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# **Summaries of FY 1977 Research in the Chemical Sciences**

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**February 1978**

**U.S. Department of Energy**

Office of Energy Research  
Division of Chemical Sciences

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Office of Energy Research  
Division of Chemical Sciences  
Washington, D. C. 20545

## FOREWORD

In the Chemical Sciences basic energy research program, scientists at government, university and corporate laboratories conduct research on fundamental interactions, processes and techniques important to the production, use and conservation of energy. The goal is to provide, within the scientific disciplines encompassed by Chemical Sciences, the necessary base of scientific knowledge required to advance the nation's energy technology programs. The research covers a spectrum of scientific and engineering areas and is conducted generally by personnel trained in the disciplines of chemistry, analytical chemistry, chemical engineering, chemical physics, physical chemistry and physics.

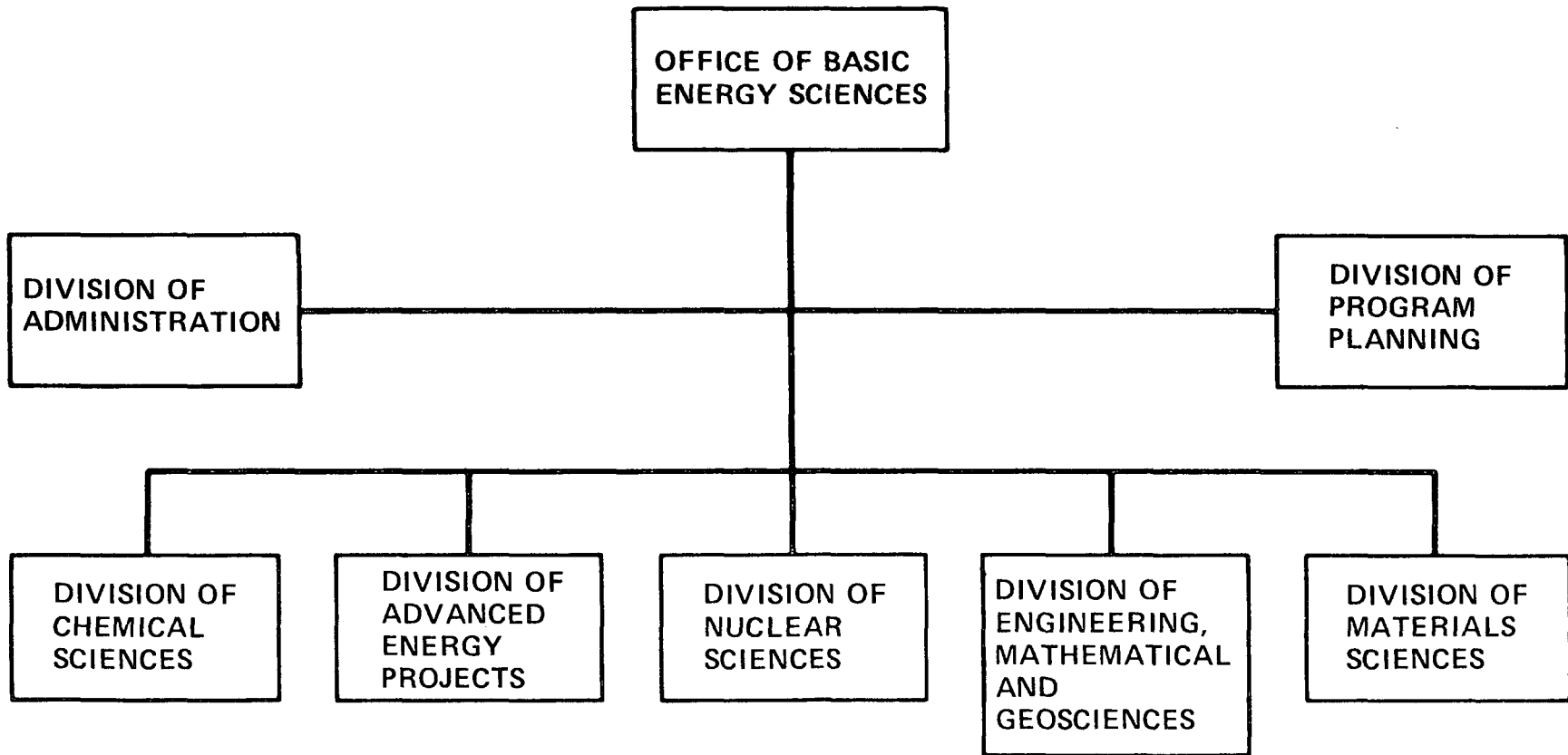
The research projects documented in this report were conducted under the aegis of the U.S. Energy Research and Development Administration (ERDA). They constituted the program of the Office of Chemical Sciences in the Division of Basic Energy Sciences.

During FY 1977 a Department of Energy was proposed by the President and enacted by Congress. The new Department of Energy (DOE) came into existence on October 1, 1977. ERDA was incorporated into DOE along with other agencies and elements of the Federal Government. The Chemical Sciences basic energy research program now constitutes the program of the Division of Chemical Sciences in the Office of Basic Energy Sciences (BES) under the Director of the DOE Office of Energy Research.

This program constitutes one element of a wide range of research activity supported by the Office of Basic Energy Sciences. Other basic energy research programs are administered by the BES Divisions of Materials Sciences; Nuclear Sciences; Engineering, Mathematical and Geosciences; and Advanced Energy Projects. The structure of the Office of Basic Energy Sciences is given in the following chart.

This report documents all of the Chemical Sciences basic energy research projects underway during FY 1977 and provides a summary of funding levels and appropriate indexes.

Elliot S. Pierce  
Acting Director  
Division of Chemical Sciences  
Office of Basic Energy Sciences



## INTRODUCTION

The purpose of this report is to provide a convenient compilation and index of the DOE basic energy research program in the Chemical Sciences. This compilation is intended for use by administrators, managers and scientists to help coordinate research and as an aid in selecting new research projects.

The report is divided into Sections A and B describing each of the projects; Section C, a summary and analysis of funding levels; Section D, an index of investigators; and Section E, an index of projects grouped by programmatic area.

Each project carries a number (underlined) for reference purposes. The FY 1977 funding level, title, personnel, budget activity number (e.g. 01-01) and a summary description of the project accompany each project number. The first two digits of the budget number refer to either Fundamental Interactions (01) or Processes and Techniques (02). The budget numbers carry the following titles for FY 1977:

01-01 - Radiation Sciences

01-02 - Chemical Physics

01-03 - Atomic Physics

02-01 - Chemical Energy

02-02 - Separations

02-03 - Analysis

02-04 - Engineering Sciences

In the indexes, Sections D and E, the references are to the project numbers appearing in Sections A and B.

It should be recognized that it is impossible to include in this report all the technical data available for such a wide variety and large number of research projects. By the time it could be compiled it would be outdated. The approach taken here was to briefly summarize the actual scope of each project for FY 1977. The best method for obtaining more detailed information about any of the projects is to contact directly the investigators listed.

We wish to express our appreciation to Dr. Jerome Hudis, Brookhaven National Laboratory, and to Dr. Raymond Wymer, Oak Ridge National Laboratory, for their most generous assistance in reviewing, condensing and editing almost all of the original project summary statements, in order that we might achieve the necessary modicum of uniformity in the text of the report.

Thomas W. Buttery  
Division of Chemical Sciences  
Office of Basic Energy Sciences



## TABLE OF CONTENTS

### SECTION A

	<u>Page</u>
Laboratories	
Ames Laboratory .....	1
Argonne National Laboratory .....	8
Atomics International .....	21
Bartlesville Energy Research Center .....	22
Brookhaven National Laboratory .....	23
Lawrence Berkeley Laboratory .....	36
Lawrence Livermore Laboratory .....	45
Los Alamos Scientific Laboratory .....	46
Morgantown Energy Research Center .....	50
Mound Laboratory .....	52
Notre Dame, University of .....	54
Oak Ridge National Laboratory .....	60
Pacific Northwest Laboratory .....	72
Sandia Laboratories (Livermore) .....	76

### SECTION B

#### Corporations

Aerochem Research Laboratories, Inc. ....	77
Aerospace Corporation .....	77
Bend Research, Inc. ....	77
General Electric Company .....	78
Stanford Research Institute .....	79

#### Other Government Agencies

National Bureau of Standards/Washington .....	80
National Bureau of Standards/Boulder .....	81

#### Universities

University of Alabama .....	82
University of Arizona .....	82
Baylor University .....	82
Boston University .....	83
Brandeis University .....	84
Brown University .....	85
University of California/Davis .....	86
University of California/Irvine .....	86
University of California/Los Angeles .....	88
University of California/Riverside .....	89
University of California/Santa Barbara .....	89

	<u>Page</u>
University of California/Santa Cruz .....	91
California Institute of Technology .....	92
University of Chicago .....	93
Cornell University .....	94
University of Delaware .....	94
Drexel University .....	94
University of Florida .....	95
Florida State University .....	95
George Washington University .....	96
University of Georgia .....	96
Harvard University .....	97
Howard University .....	98
University of Illinois/Chicago Circle .....	99
University of Iowa .....	99
John Hopkins University .....	99
University of Kansas .....	100
Kansas State University .....	100
Louisiana State University .....	101
Marquette University .....	101
University of Maryland .....	102
University of Massachusetts .....	102
Massachusetts Institute of Technology .....	103
Michigan State University .....	104
University of Minnesota .....	105
University of Mississippi .....	107
University of Missouri/St. Louis .....	107
University of Nebraska/Lincoln .....	108
University of Nevada .....	110
University of New Mexico .....	110
City University of New York/Brooklyn College .....	110
State University of New York/Buffalo .....	111
Northwestern University .....	111
Ohio State University .....	112
University of Pennsylvania .....	113
Pennsylvania State University .....	113
University of Pittsburgh .....	114
Princeton University .....	115
Purdue University .....	116
Rice University .....	116
University of Rochester .....	117
University of South Carolina .....	117
Stanford University .....	117
University of Tennessee .....	118
University of Texas .....	118
Texas A&M University .....	119
Texas Southern University .....	120
University of Utah .....	120
Virginia Polytechnic Institute and State University .....	121
Washington University .....	121
Wayne State University .....	122
College of William and Mary .....	122



	<u>Page</u>
University of Wisconsin .....	123
Worcester Polytechnic Institute .....	124
Wright State University .....	124
Yale University .....	124

SECTION C

Summary of Funding Levels .....	127
---------------------------------	-----

SECTION D

Index of Investigators .....	129
------------------------------	-----

SECTION E

Index of Projects Grouped by Programmatic Area .....	135
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SECTION A

LABORATORIES

The information was taken from current Laboratory program budget submissions and project summaries. Most of these projects are of a continuing nature.

AMES LABORATORY  
Iowa State University  
Ames, Iowa 50010

Molecular Sciences -01-

J. H. Espenson - Phone: (FTS) 865-5730 or (515) 294-5730

V. A. Fassel - Phone: (FTS) 865-2112 or (515) 294-2112

- |  |          |       |
|--|----------|-------|
| <u>1.</u> PHOTOCHEMISTRY AND<br>SPECTROSCOPY<br>G. Small | \$82,000 | 01-01 |
|--|----------|-------|

Photophysics of organic molecules and solids, mechanisms by which light quanta are converted into heat, chemical energy and different light quanta. The effects of strain, site inhomogeneity and the electron-phonon interaction of vibronic absorption band profiles of molecular solids. Survey of photochemistry and spectroscopy of selected organic compounds, e.g., organosilicon, isotopically selective solid state photochemistry. Solid state photochemical hole burning as a tool for probing the dynamics of photochemical processes as well as the structures of photoreactive states. Specific systems include organosilicon (germanium) compounds and halogen diatomics, e.g., I<sub>2</sub> and ICl. Polariton effects in naphthalene, controlling crystal perfection by chemical doping so that the dynamics of electronic energy transfer can be probed.

- |  |          |       |
|--|----------|-------|
| <u>2.</u> RADIATION AND SOLID STATE<br>SPECTROSCOPY<br>D. Martin | \$28,000 | 01-01 |
|--|----------|-------|

Chemical fate of radioactive nuclides formed in solid, inert covalently-bonded compounds of transition-metal elements, including cluster compounds with metal-metal bonds. Szilard-Chalmers processes; chemical changes in the radioactive components upon thermal or radiation annealing, kinetic parameters for defect-induced reactions; activation energies for the transfer of defect-energy by promotion of trapped electrons into the conduction band together with the dependence of such energy transfer upon structural and compositional factors.





## AMES LABORATORY

Molecular Sciences -02-

H. J. Svec - Phone: (FTS) 865-6487 or (515) 294-6487

V. A. Fassel - Phone: (FTS) 865-2112 or (515) 294-2112

8. CHEMICAL KINETICS AND REACTIVITY OF TRANSITION METAL COMPLEXES  
J. Espenson \$118,000 02-01

Transition metal complexes in reactions pertinent to coal use and conversion. Kinetics of rate-limiting molecular processes through model compounds and idealized reactions. Metal-carbon bonds and alkyl transfer reactions. Results contribute to design of syntheses of new hydrocarbon derivatives of transition metals for further study.

9. PROPERTIES OF RARE EARTH ELECTROLYTES  
F. Spedding \$17,000 02-01

Basic study of aqueous solutions of electrolytes taking advantage of the special aspect of the rare earth cations as predominately changing cation size only. This limits the number of parameters and hopefully will shed light on water itself which is one of the most complicated common solvents.

10. METALLIC AND INORGANIC HYDRIDES WITH POTENTIAL APPLICATION IN HYDROGEN STORAGE  
J. Espenson \$200,000 02-01

Structural and electronic properties for high hydrogen affinity and capacity. Chemistry-physics-metallurgy of metal-hydrogen interactions for hydrogen storage.  $\text{LaNi}_5$  and other RE-transition metal compounds and alloys, low-valent Group IV and V metal compound matrices, metal cluster compounds. Enthalpy and free energy of  $\text{H}_2$  uptake; low-temperature heat capacities; structure by X-ray, neutron diffraction, NMR; partial molal volumes, hydrogen interaction parameters; hydrogen mobility by NMR and kinetics; UPS and XPS measurements.







AMES LABORATORY  
Molecular Sciences -01- (Continued)

18. ACTIVATION ANALYSIS \$59,000 02-03  
A. Voigt

Application of neutron activation and neutron capture gamma ray analysis to energy and health problems. Trace element characterization of coals, interrelation of coal deposits; potential on-line plant analysis for S, Fe, moisture. Trace elements in blood, correlation with pathologies, removal of interferences due to Na and Br.

19. LASERS IN ANALYTICAL CHEMISTRY \$96,000 02-03  
E. Yeung

Identification and demonstration of improved analytical sensitivity and reliability through use of lasers and modern optics. Development of Fabry-Perot detection (atomic emission from spark sources) and laser-excited atomic fluorescence (flame and non-flame sources) for improved sensitivity in element detection; finding paths of trace elements from fossil fuels; Raman and Stokes-Raman scattering for combustion studies; time-synchronous Raman scattering for remote monitoring of combustion chambers.

20. ATMOSPHERIC POLLUTION \$96,000 02-03  
MONITORING BY DIODE LASERS  
E. Yeung

Determination of reliable spectral line widths and positions for atmospheric components in order to realize the potential high resolution for pollutants available with infrared diode lasers. Experimental comparisons (diode lasers vs conventional IR spectrometers) plus theoretical models to provide dependable line information. Evaluation of monitoring at an actual source. Spectral interferences identified and perhaps eliminated; long-path measurements; remote sampling.

ARGONNE NATIONAL LABORATORY  
9700 South Cass Avenue  
Argonne, Illinois 60439

Chemistry Division -01-

J. Unik - Phone: (FTS) 388-2681 or (312) 739-2681

21. RADIATION CHEMISTRY OF AQUEOUS SYSTEMS AND OTHER SOLUTIONS \$434,000 01-01  
M. S. Matheson

The program includes: chemical reactions of  $e_{aq}^-$  and OH radicals and their precursors on the picosecond time scale; chemical consequences of inhomogeneous deposition of ionizing radiation ( $e_{aq}^-$  completed, OH being studied); solvation of the electron in various solvents; magnetic field effects on ion recombination; radical-radical interactions studied by NMR and ultrafast EPR spectroscopy; activation energies for reactions between radiolytic products in solution; pulse radiolysis using high LET ions. Linac accelerator with associated optical detection methods extending down into the 50 picosecond range, streak camera technique, ultrafast EPR and fast-flow NMR methods. The fast pulse radiolysis program studies energy deposition processes that result from the absorption of radiation, the kinetics of the very fast chemical processes initiated by radiation, and the temperature dependence of reactions occurring among the radiolytic products of water.

22. FUNDAMENTAL PROCESSES IN RADIATION CHEMISTRY \$384,000 01-01  
J. R. Miller, M. C. Sauer

Phenomenon of electron tunneling and the mechanisms of energy transfer and radical reactions in the gas phase; electron transfer between molecules separated by 10-40 Å of inert solvent; effect of molecular structure and thermal energy on the rates of intermolecular electron transfer. Study of electron tunneling reactions as mechanisms for molecular rectification essential to the separation of positive and negative charge in photosynthesis and possible utility in man-made solar energy conversion devices. Energy absorption and transfer in irradiated gas mixtures; light emission from excited states used to probe the kinetics and mechanisms of processes occurring; choice of possible mechanisms of excited state formation (i.e., direct excitation, intramolecular relaxation processes, energy transfer, and ion recombination) on the basis of time-resolved fluorescence measurements; rare gases and rare gas-iodine mixtures.

ARGONNE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

23. PHOTOCHEMISTRY IN AQUEOUS SOLUTION AND CHEMICAL STORAGE OF SOLAR ENERGY  
M. S. Matheson \$282,000 01-01

Solutions containing solutes such as ferricyanide, which upon photolysis produce hydrated electrons are studied to optimize  $e_{aq}^-$  production with longer wavelength light as a means for  $H_2$  production. Investigation of systems in which sunlight stimulates oxidation-reduction reactions in pairs of solutes wherein some of the products can be kept from recombining, thus storing energy;  $MnSO_4$ - $ZnSO_4$  system with storage products being  $H_2$  and  $MnO_2$ .

24. RESEARCH IN COMBUSTIBLE FUELS  
S. Gordon \$232,000 01-01

Research in free radical processes applied to reactions with coal model compounds, hydrogen production by direct reaction of carbon with water, and hydrogen production from water utilizing ultraviolet light; elimination of organically bound sulfur. Pulse radiolysis of coal model compounds in a variety of liquids to study kinetics and to observe intermediates; final products for identification obtained by steady gamma radiolysis; reactions of  $OH$ ,  $O^{\cdot -}$ ,  $H$  and solvated electrons with various thiopenes

25. COMBUSTION, ATMOSPHERIC AND ENVIRONMENTAL CHEMISTRY  
S. Gordon, L. Kaplan \$185,000 01-01

Pulse radiolysis techniques to study reactions involving radical species  $OH$ ,  $HO_2$  and  $Cl$  with compounds (organic and inorganic) introduced into the atmosphere by the combustion of fossil fuels and by the widespread use of pesticides and aerosol propellants. Development of a condensation nucleus size analyzer capable of determining the size and number of particles from 5 to 500 Å in size; study of the chemistry and physics of aerosols generated from various atmospheric pollutants.

