Carter M. Sc. Research Proposal

Davin Carter

OKANAGAN
ORCAC
May 15, 2008

Carter Thesis Committee

Dr. Rob O'Brien

Dr. Al Vaisius

Dr. Paul Shipley

THE UNIVERSITY OF BRITISH COLUMBIA

UBC OKANAGAN

I agree to serve on the Advisory Committee for

Davin Carter (M.Sc.)

Supervisor		
Rob O'Brien		July 12, 2007
Print Name	Signature	Date
Al Vaisius		2.VIII.07
Print Name	Signature	Date
PAUL SHIPLEY		Aug 9, 2007
Print Name	Signature	Date

The role of the student advisory committee is defined in the Chemistry Graduate Program, as reproduced below.

STUDENT ADVISORY COMMITTEES

A student's advisory committee consists of three members of the graduate program committee, one of whom is the student's thesis supervisor. The composition of a committee is determined by the Graduate Program Coordinator (GPC) in consultation with the student's thesis supervisor. The GPC will endeavour to ensure that at least one of the members of each M.Sc. advisory committee has successfully supervised a student through the completion of a M.Sc. or Ph.D. degree. Similarly, the GPC will arrange, when possible, that at least one of the members of each Ph.D. advisory committee has successfully supervised a student through the completion of a Ph.D. degree. Although, primary supervision of a student rests with the student's thesis supervisor, the advisory committee must conduct an annual review of the student's progress and file a report with the GPC. The report may include recommendations such as, transfer of the student to the Ph.D. program, or require the student take additional courses or seminars above and beyond the program requirements, or request the withdraw of a student from the program in the case of unsatisfactory progress. The advisory committee will also form the core of a student's Comprehensive Examination Committee and Oral Examination Committee in accord with the College of Graduate Studies guidelines.

Carter research proposal overview

Atmospheric pressure ionization

electrical discharge in nobel gas (glow discharge)

Atmospheric Pressure Photo Ionization (APPI)
Direct Analysis in Real-Time (DART)

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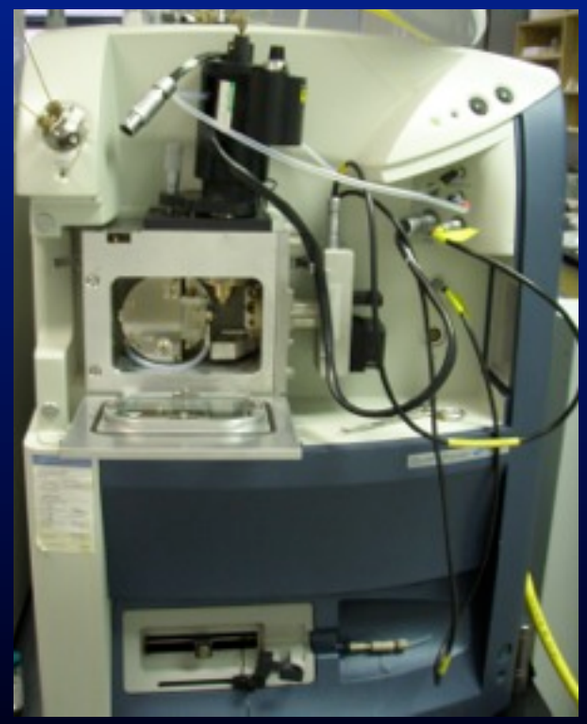

Waters MS/MS

Carter research proposal overview

Four closely related studies, electrical discharge in noble gases:

- examine ionization mechanisms of APPI

- increase APPI ionization efficiency with new sample introduction method

- increase APPI ionization efficiency with by photon focusing

- examine mechanisms of Glow Discharge

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Carter research proposal background

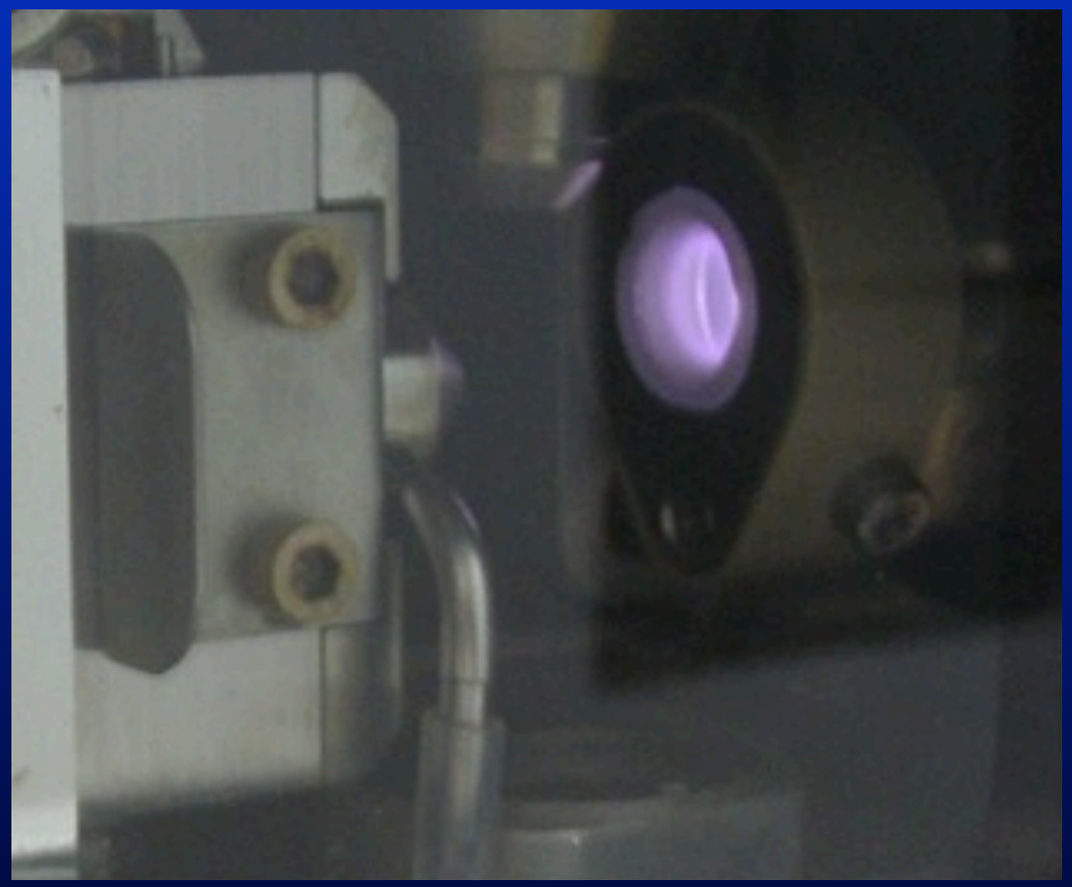
Mass spectrometer- molecular weight, structural details, fingerprint
requires ionized analytes for electrical & magnetic fields to be effective

Ionization energy: energy to remove e^- from highest occupied orbital
IE_{1st}: 6-10 eV
IE_{2nd}: 20-30 eV

Electron ionization (EI): hard ∴ fragmentation
Electrospray Ionization (ESI): soft, limited (1/10,000 molecules into MS)
Atmospheric Pressure Chemical Ionization (APCI): Soft, matrix dependent
Atmospheric Pressure Photo Ionization (APPI): soft, more universal, matrix independent, ions formed cold
Glow Discharge: related to APPI

Carter research proposal background

APPI & Glow discharge are related
electrical discharge across noble gas $Rg + e^- \rightarrow Rg^+ + 2\ e^- \rightarrow Rg^* + e^- \rightarrow Rg^* + h\nu$
APPI source is contained with a LiF window for photons, glow discharge open

