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1. SCIENTIFIC PROGRESS

Over the period covered by this report, significant progress has been made in the research supported by this contract. Twenty-seven papers were published or submitted for publication during that period. The four kinds of experiments involved in this research are unified by the common objective of helping to elucidate fundamental collision processes which are of importance for radiation chemistry, hot-atom chemistry, photochemistry, plasmas, lasers, and combustion, fields which are related to the development of new energy utilization and storage technologies. A description of the progress made follows.

1.1 Low-Energy Electron Scattering

Low-energy electron-impact is quite effective in causing atomic and molecular transitions which are optically forbidden. Electronic states of molecules which cannot be reached from the ground state by optically allowed transitions nevertheless play an important role in understanding the structure and dynamics of molecules. For example, triplet excited states of molecules which have singlet ground states have in general quite different structural parameters, potential energy surfaces, and radiative lifetimes. The measurement of the corresponding excitation energies furnishes some information about these differences and is useful in testing the validity of approximate quantum mechanical calculations of these quantities. In addition, the chemical properties of these triplet states are different from those of the ground state and are of importance in understanding the chemical effects of systems in which low-energy electrons are present, such as in radiation chemistry and in plasmas. In these systems, triplet states can be formed either by direct electron-impact

excitation or by ion-electron recombination. Finally, triplet states are also important in understanding sensitized photochemical reactions in which spin-allowed electronic excitation is produced in a sensitizer molecule (whose ground state is a singlet) by absorption of light. This molecule then may undergo intersystem crossing to a triplet state which can transfer its triplet excitation to a sensitized molecule. The latter then undergoes chemical reactions characteristic of a triplet state. These processes are also important for solar energy utilization technologies.

During this period, the new electron-impact spectrometer, EIS III was prepared for operation. The electron optics were photographed for documentation, baked, assembled, and wired. The whole apparatus was inserted into the vacuum system and pumped down. The vac-ion system for pumping the differential chambers was put into operation. The Nuclear Data Corporation data collection system was then tested and shown to have developed defects associated with its old age (12 years). It was returned to the factory for repair and has just recently been returned to us. In the interim, delivery of some of the components of a new microprocessor-based data acquisition system, which will replace the aging Nuclear Data one, was received. Design of the interface to the apparatus is nearly complete. This new data system should be operational soon, and permit more reliable and flexible data taking. In the interim, debugging of the new spectrometer is proceeding without the utilization of either of these systems.

Extensive amounts of accumulated data analyses and paper writing took place while the new system was being put into operation. Since the last technical report, 11 new papers on this work were submitted for publication. They include papers on cyclooctatetraene (Paper No. 5 of the list given in Section 3.1 of this report), CS_2 , OCS , and SO_2 (No. 11), propyne and butyne (No. 6), a

review paper (No. 14), UF_6 and WF_6 (No. 16), thiophosgene (No. 9), 1,3,5-hexatriene (No. 10), benzene and the fluorobenzenes (No. 21), 1,3-cyclopentadiene, 1,3-cyclohexadiene, and 1,3-cycloheptadiene (No. 23), cyclohexene, 1,4-cyclohexadiene, norbornene, and norbornadiene (No. 24), and nitromethane (No. 25). Reprints of the papers which have appeared in print since the last progress report are attached to the present one, as well as abstracts of those which have been submitted for publication but have not yet been published.

1.2 Variable-Angle Photoelectron Spectroscopy

Differential cross sections $d\sigma/d\Omega$ for photoionization of atoms or molecules by nonpolarized electromagnetic radiation vary with the angle θ between the directions of the incident photon beam and the ejected electron according to

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi} \left[1 - \frac{\beta}{2} P_2(\cos \theta) \right],$$

where σ is the total ionization cross section for the process under consideration and P_2 the second-order Legendre polynomial. The anisotropy parameter β lies in the range -1 to +2 and is influenced by several factors such as the angular momentum of the orbital from which the electron is ejected, the energy of that electron and the nature of the electronic interactions in the initial molecule and in the excited ion. We have previously constructed a photoelectron spectrometer capable of determining β . It consists of a resonance discharge lamp for generating monochromatic vacuum ultraviolet radiation, a scattering chamber containing the gaseous sample to be studied, an electrostatic energy analyzer for determining the energy of the photoelectrons and an electron multiplier for detecting them. The analyzer and multiplier can rotate around the scattering center so as to vary the angle θ . Spectra are taken at several

θ and from those β for each photoelectron transition is determined. Very few such machines exist, and the present one is of very high quality.

