

Sixteenth International Conference on the Physics of Electronic and Atomic Collisions

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Program Changes

General Information

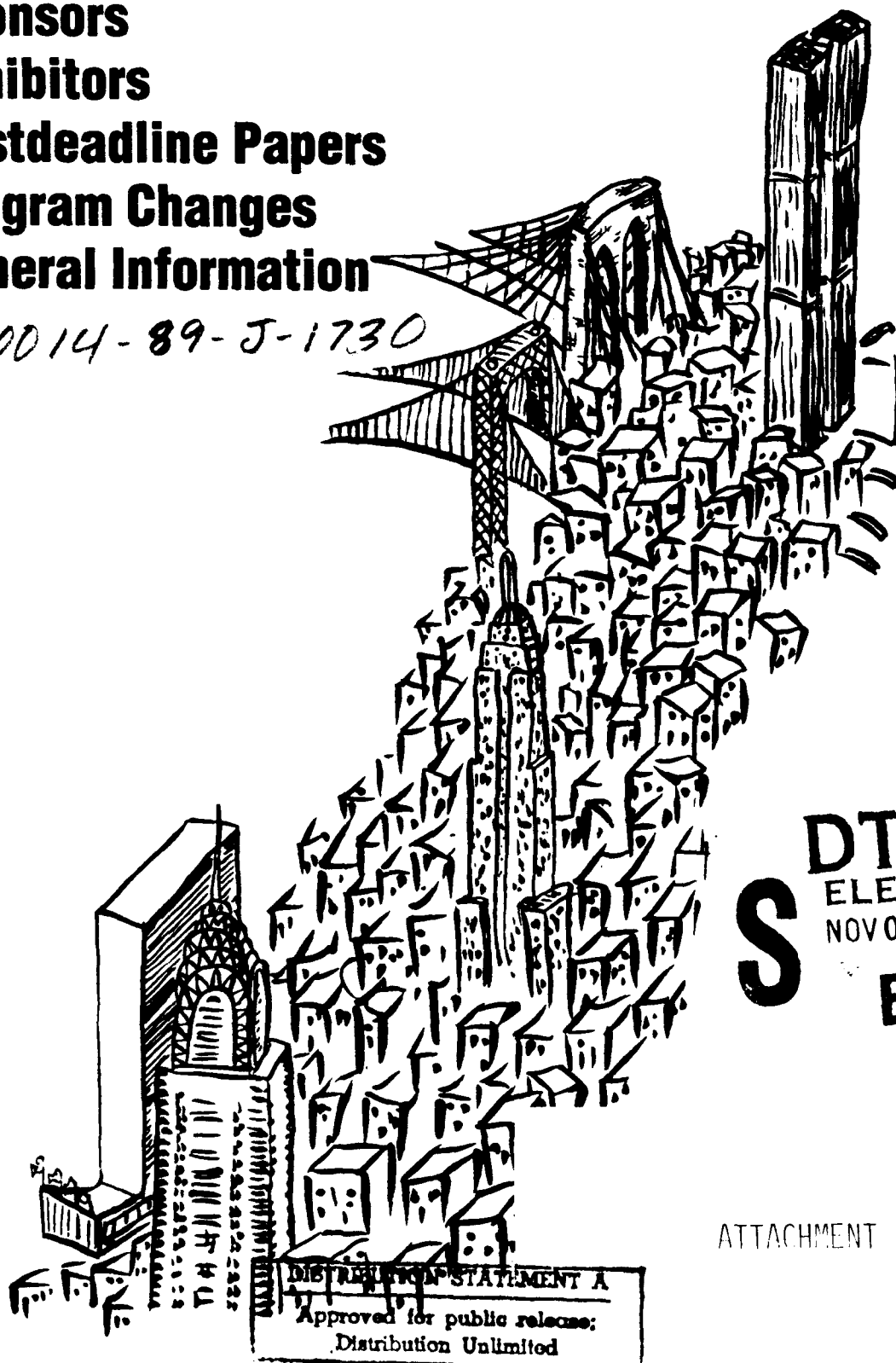
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XVI ICPEAC



30th Anniversary



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ATTACHMENT D

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Grand Hyatt Hotel • New York, New York • 26 July - 1 August 1989

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July 26 - August 1, 1989

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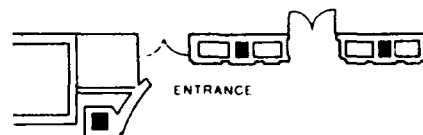
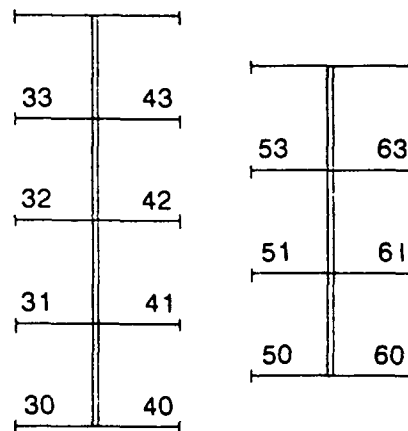
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EXHIBITS

LAYOUT OF EXHIBITS

BALLROOM B



1989 ICPEAC SHOW
16th International Conference on the Physics of
Electronic and Atomic Collisions
Grand Hyatt Hotel, New York, New York, U. S. A.
July 26-27, 1989

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GENERAL INFORMATION

GENERAL INFORMATION

16th INTERNATIONAL CONFERENCE ON THE PHYSICS OF ELECTRONIC AND ATOMIC COLLISIONS JULY 26 - AUGUST 1, 1989

WELCOME!

