RESEARCH IN NUCLEAR CHEMISTRY

Final Report

MASTER

T. Darrah Thomas

Oregon State University
Corvallis, Oregon 97331

Sept. 1, 1971 - Aug. 31, 1976

Date Published - December 1977

Prepared for the U.S. Department of Energy under Contract
EY-76-S-06-2227, Task agreement No. 14.

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately-owned rights.

DISCLAIMER

This book was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MGW

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Research in Nuclear Chemistry
EY-76-S-06-2227
Task Agreement No. 14
T. Darrah Thomas, Principal Investigator
FINAL REPORT

Progress during the first three years of this contract has been reported in reports RLO-2227-T14-1, RLO-2227-T14-11, and RLO-2227-T14-15.

The major focus of the work done on this project was investigation of the core-ionization potentials and X-ray photoelectron spectra of small molecules in the gas phase. A significant effort was also devoted to studies of nuclear reactions of heavy ions with heavy nuclei at the Berkeley HILAC, in collaboration with a group from the University of Washington. A relatively small amount of time was spent on finishing work that had been started at Princeton under an earlier contract with the AEC. A list of publications resulting from our efforts in each of these areas is included in this report. Progress in the two major areas is discussed in more detail below.

NUCLEAR REACTIONS INVOLVING HEAVY IONS

The original intent of this work was to investigate the effect of nuclear deformability on reaction cross sections. Measurements were made on the elastic scattering of ^{84}Kr from ^{208}Pb (a rigid spherical nucleus) and ^{194}Pt (a deformable spherical nucleus). The results were inconclusive and no publication has yet come out of this work.

Attention was shifted to the phenomenon of deeply inelastic scattering. Experiments with ^{84}Kr on ^{208}Pb and with ^{86}Kr on ^{139}La have helped to map out the dependence of this phenomenon on the target-projectile combination and on the projectile energy. Studies of Xe incident on Ta and Pb targets were among the first to show the relationship between the charge distribution of the reaction products and the energy loss.

Six publications have resulted from this work.

X-RAY PHOTOELECTRON SPECTROSCOPY

Research in photoelectron spectroscopy has emphasized four areas: (1) The relationship between core ionization potentials and chemical properties. (2) The accurate measurement of core ionization potentials. (3) Satellite peaks in photoelectron spectra. (4) Auger spectra of molecules isoelectronic with neon.

In the first of these we have played a significant role in the development of a point-charge model for assigning charges to the atoms in molecules. Investigations of the fluorinated benzenes showed results that are in accord with conventional ideas about the charge distribution in these molecules. Similar studies of trifluoromethylbenzene led, however, to the unexpected conclusion that the CF_3 is not an electron-withdrawing group, but owes its chemical effects to its large dipole moment. Work on ClF_3 , SF_4 , and PF_5 demonstrated the inequivalence of the axial and equatorial fluorines and showed that the axial fluorines are more negatively charged than are the equatorial fluorines, in agreement with accepted views of the bonding in these molecules.

Investigations of core ionization potentials in a number of organic compounds have established relationships between these ionization potentials and solution phase acidities. Our studies of oxygen-containing organic compounds have extended the correlations between core-ionization potentials and proton affinities and have established the site of protonation in esters to be the carbonyl oxygen.

Using a computer-based spectrometer control system developed under this project, we have made very accurate measurements of the core-ionization potentials in neon and carbon monoxide. These provide results against which theory can be tested as well as standards for calibration of photoelectron spectra.

In order to test theoretical calculations of satellite positions and intensities, we have measured the satellite structure in the photoelectron spectra of formaldehyde. Studies of the Auger spectra of HF and NH_3 (both isoelectronic with Ne) have also provided useful tests of theoretical calculations.

PUBLICATIONS

I. Completion of work begun at Princeton

1. Emission of Alpha Particles in the Fission of ^{238}U with 16- and 42-MeV Protons (with M. Rajagopalan), Phys. Rev. C5, 1402-1409 (1972).
2. Angular Distribution of Alpha Particles Emitted in the Fission of ^{252}Cf (with M. Rajagopalan), Phys. Rev. C5, 2064-72 (1972).
3. ^{127}I Mossbauer Studies of Some Fluoro Substituted Organo Iodine Compounds (with M. S. Lazarus), J. Chem. Phys., 60, 4682-89 (1974).
4. Li, Be, and B Production in the 3-GeV Proton Bombardment of Ni (with G. M. Raisbeck, P. Boerstling, and R. Klapisch) Phys. Rev. C 12, 527-532 (1975).

