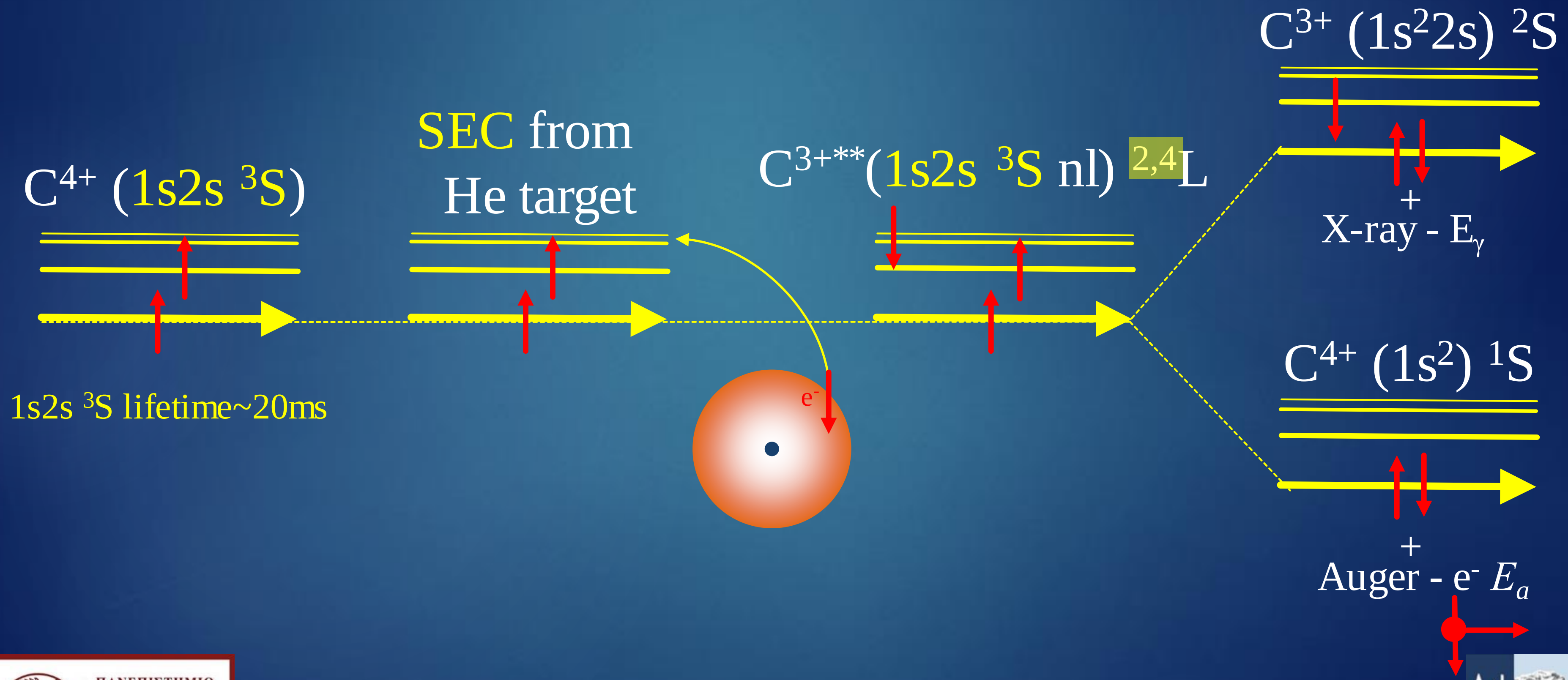
Introduction to Ion-Atom collisions and Auger projectile spectroscopy

Single Electron Capture to $1s^2$ ground state ions (~80% of He-like mixed beam)



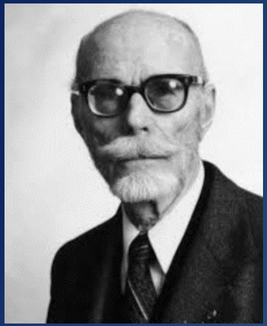
Introduction to Ion-Atom collisions and Auger projectile spectroscopy

Single Electron Capture to open-shell, 1s2s ^3S ions (~20% of He-like mixed beam)

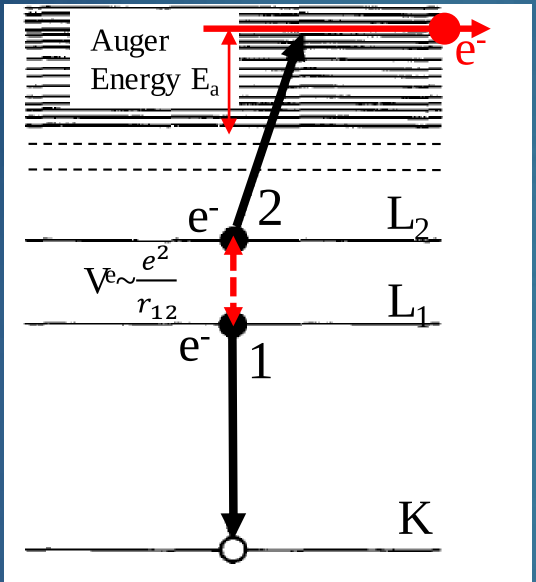


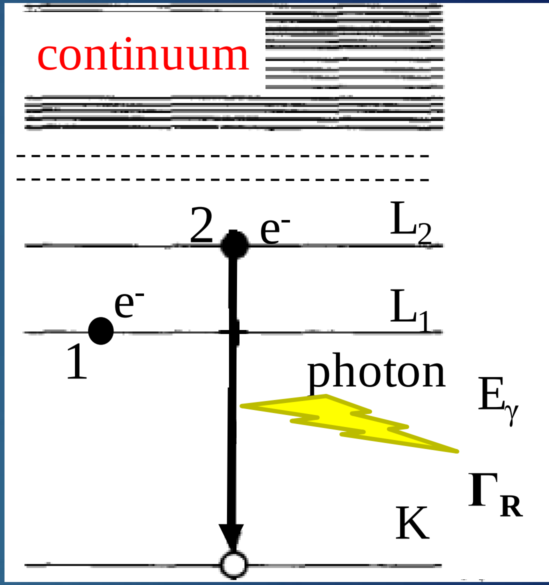
Introduction to Ion-Atom collisions and Auger projectile spectroscopy

Auger effect/spectroscopy



Pierre Auger
1899-1993





$E_a = B_K - B_{L1} - B_{L2}$

$E_\gamma = B_K - B_L = \hbar\omega$

$\Gamma_A \sim \left| \left\langle f \left| \frac{e^2}{r_{12}} \right| i \right\rangle \right|^2$ - no Z dep.

$\Gamma_R \sim \omega^3 |\langle K|\boldsymbol{r}|L\rangle|^2 \sim Z^4$

Competitive channels, but for low-Z ions,
Auger spectroscopy preferred - Efficiency

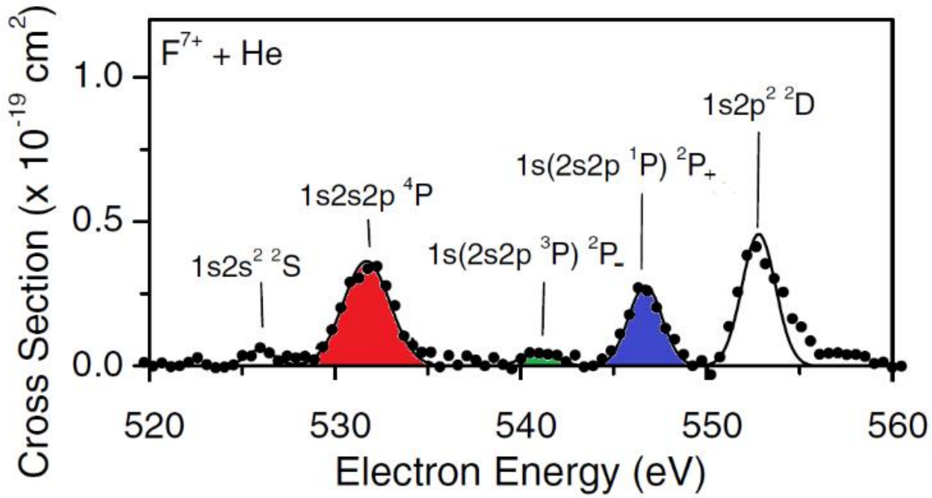
Motivation

Problem: Discrepancy between data and theory

VOLUME 92, NUMBER 13 PHYSICAL REVIEW LETTERS week ending 2 APRIL 2004

Evidence for Pauli Exchange Leading to Excited-State Enhancement in Electron Transfer

J. A. Tanis,[1] A. L. Landers,[1] D. J. Pole,[1] A. S. Alnaser,[1] S. Hossain,[1] and T. Kirchner[2]



$R_m = \frac{{}^4P}{{}^2P_- + {}^2P_+}$ of same configuration

Spin statistics

Experiment:2.9

Spin Statistics:1 (Revised to “2” in the frozen core approximation)

Pauli Exchange Interaction

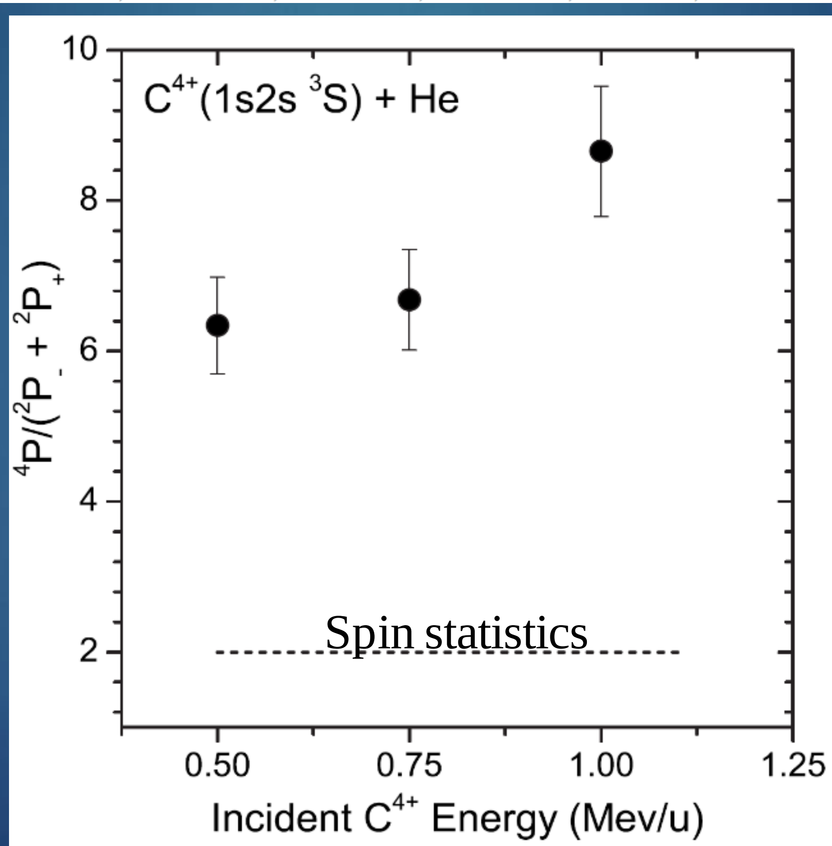
Motivation

Problem: Discrepancy between data and theory

PHYSICAL REVIEW A **77**, 022706 (2008)

Nonstatistical enhancement of the 1*s*2*s*2*p* ^4P state in electron transfer in 0.5–1.0-MeV/u $C^{4,5+}$ + He and Ne collisions