The staff at the Conference Desk will be pleased to assist you. Hostesses at the Registration and Information Desks speak five languages -- English, French, German, Russian, and Spanish.

Welcome Reception: A Welcome Reception will provide an opportunity for greeting old friends and meeting new ones on Tuesday, July 25, from 5:30 to 6:30 p.m., in Ballroom C of the Grand Hyatt Hotel, adjacent to the ICPEAC Registration Area. Wine, beer, soft drinks and light *hors d'oeuvres* will be served.

Meeting Place: The Booth/Imperial Room, on the Conference Room level of the hotel, will serve as a Meeting Place, available throughout the Conference. All activities for the Accompanying Persons' Program will take place here, and this will be the starting point for all tours. The room will be open from 8 a.m. to 10 p.m. each day, including Saturday and Sunday.

Bederson Award Book: A book citing Ben Bederson's contributions to ICPEAC, atomic physics, and scientific publishing will be available for a signature gathering at the ticket exchange table until noon on Thursday, July 27, and at the main Registration Desk thereafter. The book, produced by Academic Press, will be presented to Ben at the Awards Session on Tuesday, August 1, at 9:45 a.m.

Messages: Please check the message boards, located near the Information Desk in Ballroom Foyer FREQUENTLY. Messages will be placed in alphabetically-marked sections of the bulletin boards. The telephone numbers for connecting with the message center are 212/883-1234, ext. 3603 and 3604.

FAX Facilities: If you need to have material sent to you by Facsimile machine, you should have it sent to you, in care of XVI ICPEAC, to the FAX machine at the concierge desk in the hotel lobby. The number is 212/697-3772.

BITNET Facilities: Electronic mail facilities will be available starting Thursday, July 27 in the Majestic Room at the hours posted on the door. You may receive mail at the following BITNET address: MIACC@CUNYVM. If you wish electronic mail from the terminal in the Majestic Room, the dial-up number for the CUNY node is 974-8600. The log-on ID is MIACC, and the password is "Tuesday."

XVI ICPEAC Posters: XVI ICPEAC Posters will be available for sale in the Registration Area beginning on Thursday morning. The cost is \$6 each.

Accompanying Persons' Program: The accompanying persons' program contains many tours and visits outlined in the third announcement. To begin the week, there will be a general orientation on sightseeing in New York City, with a service of coffee and pastries, in the Booth/Imperial Room at 9 a.m. on Wednesday, July 26. A representative of the New York Convention and Visitors Bureau will be there to answer questions and distribute special sightseeing information. Informal walking tours of New York City will be arranged, and visitors may sign-up for general sightseeing tours. On Monday, July 31, Professor David Markowitz will speak on "What are They Doing When They're Not at Home?" The talk, scheduled for 9:30 a.m. in the Booth/Imperial Room, will provide a look at what's important in physics today for spouses of physicists.

Children's Hospitality: The Winter Garden and Edison Rooms, also on the Conference Room Level, have been set aside as hospitality rooms for accompanying children. The Winter Garden Room is set up as a playroom for small children, and the Edison, as a lounge for older children and teens. The rooms will be open during the sessions to facilitate parents' attending sessions. The rooms will NOT be open during lunch breaks. Register for children's hospitality and check for exact schedules in the Winter Garden Room from 5:30 - 7 p.m. on Tuesday evening and from 8:30 a.m. to 11 a.m. each meeting day.

Tours and Theater Tickets: Tickets for tours or the theater that have been ordered in advance may be picked up at the Tour/Theater Desk adjacent to Registration in the Ballroom Foyer of the Hyatt. Representatives of Convention Tours Unlimited will also sell tour and theater tickets Tuesday evening and Wednesday morning. Places are still available on each tour, and theater tickets are still available for "Cats" and "Les Miserables."

McGraw-Hill, AT&T Reception: The McGraw-Hill, AT&T Reception will be held in the Astor Hall of the New York Public Library on Thursday, July 27, from 7 to 8:30 p.m. Drinks and *hors d'oeuvres* will be served. The Library is located on the west side of Fifth Avenue, between 40th and 42nd Streets, a short three-block walk from the Grand Hyatt. Enter the Library through the main entrance, at the top of the steps on Fifth Avenue.

Conference Dinner: The Conference Dinner will be held on a boat, the "Dayliner", on Monday, July 31. The cruise will include music and dancing, as well as dinner, and spectacular views of New York City. For regular participants and others who have elected the banquet option, yellow invitations (exchange tickets) for the banquet are included in your registration packet. These invitations will not admit you to the cruise. To receive admission tickets, turn in your yellow invitations in for brown tickets at the Ticket Exchange Desk located in the Ballroom Foyer no later than 12 noon on Thursday, July 27. **Please note: You MUST exchange the tickets to be admitted to the cruise. ONLY THE BROWN TICKET WILL BE VALID.** This will allow the conference organizers to receive an accurate head count for the event.

Conference Dinner Buses: Buses will depart from the Park Avenue entrance on the Mezzanine Level of the Grand Hyatt on Monday, July 31, from 6 p.m. to 7:15 p.m. The "Dayliner" is docked at the Circle Line Pier, # 81, Hudson River, at the West end of 42nd Street.