In the past we used this instrument to determine the values of β for argon, hydrogen, nitrogen, ethylene, methylated ethylenes, and other molecules. These studies established the differences in β for ionization of π and σ electrons, the effect on this parameter of methyl substitution, and their sensitivity to autoionization processes and σ - π interactions.

During the last year, 16 molecules were investigated. They include carbon monoxide (Paper No. 15), benzene and its monohalogenated derivatives (No. 7), and ethylene and its fluorinated derivatives (No. 26). Studies were also initiated on acetylene. In addition, past work on nitrogen (No. 13), SF_6 (No. 8), furan, thiophene, and pyrrole (No. 20), and ethylene and its methylated derivatives (No. 27) were written up and submitted for publication. Reprints or abstracts of these seven papers are attached to the end of this report.

In summary, the variable-angle photoelectron spectrometer has been extensively used over the period covered by this report and has furnished new and exciting information about many molecules, indicating that it is rapidly becoming a powerful tool for the elucidation of the nature of the binding in and the electronic structure of molecules.

1.3 Laser Photochemistry and Spectroscopy

Work on three different kinds of experiments involving the use of a pulsed dye laser was done during the last year, as described below.

1.3.1 Study of the Reactions of Photochemically Produced Atoms. We are studying the reactions of fluorine atoms of variable translational energy, produced by the photodissociation of UF_6 , with hydrogen molecules. The

experiments consist of photolyzing a mixture of UF_6 and H_2 with monochromatic light from a tunable dye laser and detecting the infrared chemiluminescence emitted from the vibrationally excited states of FH formed from the $\text{F} + \text{H}_2 \rightarrow \text{FH} + \text{H}$ reaction. In preliminary experiments, we attempted to detect photons emitted by $\Delta v = 2$ transitions. The energy of these photons is high enough to permit their observation with low noise detectors. However, the probability of these two-quantum state jumps is low, and this light was not detected.

During the past year we have upgraded our detection system to allow detection of photons from $\Delta v = 1$ transitions which have a much higher probability than those from $\Delta v = 2$ ones. Such a scheme has recently been successful in the detection of F atoms formed by the infrared multiphoton photodissociation of SF_6 . Calculations indicated that the intensity of photons emitted by the vibrationally excited FH molecules expected in our experiments would be slightly too low to detect with inexpensive room temperature detectors. After consideration of the importance of this experiment, we decided to invest in a much more sensitive indium-arsenide detector operated at liquid nitrogen temperatures. An impedance-matched preamplifier designed especially for this detector was also purchased. A cooled narrow-band interference filter was installed inside the liquid nitrogen dewar to discriminate against background black-body radiation. The fast response time of the indium-arsenide detector will allow observation of the time dependence of the infrared chemiluminescence. Experimental determination of state-to-state rate constants as a function of the fluorine atom translational energy for the $\text{F} + \text{H}_2 \rightarrow \text{FH} + \text{H}$ reaction will provide useful comparisons for theoretical calculations.

The addition of a floppy disk drive to the computer which controlled the laser scan and data collection during the past year will greatly simplify digital signal processing. Since we expect to observe extremely weak signals, the

ability to store and digitally process spectra is essential.

1.3.2 Multiphoton Photoionization Spectroscopy. During the past year we interfaced a small microprocessor system to our dye laser, which provided us with wavelength scan control and digital data acquisition capability. The apparatus now consists of a Molelectron tunable dye laser pumped by a nitrogen laser. It is capable of producing monochromatic light in the wavelength region 760 nm to 360 nm and, with frequency doubling, this range can be extended to 260 nm. The absorption cell is made of stainless steel and has windows at both ends. The absorption process is a two-photon excitation, followed by a two- or three-photon photoionization. The ions formed are detected by placing in the cell two parallel square electrodes, with edges 3/4" long, and separated by 3/4". Sample pressures are typically in the range 5 to 20 Torr and the voltage across the electrodes ranges from 1000 V to 1500 V. The pulse of ions produced by a laser pulse is amplified by a charge-sensitive preamplifier and directed to a dual channel differential gated integration system.