D. Strohschein,[1] D. Röhrbein,[2] T. Kirchner,[2] S. Fritzsche,[3,4] J. Baran,[1] and J. A. Tanis[1]



Huge discrepancy
Even larger than F^{7+} results

Motivation

Problem: Discrepancy between data and theory

PHYSICAL REVIEW A **77**, 022706 (2008)

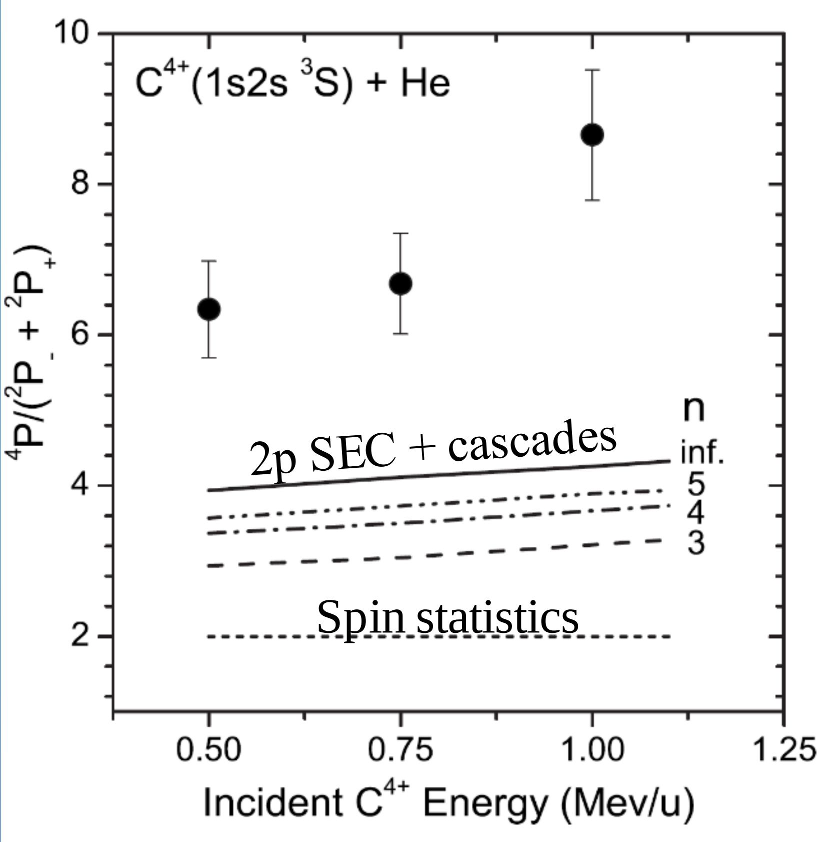
Nonstatistical enhancement of the $1s2s2p\ ^4P$ state in electron transfer in 0.5–1.0-MeV/u $C^{4,5+}$ + He and Ne collisions

D. Strohschein,[1] D. Röhrbein,[2] T. Kirchner,[2] S. Fritzsche,[3,4] J. Baran,[1] and J. A. Tanis[1]

PHYSICAL REVIEW A **77**, 050701(R) (2008)

Selective enhancement of $1s2s2p\ ^4P_J$ metastable states populated by cascades in single-electron transfer collisions of $F^{7+}(1s^2/1s2s\ ^3S)$ ions with He and H_2 targets

T. J. M. Zouros,[1,2] B. Sulik,[3] L. Gulyás,[3] and K. Tőkési[3]



Not even cascades could close the gap

PHYSICAL REVIEW A **81**, 042701 (2010)

Role of cascade and Auger effects in the enhanced population of the $C^{3+}(1s2s2p\ ^4P)$ states following single-electron capture in $C^{4+}(1s2s\ ^3S)$-He collisions

D. Röhrbein*
Institut für Theoretische Physik, Technische Universität Clausthal, D-38678 Clausthal-Zellerfeld, Germany
T. Kirchner†
Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, Canada
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GSI Helmholtzzentrum für Schwerionenforschung, D-64291 Darmstadt, Germany and Department of Physics, Post Office Box 3000, University of Oulu, FIN-90014 Oulu, Finland

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1s2l2l´ states: Production and Properties

Strong 1s2s2p ^{4}P cascade feeding

PHYSICAL REVIEW A **77**, 050701(R) (2008)

Selective enhancement of $1s2s2p\ ^4P_J$ metastable states populated by cascades in single-electron transfer collisions of $F^{7+}(1s^2/1s2s\ ^3S)$ ions with He and H_2 targets

T. J. M. Zouros,[1,2] B. Sulik,[3] L. Gulyás,[3] and K. Tőkési[3]
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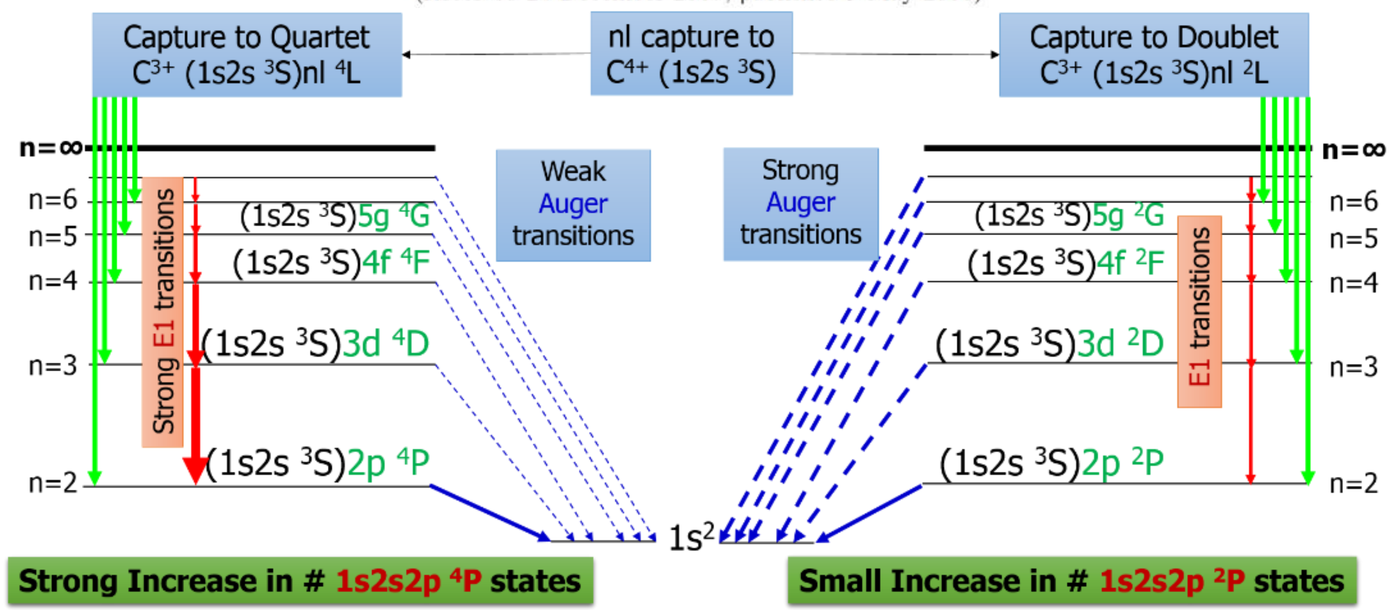
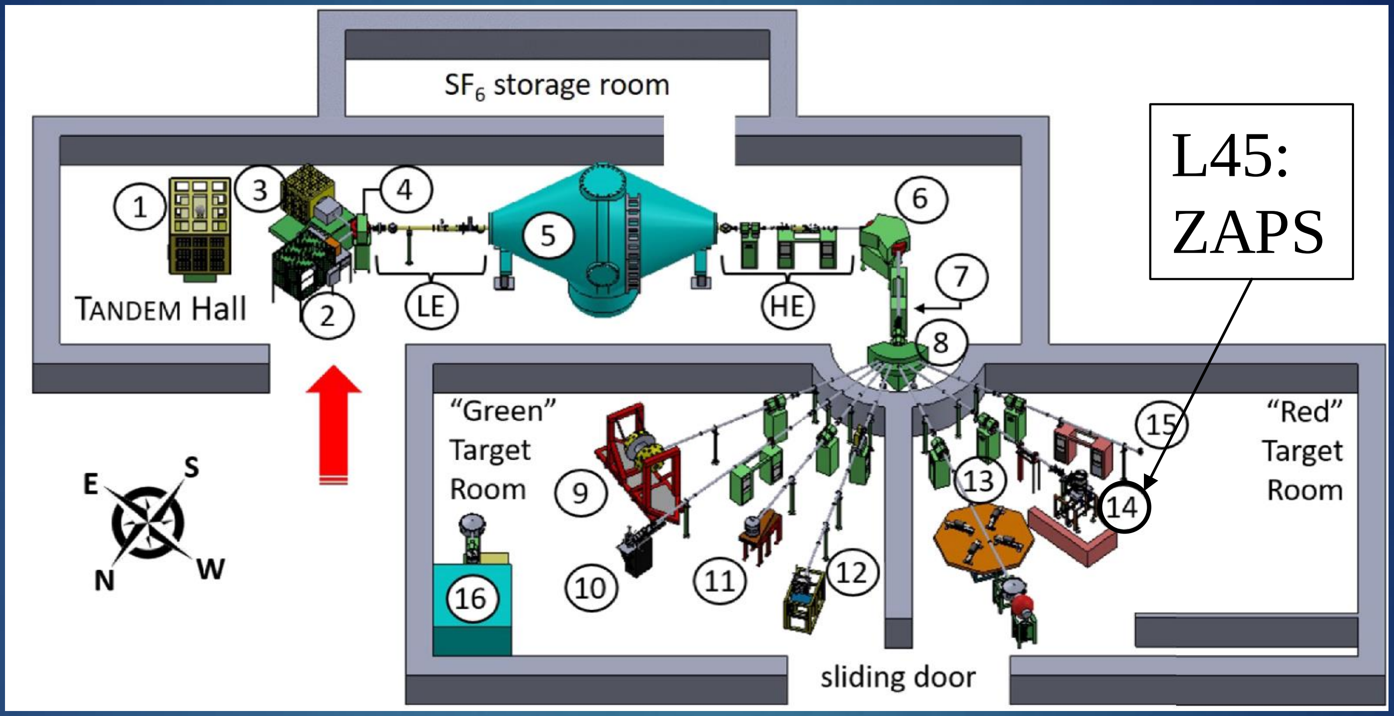
(Received 24 December 2007; published 9 May 2008)



The L45 beam line at the INPP

Building the new atomic physics beam line



- INPP Tandem - The only heavy-ion accelerator in Greece
- ZAPS: Zero-degree Auger Projectile Spectroscopy