Concert: A chamber music concert by the Manchester String Quartet of Washington, DC, will be held on Sunday, July 30, at 4 p.m. at the Tishman Auditorium, in the New York University Law School Building (Vanderbilt Hall, 40 Washington Square South). Admission is free. However, advance tickets are required for admittance. A limited number of tickets are available at the Ticket Exchange Desk, and will be distributed on a "first-come-first-served" basis.

Weekend Activities: A number of weekend activities were mentioned in the Third Announcement -- including tickets to the New York Yankees baseball game on Saturday, July 29; an excursion to the beach on Saturday; a jog in Central Park, followed by a picnic lunch; guided tours to the Botanical Gardens and the Statue of Liberty and a Tour of galleries and studios. Watch for notices about these and other weekend activities on the Message Board.

Restaurant Reviews: Reviews and ratings of New York restaurants will be available for your perusal at the Information Desk.

Smoking with not be permitted in the meeting rooms. Ashtrays will be provided in the foyer outside of each room.

PROGRAM CHANGES

PROGRAM CHANGES

Plenary Lecture

As a result of unexpected circumstances, Professor Y. T. Lee is unable to deliver the previously announced Plenary Lecture for 13:00 on Friday. We are grateful to Professor D. M. Neumark of the Chemistry Department of the University of California at Berkeley for agreeing at a late date to deliver a Plenary Lecture entitled "Spectroscopy of Transition States of Hydrogen Transfer," which will include results of collaborative work with Professor Lee.

Poster Sessions

- The Poster "Orientation of p-States in Ion-Atom Collision Propensity Rules for Excitation and Capture" by S. E. Nielsen, J. P. Hansen and A. Dubois will be presented twice: at the scheduled time on Friday (Fri 157) and in Tuesday's session on **Ion-Atom Collisions** as Poster (Tue 114).
- The Poster "Dissociation of Hydrogen Molecules in H₂-Ar Discharge" (Mon 13) by M. A. Islam, has been withdrawn.
- The Poster "Bremsstrahlung of Electrons Scattered by Xenon Atoms" (Thu 64) by E. T. Verkhovtseva, listed as "abstract withdrawn" has been resubmitted. It is reproduced here as the first abstract and will be presented in the originally scheduled session (Thu 64).
- Post-deadline Contributions: The book of Abstracts contains 31 post deadline contributions. These, along with the eight contributions reproduced in this booklet, will be presented in the **Post Deadline Session** on Tuesday afternoon.

POST-DEADLINE ABSTRACTS

BREMSSTRAHLUNG OF ELECTRONS SCATTERED BY XENON ATOMS

E.T. Verkhovtseva, E.V. Gnatchenko, and A.A. Tkachenko

Institute for Low Temperature Physics and Engineering,
UkrSSR Academy of Sciences, 310164, Kharkov, USSR

Modern theoretical concepts¹ suggest that the bremsstrahlung (BS) spectrum of electrons scattered by atoms is generated by two mechanisms. The first mechanism is radiation of photons by an incoming electron when braking in a static atomic field, i.e. "electron" BS, and the second one is radiation by an atom due to its dynamic polarization by the incoming electron field, i.e. "polarization" BS.

The polarization BS was first observed in purposive experiments with 0.6 keV electron scattering by Xe atoms in the region of 4d threshold². This paper deals with the BS dependences on the energy of electrons scattered by xenon atoms.

The experiments were carried out by using a setup comprising an X-ray tube with a supersonic gas jet as an anode and a grazing-incidence spectrometer RSM-500. The angle between the direction of the incoming electrons and that of the photons examined was 97°. The experimental technique and procedure are given in detail in³. The figure shows total BS spectra taken with 0.3, 0.6 and 0.9 keV electron scattering by Xe atoms. Analysis of the spectra permits us to ascertain that: 1) as the electron energy is increased from 0.3 to 0.9 keV, the BS curve shifts to smaller photon energies, i.e. the experimental BS maximum approaches both the resonance in the photoabsorption spectrum and the maximum of the theoretical BS curve calculated in the logarithmic approximation;¹ 2) as the electron energy is increased the spectrum profile is modified: the band on a smaller photon energy side becomes more asymmetric. Moreover, for the electron energies of 0.3 and 0.6 keV, the BS spectra display a branch in the photon energy range above 145 eV due to virtual excitations of Xe atoms into an ionization continuum above the 4p threshold.

Based on the modern theoretical concepts, the analysis of the results permits us to suggest that the BS curve profile and the maximum position are affected both by the interference

of the "electron" and "polarization" BS and the transferred momentum dependence of atomic polarizability in the scattering process. This suggestion is supported by the theoretical calculations made in the Born approximation with taking the above dependence and interference into account.

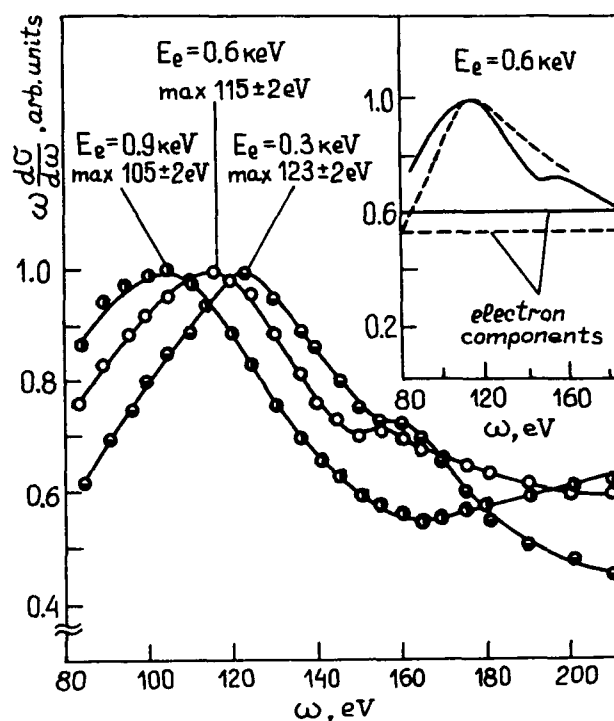


Figure 1. BS spectra of electrons on Xe atoms. Inset: comparison of the experimental BS spectrum (—) and the theoretical one¹ (---)

