GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ____

Project No./(Center No.) G-41-642 (R6351-0A0) GTRC/GIT DATE 7 / 23 / 87

Project Director: Dr. Edward W. Thomas School/GIT Physics

Sponsor: U.S. Department of Energy
Oak Ridge Operations, Oakridge, Tenn

Agreement No.: Grant No. DE-FG05-87ER13745

Award Period: From 7/1/87 To 6/30/90 (Performance) 9/30/90 Reports

Sponsor Amount:	New With This Change	Total to Date
Contract Value:	$ 231,972	$ 231,972
Funded:	$ 76,920	$ 76,920 /through 6/30/88

Cost Sharing No./(Center No.) G-41-369 (F6351-0A0) Cost Sharing: $ 47,617

Title: Metastable Enhancement of C+ and O+ Capture Reactions

ADMINISTRATIVE DATA

OCA Contact Brian J. Lindberg X4820

1) Sponsor Technical Contact:

Dr. J.V. Martinez
Division of Chemical Sciences
U.S. Department of Energy
19901 Germantown Road
Germantown, MD 20874
(301)353-5820

2) Sponsor Issuing Office:

Marlena Clark (615)576-7599
Contract Specialist
U.S. Department of Energy
Oak Ridge Operations
Procurement and Contracts Division
P.O. Box E, Oak Ridge, TN 37831

Military Security Classification: N/A
(or) Company/Industrial Proprietary: N/A

ONR Resident Rep. is ACO: ____ Yes X No
Defense Priority Rating: N/A

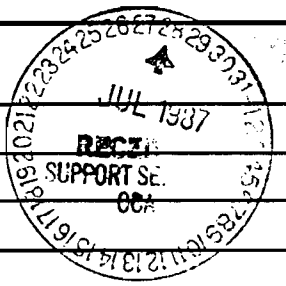
RESTRICTIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval — Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with GIT. However, sponsor retains the right to transfer ownership of any item of equipment having a unit acquisition cost of $1,000 or more.

COMMENTS:



SPONSOR'S I.D. NO. 02.141.002.86.R06

COPIES TO:

Project Director
Research Administrative Network
Research Property Management
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Procurement/GTRI Supply Services
Research Security Services
Contract Support Div.(OCA)(2) Pat
Research Communications
GTRC
Library
Project File
Other ____

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 09/19/90

Project No. G-41-642 Center No. R6351-0A0

Project Director THOMAS E W School/Lab PHYSICS

Sponsor US DEPT OF ENERGY/DOE OAK RIDGE - TN

Contract/Grant No. DE-FG05-87ER13745 Contract Entity GTRC

Prime Contract No.

Title METASTABLE ENHANCEMENT OF C+ AND O+ CAPTURE REACTIONS

Effective Completion Date 900831 (Performance) 900930 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	
Final Report of Inventions and/or Subcontracts	Y	
Government Property Inventory & Related Certificate	Y	
Classified Material Certificate	N	
Release and Assignment	Y	
Other	N	

Comments

Subproject Under Main Project No.

Continues Project No.

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

NOTE: Final Patent Questionnaire sent to PDPI.

A. Progress Report

The program objective is to study C^+ and O^+ charge transfer in gases (H, H_2 and He) separately for ground and metastable excited states of the projectile. Also we will study secondary electron ejection and particle ejection (sputtering) from surfaces by these same incident species to determine whether processes on surfaces are in any way influenced by the projectile being in a metastable state. Projectile energies are to be in the region of 20 eV to a few keV. The choice of experimental parameters, collision energy and chemical species, encompases circumstances where charge changing processes may be understood in terms of curve crossings in the temporary molecular state formed by the colliding species and where internal excitation is known to have a significant impact on cross sections. Moreover, the data are of interest to edge and wall conditions in Magnetic Fusion Energy Devices. Existing work in this area is due largely to Moran and Wilcox[1,2] who have shown how to prepare beams containing known fractions of metastable species and made accurate measurements for the charge transfer process in certain gases (including H_2 but excluding He) at energies from 500 to 2500 eV; metastable cross sections are 3 to 10 times greater than ground state but both have approximately the same energy dependence in this region. There is also some "rough" data[3] that shows the two cross sections become equal at about 10 keV energy. There is no published information on the surface collision processes. One would anticipate that at low impact energies, where cross section is closely related to energy defect one would observe significant

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1. T. F. Moran, J. P. Wilcox, J. Chem. Phys. 69, 1397 (1978).
2. T. F. Moran, J. P. Wilcox, J. Chem. Phys. 68, 2855 (1978).
3. J. M. Hoffman, G. H. Miller, G. J. Lockwood, Phys. Rev. A 25, 1930 (1982).

differences in magnitude and energy dependence between cross sections for ground and (metastable) excited states. It is these low energies that are the principal focus of the present work and they are of course of most relevance to MFE, reactive etching and other practical plasma related problems.

The work has progressed somewhat more slowly than expected. The original proposal was predicated on the assumption that we would have the services of Dr. C. F. Barnett (an adjunct faculty member, recently retired from ORNL) and the use of apparatus to be transferred to us from ORNL. While lack of both these items was forseen at the inception of the project, their impact had not been properly digested. Some modest changes to plans have been made, work is now well on track, and we forsee a more useful project than was originally envisaged. Prof. Tom Moran (School of Chemistry at this institution) is now working actively on the project instead of Barnett; it should be noted that Moran is the author of the two papers[1,2] that represent the sole existing study of metastable cross sections. An excellent, new, accelerator system has been constructed (and is operating) that is far more versatile (and simple) than the device which would have been obtained from ORNL. Collision measurements will be started shortly and will be well under-way before the end of the present contract period. Preliminary studies of metastable sputtering have been completed, are described below and reveal that metastable oxygen enhances chemical sputtering of C; this observation may be of some significance in the modelling of first wall conditions in MFE devices which employ carbon coated walls or limiters.

Low Energy Gas Phase Collisions

The general scheme of the experiment follows the very early work of

Turner et al.,[4] as developed by Moran and Wilcox[1,2]; it was extensively discussed in our original proposal and will not be reviewed here. Ions are produced in an electron impact source; control of electron energy determines the metastable fraction in the ion beam. Metastable fraction is assayed by analysis of ion beam attenuation in a gas cell; this same procedure also gives the charge transfer cross sections for ground and metastable species.

Construction of an ion source is quite straightforward and the main experimental challenge is producing a well defined ion beam of low energy. We had originally intended to use an ion accelerator similar to that of Van Zyl et al.,[5] where formation, focusing, and mass analysis of the ions is performed at high energy (1-2 keV) followed by decelleration and refocussing to the energy of interest. Such a system requires complex decelleration lenses and involves a fairly massive piece of equipment. Our original proposal envisaged eventually (year 3) a crossed C^+ (or O^+) + H experiment where the ion accelerator would be taken to an atomic H source (e.g., at ORNL). The accelerator originally envisaged would not be at all portable rendering the C^+ + H experiment mechanically very difficult.

We performed a general reappraisal of the design and have moved instead to a device that produces and analyzes the ions at low potential and accelerates them into the target at the required energy; this is to be compared with the original concept of producing ions at high energy and

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4. B. R. Turner, J. A. Rutherford, D. M. J. Compton, J. Chem. Phys. 48, 1602 (1968).

5. B. Van Zyl, N. G. Utterback, R. C. Amme, Rev. Sci. Instrum. 47, 814 (1976).

decellerating to the required energy. The device has been constructed with a simple source and a rf quadrupole as a mass analyzer. Ion currents of μA at 20 eV energy are routinely obtained; this easily meets our objectives for the critical and difficult low energy range. Beam currents are three orders of magnitude greater, and lowest energies one fifth lower, than those quoted via the decelleration approach.[5] The apparatus is compact and portable so it can readily be attached to an atomic H beam apparatus at some other location. Controls are simple, operation reliable. The equipment is far more satisfactory than the device envisaged in our original proposal.

We are currently designing the target gas cell (again a simple concept) and anticipate its fabrication within 30 days. Preliminary studies of attenuation should then start immediately. We expect first to repeat a few of Moran's earlier measurements[1,2] of C^+ and O^+ in H_2 at energies of 500 eV and above as a check of operation. The data would then be extended down to the lowest operating energies where cross sections will be very sensitive to internal excitation. We would expect to follow cross sections down to the threshold for charge transfer.

The remaining experimental concern is that angular scattering of projectiles at low energies may be large so that a significant fraction of the beam does not emerge through the exit aperture of the target gas cell. We have performed a number of theoretical estimates on the problem based on work by Inouye and Noda[6] which suggests that there should be no problems at energies down to 200 eV. In the following section we describe a strategy for assessing and if necessary overcoming the problem at lower energies.

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6. H. Inouye and K. Noda, Phys. Rev. A 24, 3261 (1981).

Surface Collisions

Considerable progress has been made on the study of how sputtering is influenced by the internal excitation of a projectile. We are using a commercial Secondary Ion Mass Spectrometer - or SIMS system by ATOMIKA of Munich. The cold cathode discharge source has been replaced by a filament source. We are tentatively assuming (and will check later) that the metastable content of the ion beam varies with electron energy in the same way as that shown by Moran and Wilcox.[1,2] The mass spectrum of ions ejected from a surface is monitored as a function of metastable content of the incident ion beam.

For the sputtering of Si the ejected species for ground and metastable O^+ impact are identical in magnitude and mass spectrum; moreover most of the ejected material is silicon and there is little evidence of oxide formation. This indicates that collisional ejection is related only to the energy of projectile impact; the mechanisms involve only physical (i.e., collisional) sputtering. This result was expected. For the case of a carbon target, however, the ejected flux includes a substantial component of CO and the oxide component is significantly higher for metastable ions than for the ground state; we assess the enhancement to be 100% (i.e., metastable O^+ is twice as efficient in ejecting CO than is ground state O). The ejection of CO is likely to be through "chemical" sputtering where the collision process leads to formation of a volatile species on the surface which is then thermally desorbed. Thus we would conclude that metastable O^+ impact produces an enhanced amount of CO leading in turn to a higher rate of erosion. This is a rather significant observation. In general terms it implies that chemical erosion/etching of surfaces may be enhanced by the excitation of the incoming species. Hints of this phenomenon come from reactive etching of micro-electronic device materials (principally Si etched by fluorides) where laser excitation is known to enhance etch rate.

These initial results are very promising and show at least that internal excitation influences chemical sputtering. Further work is required to properly document the enhancement and understand the chemistry of why CO formation is increased by metastable impact.

Georgia Tech

Office of Grants and Contracts Accounting

Georgia Institute of Technology
Lyman Hall/Emerson Building
Atlanta, Georgia 30332-0259
404•894•4624; 2629
Fax: 404•894•5519

November 2, 1989

Ms. Melissa Y. Johnson, Contract Specialist
U. S. Department of Energy-Oak Ridge Operations
Contract Management Branch
P. O. Box 2001
Oak Ridge, Tn 37831-8758

REFERENCE: Grant #DE-FG05-87ER13745

Dear Ms. Johnson,

Enclosed in triplicate is the Financial Status Report (SF-269) for Grant No. DE-FG05-87ER13745 covering the period July 1, 1988 through August 31, 1989.

If you should have questions or need additional information, please contact Geraldine Reese of this office at (404) 894-2629.

Sincerely,

David V. Welch
Director

DVW/GMR/djt

Enclosures

cc: Dr. E. W. Thomas, Physics 0430
Ms. Mary Wolfe, OCA 0420
File G-41-642/R6351-0A0

FINANCIAL STATUS REPORT

(Short Form)

(Follow instructions on the back)

1. Federal Agency and Organizational Element to Which Report is Submitted	2. Federal Grant or Other Identifying Number Assigned By Federal Agency	OMB Approval No.	Page	of
U. S. Department of Energy	DE-FG05-87ER13745	0348-0039	1	1 pages

3. Recipient Organization (Name and complete address, including ZIP code)

Georgia Tech Research Corporation
P. O. Box 100117
Atlanta, GA 30384

4. Employer Identification Number	5. Recipient Account Number or Identifying Number	6. Final Report	7. Basis
58-0603146	G-41-642/R6351-0A0	☐ Yes ☒ No	☒ Cash ☐ Accrual

8. Funding/Grant Period *(See Instructions)* From: (Month, Day, Year)	To: (Month, Day, Year)	9. Period Covered by this Report From: (Month, Day, Year)	To: (Month, Day, Year)
July 1, 1987	August 31, 1990	July 1, 1988	August 31, 1989

10. Transactions:	I Previously Reported	II This Period	III Cumulative
a. Total outlays	$62,258.32	$131,503.29	$193,761.61
b. Recipient share of outlays	34,968.96	36,328.92	71,297.88
c. Federal share of outlays	27,289.36	95,174.37	122,463.73
d. Total unliquidated obligations			6,467.38
e. Recipient share of unliquidated obligations			-0-
f. Federal share of unliquidated obligations			6,467.38
g. Total Federal share *(Sum of lines c and f)*			128,931.11
h. Total Federal funds authorized for this funding period			134,498.00
i. Unobligated balance of Federal funds *(Line h minus line g)*			$ 5,566.89

11. Indirect Expense

a. Type of Rate *(Place "X" in appropriate box)* ☐ Provisional ☐ Predetermined ☐ Final ☒ Fixed

b. Rate	c. Base	d. Total Amount	e. Federal Share
See Attached	MTDC	$49,565.26	$35,941.42

12. *Remarks: Attach any explanations deemed necessary or information required by Federal sponsoring agency in compliance with governing legislation.*

Questions pertaining to this report should be directed to: Geraldine Reese (404) 894-2629

GEORGIA TECH FISCAL YEAR ENDS JUNE 30

13. Certification: **I certify to the best of my knowledge and belief that this report is correct and complete and that all outlays and unliquidated obligations are for the purposes set forth in the award documents.**

Typed or Printed Name and Title	Telephone (Area code, number and extension)
David V. Welch, Director Office of Grants and Contracts Accounting	(404) 894-2629
Signature of Authorized Certifying Official	**Date Report Submitted**
	November 2, 1989

Previous Editions not Usable

Standard Form 269A (REV 4-88)
Prescribed by OMB Circulars A-102 and A-110

Attachment

U. S. Department of Energy
Grant # DE-FG05-87ER13745
July 1, 1988 through August 31, 1989

G-41-642/R6351-0A0

	Direct Costs	Indirect Costs
FY'88 @ 60.0%	$17,055.85	$ 10,233.51
FY'88 @ 60.0%	43,133.91	25,880.34
FY'90 @ 62.5%	16,098.53	10,061.59

REPORT PERIOD

	Direct Costs	Indirect Costs
07/01/88-06/30/89	$43,133.91	$25,880.34
07/01/89-08/31/89	16,098.53	10,061.59

DOE F538 (5-86)

OMB Control No. 1910-1400

U. S. DEPARTMENT OF ENERGY

NOTICE OF ENERGY RD&D PROJECT

1. Descriptive TITLE of work (150 characters including spaces)

METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS

2. CONTRACT or grant number: DE-FG05-87ER 13745

2A. MASTER contract number (GOCO's):

2B. Responsible PATENT office: OAK RIDGE

3. Performing organization CONTROL number (internal): G-41-642

3A. Budget and Reporting code:

3B. Funding YEAR for this award:

4. Original contract start date: 7/1/87

4A. Current contract start date: 30/9/90

4B. Current contract close date: 30/9/90

4C. Anticipated project termination date: 30/9/90

5. Work STATUS

- ☐ Proposed
- ☒ Renewal
- ☐ New
- ☐ Terminated

5A. Manpower (FTE): 1.22

5B. CONGRESSIONAL district: 5th

5C. STATE or Country where work is being performed: GEORGIA

5D. COUNTRY sponsoring research: USA

6. Name of PERFORMING organization: GEORGIA INSTITUTE OF TECHNOLOGY

6A. DEPARTMENT or DIVISION	6B. Street Address	6C. City, State, Zip Code
PHYSICS	GEORGIA INSTITUTE OF TECHNOLOGY	ATLANTA, GA 30332

7. Circle only one code for TYPE of Organization Performing R&D:

(CU) - College, university, or trade school
FF - Federally funded RD&D centers or laboratory operated for an agency of the U. S. Government
IN - Private industry
NP - Foundation or laboratory not operated for profit
ST - Regional, state or local government facility
TA - Trade or professional organization
US - Federal agency
XX - Other
EG - Electric or gas utility

8A. Contractor's PRINCIPAL INVESTIGATOR/s or project manager Name/s (Last, First, MI): THOMAS EDWARD W.