The L45 beam line at the INPP

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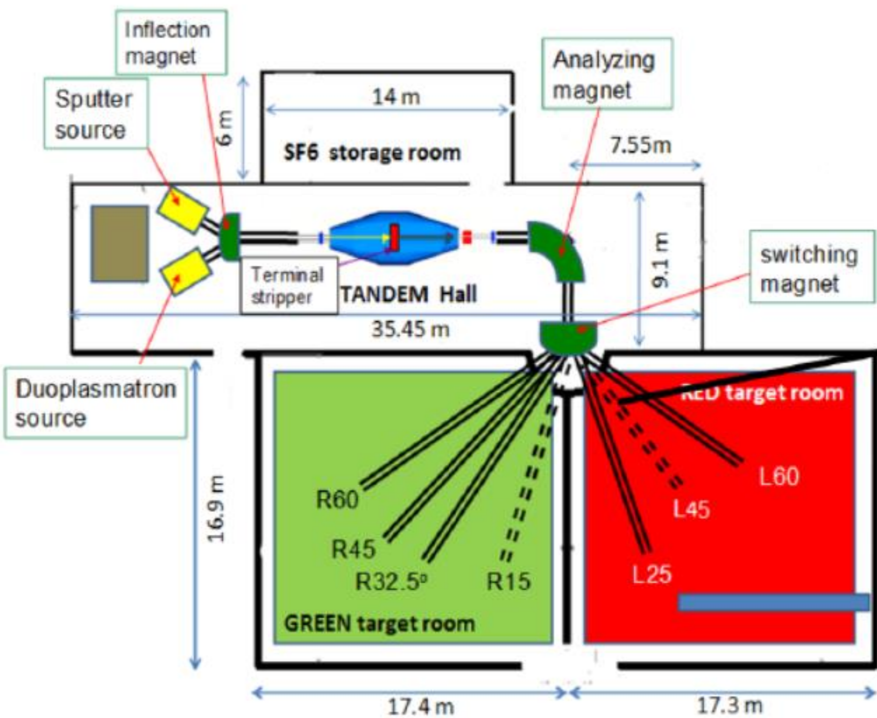
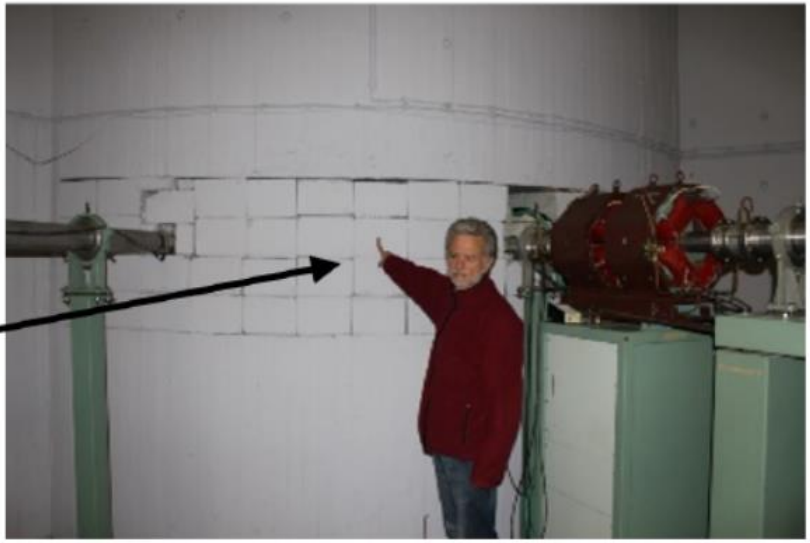


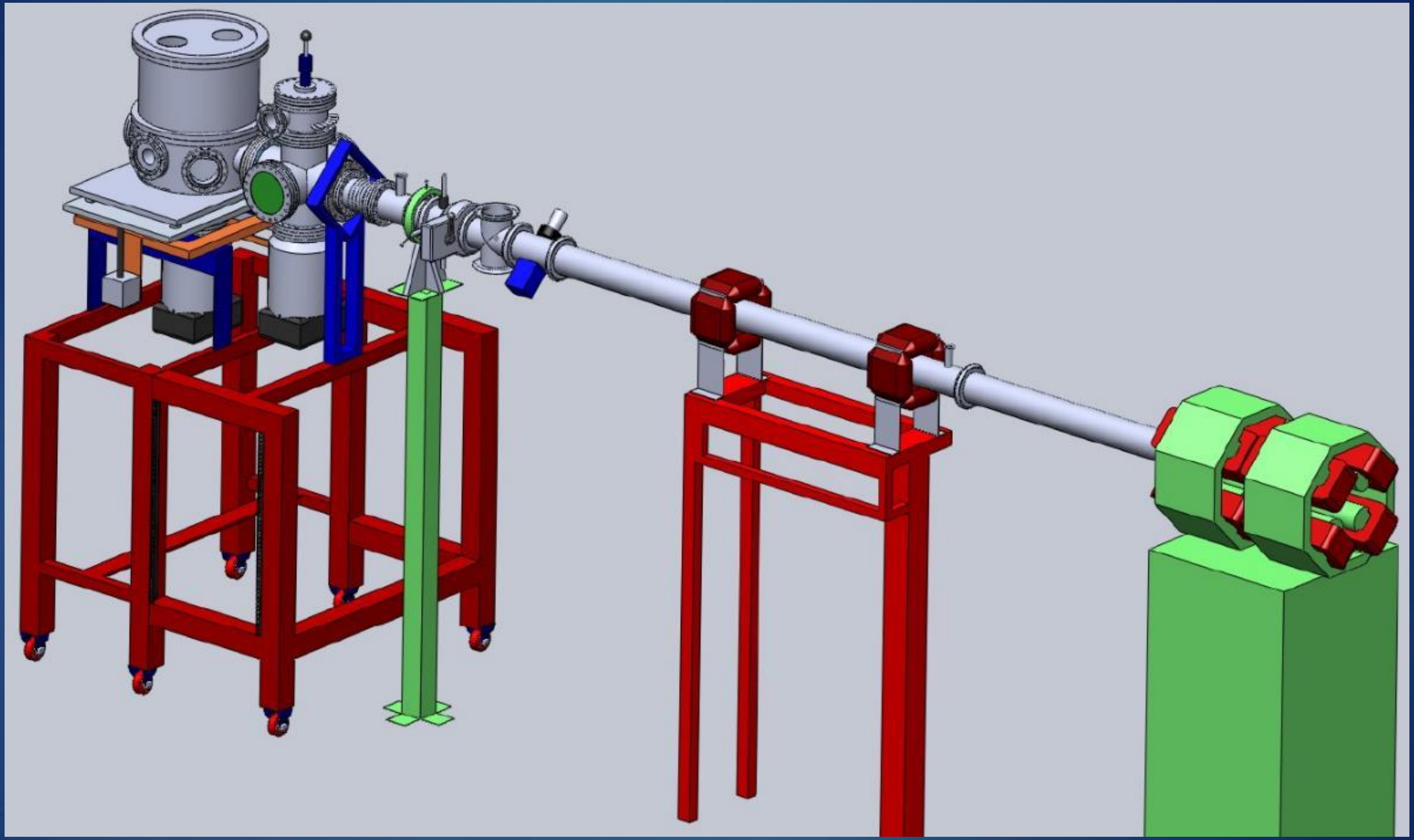


November
2012

Historic photo – Before building the new beam line of the Atomic Physics with Accelerators: Projectile Electron Spectroscopy (APAPES) project

The L45 beam line at the INPP

Building the new atomic physics beam line



SolidWorks original design

The L45 beam line at the INPP
Building the new atomic physics beam line

Doubly differentially pumped gas cell chamber
10^{-7} Torr attainable with 10 mTorr loaded gas cell

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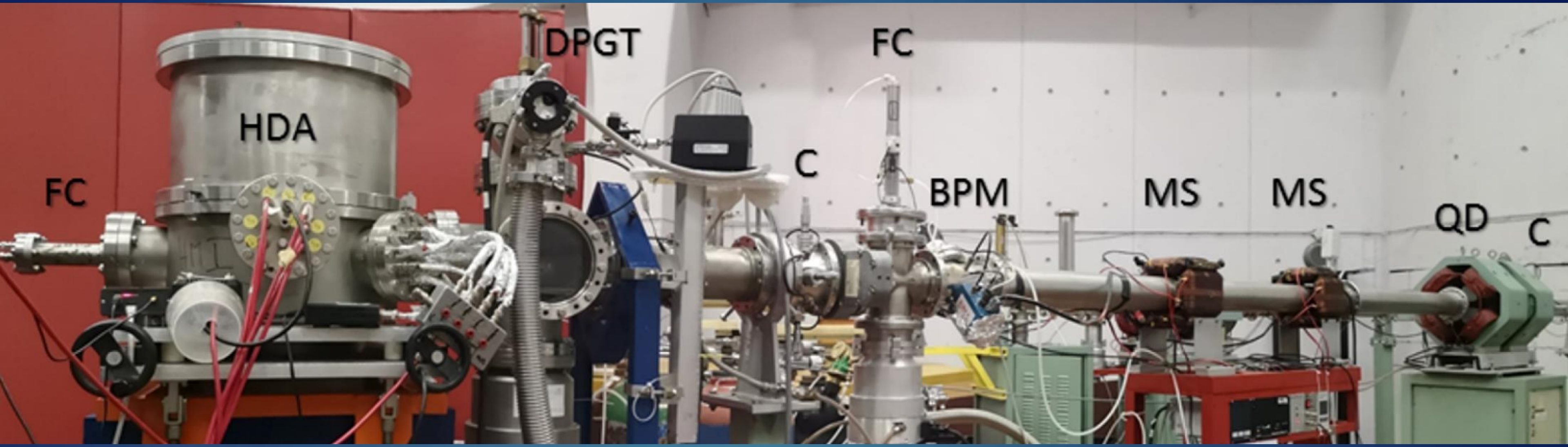
The L45 beam line at the INPP

Building the new beam line



C: Collimator
QD: QuaDrupole
MS: Magnetic Steerer
BPM: Beam Profile Monitor
FC: Faraday Cup
DPGT: Differentially Pumped Gas Target
HDA: Hemispherical Deflector Analyzer

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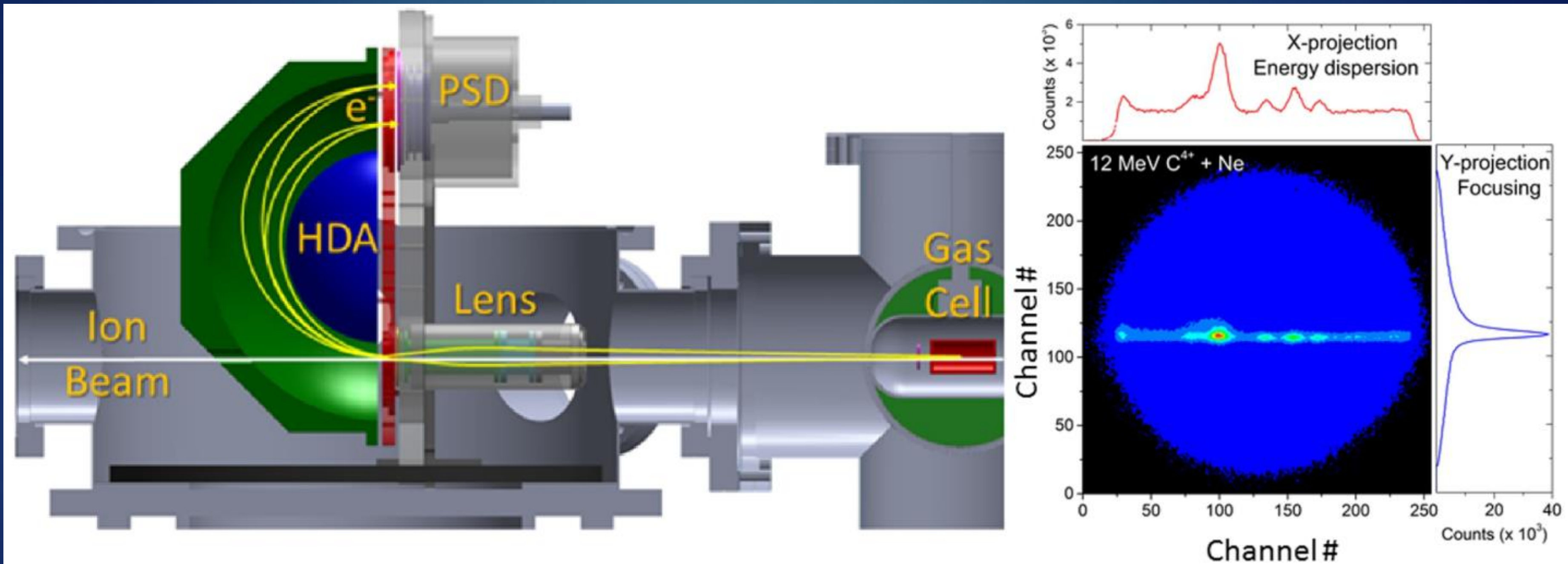
Zero-degree Auger Projectile Spectroscopy (ZAPS):