References

1. M.Ya. Amusia, V.M. Byimistrov et al., Polarization Bremsstrahlung of Particles and Atoms (Nauka, Moscow, 1987).
2. E.T. Verkhovtseva et al., J. Phys. B16 1613 (1983).
3. E.T. Verkhovtseva et al., J. Phys. B19 2089 (1986).

SEARCH FOR A JOINT SPIN-ORBIT AND EXCHANGE ASYMMETRY IN ELASTIC ELECTRON SCATTERING FROM SODIUM

J.J. McClelland, M.H. Kelley, S.J. Buckman* and R.J. Celotta

Electron Physics Group, National Institute of Standards and Technology
Gaithersburg, MD 20899, USA

The existence of an azimuthal asymmetry in the elastic scattering of unpolarized electrons from spin-polarized one-electron atoms was first proposed by Farago¹. He demonstrated that such an effect may be measurable when both spin exchange effects and the spin-orbit interaction are present. Walker² further developed this concept, which he termed an "interference" between the exchange and spin-orbit processes, with some exploratory calculations of asymmetries for several one-electron targets. He found evidence for substantial effects (~15%) in the heavier alkalis, particularly cesium, and predicted the effect should be negligible in the lighter alkalis and hydrogen.

As part of a program of measurements of spin-polarized electron scattering from spin-polarized sodium we have measured this asymmetry, which we shall term the "joint asymmetry", defined by

$$A_{\text{joint}} = \frac{1}{P_a} \frac{(I^{\uparrow\uparrow} + I^{\downarrow\uparrow}) - (I^{\uparrow\downarrow} + I^{\downarrow\downarrow})}{(I^{\uparrow\uparrow} + I^{\downarrow\uparrow}) + (I^{\uparrow\downarrow} + I^{\downarrow\downarrow})}$$

where P_a is the atom beam polarization and I is the scattered electron intensity, the arrows representing electron and atom beam polarizations respectively. Note that although these experiments are carried out with a polarized electron beam, the asymmetry represents an average over the electron spin.

These measurements have been conducted at incident electron energies of 20, 54.4 and 70 eV. The latter energy was chosen as the result of a search for the energy at which the deepest minimum in the elastic differential cross section occurred. The joint asymmetries are shown in Figure 1. It would appear that if this effect is present at these energies, then it is at a level of less than 1%.

This work is supported in part by the U.S Dept. of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences.

*Permanent address: Electron Physics Group, Australian National University, Canberra, Australia

