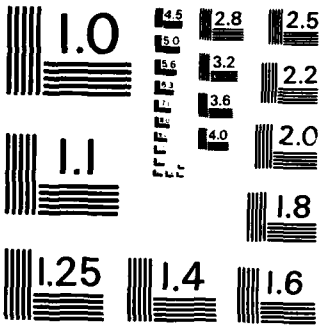
AD-A160 507 TRIPLY DIFFERENTIAL STUDIES OF ATOMIC AND MOLECULAR PHOTOIONIZATION USING..(U) NATIONAL BUREAU OF STANDARDS WASHINGTON DC NATIONAL MEASUREME.. A C PARR ET AL. 1/1

UNCLASSIFIED 17 OCT 85 N00014-85-F-0016 F/G 7/4 NL



12

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1 REPORT NUMBER	2 GOVT ACCESSION NO. / 3 RECIPIENT'S CATALOG NUMBER
4 TITLE (and Subtitle) TRIPLY DIFFERENTIAL STUDIES OF ATOMIC AND MOLECULAR PHOTOIONIZATION USING SYNCHROTRON RADIATION	5 TYPE OF REPORT & PERIOD COVERED: Final Report, 1 June 1980 - 30 Sept. 1985 / 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Albert C. Parr, J. L. Dehmer (Argonne National Laboratory)	8 CONTRACT OR GRANT NUMBER(s) N00014-85-F-0016
9. PERFORMING ORGANIZATION NAME AND ADDRESS National Measurement Laboratory, National Bureau of Standards, Gaithersburg, MD 20899	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: Program Element # 61153N, Project-Task Area #RR0110301, Work Unit # NR 393-051
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research, Physics Division (Code 412), Arlington, Virginia 22217	12. REPORT DATE: 17 October 1985 / 13. NUMBER OF PAGES: 15
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report): Unclassified / 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Photoionization, atoms, molecules, photoelectron branching ratio, photoelectron angular distribution, synchrotron radiation, VUV spectroscopy, autoionization, shape resonance, continuum-continuum coupling, electronic-vibrational coupling, photoelectron spectroscopy, photoelectron spectrometer.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Basic studies of photoionization processes in atoms and molecules have been carried out using triply differential (differential in incident wavelength, ejected electron energy, and ejection angle) photoelectron spectroscopy with synchrotron radiation as the excitation source. Measurements have been conducted in the vacuum ultraviolet wavelength range up to $h\nu \sim 35$ eV on a variety of atomic and molecular systems. Photoelectron branching ratios (partial photoionization cross sections) and photoelectron angular distribu-

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-LF-014-6601

FINAL REPORT

TRIPLY DIFFERENTIAL STUDIES OF ATOMIC AND MOLECULAR PHOTOIONIZATION USING SYNCHROTRON RADIATION (Contract No. N00014-85-F-0016)

Principal Investigators:

Dr. Albert C. Parr
Synchrotron Ultraviolet Radiation Facility
National Bureau of Standards
Gaithersburg, MD 20899
Tel.: 301-921-2031

and

Dr. J. L. Dehmer
Argonne National Laboratory
Argonne, IL 60439
Tel.: 312-972-4194

Submitted to

Office of Naval Research
Physics Division (Code 412)
Department of the Navy
Arlington, VA 22217

Attn: Prof. Douglas Klein

Submitted by

National Measurement Laboratory
National Bureau of Standards
Gaithersburg, MD 20899
17 October 1985

I. SCIENTIFIC PROBLEM

The research supported by this contract involves basic studies of vacuum ultraviolet (VUV) photoionization processes in atoms and molecules. Using advanced experimental approaches, described in Section II, we seek to develop new insight and basic data concerning the spectroscopy and dynamics of atomic and molecular photoionization by observing complementary observables, e.g., partial photoionization cross sections, photoelectron branching ratios, and photoelectron angular distributions. These studies have led to novel measurements and to new insight into photoionization mechanisms, particularly regarding the effects of shape resonances and autoionization on vibrational ionization channels.

In addition to our prime goal of developing a clear understanding of photoionization spectroscopy and dynamics, this work impacts on at least three other areas: First, we seek to develop new probes of the photoionization process. In recent annual periods, this project has introduced the techniques of fluorescence polarization spectroscopy of molecules and photoelectron-photoion coincidence spectroscopy of clusters formed in a supersonic expansion. At the present time, attention is focussed on use of a new, high-resolution angle-resolved, dual photoelectron spectrometer system (discussed below). Future work will be aimed at such experiments as electron-electron coincidence studies, VUV photoionization of laser-excited states, and photoelectron-photoion coincidence studies of molecular fragmentation using synchrotron radiation. Second, this project produces data crucial for testing theoretical predictions and, thus, contributes to the development of realistic theories of atomic and molecular photoionization. Third, the data produced by this project contribute to characterizing the alternative pathways by which radiation interacts with matter, and hence contributes to the macroscopic modeling of such microscopic interactions.