8B. PHONE/s (in order of PI names with commercial followed by FTS)

Comm. (404) 894-5200 ; FTS --- ; Comm. --- ; FTS ---

8C. PI/s address (if different from that of Performing Organization)

SAME

9. DOE SUPPORTING Organization (DOE Assistant Secretary and office sponsoring the work; technical monitor; and administrative monitor).

9A. PROGRAM division or office
(full name) DIVISION OF CHEMICAL SCIENCES — Program Office Code

9B. TECHNICAL monitor (Last, First, MI) MARTINEZ JOE V.

9C. Address U.S. DOE
19901 GERMANTOWN ROAD
GERMANTOWN, MD 20874

9D. Phone Comm. (301) 353-5820
FTS

9E. ADMINISTRATIVE monitor (Last, First, MI) CLARK, MARLENA

10. FUNDING in thousands of dollars (K$). Funds represent budget obligations for operating and capital equipment (FY runs October 1 – September 30).

Funding organization(s)	Current FY 90	Next FY ____
A. DOE	$ 57,417	0
B.		
C.		

10D. Does the current FUNDING cover more than one year's work? Yes ____ No X

E. If yes, provide dates (from when to when). ____

11. Descriptive SUMMARY of work. Enter a Project Summary using complete sentences limited to 200 words covering the following: Objective(s), state project objectives quantifying where possible (e.g., "The project objective is to demonstrate 95% recovery of sulphur from raw gas with molten salt recycling at a rate of one gallon per minute."); approach, describe the technical approach used (how the work is to be done); expected product/results, describe the final products or results expected from the project and their importance and relevance.

The project objective is to measure cross sections for neutralization of metastable C^+ and O^+ in H_2 and H targets. The result is important to the understanding of impurity ion transport in the edge of Thermonuclear Plasmas. Cross sections for metastables in H_2 are 10 to 20 A^2 at eV energies; twenty times that of the ground state. As energy increases the two cross sections become equal above about 20 KeV. The high metastable cross section may be due to an accidental energy resonance in the target H_2^+ state. Discrepancies between previously published reports are due to use of mixed metastable and ground state beams and failure to account for the different processes.

The experiments are being repeated for an atomic H target; a far more complex experimental problem. Here no resonance is anticipated and metastable cross sections are likely to be much lower.

12. PUBLICATIONS available to the public. List the five most descriptive publications that have resulted from this project in the last year that are available to the public. (Include author, title, where published, year of publication, and any other information you have to complete full bibliographic citation.) Use the back of this form or additional sheets if necessary.

None this last year.

13. KEYWORDS (Listed five terms describing the technical aspects of the project. List specific chemicals and CAS number, if applicable.)

Capture C^+, O^+, Metastable, Collisions

4. RESPONDENT. Name and address of person filling out the Form 538. Give telephone number, including extension (if you have FTS number, please include it) at which person can be reached. Record the date this form was completed or updated. The information in Item 14 will not be published.

Respondent's Name: EDWARD W. THOMAS Phone No.: (404) 894-5200 Date: Sept. 12, 1989

Street: SCHOOL OF PHYSICS, GEORGIA TECH

City: ATLANTA State: GA Zip: 30332

15. Additional space for furnishing information in items 1 to 14. (Indicate item numbers to which answers apply.)

Item No.	

NOTICE: Return this form to the office indicated in the reporting requirements for your award agreement covering this project. If you have completed a similar programmatic office project description during the current Fiscal Year, complete only the new data elements on this form and send it and a copy of the description completed earlier to Department of Energy, Office of Scientific Information, P. O. Box 62, Oak Ridge, TN 37831.

DOE F538 (5-86)

OMB Control No. 1910-1400

U. S. DEPARTMENT OF ENERGY

NOTICE OF ENERGY RD&D PROJECT

1. Descriptive TITLE of work (150 characters including spaces)
   Metastable Enhancement of C^+ and O^+ Capture Reactions

2. CONTRACT or grant number: DE-FG05-87ER13745
   2A. MASTER contract number (GOCO's):
   2B. Responsible PATENT office: Oak Ridge

3. Performing organization CONTROL number (internal): G-41-642
   3A. Budget and Reporting code:
   3B. Funding YEAR for this award: FY 88

4. Original contract start date: 7/1/87
   4A. Current contract start date: 7/1/87
   4B. Current contract close date: 6/30/88
   4C. Anticipated project termination date: 6/30/90

5. Work STATUS
   ☐ Proposed ☐ Renewal
   ☒ New ☐ Terminated
   5A. Manpower (FTE): 1.22
   5B. CONGRESSIONAL district: 5th
   5C. STATE or Country where work is being performed: Georgia
   5D. COUNTRY sponsoring research: USA

6. Name of PERFORMING organization: Georgia Institute of Technology

6A. DEPARTMENT or DIVISION	6B. Street Address	6C. City, State, Zip Code
Physics	Georgia Institute of Technology	Atlanta, GA 30332

7. Circle only one code for TYPE of Organization Performing R&D:

(CU) - College, university, or trade school
FF - Federally funded RD&D centers or laboratory operated for an agency of the U. S. Government
IN - Private industry
NP - Foundation or laboratory not operated for profit
ST - Regional, state or local government facility
TA - Trade or professional organization
US - Federal agency
XX - Other
EG - Electric or gas utility

8A. Contractor's PRINCIPAL INVESTIGATOR/s or project manager Name/s (Last, First, MI): Thomas, Edward W.

8B. PHONE/s (in order of PI names with commercial followed by FTS)
Comm. 404-894-5200 ; FTS -- ; Comm. -- ; FTS --

8C. PI/s address (if different from that of Performing Organization)
same

9. DOE SUPPORTING Organization (DOE Assistant Secretary and office sponsoring the work; technical monitor; and administrative monitor).

9A. PROGRAM division or office
(full name) Division of Chemical Sciences — Program Office Code

9B. TECHNICAL monitor (Last, First, MI) Martinez, Joe V.

9C. Address U. S. DOE
19901 Germantown Rd.
Germantown, MD 20874

9D. Phone Comm. (301) 353-5820
FTS

9E. ADMINISTRATIVE monitor (Last, First, MI) Clark, Marlena

10. FUNDING in thousands of dollars (K$). Funds represent budget obligations for operating and capital equipment (FY runs October 1 – September 30).

Funding organization(s)	Current FY 88	Next FY 89
A. DOE	76,920	75,285
B.		
C.		

10D. Does the current FUNDING cover more than one year's work? Yes ____ No x

E. If yes, provide dates (from when to when). ____

11. Descriptive SUMMARY of work. Enter a Project Summary using complete sentences limited to 200 words covering the following: Objective(s), state project objectives quantifying where possible (e.g., "The project objective is to demonstrate 95% recovery of sulphur from raw gas with molten salt recycling at a rate of one gallon per minute."); approach, describe the technical approach used (how the work is to be done); expected product/results, describe the final products or results expected from the project and their importance and relevance.

It is anticipated that capture cross sections for C^+ and O^+ will differ greatly depending on whether the initial ion species is in a ground or metastable excited state. The difference is at least an order of magnitude and therefore has a substantial bearing on the modelling of impurity C^+ and O^+ transport in the edge plasma of Tokamaks. We propose to prepare beams of known metastable and ground state composition which will then be used to measure electron capture reactions in H_2, He and H at energies from 20 to 1000eV. Of particular interest is $O^+ + H \rightarrow O + H^+$ where the reaction is accidentally resonant when the O^+ is in the metastable state; the reaction should have a very large cross section at low energies and represents a challenging problem for theoretical treatment.

We propose also to study how the metastable species of C^+ and O^+ interact with surfaces. Secondary electron ejection by potential processes is governed in part by exchange processes and should differ greatly between metastable and ground states. Chemical erosion of carbon by O^+ will also be studied to determine whether the initial excited state of the O^+ influences the erosion rate.

12. PUBLICATIONS available to the public. List the five most descriptive publications that have resulted from this project in the last year that are available to the public. (Include author, title, where published, year of publication, and any other information you have to complete full bibliographic citation.) Use the back of this form or additional sheets if necessary.

None. This is a new project.

13. KEYWORDS (Listed five terms describing the technical aspects of the project. List specific chemicals and CAS number, if applicable.)

Capture, C^+, O^+, Metastable, Collisions

14. RESPONDENT. Name and address of person filling out the Form 538. Give telephone number, including extension (if you have FTS number, please include it) at which person can be reached. Record the date this form was completed or updated. The information in Item 14 will not be published.

Respondent's Name: Edward W. Thomas Phone No.: 404-894-5200 Date: July 29, 1987

Street: School of Physics, Georgia Tech

City: Atlanta State: GA Zip: 30332

15. Additional space for furnishing information in items 1 to 14. (Indicate item numbers to which answers apply.)

Item No.	

NOTICE: Return this form to the office indicated in the reporting requirements for your award agreement covering this project. If you have completed a similar programmatic office project description during the current Fiscal Year, complete only the new data elements on this form and send it and a copy of the description completed earlier to Department of Energy, Office of Scientific Information, P. O. Box 62, Oak Ridge, TN 37831.

"METASTABLE ENHANCEMENT OF

C^+ AND O^+ CAPTURE REACTIONS"

DOE F 1332.16 (10-84)
(Formerly RA-427)

OMB Approval
No. 1910-1400

U. S. DEPARTMENT OF ENERGY

UNIVERSITY CONTRACTOR, GRANTEE, AND COOPERATIVE AGREEMENT RECOMMENDATIONS FOR ANNOUNCEMENT AND DISTRIBUTION OF DOCUMENTS

See Instructions on Reverse Side

1. DOE Report No.
DOE/ER/13745-2

2. DOE Contract No.
DE-FG05-87ER13745

3. Title
Metastable Enhancement of C^+ and O^+ Capture Reactions

4. Type of Document ("x" one)
- [X] a. Scientific and technical report
- [ ] b. Conference paper:
  - Title of conference _____
  - Date of conference _____
  - Exact location of conference _____
  - Sponsoring organization _____
- [ ] c. Other (Specify) _____

5. Recommended Announcement and Distribution ("x" one)
- [X] a. Unrestricted unlimited distribution.
- [ ] b. Make available only within DOE and to DOE contractors and other U. S. Government agencies and their contractors.
- [ ] c. Other (Specify) _____

6. Reason for Recommended Restrictions

7. Patent and Copyright Information:
Does this information product disclose any new equipment, process, or material? [X] No [ ] Yes If so, identify page nos. _____
Has an invention disclosure been submitted to DOE covering any aspect of this information product? [X] No [ ] Yes
If so, identify the DOE (or other) disclosure number and to whom the disclosure was submitted.
Are there any patent-related objections to the release of this information product? [X] No [ ] Yes If so, state these objections.
Does this information product contain copyrighted material? [X] No [ ] Yes
If so, identify the page numbers _____ and attach the license or other authority for the government to reproduce.

8. Submitted by — Name and Position (Please print or type)
E. W. Thomas

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DOE/ER/13745-2

METASTABLE ENHANCEMENT OF C+ AND O+ CAPTURE REACTIONS

ANNUAL REPORT

PERIOD COVERED 7/1/88 THROUGH 6/30/89

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10 MAY 1989

Prepared for:

U. S. DEPARTMENT OF ENERGY
DIVISION OF CHEMICAL SCIENCES
OFFICE OF BASIC ENERGY SCIENCES
CONTRACT NO: DE-FG05-87ER13745

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METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS

ABSTRACT

The project seeks to study the charge capture reactions of C^+ and O^+ in various gases (principally H_2 and He) to determine the difference between cross sections for the ground and metastable excited states of the projectile species. Emphasis is on very low energy collisions close to threshold and data in practise extends over collision energies from 10 to 500 eV; comparison can be made with data from other sources at higher energies. In general terms cross sections for the metastable species are higher by a factor of ten than for the ground state at low energies (10 eV), are surprisingly invariant with energy, are approached by the ground state cross sections at about 10^5 eV, after which both cross sections fall. We have shown also that the metastable content of C^+ and O^+ fluxes produced by dissociative ionization of various carbon containing molecules is 15 to 30%.

We conclude that in the consideration of a situation involving neutralization of C^+ and O^+ (as for example in the edge of a fusion plasma) the metastable content may be high and will influence the net cross section significantly. Present data is not always in agreement with previously published results.

INTRODUCTION

The majority of charge transfer reactions studied to date have assumed that only ground state ions contribute to the formation of the product species. In the case of C^+ and O^+ ions it is well known that there are long lived metastable species that may be created in some abundance by a process of electron induced dissociation of molecules. These metastables, as we will see shortly, may have transfer neutralization cross sections that are an order of

magnitude greater than the ground state at low energies (0.01 to 1 keV). We shall also demonstrate that the metastable fluxes range from 15 to 30% of the total ion production by dissociation and are therefore quite significant.

The present project studies, experimentally, the charge transfer neutralization of C^+ and O^+ in gases (principally H_2 and He) at low energies (10 to 500 eV) where cross section differences between metastable and ground states are expected to be most significant. The reactions are probably best described in terms of an adiabatic energy diagram of the complex formed by the incoming and target species. By selecting first the ground state alone and then the metastable state alone, as the incoming species, one is probing two separate state selected input channels, involving significantly different energy defects for the mechanism. Comparison of these results should possibly give some insignt into the details of the transfer process at energies close to threshold.

A major motivation for these studies is to contribute to the understanding of charge balance effects in the edge of a fusion plasma. C^+ and O^+ ions are significant impurities in a fusion device and as they emerge to the plasma edge undergo transfer neutralization in the cold H_2 gas giving rise to cold H_2^+ which in turn may recycle into the main device volume giving rise to reduction of ion temperature. The C^+ and O^+ fluxes will probably contain significant fractions of metastable species the cross sections for which may be an order of magnitude higher than for the ground state. Thus the principal contribution to the production of cold H_2^+ is likely to be neutralization of the minor metastable component rather than neutralization of the major ground state component. To properly model the situation and to ascertain the maximum level of impurities that may be tolerated one needs to base the anlysis on the metastable ion behaviour rather than ground state. A motivation for the

present work is to provide a basis for estimating the possible metastable content of the ion fluxes and to determine the cross sections so that plasma edge modelling might be more complete. The relevant energy range is from zero to some hundreds of eV and is largely determined by acceleration of the ions in the plasma sheath. There is no previous work in this region although it is here that cross sections for ground and metastable states are likely to be most significantly different. There is some data at higher energies (500 eV to 10^5 eV) but often there are discrepancies between different reports. Of even more concern is the availability in the literature of cross section data obtained without analysis of metastable content; these may be just plain misleading and lead to a completely erroneous conclusions. The objective of the present work is to clear up the potential confusion and to provide a proper basis for device modelling.

PROGRESS TO DATE AND ORGANIZATION OF THE REPORT.

The objective of the present reporting period was to study charge transfer neutralization of C^+ and O^+ ions in H_2 and He at energies from 10 eV (or lower) to 500 eV with separate measurements of the ground and metastable excited state cross section. We also found it desireable to investigate briefly the fraction of ions in the metastable state produced by electron impact dissociation of a variety of molecular species; this gives an indication of how significant the metastable content might be in various situations. These objectives have been largely achieved and are being brought to a conclusion by the writing of a group of papers for publication. We have chosen to present our report as a group of publication drafts, appended hereto as Appendixes A, B, C and D. We will report the progress to date in summary form with frequent reference to these appendixes.