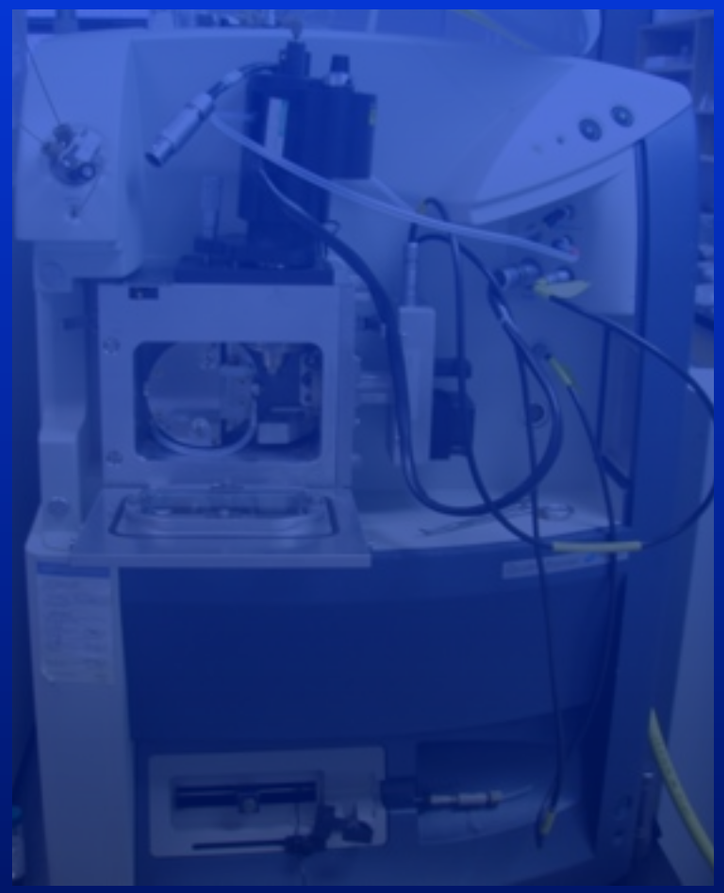


APPI Source

Glow Discharge
* Andrade et al

Carter research proposal background

Waters MS/MS



Waters MS/MS
naked

ionization chamber

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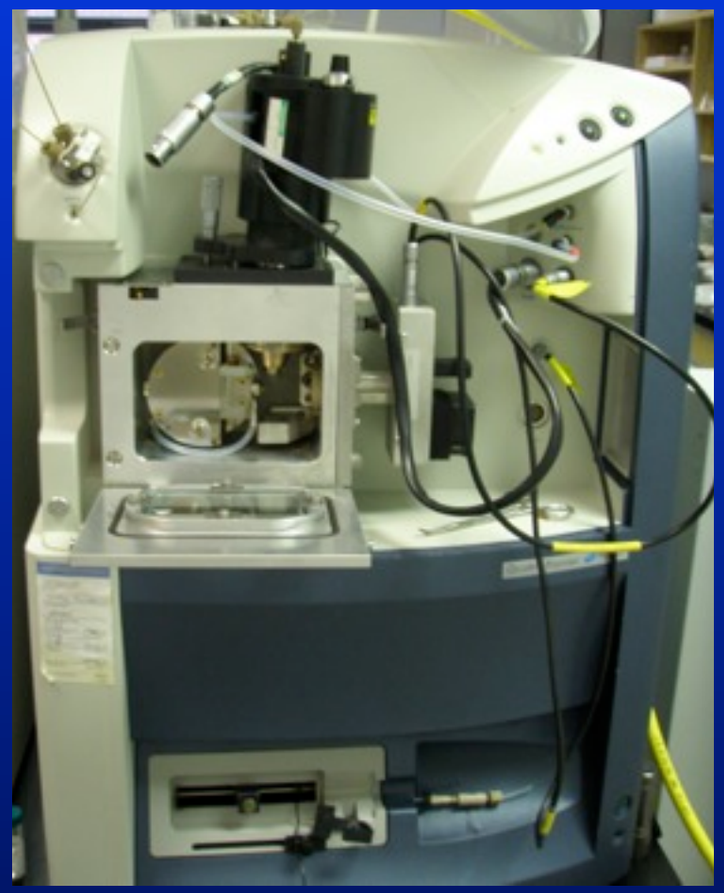
Carter research proposal background

Waters MS/MS



Waters MS/MS
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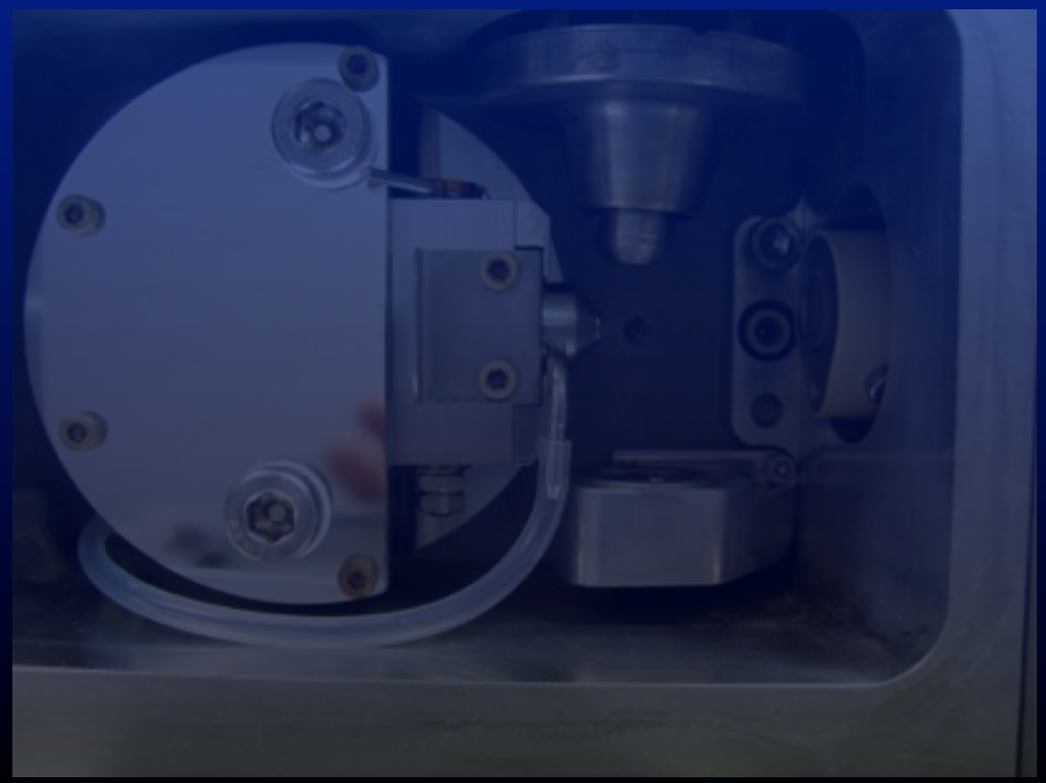
ionization chamber



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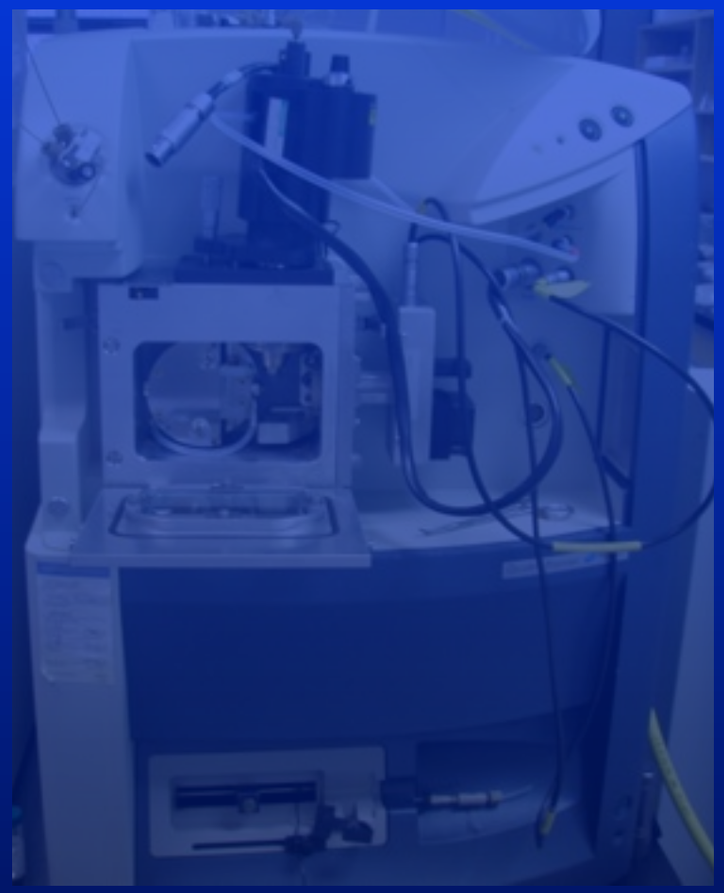
Waters MS/MS