II. SCIENTIFIC AND TECHNICAL APPROACH

The main experimental approach used in this work involves triply differential photoelectron measurements using synchrotron radiation as the continuously tunable source of ionizing radiation. By triply differential photoelectron studies, we mean that photoelectron intensity measurements are made as a function of three completely independent variables -- the incident wavelength, λ, the kinetic energy of the ejected electron, T, and the angle of ejection, θ, relative to the polarization direction of the light. Variation of λ permits the systematic mapping of photoionization properties throughout the vacuum-ultraviolet wavelength range, including probing important spectral features such as autoionizing states, shape resonances, and near-threshold phenomena. Variation of T permits the selection of particular electronic-vibrational-(rotational) states formed in the photoionization process. Hence, by monitoring the whole manifold of final states (different T's), one can determine the effect of alternative photoionization mechanisms (selected by choosing λ, as discussed above) on relative probabilities of forming the various final states. Variation of θ permits the characterization of the angular distribution of photoelectrons for each final state and λ. In photoionization of free atoms and molecules the angular dependence of photoelectron intensity has the simple form

$$\frac{d\sigma}{d\theta} = \frac{\sigma_{tot}}{4\pi}\left[1 + \beta P_2(\cos\theta)\right],$$

where σ_{tot} is the integrated cross section and β is called the asymmetry parameter. Therefore, the angular distribution as a function of (T,λ) can be characterized by β, which in turn can be measured by recording peak strengths at as little as two angles. While it is true that most applications of photoionization data hinge primarily on partial cross sections (or branching ratios), angular distributions play an indispensable role in testing theoretical models and in the fundamental understanding of the photoionization process. Hence, both branching ratios and β's are critical to sound scientific study of photoionization processes.

In addition, this project introduced two techniques to address new types of problems in molecular photoionization. These are fluorescence polarization spectroscopy of molecules and photoelectron-photoion coincidence spectroscopy on selected clusters formed in mixtures in supersonic expansions. Expertise in these techniques is available for use in future research as the need arises. Further development of our measurement capabilities is under consideration but is also subject to staffing levels. Experimental approaches of interest include electron-electron coincidence measurements of double electron ejection, VUV photoionization of laser excited states, and photoelectron-photoion coincidence studies of molecular fragmentation using synchrotron radiation.

III. WORK ACCOMPLISHED

The work accomplished during the 5 1/4 years of this project are reflected, in part, in the 36 papers, 36 abstracts of contributed talks, and 37 invited lectures listed in Section IV. In this section, we briefly describe the highlights of this body of work in eleven categories:

(1) This project pioneered the vibrationally-resolved study of the effects of autoionizing resonances on photoionization branching ratios and photoelectron angular distributions.

(2) This project pioneered the equivalent type of study on shape resonances, although two of the initial measurements were reported immediately prior to the beginning of this contract.

(3) This project produced important studies of shape resonance effects in large molecules, e.g., SF_6 and BF_3, in which detailed comparisons with recent calculations indicated the state-of-the-art in understanding the photoionization dynamics of large molecules, as well as points to be resolved in future experimental and theoretical work.

(4) This project was the first to investigate the effects of both shape resonances and autoionizing resonances in excitation of bending vibrations in polyatomic molecules. This will be a significant theme in future studies of molecular photoionization with synchrotron radiation.

(5) This project first introduced the technique of polarization of fluorescence to study the dynamics of molecular photoionization, including unique ability to measure such quantities as branching ratios between degenerate photoionization channels.

(6) This project produced a substantial amount of data on photoionization branching ratios and photoelectron angular distributions of a variety of molecules, including N_2, CO, NO, H_2, CO_2, C_2H_2, SO_2, HCN, C_2N_2, CH_3CH, BF_3, and SF_6.

(7) This project produced the first (and, as of yet, only) photoelectron spectrum of a rare gas trimer by means of photoelectron-photoion coincidence techniques.

(8) This project produced two types of data on photoionization branching ratios and angular distributions for rare gas atoms. In one type of study, variations of these dynamical parameters within autoionizing resonances were measured. In the other type of study, the accurate, absolute β parameters for all the rare gases in the open continuum were measured as a point of reference for theory and spectrometer angular calibration in other labs.

(9) The mechanism of continuum-continuum coupling, leading to the transfer of shape resonant behavior between channels, was deduced by this project in a study on SF_6 and, subsequently, a study on N_2 confirmed a prediction of the effect in that system. These are initial studies of what is believed to be an important widespread phenomenon in molecular photoionization.

(10) This project developed a second generation triply differential photoelectron spectrometer which is the highest resolution and most sensitive electron spectrometer for use with synchrotron radiation.

(11) Finally, we have written several major book chapters giving detailed discussions of principles, bibliographies, and case studies of resonance processes in molecular photoionization.