The microprocessor system allows the operator to select the laser wavelength drive speed, acquire data from the boxcar integrator every 0.1 Å, store the data and display the ratio of the signal intensity to the incident laser intensity on an XY recorder and a storage oscilloscope. Initial studies of the two-photon absorption spectrum of benzene were made, since this molecule has been studied previously. We obtained spectra of its $\tilde{A}^1B_{2u}$ state, from 38460 cm^{-1} to 43500 cm^{-1} (exciting wavelength from 520 nm to 460 nm). The $\tilde{X}^1A_{1g} - \tilde{A}^1B_{2u}$ transition is symmetry-forbidden but vibronically allowed in one- and two-photon processes. Our two-photon results agree with those of Frederice and McClain [Chem. Phys. Lett. 32, 541 (1975)], who use a fluorescence detection technique. The quality of our data is, however, better in spectral ranges where the fluorescence quantum yield decreases, since we use an ionization detection

scheme. We also examined the region in the two-photon benzene spectrum around 50000 cm^{-1} (exciting wavelength $\sim 390\text{ nm}$) which had previously been reported by P. M. Johnson [J. Chem. Phys. 64, 4143 (1976)] as a $^1E_{1g}$ or $^1E_{2g}$ state. Our data are in excellent agreement with his. Johnson suggested that this state may be Rydberg in nature but he was unable to definitely assign it. We are currently studying this same region in several fluorinated benzenes in an effort to determine the nature of this state and possibly the appropriate symmetry designation.

We have also obtained the two-photon spectrum of p-difluorobenzene in the exciting wavelength region of 530 nm to 480 nm. This spectrum exhibits rich vibronic structure in excellent agreement with the results of Robey and Schalg [Chem. Phys. 30, 9 (1978)] in their reported region from 555 nm to 500 nm. We observe a great number of peaks between 500 nm and 480 nm which have not been previously reported. Assignment of this spectrum is currently underway.

In summary, our multiphoton photoionization system is now fully operational and giving results in agreement with other laboratories, and of quality equal to or better than that of previous work. We will now proceed to use it to study transitions in other molecules which are symmetry-forbidden in one-photon excitations. These studies will nicely complement our electron-impact work.

1.3.3 Photoacoustic Spectroscopy. During the past year we have become involved in the design, construction, and utilization of a photoacoustic cell designed specifically for operation with a pulsed tunable dye laser. The photoacoustic technique is a highly sensitive method for detecting the absorption of light by molecules. It relies on the heating of a gaseous sample after the absorption of photons from an intensity-modulated light source. The heating

produces a corresponding pressure increase in the cell which is detected by the movement of the diaphragm of a condenser microphone mounted in the cell. Since the heating in the cell is proportional to the incident intensity, it is natural to employ the output of a high-intensity laser as the excitation source. In the visible and ultraviolet regions of the spectrum, most researchers have relied solely on continuous wave argon or krypton ion pumped dye lasers, using a mechanical chopper to modulate the intensity.

Our technique employs a pulsed, nitrogen-pumped dye laser. The advantages of this light source are threefold. First, it offers a wider range of accessible wavelengths than the conventional cw dye lasers. With the higher peak powers associated with the pulsed mode, frequency doubling or harmonic generation becomes a much more efficient process, allowing production of coherent radiation at photon energies as high as 5 eV. Second, the pulsed nature of the excitation offers unique possibilities for time-dependent spectroscopy. By measuring the time between the laser pulse and the appearance of a pressure wave at the microphone diaphragm, we can obtain a direct measurement of collisional deactivation rates. Preliminary experiments indicate a useful range of 1 to $10^5 \mu\text{sec}$. The photoacoustic technique offers an additional unique characteristic in that it actually measures the energy flowing out of the excited state molecules, rather than the number of photons absorbed. In the complex scheme of energy transfer, randomization, and luminescence in gaseous systems, this technique allows a direct measurement of the overall rates of nonradiative processes.