Waters MS/MS
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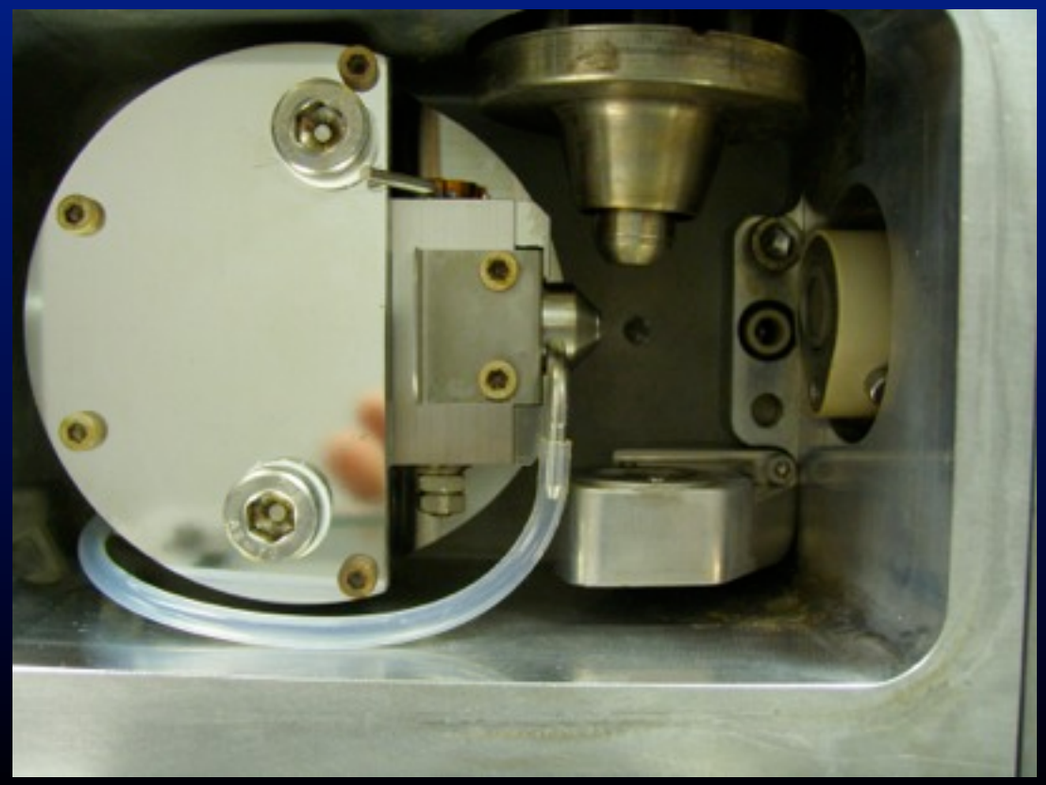


Carter research proposal background APPI

Primary APPI

$h\nu + A \rightarrow A^+ + e^-$ photoionization (+) tive

$e^- + A \rightarrow A^-$ photo induced e^- capture (-) tive

Secondary APPI

$h\nu + D \rightarrow D^+ + e^- \rightarrow D^+ + A \rightarrow A^+ + D$ dopant assisted (+) tive

$e^- + D \rightarrow D^- \rightarrow D^- + A \rightarrow A^- + D$ dopant assisted (-) tive

$h\nu + C_7H_8 \rightarrow C_7H_8^{\bullet+} + e^- \rightarrow C_7H_8^{\bullet+} + (CH_3OH)_3 \rightarrow C_7H_7^{\bullet} + (CH_3OH)_3H^+$

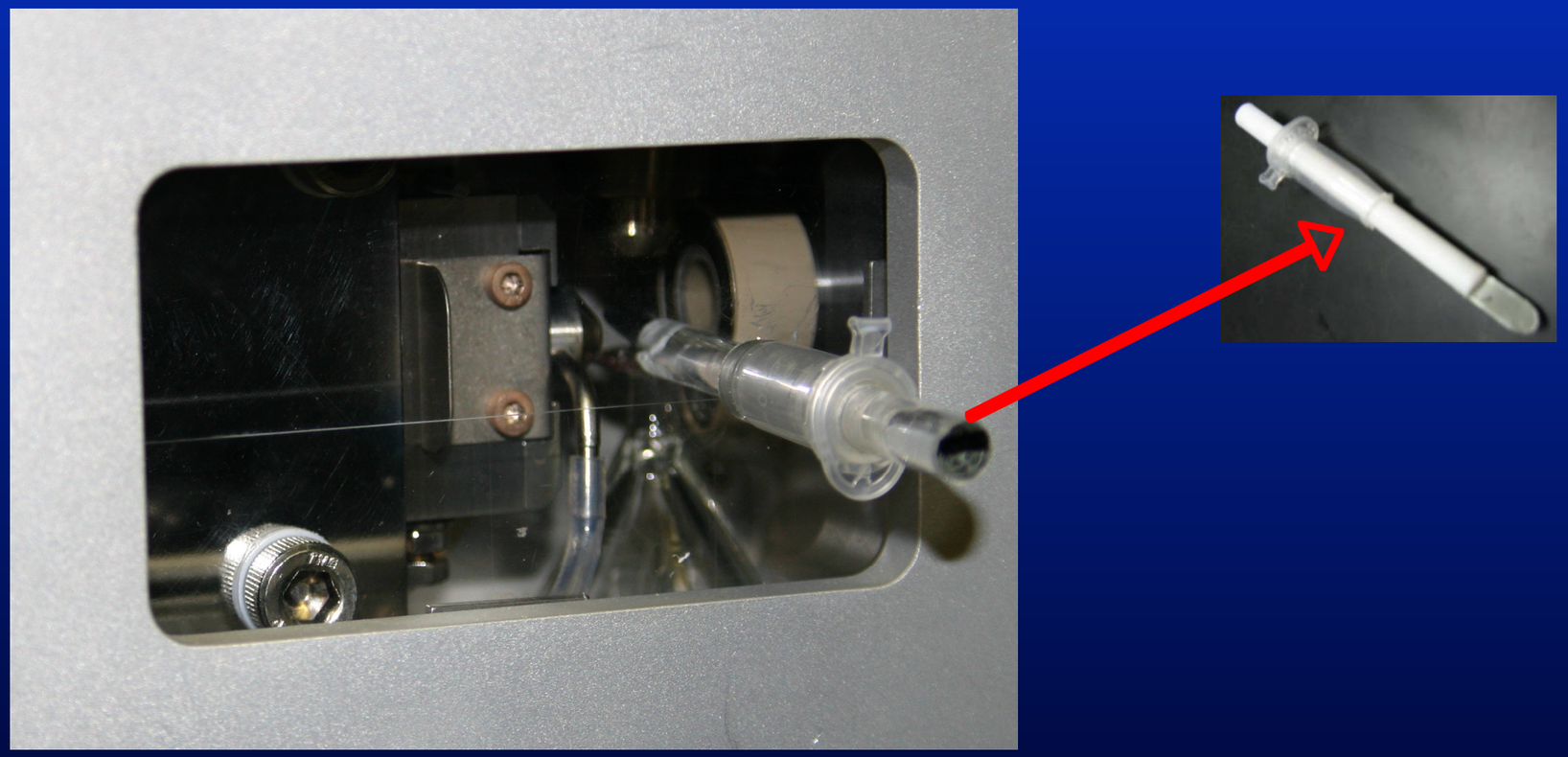
$(CH_3OH)_3H^+ + A \rightarrow AH^+ + 3CH_3OH$ Dopent Assisted Ionization (Toluene/ MeOH)

Carter research proposal background APPI

Radical APPI

$SH + hv \rightarrow S^{\bullet} + H^{\bullet} \rightarrow S^{\bullet +} + A \rightarrow AH^{\bullet} + hv \rightarrow AH^{-} + e^{-}$