ARGONNE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

26. SPECTROSCOPIC AND THEORETICAL \$321,000 01-01  
STUDIES ON CHLOROPHYLL, PHOTO-  
SYNTHESIS, AND ENERGY TRANSFER  
J. J. Katz

Laboratory studies on chlorophyll by nuclear magnetic resonance spectroscopy; nature of intermolecular chlorophyll interactions;  $^1\text{Hmr}$ ,  $^{13}\text{Cmr}$  and  $^{15}\text{Nmr}$  spectroscopy to delineate the role of the central magnesium atom in chlorophyll and the general nature of chlorophyll-chlorophyll and chlorophyll-ligand interactions. New methods developed to record nmr spectra under light irradiation to determine chlorophyll triplet hyperfine coupling constants.  $^{13}\text{Cmr}$  studies on chlorophyll incorporated into lipid vesicles and photosynthetic membranes to ascertain the state of the chlorophyll in these systems. Optical studies on ordered monolayer arrays of chlorophyll to deduce the spectral consequences of particular geometries; photoelectron spectroscopy to establish the energy of binding of valence and structural electrons in chlorophyll aggregates; chlorophyll lasers to investigate the origins and significance of fluorescence in photosynthesis and excited chlorophyll states generally. Ab initio calculations, exciton, and Förster transfer theory to study excited state properties, light absorption, and energy transfer properties of chlorophyll.

27. STUDY OF PHOTOSYNTHESIS \$134,000 01-01  
WITH ESR AND ENDOR  
J. R. Norris

Time-resolved esr spectroscopic studies of photosynthesis; development of spin echo esr spectrometer with ten nanosecond time resolution to permit direct observation by esr of primary energy production steps in photosynthesis. Goals are to determine the distance of electron transfer, identification of necessary transient stages in photochemistry, and determination of whether photochemistry proceeds from the singlet or triplet state. Esr used to measure energy degraded to heat during photosynthesis; newly developed endor procedures used to measure coupling constants of doublet and triplet chlorophyll states important in photosynthesis.

ARGONNE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

28. SOLAR ENERGY CONVERSION \$226,000 01-01  
 J. J. Katz

Development of devices which mimic the photosynthetic apparatus of plants and photosynthetic bacteria; artificial photosynthesis systems that successfully mediate electron transfer between electron donors and acceptors; successful generation of voltages as high as 400 mV. Use of artificial-linked photoreactive chlorophyll dimers as the working elements in the "synthetic leaf"; attachment of an antenna to the synthetic reaction centers to duplicate the photosynthetic light conversion apparatus of a green plant. Electrochemical studies on chlorophyll; interaction of charged chlorophyll species with electron donors and acceptors; energetics of chlorophyll excited states produced electrochemically; oxidation-reduction properties of in vivo and synthetic reaction centers.

29. PREPARATION OF BIOLOGICAL MATERIALS OF UNUSUAL ISOTOPIC COMPOSITION AND ASSOCIATED NEUTRON AND X-RAY STRUCTURAL STUDIES \$147,000 01-01  
 J. J. Katz

Large-scale culturing of unusual isotopic composition; organisms highly enriched in deuterium, carbon 13, and nitrogen 15; chlorophylls, chlorophyll-protein complexes, electron-transfer proteins, chloroplasts, and chromatophores. Development of new methods for isolating chlorophyll-protein complexes and photoreaction centers, using fluorinated surfactants and other exotic surface-active agents. Procedures for disaggregating and then reaggregating photosynthetic membranes with deuterated or  $^{13}\text{C}$ -chlorophyll and a lipid matrix of ordinary isotopic composition for nmr and small-angle neutron scattering studies. Preparation of the halophilic bacterium *Halobacterium halobium* (an organism that carries out photosynthesis using the pigment bacteriorhodopsin instead of chlorophyll) in fully deuterated form, for the study of bacteriorhodopsin and the light-utilizing apparatus of this organism by small-angle neutron scattering, nmr, and resonance enhanced Raman spectroscopy.

ARGONNE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

30. HIGH RESOLUTION SPECTROSCOPY                      \$218,000                      01-02  
           H. M. Crosswhite

Examination near the ionization threshold of energy levels of atomic uranium, plutonium and several lighter elements such as Ba, including transition probability determinations (hook method) and quadratic Zeeman effects. Relations between energy level positions and transition rates analyzed by the multichannel quantum defect theory. Theoretical analysis of empirical energy levels of U, Np, Pu and Es atomic and singly-ionized spectra, emphasis on configuration-mixing modeling relating to isotope-shift analysis and development of a systematic model for prediction of the electronic and thermodynamic properties of heavy and superheavy materials and plasmas. Experimental and theoretical studies of actinide ions (U through Es) in crystals; development of a model of 5f electronic energies for use in atomic and solid-state energy level calculations. Fundamental problems of simple diatomic molecular systems such as H<sub>2</sub>, D<sub>2</sub>, T<sub>2</sub>, OH, OT, N<sub>2</sub> and N<sub>2</sub><sup>+</sup> relating to verification of ab initio calculation methods and energy-transfer phenomena in atmospheric species.

31. CROSSED-BEAM STUDIES OF                              \$193,000                      01-02  
       REACTIONS OF ACCELERATED  
       ATOMS AND MOLECULES  
       S. Wexler

Dynamics and energetics of chemi-ionization and other (usually) endoergic reactions. Accelerated crossed-molecular beams; ionic (and sometimes neutral) collision products analyzed in flight in two "chemical accelerator" machines; chemi-ionization and other hyperthermal processes. Reactions investigated are associative ionization, rearrangement (reactive) ionization, electron transfer, collision-induced ion pair formation (polar dissociation), and inelastic scattering. Energy transfer in collision processes.

32. THEORETICAL CHEMISTRY                              \$286,000                      01-02  
       AND MODELING  
       A. C. Wahl

Chemical dynamics theories developed and applied both to efforts in chemi-ionization and isotope separation, and to evaluate the reliability of current methods of calculating potential energy curves and surfaces. The fundamental properties of atmospheric molecules calculated on a consistent basis to provide molecular characteristics as input to aeronomic modeling. New methods of calculating the fundamental properties of molecules, particular emphasis on heavy atom systems. Computer code development; a library of computer codes in molecular quantum mechanics, scattering theory, and graphics display. Function of chlorophyll in photosynthesis at the molecular level by a variety of computational techniques.









## ARGONNE NATIONAL LABORATORY

Chemistry Division -02-

J. Unik - Phone: (FTS) 388-2681 or (312) 739-2681

40. INORGANIC CHEMISTRY \$276,000 02-01  
E. H. Appelman, J. G. Malm,  
L. Stein

The inorganic chemistry program continues its strong emphasis on fluorine chemistry and on studies of the basic chemistry and applications of unusual oxidizing and fluorinating agents, such as the compounds of the noble gases. Strong support is being given to the solution of chemical problems arising from the chemi-ionization process for uranium isotope separation now under development. Methods for maintaining  $UF_5$  in solution have been discovered, a fact that may be useful for the separation of uranium isotopes by chemical exchange with  $UF_6$  in the gas phase. This possibility will be investigated further. Work continues on development of solid absorbers for the chemical trapping of radon, xenon, and, perhaps, krypton.

41. THE CHEMICAL NATURE OF COALS AND COAL PRODUCTS \$130,000 02-01  
M. H. Studier

Investigation of logical diagenesis: biological materials - peat - lignite - sub-bituminous - bituminous - anthracite. Correlation with chemical structures of petroleums, shale oil, Fischer-Tropsch products, for contribution to coal conversions. Vacuum-distillation and solvent-extraction isolation of trapped compounds in coals for clues to the formation and nature of the coal. Pyrolysis, hydrocracking and oxidative degradation to produce identifiable compounds; isolation and identification by chromatography and fractional distillation.



ARGONNE NATIONAL LABORATORY  
Chemistry Division -02- (Continued)

43. CHEMICAL SEPARATIONS SCIENCE                      \$500,000                      02-02  
       E. P. Horowitz

Liquid-liquid extraction, liquid and bonded-phase chromatography, interfacial mass transfer, adsorptive bubble separation, exclusion chromatography, and field flow fractionation. Synthesis, purification, and testing of reagents. Identification and evaluation of the system variables to elucidate equilibria. Kinetics. Crown ethers on supports for chromatography. Applications to separation of actinides and the fission products  $^{99}\text{Tc}$  and  $^{129}\text{I}$  from nuclear wastes, separation of polymers and colloids (Pu polymer, nonextractable Zr), kerogen and bitumen from shale oil, coal constituents.

44. ANALYTICAL DEVELOPMENTS                      \$135,000                      02-03  
       IN MASS SPECTROMETRY-  
       CHROMATOGRAPHY AND  
       SUPPORTING SYSTEMS  
       M. H. Studier

Improvement of instruments, procedures, and data handling systems for support of programs in (particularly) fossil energy. Time-of-flight mass spectrometers in combination with chromatographic and high vacuum techniques of separations. Aromaticity of fossil fuels by fluorination.

45. STUDY OF ATMOSPHERIC                      \$110,000                      02-03  
       TRACE GASES BY MASS  
       SPECTROMETRY  
       C. M. Stevens, E. H. Appelman

Isotopic composition of atmospheric CO to determine its principal source. Mass spectrometric measurement of  $^{14}\text{C}$  in atmospheric CO to determine the ratio of dead carbon to live carbon sources. Laboratory measurements of isotope fractionation in OH oxidation of  $\text{CH}_4 \rightarrow \text{CO}$  and  $\text{CO} \rightarrow \text{CO}_2$  to aid in analysis of data on samples of atmospheric CO. Isotopic composition in southern hemisphere to explain lower level. Analysis for tropospheric and stratospheric concentrations of OH and  $\text{HO}_2$  important in validating photochemical models of effects of trace gas pollutants. The analysis involves tagged reactants and mass spectrometry.

ARGONNE NATIONAL LABORATORY  
Chemistry Division -02- (Continued)

46. RADIOACTIVE ISOTOPES AND \$15,000 02-03  
NUCLEAR TECHNIQUES AS ANALYTICAL  
TOOLS FOR BIOLOGICAL PROBLEMS  
A. M. Friedman

Development of nuclear analytical techniques for biological systems.  
Investigation of mechanism of sulfur uptake into peat, pertinent also  
to lignite and coal; possibly useful in sulfur elimination from coal.  
Previous development completed on preparation of immunologically competent  
<sup>211</sup>At-tagged antigens.

## ARGONNE NATIONAL LABORATORY

Chemical Engineering Division -02-

F. A. Cafasso - Phone: (FTS) 388-3672 or (312) 739-3672

47. FLUID CATALYSIS

\$130,000

02-01

F. A. Cafasso, H. M. Feder

Critical test of reaction catalysis in a fluid stream by a suspension of immiscible liquid droplets; reversible reaction to transfer homogeneous catalyst from a carrier phase to a working phase (partition catalysis); formation of surface-active catalyst at interfacial film between the carrier and working phases (surfactant catalysis); emphasis on hydrogenation of aromatic molecules and valence isomerization of highly-strained molecules; comparison of homogeneous and two-phase systems using understood test reaction.

ATOMICS INTERNATIONAL  
8900 DeSoto Avenue  
Canoga Park, California 91304

Atomics International Division -02-

C. A. Trilling - Phone: (213) 341-1000, Extension 1325

<u>48.</u> MOLTEN SALT INTERACTIONS	\$115,000	02-01
IN COAL PROCESSING		
S. J. Yosim		

Investigation of reactions in molten sodium carbonate; different catalytic effects of sulfide and sulfate compounds in sodium carbonate on the air or CO<sub>2</sub> oxidation of reactive carbon and of carbon in coal; reactions between typical coal ash components (alumina, iron oxides, iron sulfide, silicon dioxide) and molten sodium carbonate; reactions of calcium oxide and sodium silicates with molten sodium carbonate.

BARTLESVILLE ENERGY RESEARCH CENTER  
P. O. Box 1398  
Bartlesville, Oklahoma 74003

Bartlesville Energy Research Center -02-

W. D. Good - Phone: (FTS) 735-4210 or (918) 336-2400, Ext. 210

<u>49.</u>	THERMODYNAMIC CHARACTERIZATION	\$75,000	02-01
	OF CONDENSED-RING COMPOUNDS		
	W. D. Good, S. H. Lee,		
	D. R. Douslin		

Determination of thermodynamic property data for condensed-ring aromatic and hydrosubstituted compounds present in syncrudes from coal, shale oil, and heavy petroleum ends; preparation of broad-range correlative equations based on chemical structure; basic data measurements include enthalpy of combustion, low-temperature calorimetry, vapor-flow heat capacity calorimetry, PVT relations, vapor pressures, and Raman and infrared spectroscopy.



BROOKHAVEN NATIONAL LABORATORY  
Upton, Long Island, New York 11973

Chemistry Department -01-

J. Hudis - Phone: (FTS) 664-4301 or (516) 345-4301

50. RADIATION CHEMISTRY \$480,000 01-01  
B. H. J. Bielski, R. W. Dodson,  
R. A. Holroyd, H. A. Schwarz

Behavior and reactions of transient chemical species (ions, electrons, free radicals, and excited states of molecules); theories to explain their behavior; development of new or improved techniques; radiolysis and photolysis to produce the transient species, usually by pulse techniques. Principal areas of investigation are: properties and reactions of electrons in dielectric fluids; superoxide radicals in biological systems; infrared spectra of protonated molecular clusters in gas phase; reactive metal ion intermediates in redox reactions.

51. CHEMISTRY OF ENERGETIC \$590,000 01-01  
ATOMS WITH APPLICATIONS  
TO NUCLEAR MEDICINE  
A. P. Wolf, J. Fowler,  
R. M. Lambrecht, G. Harbottle

Chemistry of energy-rich atomic and molecular species studied with neutral and charged reactants in either their ground or electronically excited states or as entities with high kinetic energies. Reactive intermediates produced by nuclear processes; carbon, nitrogen, oxygen, and halogen atoms both kinetically and electronically excited; probe details of atom-atom and atom-molecule reactions in an energy range inaccessible to conventional methods. Microwave plasma generation of atomic species provide the same atomic species in known electronic states and temperature distributions; spectroscopic techniques to identify reactants and products and to determine rates of gas phase reactions. Applications include: relation of spin state of carbon-11 atoms and their chemical reactivity; facile reaction rate determinations of atomic species such as carbon, silicon, and the halogens with a broad spectrum of substrates; and a variety of techniques for labeling compounds of medical and biological interest.

BROOKHAVEN NATIONAL LABORATORY  
Chemistry Department -01- (Continued)

52. ENERGY TRANSFER IN CHEMICAL KINETICS  
R. E. Weston \$120,000 01-01

Effects on chemical reaction rates by the distribution of reactant energy among translational, rotational, vibrational, and electronic degrees of freedom; energy distribution in the products as a probe of the reaction mechanism; collisional transfer of energy from excited atoms or molecules. Reactions where the well-defined electronic energy of a photoexcited atom or molecule can be transferred to a ground-state atom or molecule, or the excited species can spontaneously lose energy by emission of fluorescence radiation at a rate determined by the natural lifetime of the excited species; competition between energy transfer and emission; fluorescence lifetime; bimolecular rate constant for energy transfer. Direct measurements of lifetimes in the range 1-100 nsec by the single-photon time correlation method.

53. PHOTOCHEMICAL ENERGY CONVERSION AND SOLUTION KINETICS  
C. Creutz, N. Sutin \$330,000 01-01

Transition metal complexes as mediators in solar energy conversion and storage; photochemical investigations of such complexes and elucidation of the electron-transfer properties of charge-transfer excited states through studies of their reactions with inorganic oxidants and reductants in solution and through their electrochemical behavior at wide band-gap semiconductors. Decomposition of water into hydrogen and oxygen. Quantitative study of the physical and chemical deactivation processes such as luminescence, radiationless decay, and chemical "back-reactions"; lifetimes and other physical properties of excited states; rates of chemical back reactions of transition metal complexes.

BROOKHAVEN NATIONAL LABORATORY  
Chemistry Department -01- (Continued)

54. SELECTIVE LASER-INDUCED CHEMISTRY  
 D. Brenner \$40,000 01-01

A new program in selective laser-induced chemistry; chemistry of excited-state molecules; criteria for selectivity in photochemical reactions involving specific bond cleavages or isotope enrichments. Reactions of vibrationally excited molecules; rate of intramolecular energy flow among the vibrational modes; V-V and V-T/R energy transfer; intramolecular chemical dynamics after the absorption of a photon in the absence of collisions. Excess energy of reactions in exothermic processes, i.e., how is the exothermicity partitioned among products and to what extent is the energy distribution statistical; measurement of transfer of energy from visible and UV photons to photochemical products. Laser-induced fluorescence for measuring internal energy distributions, arrested relaxation and isotope separation for examining mode specific phenomena, photodissociation in molecular beams.

55. PICOSECOND SPECTROSCOPY  
 T. Netzel \$15,000 01-01

Exploration of sub-nanosecond photochemical processes; picosecond absorption spectroscopy; development of picosecond Raman spectrometric methods; modeling of electron photoejection; excited state geometries and reactions.

56. NEUTRON AND X-RAY STUDIES OF MOLECULAR STRUCTURE AND DYNAMICS  
 H. Bernstein, T. Koetzle,  
 R. McMullan, R. Thomas \$825,000 01-02

Methods of x-ray and neutron diffraction combined with computing and computer graphic techniques to solve significant problems in molecular structure. Emphasis on crystal structures where hydrogen atoms are important and on disordered or partially-ordered structures, since this is where neutron diffraction, alone or in combination with x-ray diffraction, has unique advantages for determining molecular structure and investigating chemical bonding. Systems being investigated are transition metal hydride coordination complexes, hydrates, ferroelectrics, and organic crystals. Combined x-ray and neutron diffraction (X-N) methods to examine the molecular charge-density distributions associated with formation of hydrogen bonds. Improved techniques for on-line network access to structural data bases, and use of interactive computer graphics to evaluate crystallographic results.

BROOKHAVEN NATIONAL LABORATORY  
Chemistry Department -01- (Continued)

57. THEORETICAL CHEMISTRY \$370,000 01-02  
S. Ehrenson, J. Muckerman,  
M. Newton

Theoretical elucidation of mechanisms of energy flow in chemical reactions; theoretical models for the role of molecular interactions in the storage and interconversion of energy, both in the gas phase and in condensed phases; phenomena associated with charged spheres, such as solvation and charge-transfer processes. Development and implementation of techniques for ab initio and semiempirical calculation of the energetics and equilibrium nuclear geometry (structure) of a variety of chemical systems in specific electronic states; classical and semiclassical treatments of the nuclear motion in kinetic processes involving these systems; aqueous electron transfer reactions, hydrogen bonding in hydroxylic systems, ab initio models for nickel surfaces, dielectric effects of solvents surrounding cavities of various shapes, dynamics and energetics of hydrogen combustion reactions and the development of a unified semiclassical theory of non-adiabatic transitions in molecular collisions.

58. ION-MOLECULE REACTIONS AND \$275,000 01-02  
THEIR APPLICATION TO CTR-  
RELATED STUDIES  
R. Beuhler, L. Friedman

Mechanisms of evaporation of large molecular systems from rapidly heated solid surfaces, energy transfer in such processes and energy transfer in the collisions of molecular ions with solid surfaces; development of mass spectrometric techniques for identification and structural analysis of large fragile molecular systems; auxiliary pigment responsible for the adsorption of radiant energy in the photosynthetic processes in blue-green algae. Nondestructive evaporation, gentle ionization and highly sensitive detection for the characterization of these compounds by mass spectrometric techniques. Evaporation mechanisms in systems suddenly heated to high temperatures relevant to attempts to develop controlled thermonuclear reactions; very intense sources of highly charged macromolecular weight ions; rapidly produced phase transitions. Detection of molecular aggregates and methods of determination of their charge as well as their mass to charge ratio; individual singly ionized particles that have molecular weight in excess of a few thousand; development of techniques for the sensitive detection of very heavy energetic ions of the kinds that may be required for heating and compression of thermonuclear reaction fuel elements.