The extreme sensitivity of the photoacoustic technique (some investigators claim they can observe transitions with oscillator strengths as low as 10^{-15}) implies that highly forbidden transitions could be easily observed. Indeed, this appears to be the case. We have taken preliminary spectra of several

high overtone and combination vibrational bands in acetylene with little difficulty. We also observed the 3A_2 state of CS_2 in a cell 10 cm long and a sample pressure of 300 Torr. This state involves a spin-forbidden transition from the singlet ground state. Previous observations of this state at 80 Torr pressure used 88 m path lengths and photographic plates exposed for up to one hour periods, about an order of magnitude longer than our observation times. The large signal-to-noise ratio of our spectra implies the ability to detect much weaker spin-forbidden transitions while still retaining the inherent high resolution associated with laser spectroscopy.

During the past several years, our group has investigated a large number of low-lying triplet states in a variety of molecules using angle-resolved electron-impact spectroscopy. A large number of these states are accessible to the wavelength range of our nitrogen-pumped dye laser. Experiments are currently in progress to observe these states optically using the extreme sensitivity of our photoacoustic detection system coupled with the narrow bandwidth light from our pulsed tunable dye laser. The increased resolution will give more detailed knowledge about the structure and energy levels of the excited electronic states of these molecules.

The photoacoustic detector we are currently using has ideal characteristics for operation in the pulsed mode. The gas chamber has a cylindrical geometry with a small radius to maximize the transfer of energy to the microphone diaphragm. Holes in the walls of the cylinder allow the pressure waves to strike an aluminized mylar diaphragm wrapped around the circumference. The cylindrical geometry insures that the pressure wave which moves radially outward from the laser beam strikes the diaphragm everywhere at the same time. A transducer is mounted on the inlet of the cell to allow constant monitoring of the pressure in the cell during evacuation and filling. This is necessary

to prevent a sudden pressure change from rupturing or stretching the fragile mylar diaphragm.

A charge-sensitive preamplifier, originally designed for high time resolution gamma spectroscopy using germanium solid state detectors, is used to bias the capacitor microphone as well as amplify the small current produced as the diaphragm moves. The signal is processed with a boxcar integrator and then digitized, normalized to the laser intensity, and stored on diskette by an on-line microcomputer.

The tentative conclusion from these preliminary studies is that spin- and symmetry-forbidden electronic transitions up to 260 nm excitation wavelength (4.75 eV) can be studied at high resolution with currently available dye laser sources. Such studies should greatly enhance our knowledge of forbidden states of molecules.

1.4 Collisions in Crossed Molecular Beams

In order to study elementary bimolecular collision processes, we have in the past built a crossed molecular beam apparatus which uses as a detector a high-efficiency electron-bombardment ionizer coupled to a quadrupole mass filter. This detector can move up and down a quadrant which can rotate around a vertical axis. The net effect is to permit the detector to view the crossing point between the molecular beams from any direction within a solid angle of the order of one steradian, which includes the two primary beams. We have used this apparatus to study collisions between two room-temperature beams, the primary one of H_2 , D_2 , or He, and the secondary one of N_2 , O_2 , NH_3 , CH_4 , CO, CO_2 , SF_6 , H_2O , Ar, or NO. Quantum oscillations were observed and used to determine spherically symmetric intermolecular potentials.

Over the last year we have installed a PDP-11/03 minicomputer data acquisition system to replace our old (10 years) SCC 4700 one which completely collapsed of old age. Appropriate software systems were developed for control of the experiment and data acquisition. The reliability of this new data system was determined by rerunning the He + Ar system, which now serves to calibrate our apparatus. Extensive maintenance work on the several pumping systems of the apparatus was performed. A severe impurity contamination of the apparatus developed and was eliminated after appreciable effort.