References

1. P.S. Farago, J. Phys. B7, L28 (1974).
2. D.W. Walker, J. Phys. B7, L489 (1974).

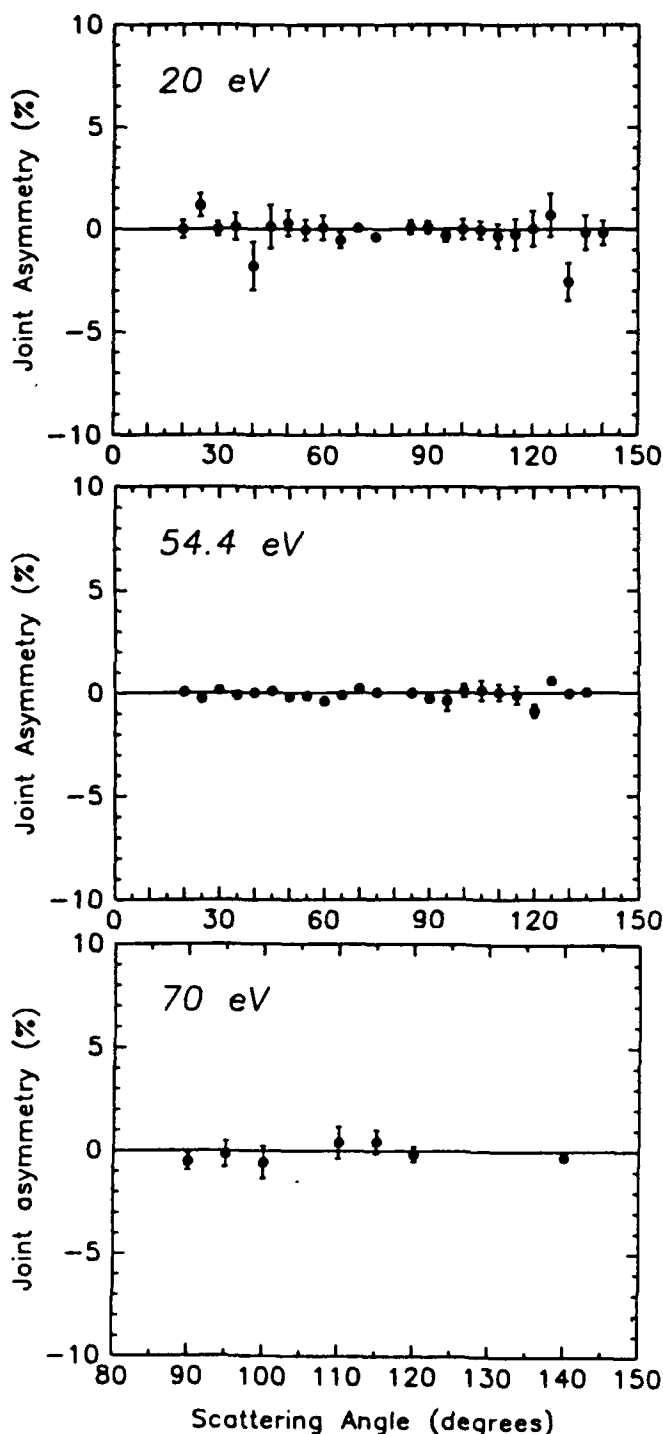


Figure 1. Joint asymmetry as a function of electron scattering angle at 20, 54.4 and 70 eV.

THE $\text{Cs}(7P) + \text{H}_2 \rightarrow \text{CsH} + \text{H}$ REACTIVE COLLISION : ROTATIONALLY-RESOLVED CROSS SECTIONS

Jean-Marc L'Hermite, Gabriel Rahmat and Raymond Vetter

Laboratoire Aimé Cotton, Bât. 505, 91405 Orsay cedex, France

The $\text{Cs}(7P_{1/2}) + \text{H}_2 \rightarrow \text{CsH}(v''=0, J'') + \text{H}$ photochemical reaction at thermal energies is studied in a crossed-beam experiment, with laser-induced fluorescence detection of CsH products ^{1,2}. A supersonic beam of H_2 and an effusive beam of Cs atoms cross at right angle; two single mode tunable laser beams intersect the collision volume, the first one is locked on a given $6S \rightarrow 7P$ hyperfine transition of cesium and the second one is scanned over a definite $X^1\Sigma^+(v''=0, J'' < 17) \rightarrow A^1\Sigma^+(v'=5, J')$ transition of CsH molecules. Figure 1 shows a recorded fluorescence profile for $J''=11$, at 0.09 eV collision energy, when the analysis laser beam propagates along the collision axis: its shape yields the differential cross section, and its area the total cross section.

The rotational distribution of products at 0.09 eV collision energy is pointed on figure 2: the 17 first rotational levels only are populated in $v''=0$, as expected from the energy balance of this isoenergetic reaction. Figure 3 shows the total cross section relative to $J''=6$ as function of the collision energy that we varied by heating or cooling the hydrogen beam nozzle and by seeding hydrogen in helium; its variation agrees with calculations of the reaction dynamics involving spin-orbit couplings at 8-11 a.u.internuclear distance between the incoming covalent channels and the ionic Cs^+-H_2^- intermediate³. As expected from calculations of potential energy surfaces⁴, there is no barrier higher than 0.015 eV in the $\text{Cs}(7P_{1/2}) + \text{H}_2$ entrance channel.

High resolution scanning of fluorescence Doppler profiles using two different arrangements of the analysis laser beam (parallel and perpendicular to the collision axis) leads to rotationally-resolved differential cross sections. The angular analysis is possible because the velocity of products is the same for a given J'' value. In spite of a good spectral resolution of 30 MHz F.W.M.H., the angular resolution is 25° only in the example of figure 1, where the velocity of CsH products in the center of mass is 22 m/s, and the corresponding full Doppler width 70 MHz; the fluorescence Doppler profile peaks toward the red, indicating a pronounced "forward" scattering of CsH products; this result is consistent with the harpooning process. The angular scattering probability is drawn on figure 4 for different energies: "forward" scattering increases with collision energy but does not vary much with J'' .

References

1. Rahmat et al. Chem. Phys. Lett., **135**, 459, (1987).
2. Rahmat et al. J. de Physique, Sup. n°12, **48**, 601, (1987).
3. Gadéa et al. Chem. Phys. Lett., **138**, 43, (1987).
4. Gadéa et al. J. Chem. Phys., **84**, 4872, (1986).