## BROOKHAVEN NATIONAL LABORATORY

Department of Applied Science -01-

D. J. Metz - Phone: (FTS) 664-3054 or (516) 345-3054

D. H. Gurinsky - Phone: (FTS) 664-3504 or (516) 345-3504

61. INVESTIGATIONS OF THE CHEMISTRY OF ENERGETIC COMPOUNDS  
M. Hillman \$160,000 01-01

Preparation, structure and chemistry of energetic compounds; possibilities of both photoconductivity and superconductivity in organic molecules; preparation of three-dimensional organic arrays that are potential conductors; photoconductivity studies of intensely colored derivatives of compounds that are already known to have some conductivity properties; ferrocene.

62. KINETICS AND MECHANISMS OF CHEMICAL PROCESSES RELATED TO THE DEVELOPMENT AND USE OF ENERGY  
J. W. Sutherland \$145,000 01-01

Basic kinetic and mechanistic details in specific chemical systems associated with the development and use of energy sources for which present data are inadequate or unavailable; input data for energy models. Flash photolytic and pulse radiolytic techniques to characterize short-lived transient chemical species; steady-state photolytic, steady-state radiolytic and standard kinetic techniques to identify and measure yields of final products of a particular overall reaction. Chemical reactivity of sulfur dioxide in the gas phase and in aqueous solution and chemistry of transient intermediate nitrogen-hydrogen compounds.

63. PORPHYRIN CHEMISTRY  
J. Fajer \$358,000 01-01

Synthetic, structural, theoretical and physical chemistry of porphyrins; electronic structure and chemical properties of porphyrins and their radicals; biological role of porphyrin ions in photosynthetic and metabolic reactions; applications of these catalytic reactions to energy conversion systems such as solar energy production of electricity by photo-excitation of porphyrins deposited on solid interfaces or isolated in micelles, the production of hydrogen and/or oxygen in solution using porphyrins to mimic the photosynthetic cell and photo-decompose water, and also to fix nitrogen photochemically via porphyrin derivatives. Techniques include optical absorption, electron spin resonance (esr), nuclear magnetic resonance (nmr) and electron nuclear double resonance (ENDOR). Redox reactions induced chemically, photochemically and electrochemically.

BROOKHAVEN NATIONAL LABORATORY  
Department of Applied Science -01- (Continued)

64. BIOELECTROCHEMISTRY AND ELECTROCHEMISTRY  
S. Feldberg \$109,000 01-02

Ion location and translocation in bilayer lipid membranes (BLM's); theory as well as several novel experimental techniques (charge pulse and inner voltage clamping) for determining the position of ions absorbed with a BLM. Electron transfer through and/or within BLM's; kinetics and mechanisms of electron transfer between excited states of molecules (porphyrins or ruthenium complexes) within the BLM and electron acceptors or donor located either within the BLM or in the aqueous phase. Computer-simulation and analysis of the behavior of photoelectrochemical transducers to test both the validity of the theory as well as the performance of the device.

65. MOLECULAR STRUCTURE OF PORPHYRINS AND PHOTOENERGY TRANSDUCING SYSTEMS  
L. Spaulding \$62,000 01-02

X-ray diffraction techniques in conjunction with other structural probes to determine the molecular and crystal structures of porphyrins, chlorins, and other energy transducing systems; compounds that are models of the natural solar energy conversion systems to fully interpret electron spin resonance (ESR), nuclear magnetic resonance, Raman spectroscopy, and theoretical calculations of these systems.

66. COMBUSTION STUDIES ON ALTERNATE FUELS  
R. Klemm \$206,000 01-02

Investigation of unconventional or alternate fuels that may be used to supplement or replace petroleum derived fuels for operation in internal combustion engines and stationary combustion devices; study of the combustion and pollutant formation processes that occur during the use of these fuels. Single cylinder test engine (ASTM-CFR engine) and flat-flame burners used to provide realistic test bases for measuring the effects of operating parameters, such as fuel type and air-fuel ratio, on the pressure, temperature and concentration profiles for stable and transient species that exist during the combustion of various fuels; potential importance of specific elementary chemical reactions that occur during the combustion process. Specific modes and rates of the indicated chemical reactions determined in controlled and isolated experiments that eliminate the complexities of actual combustion devices; combustion modeling studies.

## BROOKHAVEN NATIONAL LABORATORY

Physics Department -01-

N. P. Samios - Phone: (FTS) 664-3866 or (516) 345-3866

M. Blume - Phone: (FTS) 664-3735 or (516) 345-3735

67. ATOMIC PHYSICS RESEARCH

\$50,000

01-03

K. W. Jones

Properties of highly ionized species found as fusion plasma contaminants; mechanisms for production of inner-shell vacancies in heavy ion-atom collisions; measurements of the impact parameter dependence and total cross sections for production of characteristic x-rays; beam foil spectroscopy measurements in the x-ray and vacuum ultraviolet regions to determine lifetimes and investigate atomic structures; cross sections for electron impact excitation and ionization of highly ionized heavy ion beams for the electron energy range up to 20 keV. Three-stage MP Tandem Van de Graaff, beams of ions ranging from H to U with energies up to 250 MeV; 3.5 MV Van de Graaff for low energy, light ions.



## BROOKHAVEN NATIONAL LABORATORY

Chemistry Department -02-

J. Hudis - Phone: (FTS) 664-4301 or (516) 345-4301

68. ENZYME AND ORGANIC MECHANISMS AND ENERGY STORAGE IN ENZYME SYSTEMS  
S. Seltzer
- \$110,000
- 02-01

Mechanisms of photosensitized and enzymically and chemically catalyzed cis-trans isomerization and how they can be utilized to maximize the energy difference between photostationary and thermodynamic equilibrium states; synthetic photogalvanic cell from photoisomerization of fumaric to maleic acid.

69. STRUCTURE AND BONDING IN METAL-HYDROGEN SYSTEMS  
J. Hudis, M. L. Perlman
- \$210,000
- 02-01

Photoelectron spectroscopy and diffraction methods applied to metal hydrides and their parent metals and alloys; data combined when possible with magnetic, Mössbauer, or other information and analyzed by use of theory in terms of the configurations in valence and conduction band levels of the materials. Practical methods of storing hydrogen as hydrides.

70. LASER-INDUCED REACTIONS FOR ISOTOPE SEPARATION  
R. Weston
- \$60,000
- 02-02

Application of laser photochemistry to isotopic enrichment of lighter elements such as C, N, O, or S; unimolecular reactions, bimolecular reactions, and photodissociation processes of vibrationally excited molecules; selective removal of photo-excited molecules. Details of the laser energy absorption process and energy transfer from excited species to provide basic information needed to estimate the efficiency of the isotope separation method.



## BROOKHAVEN NATIONAL LABORATORY

Department of Applied Science -02-

D. J. Metz - Phone: (FTS) 664-3054 or (516) 345-3054

D. H. Gurinsky - Phone: (FTS) 664-3504 or (516) 345-3504

72. METAL HYDRIDES \$257,000 02-01  
R. Wiswall, J. J. Reilly

Elucidation of the thermodynamic and structural principles and behavior of metal-hydrogen systems; pressure-temperature-composition relationships; hydrogen isotope exchange between hydride and gas phases; X-ray and neutron diffraction measurements of the crystal structure and state of the hydrogen atom; methods for and synthesis of metal hydride single crystals; impact on energy storage, energy conversion, and isotope separation.

73. HIGH TEMPERATURE CHEMISTRY \$163,000 02 01  
J. J. Egan

Investigation of thermodynamic and transport properties of substances at high temperatures; atomic models; development of techniques of solid state electrochemistry; movement of electrons and electron holes in ionic crystals and molten salts; substances include solid and liquid state semiconductor alloys; application to solar cells, high energy batteries, solid and molten salt electrolytes, fuel cells, and high temperature reactor fuels.

74. CHEMISTRY AND PHYSICS OF COAL UTILIZATION \$200,000 02-01  
D. R. Mackenzie, R. T. Yang

Mechanisms of hydrogen reactions with coal including the kinetics of pyrolysis and hydrogen reactions in the competition between depolymerization (desired) and char formation in solvent refined coal (SRC) processes.

75. CYCLIC SEPARATIONS PROCESS RESEARCH \$105,000 02-02  
F. B. Hill

Application of cyclic processes to separations of interest in nuclear reactor technology; heatless fractionation, parametric pumping, cycling zone adsorption, and preparative chromatography; experimental investigations of protium-tritium separation by heatless fractionation using the hydrogen-vanadium hydride system; equilibrium and kinetic measurements; theoretical model to predict process performance. Process design studies; measurement of fluid-solid separation systems.



## BROOKHAVEN NATIONAL LABORATORY

Physics Department -02-

N. P. Samios - Phone: (FIS) 664-3866 or (516) 345-3866

M. Blume - Phone: (FIS) 664-3735 or (516) 345-3735

77. DEVELOPMENT AND APPLICATIONS                      \$105,000                      02-03  
OF NUCLEAR PARTICLE  
MICROSCOPY

K. W. Jones, H. W. Kraner

New techniques for quantitative measurement and precise spatial localization of stable isotopes; demonstration of applications in fields such as biology, medicine, marine science, solid state physics. Charged-particle beams from Van de Graaffs to produce unique atomic and nuclear effects, plus X-ray fluorescence and scanning electron microscopy; stable isotope tracers emphasized when radiotracers are not suitable.

LAWRENCE BERKELEY LABORATORY  
University of California  
Berkeley, California 94720

Materials and Molecular Research Division -01-  
D. Shirley - Phone: (FTS) 451-5619 or (415) 843-5619

78. PHOTOCHEMISTRY OF MATERIALS                      \$105,000                      01-01  
    IN THE STRATOSPHERE  
    H. S. Johnston

Study of atmospheric ozone, laboratory and field measurements, interpretation of data, and theoretical analyses; atmospheric accommodation of nitric oxide; photolysis of substances of atmospheric interest, in particular, ozone, nitric acid, nitrogen pentoxide, and the NO<sub>3</sub> free radical; atmospheric reaction rates; absorption spectra of atmospheric species; theoretical analysis by the "method of instantaneous rates."

79. RADIATION CHEMISTRY                                      \$145,000                      01-01  
    W. M. Garrison

Specific chemical information on the relative importance of ionic, free-radical and excited molecule reactions involved in the radiolysis of organic compounds with high-energy heavy-ion beams. High linear energy transfer (LET). Use of the 88-inch cyclotron and the Bevalac for the study of LET effects in radiolysis. The  $\alpha$ -amino acids, N-acyl amino acids, and oligopeptides in the solid state and in aqueous solution are compounds being investigated. Studies of radical and molecular product yields in water as a function of LET. Standard chemical dosimeters such as the Fricke and ceric sulfate systems. Basic information for use in the application of high-energy heavy-ion beams in biological and medical research.

80. ENERGY TRANSFER AND STRUCTURAL                      \$130,000                      01-02  
    STUDIES OF MOLECULES ON  
    SURFACES  
    C. B. Harris

Mechanisms for redistributing the energy in photoexcited molecules into the surface states of metals and semiconductors. Surface sensitive ellipsometry and picosecond laser spectroscopy to follow the primary steps in the redistribution of the energy from photoexcited states on a time scale as short as  $10^{-12}$  seconds. Photoelectrolysis. Emission and reflectance spectroscopy of aromatic hydrocarbons adsorbed on transition metal surfaces to characterize changes induced in the molecular and electronic structure of these molecules by physi- and chemisorption.



## LAWRENCE BERKELEY LABORATORY

Materials and Molecular Research Division -01- (Continued)

84. THEORY OF ATOMIC AND MOLECULAR COLLISION PROCESSES  
W. H. Miller \$65,000 01-02

Theoretical studies of the dynamics of chemical phenomena at a molecular level; development of theoretical models and methods to deal with atomic and molecular collision processes. Development and application of a general semiclassical mechanics that allows one to combine classical mechanics and quantum mechanics to describe many features of molecular dynamics. Quantum effects in molecular phenomena and simpler computational methods for carrying out quantitative calculations. The range of application of these various semiclassical approaches includes inelastic and reactive scattering, electronically non-adiabatic collision processes, statistical models for chemical reactions, and most recently semiclassical methods for determining the vibrational states of small polyatomic molecules.

85. PHOTOELECTRON SPECTROSCOPY  
D. A. Shirley \$620,000 01-02

Electron spectroscopy; electronic structure of matter, as determined through binding-energy measurements. Structures of high-temperature species and their interactions with radiation and surfaces, properties of both clean surfaces and adsorbate-bonded surfaces, energy transfer and lifetimes in high-energy eximers, and electronic structure of van der Waals' molecules. Development of new electron spectroscopic-techniques and synchrotron radiation applications.

86. CROSSED MOLECULAR BEAMS  
Y. T. Lee \$280,000 01-02

Investigation of the dynamics of elementary atomic and molecular processes and the energetics of exotic radicals and ion clusters using crossed molecular beams. Information on mechanism and dynamics of chemical reactions obtained from the direct identification and measurements of velocity and angular distributions of product molecules from "single collisions." Reactions of oxygen atoms and free radicals with carbon-containing molecules and radicals under single collision conditions; primary products of many important reactions of oxygen atoms; hyperthermal chemical reactions of hydrogen, deuterium and halogen atoms; reaction of electronically excited atoms and molecules; interaction potentials between atomic and molecular species; inter- and intramolecular energy transfers and the energetics of radical molecules and the spectroscopy of molecule ions.



## LAWRENCE BERKELEY LABORATORY

## Materials and Molecular Research Division -01- (Continued)

87. POTENTIAL ENERGY SURFACES FOR CHEMICAL REACTIONS \$65,000 01-02  
H. F. Schaefer

Development of new theoretical and/or computational methods for the description of electrons in molecules, with emphasis on the correlation problem, that of formulating models for going beyond the single-particle or Hartree-Fock approximation. Application of theoretical methods to significant problems of broad chemical interest: a) model theoretical studies of chemisorption, metal clusters, and catalysis and b) the potential energy surfaces which govern gas-phase chemical reactions.

88. LOW ENERGY ATOMIC PHYSICS \$220,000 01-03  
H. A. Shugart

Research on ion properties (cross sections, lifetimes, and electromagnetic constants), development of a purely-electrostatic ion trap, with possible applications for residual gas analysis, vacuum leak detection, precision spectroscopy, cross-section and ion-molecule reaction studies. Search for universal methods of detecting trace quantities of atoms or molecules; development of an ultra-sensitive, selective method employing coherent forward scattering of light to detect one part in  $10^{12}$ . Laser spectroscopic search for the possible influence of a weak neutral electron-nucleus interaction which would perturb atomic structure; ultraviolet laser development.

89. ATOMIC PHYSICS \$160,000 01-03  
R. Marrus

Atomic physics of highly-stripped heavy ions, oscillator strength and wavelength measurements; study of transitions in two-electron atoms of high Z; quenching of the metastable state of  $\text{Ar}^{+17}$  in an external electric field, study of x-ray transitions using a new method of precision x-ray measurement, search for intense UV transitions in ionized iron and molybdenum elements which are important contaminants of fusion plasmas.

## LAWRENCE BERKELEY LABORATORY

Chemical Biodynamics Division -01-

M. Calvin - Phone: (FTS) 451-6131 or (415) 843-6131

90. SOLAR ENERGY \$300,000 01-01  
J. Otvos, J. Bassham

Methods development for utilization of solar energy; green plant photosynthesis; sensitized photodecomposition of water; sensitized photovoltaic devices; hydrocarbons and energy from plants.

## LAWRENCE BERKELEY LABORATORY

Energy and Environment Division -01-

R. J. Budnitz - Phone: (FTS) 451-5410 or (415) 843-5410

91. PHOTOCHEMICAL CONVERSION                      \$110,000                      01-01  
OF SOLAR ENERGY  
L. Packer

Biotechnological applications of solar energy: photoelectric potential generation; catalytic systems in chloroplasts; light-triggered catalysts in micro-organisms such as cyanobacteria and halobacteria; hydrogen production by chloroplasts in vitro and production and consumption by cyanobacteria; applications to artificial convertors.

92. SURFACE CHEMISTRY                              \$45,000                      01-02  
BY X-RAY PHOTOELECTRON  
SPECTROSCOPY  
T. Novakov

Study of surface chemistry of materials such as graphite and activated carbon by x-ray photoelectron spectroscopy, infrared spectroscopy and laser Raman spectroscopy.

## LAWRENCE BERKELEY LABORATORY

Materials and Molecular Research Division -02-

D. Shirley - Phone: (FTS) 451-5619 or (415) 843-5619

93. FORMATION OF OXYACIDS OF SULFUR FROM SO<sub>2</sub> \$30,000 02-01  
R. E. Connick

Basic chemistry of sulfur dioxide, particularly in solution, and also the chemistry of the numerous sulfur-containing compounds formed in aqueous solutions of sulfur dioxide through reaction with bases and acids and through oxidation and reduction reactions, particularly with oxygen; spectrophotometric, Raman and NMR measurements.

94. CONVERSION OF COAL TO CLEAN LIQUID AND GASEOUS FUELS \$145,000 02-01  
G. A. Somorjai, A. T. Bell

Development of catalytic approaches for the conversion of coal to liquid and gaseous fuels; catalytic synthesis of hydrocarbons from carbon monoxide and hydrogen produced by coal gasification; factors which limit catalyst activity, selectivity, and resistance to poisoning; relationship between catalyst composition/structure and performance; synthesis and evaluation of novel homogeneous catalysts based upon mono- and polynuclear organo-metallic complexes for coal liquefaction; emphasis on developing catalysts to complex aromatic groups and selectively promote reactions with portions of aromatic substrates.

95. SYNTHETIC AND PHYSICAL CHEMISTRY \$60,000 02-01  
W. L. Jolly

X-ray photoelectron spectroscopy measurements of atomic core electron binding energies of a wide variety of inorganic and organometallic compounds; interpretation in terms of atomic charges which indicate the nature of the electron distribution and bonding in the molecules. Extent of transition metal d electron "back-bonding" in organometallic compounds. Modes of ligand metal bonding in organometallic molecules. Use of core electron binding to make thermodynamic calculations. Synthesis and characterization of simple but novel compounds of the nonmetallic elements; compounds unstable under ordinary conditions but which can be "trapped" in metastable state and used as reagents in otherwise difficult syntheses.

## LAWRENCE BERKELEY LABORATORY

Materials and Molecular Research Division -02- (Continued)

96. ELECTROCHEMICAL SYSTEMS \$45,000 02-01  
J. S. Newman

Investigation of fluid flow and electrochemical transport; transport property measurements of concentrated electrolytic solutions; analysis of mass-transfer rates and current distribution; design methods of practical electrochemical systems; impact on local and overall corrosion rates. Analysis of interacting kinetic, mass transfer, and fluid flow phenomena for semiconductor electrode systems; impact on advanced solar energy conversion systems. Configuration of liquid junction cells with polycrystalline semiconductor electrodes.

97. HIGH ENERGY OXIDIZERS AND \$90,000 02-01  
DELOCALIZED-ELECTRON SOLIDS  
N. Bartlett

Oxidation of highly ordered graphite by high-energy oxidizers to make durable and conductive (comparable to aluminum) graphite salts with intercalated anions such as  $\text{SO}_3\text{F}^-$ ,  $\text{AsF}_6^-$ ,  $\text{OsF}_6^-$ ; potential electrochemical anodes. Potentials for redox proton transfer to permit cyclic energy storage. Predict useful paramagnetic and highly conductive cations from multiring aromatics of  $\text{Ar}^+\text{X}^-$  formulation useful in synthesis.