Additional experimental work on the highly anisotropic He + CO₂, N₂O, and C₂N₂ was done, followed by extensive data analysis to obtain the corresponding potential anisotropies. A short paper on the He + CO₂ system was written (Paper No. 18). In addition, the sensitivity of the data to the several regions of the potential was explored in detail. The conclusions reached were (a) the equilibrium configuration of this system has a T shape; (b) the position and depth of the corresponding minimum is well determined by total differential cross section measurements; (c) the position of the minimum (i.e., saddle point) in the collinear configuration is determined approximately by these experiments; and (d) the potential of this last configuration is determined only very crudely by these experiments.

A series of three additional detailed papers was written and submitted for publication describing the results of recent experiments: one on the He + Ar system (Paper No. 17), a second on the He + N₂, O₂, CO, and NO systems (No. 19), and a third one on the He + CH₄, NH₃, H₂O, and SF₆ systems (No. 22). Reprints of the papers which appeared in print since the last technical progress report as well as abstracts of the papers submitted for publication since then are attached to the present progress report.

Work on the correlation chopper for a velocity analysis of the scattered beam, to be used in rotational inelasticity experiments, proceeded during the last year and that system is close to being operational.

In summary, data gathering, and extensive data analysis and paper writing have been accomplished during the last year. This constitutes satisfactory overall progress of this project.

1.5 Energy Relevance of Research Performed

We will now indicate the relevance of the research performed under this contract to the development of new energy technologies.

Almost any energy storage or utilization system involves the conversion of energy from one form to another. Nuclear power plants involve the conversion of nuclear energy to thermal to electric energy, fossil fuel plants that of chemical to thermal to electric energy, internal combustion engines that of chemical to thermal to mechanical energy, storage batteries that of electrical to chemical energy and so on. Whenever chemical energy is involved, energy states, ground or excited, play a central role, as do energy redistribution processes. All of the research described in this report involves the understanding of energy states and energy redistribution processes in the interaction of molecules with electrons, photons, atoms, or other molecules.

In the electron scattering work, we have investigated the electronically excited states of molecules, with particular attention having been paid to low-lying spin-forbidden transitions. Such states have special roles in photochemistry. If a photon is absorbed to a low-lying singlet state of a molecule, it can intersystem cross into a triplet state. Because of the relatively long radiative lifetime of the latter, varying from about a microsecond upwards, chemical reactions may occur which are of a different character from the reaction of

singlet states. Therefore, low-lying triplet states of molecules may play important roles in the chemical storage of solar energy. In addition, in plasmas in general and high pressure electrical discharges in particular, the electron energy distribution function is determined by the presence of energy sinks. Low-lying triplet states of molecules and free radicals are such sinks, and their presence helps to determine the character of the system. In radiation chemistry, triplet states can be formed by electron ion recombination, and they can affect the subsequent chemistry. In the attempt to develop high-power electronic transition lasers, triplet states play a crucial role because their long radiative lifetime is favorable for the buildup of electronic population inversions. Such lasers, if powerful enough, may be useful in the development of controlled thermonuclear fusion devices.

In the photoelectron work, we have studied the details of the ionization process, with special attention being paid to angular distributions. Photoionization and electron-impact ionization are closely related. The latter is central for the behavior of plasmas, and photoionization studies of the present type are useful for the understanding of electron-impact ionization. In addition, in high density plasmas, radiative recombination of electrons and ions generates photons which can be reabsorbed elsewhere in the system to reionize it. This provides a mechanism for propagation of the plasma, and our studies are relevant for the understanding of the ease and direction of such propagation. In addition, the understanding of the details of chemical binding in molecules promoted by these studies complements the electron-impact spectroscopy information and may be useful for solar energy utilization systems. Furthermore, the differences between the angular distributions of molecules in the gas phase and adsorbed on surfaces is also being used to furnish information on the orientation of molecules on surfaces and in energy-related technology.

In our laser photochemistry work, the study of the energy-dependence of chemical reactions is useful for the understanding of photochemical and hot-atom processes, and this is relevant for solar energy utilization, radiation chemistry, and chemical lasers. In laser two-photon and photoacoustic absorption spectroscopy, the information about symmetry- and spin-forbidden transitions nicely complements that obtained from the electron-impact work and has the same relevance as the latter.