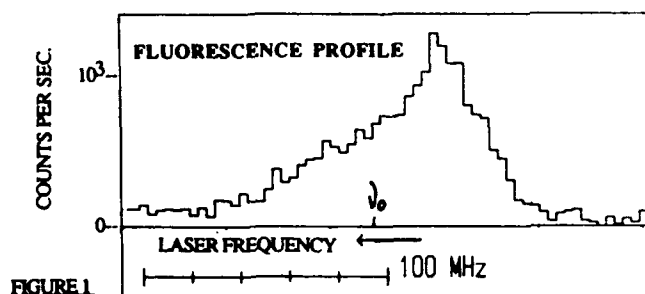


FIGURE 1

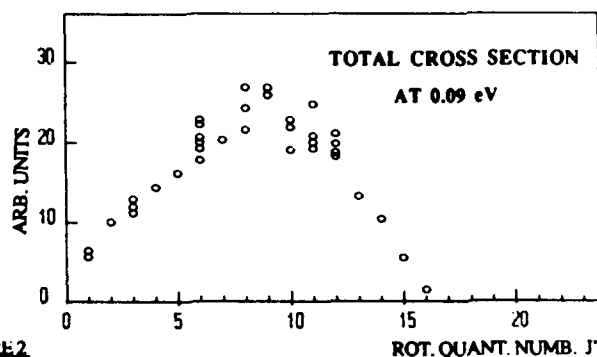


FIGURE 2

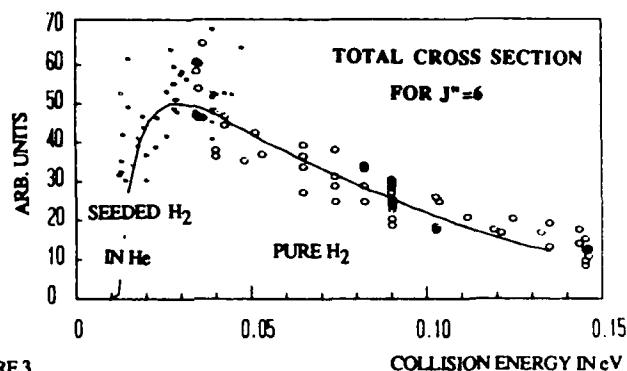


FIGURE 3

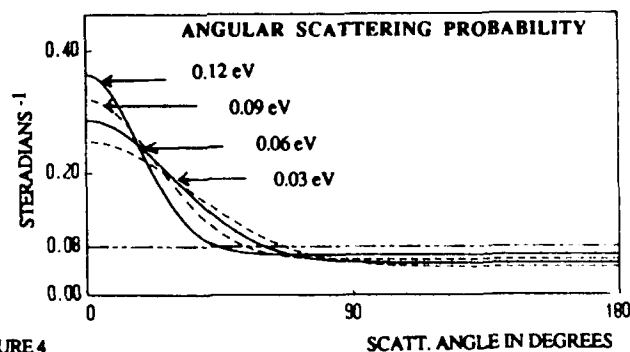


FIGURE 4

Experimental Cross Section for Dielectronic Recombination in C^{3+}

A.R. Young, L.D. Gardner, J.L. Kohl, and D.W. Savin

Harvard-Smithsonian Center for Astrophysics
60 Garden Street, Cambridge, MA 02138 U.S.A.

The interpretation of astrophysical observations and laboratory plasma diagnostics requires a detailed knowledge of the physical processes that produce the light detected. In the particular case of high temperature, low density plasmas, such as the sun's corona and in tokomaks, most of the ultraviolet light is in the form of line radiation and comes from the decay of excited ions.^{1,2} Consequently knowledge of excitation and recombination cross sections is required to understand the nature and behavior of such plasmas.

We have measured the cross section for dielectronic recombination (DR) in C^{3+} using an inclined electron/ions beams collision apparatus.^{3,4,5} DR events are counted by detecting the stabilizing photon (a satellite of the $C^{3+}(2p-2s)$ transition) in delayed coincidence with the resulting C^{2+} ion. Since the DR cross section is expected to be sensitive to the presence of electric fields, an external magnetic field, coaxial with the electron beam, was applied to the collision region. An electric field was thereby produced in the rest frame of the ions. For the present measurement, the magnetic field and ion velocities resulted in an electric field of 10 V/cm. The energy spread of the electrons was determined by measurements of the electron impact excitation (EIE) cross section for $C^{3+}(2s-2p)$ across its threshold. The EIE measurement also calibrates the energy scale of the electron gun and checks the methods used to determine photon detection efficiencies and form factors. Charge transfer cross sections were used to check the efficiency for ion detection.

A measured value will be presented for the energy averaged cross section for DR in a 10V/cm external electric field which results in the capture of an electron into a high Rydberg state of C^{2+} , excitation of the C^{3+} core, and stabilization by a satellite of the $C^{3+}(2s-2p)$ resonance line. DR events involving capture into states which are ionized by the electric field in the final charge state analyzer are not detected. Results will be compared to theoretical treatments and to previous measurements.

This work was supported by the Office of Basic Energy Science, Chemical Sciences Division, of the U.S. Department of Energy and by a Scholarly Studies Award of the Smithsonian Institution.

References

1. J.C. Raymond, *Astrophys. J.* **222**, 1114 (1978).
2. K. Davidson and H. Netzer, *Rev. Mod. Phys.* **51**, 715 (1979).
3. G.P. Lafyatis and J.L. Kohl, *Bull. Am. Phys. Soc.* **24**, 1181 (1979).
4. L.D. Gardner, J.L. Kohl, G.P. Lafyatis, A.R. Young, and A. Chutjian, *Rev. Sci. Instrum.* **57**, 2254 (1986).
5. G.P. Lafyatis, J.L. Kohl, and L.D. Gardner, *Rev. Sci. Instrum.* **58**, 383 (1987).

EXPERIMENTAL AND THEORETICAL ANALYSIS OF COLLECTIVE EFFECTS IN ELECTRON IMPACT IONIZATION PHENOMENA

G.Arena, M.Armenante, R.Bruzzese, F.Giammanco*, N.Spinelli, R.Velotta

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*Dipartimento di Fisica, Università di Pisa, Pisa, Italy

The importance of collective effects, depending on the electron-ion mutual interaction, in experiments involving the production and collection of charged particles has been investigated. Although many authors concerned with different fields of investigations and applications introduced the so called "space-charge" effect as a possible explanation of the observed "anomalous" dependences on the laser power, nevertheless, no experimental work was especially performed to carry out a detailed analysis of the collective plasma phenomena and their range of influence. We report the observation of relevant collective effects in the process of electron impact ionization of low density atomic and molecular gases (pressure 10^{-6} : 10^{-4} Torr). It has been observed a focussing ion effect on the electronic beam very similar to that observed in a different experimental condition in which, anyway, collective effects were present.