IV. LIST OF PAPERS, ABSTRACTS OF CONTRIBUTED PAPERS, AND INVITED TALKS, COLLOQUIA, AND SEMINARS

PAPERS

1. B. E. Cole, D. L. Ederer, R. Stockbauer, K. Codling, A. C. Parr, J. B. West, E. D. Poliakoff, and J. L. Dehmer, "Wavelength and Vibrational-State Dependence of Photoelectron Angular Distributions. Resonance Effects in 5σ Photoionization of CO," J. Chem. Phys. 72, 6308 (1980).

2. A. C. Parr, D. L. Ederer, B. E. Cole, J. B. West, R. Stockbauer, K. Codling, and J. L. Dehmer, "Triply-Differential Photoelectron Studies of Molecular Autoionization Profiles," Phys. Rev. Letters 46, 22 (1981).

3. E. D. Poliakoff, J. L. Dehmer, D. Dill, A. C. Parr, K. H. Jackson, and R. N. Zare, "Polarization of Fluorescence Following Molecular Photoionization," Phys. Rev. Letters 46, 907 (1981).

4. K. Codling, A. C. Parr, D. L. Ederer, R. Stockbauer, J. B. West, B. E. Cole, and J. L. Dehmer, "The Effects of Autoionization on Vibrational Branching Ratios and Photoelectron Angular Distributions in Molecular Photoionization: The Formation of the Ground State of O_2^+ Between 574 Å and 600 Å," J. Phys. B 14, 657 (1981).

5. D. L. Ederer, A. C. Parr, B. E. Cole, R. Stockbauer, J. L. Dehmer, J. B. West, and K. Codling, "Vibrational-State Dependence of Partial Cross Sections and Photoelectron Angular Distributions through Autoionizing Resonances: The n = 3 Rydberg Level Converging to the $B^2\Sigma^+$ State of CO^+," Proc. Roy. Soc. Lond. A 378, 423 (1981).

6. A. C. Parr, G. Rakowsky, D. L. Ederer, R. L. Stockbauer, J. B. West, and J. L. Dehmer, "Current Research at NBS Using Synchrotron Radiation at SURF-II," IEEE Transactions on Nuclear Science, Volume NS28, 1210 (1981).

7. J. B. West, K. Codling, A. C. Parr, D. L. Ederer, B. E. Cole, R. Stockbauer, and J. L. Dehmer, "Partial Photoionization Cross Sections and Photoelectron Angular Distributions through the Hopfield Bands in N_2 Between 650 Å and 730 Å," J. Phys. B 14, 1791 (1981).

8. K. Codling, J. B. West, A. C. Parr, J. L. Dehmer, and R. L. Stockbauer, "Measurement of β Values and Branching Ratios in the Region of the $3s3p^64p\ {}^1P_1^o$ Resonance in Ar and the $5s5p^66p\ {}^1P_1^o$ Resonance in Xe," J. Phys. B 13, L693 (1980).

9. E. D. Poliakoff, P. M. Dehmer, J. L. Dehmer, and R. L. Stockbauer, "The Photoelectron Spectrum of Xe_3 by the Photoelectron-Photoion Coincidence Technique," J. Chem. Phys. 75, 1568 (1981).

10. D. M. P. Holland, A. C. Parr, D. L. Ederer, J. L. Dehmer, and J. B. West, "The Angular Distribution Parameters of Argon, Krypton, and Xenon for Use in Calibration of Electron Spectrometers," Nucl. Instr. and Meth. 195, 331 (1982).

11. E. D. Poliakoff, P. M. Dehmer, J. L. Dehmer, and R. Stockbauer, "Photoelectron-Photoion Coincidence Spectroscopy of Gas-Phase Clusters," J. Chem. Phys. 76, 5214 (1982).

PAPERS, Continued

12. A. C. Parr, D. L. Ederer, J. B. West, D. M. P. Holland, and J. L. Dehmer, "Triply Differential Photoelectron Studies of Non-Franck-Condon Behavior in the Photoionization of Acetylene," J. Chem. Phys. 76, 4349 (1982).

13. D. L. Ederer, A. C. Parr, J. B. West, D. M. P. Holland, and J. L. Dehmer, "Measurement of the Spin-Orbit Branching Ratios and the Angular Asymmetry Parameters in the Region of the $4s4p^6 5p$ Resonances in Krypton and the $5s5p^6 6p$ Resonances in Xenon, Phys. Rev. A 25, 2006 (1982).

14. A. C. Parr, D. L. Ederer, J. L. Dehmer, and D. M. P. Holland, "Characterization of Some Autoionizing Resonances in CO_2 Using Triply Differential Photoelectron Spectroscopy," J. Chem. Phys. 77, 111 (1982).