EXPERIMENTAL TECHNIQUE

The experimental arrangment and operational technique is outlined in Appendix A. The facilities consist of an electron impact ion source, a quadrupole mass analyzer to define projectile species, a target cell through which the beam proceeds, followed by a detector to monitor the transmitted ion flux by pulse counting. The whole system is collinear, exhibits a high transmission efficiency and is designed to operate at very low ion energies.

The ion flux transmitted through the gas cell is monitored as a function of gas pressure; beam attenuation is due to charge transfer neutralization of the ions and from the attenuation one may determine the neutralization cross section. If two projectile species are present, for example a ground and metastably excited ion, with significantly different cross sections, then the attenuation behavior includes two rates that can be separately unfolded to give the separate cross sections. The technique does not work if there are two (or more) species present whose cross sections are almost the same.

Use of a controlled energy electron impact ion source allows us to select the energy at which a source gas (e.g. CO) is dissociated. Dissociation processes are well understood. It is possible to select a dissociation energy where only ground state ion species will be created so that cross section measurements may be made on that species alone. One may then elevate the dissociation energy above the threshold for metastable formation and create a mixed beam of ground and metastable species. From this one may measure both the cross sections for ground an metastable states at once and also evaluate the ratio of ground and metastable flux densities.

It is possible, depending on source energy, that mixed metastable and ground state beams might contain a fraction of ions in excited states above the metastable level. In our experiment the flight time to the collision

region is sufficiently long that such states will have undergone normal radiative decay before they enter the collision cell. Thus we are quite confident that the incident beam contains only metastable and ground state species or, if below the metastable threshold, only the ground state alone.

Controlled electron impact ion sources must operate under single collision conditions and produce only very small fluxes of ions. For this reason we must operate with a pulse counting detector system. Low fluxes of ions are in fact necessary for very low energy experiments where space charge blow-up of ion beams might be a problem.

The gas CO is used in the ion source for production of C^+ beams. It had been intended to use O_2 for production of O^+ beams. We have found, however, that the CO source gas produces sufficent quantities of O^+ and that control of metastable population is quite easy; consequently the CO has been use for both species.

METASTABLE FRACTIONS

As a sideline activity we undertook a brief study of the metastable fractions of ions produced in the electron impact dissociation of various carbon containing molecules; this is described in Appendix B. For six precursor molecules containing C, O, and H, the metastable fraction is in the range 0.22 (C_6H_6) to 0.29 (CH_3OH). The only molecule to stand significantly outside this range is CH_3CN where the fraction is quite low at 0.15. We have not yet determined why this low fraction occurs.

In general terms one might conclude that the metastable fraction of C^+ ions produced by dissociation of the contaminant species anticipated in a fusion plasma, or of precursors that one might expect to use in a simple ion source, are likely to be in the region of 0.22 to 0.29 or about one quarter of

the total ion flux.

NEUTRALIZATION OF C^+ IN H_2

The results for this case have now been fully documented and are complete; they are shown in Appendix A. The measured cross section are in the energy range 10 to 500 eV, lower than anything presented in the past. Comparing with data from four other groups at higher energies we find that all the published data is consistent within error limits giving a comprehensive picture from 10 to 10^5 eV. At low energies (10 to 100 eV the metastable cross section is about 5 A^2 and the ground state about a factor of ten lower. As energy increases toward 10^5 eV the ground state cross section increases regularly towards a value of 10 A^2 while the metastable state increases by only a factor of two to equal the ground state cross section. At yet higher energies the two cross sections fall, and are identical so that there is no difference between the neutralization behaviour of the ground and metastable states.

The cross section behaviour can be broadly understood interms of the energetics of the reactions. Electron transfer from H_2 to neutralize the metastable is almost resonant with the formation of the post collision H_2^+ in the fourth vibrational state; so cross sections are expected to be high. By contrast the neutralization of the ground state is a reaction that is 4.17 eV endothermic and therefore would be expected to have a much lower cross section; this should increase with impact energy as we observe. It is not immediately clear why the cross section for the metastable neutralization should remain almost constant with energy but this might be due to competition in the formation of different post collision state in the H_2^+ ion; this present experiment does not define the post collision state.

NEUTRALIZATION OF C^+ IN HE

Our experience with this case is limited. The cross section is exceedingly small, less than 0.1 A^2, and therefore lower than any of the other cross sections we have attempted to measure; measurement will be very sensitive to trace impurities in the gas cell and accelerator. It is not clear whether that case can be reliably measured with the present arrangement. Our limited conclusions on the case are given in Appendix C.

NEUTRALIZATION OF O^+ IN H_2.

Our results on this case are quite smilar to the experience on neutralization of C^+ with low cross sections for the ground state (about 0.5 to 0.6 A^2) and metastable cross sections about ten times higher. A major practical problem here is that the present data, previous work by Moran and Wilcox (at 0.6 to 3 keV), and work by Hoffman et al. (3.1 to 99 keV), are not in agreement at the places where they overlap in energy. Differences in one case are a factor of ten. It is not at all clear why this problem occurs since the same groups of authors are in apparent agreement for data on the C^+ case taken with identical experimental procedures. While we are confident in the present data the matter remains under review.

SUMMARY

The data for neutralization of C^+ and O^+ in H_2 seems quite satisfactory and shows that the metastable state gives rise to very large cross sections. The data has been extended to much lower energies than in the past and is directly applicable to the regime for modelling the fusion plasma edge region. The data for the same processes in He is somewhat unclear. Nevertheless it is quite certain that the cross sections are very small and neutralization in He

(the reaction ash) for a fusion device is probably irrelevant.

PERSONNEL

Co-Principal investigators on the project during the reporting period were Prof. Thomas Moran of the School of Chemistry and Prof. Edward W. Thomas of the School of Physics. The project involved two graduate students, Mr. R. Whelton of Physics and Mr. Yaodong Xu of Chemistry. Mr. James Cagle of Physics also assisted in technical matters.

PUBLICATIONS

No publications were submitted during the present reporting period. We are at the present time, however, preparing Appendixes A, B and D as papers for publication.

APPENDIX A

REACTIONS OF GROUND $C^+(^2P)$ AND METASTABLE $C^+(^4P)$ IONS WITH H_2 MOLECULES

INTRODUCTION

The majority of charge transfer reactions measured to date have assumed that only ground state ions contribute to the formation of product species. However, ion beams formed by high energy electron impact ionization may contain a component of long lived excited states and these states may significantly affect measured cross sections.

Early experiments of Lindholm and co-workers [1,2] have shown the C^+ ions, produced by electron impact ionization of CO, are formed in both the ground ^2P state and the excited ^4P state. These workers [1,2] employed a tandem mass spectrometric apparatus in which ionic products from organic molecule decompositions have been monitored after collisions with mass analyzed C^+ ion beams. The features of this product ion spectra led these investigators to the conclusion that the abundances of $C^+(^2P)$ and $C^+(^4P)$ state ions were approximately 0.6 and 0.4 respectively. THe state distribution of ions in a C^+ beam has been examined also by Lao et al [3] who used a beam attenuation technique to measure a relative abundances of 0.68 and 0.32 for $C^+(^2P)$ and $C^+(^4P)$ ions formed by 100 eV ionization of CO. Nagatani et al [4] have estimated that 20% of the C^+ ions produced by 70 eV electron impact of CO_2 are formed in the ^4P state.

The purpose of the present paper is to report the results of an examination of charge transfer reactions of both ground and excited state C^+ ions with H_2 at low ion kinetic energies.

EXPERIMENTAL

A schematic diagram of the experimental apparatus used in this investigation is shown in Fig.1. The reactant C^+ ions have been formed by 100 eV electron impact ionization of high purity CO in a Nier type ion source. The ionizing electrons have been emitted from a directly heated tungsten filament, collimated into a beam, and accelerated into the source where ionization occurs. The ionizing electron beam current has been stabilized using an electron trap current / filament current feedback circuit control supply. The energy of ionizing electrons has been determined by applied voltages and checked by measurement of the known Ar and CO ionization potentials. Care has been taken to physically shield the filament and ion source to prevent stray electrons and/ or ions from reaching the acceleration region. In order to repel ions out of the electron beam in the ion source region, a small voltage has been applied to the ion repeller electrode. Ions gently repelled out of the source region have been collimated, slightly accelerated and focused on the entrance aperture of a quadrupole mass filter. Mass analyzed C^+ ions emerging from the quadrupole have been focused and accelerated to terminal velocities by circular defining and split focusing plates. This C^+ ion beam has interacted with target gas H_2 in a collision chamber where C^+ charge-transfer reactions occur.

$$C^+ (^2P, ^4P) + H_2 (^1\Sigma_g^+, v''=0) \longrightarrow C (^3P) + H_2^+ (^2\Sigma_g^+, v') \qquad (1)$$

Fine control needle valves have been used to allow high purity gases into the respective ion source and collision chamber. Target gas pressures in the cylindrical collision chamber have been determined by a MKS baratron pressure gauge (Type 220A). Ions exiting from the collision chamber are then postaccelerated to approximately 3 KV and detected using a Bendix channeltron electron multiplier. The channeltron output has been measured using both a counting (Ortec) and current amplification

(Keithly picoammeter) techniques. The detector has been shielded in a separate container to prevent stray photons and/or ions from reaching the channeltron. The entire apparatus has been contained in a stainless stell vacuum chamber which has been evacuated by a 6" 3000 l/min diffusion pump and 500 l/min mechanical roughing pump. Background pressures in the vacuum chamber were approximately 6×10^{-7} Torr.

RESULTS AND DISCUSSION

Since the electron impact ionization energy required to produce metastable state $C^+(^4P)$ ions is 5.33 eV higher than that for the ground state $C^+(^2P)$ ions, the minimum electron energies used to form $C^+(^2P)$ and $C^+(^4P)$ ions from CO ($X^1\Sigma^+$, v=0) in the reactions

$$e\ (22.4\ V) + CO\ (X^1\Sigma^+,\ v=0) \longrightarrow C^+(^2P) + O\ (^3P) \qquad (2)$$

$$e\ (27.7\ V) + CO\ (X^1\Sigma^+,\ v=0) \text{ ------ } C^+(^4P) + O\ (^3P) \qquad (3)$$

are 22.4 eV and 27.7 eV respectively. The fraction of excited $C^+(^4P)$ state in a C^+ beam has been shown [3] to increase rapidly from a value of 0.05 near the 27.7 eV threshold to 0.28 at 100 eV. An ionizing electron energy of 100 eV was employed in this investigation and consequently our C^+ ion beam entering the collision cell is expected to have a significant fraction of metastable ions.

When an ion beam passes through a target gas in a collision chamber, the beam is attenuated exponentially as a function of gas concentration. The cross section for ion loss σ can be estimated from the ion beam flux I_o determined without collision gas and the flux I at a given gas concentration by the use of the relation

$$I/I_o = \exp(-nl\sigma) \qquad (4)$$

where n is the number density of the target gas and l is the effective length of the collision chamber. A plot of $\ln(I/I_o)$ verses n should be linear with slope $l\sigma$, from which σ can be determined. Since the electron impact energies in our ion source are much larger than the threshold of the long-lived excited $C^+(^4P)$ state ions, the mixed state C^+ ion beams (with ground state fraction f_g and metastable state fraction f_m) follow the attenuation relation

$$I = I_o \left[f_g \exp(-nl\sigma_g) + f_m \exp(-nl\sigma_m) \right] \qquad (5)$$

where $f_m = 1 - f_g$ and σ_g and σ_m refer to cross sections for ground and metastable states respectively. In the case where the cross sections for reactions of ground and metastable state ions are significantly different, it is possible to resolve the curve of $\ln(I/I_o)$ verses n into two components, one from reactions of ground $C^+(^2P)$ state ions at high pressures, and another at low pressures from reactions of ground and metastable state ions. Cross sections for metastable $C^+(^4P)$ - H_2 reactions are an order of magnitude larger than the corresponding ground state $C^+(^2P)$ - H_2 cross sections. The values of I/I_o drop very rapidly at low target gas concentration due to the exponential $(-nl\sigma_m)$ term and as a result the $\ln(I/I_o)$ values at high (nl) are due only to ground state reactions. the slope of the $\ln(I/I_o)$ curve at large (nl) is essentially governed by σ_g. Extropolation of this curve to zero target gas concentration yields an intercept equal to f_g. Given the values of f_g, σ_g, and nl, the σ_m has been deduced by fitting Eq. (5) to experimental I/I_o values at low target gas concentrations.

Ground state cross sections measured in this investigation are displayed as the open circles in Fig.2 and cover the kinetic energy range of 10 to 500 eV. Measured attenuation cross sections are identified with charge trasfer processes when the ion energy is in excess of approximately 75 eV. At low ion kinetic energies, the cross sections for the $C^+(^2P) + H_2 \longrightarrow CH^+ + H$ rearrangement reactions are large and can effectively compete with charge transfer. The experimental data of Ref.5 for total CH^+ formation is given by the dash line in Fig.2. The CH^+ data of Ref.5 has been multiplied by 0.1 for convenient display. Product CH^+ angular distributions measured by Mahan and Sloan (6) and Jones et al (7) have shown that CH^+ products can be scattered into angles in excess of the 5° average acceptance angle in our system and will not reach our collector system. As a result the ground $C^+(^2P)$ state attenuation cross sections below

75 eV kinetic energy are a composite of charge transfer and rearrangement reactions.

The ground state $C^+(^2P)$ — $H_2(^1\Sigma_g^+, V''=0)$ cross sections obtained in this work are compared with charge trasfer cross sections obtained by other investigators in Fig.3. The closed circles representing ion beam attenuation data of this work at low ion kinetic energies smoothly ~~extrapolate~~ join to ground $C^+(^2P)$ state charge trasfer cross sections measured in Ref.8 at higher (0.7 to 3.0 keV) kinetic energies. Time-of-flight techniques were used by Ref.8 to monitor fast C neutrals produced in $C^+(^2P)$ — H_2 charge trasfer collisions. The cross sections measured by Hoffman, Miller and Lockwood over the 3 to 100 keV energy range were obtained by detection of the fast neutrals from a magnetically selected ground state C^+ ion beam [9]. Although the three different sets of ground state cross section data were obtained using different experimental arrangements at different ion kinetic energies, the trend in the charge transfer cross sections as a functin of ion kinetic energy is clear. Cross sections approximating 0.2 $Å^2$ at eV energies tend to smoothly increase with ion energy to a maximum around 10 $Å^2$ at 7×10^4 eV and then start to decrease at higher energies.

The cross sections of charge transfer reaction $C^+(^4P)$ -- $H_2(^1\Sigma_g^+, v''=0)$, which have been measured in our labolatory, are at least one order of magnitude larger than those involving $C^+(^2P)$ ground state ions.[7] The increased reactivity of the metastable state $C^+(^4P)$ ions over that of the ground state $C^+(^2P)$ ions can be rationalized considering the energetics of those two reactions. The recombination energy of $C^+(^2P)$ ions is only 11.26 eV and the electron transfer reaction producing H_2^+ is 4.17 eV endothermic. As such, this reaction is not expected to occur with high probability at low reactant ion kinetic energies. However, there is reasonably close energy balance between the $C^+(^4P)$ 16.59 eV

This data is shown in Fig. 5.

recombination energy and the energy required to form product H_2^+ in the 4th or 5th vibrational levels with the result that much larger cross sections are expected for this near resonant charge transfer reaction. The energetics and vibrational overlaps for the investigated system are shown in Fig. 6 where the recombination energies of the ground state and metastable state C^+ ions are given along with the transition energies from the $v''=0$ vibrational level of H_2 molecules to different v' levels of H_2^+ formed by charge transfer reactions.

In conclusion, the cross sections in a low ion kinetic energy range for charge transfer reactions of $C^+(^2P)$ and $C^+(^4P)$ ions with target molecule H_2 have been determined. Reaction cross sections are much larger for reactant C^+ ions in the metastable state than those in the ground state.

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FIGURE CAPTIONS

Fig.1 Schematic diagram of collision apparatus used to study metastable enhancement of C^+ capture reactions.