Finally, the energy-transfer processes studied with the crossed molecular beam apparatus furnishes important information about energy redistribution and relaxation in energy-rich systems, which are important in energy-related technologies such as lasers, combustion, flames, hot-atom reactions, and plasmas.

In summary, the research performed has a basic relevance for many classes of energy storage and utilization technologies, in addition to providing fundamental information about elementary processes of importance to chemistry.

2. SCIENTIFIC AND OTHER PERSONNEL

During part or all of the period covered by the present technical progress report, in addition to the Project Director, the following people have been associated with the project:

David A. Edmonson, postdoctoral research fellow, electron scattering

Dorothy J. Flanagan, graduate student, photoelectron spectroscopy

Robert P. Frueholz, graduate student, electron-impact and two-photon spectroscopy

James F. Garvey, graduate student, molecular beams

Mark H. Keil, graduate student, molecular beams

David J. Moll, graduate student, laser photochemistry and photoacoustic spectroscopy

Ronald Rianda, graduate student, electron-impact and two-photon spectroscopy

Jeffrey A. Sell, graduate student, photoelectron spectroscopy

Capt. J. Thomas Slankas, graduate student, molecular beams

Jaroslav W. Winniczek, graduate student, molecular beams

William Schuelke, instrument shop supervisor, general

Adria McMillan, secretary

Robert P. Frueholz, Mark Keil, Jeffrey A. Sell, and Capt. J. Thomas Slankas all obtained their Ph.D. 's during the last year. Frueholz is now at the Aerospace Corporation, Keil is at the University of Toronto, Sell is working for the General Motors Research Laboratories, and Capt. Slankas is at the Air Force Weapons Laboratory in Albuquerque, New Mexico.

3. PUBLICATIONS

3.1 The papers published or submitted for publication since the last technical progress report are:

1. Doublet-Quartet Transitions in Nitric Oxide as Detected by Electron-Impact Spectroscopy.
R. P. Frueholz, R. Rianda, and A. Kuppermann.
J. Chem. Phys., 68, 775 (1978).
2. Doublet-Quartet Transitions in Nitric Oxide by Low-Energy, Variable-Angle Electron Scattering.
R. P. Frueholz, R. Rianda, and A. Kuppermann.
Chem. Phys., 31, 315 (1978).
3. Excited Electronic States of 1,3,5-Cycloheptatriene.
R. P. Frueholz, R. Rianda, and A. Kuppermann.
Chem. Phys. Lett., 55, 88 (1978).
4. Electron-Impact Investigation of Excited Singlet States in 1,3-Butadiene.
W. M. Flicker, O. A. Mosher, and A. Kuppermann.
Chem. Phys., 30, 307 (1978).
5. Electronic Spectroscopy of 1,3,5,7-Cyclooctatetraene by Low-Energy, Variable-Angle Electron Impact.
R. P. Frueholz and A. Kuppermann.
J. Chem. Phys., 69, 3614 (1978).
6. Electron-Impact Spectroscopy of the Alkynes: A Comparison of Propyne and 1-Butyne with Acetylene.
W. M. Flicker, O. A. Mosher, and A. Kuppermann.
J. Chem. Phys., 69, 3311 (1978).
7. Angular Distributions in the Photoelectron Spectra of Benzene and Its Monohalogenated Derivatives.
J. A. Sell and A. Kuppermann.
Chem. Phys., 33, 367 (1978).
8. Angular Distributions in the Photoelectron Spectroscopy of SF₆.
J. A. Sell and A. Kuppermann.
Chem. Phys., 33, 379 (1978).
9. Detection of a Second Triplet State in Thiophosgene by Electron-Impact Spectroscopy.
W. M. Flicker, O. A. Mosher, and A. Kuppermann.
Chem. Phys. Lett., 57, 183 (1978).
10. Vibronic Structure of the Second Triplet State of 1,3,5-Hexatriene.
R. P. Frueholz and A. Kuppermann.
J. Chem. Phys., 69, 3433 (1978).