LAWRENCE LIVERMORE LABORATORY  
 P. O. Box 808  
 Livermore, California 94550

Scientific Support Departments -02-

G. Dorough - Phone: (FTS) 457-3767 or (415) 447-1100

S. Fernbach - Phone: (FTS) 457-3767 or (415) 447-1100

102. THERMOCHEMICAL PRODUCTION                      \$150,000                      02-01  
 OF HYDROGEN FROM WATER  
 O. Krikorian

Investigation of the scientific feasibility and economic potential of closed-cycle thermochemical processes for producing hydrogen from water using nonhydrocarbon energy sources; identification of at least three promising cycles leading to one or more bench-scale studies and economic evaluations; scientific feasibility and some detailed cycle chemistry established for ZnSe cycle; cycle process design optimization and development of alternative chemical approaches to reduce heat requirements at high temperatures shown to be needed; detailed research on rates, yields, and mechanisms in ZnSe cycle.

103. ENGINEERING ANALYSIS OF                      \$75,000                      02-04  
 COMBUSTION PROCESSES  
 J. W. Routh

The objective of this project is to develop models of the physical and chemical processes in combustion. The models will be tested against existing and future experimental results with the goal of providing a basic scientific resource which can be applied in improving the technology and machinery of combustion. Included are those efforts which form the basic research part of the laboratory's Combustion Research Program.

The work included in this project involves the development of detailed computer code descriptions of the combustion process; their purpose will be to investigate in detail specific mechanisms and experiments in order to provide understanding at the most fundamental level.

LOS ALAMOS SCIENTIFIC LABORATORY  
University of California  
P. O. Box 1663  
Los Alamos, New Mexico 87545

Q Division -01-

W. A. Ranken - Phone (FTS) 843-6578 or (505) 667-6578

<u>104.</u>	VAPOR PHASE HEAT TRANSFER	\$55,000	01-03
	J. E. Kemme		

Heat pipes offer unique advantages for efficiently carrying heat from one location to another. This effort extends and improves the existing description of heat transfer phenomena in heat pipes in order to achieve improved design codes for high heat transfer rates with liquid metal working fluids at temperatures ranging from 700-1800 K. Substantial revision in heat pipe theory and reformulation of heat pipe design codes is being applied to the development of vertically oriented, gravity assisted heat pipes. Continued theoretical and experimental work is being directed towards improved understanding of transition region, turbulent flow in wick structures, in variable-mass turbulent vapor-phase flow, and in capillary pumping force predictions.



## LOS ALAMOS SCIENTIFIC LABORATORY

P Division -01-

H. T. Motz - Phone: (FTS) 843-4117 or (505) 667-4117

105. RADIATION FROM HIGH TEMPERATURE      \$60,000      01-03  
PLASMAS SEEDED WITH HIGH-Z  
ELEMENTS

L. Jones, D. B. Thomson

Ionization rates of multiply ionized (five to thirty times) species are being furnished in order to understand the behavior of impurity ions in current magnetic fusion plasma experiments and to estimate the radiative cooling and energy balance in future confinement devices. The extremely high temperature environment obtainable only at the LASL theta pinch is being used to determine the ionization rates of neon VI-VIII, nitrogen V, oxygen VI, and line identification and ionization rates for krypton IX-XII. Time histories of successive ionization stages in the theta pinch seeded with the selected element are being compared to expected values in order to improve estimation procedures along isoelectronic sequences.

106. A STUDY OF ENERGY CONVERSION      \$60,000      01-03  
AND TRANSPORT IN SPACE PLASMAS  
W. C. Feldman

The solar wind, lower solar corona, and Earth's bow shock magnetopause provide a unique plasma in which any spacecraft approaches a truly nonperturbing diagnostic probe. This effort seeks to make use of existing satellite data to yield information and understanding of plasma and heavy ion physics processes - evolution and saturation of heat flux mechanisms, ion beam and thermal driven anisotropy-driven instabilities, and various sources of the free-energy in particle velocity distributions in the earth's magnetically confined upper atmosphere. Special attention is given to those phenomena which occur in magnetically confined fusion plasmas.



## LOS ALAMOS SCIENTIFIC LABORATORY

CMB Division -02-

M. G. Bowman - Phone: (FTS) 843-6014 or (505) 667-6014

108. SYNTHESIS OF THERMOCHEMICAL                      \$290,000                      02-01  
CYCLES FOR HYDROGEN  
PRODUCTION  
J. D. Farr

Theoretical and laboratory work to survey thermochemical cycles for hydrogen production from water using heat from nuclear reactors and solar collectors; identification of improved chemical systems; testing of reactions in potential cycles to determine thermochemical parameters, reaction rates, and practical yields; hybrid thermochemical-electrochemical cycles identified which may facilitate processes requiring lower maximum temperatures and less corrosive chemicals.

MORGANTOWN ENERGY RESEARCH CENTER  
P. O. Box 880  
Morgantown, West Virginia 26505

Energy Conversion and Utilization Division -02-  
R. J. Belt - Phone: (FTS) 923-7747 or (304) 599-7747

109. CHEMICAL KINETICS AND SURFACE CHEMISTRY \$40,000 02-01  
G. L. Karapinka

Determination of chemical reaction mechanisms and kinetics, and catalyst surface chemistry and activity during hydrodenitrogenation of model coal-derived organic nitrogen compounds, such as quinoline; comparison of catalysts such as cobalt molybdate on alumina, and transition metal organo-metallic compounds (molybdenum, iron, tungsten); determination of effect of valence state of metals (degree of reduction) on activity and selectivity for hydrogenation (insertion of hydrogen), hydrogenolysis (carbon-carbon bond cleavage), and hydrodenitrogenation (formation of ammonia); determination of back-reactions of ammonia; suggested applications to hydroliquefaction of coal, and catalytic hydrotreating of coal-derived liquid fuels.

## MORGANTOWN ENERGY RESEARCH CENTER

Analytical Research Division -02-

W. E. Wallace, Jr. - Phone: (FTS) 923-7294 or (304) 599-7294

110. BASIC STUDIES OF HIGH GRADIENT MAGNETIC SEPARATION CAPTURE MECHANISMS \$40,000 02-02  
L. C. Headley, W. H. Simmons,  
W. F. Lawson, R. P. Treat

Analysis of the dynamics of attraction and capture of magnetic particles by magnetized fibers; separation of sulfur-bearing particles from coal conversion and combustion streams in a high-gradient magnetic field; equation of motion for magnetic particle when acted on by magnetic, viscous, and gravitational forces; particle capture when trajectory intersects the fiber with a favorable static force balance; calculation of trajectories and capture distances for multifiber configurations; experimental determination of trajectories. Inertial terms are included in theoretical equation of motion.

MOUND LABORATORY  
P. O. Box 32  
Miamisburg, Ohio 45342

Nuclear Operations Department -02-

R. J. DeSando - Phone: (FTS) 774-3137 or (513) 866-7444

R. A. Schwind - Phone: (FTS) 774-7147 or (513) 866-7444

111. FUNDAMENTAL INVESTIGATION                      \$180,000                      02-01  
OF METAL-HYDROGEN SYSTEMS  
G. C. Abell, R. C. Bowman, Jr.,  
J. L. Ivey, C. M. Love

Identification and evaluation of factors to permit improved metal hydrides as energy storage systems; Ti, V, Li-transition metal systems. Determine hydrogen transport mechanism via crystal structure, composition, phase transformation; changing electronic structure via hydride formation, nature of metal-H bonds; effects of dopants. Hartree-Fock computer calculations of metal and metal-H clusters.

112. ISOTOPE SEPARATION                                      \$210,000                      02-02  
RESEARCH AND DEVELOPMENT  
B. E. Jepson, E. D. Michaels  
W. M. Rutherford

Investigation of isotope separation by liquid phase thermal diffusion and by chemical exchange; multiple column liquid thermal diffusion cascades with annular column spacings of 250  $\mu\text{m}$  and less; thermal diffusion factors (chlorine, sulfur, and bromine isotopes); influence of vertical temperature gradients and coolant hydrodynamics on stability of thermogravitational circulation. Separation of metal isotopes (calcium, lithium, molybdenum, and iron) by chemical exchange with polyethers; countercurrent isotope exchange processes and single-stage separation factors. Derive empirical relations to describe separations in terms of basic parameters.



NOTRE DAME, UNIVERSITY OF  
Notre Dame, Indiana 46556

Radiation Laboratory -01-

R. H. Schuler - Phone: (FTS) 332-7308 or (219) 283-7502

115. SPECTROSCOPY OF REACTION                      \$133,000                      01-01  
INTERMEDIATES  
S. J. Sheng

Spectroscopic studies of intermediates present in systems exposed to ionizing radiation and light to provide detail on the molecular and electronic configurations of these intermediates. Examples examined include free radicals, carbenes, radical ions and carbonium ions and excited states of both radicals and neutral molecules. Methods employed include absorption and emission spectroscopy, Raman studies, spectroscopic examination of Stark and Zeeman effects, and optical detection of both electrical and magnetic properties. Many of these studies carried out in doped solids at temperatures down to 4°K to provide the optical resolution required. Vibronic analysis to identify intermediate states present and to understand the electronic transitions involved.

116. THEORETICAL ASPECTS OF                      \$191,000                      01-01  
RADIATION CHEMISTRY  
K. P. Funabashi,  
A. Mozumder

Theoretical studies of the effects of the absorption of ionizing radiation in condensed systems; events which occur in times less than  $10^{-9}$  sec. Dynamic properties of electrons produced by radiation; mechanisms for electron localization in solvent traps and reaction with solutes. Role of electron-phonon (vibronic) interaction in addition to that of the structural disorder of the system as localization mechanisms; time-dependent optical absorption spectrum of trapped electrons and its decay pattern; chemical reactions involving localized electrons examined at early times using, in addition to the Smoluchowski equation, the continuous-time-random-walk (CTRW) model of Montroll-Weiss.



NOTRE DAME, UNIVERSITY OF  
Radiation Laboratory -01- (Continued)

117. CHEMICAL PHYSICS OF REACTING SYSTEMS \$85,000 01-01  
J. J. Kozak, M. E. Schwartz

Quantum mechanics, statistical mechanics and non-equilibrium thermodynamics to interpret phenomena and chemical-dynamic processes of interest in radiation chemistry, both at the molecular and macroscopic levels. Electronic structure calculations; model potential methods, self-consistent-field valence bond theory, direct methods for examining ionization phenomena, studies on the conceptual basis of exchange interactions. Theoretical studies of chemisorption, cluster stability, electron-solvent interactions, electron binding energies, photoionization cross sections, spin densities in radicals, and various spectroscopic properties. Dynamical aspects of the interaction of radiation with matter, and in particular, the temporal decay of excited states of two- and three-level atomic and molecular systems by an analytical study of the time-dependent Schrödinger equation. Statistical-mechanical theory of electrolytes applied to micellar kinetic processes. Non-equilibrium thermodynamics and non-linear kinetics applied to numerical studies of the cooperative effects associated with examples of coupled chemical reactions.

118. CHEMICAL STUDIES OF RADIATION INDUCED REACTIONS \$169,000 01-01  
R. H. Schuler

Chemical approaches to examine radiation induced reactions; effects of track structure and ion and radical recombination processes on the overall chemistry; liquid chromatographic methods; radiolysis of aqueous solutions; gas chromatography and radio chromatography to examine reactions in organic systems. Computational methods to simulate the course of radiation chemical reactions; effects of the different kinetic variables; effect of solute concentration on product formation (chemical scavenger studies) transformed to give descriptions of the time dependence of intermediates; track and ion recombination processes.

NOTRE DAME, UNIVERSITY OF  
Radiation Laboratory -01- (Continued)

<u>119.</u>	RADIATION CHEMICAL AND PHOTOCHEMICAL STUDIES OF REACTIONS AT CHEMICAL INTERFACES	\$94,000	01-01
	J. K. Thomas		

Radiation chemical and photochemical effects in micellar systems; catalytic or inhibitive effects of micellar isolation; transport of reaction intermediates across interfacial barriers. Reaction control by aqueous-lipid interface; development of micellar methods to examine kinetic details of chemical reactions; pulse radiolysis and laser photolysis techniques.

<u>120.</u>	PHOTOCHEMICAL STUDIES	\$236,000	01-01
	A. M. Trozzolo		

Photochemical studies on organic and inorganic systems to study the mechanism of which absorbed light energy ultimately produces chemical effects. Valence isomerization of heterocyclic compounds; chemistry of photolytically produced biradicals; photochemistry of organometallic compounds and inorganic complexes; electron transfer reactions of singlet oxygen and superoxide anion. Studies on photochromic systems in which a relatively strained heterocyclic ring is either open or closed photochemically to produce a high energy intermediate, whose stability can be controlled, as models for energy storage devices. Biradicals, which are important intermediates in a variety of photo-cleavage reactions of ketones, characterized by direct spectroscopic methods where electron-transfer trapping of these species allows the direct determination of biradical lifetimes. Photochemical studies on organometallic compounds and inorganic complexes for possible efficient photocatalytic systems; electron transfer reactions of singlet oxygen and superoxide anion. A primitive photovoltaic cell based on electron concentration differentials is being investigated.

NOTRE DAME, UNIVERSITY OF  
Radiation Laboratory -01- (Continued)

121. RADIATION CHEMISTRY DATA                      \$57,000                      01-01  
          CENTER  
          A. Ross

Continuous survey of the literature of radiation and photochemistry, the assembly of appropriate bibliographic information on computer readable keyworded files and the critical examination and compilation of experimental data on radiation produced reaction intermediates. Preparation of a variety of information services including literature searching, preparation of current-awareness aids and bibliographic searching. Bibliographic publications issued regularly are the Biweekly List of Papers on Radiation Chemistry and its annual cumulations and indexes. Evaluated compilations of kinetic and spectroscopic information on reaction intermediates; compilations made available to interested scientists by publication in the NSRDS-NBS series.

122. ESR STUDIES ON RADIATION                      \$247,000                      01-01  
          CHEMICALLY AND PHOTOCHEMICALLY  
          PRODUCED INTERMEDIATES  
          R. W. Fessenden

Electron spin resonance spectroscopy (ESR) studies of free radical intermediates present in reacting systems in both continuous and pulsed radiolysis and photolysis experiments. Steady state experiments used in situ radiolysis with 3-MeV electrons; intermediates produced by ionizing radiation in organic systems and in aqueous solutions. Time resolved studies using pulsed electron beams to yield kinetic behavior of intermediates on the microsecond time scale and also on chemically induced dynamic polarization of the radicals (CIDEP); spin selective reactions of the radicals; also photochemical experiments using continuous and mechanically and electronically modulated light beams and also with time resolved studies using laser pulses. Data give information on the electronic and geometric structure of radicals such as acidity and rates of protonation and on the rates for electron exchange between radical anions and their neutral parent molecules; data examined and integrated with results from optical studies and chemical approaches to give a more complete picture of the mechanisms of radiation chemical and photochemical reactions.

NOTRE DAME, UNIVERSITY OF  
Radiation Laboratory -01- (Continued)

123. PULSE RADIOLYSIS STUDIES \$148,000 01-01  
OF RADIATION CHEMICAL  
REACTIONS  
P. Neta, L. K. Patterson

Kinetic behavior and spectroscopic properties of transient species which absorb light in the UV, visible or near-infrared region by optical pulse radiolysis techniques; processes occurring in the range of  $10^{-7}$  to  $10^2$  seconds; absorption spectra of the intermediates; time resolution of  $10^{-8}$  sec; extension of time resolution of the automated system down to  $10^{-9}$  sec. Studies of radiation induced reactions of various organic substrates in aqueous solution; examination of the redox reactions in metal ion-organic ligand complexes with emphasis on examining the cleavage of various inorganic anions and reactivities of the resultant oxidizing intermediates; studies of the effects of local molecular organization on radical kinetics in heterogeneous systems; investigation of the oxidation of organic radicals by electron transfer and determination of the one electron redox potentials of radicals.

124. ENERGY TRANSFER IN \$55,000 01-01  
ATOMIC AND MOLECULAR  
SYSTEMS  
D. H. Winicur

Molecular beam methods to determine the mechanisms, cross sections, and intermediate species involved in the transformation of energy from one form to another. Crossed beams to measure differential scattering of electronically-excited metastable rare-gas atoms by various small molecules (e.g.,  $H_2O$ ,  $CO_2$ ,  $HBr$ ,  $C_6H_6$ ,  $N_2$ ,  $Br_2$ ). Time-of-flight techniques to measure the velocities and the identities of the scattered species; detailed information on the cross sections for energy transfer between atoms and molecules; identification of states formed immediately after the initial energy transfer; determination of the potential-energy curves for the interacting atoms and molecules. Examination of the magnitudes and velocity dependences of the integral energy exchange cross sections between excited argon and  $HBr$  or  $CO_2$  by examining quenching of the differential scattering at large angles; potential-energy curves for the electronically-excited states of atom-molecule complexes to examine the qualitative differences between these and the ground-state curves; effects of the initial relative kinetic energy and of the electronic excitation energy of the atom on the transfer of energy to small molecules.





OAK RIDGE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

128. SURFACE EFFECTS- \$50,000 01-01  
HYDROGEN RECYCLE  
CHEMISTRY  
S. H. Overbury

The goal is complete understanding of the processes of energy transfer, chemical reactivity, and re-emission of hydrogen at the first wall of MFE reactors. Apparatus development for study of chemical reactivity of atomic hydrogen with various substrates including isotope effects; study of the hydrogen-carbon system: energy distributions of back-scattered ions, detection of molecular species formed.

129. ATOMIC AND MOLECULAR \$240,000 01-02  
COLLISION DYNAMICS  
J. T. K. Cheung,  
P. F. Dittner, H. F. Krause

Atomic and molecular collision processes including chemical reactivity and intermolecular energy transfer at thermal and epithermal energies; ion pair formation and electron transfer at energies of 1-100 eV; electron transfer, inner shell quasi-molecular effects, penetration phenomena at very high energies. Study of single collision phenomena in atomic and ionic beams using model systems, application to more general systems and to problems of programmatic interest. Apply understanding of electronic excitation in the chemical reactivity of mercury atoms to the reactivity of excited carbon atoms where low lying electronic states are populated at thermal energies; surface and chemi-ionization of UF<sub>6</sub>.

130. PHOTOCHEMICAL, PYROLYTIC, AND \$150,000 01-02  
REACTIVE INTERMEDIATES BY  
ELECTRON SPIN RESONANCE  
R. Livingston, H. Zeldes

Chemical free radicals in liquids studied by electron spin resonance; methods of forming radicals include photolysis, pyrolysis, and chemical reaction in molten salts. The radicals with lifetimes ranging down to less than a millisecond observed at steady state concentration as the liquid flows through the spectrometer; radicals identified and features of their electronic structure elucidated. Changes in the nature of the liquid (temperature, pH, solvent, etc.); mechanisms of reactions, motional effects, exchange of protons, pK for ionization, etc.: kinetic studies on the rates of formation and disappearance of radicals. Studies of pyrolytic processes and molten salt solutions and photolytic reactions.