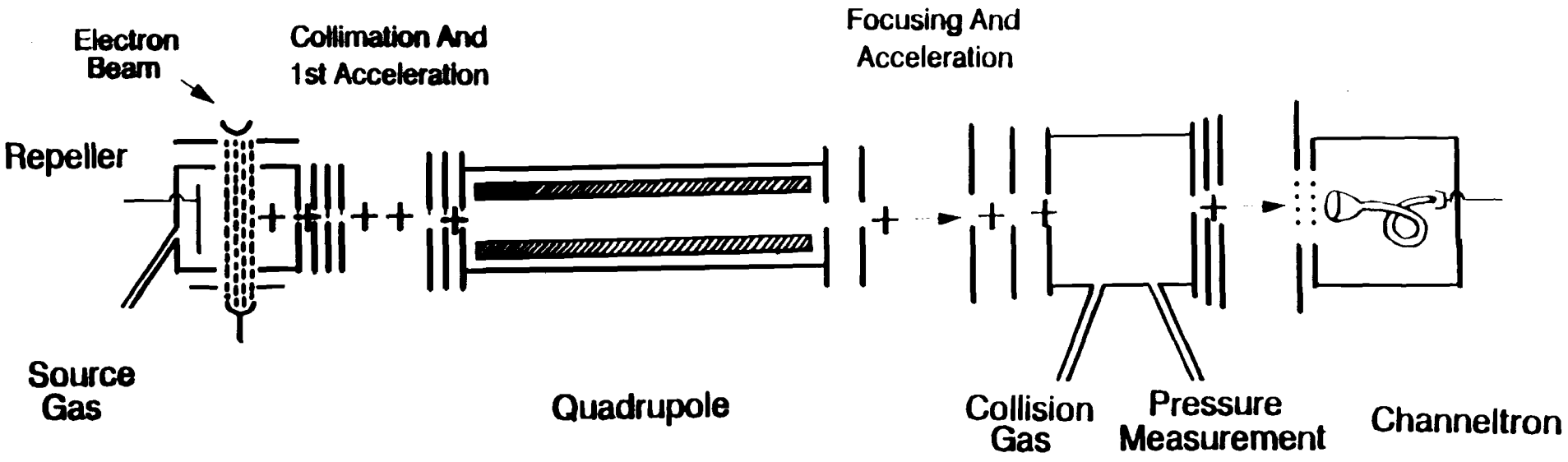
Fig.2 Charge transfer crss sections ($\mathring{A}^2$) as a function of reactant ion kinetic energy (eV) in $C^+(^2P) + H_2$ reactions. The open circles represent the cross sections obtained in this investigation while the dash line gives the cross sections measured for the rearragement channel $C^+(^2P) + H_2 \longrightarrow CH^+ + H$ by Ervin and Armentrout [5] which have been multiplied by 0.1 for display purposes.

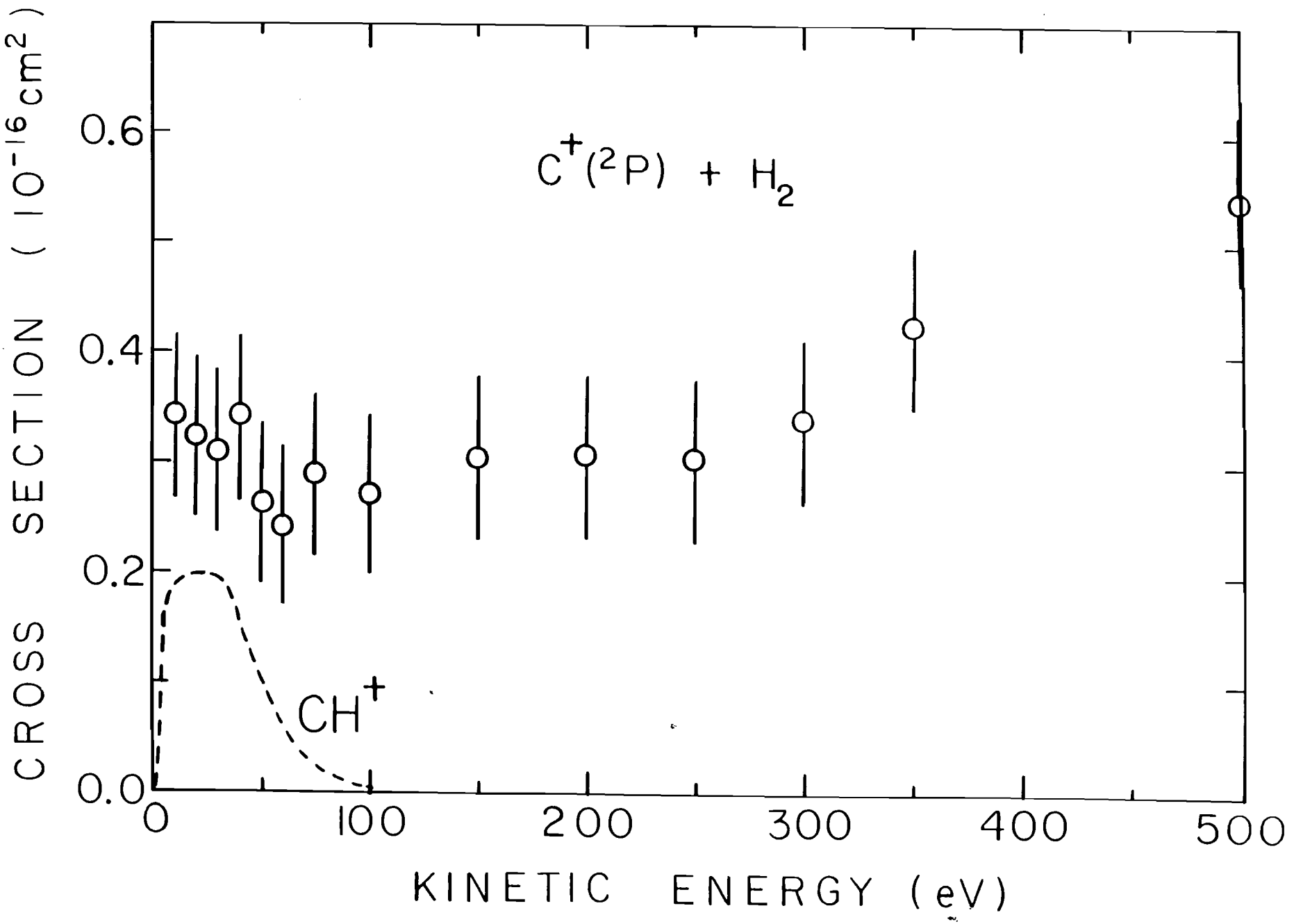
Fig.3 Charge transfer cross sections ($\mathring{A}^2$) as a function of reactant kinetic energy (eV) in $C^+(^2P) + H_2$ reactions. Closed circles at low ion kinetic energies are the cross sections measured in this investigation. The open circles labeled MW represent data of Ref.8 while the closed circles labeled HML represent data of Ref.9.

Fig.4 Transition energies (eV) for neutralization of reactant $C^+(^2P)$ and $C^+(^4P)$ ions and the ionization energies of target molecule H_2 to produce H_2^+. The relative magnitudes of vibrational overlaps from the $v''=0$ level of H_2 to different v' levels are represented by the lengths of the respective lines.

Fig. 4 Charge transfer cross sections ($\mathring{A}^2$) as a function of reactant kinetic energy (eV) in $C^+(^4P) + H_2$ reactions. Closed circles at low ion kinetic energies are the cross sections measured in this investigation. The open circles labeled MW represent data of Ref. 8 while the closed circles labeled LMH represent data of Ref 10.

Ion Production | Mass Analysis | Acceleration | Collision | Detection

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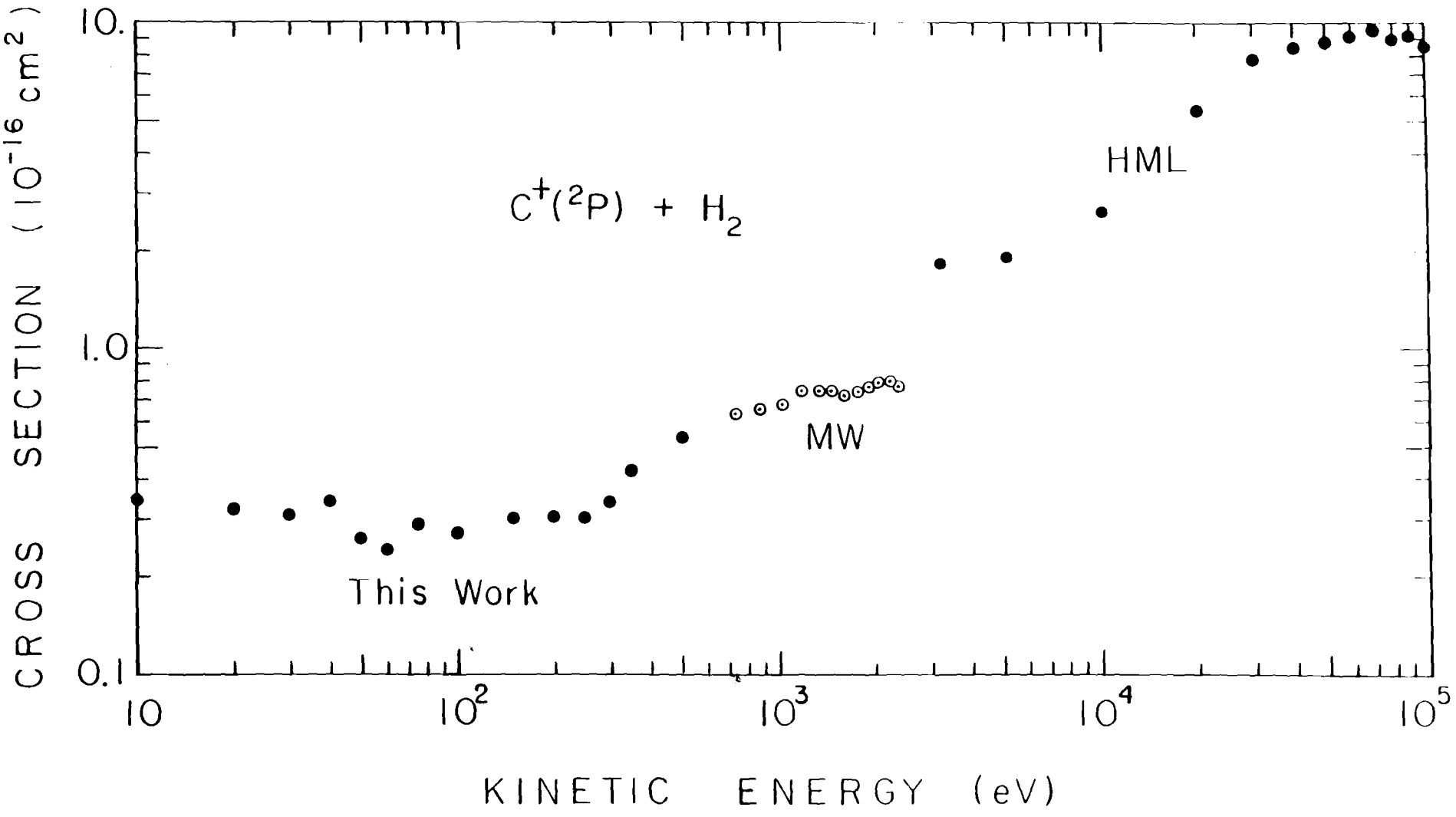
CH^+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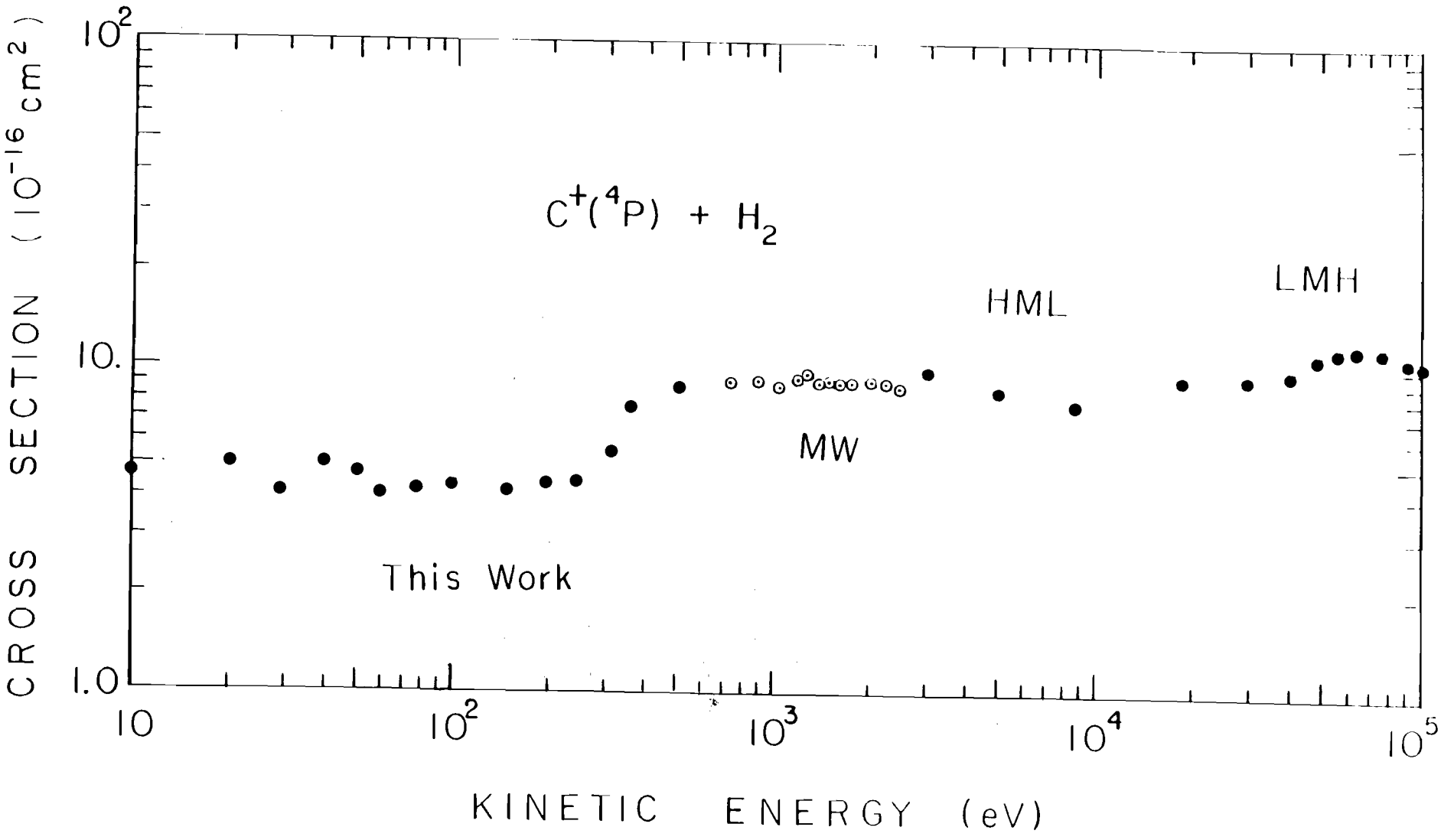
HML
MW
This Work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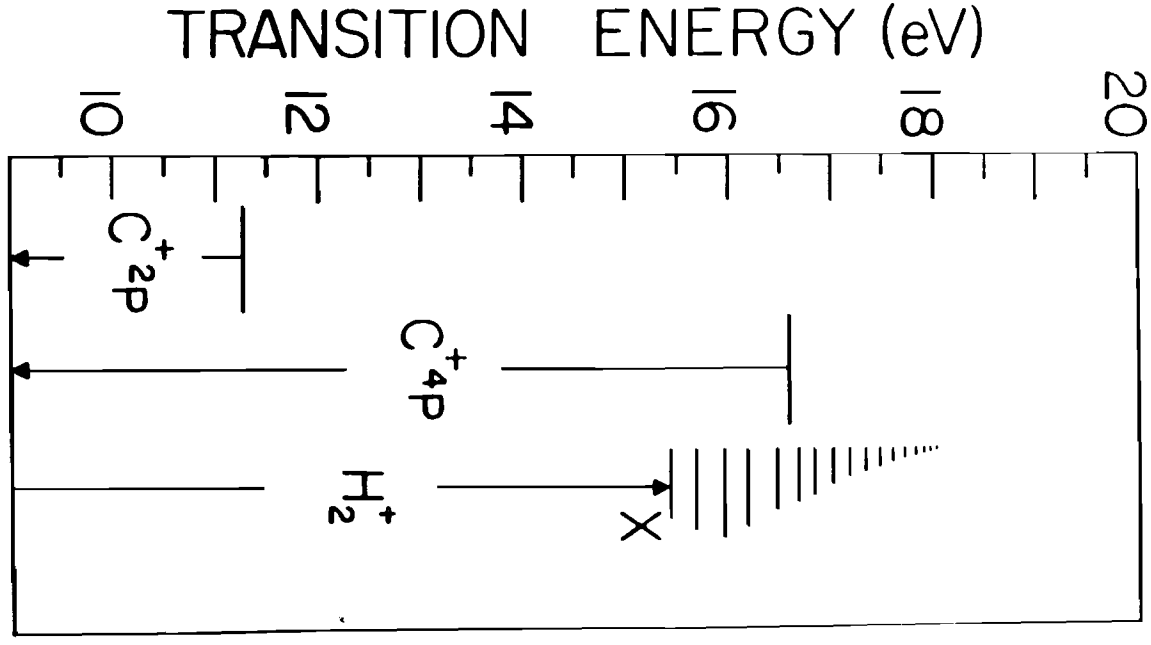
KINETIC ENERGY (eV)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4
6
8
20
C^+_{2P}
C^+_{4P}
H_2^+
X

APPENDIX B

THE ABUNDANCE OF METASTABLE $C^+(^4P)$ IONS PRODUCED IN ELECTRON IMPACT IONIZATION OF CARBON CONTAINING MOLECULES

The electron impact ionization of carbon containing molecules results in the formation of C^+ ions but to date there is no information concerning the state distribution of these C^+ ions for a wide range of compound types. It is possible for both ground $C^+(^2P)$ state and metastable $C^+(^4P)$ state ions to be formed in the electron impact ionization of molecules containing carbon. An approximate measure of the $C^+(^4P)$ metastable fraction produced in ionization of different carbon compounds, as well as the reactions these ions undergo, is useful in plasma modeling.