$[M+4H-2F]^{-}$ observed → points to 2x H_2 → radical



Solvent free probe introduction

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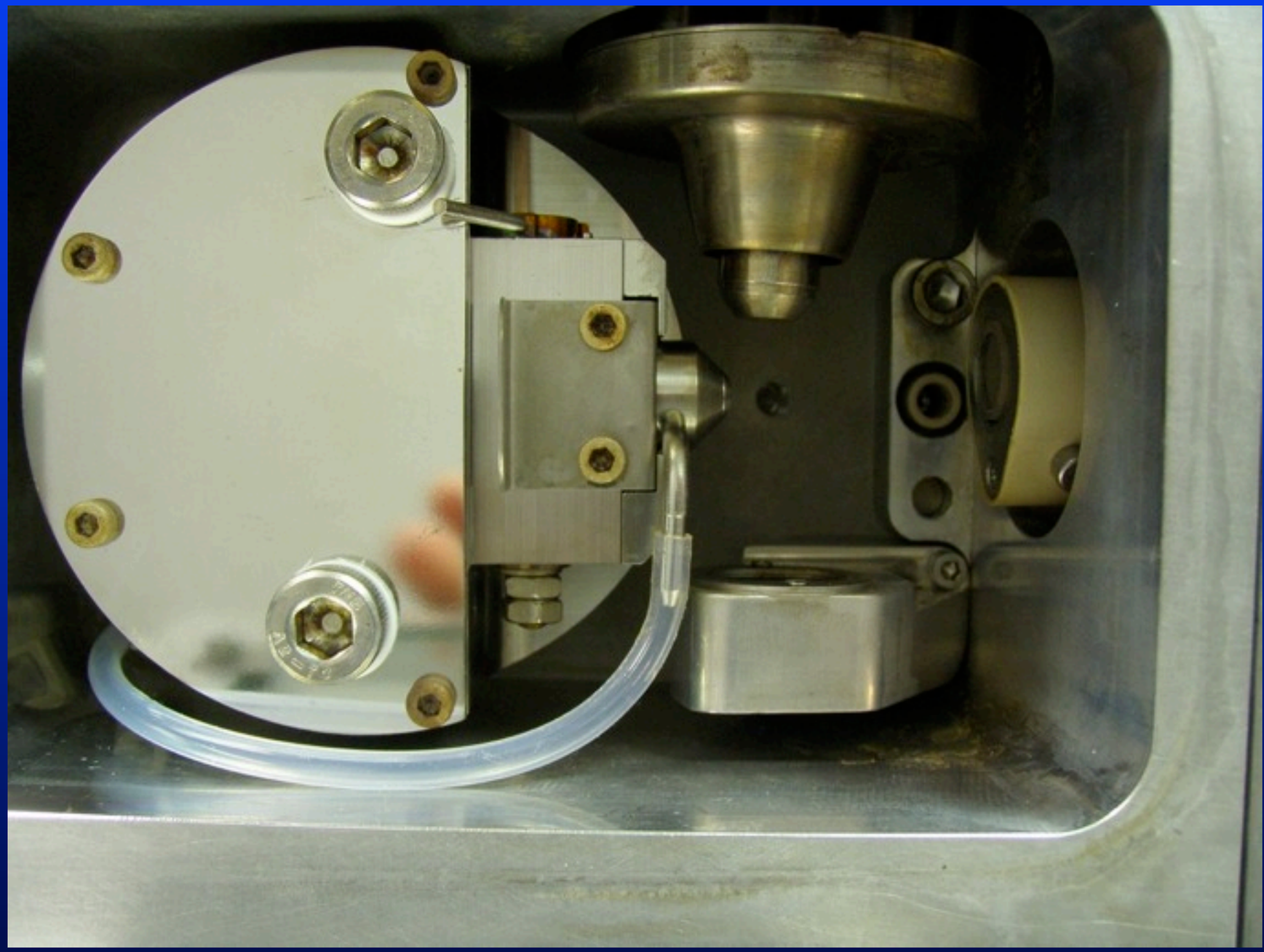
Carter research proposal VUV transparent Plate