Operating Principle



$$\frac{\Delta E}{E} \leq 0.15\%, \quad \left.\frac{\Delta E}{E}\right|_{\substack{acceptance\\ window}} = \pm 10\%, \quad \frac{\Delta\Omega}{4\pi} = 1.2\times 10^{-5}$$

Overall efficiency gain ~ 100-200

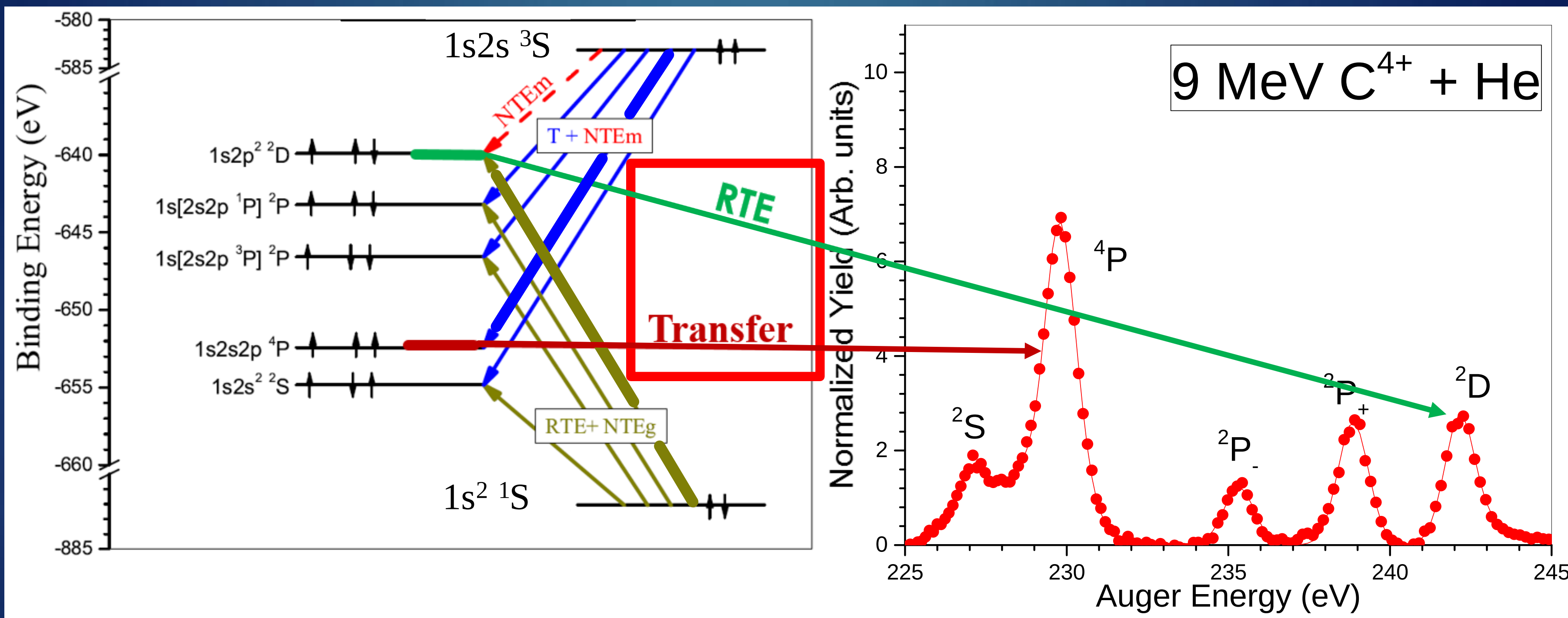
High Transmission ~ 90%

PSD: Position Sensitive Detector

HDA: Hemispherical Deflector Analyser

1s2l2l´ states: Production and Properties

KLL spectrum production



^{4}P populated exclusively from the 1s2s ^{3}S component

^{2}D populated exclusively from the 1s^2 ^{1}S component

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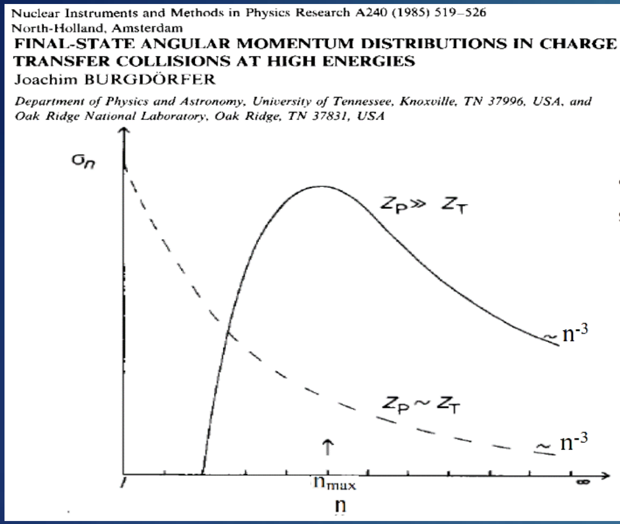
1s2l2l′ states: Production and Properties

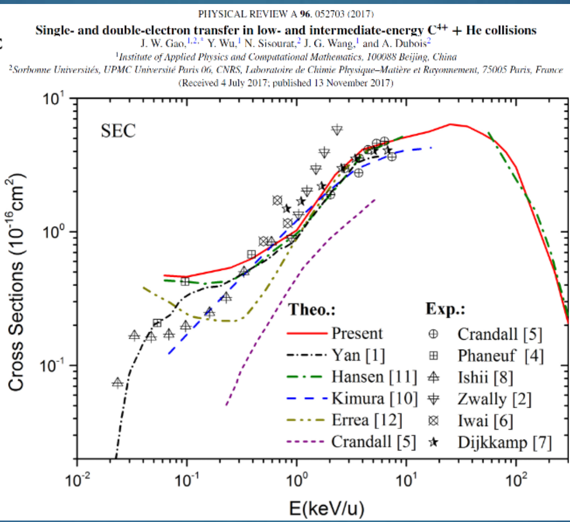
Single Electron Capture (Transfer)

(A)



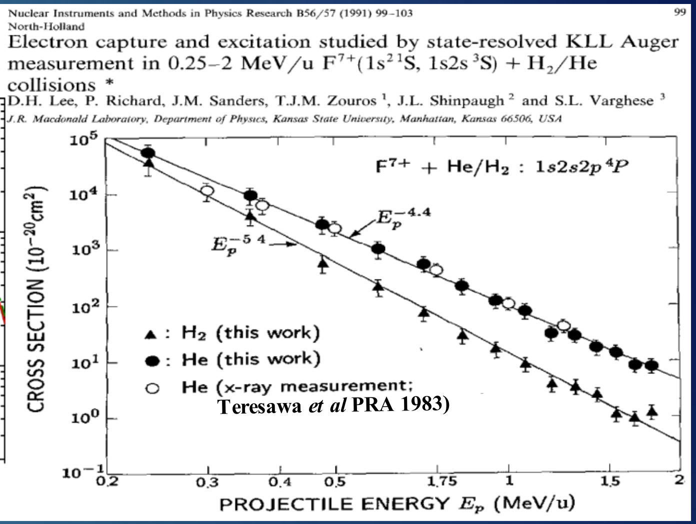
Symmetry of collision partners affects cascades

(B)



Maximizes at velocity matching

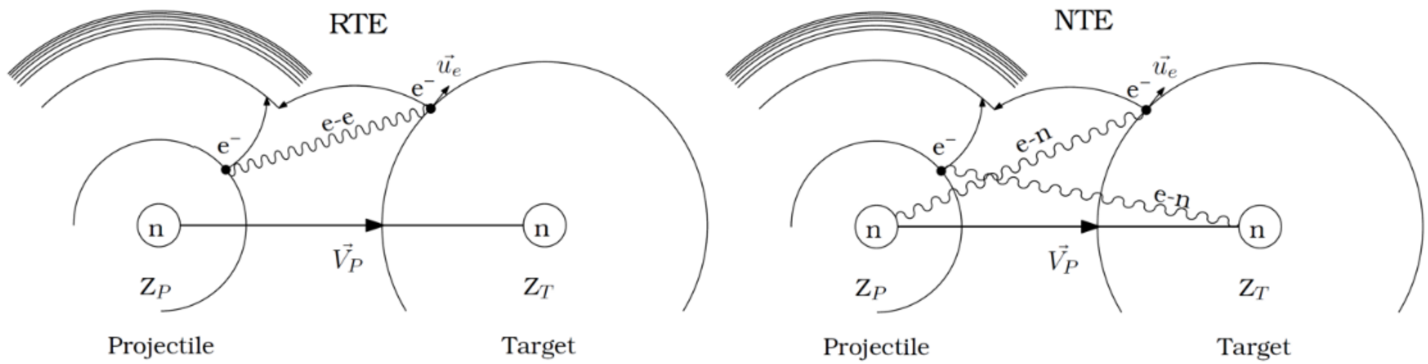
(C)



Exponential decrease at velocity regime of interest

1s2l2l´ states: Production and Properties

Resonant/Non-resonant Transfer-Excitation

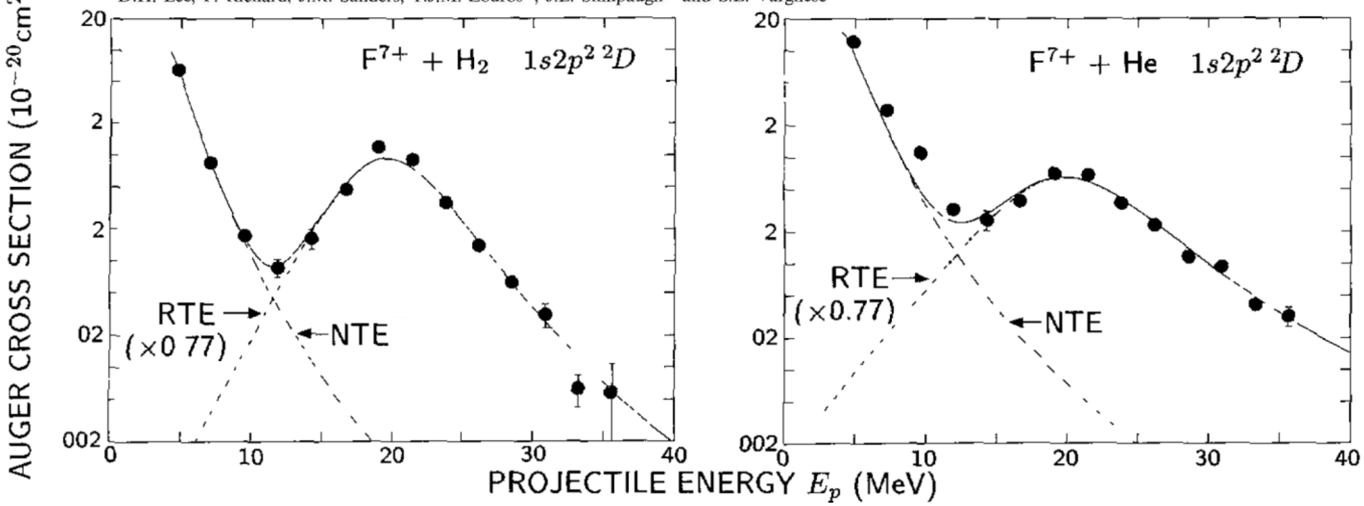


Resonance @V_p=v_A

Nuclear Instruments and Methods in Physics Research B56/57 (1991) 99-103
North-Holland