OAK RIDGE NATIONAL LABORATORY  
Chemistry Division -01- (Continued)

131. THEORETICAL CHEMISTRY \$65,000 01-02  
O. H. Crawford

A new program to develop strong capability in theoretical chemistry and to give theoretical guidance and support to the experimental programs including atomic and molecular structure, and chemical reactions. Theory will be used to calculate chemical reaction cross sections, energy distribution in reaction products, potential energy surfaces for atomic and molecular collisions, the structure of molecular fluids, and structures of molecules and ions.



## OAK RIDGE NATIONAL LABORATORY

Physics Division -01-

P. H. Stelson - Phone: (FTS) 850-6402 or (615) 483-8611

132. MOLECULAR RESEARCH WITH ELECTRON SPECTROSCOPY  
T. A. Carlson \$160,000 01-03

Development of electron spectroscopy as a useful tool in the study of molecular physics and general chemical behavior; orientation and bonding of molecules on surfaces; combined use of x-ray, uv, and photon-induced Auger spectroscopy to study chemical bonding and spatial orientation; development of ultra high vacuum compatible uv lamp for production of polarized HeI radiation.

133. COLLISIONS OF LOW ENERGY MULTICHARGED IONS  
C. F. Barnett, D. H. Crandall \$160,000 01-03

Measurement of electron impact excitation and ionization cross sections for multicharged ions using electron-ion cross beam techniques; charge exchange measurements of low mass ions with atomic hydrogen in the velocity range  $0.1$  to  $1 \times 10^8$  cm/sec; calculation of charge exchange cross sections for energetic ions colliding with hydrogen atoms.

134. HEAVY ION ATOMIC PHYSICS RESEARCH  
C. D. Moak, P. D. Miller \$180,000 01-03

Ion stripping in gases and solids; ionic states inside solids; inner shell and outer shell excitation of multiply charged ions; radiative and non-radiative electron capture by multiply charged ions; beam foil spectroscopy and target atom radiation; Auger and auto-ionization processes; stopping powers of heavy ions in gases, solids, and in crystal channels; Coulomb excitation and molecular orbital promotion of atomic states of heavy atoms; electron ejection from solids; quasi-molecular x-ray studies.

135. MOLECULAR INFRARED SPECTROSCOPY  
H. W. Morgan \$120,000 01-03

Solid state studies in the infrared spectra region on: the behavior of dopants and impurities, the formation of solid solutions by foreign ions in alkali halide lattices, and the occurrence of solid phase chemical reactions; examination and recalculation of the rotational spectra of small molecules together with Stark effects and energy shifts due to centrifugal distortion; supportive research in the development of submillimeter lasers.

## OAK RIDGE NATIONAL LABORATORY

Chemistry Division -02-

O. L. Keller, Jr. - Phone: (FTS) 850-6444 or (615) 483-8611

136. RESEARCHES ON THERMAL GENERATION OF HYDROGEN \$140,000 02-01  
C. E. Bamberger, D. M. Richardson

Hydrogen production from water splitting by thermochemical reactions; new or improved chemical reactions, chemical compounds, thermodynamic data, and process kinetics to develop viable and economical thermochemical cycles; minimization of temperatures, work and heat requirements, corrosiveness, and cost of recycled chemicals; impact on solar energy, synthetic fuels, and energy storage.

137. AQUEOUS CHEMISTRY AND THERMODYNAMICS TO ELEVATED TEMPERATURES AND PRESSURES \$335,000 02-01  
C. F. Baes, H. F. Holmes,  
M. H. Lietzke, W. L. Marshall

Thermodynamics of aqueous systems at elevated temperatures and pressures for ERDA technological applications using potentiometry, conductance, isopiestic experiments, and solubility measurements; understanding of temperature and pressure on equilibria, acid-base buffering systems, and electrolyte behavior; basis for accurate equations of state; hydrolysis and solubility of metal ions; solutions of alkali and alkaline earth halides; impact on steam generators, geothermal chemistry, environmental chemistry, and processing chemistry.

138. COMPARATIVE INORGANIC CHEMISTRY \$135,000 02-01  
D. H. Smith

Fundamental thermodynamic and kinetic information on inorganic systems; individual system details complemented through comparisons with related systems; contributions to separations methods. Distribution equilibria between aqueous solutions and fixed phases (ion exchangers, hydrous oxides, metal sulfides, activated carbon). Mass transport at interfaces of two-phase systems, including colloids. Effects of surfactants, micelles, microemulsions; salting effects, including polyvalent counterions. Adsorption of organics on inorganic solids.

OAK RIDGE NATIONAL LABORATORY  
Chemistry Division -02- (Continued)

139. HETEROGENEOUS CATALYSIS                      \$145,000                      02-01  
RELATED TO ENERGY  
SYSTEMS  
E. L. Fuller, W. C. Waggener  
P. A. Agron, R. A. Strehlow

Model reactions, studied by microreactor with mass spectroscopy and gas chromatography, for understanding and control of non-metallic coal conversion catalysts, commercial and specially prepared. Catalysts studied by ESCA, chemisorption, infrared spectroscopy and gravimetric measurements. Simplified catalyst surface studied by new technique for directional resolution of forces between clean metal surface and adsorbed molecule. Luminescence used to study catalyzed reactions in molecular beams.

140. ORGANIC CHEMISTRY AND THE                      \$330,000                      02-01  
CHEMISTRY OF FOSSIL FUELS  
C. J. Collins, B. M. Benjamin,  
V. F. Raaen, E. W. Hagaman

Identification of "scissile bonds" modified or cleaved in 400° conversion, with hydrogen donor, to preasphaltenes, asphaltenes, oils; better means to attack the bonds leading to coal liquefaction. Investigations with <sup>14</sup>C labels of separated vitrinite and of compounds analogous to coal structures. Search for free radical processes. Product identification by gas chromatography, radioactivity assay, proton and <sup>13</sup>C nmr spectroscopy.

OAK RIDGE NATIONAL LABORATORY  
Chemistry Division -02- (Continued)

141. FUNDAMENTALS OF SEPARATIONS . \$170,000 02-02  
CHEMISTRY  
W. D. Arnold, F. J. Hurst

Chemical knowledge of important separations methods, their mechanisms, and applications. Investigation and improvement of methods for the studies; preparations and purifications; application of fundamental information to separations process development. Difficult-pair separations (Zr-Hf; Ta-Nb) using high pressure liquid chromatography. Continued improvement of process for uranium recovery from wet-process phosphoric acid, and interaction with commercial users.

142. SPECTROPHOTOMETRIC STUDIES \$150,000 02-02  
OF SOLUTIONS WITH ALPHA-  
ACTIVE MATERIALS  
J. T. Bell, L. M. Toth

Chemistry of actinides and fission products under conditions related to development of nuclear fuel cycles. Redox, photochemical, corrosion reactions; distribution coefficients. Demonstration of reversible (light-dark) photosensitive redox reaction in aqueous solution. Photochemistry of uranium and plutonium in selected aqueous solutions; application to separation method and to improvement of fuel reprocessing. Chemistry of gaseous fission products. Plutonium polymerization in nitric acid solutions.

143. FLOW THROUGH POROUS \$155,000 02-02  
BODIES  
J. S. Johnson, A. J. Shor

Transport of solutions through packed beds (ion-exchange kinetics), fluidized beds, hyperfiltration and ultrafiltration membranes, and cakes formed in filtration processes; flow instabilities arising from density, viscosity, and interfacial tension gradients in aqueous-hydrocarbon systems (enhanced oil recovery); mass transport effects on microbiological kinetics; impact on nuclear fuel production, waste processing, coal conversion processes; fossil fuel conversion.

## OAK RIDGE NATIONAL LABORATORY

Chemical Technology Division -02-

D. E. Ferguson - Phone: (FTS) 850-6051 or (615) 483-8611

144. MOLTEN SALT CATALYSTS FOR \$260,000 02-01  
 CLEAN FUEL SYNTHESIS  
 G. P. Smith, A. S. Dworkin,  
 J. Brynestad, L. O. Gilpatrick

Solvation and reactions of polycyclic aromatic hydrocarbons in molten halide hydrocracking catalysts, to determine reaction patterns and origins of catalytic activity. Solvent salts:  $SbCl_3$ ;  $AlCl_4^-$ -- $Al_2Cl_7^-$  with inert cations. Substrates contain 2 to 5 fused aromatic rings. Studies of possible salt-hydrocarbon complexation, conditions for protonated and radical cations from neutral molecules; applicability of cyclic voltammetry and electron spin resonance analyses to augment nmr, spectroscopy and quenching.

145. CHEMISTRY OF SELECTED \$110,000 02-01  
 FISSION PRODUCT ELEMENTS  
 J. C. Mailen

Basic data needed in development of nuclear reactor fuel reprocessing systems. Development of new chemical processes, solutions to problems arising in existing processes. Identification and study in solvent extraction organic phases of fission product complexes with complexes typically present or intentionally added. Characterization of insoluble particulates encountered in fuel dissolutions in order to mitigate resulting problems. Possible volatilizations during head-end operations. Investigation of techniques to preclude diversion of fissionable material, such as co-processing, seeding with strong gamma-emitters.

146. KINETICS OF ENZYME-CATALYZED \$110,000 02-01  
 PROCESSES  
 B. Z. Egan

Investigation of kinetics and enzyme catalysis related to hydrogen and ammonia production and energy production processes; catalytic processes for environmental control of waste effluents; hydrogen production from water (catalysts ferredoxin and hydrogenase) with thermal recycle of reducing substrate or by photooxidation; optimization of reaction rates; isolation, purification and immobilization of necessary enzymes; stabilization of enzymes and substrates; kinetics of redox reactions of ferredoxin.



OAK RIDGE NATIONAL LABORATORY  
Chemical Technology Division -02- (Continued)

150. WASTE STREAM PROCESSING                      \$225,000                      02-02  
STUDIES  
M. H. Lloyd, J. B. Knauer

Investigation of plutonium losses due to instabilities and solids formation in anticipated LWR reprocessing solutions; plutonium loss mechanisms include precipitates due to zirconium hydrolysis and zirconium-molybdenum and plutonium-molybdenum compound formation; plutonium stripping loss mechanisms in Purex process; formation of polymeric plutonium in reprocessing solutions.





OAK RIDGE NATIONAL LABORATORY  
Analytical Chemistry Division -02- (Continued)

154. MASS SPECTROMETRY R&D \$140,000 02-03  
FOR ORGANIC ANALYSIS  
W. T. Rainey, D. C. Canada,  
J. C. Franklin

Development of mass spectrometry and separations for identification and quantification of major, intermediate, and trace organic constituents in complex mixtures such as coal liquids and gases. Improved ion sources and associated components; instrumentation and software for data acquisition. MS50/DS50 system: ultra-high resolution, high sensitivity, exact mass measurement. Use of soft ionization techniques (field ionization, low-voltage electron bombardment, energy transfer ionization).

155. ADVANCED SPECTROSCOPIC \$200,000 02-03  
METHODOLOGY FOR CHEMICAL  
ANALYSIS  
L. D. Hulett, J. M. Dale,  
R. W. Shaw, L. Klatt

Development of spectroscopic methods applicable to ERDA programs; design and fabrication of laser-excited opto-acoustic spectrometer for coal and other (opaque, etc.) materials not amenable to conventional techniques. Rapid-scan spectrometry, initially for molecular absorption for liquid chromatography and atomic emissions for gas chromatography. Development of electron spectroscopy (ESCA, Auger, diffraction) for catalyst, corrosion and other energy-related problems. Two new electron spectrometers built for in situ surface studies. Absolute alloy analysis by x-ray fluorescence extended to other samples.

PACIFIC NORTHWEST LABORATORY  
 P. O. Box 999  
 Richland, Washington 99352

Chemical Technology Department -02-

R. E. Nightingale - Phone: (FTS) 444-7511 Ext. 946-2597 or (509) 946-2597

156. STUDY OF THE CHEMICAL BEHAVIOR OF COAL AND ITS RELATIONSHIP TO MODEL COMPOUNDS

\$120,000

02-01

J. R. Morrey, G. L. Tingey

Phenolic depolymerization of coal to identify important functional groups, define appropriate model compounds for coal conversion studies. Kinetics (solubility,  $^{13}\text{C}$  NMR) indicate depolymerization followed by slow repolymerization. Nitrogen, sulfur functional groups, current emphasis.

157. A FUNDAMENTAL INVESTIGATION OF HOMOGENEOUS CATALYTIC SYSTEMS FOR THE SYNTHESIS OF HYDROCARBONS FROM SYNTHESIS GAS

\$93,000

02-01

J. L. Cox

Investigation of the homogeneous catalytic synthesis of hydrocarbons and oxygenates from hydrogen and carbon monoxide; homogeneously catalyzed hydrogenation of coal with group VIII metals; carbonylation-decarbonylation reactions as possible reversible chain growth-shrinkage mechanisms; decarbonylation of formaldehyde; deoxygenation of carbon monoxide in the presence of polynuclear complexes.

158. THERMOCHEMICAL CONVERSION OF CELLULOSIC WASTES INTO LIQUID FUELS

\$117,000

02-01

T. F. Demmitt, P. M. Molton

Investigate chemistry of thermochemical processes for direct conversion of cellulosic materials into liquid fuels; determination of process variables on reaction chemistry and reaction product properties; conversion of aqueous cellulose slurries (with dissolved alkali materials) to liquid fuels; variation of oil yields and properties with temperature (300 to 365°C) and alkali addition; carbon monoxide addition not required to achieve liquefaction; mathematical modeling.



## PACIFIC NORTHWEST LABORATORY

Radiological Sciences Department -02-

N. E. Ballou - Phone: (FTS) 444-3061 or (509) 946-3061

161. COMBINED ATOMIC ABSORPTION- \$69,000 02-03  
MASS SPECTROMETRIC ANALYTICAL  
TECHNIQUES  
J. H. Kaye

Improvement of flameless atomic absorption and mass spectrometric trace analyses through correlation of emitted neutral atoms, ions, and molecular species with nature and temperature of emitting surface; investigation by simultaneous atomic absorption of neutral atoms and mass spectrometric analysis of ionized species.

162. ULTRASENSITIVE LASER-BASED \$60,000 02-03  
SPECTROMETRIC ANALYTICAL  
TECHNIQUES  
R. W. Gales

Development of ultrasensitive and selective laser-based analytical techniques for detection, identification, and measurement of trace substances; detection and identification of chemical forms; laser operating and measuring modes: fluorescence, absorption, cavity-amplified absorption, cavity-induced selective extinction, and coherent anti-Stokes Raman spectroscopy; frequency modulation techniques; digital and phase sensitive techniques along with photon source regulation and source compensation methods for sensitivity enhancement; frequency stabilization for selectivity enhancement.

163. ULTRASENSITIVE RADIOACTIVITY \$74,000 02-03  
SPECTROMETRIC ANALYTICAL  
TECHNIQUES  
F. P. Brauer

Development of ultrasensitive and selective radioactivity spectrometric techniques; exploitation of unique and extremely specific correlations between decay emissions; multiparameter nuclear spectrometric measurements of x-rays, gamma-rays, alpha particles, electrons, neutrons, and time relationships between decay events; improved data analysis, background reduction, and detector efficiency and selectivity; methods for in situ real-time determinations; impact on nuclear processing, waste management, nuclear safeguards, and environmental programs.



SANDIA LABORATORIES (LIVERMORE)  
Livermore, California 94550

Systems Development -01-

D. L. Hartley - Phone: (FTS) 469-2747 or (415) 455-7011

<u>167.</u>	COMBUSTION ANALYSIS BY ADVANCED RESEARCH METHODS	\$195,000	01-02
	W. T. Ashurst, R. J. Cattolica, R. A. Hill, D. R. Hardesty, R. J. Kee, J. A. Miller, L. A. Rahn, R. E. Setchell, R. E. Mitchell, J. R. Smith		

Advanced research methods, including laser-based diagnostics and new computational schemes, for application to research on combustion processes. Studies of flat flame kinetics and diffusion flame transport using laser Raman, Doppler, and fluorescence techniques; diffusion flame facility for combining several conventional and laser-based diagnostics for the study of turbulent reaction flow; models of those flames with finite rate chemistry and reasonable turbulent transport models. Development of advanced diagnostics including resonance scattering, nonlinear optical and multi-photon techniques.

SECTION B

Corporations  
Other Government Agencies  
Universities

The information was taken from current 200-Word Summaries provided by the contractors. There is considerable (about 10%) turnover in these research projects and some may not be continued beyond the current contract period.

## AEROCHEM RESEARCH LABORATORIES, INC.

201. HIGH TEMPERATURE PHOTOLYSIS                      \$60,000                      01-02  
 STUDIES OF COMBUSTION REACTIONS  
 A. Fontijn - Reaction Kinetics Group

A new program to measure the rate coefficients of combustion reactions over a wide temperature range, i.e., from about 1800 to 300 K (2800 to 100°F) or to as low a temperature as is of practical interest. Development of a new experimental technique, high temperature photolysis (HTP) which combines two individually well-tested techniques: (i) the high-temperature fast-flow reactor developed to study the kinetics of metal atom/oxide reactions over about the 300 to 1800 K temperature range and (ii) the photolysis technique used in many laboratories for kinetic measurements of combustion intermediates (free radicals), but only near room temperature. The initial experiments will concern the reaction of oxygen atoms with methane, a reaction of major interest and one that is also conducive to development of the HTP technique. Subsequent studies will concern reactions of increasing complexity, culminating in radical-radical reactions of higher hydrocarbon and oxidizer radical combinations.

## AEROSPACE CORPORATION

202. EXPERIMENTAL STUDY OF                      \$71,628                      02-02  
 IMPORTANT PARAMETERS IN  
 TWO PHOTON (TWO-STEP)  
 ISOTOPE ENRICHMENT  
 P. F. Zittel - Chemical Physics Department

Investigation of a two-photon isotope separation technique using an infrared laser to vibrationally excite molecules and an ultraviolet laser to photodissociate the excited isotopes; collection of photodissociation fragments by chemical reactions; theoretical model and experimental system for laser isotope separation of molecules containing <sup>79</sup>Br and <sup>81</sup>Br; mass spectrometric sampling system for monitoring products.

## BEND RESEARCH, INC.

203. COUPLED TRANSPORT MEMBRANES                      \$45,100                      02-02  
 FOR URANIUM SEPARATIONS  
 H. K. Lonsdale - President

The effect of the nature of the exchanger, the effect of diluents, the make up of the rate limiting effect, the nature of the coupled ion, and the effect of external conditions such as pH, ionic strength and desired and contaminating ion concentrations on the flux and selectivity of liquid membranes, which are made by filling the pores of a microporous solid with a water immisible organic liquid complexing agent. A basic parametric study including both cation and anion transport, however, it will concentrate at first on anion transport using principally uranium.



## GENERAL ELECTRIC COMPANY

204. PHOTO-INDUCED ELECTRON \$80,000 01-01  
TRANSFER REACTIONS ACROSS  
PHASE BOUNDARIES  
S. J. Valenty, G. L. Gaines - Chemistry  
Laboratory, Research and Development  
Center, Schenectady, N.Y.

Experimental studies of photo-induced electron transfer reactions of ruthenium complexes and related compounds in the presence of phase boundaries for the purpose of achieving useful charge separation. Preparation and characterization of Cr(III) analogs of Ru(bipy) complexes in both water soluble and surfactant forms; study of the luminescence quenching of Ru and Cr complexes as water soluble and surfactant derivatives in water and inorganic solvents; study of the luminescence quenching of surfactant complexes in monolayers at the air-water interface; transfer of monolayers to glass supports and study of luminescence on such films; testing of promising systems and configurations for their ability to dissociate water.