We have employed a magnetic mass spectrometer system to deliver a well defined beam of keV C^+ ions. These ions were formed by 100eV electron impact ionization of neutral molecules in a Nier type ion source. The source was operated a low pressure to prevent collisional deactivation of the excited $C^+(^4P)$ state ions as they were accelerated and momentum analyzed. The mass spectrometer system was operated at approximately 8,000 resolution in order to produce an ion beam composed of only C^+ ions. These ions were directed at a collision chamber containing H_2 where

$$C^+(\,^2P,\,^4P\,) + H_2(\,^1\Sigma_g^+, v''=0) \rightarrow C^0 + H_2^+(\,^2\Sigma_g^+, v')$$

charge transfer reactions occurred. A schematic of the experimental apparatus is shown in the attached figure.

The fast neutral C^0 product and unreacted C^+ ions emerging from the collision region proceed into a short drift space containing deflection electrodes before proceeding to the electron multiplier detector. Without voltage on the deflection electrodes, both the C^0 product and unreacted ion beam impinge on the multiplier. With sufficient voltage on the deflection electrodes, only the neutral C^0 product strikes the multiplier since the unreacted C^+ ions are rejected. Thus, the reactant C^+ ion beam and neutral C^0 product can be determined (the secondary electron emission coefficient of the first dynode of the multiplier has been obtained using a calibration reaction). The

total amount of C^0 product flux, i_s, is related to the reactant C^+ beam flux, i_p, by means of the relation

$$i_s = i_p n \ell \sigma = f_g i_p n \ell \sigma_g + f_m i_p n \ell \sigma_m$$

where n is the target gas concentration, ℓ the reaction path length, f_g the fraction of ground state $C^+(^2P)$ ions, f_m the fraction of metastable $C^+(^4P)$ ions, σ_g the ground state charge transfer cross section and σ_m the metastable state charge transfer cross section. The above equation can be rearranged to the forms

$$(i_s / i_p n \ell) = \sigma = f_g \sigma_g + f_m \sigma_m$$

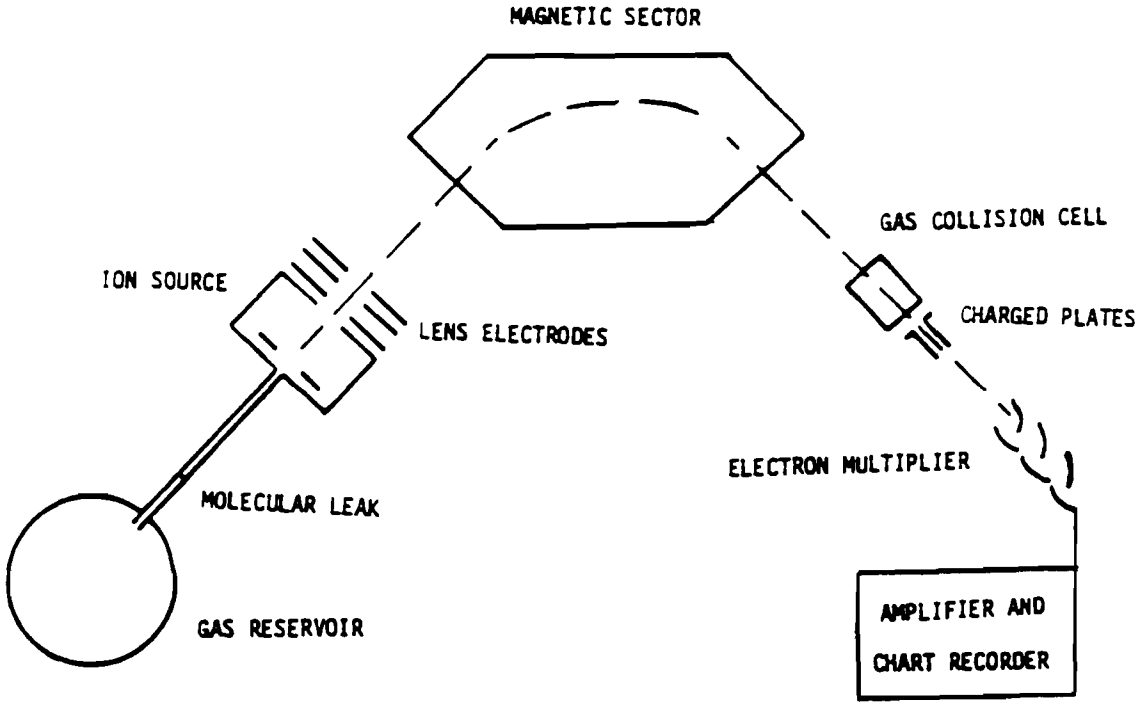
$$\sigma = (1 - f_m) \sigma_g + f_m \sigma_m \qquad (A)$$

where $f_g + f_m = 1$. For the $C^+ + H_2$ charge transfer reaction, both the σ_g and σ_m are known and we have measured σ using the magnetic mass spectrometer system described. With the aid of equation (A), the fraction f_m of metastable $C^+(^4P)$ ions present in C^+ ion beams have been determined for a range of precursor molecules. This data is given in the Table below where the f_m's range from 0.29 in the case of methanol to 0.15 for C^+ ions produced in the ionization of acetonitrile.

TABLE

METASTABLE $C^+(^4P)$ FRACTION FOR C^+ IONS PRODUCED BY 100 eV ELECTRON IMPACT IONIZATION OF DIFFERENT CARBON CONTAINING MOLECULES

COMPOUND	FRACTION OF ION IN METASTABLE $C^+(^4P)$ STATE
CH_3OH	0.29
C_2H_5OH	0.22
C_3H_7OH	0.24
CH_3COCH_3	0.22
CH_3CN	0.15
C_6H_6	0.22
C_5H_{12}	0.25



Schematic diagram of single focusing mass spectrometer used in the investigation of charge transfer

APPENDIX C

REACTIONS OF C^+ IONS WITH HELIUM

The low energy charge transfer cross sections for the C^++He system are significantly below 0.1 $Å^2$. Small cross section values are expected in this system because of the large endothermicities for both the $C^+(^2P)$ and $C^+(^4P)$ state reactions. Reliable estimates of the cross sections have proven elusive and can only be obtained using high purity He gas in the absence of impurities contributed from the He gas itself or [redacted] outgassing of very small amounts of water vapor or other contaminents in the inlet lines, collision chamber, etc.

APPENDIX D

REACTIONS OF O^+ IONS WITH H_2 MOLECULES

RESULTS AND DISCUSSION

Since the electron impact ionization energy required to produce metastable state $O^+(^2D)$ ions is 3.32 eV higher that for the ground state $O^+(^4S)$ ions, the minimum electron energies used to form $O^+(^4S)$ and $O^+(^2D)$ ions from CO ($X^1\Sigma^+$, v=0) in the reactions

$$e\ (24.7\ V) + CO\ (X^1\Sigma^+,\ v=0) \text{ ------ } O^+(^4S) + C \qquad (1)$$

$$e\ (28.0\ V) + CO\ (X^1\Sigma^+,\ v=0) \text{ ------ } O^+(^2D) + C \qquad (2)$$

are 24.7 eV and 28.0 eV respectively. When the electron impact ionization energy is increased, the probability for producing metastable $O^+(^2D)$ state ions is also increased. An ionizing electron energy of 100 eV was employed in this investigation and consequently our O^+ ion beam entering the collision cell is expected to have a significant fraction of metastable ions.

When an ion beam passes through a target gas in a collision chamber, the beam is attenuated exponentially as a function of gas concentration. The cross section for ion loss σ can be estimated from the ion beam flux I_o determined without collision gas and the flux I at a given gas concentration by the use of the relation

$$I/I_o = \exp\ (-nl\sigma) \qquad (3)$$

where n is the number density of the target gas and l is the effective length of the collision chamber. A plot of $\ln(I/I_o)$ verses n should be linear with slope $l\sigma$, from which σ can be determined. Since the electron impact energies in our ion source are much larger than the threshold of the long-lived excited $O^+(^2D)$ state ions, the mixed state O^+ ion beams (with ground state fraction f_g and metastable state fraction f_m) follow the attenuation relation

$$I = I_o \left[f_g \exp(-nl\sigma_g) + f_m \exp(-nl\sigma_m) \right] \qquad (4)$$

where $f_m = 1 - f_g$ and σ_g and σ_m refer to cross sections for ground and metastable states respectively. In the case where the cross sections for reactions of ground and metastable state ions are significantly different, it is possible to resolve the curve of $\ln(I/I_o)$ verses n into two components, one from reactions of ground $O^+(^4S)$ state ions at high pressures, and another at low pressures from reactions of groud and metastable state ions. Cross sections for metastable $O^+(^2D)$ - H_2 reactions are an order of magnitude larger than the corresponding ground state $O^+(^4S)$ - H_2 cross sections. The values of I/I_o drop very rapidly at low target gas concentration due to the exponential $(-nl\sigma_m)$ term and as a result the $\ln(I/I_o)$ values at high nl are due only to ground state reactions. the slope of the $\ln(I/I_o)$ curve at large nl is essentially governed by σ_g. Extropolation of this curve to zero target gas concentration yields an intercept equal to f_g. Given the values of f_g, σ_g, and nl, the σ_m has been deduced by fitting Eq. (4) to experimental I/I_o values at low target gas concentrations.

Table 1 shows the charge transfer cross sections ($\AA^2$) as a function of ion kinetic energy covered a range of 10 to 500 eV for the reaction

$$O^+(^4S) + H_2(X^1\Sigma_g^+,\ v''=0) \longrightarrow O(^3P) + H_2^+(X^2\Sigma_g^+, v')$$

which is 1.81eV endothermic. Our investigation shows as the ion kinetic energy increases, the charge transfer cross sections slightly increase.

Table 2 gives the cross sections for the charge transfer interaction $O^+(^4S) + H_2$, which were obtained by other workers. The results obtained in this investigation and in Ref. 10 are lower than that in Ref. 2. At present stage, we cannot explain why the cross section values obtained by different investigators are not in harmony.

Table 1 Cross sectins ($\mathring{A}^2$) for charge transfer reactions

$O^+ (^4S) + H_2 \longrightarrow O\ (^3P) + H_2^+$ in this investigation

Ion kinetic energy (eV)	Cross sections ($\mathring{A}^2$)
10	.505
20	.596
30	.558
40	.471
50	.596
60	.574
75	.555
100	.613
150	.613
200	.679
250	.716
300	.734
350	.690
500	.904

Table 2 Cross sections ($\mathring{A}^2$) for charge transfer reactions

$O^+ (^4S) + H_2 \longrightarrow O(^3P) + H_2^+$ in other investigations

Ion kinetic energy (keV)	Cross sections (A)	Authors
.61	.324	
.81	.412	
1.00	.441	
1.20	.441	Moran and
1.40	.471	Wilcox Ref. 1
1.60	.471	
1.80	.471	
2.00	.471	
2.20	.515	
2.40	.559	
2.60	.559	
2.80	.559	
3.00	.588	
3.13	4.79	
5.15	4.39	
10.04	8.40	
20.02	11.6	Hoffman
30.04	12.1	et al Ref. 2
40.22	12.8	
50.01	11.5	
60.01	11.1	
70.17	10.3	
80.14	9.34	
90.04	8.28	
99.91	8.35	

REFERENCES

1. T. F. Moran and J.B. Wilcox, J. Chem Phys. 69,1397(1978).
2. J.M.Hoffman, G.H. Miller and G.J.Lockwood, Phys. Rev. A, 25,1930(1982).

DOE F538 (5-86)

OMB Control No. 1910-1400

U. S. DEPARTMENT OF ENERGY

NOTICE OF ENERGY RD&D PROJECT

1. Descriptive TITLE of work (150 characters including spaces)

Metastable Enhancement of C^+ and O^+ Capture Reactions

2. CONTRACT or grant number: DE-FG05-87ER13745

2A. MASTER contract number (GOCO's):

2B. Responsible PATENT office: Oak Ridge

3. Performing organization CONTROL number (internal): G-41-642

3A. Budget and Reporting code:

3B. Funding YEAR for this award: FY 89

4. Original contract start date: 7/1/87

4A. Current contract start date: 7/1/88

4B. Current contract close date: 6/30/89

4C. Anticipated project termination date: 6/30/90

5. Work STATUS

☐ Proposed ☒ Renewal

☐ New ☐ Terminated

5A. Manpower (FTE): 1.22

5B. CONGRESSIONAL district: 5th

5C. STATE or Country where work is being performed: Georgia

5D. COUNTRY sponsoring research: USA

6. Name of PERFORMING organization: Georgia Institute of Technology

6A. DEPARTMENT or DIVISION	6B. Street Address	6C. City, State, Zip Code
Physics	Georgia Institute of Technology	Atlanta, Georgia 30332

7. Circle only one code for TYPE of Organization Performing R&D:

(CU) College, university, or trade school
FF - Federally funded RD&D centers or laboratory operated for an agency of the U. S. Government
IN - Private industry
NP - Foundation or laboratory not operated for profit
ST - Regional, state or local government facility
TA - Trade or professional organization
US - Federal agency
XX - Other
EG - Electric or gas utility

8A. Contractor's PRINCIPAL INVESTIGATOR/s or project manager Name/s (Last, First, MI): Thomas, Edward W.

8B. PHONE/s (in order of PI names with commercial followed by FTS)

Comm. (404) 894-5200 ; FTS -- ; Comm. -- ; FTS --

8C. PI/s address (if different from that of Performing Organization)

same

9. DOE SUPPORTING Organization (DOE Assistant Secretary and office sponsoring the work; technical monitor; and administrative monitor).