Electron capture and excitation studied by state-resolved KLL Auger measurement in 0.25–2 MeV/u $F^{7+}(1s^2\,{}^1S,\ 1s2s\,{}^3S)$ + H_2/He collisions *

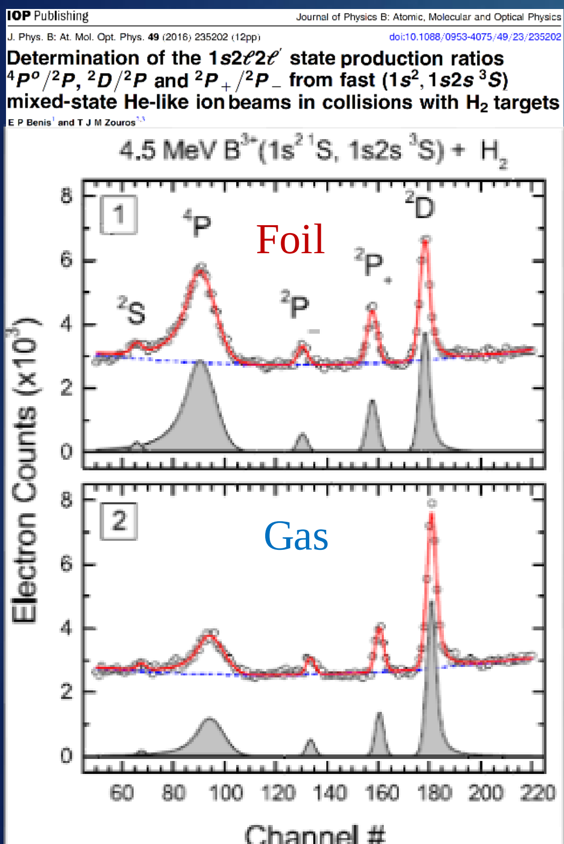
D.H. Lee, P. Richard, J.M. Sanders, T.J.M. Zouros [1], J.L. Shinpaugh [2] and S.L. Varghese [3]



1s2l2l′ states: Production and Properties

Dual spectra technique

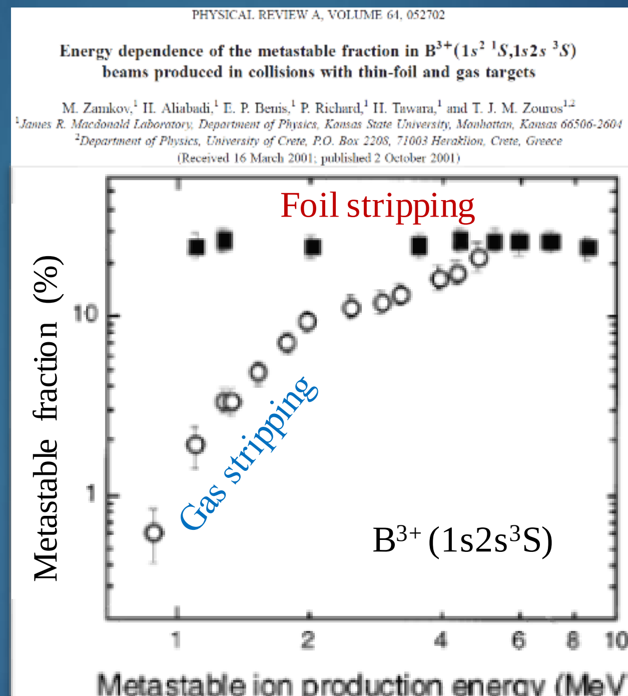
Two measurements with different 1s2s ^3S metastable fractions


IOP Publishing — Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. 49 (2016) 235202 (12pp) doi:10.1088/0953-4075/49/23/235202

Determination of the $1s2\ell2\ell'$ state production ratios $^4P^o/^2P$, $^2D/^2P$ and $^2P_+/^2P_-$ from fast $(1s^2, 1s2s\,^3S)$ mixed-state He-like ion beams in collisions with H_2 targets

E P Benis[1] and T J M Zouros[1,2]


PHYSICAL REVIEW A, VOLUME 64, 052702

Energy dependence of the metastable fraction in $B^{3+}(1s^2\,^1S, 1s2s\,^3S)$ beams produced in collisions with thin-foil and gas targets

M. Zamkov,[1] H. Aliabadi,[1] E. P. Benis,[1] P. Richard,[1] H. Tawara,[1] and T. J. M. Zouros[1,2]

[1]James R. Macdonald Laboratory, Department of Physics, Kansas State University, Manhattan, Kansas 66506-2604

[2]Department of Physics, University of Crete, P.O. Box 2208, 71003 Heraklion, Crete, Greece

(Received 16 March 2001; published 2 October 2001)

$$R_m = \frac{\dfrac{N[^4P,^2D]}{G_\tau}}{N[^2P_+,^2D] + N[^2P_-,^2D]}$$

$$N[x,y] \equiv \left(\frac{N_1^e[x]}{N_1^e[y]} - \frac{N_2^e[x]}{N_2^e[y]}\right)$$

- Only relative peak intensities in R_m normalized to ^2D
- Independent of all the experimental parameters
- No need to determine actual metastable fraction

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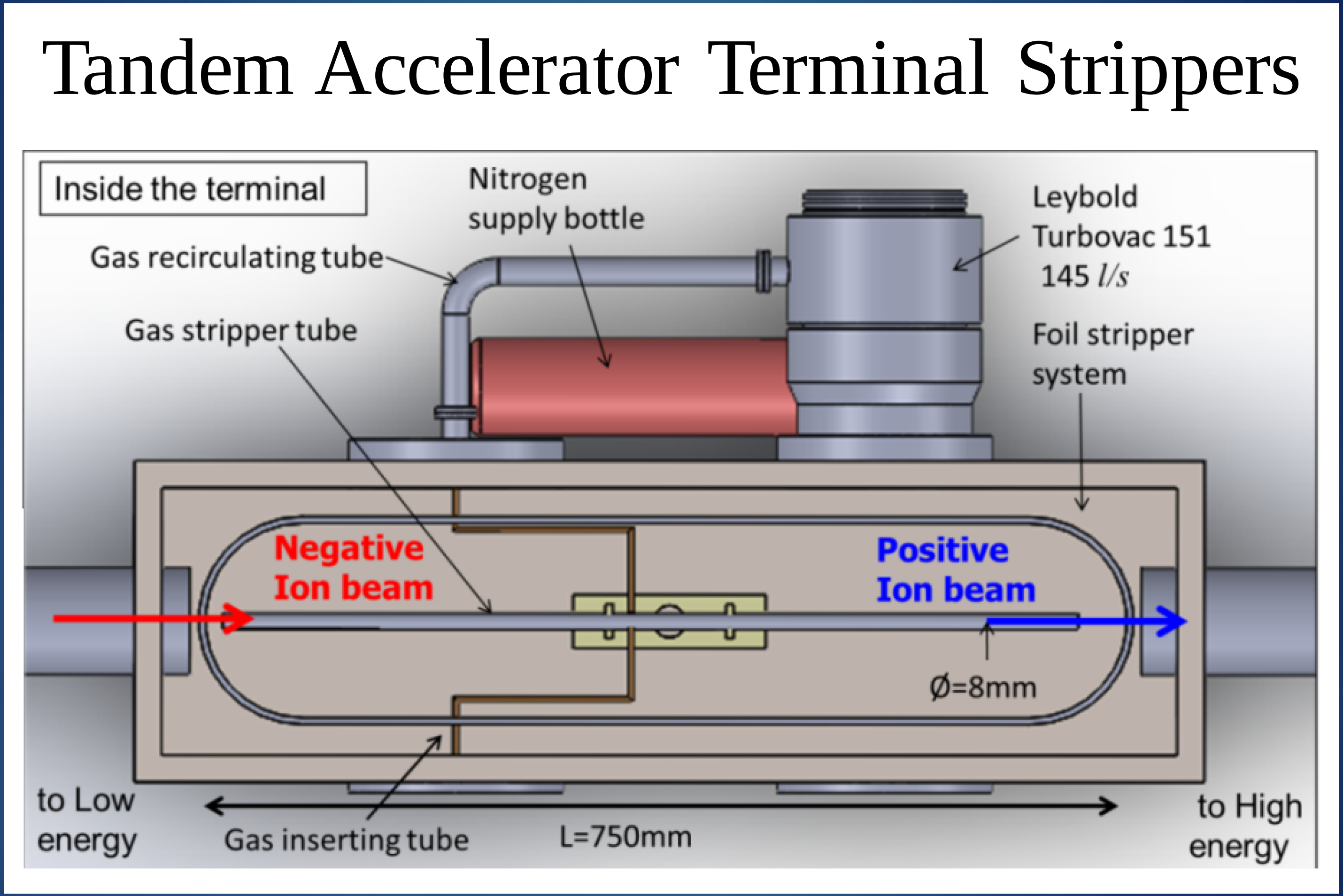
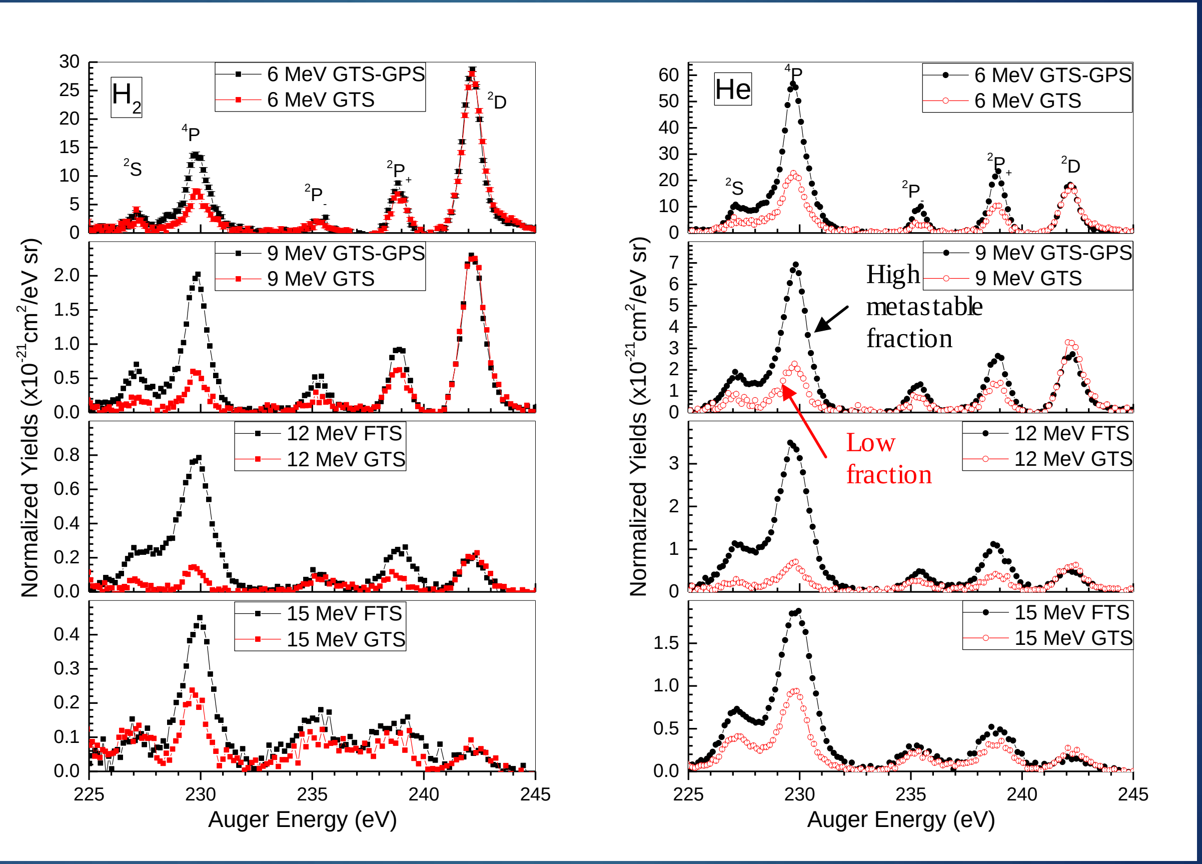
The L45 beam line at the INPP