205. STUDY OF PHOTOCHEMICAL EFFECTS \$45,000 01-01  
USING STABLE SEMICONDUCTOR  
ELECTRODES  
R. H. Wilson, L. A. Harris,  
R. H. Wentorf, Jr. - Energy  
Sciences Branch, Research and  
Development Center, Schenectady, N.Y.

Studies in which a new technique for investigating layers of organometallic compounds will be evaluated. The material to be investigated will be deposited on the surface of stable semiconductor electrodes of known behavior. The semiconductor will be excited by light of sufficient energy to produce bandgap transitions and this energy will be transferred via minority carriers to the surface coating. Initially, previously investigated compounds, such as chlorophyll-a and ruthenium tris-bipyridyl, will be examined using lower energy light for comparison with previous results. The measurements will then be extended with the new techniques using higher energy light.

## STANFORD RESEARCH INSTITUTE

206. HIGH TEMPERATURE CHEMISTRY                      \$32,475                      02-01  
OF HYDROGEN PRODUCTION CYCLES  
D. L. Hildenbrand - Physical  
Sciences Division

This research consists of a study of the high temperature chemistry of a class of reactions which are common to a number of the more attractive thermochemical cycles for generating hydrogen; namely the decomposition of metal sulfates. This includes both kinetic and thermodynamic property experimental measurements. Of particular interest is the observation that small amounts of  $\text{Fe}_2\text{O}_3$  affect significantly the decomposition pressure of  $\text{MgSO}_4$ . The proposed research is expected to provide understanding of this catalyzed reaction which is relevant to the development of a viable sulfate cycle as well as pertinent thermodynamic values for the sulfates involved.

207. THERMODYNAMICS OF SULFUR                      \$55,000                      02-01  
ADSORBATES ON METAL CATALYST  
SURFACES  
H. Wise - Materials Research  
and Catalysis Laboratory

This research is to establish the upper limit of sulfur-bearing compounds in the gas phase, above which deactivation of a given catalyst begins and below which catalyst reactivation becomes feasible. The emphasis of this research is the measurement of the thermodynamic properties of the metal surface-gas interface for sulfur chemisorbed on supported iron, cobalt, nickel and copper catalysts as well as on selected single-crystal faces of these metals.





## UNIVERSITY OF ALABAMA

212. ELDOR INVESTIGATIONS OF RADIATION PROCESSES \$40,000 01-01  
L. D. Kispert, T. C. S. Chen -  
Chemistry Department

Role of a host lattice in determining the type and yield of radicals produced by x-irradiation of a crystalline material as a function of temperature; heavy atom substitution techniques, x-ray crystallography and magnetic resonance measurements, electron-electron double resonance (ELDOR), electron-nuclear double resonance (ENDOR), and electron spin resonance (ESR).

## UNIVERSITY OF ARIZONA

213. CHELATING EXTRACTANTS OF IMPROVED SELECTIVITY \$44,925 02-02  
H. Freiser - Department  
of Chemistry

Development of chelating extractants by application of pattern recognition techniques to the existing data base of metal chelate stability and extraction equilibrium constants; determination of extraction characteristics of selected alkylated 1,2-dihydroxybenzenes and salicylic and phenylarsonic acids with La(III), Th(IV), and U(VI); design of more selective reagents; use of high pressure liquid chromatography to determine fundamental extraction equilibrium and kinetic parameters.

## BAYLOR UNIVERSITY

214. RADIATION CHEMISTRY OF HIGH POLYMERS \$22,500 01-01  
M. Dole - Chemistry Department

Study of the kinetics of the radiation-induced crosslinking process of polyethylene by means of electron spin resonance measurements of the decay of the highly reactive free radicals produced by gamma radiation. Polyethylene treated so as to produce single crystals, extended chain crystals, etc.; kinetics of the decay in these different forms of the PE of the two different types of free radicals produced by the irradiation and by transformations subsequent to the irradiation interpreted in terms of a fast and a slow decay process, with or without diffusion control.

## BOSTON UNIVERSITY

215. INVESTIGATION OF THE \$52,974 01-01  
TRIPLET STATES OF  
CHLOROPHYLLS  
R. H. Clarke - Department of Chemistry

The characterization of the structures assumed by chlorophyll molecules upon aggregation in photosynthetic systems is important for an understanding of the mechanisms of energy conversion in photosynthesis. Since the properties of the excited triplet state of the pigment molecules, such as the electron distribution and excited state dynamics, are sensitive to the surrounding interactions and to the state of aggregation, triplet state properties, serve as a convenient (non-destructive) probe into the makeup of photosynthetic systems. Our research program utilizes optical detection of magnetic resonance spectroscopy to investigate the triplet state properties of the isolated molecule and solutions of aggregated chlorophylls. These measurements allow an evaluation of in vitro chlorophyll systems for structural features proposed as models for the antenna and reaction center of photosynthetic systems in vivo and for their general applicability as model systems for photosynthesis.

216. ELECTRON TRANSFER \$55,714 01-01  
REACTIONS OF EXCITED  
DYES WITH METAL COMPLEXES  
N. N. Lichtin, M. Z. Hoffman -  
Chemistry Department

Study of factors which determine the quantum efficiency of transfer of reducing equivalents between excited dye molecules and metal complexes in their ground state as well as other factors which determine the composition and dynamics of formation and decay of the photostationary state of such photoredox systems. Aspects of interest include structures of dyes and ground state reagents, photophysical properties of dyes, ground state redox potentials of dyes and metal complexes, sensitization, and the influence of solvent and solution composition on dynamic and steady state properties. Objective is to provide a rational basis for selecting photoredox systems for incorporation in photogalvanic solar cells; identify combinations of dyes, metal complexes, sensitizers and solution composition which possess properties consistent with efficient photogalvanic conversion of solar energy; laser flash photolysis; conventional flash photolysis; dynamics of photoredox reactions involving thiazine dyes and complexes of iron as well as of corresponding ground state back reactions.

## BOSTON UNIVERSITY (Continued)

217. ORGANIC PHOTOCHEMICAL STORAGE OF SOLAR ENERGY \$45,000 01-01  
G. Jones, II - Department of Chemistry

Study of organic photochemical reactions with the capability of converting solar energy into chemical energy: study of valence isomerization of hydrocarbon dienes induced by visible-absorbing photosensitizers which are electron acceptors; similar work with norbornadienes and visible-absorbing electron donors; study of luminescence quenching and its role in donor-acceptor interactions; role of charge transfer complexes in valence photoisomerization; reactivity of caged valence isomers in the presence of catalysts; development of photocalorimeter for measurement of heats of photoisomerization; use of photocalorimeter to get thermochemical data for unstable molecules.

## BRANDEIS UNIVERSITY

218. PHOTOCHEMICAL REACTIONS OF COMPLEX MOLECULES IN CONDENSED PHASE \$64,834 01-01  
H. Linschitz - Chemistry Department

Elucidation of the sources of inefficiency in photo-redox reactions involving electron or H-atom transfer to or from light-excited molecules. Laser flash photolysis and luminescence used to observe each stage of the overall redox process; reaction rates and products and intermediates yields allow identification of energy-storing and energy dissipating processes. Correlations made with solvent structure and polarity, redox potentials and nature of excited states. Test substances include metalloporphyrins, including chlorophyll, and aromatic ketones.

## BRANDEIS UNIVERSITY (Continued)

219. HYDROGEN TRANSFER AND CHARGE TRANSFER IN PHOTO-CHEMICAL AND RADIATION INDUCED REACTIONS  
S. G. Cohen - Chemistry Department
- \$33,834
- 01-01

Electron transfer and hydrogen transfer caused by absorption of ultraviolet or visible light are studied. Reaction of photoexcited carbonyl compounds with amines and other electron donors; sulfur compounds--mercaptans, thioethers and disulfides; quenching of excited carbonyl compounds. Quantitative study of quenching and formation of radicals from reaction of photoexcited carbonyl compounds and dyes with alcohols, amines and sulfur compounds, and on the effects of sulfur compounds in retarding and enhancing reactions in the other systems. Results will be compared with analogous systems subjected to high energy  $^{60}\text{Co}$  gamma radiation and to peroxides.

## BROWN UNIVERSITY

220. EXPERIMENTAL CHEMICAL KINETICS  
A STUDY OF CHEMICAL REACTIONS  
BY MEANS OF MOLECULAR BEAM  
TECHNIQUES  
E. F. Greene - Chemistry Department
- \$59,974
- 01-02

Inelastic scattering of atoms by diatomic molecules;  $\text{CsI} + \text{Ar}$  and  $\text{CsI} + \text{Xe}$  systems; study of effect in which at low densities neutral atoms and molecules are trapped by a beam of electrons and move preferentially parallel to its direction; details of the interaction; possible practical application in increasing the sensitivity of mass spectrometers and detectors for molecular beams. Measurements of angular distributions of atoms elastically scattered off of crystal surfaces to show features of the structure of the surfaces.



## UNIVERSITY OF CALIFORNIA/DAVIS

221. NUCLEAR METHODS IN CHEMICAL KINETICS \$55,000 01-01  
J. W. Root - Department of Chemistry

Experimental chemical kinetics investigations of low-energy fluorine and chlorine atom reactions with gaseous hydrocarbons and halogenated hydrocarbons. The information sought includes the relative rapidities of hydrogen abstraction and olefin addition reactions and the effect of temperature upon these relative reaction rates. An unusual aspect of this research is that radiotracer techniques are exclusively utilized in order to prevent the occurrence of severe experimental complications that would otherwise result from the extreme reactivities of atomic and molecular fluorine reagents.

## UNIVERSITY OF CALIFORNIA/IRVINE

222. INTERMOLECULAR ELECTRONIC ENERGY TRANSFER PROCESSES \$46,358 01-02  
E. K. C. Lee - Chemistry Department

Rates and mechanisms of energy transfer and storage involving molecular excited states which are important in energy conversion processes. Excitation of molecular vibrations and rotations accompanying an intermolecular electronic energy transfer process are investigated to determine the resulting energy distribution and hence establish the physical and chemical mechanisms. The involvements of chemical quenching, charge transfer complex, excimer/exciple formation, isotope effect, reactive intermediates, long and short range interactions, etc., will be studied by luminescence spectroscopy and chemical kinetics.

## UNIVERSITY OF CALIFORNIA/IRVINE (Continued)

223. RESEARCH IN CHEMICAL KINETICS                      \$187,500                      01-01  
F. S. Rowland - Department  
of Chemistry

Research on the photochemistry of chlorine compounds, particularly those found in the earth's atmosphere. Ultraviolet cross sections and reaction rates with  $O(^1D)$  atoms are being measured for many different halocarbons, and for subsequent decomposition products including  $CClFO$ ,  $CF_2O$ ,  $ClONO_2$  and  $BrONO_2$ . The photochemistry of  $ClONO_2$  is being studied at 302.5 nm. Heterogeneous decomposition reactions are also being studied for  $ClONO_2$  and other chlorinated species.

Fundamental reaction rate studies of chlorine atoms are being made with the radioactive  $^{38}Cl$  atoms thermalized by multiple collisions with  $CClF_3$ . Substrates for  $^{38}Cl$  reaction include several alkenes and alkynes and some organometallic compounds. Intramolecular chlorine atom shifts are being studied with  $C_3H_6Cl$  and  $C_3H_4Cl$ . The rates of hydrogen abstraction by  $^{38}Cl$  are being measured indirectly through competition with vinyl bromide. The method is being extended to 240-360°K.

Fundamental fluorine atom reactions are being investigated with  $^{18}F$  atoms. Substrates include alkenes and alkynes with emphasis on isotopic differences. The effects of radiation damage at high fast neutron flux are being studied.

Studies have been initiated on the reactions of energetic recoil tritium atoms with graphite and lithium chloride.

224. STUDY OF ISOTOPIC MASS                                      \$67,342                                      02-02  
EFFECTS IN CHEMISTRY  
M. Wolfsberg - Department  
of Chemistry

Investigation of isotopic mass effects via isotopic effects on corrections to Born-Oppenheimer approximation; complete wave equation of molecular system. Experimental vs theoretical isotope effects on equilibrium constants. Energy transfer in collisions. Statistical mechanical perturbation theory to elucidate factors influencing isotope effects on chemical equilibria and chemical kinetics.

## UNIVERSITY OF CALIFORNIA/LOS ANGELES

225. CHEMISTRY OF HYDROCARBON SOLIDS AT HIGH PRESSURES \$52,000 01-02  
M. F. Nicol - Chemistry Department

Effect of pressure on chemical properties, reactions, optical spectra, and photochemistry of hydrocarbons; solids and fluid solutions; the absorption spectrum of anthracene upon application of 30,000 atmospheres. Development of technology for studying extremely high pressures at very low and very high temperatures and for observing reactions on the picosecond time scale.

226. MECHANISMS OF ENERGY TRANSFER AND PHOSPHORESCENCE-MICROWAVE MULTIPLE RESONANCE TECHNIQUES \$62,069 01-02  
M. A. El-Sayed - Chemistry Department

Development and application of phosphorescence microwave double resonance (PMDR) to follow the path of energy flow in a molecule and thus determine the mechanism of the energy transfer processes involved in the intramolecular energy conversion. The method determines the direction of the spins of triplet molecules formed by energy transformation of the excited singlet states formed by light absorption. The method is applied to a number of aromatic hydrocarbons and their halogenated derivatives, nitrogen heterocyclics, and aromatic carbonyl compounds. The dependence of this conversion process on the type of electronic states involved, the molecular structure, the effects of vibrations and the solvents are all being examined.

227. MULTIHETEROMACROCYCLES THAT COMPLEX METAL IONS \$70,040 02-02  
D. J. Cram - Department of Chemistry

Studies to design, synthesize and evaluate cyclic organic compounds that selectively complex metal salts and solubilize them in organic solvents. These cyclic organic ligands are applicable to procedures for separating metal salts by differential distributions between water and organic solvents containing the ligands. The organic compounds possess charged cavities that match the sizes and charges of the metal ions they are designed to encapsulate. Compounds that will differentiate between actinides, lanthanides and the other products of spent reactor fuels are being sought.

## UNIVERSITY OF CALIFORNIA/RIVERSIDE

228. ION-ION CHARGE EXCHANGE PROCESS           \$33,187           01-03  
R. T. Poe - Department of  
Physics

Direct charge exchange between individual ions is expected to be the principal loss mechanism and limiting design factor in any heavy ion driven inertial fusion energy production scheme. Estimates are required of the direct charge exchange cross sections between singly ionized heavy elements in the keV energy range. This project supports calculations using a semiclassical impact parameter approach using independent particle basis functions. The method will be used to calculate charge exchange cross sections for singly charged ion species helium and lead in the 5-50 keV energy range and these results compared with those obtained by other methods.

## UNIVERSITY OF CALIFORNIA/SANTA BARBARA

229. METASTABLE RARE GAS                       \$40,942           01-02  
CHEMILUMINESCENT REACTION  
CROSS SECTIONS  
R. M. Martin - Department  
of Chemistry

Studies of the cross sections and emission spectra of metastable rare gas chemiluminescent and excitation transfer reactions; the reactions take place in crossed molecular beams under single collision conditions, permitting definitive identification of primary products. Initial emphasis on reactions of metastable krypton and xenon producing halide excimers with emission spectra in the visible and ultraviolet regions.

## UNIVERSITY OF CALIFORNIA/SANTA BARBARA (Continued)

230. THE DETAILED COMBUSTION OF SULFUR COMPOUNDS \$55,000 01-02  
H. P. Broida - Department  
of Physics

A quantitative spectroscopic investigation will be made of the role played by free radical sulfur intermediates in the combustion of sulfur bearing fuels.

Previous experimental difficulties will be overcome by applying new absorption and fluorescence techniques. The former of these is based on gain measurements of a radiating system when placed in a laser cavity and relates to the absorption in the system. By this means, absolute concentrations of  $S_2$ , SH and CS will be obtained for the first time in flames. In addition, the concentrations of S,  $S_2$ , SO, SH, CS, and  $SO_2$  will also be measured using recently developed fluorescence techniques. Being able to monitor some of the species by both techniques provides a powerful built-in self consistency check. Coupled to more conventional emission measurements of  $S_2$ , SO, SH, CS and the  $SO+O$  continuum, a measure of both ground and electronically excited state populations will emerge.

Studies will be made using two separate laboratory combustion systems designed for reduced pressure and atmospheric pressure flames. These currently available burners will be used to examine hydrogen and propane/air flames containing trace additions of  $H_2S$  or thiophen,  $C_4H_4S$ .

231. HOMOGENEOUS CATALYSIS OF THE WATER GAS SHIFT REACTION \$36,600 02-01  
P. C. Ford - Department of  
Chemistry

Studies of transition metal carbonyl compounds which may be suitable for use as homogeneous catalysts in supported liquid phase systems: investigations of homogeneous, solution phase catalysts for the production of hydrogen from water via the water gas shift reaction; exploratory studies to identify active systems; characterization of reaction kinetics and mechanisms; testing for practical application as a supported liquid bed catalyst in fixed bed flow reactors.

## UNIVERSITY OF CALIFORNIA/SANTA BARBARA (Continued)

232. MASS TRANSFER AND CHEMICAL REACTION OF GASEOUS SPECIES IN NON-CATALYTIC AND CATALYTIC POROUS MEDIA SUPPORTING CATALYTIC AND NON-CATALYTIC LIQUIDS

\$30,465

02-04

R. G. Rinker - Department of  
Chemical and Nuclear Engineering

Investigation of homogeneous organometallic catalysts dissolved in non-volatile liquids supported as thin films on porous solids; immobile catalyst with high contact area and free molecular motion; liquid partitioning agent for selective absorption of gaseous reactants; valence isomerization of quadricyclene to norbornadiene with cobalt tetraphenyl porphyrin catalyst dissolved in 1-chloronaphthene on alumina pellets; water-gas shift reaction; decomposition of formic acid vapor; steady-flow diffusion cell; impact on hydrogen production.

## UNIVERSITY OF CALIFORNIA/SANTA CRUZ

233. PHOTOINDUCED ELECTRON TRANSFER IN MIXED ORGANIC-INORGANIC SYSTEMS

\$38,029

01-01

G. S. Hammond - Division of  
Natural Sciences

Absorption of light by molecules produces electronically excited states. These excited states have much enhanced reactivity as electron acceptors and electron donors and react with other substances by electron transfer. The products of these photoinduced electron transfers are high energy substances. If the energetic products can be separated even briefly from each other it may be possible to cause them to undergo still further changes which will result in storage of the light energy in usable form. One form of storage might involve reaction of the high energy photo products with electrodes to produce photo-potentials and enable storage as electrical power. Studies of the efficiency of the primary electron transfer reactions, the efficiency of first-formal reaction products and the transport of high energy photoproducts to suitable electrodes are being pursued.

## CALIFORNIA INSTITUTE OF TECHNOLOGY

234. STUDIES IN CHEMICAL DYNAMICS \$128,275 01-01  
A. Kuppermann - Division of  
Chemistry

Study of molecular collisions: energy flow; determination of intermolecular forces and cross sections; energy-loss spectra; angular distribution of molecular photoelectrons; angular distributions in elastic, inelastic and reactive scattering. Study of the effect of photon energy on the photochemistry of important molecules including  $UF_6$ . The unifying goal of these studies is the understanding of the effect on a molecule of a collision with an electron, a photon, or another molecule.