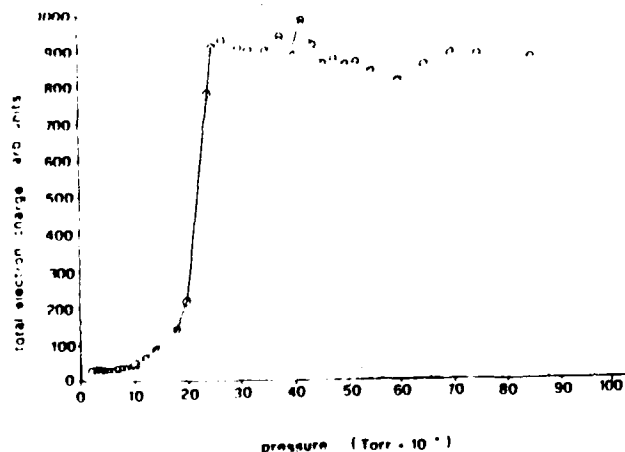


Figure 1. Total collected charge of the electron beam pulse as a function of the gas pressure.

The focussing effect results, in the present case, in an increase of the axial current measured by an electron detector, whose radius is smaller than the radial width of the unperturbed electron beam,

which monitors the electron beam current after it has passed through the target gas.

The observed effect shows a strong dependence on the gas pressure, i.e. on the degree of ionization produced. Actually, the peak and the total charge of the electron current exhibit a sudden growth in a very small range of pressure variation and subsequently the behavior is quite flat, except for a non-regular modulation.

The total ion count rate exhibits a change in the slope in correspondence of the same range of pressure.

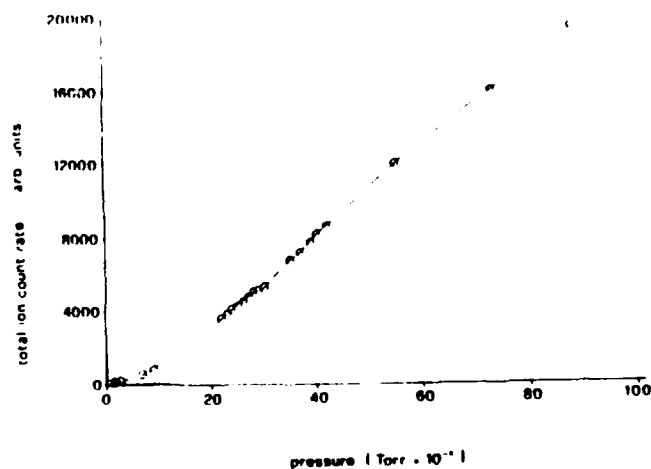


Figure 2. Total ion count rate as a function of the gas pressure.

Moreover, the shape of the peaks in the time of flight (TOF) spectrum of the produced ions changes as a function of the gas pressure, showing a growing tail in the region of increasing time of flight. By adapting the theoretical approach described in ref.1 in order to include the specific features of the experiment, an analysis of the phenomena has been carried out, as well as a detailed comparison with the experimental results.

References

1. F.Giammanco-Phys. Rev.A 36,5658(1987).

DATABASING ATOMIC COLLISION DATA FOR ATOMIC PHYSICS MODELING*

Robert Cauble

Lawrence Livermore National Laboratory
Livermore, California

Atomic modeling is a key component in the overall study of the physics of plasmas, whether in the laboratory or in astrophysical applications. Often most of the model consists of information on collision physics, so it is essential to have a method by which this information can be searched, selected, and retrieved. We describe here a way of accomplishing this in the context of an application for building atomic models from databased information.

An atomic model is a collection of labeled energy levels for one or more ion stages of an atom of charge Z , along with rates (or cross sections plus a method of generating rates) for all relevant processes connecting the energy levels, i.e., a rate matrix. The model may contain a few levels or several thousand. A small subset of the levels may be connected by processes (i.e., collisional excitation) or all of the levels may be. The rates may have been calculated by simple approximations or may be actual experimental data. The size and sophistication of the model are entirely dependent on the problem or the experiment. The rate matrix can be inverted to directly obtain relative electronic populations of the energy levels or the inversion may be one package in a large radiation-hydrodynamics code. Often a small model suffices to determine the dominant features in spectral data, thus allowing temperature and density diagnostics to be quickly performed. For more detailed problems (such as plasma material opacities), a more complete model is necessary.

Given this wide variety of tasks, we are attempting to build a system which (1) provides a relational database of all relevant atomic data and approximate calculations - along with the database's ability to search and compare disparate but related information - and (2) gives the user enough software tools to take selected information and actually construct an atomic model with it.

Data to be stored in the database include: energy levels and associated statistical weights; dominant and less dominant configurations including all intermediate quantum numbers, parities, elements and isoelectronic sequences; oscillator strengths; collisional excitation

and ionization cross sections and/or rates; photoionization cross sections and/or rates; dielectric recombination rates; source information (what code provided these numbers when, who ran the code, etc. or what experiment by which group provided what kind of data, etc.); and the possibility to include data for other processes. No bibliographic information will be maintained, since this is being better taken care of elsewhere. In addition, we are communicating with other atomic data centers (NIST and IAEA) about exchange of information.