9A. PROGRAM division or office (full name) Division of Chemical Sciences — Program Office Code

9B. TECHNICAL monitor (Last, First, MI) Martinez, Joe V.

9C. Address U. S. DOE
19901 Germantown Rd.
Germantown, MD 20874

9D. Phone Comm. (301) 353-5820
FTS

9E. ADMINISTRATIVE monitor (Last, First, MI) Clark, Marlena

10. FUNDING in thousands of dollars (K$). Funds represent budget obligations for operating and capital equipment (FY runs October 1 – September 30).

Funding organization(s)	Current FY 89	Next FY 90
A. DOE	$ 57,578	$ 57,417
B.		
C.		

10D. Does the current FUNDING cover more than one year's work? Yes ____ No X

E. If yes, provide dates (from when to when). ____

11. Descriptive SUMMARY of work. Enter a Project Summary using complete sentences limited to 200 words covering the following: Objective(s), state project objectives quantifying where possible (e.g., "The project objective is to demonstrate 95% recovery of sulphur from raw gas with molten salt recycling at a rate of one gallon per minute."); approach, describe the technical approach used (how the work is to be done); expected product/results, describe the final products or results expected from the project and their importance and relevance.

It is anticipated that capture cross sections for C^+ and O^+ will differ greatly depending on whether the initial ion species is in a ground or metastable excited state. The difference is at least an order of magnitude and therefore has a substantial bearing on the modelling of impurity C^+ and O^+ transport in the edge plasma of Tokamaks. We propose to prepare beams of known metastable and ground state composition which will then be used to measure electron capture reactions in H_2, He and H at energies from 20 to 1000eV. Of particular interest is $O^+ + H \rightarrow O + H^+$ where the reaction is accidentally resonant when the O^+ is in the metastable state; the reaction should have a very large cross section at low energies and represents a challenging problem for theoretical treatment.

We propose also to study how the metastable species of C^+ and O^+ interact with surfaces. Secondary electron ejection by potential processes is governed in part by exchange processes and should differ greatly between metastable and ground states. Chemical erosion of carbon by O^+ will also be studied to determine whether the initial excited state of the O^+ influences the erosion rate.

12. PUBLICATIONS available to the public. List the five most descriptive publications that have resulted from this project in the last year that are available to the public. (Include author, title, where published, year of publication, and any other information you have to complete full bibliographic citation.) Use the back of this form or additional sheets if necessary.

None.

13. KEYWORDS (Listed five terms describing the technical aspects of the project. List specific chemicals and CAS number, if applicable.)

Capture, C^+, O^+, Metastable, Collisions

14. RESPONDENT. Name and address of person filling out the Form 538. Give telephone number, including extension (if you have FTS number, please include it) at which person can be reached. Record the date this form was completed or updated. The information in Item 14 will not be published.

Respondent's Name: Edward W. Thomas Phone No.: (404) 894-5200 Date: July 29, 1987

Street: School of Physics, Georgia Tech

City: Atlanta, State: Georgia Zip: 30332

15. Additional space for furnishing information in items 1 to 14. (Indicate item numbers to which answers apply.)

Item No.	

NOTICE: Return this form to the office indicated in the reporting requirements for your award agreement covering this project. If you have completed a similar programmatic office project description during the current Fiscal Year, complete only the new data elements on this form and send it and a copy of the description completed earlier to Department of Energy, Office of Scientific Information, P. O. Box 62, Oak Ridge, TN 37831.

DOE F538 (5-86)

OMB Control No. 1910-1400

U. S. DEPARTMENT OF ENERGY

NOTICE OF ENERGY RD&D PROJECT

1. Descriptive TITLE of work (150 characters including spaces)

METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS

2. CONTRACT or grant number DE-FG05-87ER 13745

2A. MASTER contract number (GOCO's)

2B. Responsible PATENT office OAK RIDGE

3. Performing organization CONTROL number (internal) G-41-642

3A. Budget and Reporting code

3B. Funding YEAR for this award

4. Original contract start date 7/1/87

4A. Current contract start date 7/1/87

4B. Current contract close date 4/30/92

4C. Anticipated project termination date 4/30/92

5. Work STATUS

☐ Proposed ☒ Renewal

☐ New ☐ Terminated

5A. Manpower (FTE) 0.66

5B. CONGRESSIONAL district 5th

5C. STATE or Country where work is being performed GEORGIA

5D. COUNTRY sponsoring research USA

6. Name of PERFORMING organization GEORGIA INSTITUTE OF TECHNOLOGY

6A. DEPARTMENT or DIVISION	6B. Street Address	6C. City, State, Zip Code
PHYSICS	GEORGIA INSTITUTE OF TECHNOLOGY	ATLANTA, GEORGIA 30332

7. Circle only one code for TYPE of Organization Performing R&D:

CU - College, university, or trade school
FF - Federally funded RD&D centers or laboratory operated for an agency of the U. S. Government
IN - Private industry
NP - Foundation or laboratory not operated for profit
ST - Regional, state or local government facility
TA - Trade or professional organization
US - Federal agency
XX - Other
EG - Electric or gas utility

8A. Contractor's PRINCIPAL INVESTIGATOR/s or project manager Name/s (Last, First, MI) THOMAS, EDWARD W.

8B. PHONE/s (in order of PI names with commercial followed by FTS)

Comm. (404) 894-5249 ; FTS _____ ; Comm. _____ ; FTS _____

8C. PI/s address (if different from that of Performing Organization)

SAME

9. DOE SUPPORTING Organization (DOE Assistant Secretary and office sponsoring the work; technical monitor; and administrative monitor).

9A. PROGRAM division or office (full name) DIVISION OF CHEMICAL SCIENCES — Program Office Code

9B. TECHNICAL monitor (Last, First, MI) MARTINEZ JOE V.

9C. Address U.S. DOE
19901 GERMANTOWN ROAD
GERMANTOWN, MD 20874

9D. Phone Comm. (301) 353-5820
FTS

9E. ADMINISTRATIVE monitor (Last, First, MI) CLARK, MARLENA

10. FUNDING in thousands of dollars (K$). Funds represent budget obligations for operating and capital equipment (FY runs October 1 – September 30).

Funding organization(s)	Current FY 91	Next FY 92
A. DOE	17,985	
B.		
C.		

10D. Does the current FUNDING cover more than one year's work? Yes ____ No X

E. If yes, provide dates (from when to when). ____

11. Descriptive SUMMARY of work. Enter a Project Summary using complete sentences limited to 200 words covering the following: Objective(s), state project objectives quantifying where possible (e.g., "The project objective is to demonstrate 95% recovery of sulfur from raw gas with molten salt recycling at a rate of one gallon per minute."); approach, describe the technical approach used (how the work is to be done); expected product/results, describe the final products or results expected from the project and their importance and relevance.

The project studies neutralization of C^{q+} and O^{q+} ions in H and H_2 at energies of 10 to 500 eV. Separate cross sections are measured for incoming ground and metastable state ions. The experimental technique involves analysis of the alternation of a mixed metstable and ground state ion beam in the target. For low states of ionization metastable states show ten times the cross section of the ground state. Errors in previous work have been identified and explained. The high cross sections are probably related to near resonance of the electron transfer process. An ECR source to produce the higher charge states has been completed and is operational.

12. PUBLICATIONS available to the public. List the five most descriptive publications that have resulted from this project in the last year that are available to the public. (Include author, title, where published, year of publication, and any other information you have to complete full bibliographic citation.) Use the back of this form or additional sheets if necessary.

"Charge Transfer Reactions of Ground $C^+(^2P)$ and Metastable $C^+(^4P)$ Ions with H_2 Molecules", Yaodong Xu, T.F. Moran and E. W. Thomas, Phys. Rev. A 41, 1408 (1990).

"Charge Transfer Reactions of Ground $O^+(^4S)$ and Metastable $O^+(^2D,^2P)$ Ions with H_2 Molecules", Yaodong Xu, T.F. Moran and E. W. Thomas, J. Phys. B: At. Mol. Opt. Phys. 23, 1235 (1990).

"Simple Method to Calculate the Operating Frequency of a Helical Resonator/RF Discharge Tube Configuration", R.F. Welton, E.W. Thomas, R. K. Feeney, and T.F. Moran, Meas. Sci. Technol. 2, 242 (1991).

"Metastable CII Ion Abundances from Electron Impact of Molecules", R. F. Welton, Y. Xu, E.W. Thomas and T. F. Moran, Physica Scripta, (in publication).

"Metastable State Abundances in Multipy Charged Ion Beams", R. F. Welton, T. F. Moran and E. W. Thomas, J. Phys. B (in publication).

13. KEYWORDS (Listed five terms describing the technical aspects of the project. List specific chemicals and CAS number, if applicable.)

Capture, C^+, O^+, Metastable, Charge Transfer

14. RESPONDENT. Name and address of person filling out the Form 538. Give telephone number, including extension (if you have FTS number, please include it) at which person can be reached. Record the date this form was completed or updated. The information in Item 14 will not be published.

Respondent's Name: EDWARD W. THOMAS Phone No.: (404) 894-5249 Date: 8/21/91

Street: SCHOOL OF PHYSICS, GEORGIA TECH

City: ATLANTA State: GA Zip: 30332

15. Additional space for furnishing information in items 1 to 14. (Indicate item numbers to which answers apply.)

Item No.	

NOTICE: Return this form to the office indicated in the reporting requirements for your award agreement covering this project. If you have completed a similar programmatic office project description during the current Fiscal Year, complete only the new data elements on this form and send it and a copy of the description completed earlier to Department of Energy, Office of Scientific and Technical Information, P. O. Box 62, Oak Ridge, TN 37831.

DOE F 1332.16 (10-84)
(Formerly RA-427)

OMB Approval
No. 1910-1400

U. S. DEPARTMENT OF ENERGY

UNIVERSITY CONTRACTOR, GRANTEE, AND COOPERATIVE AGREEMENT RECOMMENDATIONS FOR ANNOUNCEMENT AND DISTRIBUTION OF DOCUMENTS

See Instructions on Reverse Side

1. DOE Report No.	3. Title
DOE/ER/13745-3	METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS
2. DOE Contract No. DE-FG05-87ER13745	

4. Type of Document ("x" one)
   - ☒ a. Scientific and technical report
   - ☐ b. Conference paper:
     - Title of conference _____
     - Date of conference _____
     - Exact location of conference _____
     - Sponsoring organization _____
   - ☐ c. Other (Specify) _____

5. Recommended Announcement and Distribution ("x" one)
   - ☒ a. Unrestricted unlimited distribution.
   - ☐ b. Make available only within DOE and to DOE contractors and other U. S. Government agencies and their contractors.
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8. Submitted by	Name and Position (Please print or type)	
E. W. Thomas	Director, School of Physics	
Organization: Georgia Institute of Technology		
Signature	Phone: 894-5200	Date: 10/90

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9. Patent Clearance ("x" one)
   - ☐ a. DOE patent clearance has been granted by responsible DOE patent group.
   - ☐ b. Report has been sent to responsible DOE patent group for clearance.

METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS.

FINAL TECHNICAL REPORT
COVERING THE PERIOD JUNE 87 THROUGH SEPTEMBER 90

DOE GRANT NO DE-FG05-87ER13745

TO DEPARTMENT OF ENERGY,
DIVISION OF CHEMICAL SCIENCES,
WASHINGTON DC 20874

by

E. W. THOMAS[+] &

T. F. MORAN[++]

Schools of Physics[+] and Chemistry,[++]
Georgia Institute of Technology
Atlanta, Ga 30332

SEPTEMBER 1990

ABSTRACT

We have studied single electron capture by 10 to 500 eV singly charged C and O ions traversing targets of H_2 and H with emphasis on comparing cross sections for metastable species with those for the ground state. For an H_2 target cross sections are of the order 10 $\AA^2$ and 20 to 30 times larger than for ground state species. Electron impact ion sources typically produce 5 to 30% of their output in the metastable state. Previous published work has largely ignored (or failed to detect) the presence of metastables and is incorrect by as much as an order of magnitude. Discrepancies between data sets have been resolved and a reliable data set provided for energies from 10 to 10^5 eV. Similar experiments for an atomic H target are underway. We propose to extend the program to similar studies with multiply charged projectile species.

INDEX

A. INTRODUCTION

The present work involves measurement of the charge transfer neutralization of carbon and oxygen ions in H_2 and H targets which can be described by the general equations:

$$C^+ \text{ (or } O^+) + H_2 \text{ (or H)} \rightarrow C^o \text{ (or } O^o) + H_2^+ \text{ (or } H^+) \qquad (1)$$

We concentrate on impact energies from near threshold to a few hundred eV. This is an energy region where processes are expected to be adiabatic and described in terms of curve crossings of the projectile-target complex. The reactants represent species where adiabatic potential energy curves are available from molecular spectroscopy. Thus there is a good opportunity to formulate and test theoretical predictions. Apart from theoretical interest these processes are very important to the modelling and understanding of processes occuring in the sheath of a plasma such as a tokamak device. The choice of carbon and oxygen represents common plasma impurities and the target H_2 or H represents fuel that is found in the wall region. Our choice of energies represents the sheath potential of a typical plasma device where impurity ions emerging from a plasma acquire most of their energy.

The cross section for a process described by Eq. 1 is very sensitive to the internal excitation state of the incoming projectile. For example when C^+ is incident on H_2 the cross section for metastable impact is a factor of ten greater than for the ground state. Hints of such behaviour have long been in the literature (for example Moran and Wilcox[1]) but have been largely ignored. There are a number of confusing consequences. A typical ion flux, whether from an ion source or from the center of a plasma, will contain a significant fraction of ions in metastable states (up to 20 to 30 % in some cases). The apparent cross section for neturalization will then be dominated by the

metastable component which is often undiagnosed and ignored. Different sources produce different metastable fractions which in turn gives rise to different apparent cross sections. Most of the recent experimental measurements ignore the presence of metastables. As a result data from different groups disagrees by factors of three to ten and is quite unreliable. Data are often described as being for ground state beams (which is incorrect) leading theoreticians to compare with ground state theoretical calculations; any conclusions are likely to be irrelevent. Use of any of this information for modelling fusion or other plasmas is likely to give misleading results.

The major objective of the present work was to study the charge transfer process of Eq. (1) separately for the ground and metastable states of the projectile. This should provide correct data for modelling purposes, resolve differences in data published by different groups and provide a firm basis for the comparison with theory.

The present work represents a study of the charge transfer process with two defined states of the incoming projectile; the metastable state and the ground state. Thus we capitalize on the opportunity to vary the pre-collision channel. This provides an opportunity to see how the input channel influences cross section. In the present study the transfer of a single electron from H_2 to a incoming metastable C^+ involves an energy change of only a fraction of an eV; if the resulting target H_2^+ is left in a vibrationally excited state the energy transfer can be essentially zero leading to an accidentally energy resonant situation. For low energy impact this is likely to give a large cross section and that, we shall see, is what is observed. By contrast the transfer of a single electron from H_2 to ground state C^+ involves an energy defect of many eV, it is certainly not resonant and the cross sections at low energy are likely to be small; again this is what we observe. As best we can tell there is not a single theoretical treatment of how a change in the

incoming channel (e.g. by excitation) can alter the cross sections for a process. There are of course many studies of cross section as a function of the post collision channel (through measurement of excited state formation) but none on the prior collision channnel.

The work to date can be considered in two parts. First we have studied the charge transfer neutralization of C^+ and O^+ in H_2 separately measuring cross sections for ground and metastable excited projectile states. These studies are complete and have been published.[2,3] We briefly describe the results below and refer the reader to the published articles for details. Secondly, we have started studies of the same process but with an atomic H target. There is need for a change of technology here with the provision of an atomic H target in the form of a beam from an RF discharge device. Substantial work has been done on this project, a paper on design considerations has been published, but final data on the cross sections are not yet in hand. We will describe the present status of the work. Finally we will discuss briefly the work that is contained in a renewal proposal to DOE which proposes to extend these studies to multiply charge projectile ions.