235. APPLICATION OF ION CYCLOTRON \$40,000 01-01  
RESONANCE SPECTROSCOPY,  
PHOTOIONIZATION MASS  
SPECTROSCOPY AND PHOTOELECTRON  
SPECTROSCOPY TO STUDY THE  
PROPERTIES AND REACTIONS OF  
IONS IN GASES  
J. Beauchamp - Division of  
Chemistry & Chemical Engineering

Experimental methods of atomic and molecular physics, including ion cyclotron resonance spectroscopy, photoionization mass spectrometry and photoelectron spectroscopy; properties, reactions and photochemistry of metal ions and their complexes in the gas phase; transition metal ions; metal hydrides for information such as metal-hydrogen bond dissociation energies and the cross sections for photoproduction of atomic and molecular hydrogen. Ionic processes occurring in ultraviolet rare gas eximer lasers are characterized to facilitate complete modeling of these devices; data include parameters such as the ionization potential of  $KrF^*$  and the photodestruction cross sections of atomic and diatomic halogen anions. Photoelectron spectroscopy is being developed as a technique for detecting, characterizing, and monitoring transient species such as excited states and free radicals which are produced in high energy environments.

## UNIVERSITY OF CHICAGO

236. BASIC STUDIES OF ATOMIC DYNAMICS \$80,000 01-03  
U. Fano - Department of Physics

Quantum-physical study of the conditions that favor and control atomic shifts, i.e., chemical reactions. More specifically, studies of the joint motion of electrons around atoms, the joint motion which binds electrons into molecules and hence controls their rearrangements. Past studies have been concerned with atoms of helium and hydrogen molecules. A tentative interpretation of the mechanism by which electrons dislodge one another and thus loosen chemical bonds has been outlined; these ideas are not yet formulated into a mathematical theory.

237. SYNTHESIS, CHEMISTRY AND ANALYTICAL ACTIVITY OF COMPLEXES OF LANTHANIDE AND ACTINIDE METALS IN UNUSUAL OXIDATION STATES AND COORDINATION ENVIRONMENTS \$38,000 02-01  
W. J. Evans - Department of Chemistry

Investigations of the synthesis of several new classes of lanthanide and actinide complexes to enable development of a more comprehensive understanding of the f orbitals which should participate in unusual catalytical transformations specific to these metals. The research is directed toward the synthesis of low and zero valent metal complexes. Examination of the reductive chemistry of these metals to develop basic information concerning the interaction of the lanthanide and actinide metals in a variety of oxidation states with ligands such as phosphines, arsines, cyanide, isonitriles, silyls, stannyls, and olefins. Application of several modern synthetic inorganic reaction techniques including electrochemistry, metal atom vaporization, activated metal synthesis, and crown ether methodology. Elaboration of the reaction chemistry of the new molecular classes with particular emphasis on the potential of the low valent species to participate in new catalytic reactions, reactions for which no precedent exists in transition metal chemistry.





## UNIVERSITY OF FLORIDA

241. RADIATION CHEMISTRY OF \$42,000 01-01  
HYDROCARBON AND ALKYL  
HALIDE SYSTEMS  
R. J. Hanrahan - Department  
of Chemistry

Characterization of primary physical and chemical steps, as well as secondary chemical reactions, which lead to formation of observed products in the gamma or pulsed electron irradiation of simple gas phase systems; chemical analysis for net products in the presence and absence of reactive chemical additives (free radical scavengers); effect of physical variables such as pressure, temperature, and radiation dose; and comparison with other modes of activation (photolysis, electron bombardment in the mass spectrometer) in order to shed light on primary processes. Studies of the radiolysis of H<sub>2</sub>-CO mixtures as well as hydrocarbon-O<sub>2</sub> systems related to interest in synthetic fuels; radiolysis of chlorofluoromethanes is motivated by the atmospheric Freon problem, and studies of systems containing CF<sub>3</sub>I and CH<sub>3</sub>I are suggested by chemical laser work.

## FLORIDA STATE UNIVERSITY

242. RADIATION INDUCED EFFECTS \$46,000 01-01  
IN ORGANIC SYSTEMS  
R. H. Johnsen - Chemistry  
Department

Reactions of high energy species generated in events involving the absorption of energetic quanta, or fast moving charged particles; excited ions, excited molecular species, free radicals and hot atoms. Systems under study include (1) molecular ions of moderate complexity whose unimolecular dissociation characteristics depend on activation by collision with metallic surfaces. The role of molecular structure in determining the fragmentation pattern is of especial interest. (2) ordered and disordered solids which in the reactivity (rates and mechanism) of large free radical species is being investigated using a variety of esr techniques. (3) gas phase aromatic hydrocarbons whose reactivity with photochemically generated OH-radicals is being investigated using a combination of photochemical and mass-spectrometric techniques in a continuous flow system. Attention is focused on end-product analysis in order to allow better interpretation of existing kinetic data.

## GEORGE WASHINGTON UNIVERSITY

243. LANTHANIDE IONS AS SENSITIVE PROBES IN ENERGY TRANSFER AND ORGANIC PHOTOCHEMISTRY  
N. Filipescu - Department of Chemistry
- \$34,000
- 01-01

Mechanism of energy migration and properties of electronically excited sensitizers, lanthanide ions, competition between phototransformation and energy transfer. Methods of study: spectroscopy (UV-visible absorption and emission, electron spin resonance, nuclear magnetic resonance, time-lapse spectrometry). Points of interest: donor-acceptor energy level matching, rate constants of fundamental steps, dependence of energy transfer on donor-acceptor separation and orientation, electrostatic interaction, correlation of theoretical quantities with experiment. Rate constants for energy transfer for organic donor--lanthanide ion acceptor systems; statistical models for exchange transfer; rigid model molecules have been synthesized and the energy studied spectroscopically and photochemically; esr spectra of new long-lived free radicals were interpreted by use of computer simulation; spectral properties of many hydroxycarbocations and their photorearrangements; energy transfer between cations.

## UNIVERSITY OF GEORGIA

244. TRANSITION METAL CHEMISTRY UNDER HIGH CARBON MONOXIDE PRESSURE: AN INFRARED SPECTROSCOPIC STUDY OF CATALYSIS IN THE FISCHER-TROPSCH REACTION  
R. B. King, A. D. King - Department of Chemistry
- \$70,000
- 02-01

Development of transition metal compounds to catalyze the synthesis of hydrocarbons from carbon monoxide and hydrogen; high pressure infrared spectroscopic cell for reactions and product analyses; simulation of the gas mixtures used for the Fischer-Tropsch synthesis of hydrocarbons from coal; exploration and systematization of metal carbonyl chemistry at high carbon monoxide pressures for possible catalytic activity; study of cluster metal carbonyl carbides.

## UNIVERSITY OF GEORGIA (Continued)

245. FUNDAMENTAL STUDIES OF SEPARATION PROCESSES \$65,000 02-02  
L. B. Rogers - Department of Chemistry

Investigation of chromatographic systems at elevated temperatures and pressures; faster chromatographic methods for analyzing large molecules (polymers); determination of conditions for isolating vanadium impurities in petroleum crudes (catalyst poison in cracking and reforming operations). Investigation of factors that control the formation rate of deposits in geothermal brine heat exchangers.

246. A STUDY OF MECHANISMS OF HYDROGEN DIFFUSION IN SEPARATION DEVICES \$44,520 02-02  
M. H. Lee - Department of Physics & Astronomy

Quantum mechanical formulation of the diffusion of hydrogen through palladium in order to ascertain if the failure of the classical treatment is due to the large difference in mass between the hydrogen and palladium atoms.

## HARVARD UNIVERSITY

247. THEORETICAL STUDIES OF HIGHLY IONIZED SPECIES \$60,914 01-03  
A. Dalgarno, G. Victor - Harvard College Observatory

Development of ways of calculating from first principles the relevant properties of highly ionized atoms for which few experimental data are available; the method developed, relativistic random phase approximation, accounts for an important part of the electron-electron interactions in the ion and includes relativistic effects in a direct way; it is being applied to many important ionic species. For less highly ionized atoms, accurate calculations using a different method, the model potential method, are being carried out in order to obtain a good understanding of the accuracy of the RRPA theory. Transition probabilities and excitation frequencies and wavelengths obtained for several energy levels of essentially all the members of the helium, beryllium and magnesium isoelectronic sequences. A simple formula for extending charge transfer cross sections of highly ionized systems has been obtained. Theoretical studies to identify the most important atomic and molecular processes that affect the energy balance of an ionized plasma. Development of simple generally applicable formulas that can be used to extrapolate from experimental measurements to a wide range of atomic systems; recombination mechanisms, particularly in dissociative recombination, which is the main removal process of molecular ions in cool plasmas.

## HOWARD UNIVERSITY

248. THEORETICAL STUDY OF RADIATIVE INTERACTION AND ENERGY TRANSFER PROCESSES OF MOLECULAR AND ATOMIC SYSTEMS  
L.-Y. C. Chiu - Chemistry Department
- \$25,000                      01-02

Theoretical studies of rotational and vibrational energy transfer; cross sections for V-V energy transfer recalculated for the reaction  $N_2(v=0) + CO_2(001)$  by treating  $q_{max}$  ( $\sim 1/d$ ) as an adjustable parameter; preliminary results on vibrational overlap between  $c^3\pi_u(v=0)$  and repulsive  $b^3\Sigma_u^+$ ; hyperfine energy expression for vibronic state  $K = v_2 + 1$ .

249. LASER INDUCED PHOTOLUMINESCENCE SPECTROSCOPY STUDIES OF THE ENERGY DISTRIBUTION OF RADICALS FROM ATOM-MOLECULE REACTIONS  
W. M. Jackson - Chemistry Department
- \$36,022                      01-02

The vibrational and rotational distribution of radicals produced from the reactions of an atom with a stable molecule will be measured using a tuneable dye laser; atoms will be produced with a low intensity flash lamp and the signal detected with a photomultiplier tube and processed with a box car integrator.

250. KINETIC, MAGNETIC AND MÖSSBAUER STUDIES ON PORPHYRIN SYSTEMS  
P. Hambright - Department of Chemistry
- \$21,000                      02-01

Basic coordination chemistry of metal ion interactions with biologically and geologically occurring porphyrin-type molecules; mechanisms of metal addition, removal, exchange, electron transfer and ligation of the metal-porphyrin. Solid state metal complexes interacting with gases ( $O_2$ ,  $N_2$ ,  $CO$ ,  $SO_2$ ) are probed by magnetic and Mössbauer means. Mechanisms of removing vanadium and nickel porphyrins from oil are studied, in order to give petro-catalysts longer lifetimes. The possibility of using such thermally stable metal-ligand species as efficient catalysts are being explored, as well as much new chemistry on unusual second and third period metals and oxidation states.

## UNIVERSITY OF ILLINOIS/CHICAGO CIRCLE

251. MEASUREMENT OF GAS PHASE REACTION RATES \$39,780 01-02  
 R. J. Gordon - Department of Chemistry

Study of hydrogen atom exchange reactions,  $D + HX \rightarrow H + DX$  using flash photolysis with resonance fluorescence and laser absorption detection. The effect of vibrational excitation of HX on the reaction rate will also be studied. Study of the reaction of NO with ozone.

## UNIVERSITY OF IOWA

252. THE DISTRIBUTION OF ENERGY IN BIMOLECULAR CHEMILUMINESCENT REACTIONS INVOLVING HYDROGEN \$42,000 01-01  
 W. C. Stwalley - Chemistry Department

Study of chemiluminescent reactions involving hydrogen atoms; light emitted observed under high vacuum conditions; result of single (rather than multiple) collisions; wavelength analysis allows one to infer the molecule which emitted the light and the condition of its energy (i.e., the amount of energy tied up in the vibration and the rotation of its atoms and the amount tied up in chemically bonding electrons). A unique 25,000°K intense source of fast hydrogen (H) atoms has been developed and characterized to provide hydrogen atoms with various high velocities. Collisions of these fast H atoms with lithium (Li, Li<sub>2</sub> and Li-coated surfaces) have been observed to produce light throughout the visible region. Species emitting the light include high energy states of Li atom and of the molecules Li<sub>2</sub> and LiH.

## JOHN HOPKINS UNIVERSITY

253. FAR INFRARED CHEMICAL LASERS \$55,000 01-01  
 D. W. Robinson - Chemistry Department

Rates and mechanisms of chemical reactions in which the energy evolved is specifically located in certain dynamic modes of the products: electronic, vibrational, rotational; inversion of equilibrium energy distributions, chemical lasers; OH + Ar, HCN + CO systems.

## JOHN HOPKINS UNIVERSITY (Continued)

254. STUDIES IN HOT ATOM AND RADIATION CHEMISTRY \$60,000 01-01  
W. S. Koski, J. J. Kaufman -  
Chemistry Department

Kinematics and dynamics of positive ion reactions such as  $Cl^+$ ,  $B^+$  and  $Br^+$  with molecular hydrogen;  $Cl^+(H_2,H)ClH^+$ ; reactivity of the ground state and first excited state of the ions; factors that determine the position of the limiting value of the translational exoergicity in the reactions  $F^+(H_2H)FH^+$  and  $C^+(H_2,H)CH^+$ ; internal energy distribution in the  $CH^+$  product.

## UNIVERSITY OF KANSAS

255. STEREOELECTRONIC PROPERTIES \$65,000 01-01  
AGGREGATED CHLOROPHYLL  
SYSTEMS  
R. E. Christoffersen, G. M. Maggiora -  
Chemistry Department

Quantum mechanical studies of electronic structural features (both for ground and for excited states) of isolated chlorophyll and related molecules; examination of the structure of and forces responsible for the formation of dimeric chlorophyll systems.

## KANSAS STATE UNIVERSITY

256. ATOMIC PHYSICS WITH \$350,000 01-03  
HIGHLY IONIZED IONS  
P. Richard, J. R. MacDonald -  
Physics Department

Use of monoenergetic ions in a pure charge state from a Van de Graaff accelerator to study processes of charge exchange (electron loss and electron capture) and ionization for gas targets as a function of the important parameters which include charge state, energy, atomic number and collision distance (impact parameter). These processes are also being investigated in solid targets and, in particular, the charge state fractions of the ions and x-ray yields of the target material are being obtained as a function of the distance into very thin foils (1-500  $\mu g/cm^2$ ). These results are important for the proper interpretation of x-ray cross sections obtained from heavy ion-atom collisions in solid samples. The primary process of radiative decay is being investigated with high resolution x-ray spectrometers in order to deduce the final stages of the collision, the fluorescence yields and the state of polarization of the emitted radiation.

## LOUISIANA STATE UNIVERSITY

257. THEORETICAL STUDIES OF EXCESS                    \$42,862                    01-01  
ELECTRONS IN FLUIDS  
N. R. Kestner - Department  
of Chemistry

Theoretical studies and formulation of models for the trapping of electrons in fluids; testing of the models against experimental data. The studies will treat, sequentially, pure solvents, fused salts, mixed solvents and, finally, electron transfer reactions leading to solvated electrons. The methods are those of ab initio and semiempirical quantum chemistry.

258. ELECTRON EXCITATION CROSS                    \$51,657                    01-03  
SECTIONS FOR MULTIPLY  
CHARGED IONS  
J. Callaway, R. J. W. Henry -  
Department of Physics & Astronomy

Theoretical calculations of the cross sections for excitation of positive ions of the lithium and helium isoelectronic sequences by electron impact. The energy range considered is from the threshold for excitation to (roughly) 4 times the ionization energy. Cross sections for the electron impact excitation of  $C^{3+}$  and  $Ar^{15+}$  using a 5 state close coupling expansion and the non-iterative integral equation method of Smith and Henry; electron energies up to three times the threshold energy. Pseudo-state calculation for  $He^+$  in which 1s, 2s, 3s and 3p functions are included in a close coupling expansion; 1s  $\rightarrow$  2s excitation.

## MARQUETTE UNIVERSITY

259. SOLID PHASE CATALYSTS                    \$40,000                    02-01  
AND REAGENTS  
S. L. Regen - Department  
of Chemistry

The proposed research is concerned with the development of efficient catalytic methods for accelerating aqueous phase-organic phase reactions and to develop polymer resins which will provide a high degree of selectivity to synthetically important catalysts and reagents. Particular interest is in the development of the triphase catalysis principle. The principal goals of this phase of the work are: (1) developing new forms of solid-phase catalysts, (2) exploration of possible synthetic applications and (3) examination of the detailed nature of the microenvironment within the resin-catalysts. A particular emphasis of these studies addresses the selectivity of these catalyst systems.



## UNIVERSITY OF MARYLAND

260. RADIATION-INDUCED EFFECTS IN POLYMERS AND RELATED COMPOUNDS \$60,000 01-01  
 J. Silverman - Laboratory for Radiation & Polymer Science

Irradiation of acrylamide-polyethylene and of methacrylonitrile-polyethylene systems to determine the possible sensitization of crosslink formation; measurement of free radical migration in irradiated single crystal alkanes; measurement of the drift mobility of fast negative carriers in irradiated CS<sub>2</sub>-solutions; measurement of the effect of the filler content on the gel fraction of irradiated polyethylene-filler systems; pulse radiolysis of styrene solutions.

261. NON-DESTRUCTIVE DETERMINATION OF TRACE ELEMENT CONCENTRATIONS \$111,000 02-03  
 W. B. Walters, G. E. Gordon, W. H. Zoller - Department of Chemistry

Development of a neutron-capture gamma-ray spectrometer to determine trace-element concentrations in a wide variety of samples; utilization of a large-volume, high-resolution germanium (lithium) detector with a split annulus Compton suppression pair spectrometer; emphasis on high sensitivity and automatic data analysis.

## UNIVERSITY OF MASSACHUSETTS

262. DYNAMICS OF, AND HEAT AND MASS TRANSFER IN, AN INDUCTION PLASMA \$37,360 02-03  
 R. M. Barnes - Department of Chemistry

Steady state solution of the fluid dynamics, transport of heat and mass and the particle dynamics of an induction plasma by formulating the solution from the general equations of transport of momentum, energy and mass and the Maxwell's equation of electromagnetic induction.

## MASSACHUSETTS INSTITUTE OF TECHNOLOGY

263. PHOTOCHEMICAL ENERGY STORAGE: \$56,114 01-01  
STUDIES OF INORGANIC  
PHOTOASSISTANCE AGENTS  
M. S. Wrighton - Department  
of Chemistry

Photoinduced oxidation-reduction chemistry at solid-liquid interfaces; factors controlling rates of photoinduced interfacial electron transfer; evaluation of such primary processes in storage of optical, including solar, energy. Photoinduced charge-transfer processes occurring at irradiated semiconductor electrode-electrolyte interfaces; surface-localized energy levels and electron transfer rate under variable conditions; role of energetics and kinetics in controlling whether given photochemistry occurs.

264. THEORY OF CHEMICAL KINETICS \$47,000 01-02  
J. Ross - Department  
of Chemistry

Research on the prediction of the dynamics of reactive collisions: reaction cross sections, disposition of exoergicity of the reaction which is of importance in the formation of energy-rich molecules, relation of reactivity to structure and complexity of the reactants. Search for well-posed approximations to formal collision theory and development of simple theoretical expressions which readily give the dependence on masses (isotope effects), on features of the potential surface, and on properties of reactants and products (vibrational frequencies, etc.); utility of generalized Franck-Condon factors in chemical reactions and energy transfer problems; reactions proceeding by direct interactions, complex formation, and electronic curve crossings; effect of symmetry on heterogeneous (surface) reactions and on reactions in the presence of external fields. Cooperative processes in potentially unstable chemical systems investigated in the rates of growth of colloidal particles.