15. J. L. Dehmer, A. C. Parr, S. Wallace, and D. Dill, "Photoelectron Branching Ratios and Angular Distributions for the Valence Levels of SF_6 in the Range $16eV<h\nu<30eV$," Phys. Rev. A 26, 3283 (1982).

16. D. M. P. Holland, J. B. West, A. C. Parr, D. L. Ederer, R. Stockbauer, R. D. Buff, and J. L. Dehmer, "Constant Photoelectron Energy Spectroscopy of Acetylene," J. Chem. Phys. 78, 124 (1983).

17. A. C. Parr, D. M. P. Holland, D. L. Ederer, and J. L. Dehmer, "Effects of Resonances in Molecular Photoionization Measured with Triply Differential Photoelectron Spectroscopy," Int. J. Mass Spect. Ion Phys. 46, 285 (1983).

18. P. M. Dehmer and J. L. Dehmer, "Observation of Bending Modes in the X $^2\Pi_u$ State of the Acetylene Ion Using HeI Photoelectron Spectrometry," J. Electron Spectrosc. 28, 145 (1982).

19. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi, "Fluorescence Polarization as a Probe of Molecular Autoionization," J. Chem. Phys. 77, 5243 (1982).

20. A. C. Parr, S. H. Southworth, J. L. Dehmer, and D. M. P. Holland, "Photoelectron Spectrometer for High Resolution Angular Resolved Studies," Nucl. Instr. and Meth. 208, 767 (1983).

21. J. L. Dehmer, D. Dill, and A. C. Parr, "Photoionization Dynamics of Small Molecules" in Photophysics and Photochemistry in the Vacuum Ultraviolet, edited by S. McGlynn, G. Findley, and R. Huebner (D. Reidel Publ., Dordrecht, Holland, 1985) p. 341.

22. E. D. Poliakoff, J. L. Dehmer, P. M. Dehmer, and A. C. Parr, "Vibrationally-Resolved Photoelectron Angular Distributions for H_2," Chem. Phys. Lett. 96, 52 (1983).

23. D. L. Ederer, R. P. Madden, A. C. Parr, G. Rakowsky, E. B. Saloman, J. Cooper, R. Stockbauer, T. E. Madey, and J. L. Dehmer, "An Overview of Research at NBS Using Synchrotron Radiation at SURF-II," IEEE Trans. Nucl. Sci. NS-30, 1020 (1983).

PAPERS, Continued

24. D. M. P. Holland, A. C. Parr, D. L. Ederer, J. B. West, and J. L. Dehmer, "Triply Differential Photoelectron Studies of the Four Outermost Valence Orbitals of Cyanogen," Int. J. Mass Spect. Ion Phys. 52, 195 (1983).

25. D. M. P. Holland, A. C. Parr, and J. L. Dehmer, "Photoelectron Asymmetry Parameters and Branching Ratios for Sulphur Dioxide in the Photon Energy Range 14 to 25 eV," J. Electron Spectrosc. 32, 237 (1983).

26. D. M. P. Holland, A. C. Parr, and J. L. Dehmer, "Photoelectron Branching Ratios and Asymmetry Parameters for the Two Outermost Molecular Orbitals of Hydrogen Cyanide," J. Phys. B 17, 1343 (1984).

27. D. M. P. Holland, A. C. Parr, and J. L. Dehmer, "Photoelectron Branching Ratios and Asymmetry Paremeters for the Two Outermost Orbitals of Methyl Cyanide," J. Electron Spectrosc. 34, 87 (1984).

28. A. C. Parr, S. H. Southworth, J. L. Dehmer, and D. M. P. Holland, "High-Resolution Angle-Resolved Photoelectron Spectrometer System," Nucl. Instr. Meth. 222, 221 (1984).

29. J. L. Dehmer, A. C. Parr, S. H. Southworth, and D. M. P. Holland, "Angle-Resolved Photoelectron Study of the Valence Levels of BF_3 in the Range $17 < h\nu < 28$ eV," Phys. Rev. A 30, 1783 (1984).

30. J. L. Dehmer, "Shape Resonances in Molecular Fields," in Resonances in Electron-Molecule Scattering, van der Waals' Complexes, and Reactive Chemical Dynamics, ACS Symposium Series, Vol. 263, D. G. Truhlar, Ed. (American Chemical Society, Washington, D.C., 1984) p. 139.

31. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi, "Fluorescence Excitation Studies of Molecular Photoionization in External Electric Fields," Chem. Phys. Lett. 111, 128 (1984).

32. J. L. Dehmer, S. H. Southworth, and A. C. Parr, "Triply Differential Photoelectron Studies of Resonances in Molecular Photoionization," Nucl. Instrum. & Meth. B10/11, 247 (1985).

33. A. C. Parr, "Synchrotron Radiation: Application to Chemistry," in New Directions in Chemical Analysis, edited by B. L. Shapiro (Texas A & M Press, College Station, 1985).