11. Electron-Impact Excitation of Low-Lying Electronic States in CS₂, OCS, and SO₂.
W. M. Flicker, O. A. Mosher, and A. Kuppermann.
J. Chem. Phys., 69, 3910 (1978).
12. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. I. Sensitivity of the Elastic Differential Cross Section to the Interatomic Potential.
M. Keil and A. Kuppermann.
J. Chem. Phys., 69, 3917 (1978).
13. Energy Dependence of the Differential Photoelectron Cross Sections of Molecular Nitrogen.
D. M. Mintz and A. Kuppermann.
J. Chem. Phys., 69, 3953 (1978).
14. Electronic Spectroscopy of Molecules by Low-Energy, Variable-Angle Electron Impact.
A. Kuppermann, W. M. Flicker, and O. A. Mosher.
Chem. Rev., accepted.
15. Angular Distributions in the Photoelectron Spectroscopy of Carbon Monoxide.
J. A. Sell, A. Kuppermann, and D. M. Mintz.
J. Electron Spectrosc., in press.
16. Electronic Spectroscopy of UF₆ and WF₆ by Electron Impact.
R. Rianda, R. P. Frueholz, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
17. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. II. The He-Ar van der Waals Potential.
M. Keil, J. T. Slankas, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
18. An Empirical Anisotropic Intermolecular Potential for He + CO₂.
M. Keil, G. A. Parker, and A. Kuppermann.
Chem. Phys. Lett., 59, 000 (1979).
19. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. III. Anisotropic Intermolecular Potentials for He + N₂, O₂, CO, and NO.
M. Keil, J. T. Slankas, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
20. Angular Distributions in the Photoelectron Spectroscopy of Furan, Thiophene, and Pyrrole.
J. A. Sell and A. Kuppermann.
Chem. Phys. Lett., 59, 000 (1979).
21. Electronic Spectroscopy of Benzene and the Fluorobenzenes by Variable Angle Electron Impact.
R. P. Frueholz, W. M. Flicker, O. A. Mosher, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).

22. Scattering of Thermal He Beams by Crossed Atomic and Molecular Beams. IV. Spherically Symmetric Intermolecular Potentials for He + CH₄, NH₃, H₂O, SF₆.
J. T. Slankas, M. Keil, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
23. Electronic Spectroscopy of 1,3-Cyclopentadiene, 1,3-Cyclohexadiene, and 1,3-Cycloheptadiene by Electron Impact.
R. P. Frueholz, W. M. Flicker,
O. A. Mosher, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
24. Excited Electronic States of Cyclohexene, 1,4-Cyclohexadiene, Norbornene, and Norbornadiene as Studied by Electron-Impact Spectroscopy.
R. P. Frueholz, W. M. Flicker,
O. A. Mosher, and A. Kuppermann.
J. Chem. Phys., 70, 000 (1979).
25. Investigation of Low-Lying Electronic States in Nitromethane by Electron-Impact Spectroscopy.
W. M. Flicker, O. A. Mosher, and A. Kuppermann.
Chem. Phys. Lett., 59, 000 (1979).
26. Variable Angle Photoelectron Spectroscopy of the Fluoroethylenes.
J. A. Sell and A. Kuppermann.
J. Chem. Phys., submitted.
27. Photoelectron Spectroscopy of Ethylene, Isobutylene, Trimethylethylene and Tetramethylethylene at Variable Angle.
D. M. Mintz and A. Kuppermann.
J. Chem. Phys., submitted.

Reprints of the published papers are attached. Preprints of the papers in press would involve several hundred pages of material and therefore only their abstracts are attached. The full preprints are available upon request.

3.2 Ph.D. Theses

1. Interaction Potentials of Helium with Atoms and Molecules from Crossed Beam Experiments.

Mark Keil
May 1978, 348 pages.
2. Electronic Spectroscopy of Various Molecular Systems by Low-Energy, Variable-Angle, Electron Impact.

Robert P. Frueholz
May 1978, 345 pages.

3. Angular Distributions in Photoelectron Spectroscopy.

Jeffrey A. Sell
August 1978, 294 pages.

4. Interaction Potentials of Atom-Molecule and Molecule-Molecule Systems from Crossed Beam Experiments.

John Thomas Slankas
September 1978, 502 pages.

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