B. METASTABLE AND GROUND STATE C^+ AND O^+ ON H_2

Under a present DOE grant we have performed a study of single electron transfer processes[2,3] for C^+ and O^+ at energies from 10 to 500 eV. Of particular interest is the case of an H_2 target where there is an opportunity for a near resonant transfer (energy defect of zero) and which is of practical importance in modelling the edge of fusion plasma devices.

Figure 1 gives the basic experimental arrangement. Ions are produced in a controlled energy electron impact source, extracted at a few eV energy, mass selected (with an RF quadrupole) accelerated to the desired energy (10 to 500 eV) focussed and directed through a cell containing the target gas. Ions that survive the transit of the target are accelerated to 5 keV and counted with a channeltron. For a two component (one metastable and one ground state) beam the flux of ions I surviving transit of the cell is given by

$$I = I_o(1-F)\exp(-n\,\sigma_{gs}\ell) + I_o\,F\exp(-n\,\sigma_m\,\ell) \qquad (4)$$

Here I_o is the transmitted current when target pressure is zero, n is the number density of target atoms in the cell of length ℓ. The cross section for charge transfer neutralization of ground state ions is σ_{gs} and that for metastables is σ_m. The fraction of the ion beam in the metastable state is F and the fraction of ground state ions 1-F. If I is measured as a function of n the resulting experimental data can be deconvoluted[2,3] to give the two cross sections σ_{gs} and σ_m as well as the fraction of metastables F. Calculation of effective absolute values for cell density n and cell length ℓ requires a correction for density gradients at the cell's entrance and exit apertures;

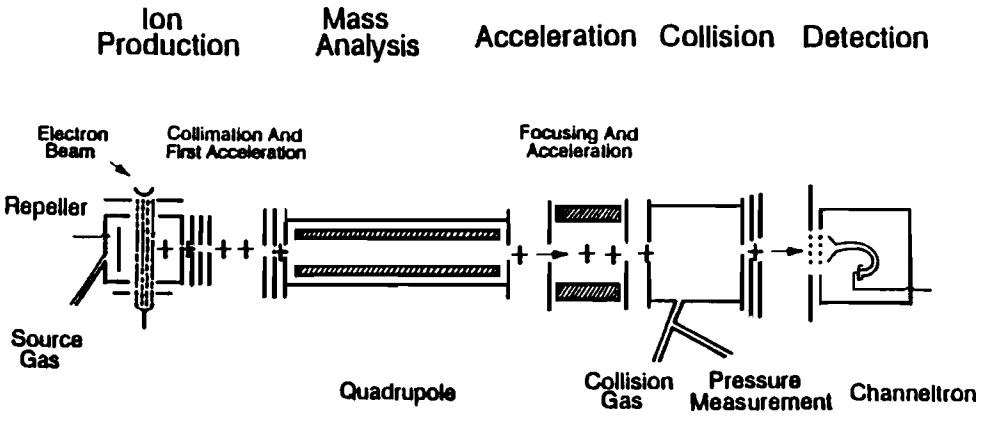

Fig. 1. Experimental arrangement used in the present study of C^+ and O^+ neutralization in H_2.

this was accomplished following a prescription by Van Zyl.[4] Precise control of electron energy and gas (CO) density in the ion source premits a reproducable metastable state fraction F. By choosing an electron energy between ground and metastable thresholds it is possible to create an ion beam of ground state ions only. In that case F = 0 and the data is represented by only a single exponential decay.

The apparatus described above has the great virtue of simplicity and through simplicity it operates reliably down to 10 eV energy, a level not previously described in the literature. A sample of the data for C^+ ions is shown in Figure 2.

The measured cross sections for metastables are about 10 Å^2 (see Fig. 2b) and vastly exceed the ground state cross sections of 1 Å^2 or less[2,3] (see Fig. 2a at low energies). We have demonstrated[2,3] that the earlier data of Moran and Wilcox at 500-2000 eV are correct and that the considerable body of data by Nutt et al.[5] are wrong. With the benefit of data from other groups[6,7] we can see that the metastable cross section for an H_2 target is about 10 Å^2 at 10 eV and remains virtually unchanged to 10^5 eV when it starts to fall. The ground state cross section is .3 Å^2 at 10 eV and rises with energy until it

equals the metastable cross section from about 10^4 eV onwards.

We originally suggested[2,3] that the high cross section for metastables might be explained by the process being near resonant (energy defect of zero) if the target H_2^+ was left in a vibrationally excited state; near resonant processes are expected to have large cross sections. By contrast the ground state process will involve a large energy defect and should have a small cross section. Recently, however, we had access to unpublished data by Winter[8] on single electron capture by ground and metastable C^{2+} in H_2; this we show as Figure 3. Here again we see a metastable cross section ten times that of the ground state (at 500 eV) but for neither case is the reaction near resonant. It seems therefore that the concept of energy resonance will not explain the large differences in cross section.

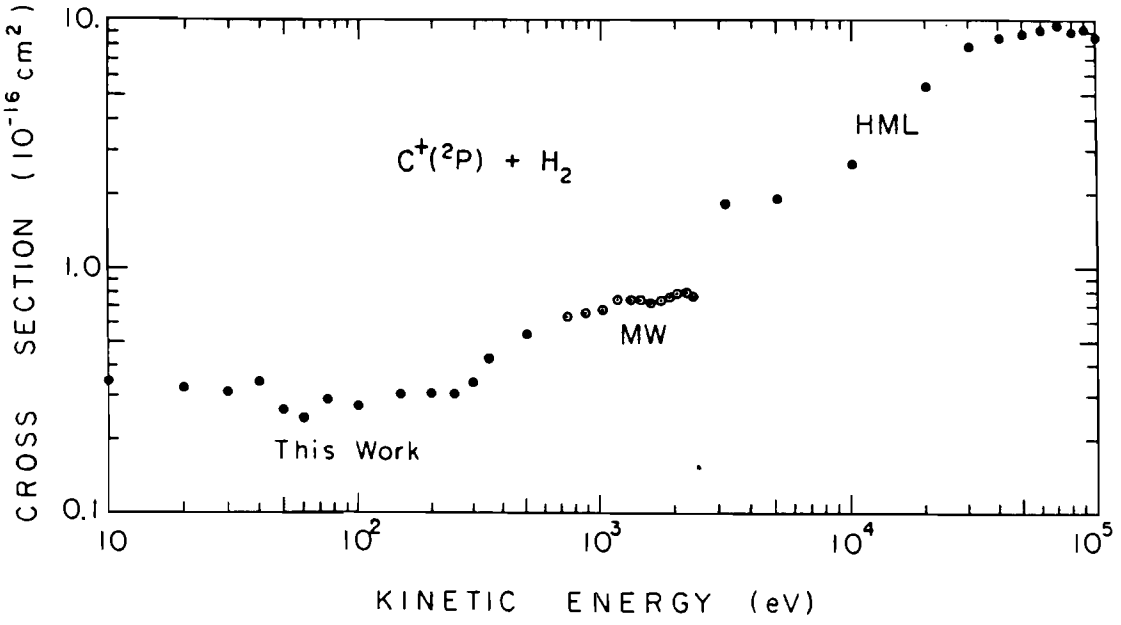

Fig. 2a. Charge transfer neutralization of ground state C^+ in H_2 as a function of energy. The present work is shown along with higher energy data. From Ref. 2.

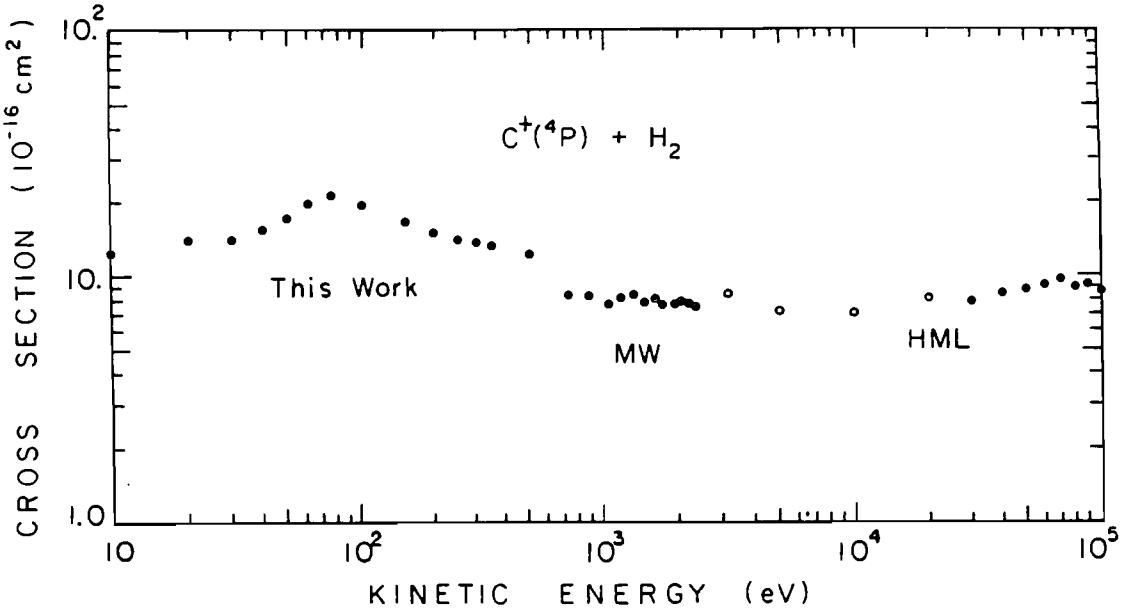

Fig. 2b. Charge transfer neutralization of metastable state C^+ in H_2 as a function of energy. The present work is shown along with higher energy data. From Ref. 2.

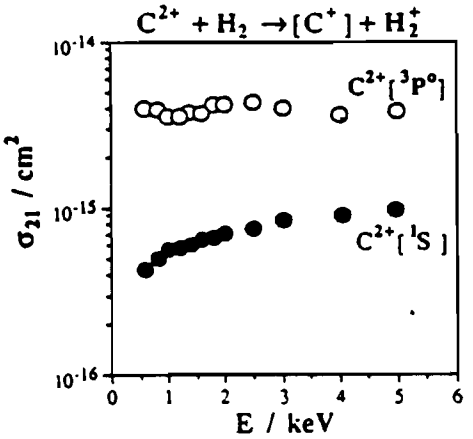

Fig. 3. Preliminary studies by Winter[8] on single electron capture by ground state (^1S) and metastable state ($^3P^o$) C^{2+} in H_2.

The general conclusion of the work is that the metastable state exhibits cross sections ten times that of the ground state at low energy. This is generally in accord with the observations of Moran and Wilcox[1] that have largely been ignored in the literature. All other studies at low energies have claimed that measured cross sections are for the ground state alone. We believe this to be incorrect and that the data are quite unreliable. For higher energies above 10 keV the cross sections for ground and metastable states become virtually the same and any neglect of metastable fractions in ions fluxes is pretty irrelevant. Discrepancies between data sets by different authors have now been resolved and we have established a reliable data set extending from 10 to 10^5 eV impact energy. The results of the work are now all fully published and the reader is referred to the relevant articles for full details.[2,3]

C. METASTABLE AND GROUND STATE C^+ AND O^+ ON ATOMIC H

We are currently performing the same type of single electron charge transfer studies on an atomic H target. The major technical change involves the provision of the atomic (rather than molecular) H source. The revised experimental system is shown in Figure 4. The H is produced as a beam by dissociation of H_2 in a Slevin type RF discharge source. We have recently analyzed the RF characteristics of this source.[9] Due to the tenuous nature of the target it is not feasible to use the attenuation technique of Eq. 4. Instead product ions are monitored and identified by a small inflection field magnetic spectrometer operating at 90^o to the incident ion beam. A small repeller voltage repells product ions out of the collision chamber and into the analyzing system. The system is rotatable through angles from 90^o to 0^o so that the incident ion beam can be monitored also as it is attenuated by the target gas. The H and H_2 components from our RF discharge source are determined using an electron beam (not shown in figure and which crosses the H/H_2 beam from the discharge) and the analyzing mass spectrometer system. Results are placed on an absolute basis by normalizing to the data for H_2 that we have recently published.[2,3] The experiment is greatly complicated by the fact that the Slevin type source produces only a 90% dissociation so that 10% of the target beam is H_2 for which cross sections can be very high. Thus one has a mixed beam of C^+ (or O^+) ground and metastable ions crossing a target beam that includes both H and H_2. By a process of elimination one can arrive at the desired cross sections for C^+ (or O^+) on H but the accuracy will inevitably be poor. We anticipate that the results will be greatly different from those of Nutt et al.,[5] since these workers normalized their H results to their H_2 data and that latter data is quite incorrect.

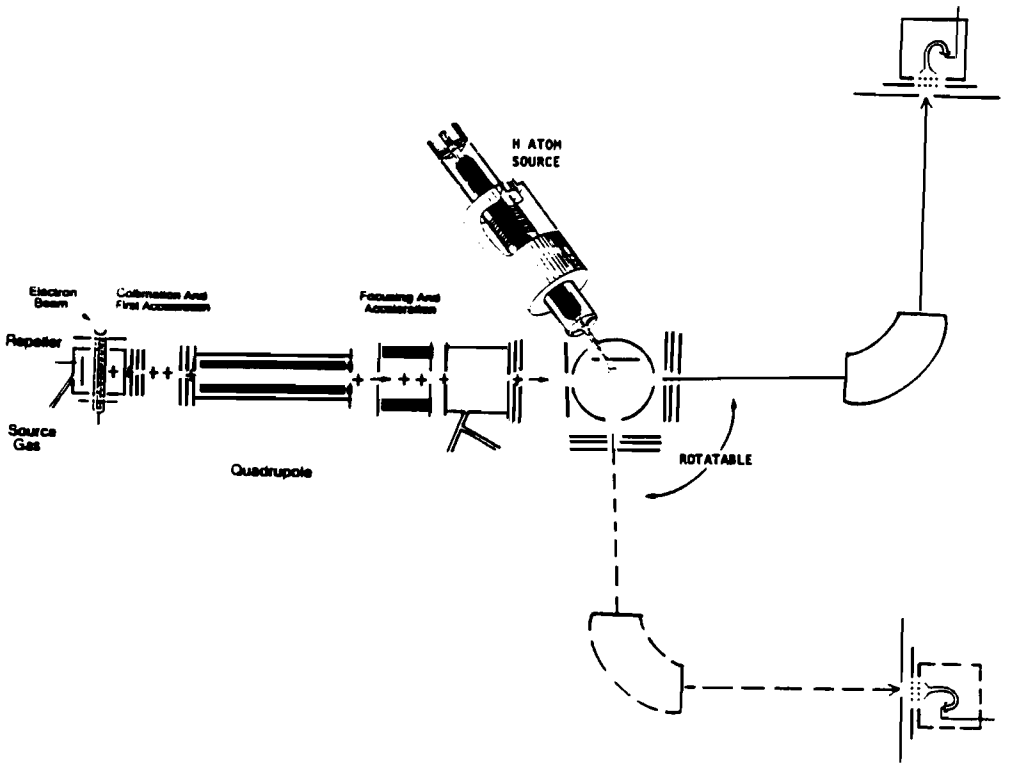

Fig. 4. Schematic of experimental apparatus used to measure charge transfer cross sections of ions with H atoms.

The apparatus is complete and preliminary data are being obtained. Some difficulties have been experienced in making the RF source produce the desired 90% dissociation of source gas (H_2) into H. Dissociation fraction of the emergent neutral flux is greatly dependent on the nature of the wall surface in the extraction capillary Various standard surface cleaning techniques have been employed and dissociation fraction of around 80% are now routinely obtained. An interesting feature is that the RF discharge seems to induce precipitation of pump oil inside the source shield. Due to the configuration of our source region that oil migrates to the extraction orifice and causes it to be periodically blocked. Other workers using this type of source seem to

have experienced the same problem. Various strategies for eliminating the problem are being employed. These include altering the surface migration path and maintaining a continuous flow of source gas even when the apparatus is not in use. The phenomenon is not related to excessive oil in the vacuum system. Preliminary data for charge transfer of singly charged C and O ions on atomic H are now being obtained and the experiment should be completed during the next few months. A paper concerning the design of the RF cavity is in course of publication.