34. J. L. Dehmer, A. C. Parr, and S. H. Southworth, "Resonances in Molecular Photoionization," in Handbook on Synchrotron Radiation, Vol. II, edited by G. V. Marr (North Holland, Amsterdam, 198X) p. XX.

35. S. H. Southworth, A. C. Parr, J. E. Hardis, and J. L. Dehmer, "Channel Coupling and Shape Resonance Effects in the Photoelectron Angular Distributions of the $3\sigma_g^{-1}$ and $2\sigma_u^{-1}$ Channels of N_2," Phys. Rev. A, submitted.

PAPERS, Continued

36. S. H. Southworth, A. C. Parr, J. E. Hardis, J. L. Dehmer, and D. M. P. Holland, "Calibration of a Monochromator/Spectrometer System for the Measurement of Photoelectron Angular Distributions and Branching Ratios," Nucl. Instr. Meth., submitted.

ABSTRACTS OF CONFERENCE PAPERS

1. A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer, R. L. Stockbauer, and J. B. West, "An Angle-Resolved Photoelectron Spectrometer for Triply-Differential Photoionization Studies," Sixth International Conference on Vacuum Ultraviolet Radiation Physics, June 2-6, 1980, Charlottesville, Va. Book of Extended Abstracts, p. III-70.

2. K. Codling, J. B. West, A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer, and R. L. Stockbauer, "Partial Cross Sections, Vibrational Branching Ratios, and Angular Distributions in the 570-600 Å Window Resonance in O_2," ibid. p. II-14.

3. R. Stockbauer, A. C. Parr, J. L. Dehmer, B. E. Cole, D. L. Ederer, J. B. West, and K. Codling, "Perturbation of Vibrational Intensities and Angular Distributions by Autoionization in Molecular Photoionization," ibid., p. II-15.

4. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, D. Dill, K. H. Jackson, and R. N. Zare, "Polarized Fluorescence Excitation Spectroscopy of N_2," ibid., p. II-25.

5. J. L. Dehmer, A. C. Parr, J. B. West, K. Codling, D. L. Ederer, B. E. Cole, E. D. Poliakoff, and R. Stockbauer, "Effects of Shape Resonances on Vibrational Branching Ratios and Photoelectron Angular Distributions in Molecular Photoionization," ibid., p. II-86.

6. A. C. Parr, R. L. Stockbauer, K. Codling, J. B. West, and J. L. Dehmer, "Photoelectron Branching Ratios and Angular Distributions in the Region of the $3s3p^64p\ {}^1P_1^o$ Resonance in Ar and the $5s5p^66p\ {}^1P_1^o$ Resonance in Xe," Annual DEAP Meeting, 1-3 December 1980, Los Angeles, CA, Bull. Am. Phys. Soc. 25, 1131 (1980).

7. J. L. Dehmer, J. B. West, K. Codling, R. Stockbauer, A. C. Parr, D. L. Ederer, and B. E. Cole, "Triply-Differential Photoionization Studies of Molecular Autoionization Profiles," ibid., p. 1136.

8. E. D. Poliakoff, J. L. Dehmer, D. Dill, A. C. Parr, K. H. Jackson, and R. N. Zare, "Polarization of Fluorescence Following Molecular Photoionization," ibid., p. 1136.

9. K. Codling, J. B. West, A. C. Parr, J. L. Dehmer, and R. L. Stockbauer, "Photoelectron Angular Distribution Measurements through Autoionizing Resonances in Argon and Xenon," Molecular Spectroscopy and Dynamics with Synchrotron Radiation-A European Workshop, Maria Laach, West Germany, 29 September-1 October 1980, Book of Abstracts, p. 52.

10. R. Stockbauer, A. C. Parr, B. E. Cole, D. L. Ederer, J. Dehmer, J. West, and K. Codling, "Effects of Two-Electron Resonances in Photoelectron Energy and Angular Distributions," presented orally at the Gordon Research Conference on Electron Spectroscopy, Wolfsboro, NH, July 1980 (no abstract available).

ABSTRACTS OF CONFERENCE PAPERS, Continued

11. A. C. Parr, D. L. Ederer, R. Stockbauer, J. B. West, K. Codling, D. M. P. Holland, and J. L. Dehmer, "Triply-Differential Photoelectron Studies of Atomic and Molecular Photoionization," Twelfth International Conference on the Physics of Electronic and Atomic Collisions, 15-21 July 1981, Gatlinburg, Tennessee, Book of Abstracts, p. 81.

12. E. D. Poliakoff, P. M. Dehmer, J. L. Dehmer, and R. Stockbauer, "The Photoelectron Spectrum of Xe_3 by the Photoelectron-Photoion Coincidence Technique," ibid, p. 97.

13. E. D. Poliakoff, J. L. Dehmer, D. Dill, A. C. Parr, K. H. Jackson, and R. N. Zare, "Polarization of Fluorescence Following Molecular Photoionization, ibid, p. 99.

