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TRIPLY DIFFERENTIAL STUDIES OF ATOMIC AND MOLECULAR PHOTOIONIZA--ETC(U)
JUL 81 J L DEHMER, A C PARR, R STOCKBAUER N00014-81-F-0005

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Photoionization, atoms, molecules, branching ratio, photoelectron spectroscopy, photoelectron angular distribution, synchrotron radiation, autoionization, shape resonance, atomic clusters, photoelectron-photoion coincidence, fluorescence polarization.

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

Basic studies of the dynamics and spectroscopy of atomic and molecular photoionization have been carried out using three experimental probes. The first and most extensively used experimental approach involves triply differential (differential in incident wavelength, electron energy, and ejection angle) photoelectron measurements using synchrotron radiation. Measurements were conducted in the vacuum ultraviolet wavelength range up to $h\nu \sim 35$ eV on

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20 (contd). several atomic and molecular species, e.g., Ar, Kr, Xe, H_2, N_2, O_2, CO, SO_2, C_2H_2, C_2N_2, HCN, CH_3CN, BF_3, and SF_6. Photoelectron branching ratios and angular distributions were obtained for all accessible states. A major emphasis of this work involved the initial exploration of novel effects of autoionization and shape resonances on alternative vibrational ionization channels. The second experimental approach entailed measuring the polarization of fluorescence following production of excited molecular ions by photoionization. This was also a novel experiment, allowing the direct measurement of the alignment of molecular ions produced by photoionization and, simultaneously, the branching ratios for degenerate photoelectron channels. The third experimental approach was, again, a novel experiment, and involved determining the photoelectron spectrum of an atomic cluster (Xe_3) in a mixture of clusters formed in a supersonic expansion by the technique of photoion-photoelectron coincidence.

SUMMARY QUESTIONNAIRE

Triply Differential Studies of Atomic and Molecular Photoionization Using Synchrotron Radiation (Contract No. N00014-81-F-0005)

Submitted to

Office of Naval Research
Physical Sciences Division
Physics Program Office
Department of Navy
Arlington, VA 22217

ATTN: Dr. Bobby R. Junker

Submitted by

National Bureau of Standards
6 July 1981

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2. Contract Description

The research covered by this contract involves basic studies of photoionization processes in atoms and molecules using three novel and/or advanced experimental approaches outlined in item 4. Topics of main interest include photoelectron branching ratios, photoelectron angular distributions, alignment of molecular ions by photoionization, and photoelectron spectra of atomic clusters.

3. Scientific Problem

This study is aimed at resolving roughly four unknown or incompletely known aspects of this problem area: First, this program seeks to characterize major aspects of photoionization dynamics, such as the effects of shape resonances and autoionizing resonances on alternative ionization channels, which can only now be studied in a definitive way with the advanced techniques employed in this work. Second, we seek to develop new probes of the photoionization process, e.g., fluorescence polarization spectroscopy and photoelectron spectroscopy of atomic clusters, which will yield new types of information. Third, this project produces data crucial to testing theoretical predictions and, thus, contributes to the development of realistic theories of atomic and molecular photoionization. Fourth, the data produced by this project contributes to characterizing all the pathways by which radiation interacts with matter, and hence contributes to the macroscopic modeling of such interactions.

4. Scientific and Technical Approach

This program utilizes three experimental approaches: First, the main effort involves measuring triply differential photoelectron cross sections using synchrotron radiation. Thus the intensity of photoelectrons ejected from atoms and molecules are measured as a function of three independent parameters — the wavelength of the incident synchrotron radiation, the kinetic energy of the photoelectron, and the ejection angle relative to the polarization direction of the light. Second, the polarization of fluorescence from excited ionic states produced by photoionization is measured as a function of the wavelength of the incident light. Third, photoelectron spectra are measured in coincidence with the mass of the ion produced in order to obtain the photoelectron spectra of specific atomic clusters in the presence of a whole range of clusters formed in a supersonic expansion.