II. Heavy-Ion nuclear reactions

1. Energy Dependence of Deeply Inelastic Scattering of ^{84}Kr from ^{208}Pb (with R. Vandenbosch and M. P. Webb), Phys. Rev. Letters 36, 459-462 (1976).
2. Elastic Scattering of ^{84}Kr by ^{208}Pb (with R. Vandenbosch, M. P. Webb, S. W. Yates, and A. M. Friedman), Phys. Rev. C 13, 1893-99 (1976).
3. Deeply Inelastic Scattering of ^{84}Kr and ^{208}Pb (with R. Vandenbosch and M. P. Webb) Phys. Rev. C 14, 143-151 (1976).
4. Nuclear Reactions in the $^{86}\text{Kr} + ^{139}\text{La}$ System at 710 MeV (with M. P. Webb and R. Vandenbosch), Phys. Lett. 62B, 407-410 (1976).
5. Energy, Angular and Charge Distributions for Deeply Inelastic Scattering of Xe by Ta and Pb (with R. Vandenbosch, M. P. Webb, and M. S. Zisman), Nucl. Phys. A269, 210-222 (1976).
6. Elastic and Deeply Inelastic Reactions in the $^{86}\text{Kr} + ^{139}\text{La}$ System at 505, 610, and 710 MeV (with R. Vandenbosch, M. P. Webb, P. Dyer, R. J. Puigh, and M. S. Zisman), submitted to Phys. Rev. C.

III. X-Ray Photoelectron Spectroscopy

1. Search for Core Electron Satellites in Carbon Monoxide (with R. W. Shaw, Jr.), Chem. Phys. Lett. 14, 121-3 (1972).
2. Chemical Effects on the Lifetime of 1s-Hole States (with R. W. Shaw, Jr.), Phys. Rev. Letters. 29, 689-91 (1972).

3. X-Ray Photoelectron Spectroscopy of Alkali Halides (with P. H. Citrin), J. Chem. Phys., 57, 4446-61 (1972).
4. Observation by ESCA of Inequivalent Fluorines in ClF_3 , SF_4 , and PF_5 (with R. W. Shaw, Jr., and T. X. Carroll), J. Am. Chem. Soc. 95, 2033-34 (1973).
5. Equivalent-Cores Analysis of ESCA Shifts of Fluorine 1s Electrons (with R. W. Shaw, Jr.), Chem. Phys. Letters 22, 127-131 (1973).
6. X-Ray Photoelectron Spectroscopy of Chlorine Trifluoride, Sulfur Tetrafluoride, and Phosphorus Pentafluoride (with R. W. Shaw, Jr. and T. X. Carroll), J. Am. Chem. Soc. 95, 5870-5875 (1973).
7. Electron Distribution in the Xenon Fluorides and Xenon Oxide Tetrafluoride by ESCA and Evidence for 'Orbital Independence' in the Xenon-Fluorine Bonding (with T. X. Carroll, R. W. Shaw, Jr., C. Kindle, and N. Bartlett), J. Am. Chem. Soc. 96, 1989-96 (1974).
8. Charge Distribution in ClF from Core-Electron Binding Energies (with T. X. Carroll), J. Chem. Phys. 60, 2186-7 (1974).
9. Accurate Core Ionization Potentials and Photoelectron Kinetic Energies for Light Elements (with R. W. Shaw, Jr.), J. Electron Spectr., 5, 1081-94 (1974).
10. Core Ionization Potentials in Dimethyl Ether and Methyl Amine (with J. S. Jen), J. Electron Spectr. 4, 43-48 (1974).
11. 1s Hole Satellite Peaks in Formaldehyde (with T. X. Carroll), J. Electron Spectr., 4, 270-271 (1974).
12. Why the Hadamard Transform is Unsuitable for a Photoelectron Spectrometer, J. Electron Spectr. 6, 81-83 (1975).
13. Correlation between Proton Affinity and Core-Electron Ionization Potentials for Double-Bonded Oxygen. Site of Protonation in Esters (with T. X. Carroll and S. R. Smith), J. Am. Chem. Soc., 97, 659-660 (1975).
14. Correlation between Acidities of Carboxylic Acids and Core Ionization Potentials (with J. S. Jen), J. Am. Chem. Soc., 97, 659-660 (1975).
15. Auger Electron Spectrum and Ionization Potentials of the HF Molecule (with R. W. Shaw, Jr.), Phys. Rev. A 11, 1491-97 (1975).
16. Electron Distribution in Trifluoromethylbenzenes. Electron Donation by the Trifluoromethyl Group (with S. A. Holmes), J. Am. Chem. Soc., 97, 2337-41 (1975).
17. Core Ionization Potentials in Carbon Monoxide (with S. R. Smith), J. Electron Spectr. 8, 45-59 (1976).

18. Shakeup Spectra and Core Ionization Potentials for Formaldehyde. The Role of Electron Spin in Shakeup (with T. X. Carroll), J. Electron Spectr. 10, 215-225 (1977).
19. Auger Spectrum of Ammonia (with R. W. Shaw, Jr., and J. S. Jen) J. Electron Spectr., 11, 91-100 (1977).

IV.. Technical Reports.

1. Annual Progress Report, Sept. 1, 1971-Aug. 31, 1972. (RLO-2227-T14-1).
2. Annual Progress Report, Sept. 1, 1972-Aug. 31, 1973. (RLO-2227-T14-11).
3. Annual Progress Report, Sept. 1, 1973-Aug. 31, 1974. (RLO-2227-T14-15).