Current orientation

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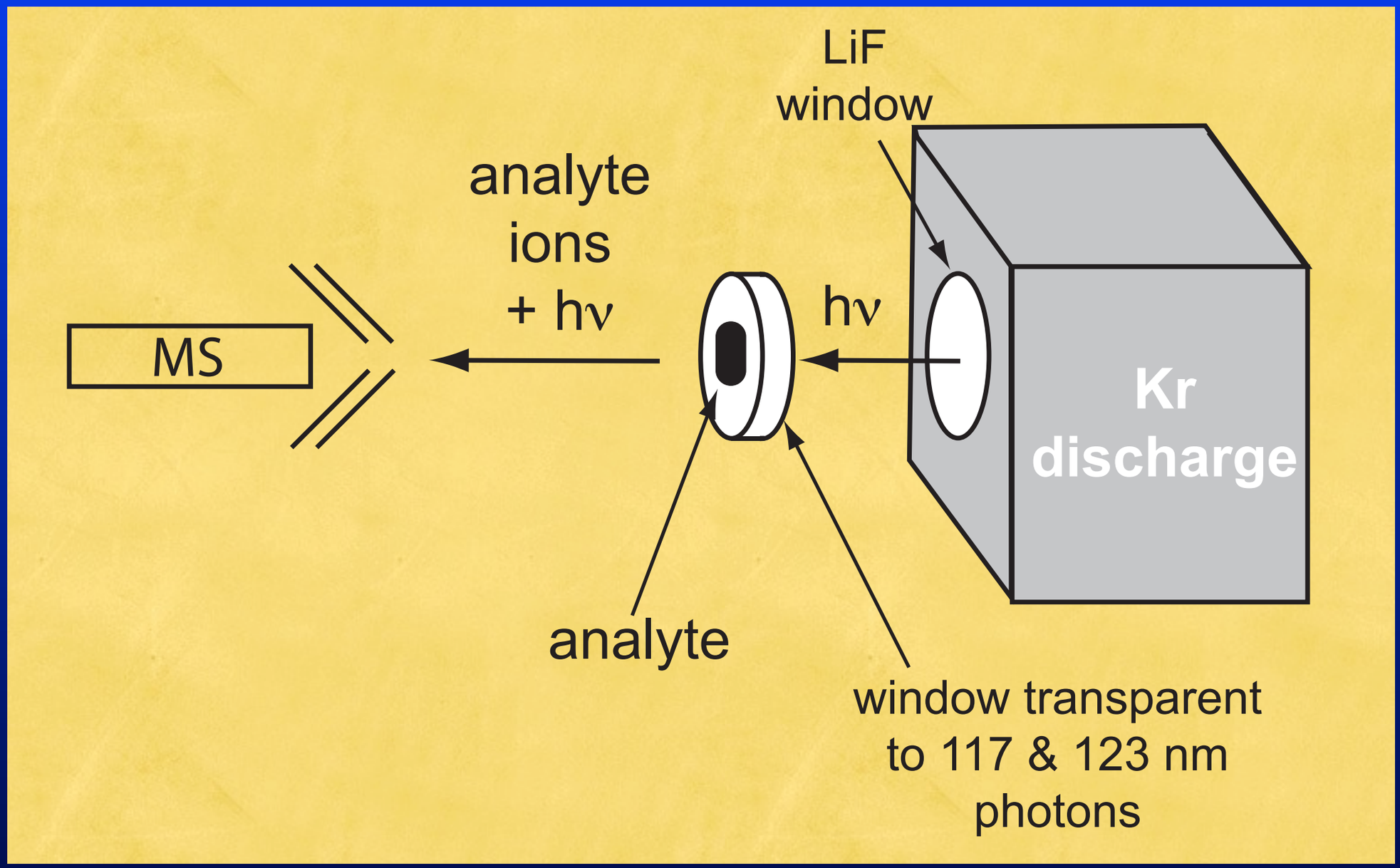
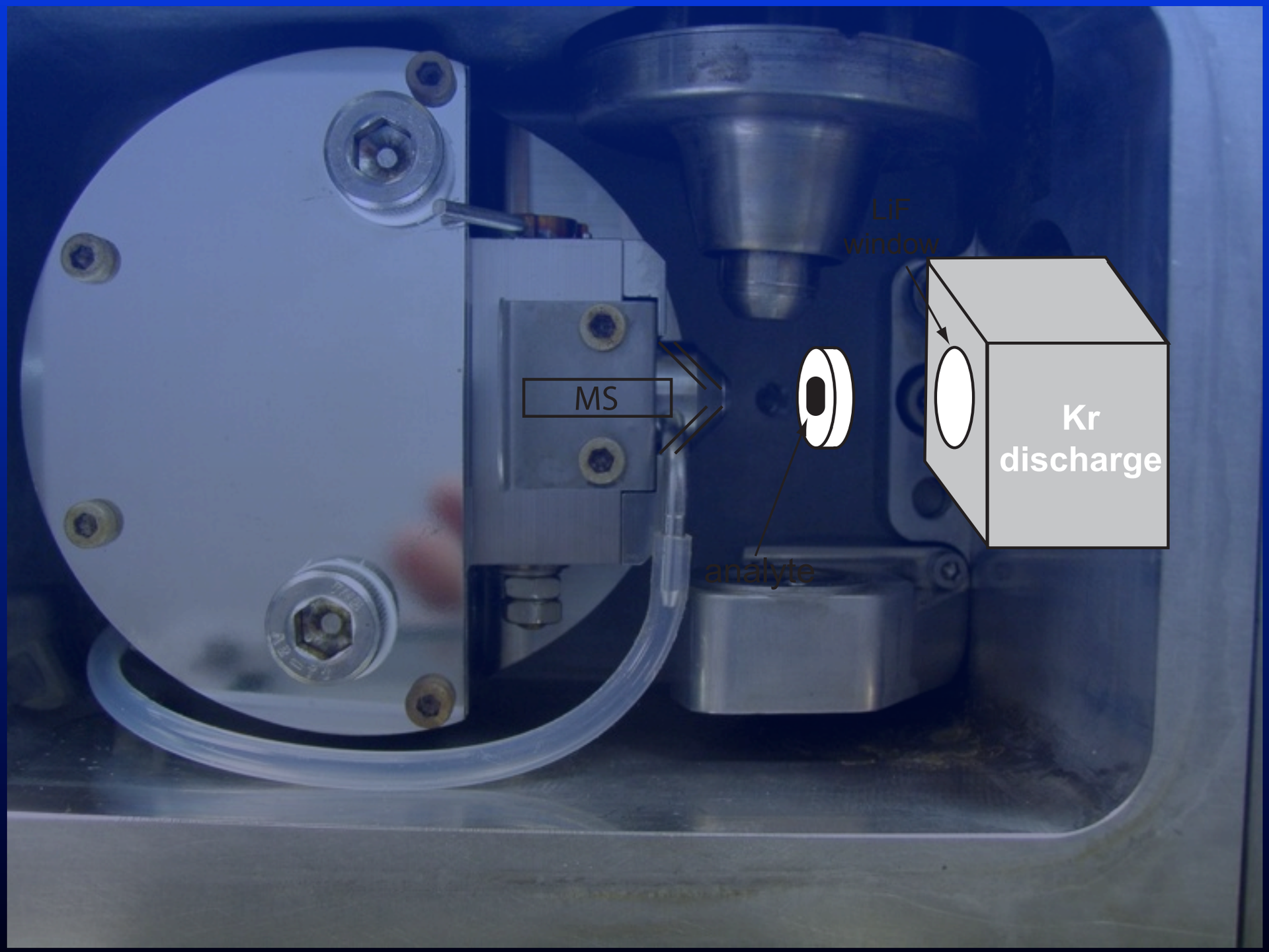
Carter research proposal VUV transparent Plate