5. Progress

Triply differential measurements were conducted in the vacuum ultraviolet wavelength range up to $h\nu \sim 35$ eV on several atomic and molecular species, e.g., Ar, Kr, Xe, H_2, N_2, O_2, CO, SO_2, C_2H_2, C_2N_2, HCN, CH_3CN, BF_3, and SF_6. Photoelectron branching ratios and angular distributions were obtained for all accessible states. A major emphasis of this work involved the initial exploration of novel effects of autoionization and shape resonances on alternative vibrational ionization channels. Prototype fluorescence polarization spectroscopy measurements were performed on the $B^2\Sigma_u^+$ state of N_2^+ formed by photoionization of N_2 in the range 450 Å < λ < 660 Å. The feasibility and theoretical interpretation of this new class of experimental probe was established. Finally, in the third part of the project, the photoelectron spectrum of Xe_3 was determined by photoelectron-photoion coincidence technique using a supersonic jet source of xenon clusters.

6. Publications

The papers, abstracts of contributed talks, and invited talks are listed on the following pages.

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. (London), in press.

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, in press.

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, accepted for publication.

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 $3s3p^6 4p\ {}^1P_1^o$ Resonance in Ar and the $5s5p^6 6p\ {}^1P_1^o$ 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., accepted for publication.

ABSTRACTS OF CONTRIBUTED 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 of 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 $3s3p^6 4p\ {}^1P_1^o$ Resonance in Ar and the $5s5p^6 6p\ {}^1P_1^o$ 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 on Photoelectron Energy and Angular Distributions," presented orally at the Gordon Research Conference on Electron Spectroscopy, Wolfsboro, NH, July 1980 (no abstract available).

ABSTRACTS OF CONTRIBUTED 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 Stodues 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.

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.

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.

14. A. C. Parr, D. L. Ederer, J. West, J. L. Dehmer, "Resonance Effects in the Angular Distribution 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.

INVITED TALKS

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, Book of Abstracts, p. 43.

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. See paper 6.

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.

7. Extenuating Circumstances

None.

8. Unspent Funds

None will remain unspent at the end of the current contract period.

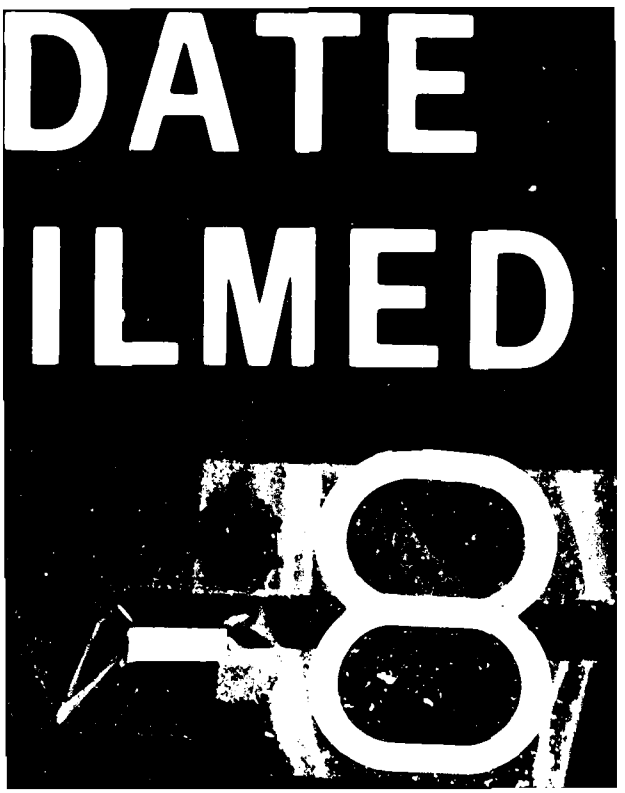
9. Graduate Students Receiving Degrees

None.

10. Other Federal Contract Support

J. L. Dehmer is a co-principal investigator of Office of Naval Research Contract N00014-81-F-0051, "Selectivity of Multiphoton Processes," 6/1/81 — 5/31/82.

R. Stockbauer is a co-principal investigator of Office of Naval Research Contract N0014-81-F0021, "Characterization of Surface Bonding Using Photon and Electron Simulated Desorption", 1 Oct 1980 - 30 Sept 1981.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