D. PROPOSED WORK.

A proposal for continuation of the work beyond the period of the present grant has been submitted to DOE. The general objective is to study the same processes of electron transfer but for multiply charged ions of C and of O; again targets will be H_2 and H. Again the emphasis is on studying the difference between ground and metastable excited species concentrating on low energies (10 to 500 eV) that are typical of a tokamak fusion plasma's edge. Experimental facilities will remain basically the same as use in the previous work reported here except that we will need to provide a source of multiply charged ions (rather than singly charged ions as at present).

As a source we propose a simple Electron Cyclotron Resonance (ECR) source following the general design of Sortais et al.[10] and Melin et al.[11] This is a very simple system designed to be added to accelerator terminals or to Molecular Beam Epitaxy systems. Part of our objectives is to diagnose the metastable fraction of the ions from such an ECR source. The literature provides very little indication of what excited state fractions might be expected from ECR sources.

The source has been fully designed and is now being constructed. It will be added to a Hitachi RMU-7L mass spectrometer that will provide both mass resolution and energy definition of the ion beam. This in a sense replaces the source-quadrupole part of the apparatus shown in Figs 1 and 4. All other parts of the experiement remain basically the same.

Very little prior work exists on the subject of how multiply charged ions in metastbale states pick up an electron by charge transfer. Most published work on this general area assumes that the ions from a source are all ground state and that metastable content is irrelevant; there is generally no evidence to support this contention.

In unpublished work Winters[8] has shown that 400 eV metastable C^{2+} in H_2

has a cross section of 40 $\mathring{A}^2$, ten times that of the ground state. The cross section gap appears to be increasing towards lower energies. The experimental arrangement was almost the same as in our own work with the ions being produced in an electron impact source. Aumayr and Winters[12] also showed that 50% of a typical C^{2+} ion beam is metastable. Studies of neutralization of O^{2+} in H_2 by two different authors[13,14] show a difference of an order of magnitude in the few hundred eV energy region. Similar differences were apparent before in data for singly charged ions and explained by us[2,3] as due to differing levels of metastable content in the various experiments along with great differences between ground and metastable state cross sections. Beyond that,the literature contains a few standard expressions of concern but no information.

The general intent is to cover O and C ions with charge states from twice ionized to completely stripped, if at all possible. Some of these species (for example completely stripped ions and ions with only three electrons remaining) do not have metastable excited states and any measurements is clearly for a ground state species. For most of the other configurations metastable states exist, are expected to be present in ion beams, and may show cross sections greatly different from the ground state.

The experiment is now in course of assembly and the pursuit of this problem is covered by the proposed three year renewal of this project.

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F. PUBLICATIONS

The following two publications have fully described the results to data.

PHYSICAL REVIEW A VOLUME 41, PAGE 1408 1 FEBRUARY 1990

Charge-transfer reactions of ground-state C^+ (^2P) and metastable-state C^+ (^4P) ions with H_2 molecules

Yaodong Xu, T. F. Moran, and E. W. Thomas

Abstract: Cross sections for charge-transfer reactions of ground state C^+ (^2P) and metastable-state C^+ (^4P) ions with H_2 have been measured in the 10- to 500-eV kinetic energy range. Ground-state reaction cross sections range from 0.3 to 0.5 x 10^{-16} cm^2, and the corresponding values for metastable state C^+ (^4P) ions vary from 20 to 12 x 10^{-16} cm^2. both sets of cross-section values smoothly extrapolate to previously measured data at higher energies.

J. PHYS. B: AT. MOL. OPT. PHYS. VOLUME 23, PAGE 1235 APRIL 1990

Charge transfer reactions of ground O^+ (^4S) and metastable O^+ (^2D,^2P) ions with H_2 molecules

Yaodong Xu, E. W. Thomas and T. F. Moran

Abstract: Cross sections for charge transfer reactions of ground O^+ (^4S) and metastable O^+ (^2D,^2P) state ions with H_2 have been measured for reactant ions with 10 to 500 eV kinetic energies. Ground-state ion cross sections range from 0.5 to 0.9 x 10^{-16} cm^2 and metastable-state ion cross sections are approximately constant at 10 x 10^{-16} cm^2.

The following article describing the design feautres of the RF discharge source of atomic H has been submitted for publication and tentatively accepted subject to some revisions.

JOURNAL OF PHYSICS E (SUBMITTED)

Simple Method to Calculate the Operating Frequency
of a Helical Resonator/RF Discharge Tube Configuration

R. F. Welton, E. W. Thomas, R. K. Feeney and T. F. Moran

Abstract: A practical technique is described to estimate the resonant frequency shift of a helical resonator due to addition of a coaxially mounted discharge tube. A simple formula is derived which relates this change in resonant frequency of the cavity to dimensions and dielectric properties of the discharge tube and its contents.

G. PERSONNEL

Edward W. Thomas of the School of Physics and Thomas F. Moran of the School of Chemistry have acted as co-PIs for the majority of the reporting period. The project was in part inspired by Mr. C. F. Barnett of the ORNL and an adjunct faculty person at Georgia Tech; Barnett was to have been co-PI with Thomas but passed away early in the period of the present grant.

Students Robert F. Welton (of Physics) and Yaodong Xu (of Chemistry) have been employed on the project for most of the reporting period. Both will use protions of this work as the basis for their PhD Theses; Xu is expected to graduate within the next twelve months and Welton in the year following.

The project has made use of technical service and shop facilities in both the schools of Physics and Chemistry as these were required.

METASTABLE ENHANCEMENT OF C^+ AND O^+ CAPTURE REACTIONS

FINAL REPORT

DOE CONTRACT NUMBER DE-FG05-87ER 13745

By
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July 31, 1992

I INTRODUCTION

The project is devoted to the study of charge transfer neutralization of Carbon and Oxygen ions in H and H_2 gases at energies from 10 to 500 eV. A major motivation was to provide cross section data to support analysis of edge plasmas in Tokamak Fusion devices.

The first objective was to measure cross sections for metastable excited singly charged ions separately from the cross sections for ground state ions. Previously published values are confusing because the beams used included unknown fractions of metastables and these metastables have cross sections greatly different from the ground states. The program was fully accomplished, metastable cross sections were found to be over an order of magnitude greater than the ground state and existing discrepancies in the literature were resolved. Considerable effort was devoted to the design and operation of ion source configurations were the metastable content of the ion beam was known.

Subsequently we have moved to study neutralization of multiply charged C and O ions in the same targets. First there has been a need to develop ion sources which can produce useful beams of multiply charged species. This has now been accomplished. The intent is to use these sources for the measurement of cross sections with again an attempt to differentiate between the behavior of ground and metastably excited species.

II PROGRESS OF THE WORK

As the project proceeded the results were rather frequently and fully published in the open literature. To summarize the results and progress we shall largely confine ourselves to the reproduction of the abstracts of these publications.

The majority of the published work relates to the study of metastable ion neutralization. The basic detection technique was to study the attenuation of the ion beam as it traversed a target gas cell. The attenuation can be related to gas pressure, cell thickness and the cross section for charge transfer neutralization. If two species are present (e.g. metastable and ground state) which exhibit greatly different cross sections then the attenuation curve can be deconvoluted to give the two separate cross sections. The deconvolution procedure also allows one to measure the metastable content of the ion beam as a ratio to the total beam. As a source of ions we used an electron impact source where the electron energy could be rather closely controlled. Thus by selecting an electron energy below the threshold for metastable ion production but above the ground state ionization threshold one may produce beams for only ground state species. These can be used for a ground state measurement free of any confusion about the presence of metastables. At higher electron energies one may produce both

metastable and ground state species for which the separate cross sections may be evaluated by the attenuation deconvolution. With the information on the ground state alone one can separate identify the metastable behavior. We should perhaps note in passing that the flight length of the apparatus was sufficient that any excited states that radiatively couple to the ground (or metastable) states will decay before the ion beam enters the collision region.

We discussed our studies of charges transfer neutralization of oxygen ions in a paper with the following abstract (1):

> Cross sections for charge transfer reactions of ground $O^+(^4S)$ and metastable $O^+(^2D,^2P)$ state ions with H_2 have been measured for reactant ions with 10 to 500 eV kinetic energies. Ground-state ion cross sections range from 0.5 to 0.9×10^{-16} cm^2 and metastable-state ion cross sections are approximately constant at 10×10^{-16} cm^2.

A similar paper with full experimental details contained our data on the neutralization of the carbon ions and had the following abstract (2):

> Cross sections for charge-transfer reactions of ground-state $C^+(^2P)$ and metastable-state $C^+(^4P)$ ions with H_2 have been measured in the 10-to 500-eV kinetic energy range. Ground-state reaction cross sections range from 0.3 to 0.5×10^{-16} cm^2, and the corresponding values for metastable state $C^+(^4P)$ ions vary from 20 to 12×10^{-16} cm^2. Both sets of cross-section values smoothly extrapolate to previously measured data at higher energies.

Typically the cross sections for the metastable state were an order of magnitude of more higher than those of the ground state at low energies. A major result of the work was to show that previous measurements of these processes by Gilbody's group were in fact totally incorrect due to inadequate assessment of the metastable content of the ion beams they utilized. Prompted by our results Gilbody repeated most of his previous work and completely confirmed the observations of the present project.

The interest in the metastable state composition led us to perform a brief general study of what metastable carbon fluxes could be obtained from ionization of various carbon containing gases. The highest fraction was found from CO, some 32 %. Gases with CH bonds generally gave metastable fractions of about 20-25% and those with a CN bond only 15%. These fractions were obtained for electron impact ionization at 100 eV; that is far above threshold. We believe at these energies the metastable fraction is rather independent of energy and probably representative of any ion source configuration including a plasma device. The results have been fully reported in a paper with the following abstract (3):

An experimental technique has been developed to determine the fraction of metastable ions present in beams. The technique involves measurement of total electron capture cross sections from neutral species where individual ground and excited state reactant ion cross sections are known. Metastable C II ion abundances from electron impact ionization of various molecules have been obtained.

We further wished to pursue these studies by seeking the same type of cross section information for highly charged ions of O and C. We first attempted to predict what sort of metastable populations would be obtained from an ECR plasma type source utilizing a stepwise ionization model. Cross sections are based on the semiempirical model of Lotz. Comparison could be made between predictions and our own measurements as well as the measurements of other groups. Good comparisons were obtained and the results are fully published in a paper with the following abstract (4):

A simple ionization model has been used to compute metastable beam populations for atomic ions formed in low density, high electron temperature ECR plasma type ion sources. Metastable fractions for each charge state of atomic carbon, nitrogen and oxygen have been evaluated. Computed metastable fractions are found to be in reasonable agreement with experimental data.

With the prediction of source operating conditions in hand we have no turned to the design of an ECR source that will produce highly ionized ions and in particular ions of all state of C and O. The intent is that the source should be compact and readily retrofitted to existing ion accelerator systems. This has been achieved with a novel magnetic mirror structure based on permanent magnets. The design has now been submitted for publication with the following abstract (5):

A novel compact electron cyclotron resonance (ECR) ion source has been constructed and its performance characteristics evaluated using a double focusing mass spectrometer system. The source is particularly well suited for applications where beams of multiply charged ions of moderate intensities are utilized as, for example, in certain atomic physics experiments. The design features an adjustable all permanent magnetic mirror structure and a low microwave (2.45 GHz) power requirement. This low cost, simple source provides a practical alternative to larger more sophisticated ECR ion sources when production of intense beams of highly charged ions is not required. Detailed analysis of the novel magnetic structure is presented. Both charge state and kinetic energy distributions of up to eight times ionized argon as well as total extracted ion currents resulting from differing source operating parameters are given. The end loss ion temperatures for each of these argon charge states has also been determined.

ECR sources, relying on multiple electron impacts, offer the opportunity to produce molecular species not readily observed in other collisional situations. This has led us to utilized our ECR design to search for the elusive CH^{2+} ion that has sometimes been reported. Our conclusion is that the species does not exist and we have provided theoretical calculations to show that the configuration should be repulsive. The work has been submitted for publication with the following abstract (6):

> Experiments with an electron cyclotron resonance ion source have been employed in a hunt for the elusive CH^{2+} ion. Our experiments do not find evidence for the existence of stable CH^{2+} ions. Different levels of ab initio molecular orbital theory have been employed to obtain potential energy curves for CH^{2+}. Although SCF calculations show a small minimum in the potential, post-Hartree-Fock computations indicate CH^{2+} states to be repulsive.

The majority of the experiments described in our various papers involved targets of molecular hydrogen. It was, however, always our intent to perform the same experiments with an atomic hydrogen target. This was to be done with the H in the form of a beam with dissociation taking place in an RF discharge. A source was designed and reported with the following abstract (7):

> A practical technique is described to estimate the resonant frequency of a helical resonator surrounding a coaxially mounted discharge tube. A simple formula is derived that relates the resonant frequency of the cavity to dimensions and dielectric properties of the discharge tube and its contents. An experimental test is performed on a resonator used to power an RF discharge, designed to produce an atomic hydrogen beam for an atomic collision experiment. The formulation adequately predicts the resonant frequency for a helical resonator that contains a discharge tube and cooling water jacket.

Unfortunately the degree of dissociation obtained in the configuration was only about 60% with the remainder being molecular hydrogen. Moreover the collision chambers available to us were of only modest vacuum quality and exhibited significant backgrounds of H_2. Inevitably the observed signals are a mixture of signals due to neutralization in the (desired) atomic beam and in the (undesired) molecular beam or background. As a result it was not possible to separate out the atomic H cross sections and the experiment is, to date, a failure.

As a subsidiary study one of us also undertook some extensive reviews of how atomic particles interact with surfaces. The principle objectives were to collect and assess data which might be required for the modelling of Plasma Fusion devices. One paper considers how hydrogen particles reflected from materials that are candidate first wall materials for Fusion devices. That work is in publication with the following abstract (8):

> Previously published data on particle backscattering from surface under normal incidence conditions is reviewed in order to arrive at a general scaling relationship in terms of projectile energy and the masses of the colliding species. A single empirical formula is proposed which, with suitable coefficients, represents the available data base and provides a basis for interpolation and extrapolation. The formula is intended for use in codes for the modeling of particle recyclying in fusion reactor devices. Attention is focused primarily on light projectile (H, D, T, He) reflection from candidate plasma facing materials and covers an energy range from tens of eV to 100 keV to encompass situations of interest in a fusion device. We also review briefly the case of self-ion reflection.

A second paper considered the available data on electron reflection from solids and coefficients for ejection of secondary electrons. That work is also fully published with the following abstract (9):

> Particle induced electron emission from the wall of a plasma device alters the sheath potential and plasma transport in the scrape-off layer. Incident electrons eject electrons from a solid by a kinetic process. The ejected electrons cannot be distinguished from the reflected electrons and so the total yield is the sum of the two processes. Heavy particles eject electrons by the kinetic mechanism; when the projectile is ionized or excited, there may also be a contribution from potential ejection processes. Available data on electron ejection and electron reflection are reviewed, the most reliable data selected and, where appropriate, formulas are proposed that represent the functional dependence of the yield on the impact energy and impact angle.

III PUBLICATIONS

Nine major publications supported wholly or in part by the DOE have been prepared and are listed as references 1 through 9 in this report. Copies of those published have already been transmitted to DOE.

IV PERSONNEL

Principal investigator for the project was E. W. Thomas of the school of Physics. Co-PI is T. F. Moran of the School of Chemistry.

Dr. Yaodong Xu obtained a Ph.D degree based on this work. Mr. R. F. Welton will shortly write a Ph.D. thesis based on some of this work with completion projected within the next six months.

The project benefitted greatly from extensive interactions with other faculty and students at Georgia Tech particularly with R.K.Feeney of EE.

V FUTURE WORK

No further support is being provided by the DOE. It is however anticipated that the study of charge transfer neutralization of highly charge ions will continue with support from other sources.

VI FINANCIAL MATTERS

All funds are now expended and financial reports have already been submitted in the required format.

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