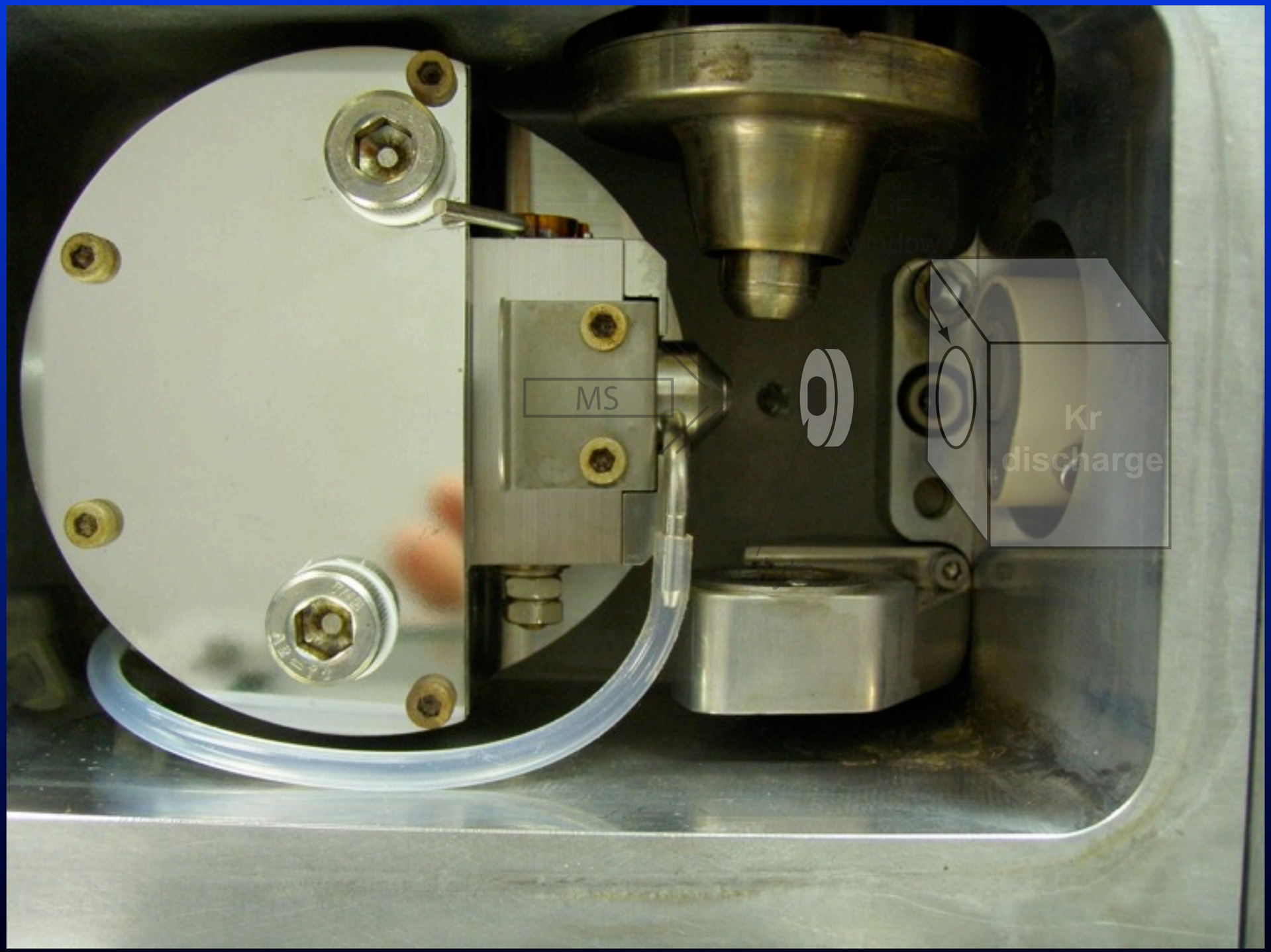


Sample evaporated on plate

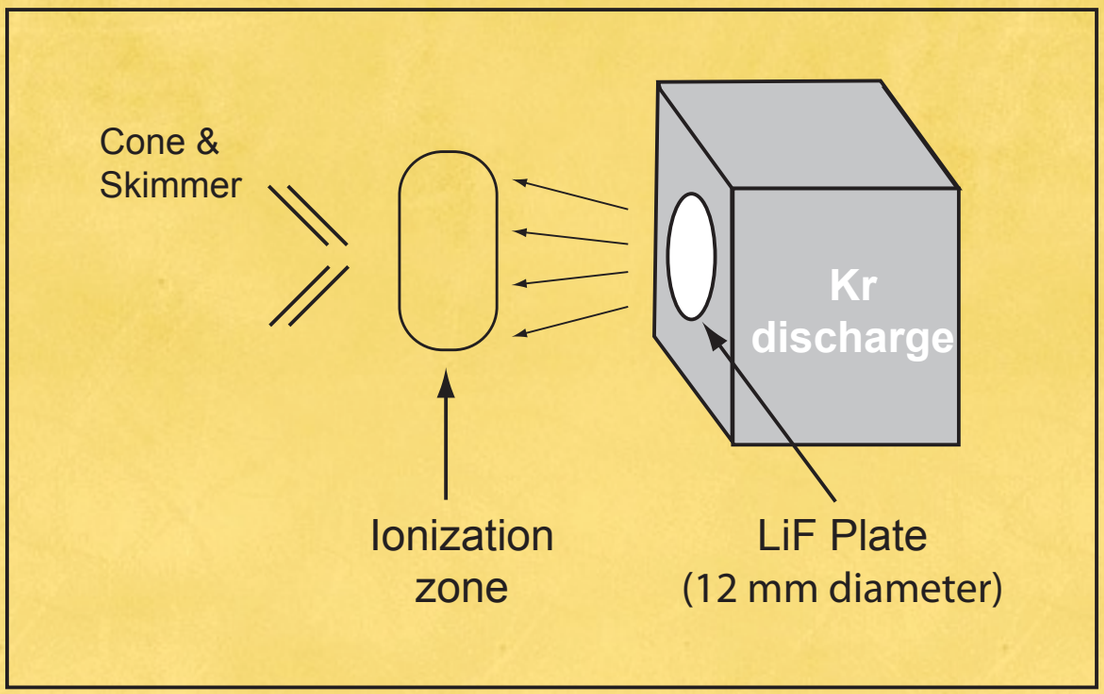
Carter research proposal VUV transparent Plate



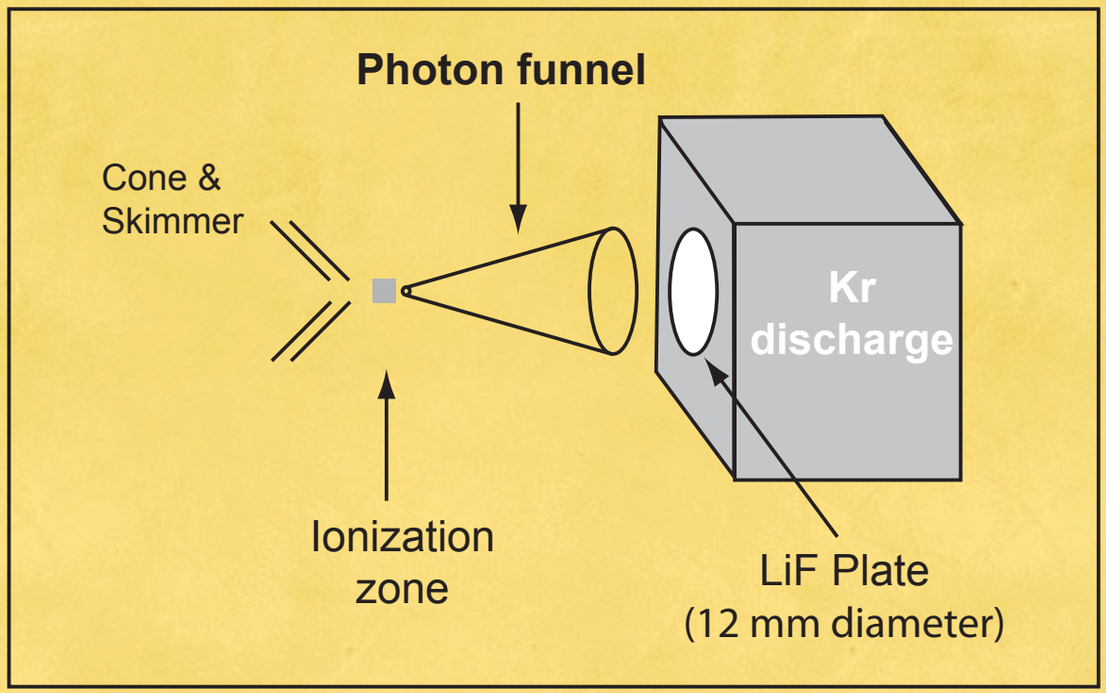
Carter research proposal VUV transparent Plate



Carter research proposal Photon Funnel



Current Orientation



Proposed Orientation

Funnel to focus photons

Carter research proposal Glow Discharge

Examine glow discharge mechanisms

1.) Penning ionization (excited Noble gas)
2.) proton transfer between hydronium produced by He & analyte
3.) Electron capture (e- released by Penning Ionization)
4.) Photo ionization

1.) Penning ionization (excited Noble gas)

$$Rg + e^- \rightarrow Rg^+ + 2\,e^- \rightarrow Rg^* + e^- \rightarrow Rg^* + A \rightarrow Rg + A^+ + e^-$$

2.) proton transfer between hydronium produced by He & analyte

$$He^* + H_2O \rightarrow H_2OH^+ + OH^- \rightarrow H_2OH^+ + A \rightarrow AH^+ + H_20$$

3.) Electron capture (e^- released by Penning Ionization)

$$He^* + N \rightarrow N^+ + He + e^- \rightarrow e^- + O_2 \rightarrow O_2^- + A \rightarrow [A\text{-}H]^- + OH$$