14. A. C. Parr, D. L. Ederer, J. West, and J. L. Dehmer, "Resonance Effects in the Angular Distributions and Branching Ratios of the Photoelectrons in C_2H_2 and C_2N_2," Annual Meeting of the American Society for Mass Spectrometry and Allied Topics, 25-29 May 1981, Minneapolis, Minn., Book of Abstracts.

15. D. M. P. Holland, A. C. Parr, D. Ederer, J. L. Dehmer, and J. B. West, "The Angular Distribution Parameters of Selected Rare Gases for Use in Calibration of Electron Spectrometers," National Synchrotron Instrumentation Conference, Cornell University, 15-17 July 1981, Book of Abstracts.

16. A. C. Parr, D. L. Ederer, R. Stockbauer, J. B. West, D. M. P. Holland, K. Codling, and J. L. Dehmer, "Triply Differential Photoelectron Studies of Autoionization and Shape-Resonance Effects in Molecular Photoionization," Annual DEAP Meeting, 3-5 December 1981, New York, New York, Bull. Am. Phys. Soc. 26, 1322 (1981).

17. E. D. Poliakoff, P. M. Dehmer, J. L. Dehmer, and R. Stockbauer, "Photoelectron-Photoion Coincidence Spectroscopy of Gas-Phase Clusters," ibid., p. 1322.

18. A. C. Parr, D. M. P. Holland, D. L. Ederer, and J. L. Dehmer, "Effects of Resonances in Molecular Photoionization Measured with Triply Differential Photoelectron Spectroscopy," Ninth International Conference on Mass Spectrometry, Vienna, Austria, July, 1982, Book of Abstracts.

19. A. C. Parr and H. M. Rosenstock, "Resonance, Autoionization, and Kinetic Effects in Photoionization," (invited talk) Annual Meeting of the American Society for Mass Spectrometry, 7-11 June 1982, Honolulu, Hawaii, Book of Abstracts.

20. J. L. Dehmer, D. Dill, and A. C. Parr, "Molecular Photoionization Dynamics with Emphasis on Shape and Autoionizing Resonances," Abstract of Invited Lecture at the NATO Advanced Study Institute on Photophysics and Photochemistry in the Vacuum Ultraviolet, 15-28 August 1982, Lake Geneva, Wisconsin, Book of Abstracts.

ABSTRACTS OF CONFERENCE PAPERS, Continued

21. A. C. Parr and J. L. Dehmer, "Photoelectron Spectrometer for High Resolution Angular Resolved Studies," International Conference on X-Ray and VUV Synchrotron Radiation Instrumentation, 9-13 August 1982, Hamburg, W. Germany, Book of Abstracts.

22. D. L. Ederer, R. P. Madden, A. C. Parr, G. Rakowsky, E. B. Saloman, J. Cooper, R. Stockbauer, T. E. Madey, and J. L. Dehmer, "An Overview of Research at NBS Using Synchrotron Radiation at SURF-II," Seventh Conf. on the Application of Accelerators in Research and Industry, 8-10 November 1982, Denton, TX, Bull. Am. Phys. Soc. 27, 809 (1982).

23. D. L. Ederer, A. C. Parr, J. B. West, K. Codling, D. M. P. Holland, J. L. Dehmer, J. M. Bizau, P. Dhez, F. Wuilleumier, J. L. Picque, J. L. LeGouet, and P. Koch, "Studies of Photoionization Processes from Ground State and Excited State Atoms and Molecules," Workshop on Techniques for the Production and Use of Polarized Radiation in the Vacuum Ultraviolet, August, 1982, Imperial College, London, Book of Extended Abstracts.

24. J. L. Dehmer, A. C. Parr, S. H. Southworth, and D. M. P. Holland, "Triply Differential Photoelectron Studies of Autoionization and Shape-Resonance Effects in Molecular Photoionization," Annual DEAP Meeting, 23-25 May 1983, Boulder, CO, Bull. Am. Phys. Soc. 28, 809 (1983).

25. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi, "Fluorescence Polarization as a Probe of Molecular Autoionization," ibid., p. 809.

26. J. L. Dehmer, A. C. Parr, S. H. Southworth, and D. M. P. Holland, "Triply Differential Photoelectron Studies of Resonant Molecular Photoionization," XIII International Conference on the Physics of Electronic and Atomic Collisions, Berlin, W. Germany, 27 July - 2 August 1983, Book of Abstracts, p. 42.

27. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi, "Fluorescence Polarization as a Probe of Molecular Autoionization," ibid., p. 43.

28. E. D. Poliakoff, J. L. Dehmer, A. C. Parr, and G. E. Leroi, "Fluorescence Excitation Studies of Molecular Photoionization in the Presence of External Electric Fields," VII International Conference on Vacuum Ultraviolet Radiation Physics, Jerusalem, Israel, 8-12 August 1982, Book of Abstracts; also in Ann. Israel Phys. Soc. 6, 204 (1983).