Recirculating Gas Terminal Stripper - GTS



Zero-degree Auger Projectile Spectroscopy (ZAPS):



High quality KLL spectra
Allow for state-selective cross section determinations
More stringent test of theories

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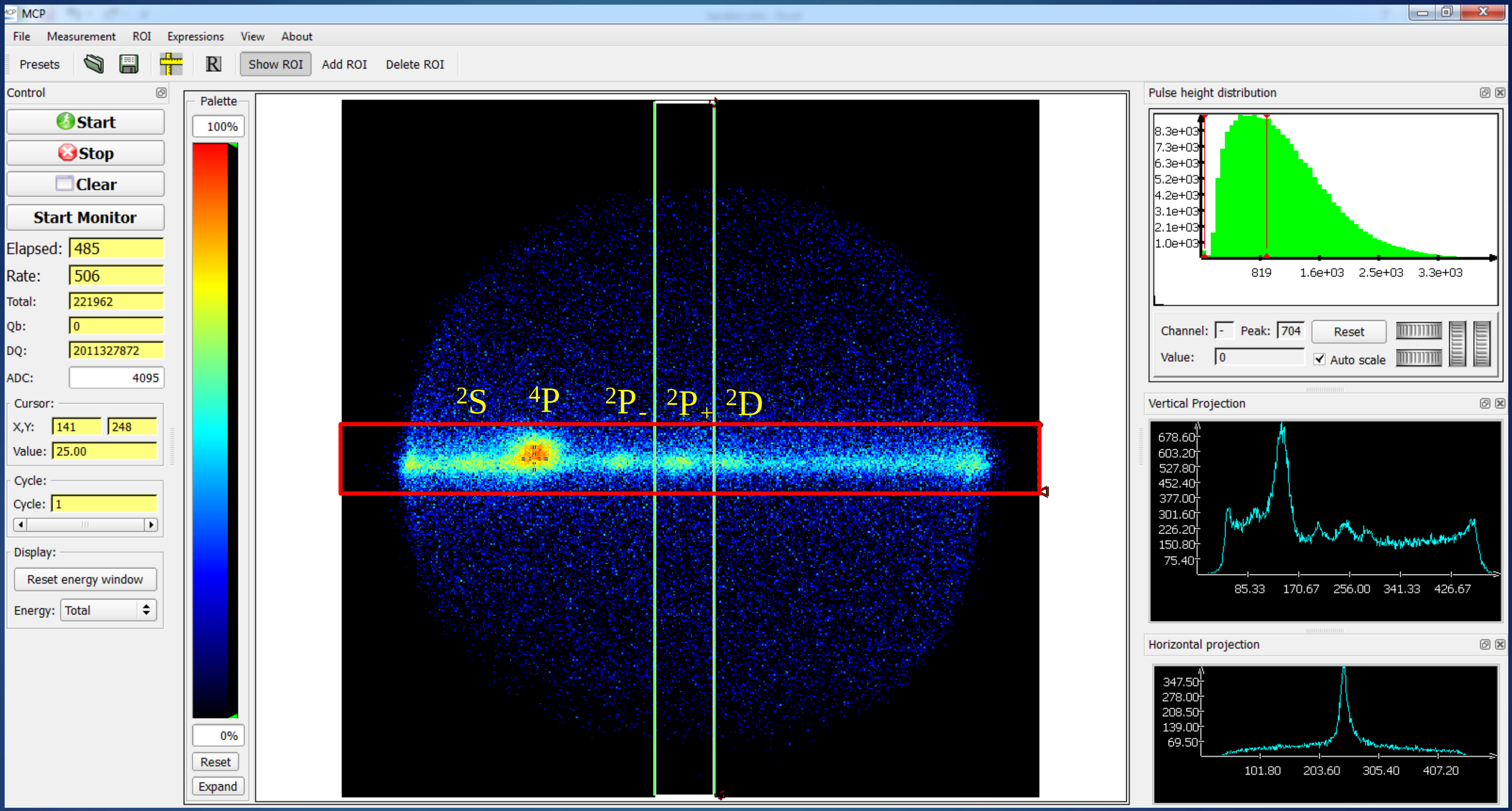
Zero-degree Auger Projectile Spectroscopy (ZAPS):



Horizontal misalignment
μ-metal shielding

First spectrum - 28th July 2014

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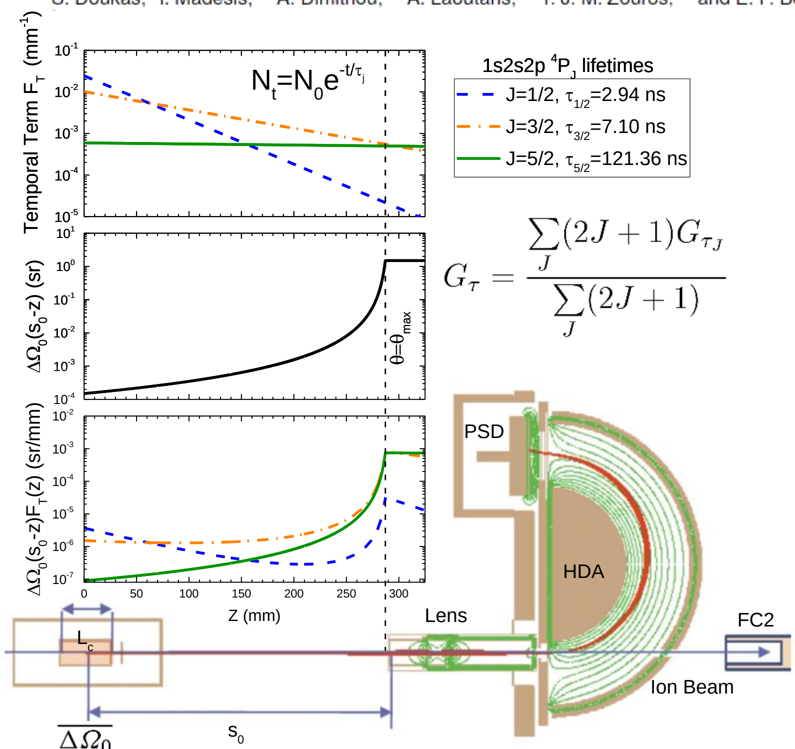
Data treatment

1s2s2p ^4P solid angle correction

REVIEW OF SCIENTIFIC INSTRUMENTS 86, 043111 (2015)

Determination of the solid angle and response function of a hemispherical spectrograph with injection lens for Auger electrons emitted from long lived projectile states

S. Doukas,[1] I. Madesis,[2,3] A. Dimitriou,[2,3] A. Laoutaris,[4,3] T. J. M. Zouros,[2,3] and E. P. Benis[5]



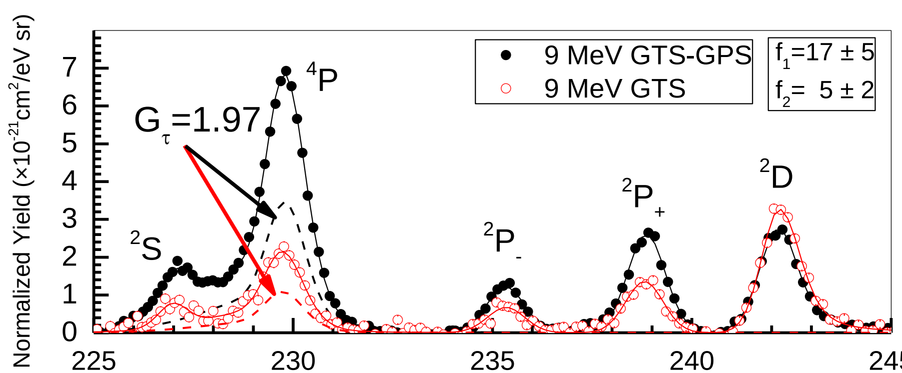
$$G_\tau = \frac{\sum_J (2J+1) G_{\tau_J}}{\sum_J (2J+1)}$$

$$\overline{\Delta\Omega_J} \equiv \overline{\Delta\Omega_0}\, G_{\tau_J}$$

$$\overline{\Delta\Omega_0} \equiv \frac{1}{L_c}\int_{z'=0}^{L_c} dz'\, \Delta\Omega_0(L_c/2 + s_0 - z')$$

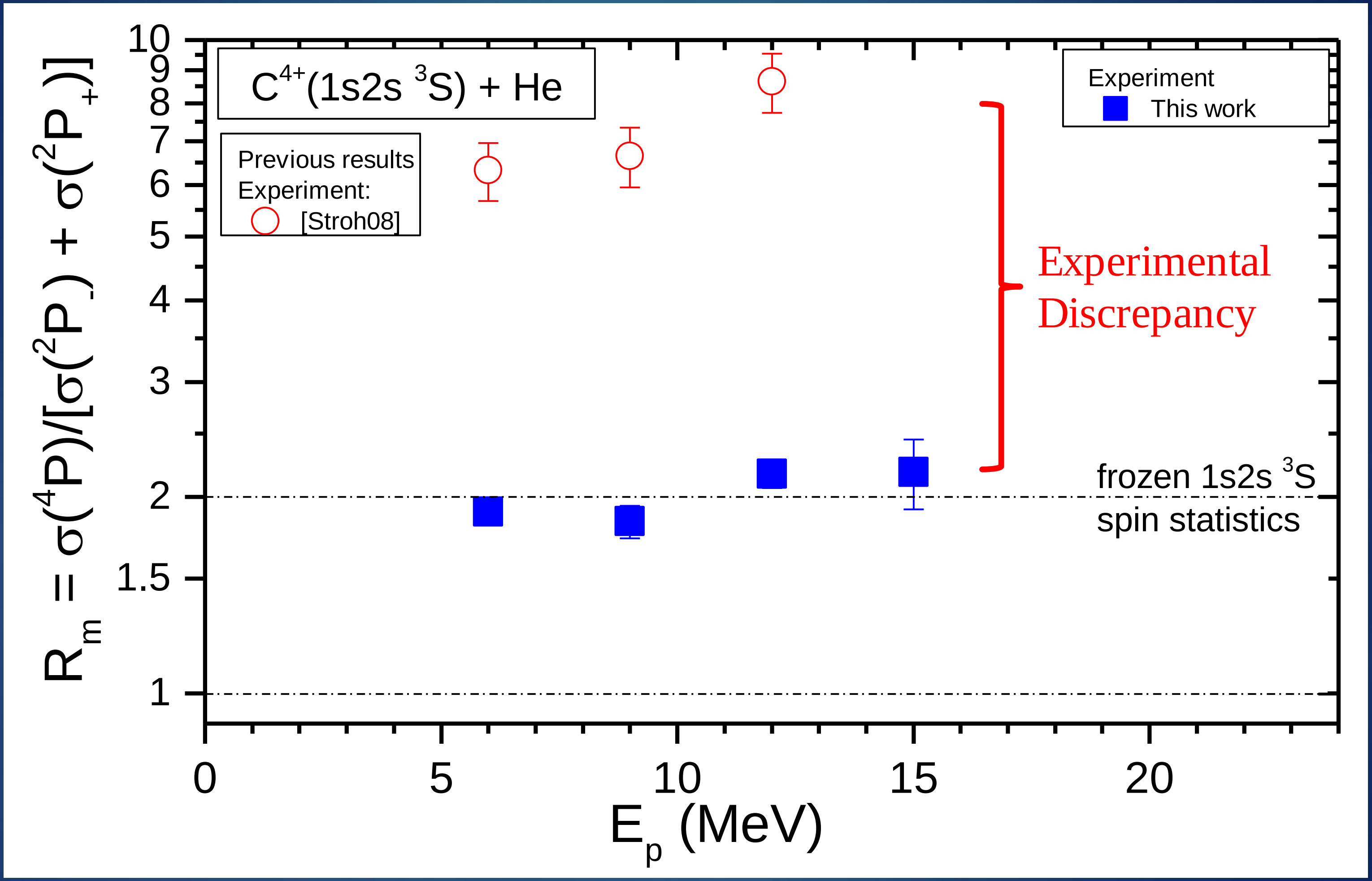
$$\overline{\Delta\Omega_J} \equiv \frac{1}{L_c}\int_{z'=0}^{L_c} dz' \int_{z=0}^{L-Z'} dz \frac{e^{-z/V_p\tau_J}}{V_p\tau_J}\Delta\Omega_0(L - z' - z)$$