The application itself is being written within a commercial database management system (INGRES) in standard computer languages. The data and the application should thus be portable to (virtually) any UNIX, VMS, or DOS system.

The effort is somewhat daunting, but a start has been made. Limiting ourselves to ionic processes (excluding, for instance, molecular interactions), we have built a modular prototype application which accomplishes the above assignments on a database testbed. The system will be described, the form for the database itself, the user interface and data display, and what we hope to do in the future.

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RESONANCES IN LOW-ENERGY ELECTRON-MOLECULE COLLISIONS

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In a series of studies on low-energy electron-molecule collisions, we have found rich resonance structures in both elastic and inelastic channels. The calculations were carried out using a multichannel Schwinger variational principle,¹ and included both diatomic and polyatomic targets. The resonances were analyzed by studying the partial wave T-matrix (or K-matrix) elements.

Resonances in the valence excitations in N₂ have been studied^{2,3} using a six-state calculation including $X^1\Sigma_g^+$, $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, and $C^3\Pi_u$, and a five-state calculation including $X^1\Sigma_g^+$, $a^1\Pi_g$, $a'^1\Sigma_u^-$, $w^1\Delta_u$, and $B^3\Pi_g$. We observed both core excited valence-type and Rydberg-type shape resonances. The nature of the negative ion responsible for the resonance was deduced by comparing the phase of the partial wave T-matrix elements for the inelastic channel as well as the elastic channels of the initial and final target states. The positions of the calculated resonances for the $X - B^3\Pi_g$, $X - A^3\Sigma_u^+$, and $X - a^1\Pi_g$ transitions are in agreement with the experimental measurements of Mazeau et al.,⁴ Sanche and Schulz,⁵ and Polley and Bailey.⁶ In addition, resonance structures also appear in excited state to excited state inelastic cross sections. Their positions can be correlated with the same negative ion states found in ground to excited transitions.

We also studied resonances in Rydberg excitations in CO, $X^1\Sigma^+ \rightarrow b^3\Sigma^+$, and in N₂, $X^1\Sigma_g^+ \rightarrow E^3\Sigma_g^+$, at the two-state level.^{7,8} Both transitions show core-excited Rydberg-type shape resonances near thresh-

old, in agreement with experiment.^{9,10} The positions of these resonances are sensitive to the treatment of differential correlation effects between the negative ion and the neutral molecule. The analysis of eigenphases indicates that both time-delayed and time-advanced scattering contribute at resonance. The time-advanced character is due to interference effects between resonant and nonresonant contributions.⁸

Resonance structures have also been found in the elastic scattering of the series of fluoromethanes CF₄,¹¹ CHF₃, CH₂F₂, and CHF₃. These calculations were carried out at the static-exchange level. Correlated treatment for CF₄ is in progress.

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ELECTRON-MOLECULE COLLISION CODES AT NASA AMES

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Two sets of electron-molecule collision codes have been developed at NASA AMES. The AMES SMC code for electron - neutral molecule collisions and the PDE code for electron - positive ion collisions.

The AMES SMC code is based on a multichannel Schwinger variational principle.¹ It can treat molecules of arbitrary geometry, spin multiplicity, closed or open shell, in the ground or excited state, and with or without target correlation. It is applicable at electron energies from threshold to ≈ 30 eV. A new version of the code, under development for the supercomputers at NASA Ames, will be described. Efficient coding of the Schwinger method depends on three critical steps: (1) The calculation of bound-free integrals. The integral code is completely vectorized. Furthermore, the use of molecular rotation symmetry reduces the number of integrals calculated by a factor of five to ten in typical calculations. The I/O overhead is also significantly reduced. (2) The calculation of Green's function matrix elements. The efficient evaluation of bound-free integrals enables us to calculate Green's function matrix elements over a numerical quadrature of the momentum vector. The matrix multiplication routine in CRAY's SCILIB enables us achieve this step efficiently. (3) Treatment of the (n+1)-electron problem in the scattering region. Here we make full use of the efficient methodology of bound state code SWEDEN at Ames.² The performance of the code at the CRAY-XMP/48, CRAY-2, and CRAY-YMP/832 will

be compared. The relative advantages of fine grain and coarse grain paralleling computing will also be studied.

The PDE method, developed by Temkin and Sullivan,^{3,4} is a non-iterative solution of the Schrödinger equation for a diatomic target by finite differences. Exchange contributions are treated exactly by defining separate differential equations for each exchange term and solving the resulting set of coupled differential equations.⁵ Partial-wave decomposition is avoided. The resulting algorithm is computationally very stable and highly vectorizable. New features of the PDE method developed for electron-positive ion collisions are (1) the use of Coulomb functions on the asymptotic PDE boundary; and (2) the explicit calculation of the continuum orbital. The PDE method is particularly suited for parallel computing. The results of tests at Ames's parallel processors will be discussed.

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Broadening and Shifts of Ca Rydberg States

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ABSTRACT

Impact broadening of Calcium Rydberg States has been studied by two photon excitation using a tunable dye laser pumped by an excimer laser. The atoms in a heat pipe were prepared in the $ns\ ^1S_0$ and $nd\ ^1D_2$ states and the pressure broadening of these states over a wide range of pressures of the inert perturber gases He, Ar and Xe were measured.

Pressure dependence of broadening and shift parameters of the even parity Rydberg states will be discussed. Interconfiguration perturbations and observation of new series due to doubly excited terms of Ca will be presented. Possible origin of the new lines due to two photon-one collision interaction and two photon-two collision interactions will be outlined.