29. G. E. Leroi, J. L. Dehmer, A. C. Parr, and E. D. Poliakoff, "Polarization of Fluorescence: A Probe of Molecular Autoionization," ibid., p. 207.

30. A. C. Parr and R. Stockbauer, "Photoelectron Spectroscopy Studies in Recent Years at NBS," Annual Meeting of the American Society for Mass Spectrometry, Boston, MA, 9-13 May 1983, Book of Abstracts.

ABSTRACTS OF CONFERENCE PAPERS, Continued

31. A. C. Parr, S. H. Southworth, J. L. Dehmer, and D. M. P. Holland, "Angle Resolved Photoelectron Spectrometers," 3rd National Conference on Synchrotron Radiation Instrumentation, Brookhaven National Laboratory, Upton, Long Island, New York, 12-14 September 1983, Book of Abstracts.

32. J. L. Dehmer, "Shape Resonances in Molecular Fields," National Meeting of the American Chemical Society, St. Louis, Missouri, 8-13 April 1983, Book of Abstracts, p. Phys.-2.

33. S. H. Southworth, A. C. Parr, J. L. Dehmer, and D. M. P. Holland, "Angle-Resolved Photoelectron Study of the Valence Levels of BF_3," XVth Annual Meeting of the DEAP, American Physical Society, Storrs, CT, 30 May - 1 June 1984, Bull. Am. Phys. Soc. 29, 800 (1984).

34. J. L. Dehmer, "Resonant Processes in Molecular Photoionization," VIII Conference on the Applications of Accelerators in Research and Industry, Denton, TX, 12-14 November 1984, Bull. Am. Phys. Soc. 29, 1089 (1984).

35. S. H. Southworth, J. L. Dehmer, A. C. Parr, and J. E. Hardis, "Channel-Coupling and Shape-Resonance Effects in the Photoelectron Dynamics of N_2 and NO," Sixteenth Annual Meeting of the Division of Electron and Atomic Physics of the American Physical Society, Norman, OK, 29-31 May 1985, Bull. Am. Phys. Soc. 30, 879 (1985).

36. S. H. Southworth, A. C. Parr, J. L. Dehmer, J. E. Hardis, and D. M. P. Holland, "Calibration of a Monochromator/Spectrometer System for the Measurement of Photoelectron Angular Distributions and Branching Ratios," Synchrotron Radiation Instrumentation Conference, Stanford University, 29 July - 2 August 1985, Book of Abstracts, p. 263.

INVITED TALKS, COLLOQUIA, AND SEMINARS

1. J. L. Dehmer and Dan Dill, "Shape Resonances in Molecular Photoionization," Plenary talk presented at Molecular Spectroscopy and Dynamics with Synchrotron Radiation-A European Workshop, Maria Laach, West Germany, September 29-October 1, 1980.

2. A. C. Parr, "Current Research at NBS Using Synchrotron Radiation at SURF-II," Invited talk presented at the Sixth Conference on the Application of Accelerators in Research and Industry, Denton, TX, November 3-5, 1980.

3. J. L. Dehmer, "Potpourri of Current and Future Studies of Molecular Photoionization-Synchrotron Radiation, Supersonic Jets, and Multiphoton Ionization," Chemistry Department Colloquium, Boston University, Boston, MA, 13 April 1981.

4. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Photoelectron-Photoion Coincidence Spectroscopy of Atomic Clusters and Fluorescence Polarization Analysis," Atomic and Molecular Science Seminar, Argonne National Laboratory, Argonne, Illinois, 6 May 1981.

5. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Molecular Spectroscopy Division Seminar, National Bureau of Standards, Gaithersburg, MD, 21 May 1981.

6. E. D. Poliakoff, "Alignment of Molecular Ions Produced by Photoionization," Seminar on Collision Experiments in Their Theoretical Frame (Fano Workshop), The University of Chicago, Chicago, IL, 23 May 1981.

7. A. C. Parr, "Status of Programs at NBS SURF-II," National Synchrotron Instrumentation Conference, Cornell University, 15-17 July 1981.

8. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Physics Department Colloquium, Georgetown University, Washington, D.C. 6 November 1981.

9. A. C. Parr, "Triply Differential Photoelectron Spectrometry of Atoms and Simple Molecules," Center Colloquium, Center for Absolute Physical Quantities, National Bureau of Standards, January 6, 1982.

10. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Fluorescence Polarization and Photoelectron-Photoion Coincidence Studies of Clusters," Brookhaven National Laboratory, December 2, 1981.

11. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Fluorescence Polarization and Photoelectron-Photoion Coincidence Studies of Clusters," Exxon Research Laboratory, January, 1982.

12. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Fluorescence Polarization and Photoelectron-Photoion Coincidence Studies of Clusters," Department of Chemistry, Dartmouth University, January, 1982.