Ion	E_p (MeV)	G_τ Exp.	G_τ SIMION
C^{2+}	6.6	2.0(4)	1.92[a]
			2.41[b]
		1.9(4)	2.47[a]
			2.80[b]
O^{4+}	17.5	1.5(4)	2.08[a]
			2.33[b]



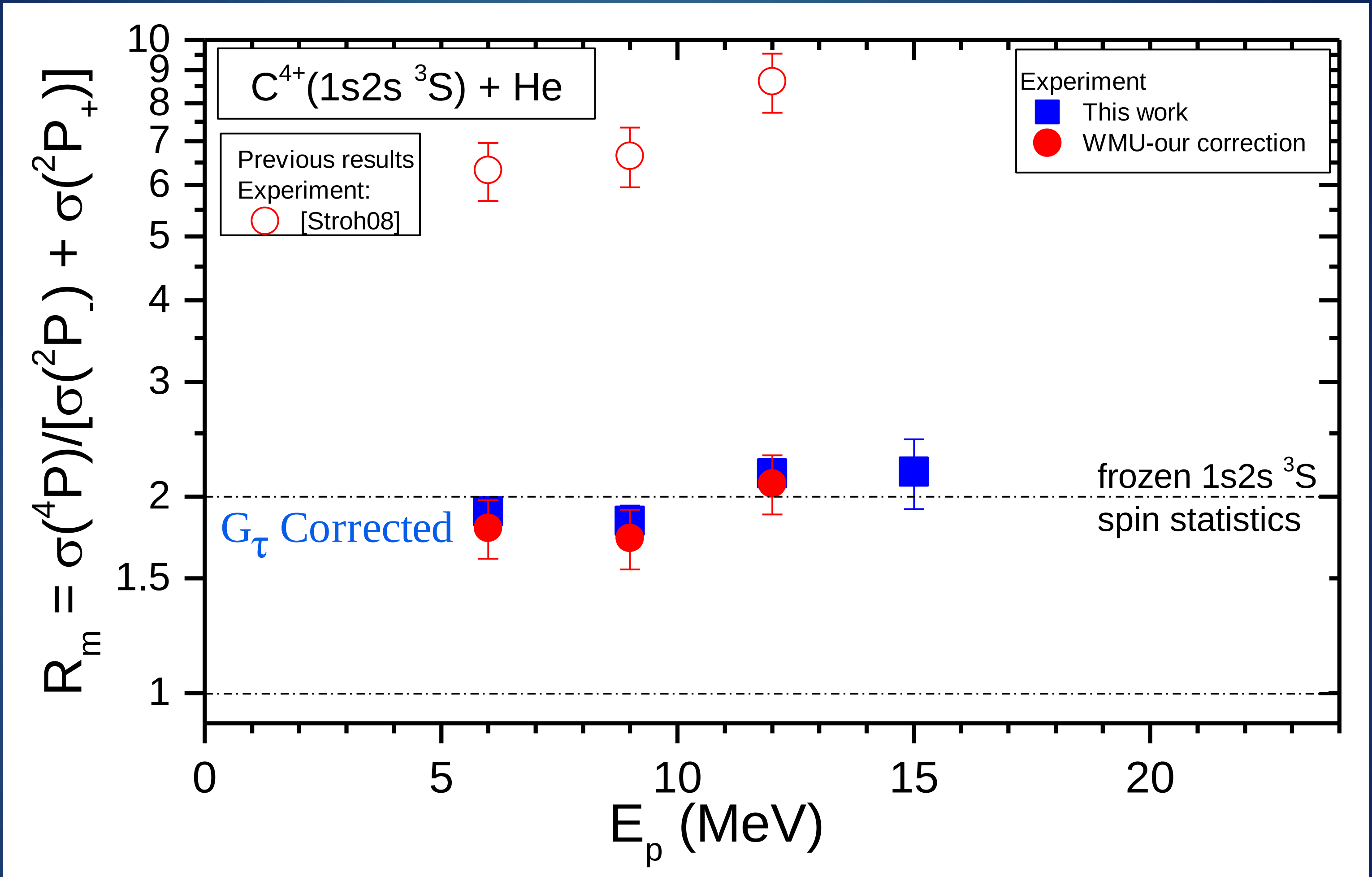
Experimental Results for SEC to ^3S

Results on R_m measurements



Experimental Results for SEC to ^3S

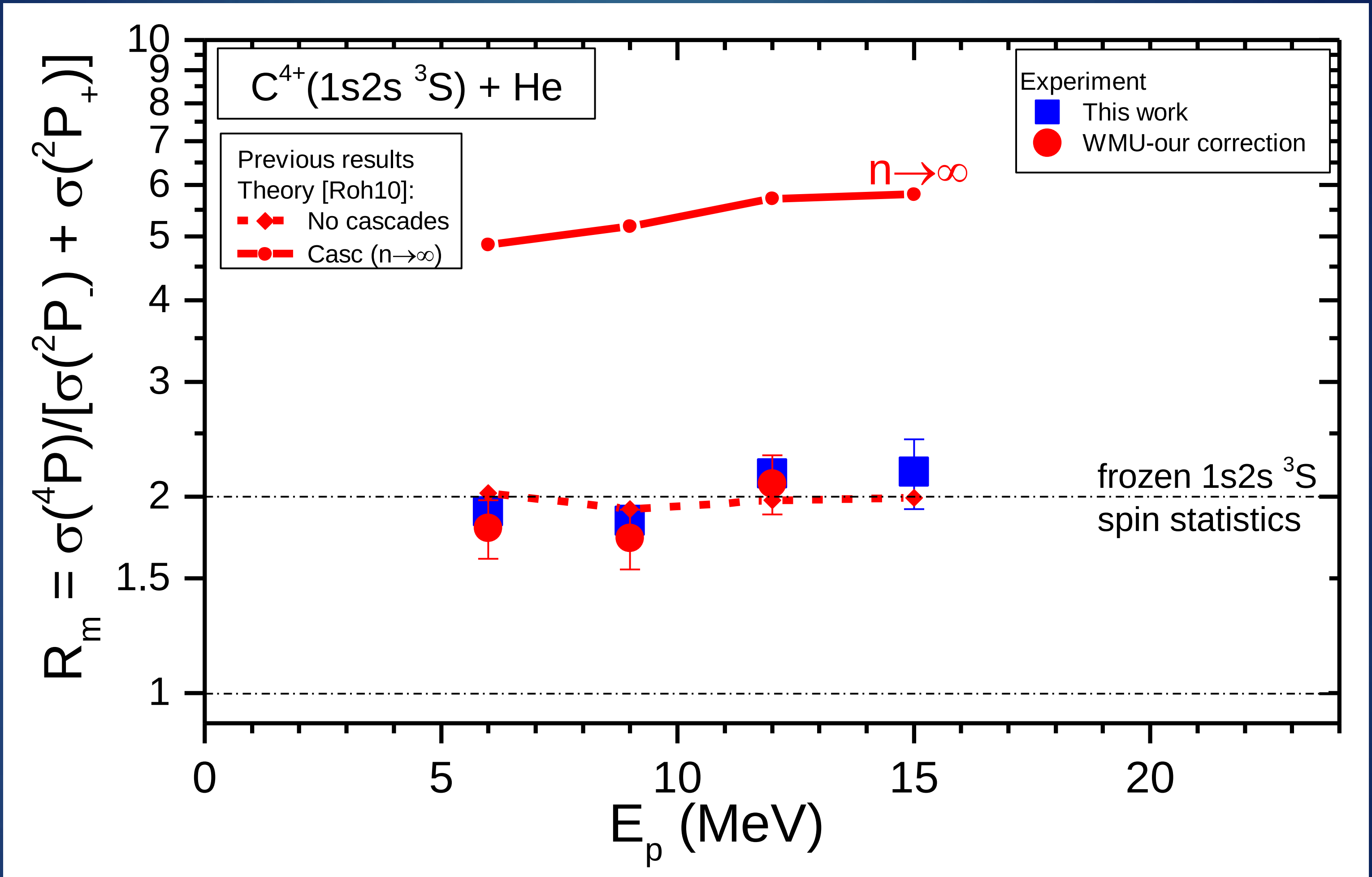
Results on R_m measurements



No discrepancy between experimental results after applying our Gτ corrections to the older measurements