$$O_2^- + A \rightarrow A^- + O_2$$

4.) Photo ionization

$$h\nu + A \rightarrow A^+ + e^-$$

$$e^- + A \rightarrow A^-$$

Carter research proposal Glow Discharge

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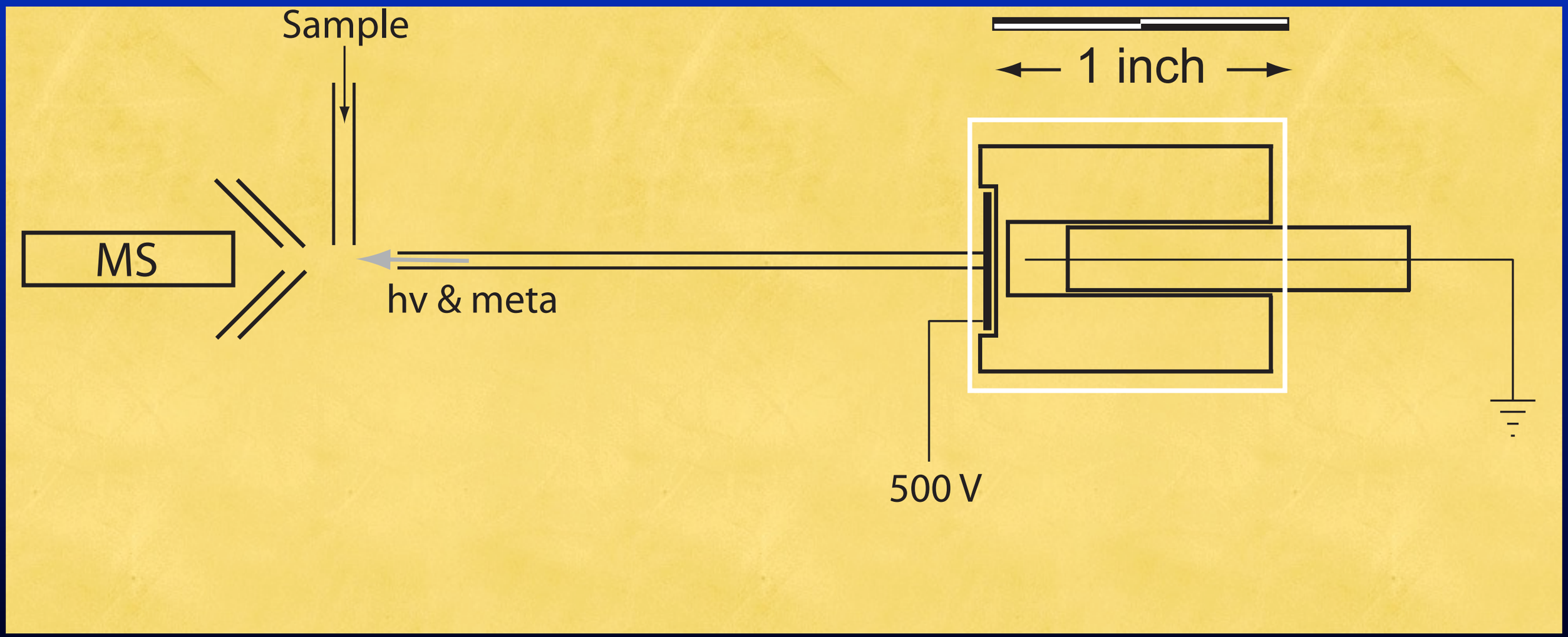
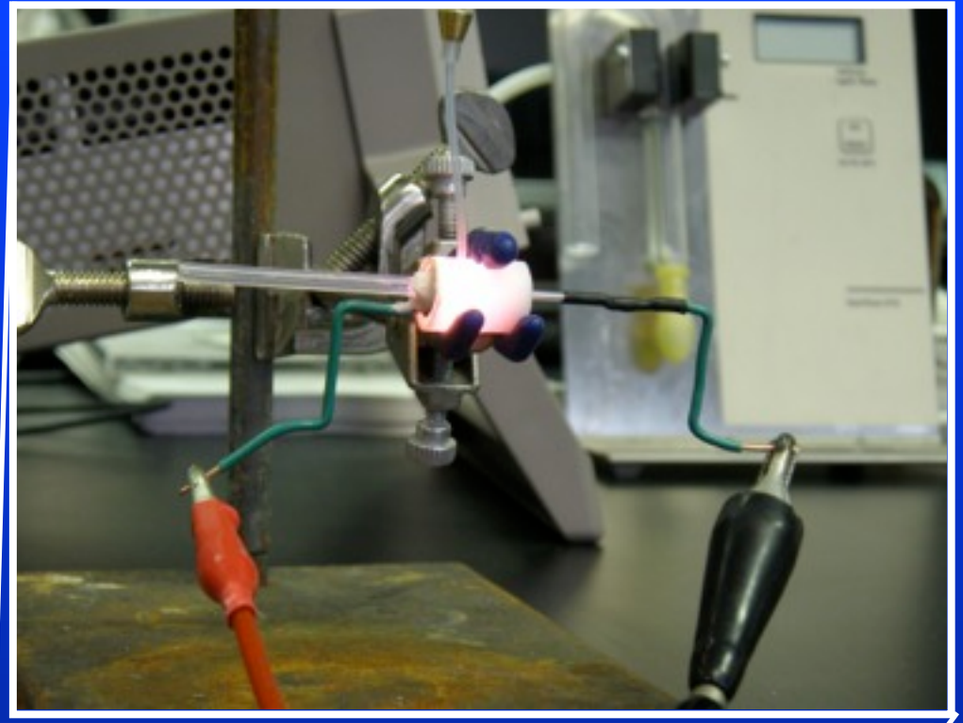
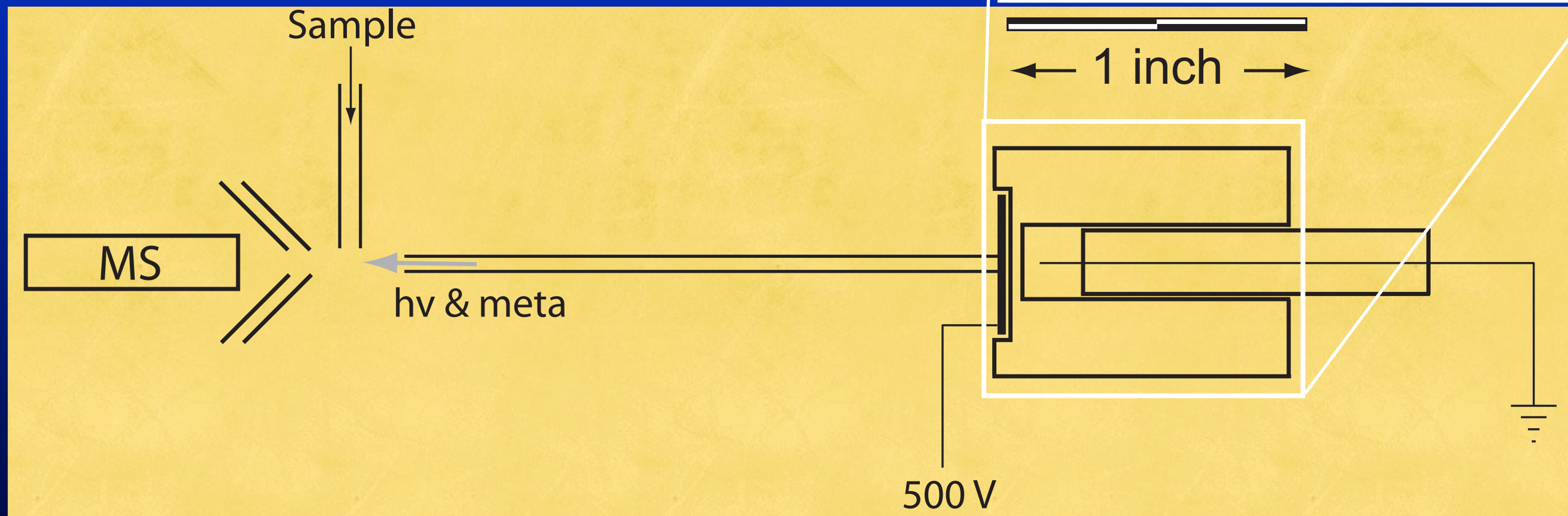
Carter research proposal Glow Discharge