INVITED TALKS, COLLOQUIA, AND SEMINARS, Continued

13. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Fluorescence Polarization and Photoelectron-Photoion Coincidence Studies of Clusters," Department of Chemistry, Boston University, January 1982.

14. E. D. Poliakoff, "Two Novel Probes of Molecular Photoionization: Fluorescence Polarization and Photoelectron-Photoion Coincidence Studies of Clusters," Department of Chemistry, University of Pennsylvania, February, 1982.

15. A. C. Parr and H. M. Rosenstock, "Resonance, Autoionization, and Kinetic Effects in Photoionization," Invited talk presented at the 30th Annual Conf. on Mass Spectrometry and Allied Topics, Honolulu, June 6-11, 1982.

16. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Department of Physics Colloquium, University of Alabama, March 31, 1982.

17. J. L. Dehmer, "Molecular Photoionization Dynamics - Progress and Prospects," Physics Colloquium, University of Chicago, May 27, 1982.

18. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," California Institute of Technology, June 14, 1982.

19. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," University of California, Santa Barbara, June 15, 1982.

20. J. L. Dehmer, "Overview of Experimental and Theoretical Studies of Resonance Processes in Molecular Photoionization by Single-Photon and Multiphoton Excitation," Gordon Research Conference on Electron Spectroscopy, Wolfeboro, New Hampshire, 19 July, 1982.

21. J. L. Dehmer, D. Dill, and A. C. Parr, "Photoionization Dynamics of Small Molecules," NATO Advanced Study Institute on Photophysics and Photochemistry in the Vacuum Ultraviolet, Lake Geneva, WI, 15-28 August 1982.

22. A. C. Parr, "Resonance Phenomena in Molecular Photoionization," Uppsala University, 17 August 1982.

23. J. L. Dehmer, "Resonant Processes in Molecular Photoionization," Meeting of the American Physical Society (Division of Condensed Matter Physics Symposium), Los Angeles, CA, 24 March 1983.

24. A. C. Parr, "Studies of Ion Fragmentation and Molecular Photoionization Using Photoelectron Spectroscopy," JILA Colloquium, Boulder, CO, 8 April 1983.

25. A. C. Parr and R. Stockbauer, "Photoelectron Spectroscopy Studies in Recent Years at NBS," Annual Meeting of the American Society for Mass Spectrometry, Boston, MA, 12 Ma, 1983.

INVITED TALKS, COLLOQUIA, AND SEMINARS, Continued

26. A. C. Parr, "Angle Resolved Photoelectron Spectrometers," 3rd National Conference on Synchrotron Radiation Instrumentation, Brookhaven National Laboratory, Long Island, NY, 12-14 September 1983.

27. J. L. Dehmer, "Shape Resonances in Molecular Fields," Symposium on Resonances in Electron-Molecule Scattering, van der Waals' Complexes, and Reactive Chemical Dynamics, National Meeting of the American Chemical Society, St. Louis, MO, 8-13 April 1983.

28. A. C. Parr, "Studies of Resonances in Molecular Photoionization Using Synchrotron Radiation," Physics Colloquium, University of Alabama, 9 March 1984.

29. A. C. Parr, "Studies of Resonances in Molecular Photoionization Using Synchrotron Radiation," BESSY Synchrotron Radiation Facility, Berlin, W. Germany, 12 April 1984.

30. A. C. Parr, "Studies of Resonances in Molecular Photoionization Using Synchrotron Radiation," LURE Synchrotron Radiation Facility, Orsay, France, 16 April 1984.

31. A. C. Parr, "Overview of Research at NBS Using Synchrotron Radiation at SURF-II," Daresbury Laboratory, England, 14 May 1984.

32. J. L. Dehmer, "Resonant Processes in Molecular Photoionization," Eighth Conference on the Applications of Accelerators in Research and Industry, Denton, TX, 12-14 November 1984.

33. J. L. Dehmer, "Molecular Photoionization Dynamics - Progress and Prospects," Physics Colloquium, University of Oregon, Eugene, OR, 29 November 1984.

34. A. C. Parr, "Synchrotron Radiation: Application to Chemistry," IUCCP Conference on Industry/University Cooperative Chemistry Programs, College Station, TX, 2 April 1985.

35. A. C. Parr, "Resonances in Molecular Photoionization," Atomic and Molecular Physics Seminar, Los Alamos National Laboratory, May 1985.

36. J. L. Dehmer, "Dynamics of Photoelectron Escape from Molecular Fields," Physics Colloquium, Los Alamos National Laboratory, Los Alamos, NM, 6 June 1985.

37. J. L. Dehmer, "Dynamics of Photoelectron Escape from Molecular Fields," Chemical Physics Seminar, Institute of Physical Science and Technology, University of Maryland, College Park, MD, 25 June 1985.

END

FILMED

12-85

DTIC