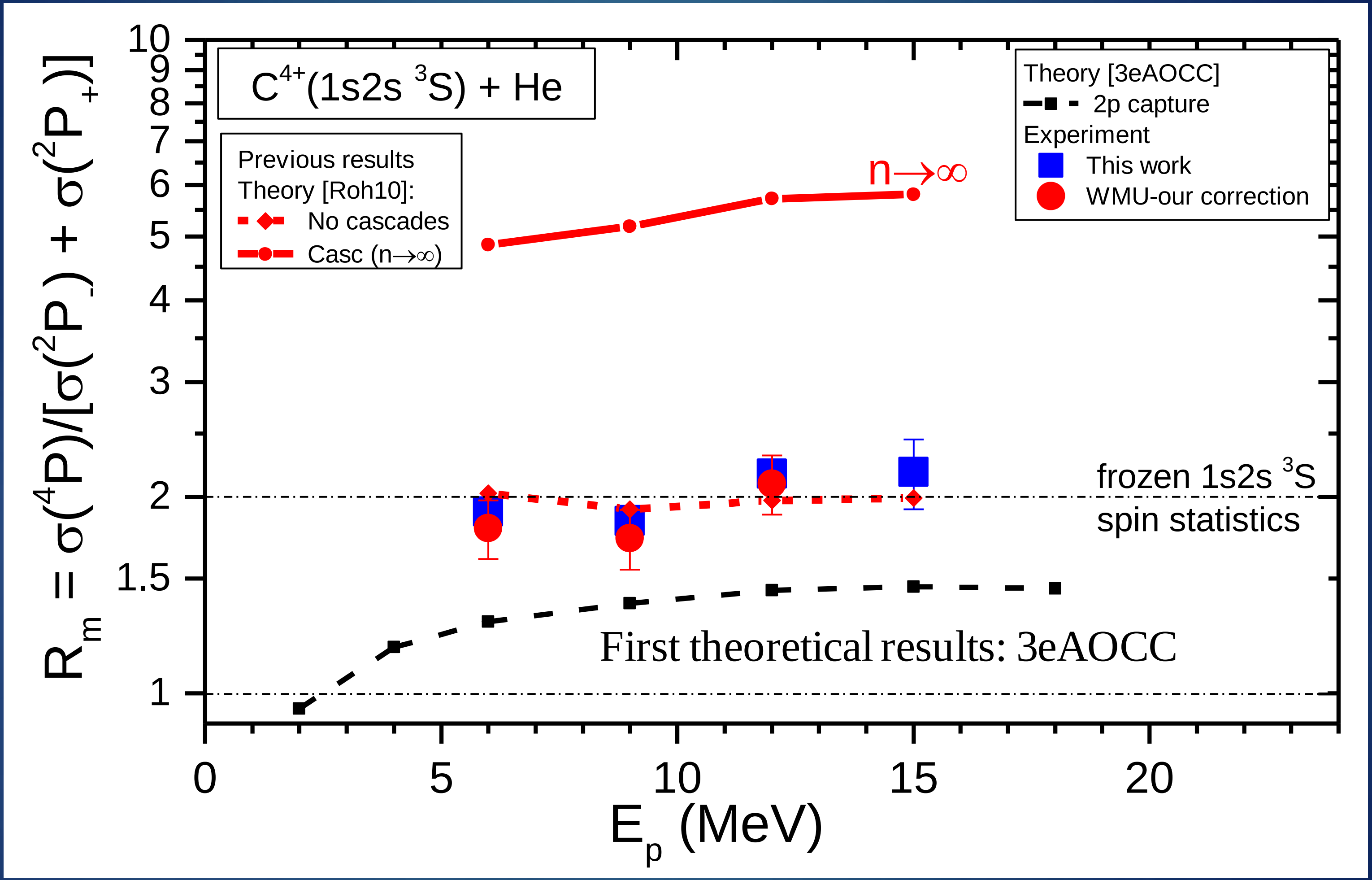
Experimental Results for SEC to ^3S

Results on R_m measurements



Experimental Results for SEC to ^{3}S

Results on R_m measurements



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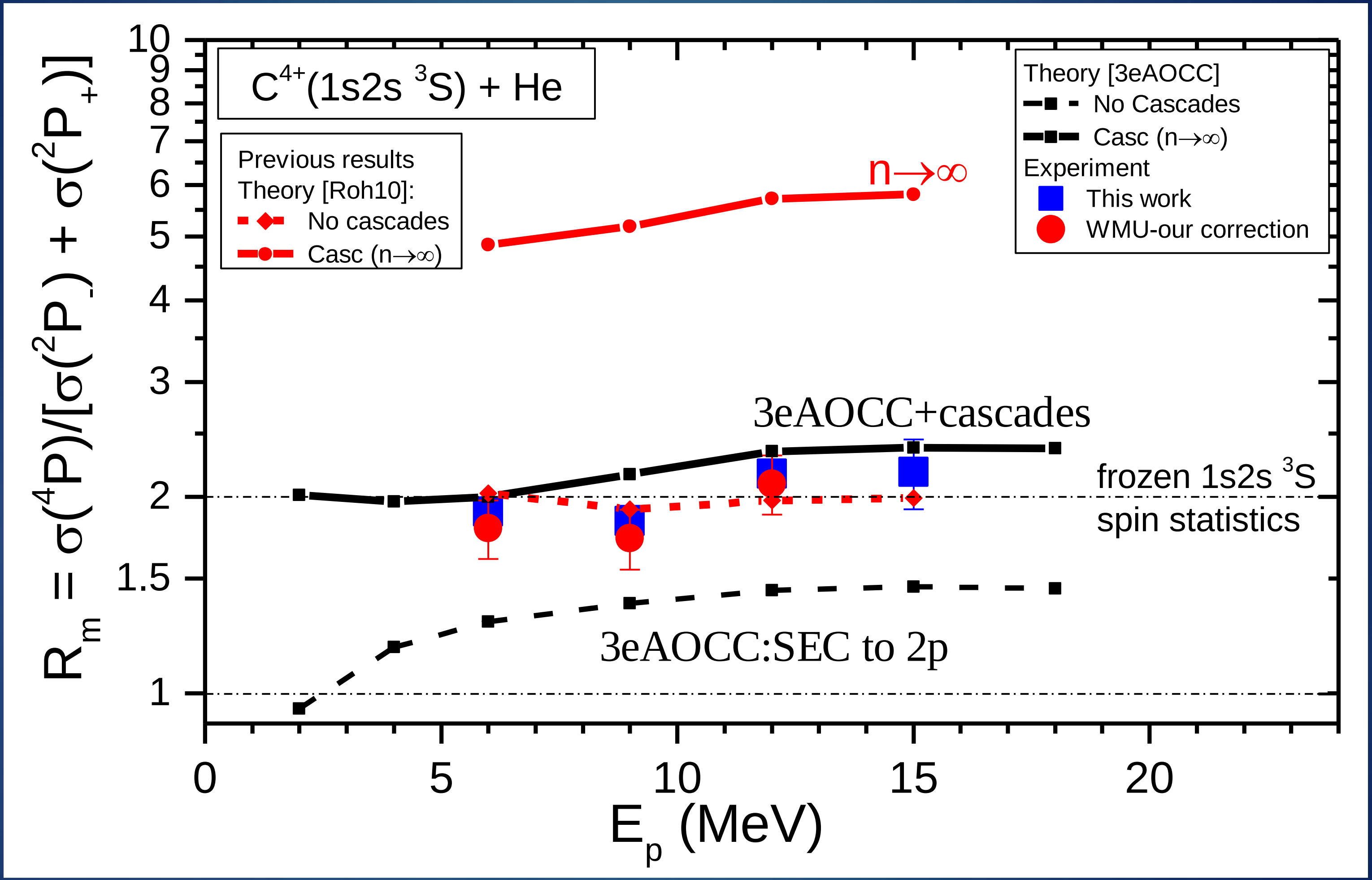
Experimental Results for SEC to ^3S

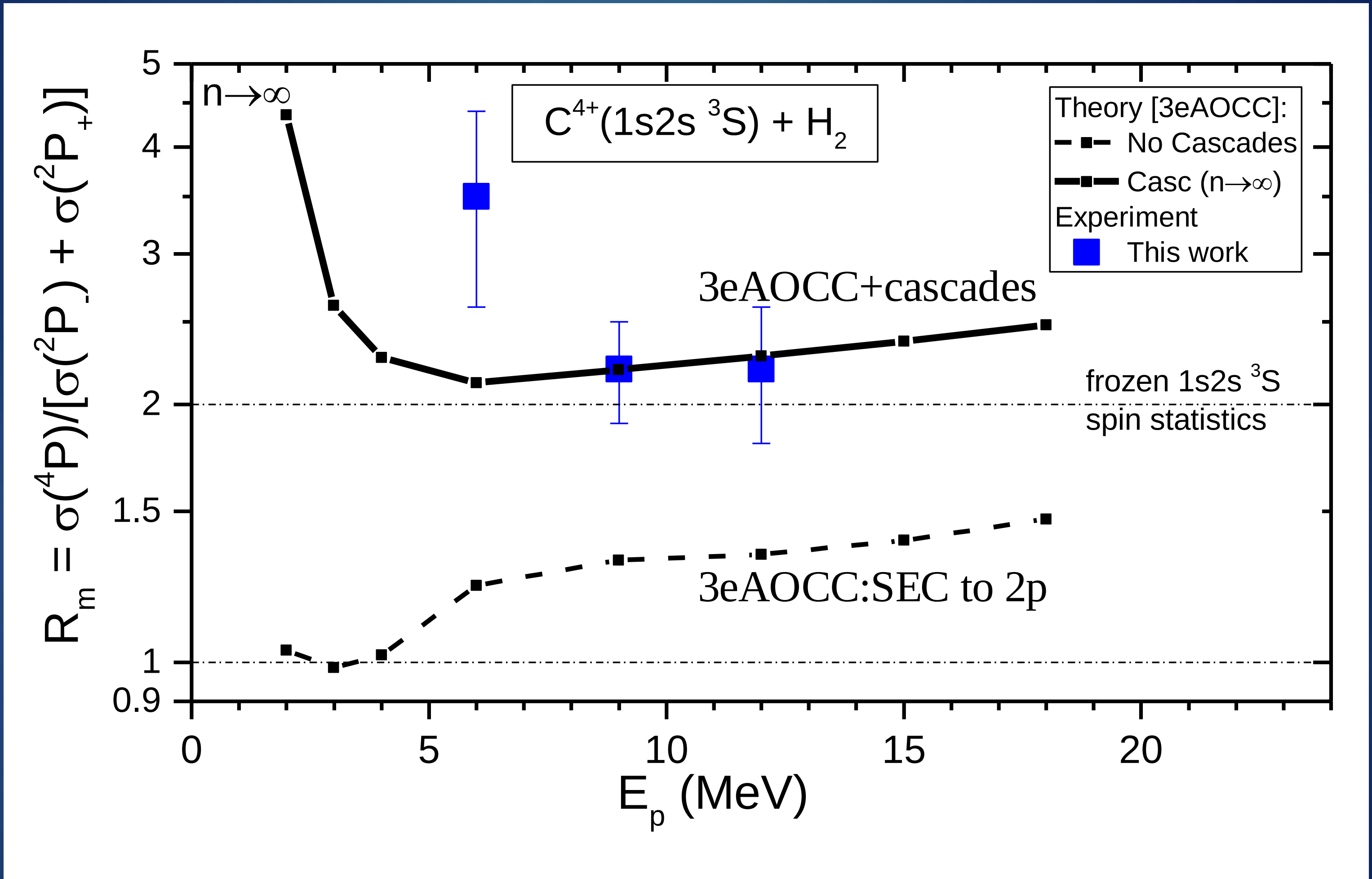
Results on R_m measurements



Very good agreement between 3eAOCC+casc and experiment

Experimental Results for SEC to ^3S

Results on R_m measurements



Very good agreement between 3eAOCC+casc and experiment

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1s2l2l´ states: Production and Properties

3-electron Atomic Orbital Close Coupling - 3eAOCC (A. Dubois - Paris)

Method:

- Ab initio dynamical calculation involving 3 electrons within full CI approach
- Semi-classical atomic orbital close-coupling approach with asymptotic description of the collision partners
- TDSE solved non-perturbatively for 3 electrons with inclusion of all couplings related to the static and dynamic inter-electronic repulsions and effects stemming from Pauli exclusion principle
- Calculated $\sigma(1s2lnl'\ ^{2,4}L$, n=2-4) – Higher n contributions (for cascade calculations)

Advantages:

- Accurate modelling of $C^{4,3+}$ electronic structures
- 3eAOCC goes much beyond the frozen core models

Disadvantages:

- Computationally demanding, e.g. for a single collision energy 5 days needed for each initial C^{4+} ion state, $1s^2$ and $1s2s\ ^3S$

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Publications

PHYSICAL REVIEW LETTERS **124,** 113401 (2020)

Pauli Shielding and Breakdown of Spin Statistics in Multielectron Multi-Open-Shell Dynamical Atomic Systems

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atoms

MDPI

Article

Radiative Cascade Repopulation of $1s2s2p\ ^4P$ States Formed by Single Electron Capture in 2–18 MeV Collisions of $C^{4+}(1s2s\ ^3S)$ with He

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Summary and Conclusions

- A new, atomic physics beam line in the INPP
- High resolution, high efficiency ZAPS setup
- Method for component contribution separation
- Experimental results for the 1s2s2p $^4P/^2P$ line ratio R_m for SEC for C^{4+} (1s2s ^3S)+He

Summary and Conclusions

- First time 3e dynamic calculation achieved (3eAOCC) (Prof. Dubois – Paris)
- Cascade calculations
- Calculated ratio R_m found to be in agreement with experiment, for the first time.
- Disagreement between theory and experiment resolved

Future Plans

Systematic isoelectronic (1s2s ^3S) measurements for further investigation:

- Calculations for F^{7+} (1s2s ^3S) recently started
- First measurements for O^{6+} (1s2s ^3S)
- Awaiting for the new negative ion sputter source (CALIBRA Tandem upgrade 2022) to also check Li^{+} and B^{3+}

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