Design to measure combination of all glow discharge ionization modes

Carter research proposal Glow Discharge





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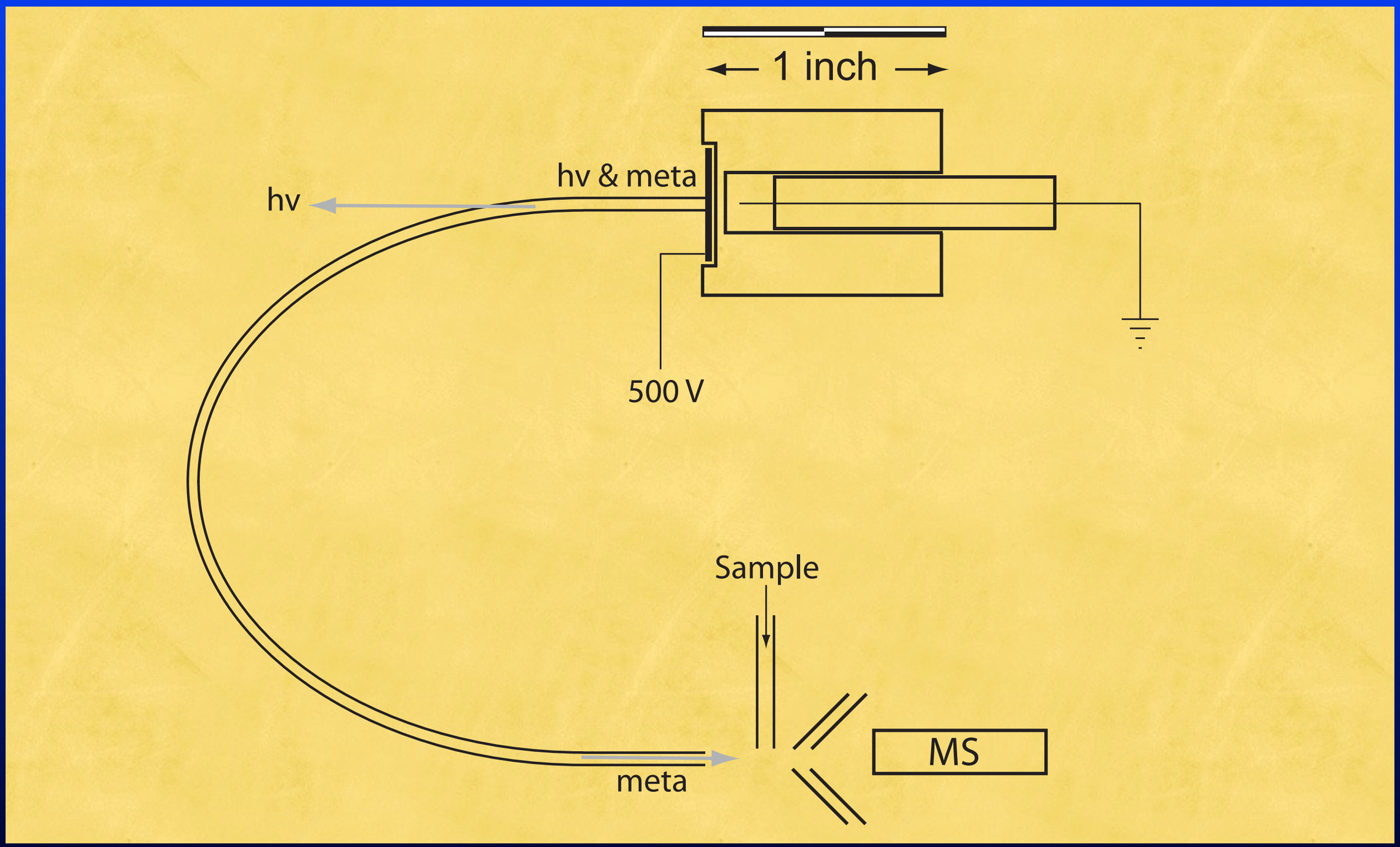
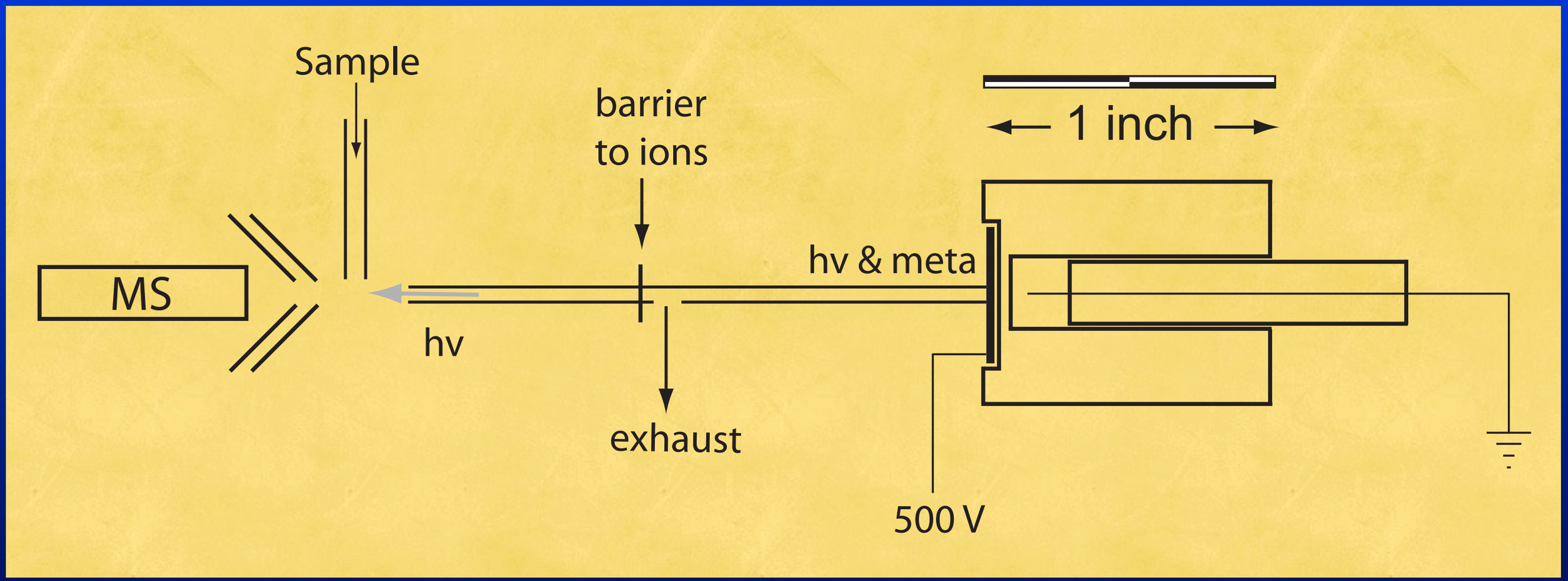


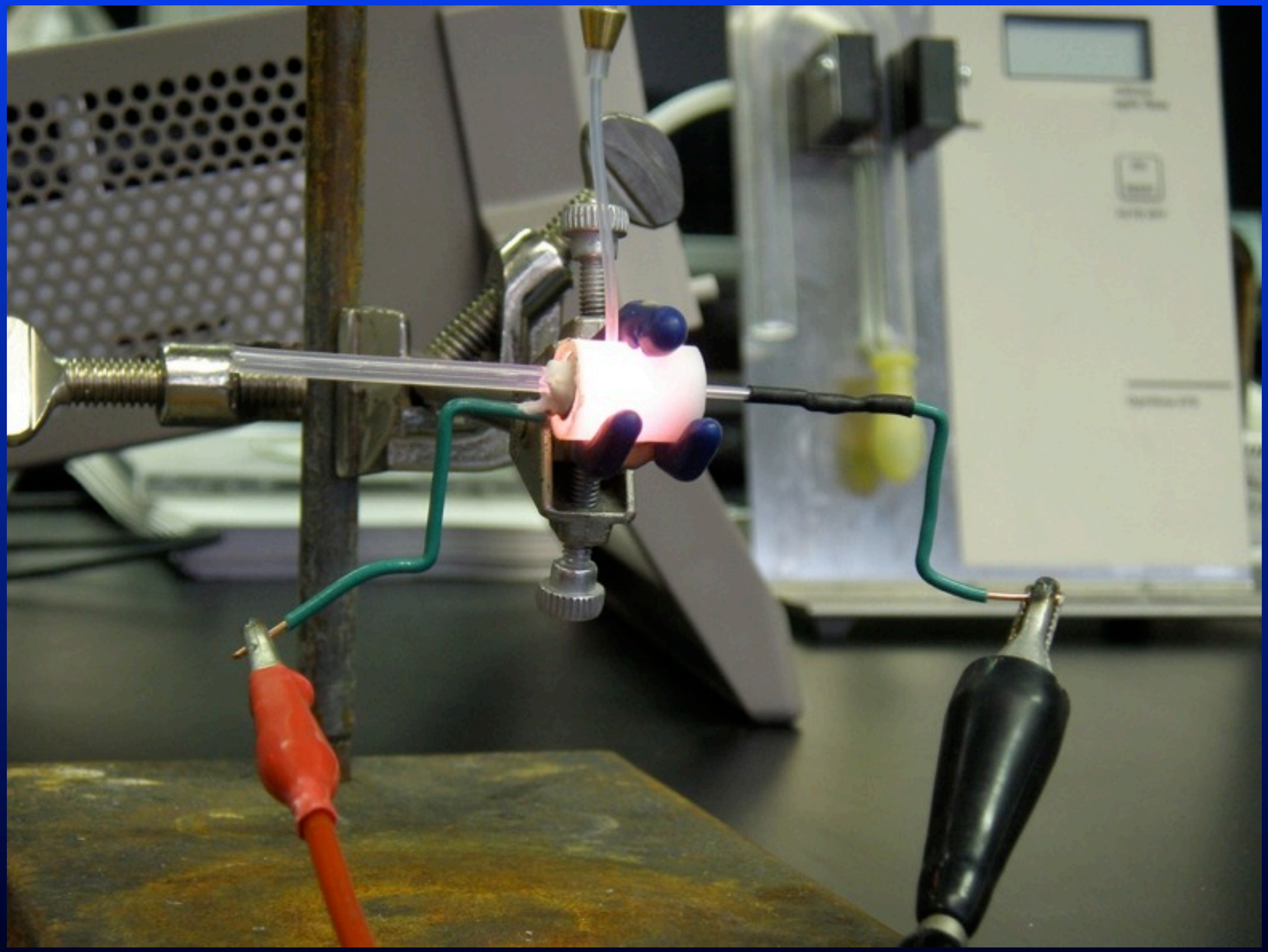
Design to measure ionization due to glow discharge metastable & ions

Carter research proposal Glow Discharge



Design to measure ionization due to glow discharge hv

Carter research proposal Glow Discharge



Carter research proposal review

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Questions

Thank you

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