## MASSACHUSETTS INSTITUTE OF TECHNOLOGY (Continued)

265. PHOTOIONIZATION AND FIELD IONIZATION OF HIGHLY EXCITED ONE- AND TWO-ELECTRON ATOMS \$80,000 01-03  
D. Kleppner - Department of Physics

Experimental studies of the structure of highly excited (Rydberg) states of one and two electron atoms in high electric fields; photoionization processes in atomic species close to their ionization limits. Such species exhibit relatively long lifetimes (compared to those atoms excited in lower levels of excitation) and offer unique opportunities to probe atomic structure and electron correlation phenomena.

## MICHIGAN STATE UNIVERSITY

266. ELECTRON SPIN RESONANCE STUDIES OF RADIATION EFFECTS \$37,000 01-01  
M. T. Rogers - Department of Chemistry

Radiation damage in various classes of organic and inorganic solids produced by  $\gamma$  rays, x rays and ultraviolet light; paramagnetic fragments or defects so identified by ESR and the ESR parameters are used to determine the molecular and electronic structures of the radicals. Temperature and time dependence of the ESR spectra to determine the stability of radicals, their structural and conformational changes, and their chemical reactions; paramagnetic species which are interesting structurally but cannot be prepared chemically in macroscopic quantities. Quantum chemical calculations of radical geometries and electron distributions. Organic materials investigated include carboxylic acids, amides, aliphatic halocarbon derivatives and alicyclic compounds. Inorganic materials studied are metal fluorides, oxyfluorides and cyanides and their paramagnetic products include metals in unusual valence states, excess-electron radicals and hole species; prediction of the nature of radiation damage in non-metallic materials.

## MICHIGAN STATE UNIVERSITY (Continued)

267. PROPERTIES OF SOLVATED ELECTRONS, \$42,000 01-02  
ALKALI ANIONS AND OTHER SPECIES  
IN METAL SOLUTIONS AND KINETICS  
OF CATION AND ELECTRON EXCHANGE  
REACTIONS

J. L. Dye - Chemistry Department

Solvated electrons produced by active metals such as sodium dissolved in amines and ethers; formation of alkali metal anions; organic "cage-type" molecules to trap the positive ions and isolate solid compounds which contain alkali metal anions which behave as semiconductors. Properties of solvated electrons and alkali metal anions and their potential as reducing agents for chemical synthesis. Conversion of light energy into solvated electrons by the sodium anion in solution; absorption of light by metal anions in solid salts; electrical energy from light energy by using these newly developed compounds.

## UNIVERSITY OF MINNESOTA

268. THE CONTRIBUTION OF ELECTRONICALLY \$70,000 01-01  
EXCITED STATES TO THE RADIATION  
CHEMISTRY OF ORGANIC SYSTEMS

S. Lipsky - Department  
of Chemistry

Photophysical properties of organic molecules that have relevance in determining their radiation-chemical and photochemical behavior: measurement of rates at which very highly excited electronic states of simple aromatic molecules non-radiatively dissipate their energy via cascade to lower electronic states and determination of the influence of the molecular environment on the magnitude of these rates; characterization, by fluorescence spectroscopy, of the lowest excited states of saturated hydrocarbons in order to understand the important influence of rather minor structural modifications on the photostability of these molecules; electron-impact spectroscopy to locate the energies of triplet states of these molecules to better predict the involvement of such states in photochemical processes and in the process of energy migration in the liquid phase of these molecules; measurement of the energy required to eject an electron from a molecule in a condensed phase and study of the influence of the nature of the solvent to alter this energy and to alter the overall efficiency of the ionization process. Absorption and emission properties of molecular Rydberg states under heavily perturbed conditions such as exist in a high pressure gas or liquid phase.

## UNIVERSITY OF MINNESOTA (Continued)

269. STUDIES IN CHEMICAL REACTIVITY \$45,000 01-01  
R. W. Carr, Jr. - Department  
of Chemical Engineering &  
Materials Science

Rates and mechanisms of hydroxyl radical reactions occurring in or related to both combustion and to pollution in the earth's atmosphere; reaction of hydroxyl radicals with propylene by steady-illumination photolysis methods. Fate of  $\text{CFCl}_2$  and  $\text{CF}_2\text{Cl}$  radicals produced when the parent species react with hydroxyl radicals in the lower atmosphere. The final environmental disposition of the chlorine and fluorine; removal of energy from highly energetic polyatomic molecules by collisions; collisional deactivation of methylcyclobutane and ethylcyclobutane by cyclobutane and cyclohexane.

270. REACTIONS OF IONS WITH ATOMIC AND MOLECULAR FREE RADICALS \$34,000 01-02  
W. R. Gentry - Chemistry  
Department

Studies of the microscopic reaction dynamics in collisions of ions with atomic and molecular free radicals, importance of electronic non-adiabaticity in chemical reactions.  $\text{H}_2^+ + \text{C,N,O,F} \rightarrow \text{CH}^+ + \text{H}$ , etc. systems, relative kinetic energy from  $\sim 0.002$  eV to  $>20$  eV, using a merged molecular beam apparatus.  $\text{D}_2^+ + \text{X} \rightarrow \text{DX}^+ + \text{D}$ , systematic variations of the reaction dynamics in the series  $\text{X} = \text{C,N,O,F}$  elucidates the reaction mechanisms.

271. CONTINUOUS CHEMICAL REACTION CHROMATOGRAPHY \$26,065 02-02  
R. Aris, R. W. Carr, Jr. -  
Department of Chemical Engineering  
& Materials Science

Investigation of a chromatographic reactor with superior product yields and continuous operation; achievement of enhanced chemical reaction yields by chromatographic separation of the products and reactants; demonstration of continuous gas chromatography with radial flow in a rotating disc; combination of convection and adsorption in design, construction, and testing of a reactor to test predictions of the theory using reactions favored by chromatographic conditions.

## UNIVERSITY OF MINNESOTA (Continued)

272. PHOTO-INDUCED CATAPHORETIC ISOTOPE SEPARATION \$69,934 02-02  
J. A. Carruthers, L. M. Chanin,  
H. J. Oskam - Department of  
Electrical Engineering

Experimental investigation of isotope separation feasibility by a radiation-induced cataphoretic segregation process in gaseous discharges; resonance excitation and subsequent ionization by electrons; separation measurement of neon isotopes using a neon 0.63  $\mu$  laser and mercury isotopes using monoisotopic resonance lamps; light-spectrometer techniques.

## UNIVERSITY OF MISSISSIPPI

273. THE RADIATION CHEMISTRY OF PLASTIC CRYSTALS \$33,456 01-01  
T. J. Kligen - Chemistry  
Department

Radiation chemistry of the carboranes, adamantanes and organometallic carbonyls in the plastic crystalline solid state; development of a modified diffusional model of the radiation chemistry to fit the liquid-like nature of this solid state of matter. Study of the radiation chemistry of a homologous series of compounds exhibiting the plastic crystalline state; determination of the effect of radiation on the electro-optical properties of various plastic crystals; investigation of the diffusion of radiation-induced impurities in the plastic crystalline state using the positron probe technique.

## UNIVERSITY OF MISSOURI/ST. LOUIS

274. OBSERVATION OF LUMINESCENT SPECTRA IN LOW ENERGY ION-NEUTRAL COLLISIONS \$47,000 01-02  
J. J. Leventhal - Physics  
Department

Internal excitation energy of atoms and molecules produced in low energy molecular collisions by observing luminescence emerging from a collision cell containing neutral molecules, into which a beam of positively charged atoms or molecules is directed; spectral distribution of the collision-produced luminescence yields microscopic details of the collision process since only single ion-molecule encounters occur in the collision cell. Determination of internal energy stored in the molecular collision products and the partitioning among the available molecular internal energy levels; efficiency of the conversion of kinetic to internal energy.



## UNIVERSITY OF NEBRASKA/LINCOLN (Continued)

277. PHOTOIONIZATION OF ATOMS                      \$59,700                      01-03  
J. A. R. Samson, A. F. Starace -  
Department of Physics & Astronomy

Experimental and theoretical study of atomic photoionization processes; cross sections in the vacuum ultraviolet region; effects of electron correlation and of spin-orbit interaction on atomic photoionization processes. Measurement and/or calculation of total and partial photoionization cross sections, photoelectron branching ratios and angular distributions, and multiple ionization cross sections either over an energy region of a few Rydbergs above threshold or over the narrow energy region of an autoionizing resonance; rare gases and open-shell atoms. Theoretical study of photoionization of hydrogen-like atoms in high laboratory magnetic fields. Rotatable vacuum UV polarizer and fixed electron energy analyzer, measure the photoelectron angular distribution of atomic oxygen at 584 Å; rotatable 127° electron energy analyzer for measurements of photoelectron angular distributions at other wavelengths. Measurements of photoelectron branching ratios across an autoionizing resonance. Construction of a photoionization mass spectrometer system to measure multiple photoionization cross sections.

278. CHARGE TRANSFER CROSS SECTION                      \$31,807                      01-03  
DETERMINATIONS IN HEAVY ION-  
HEAVY ION COLLISIONS  
J. H. Macek, G. Gallup - Department  
of Physics & Astronomy

Direct charge exchange between individual ions is expected to be the principal loss mechanism and limiting design factor in any heavy ion driven inertial fusion energy production scheme. Estimates are required of the direct charge exchange cross sections between singly ionized heavy elements in the keV energy range. This project will use the molecular perturbed stationary state approximation method to calculate charge exchange cross sections. The study will assess the need to take into account metastable, intermediate charge states. Results of this technique will be compared with those obtained by other procedures.





## CITY UNIVERSITY OF NEW YORK/BROOKLYN COLLEGE (Continued)

282. STUDIES OF CARBON ISOTOPE FRACTIONATION \$72,880 02-02  
 T. Ishida - Department  
 of Chemistry

Investigation of producing enriched isotopes efficiently and economically; isotope separation factors by reversible processes; correlation of molecular properties with isotope enrichment process efficiencies; measurement of low temperature vapor pressure differences of carbon -13 and -12 compounds; measurement of carbon isotope separation factors; optimization of the design and operation of isotope enrichment plants.

## STATE UNIVERSITY OF NEW YORK/BUFFALO

283. STUDY OF DYE LASER INTRACAVITY ABSORPTION AS A DETECTOR OF LOW DENSITY SPECIES \$35,300 01-02  
 G. O. Brink - Department  
 of Physics

The technique of dye laser intracavity absorption (ICA) will be investigated as a possible tool for studying combustion processes. An ICA instrument will be constructed, then used in preliminary work to study low concentrations of atoms and molecules. Finally real combustion systems will be studied if the preliminary studies are successful.

## NORTHWESTERN UNIVERSITY

284. THEORETICAL STUDIES ON HETEROGENEOUS COMBUSTION \$32,000 01-02  
 C. K. Law - Department of Mechanical  
 Engineering & Astronautical Sciences

Study of the various heterogeneous processes occurring within vaporizing/combusting fuel sprays in the hot, oxidizing environments of various forms of liquid-fueled combustors. The approach is theoretical and will involve (1) the vaporization, ignition, deflagration, and extinction of individual fuel droplets in a reactive fuel/oxidizer environment; and (2) the vaporization of the droplet ensemble within a spray jet. The fundamental questions to be addressed are (1) the relative importance of premixed versus diffusional burning; (2) the relative importance of homogeneous versus heterogeneous burning; (3) the possible non-existence of the individual droplet combustion mode within the spray; and (4) the ignition and extinction criteria of the various droplet burning modes.

## NORTHWESTERN UNIVERSITY (Continued)

285. THE PROPERTIES OF SUPPORTED METAL CATALYSTS \$80,000 02-01

J. B. Butt - Department of Chemical Engineering, R. L. Burwell - Department of Chemistry, J. B. Cohen - Department of Materials Science & Engineering

Chemical preparation of metal catalysts; detailed characterization of platinum, palladium, and rhodium catalyst particles and their alloys which are supported on alumina and silica; evaluation of catalytic properties by study of isotope exchange hydrogenolysis and hydrogenation reactions; elucidation of the role that the metal particle size and morphology play in determining catalytic properties.

## OHIO STATE UNIVERSITY

286. KINETICS OF IONIZING RADIATION INDUCED REACTIONS \$52,000 01-01

R. F. Firestone - Department of Chemistry

Chemical and physical mechanisms for formation and destruction of excited rare gas atoms and molecules in rare gases subjected to pulsed high energy electron beams. Procedure consists of (i) passage of electron beam through gas sample for one hundred millionth of one second, (ii) passage of beam of white light through sample for one thousandth of one second following (i), (iii) measurement of light absorbed and/or emitted by excited atoms and molecules. Measurements indicate nature of and provide details of chemical and physical reactions in the rare gas samples. Electron beam generation of highly excited rare gas atoms and atomic ions; secondary reaction population of lowest-lying excited manifold of atomic levels (Paschen 1s); reaction via collisional mechanisms to form the laser molecular level. Efficiency of formation of laser level molecules dependence upon rare gas pressure and purity of sample at pressures in 100 to 1000 torr range.

287. PULSE RADIOLYSIS STUDIES OF FAST REACTIONS IN MOLECULAR SYSTEMS \$70,627 01-01

L. M. Dorfman - Chemistry Department

Chemical kinetics of elementary processes in molecular systems studied by pulse radiolysis; mechanisms by which chemical and biological effects are produced by ionizing radiation. Formation and reactivity of organic molecular ions in solution, with special reference to carbonium ions and carbanions. Rates and mechanism of electron transport in redox proteins; specific rate and mechanism of carbon monoxide uptake by hemoglobin.

## UNIVERSITY OF PENNSYLVANIA

288. ANISOTROPIC INTERMOLECULAR                      \$38,000                      01-02  
INTERACTIONS AND ROTATIONAL  
ORDERING IN HYDROGEN  
CONTAINING SOLIDS  
D. White - Department of Chemistry

Experimental and theoretical studies of the macroscopic and microscopic behavior of molecular crystals including dynamical processes important in energy transfer: molecular hydrogens and other simple diatomic hydrogen-containing molecules, mixtures of ortho-para species in the solid hydrogens, impurity and isotope effects. Experimental techniques include measurements to 100 millidegrees Kelvin utilizing a  $^3\text{He}$ - $^4\text{He}$  dilution refrigerator: thermodynamic measurements, pulsed NMR and optical Raman studies.

289. THERMOCHEMICAL PROCESSES                      \$71,535                      02-04  
FOR HYDROGEN PRODUCTION  
BY WATER DECOMPOSITION  
D. D. Perlmutter, A. L. Myers -  
Department of Chemical &  
Biochemical Engineering

Investigation of mass and heat transfer processes, with and without chemical reactions. Involves heat transfer models derived and tested on experimental rotary reactors for solid decomposition process steps; effect of surface renewal of solids on mass transfer; and catalysis by selected additives. These studies are related to thermochemical hydrogen systems including hybrid cycles which combine low-voltage electrolysis and high temperature endothermic reactions.

## PENNSYLVANIA STATE UNIVERSITY

290. THE RADIATION CHEMISTRY                      \$46,821                      01-01  
OF VOLATILE SILANES AND  
GERMANES  
F. W. Lampe - Department  
of Chemistry

Chemical reactions that are initiated by the passage of radiation through systems containing volatile organo-silicon and organo-germanium compounds. Irradiation by gamma rays; chemical analysis of the products formed under various conditions of pressure and energy-deposition rate results in a picture of the overall chemical conversions induced by the radiation. Detailed reactions and properties of ions and free-radicals derived from silicon and germanium compounds investigated concurrently in photochemical and mass spectrometric experiments.

## PENNSYLVANIA STATE UNIVERSITY (Continued)

291. OSCILLATOR STRENGTHS FOR HIGHLY IONIZED ATOMIC SYSTEMS \$45,000 01-03  
C. F. Fischer - Computer Science Department

Theoretical study of trends in and calculation of oscillator strengths for atomic systems with one or two electrons outside closed shells, including electron correlations, spin-orbit interactions, and relativistic effects. Focus is on those atomic species of special interest as contaminants in fusion plasmas - lithium and copper isoelectronic sequences.

292. CRYSTALLITE SIZE AND SUPPORT INTERACTIONS ON CO HYDROGENATION \$55,000 02-01  
M. A. Vannice - Department of Chemical Engineering

This research deals with the ultimate development of more effective catalysts for synthesizing hydrocarbons from  $H_2$  and CO. One objective of the proposed research is to understand the relationship between (1) the catalytic metal crystallite size and (2) metal-support interactions on the reactivity of the surface for the  $H_2 + CO$  synthesis reactions. Of particular interest is the relationship between product selectivity and the CO adsorption bond strength. This work is relevant to methanation reactions; however, the emphasis is to minimize  $CH_4$  formation and maximize the production of olefins and chemical intermediates.

## UNIVERSITY OF PITTSBURGH

293. MICROWAVE-OPTICAL DOUBLE RESONANCE SPECTROSCOPY \$45,000 01-02  
D. W. Pratt - Department of Chemistry

Structure of matter and its interaction with radiation through the exploration of new physical and chemical phenomena; short-lived chemical species produced by irradiation of solids with x-rays,  $\gamma$ -rays, and ultraviolet light, and include electronically-excited molecules, free radicals, and collective excitations in solids; optical detection of magnetic resonance spectroscopy.

## UNIVERSITY OF PITTSBURGH (Continued)

294. CHARGE EXCHANGE COLLISIONS OF HIGHLY STRIPPED IONS WITH ATOMIC HYDROGEN \$85,000 01-03  
 J. E. Bayfield - Department of Physics & Astronomy

Experimental studies of charge exchange processes between highly stripped ions and between ions and atomic hydrogen. Charge exchange measurements required to assess impurity radiation loss mechanisms and auxiliary neutral beam plasma heating effectiveness in magnetic fusion systems. Charge exchange cross section measurements between carbon, nitrogen, and oxygen ions with charge state plus two to plus six and between these ions and atomic hydrogen using Oak Ridge National Laboratory and University of Pittsburgh accelerator facilities.

## PRINCETON UNIVERSITY

295. INELASTIC MOLECULAR COLLISIONS- APPLICATIONS OF THEORETICAL METHODS TO PROBLEMS IN RELAXATION PHENOMENA AND LASER OPERATION \$28,704 01-02  
 H. Rabitz - Department of Chemistry

Aspects of molecular collision phenomena; new theoretical methods capable of handling realistic collision problems; variationally based decomposition methods along with effective Hamiltonian-type techniques; vibrational relaxation of HF; rotational state participation in vibrational relaxation. Modeling of HF lasing under various experimental conditions. Analysis of key physical factors controlling various types of collision behavior; temperature and quantum number scaling of vibration-vibration exchange rates. Chemical reaction theory based on a combination of decomposition methods and special channel coupling techniques; multichannel reactive cross sections.

296. NOVEL ENERGY SOURCES AND ENERGY CONSERVATION PROCESSES BASED ON CATALYSIS \$79,603 02-01  
 J. Turkevich - Department of Chemistry

Development of supported catalysts for petroleum refining, chemical processing, and cleanup of automotive exhausts; synthesis of uniform-sized particles of platinum, palladium, and gold; adherence of catalysts on supports of uniform size and shape; characterization of catalysts in solution form by absorption spectroscopy, ultracentrifugation, light scattering, transmission electron microscopy, and in solid form by electron microscopy, gas chemisorption, poisoning of active centers and catalytic activity.

## PURDUE UNIVERSITY

297. FLASH PHOTOELECTROCHEMICAL STUDIES OF TRANSIENT ELECTRODE PROCESSES  
S. P. Perone - Department of Chemistry

\$57,568

01-01

Photochemical, electroanalytical and spectroscopic studies of the transient phenomena which are characteristic of three types of processes at electrode/solution interfaces, having potential value in solar energy conversion. The three types are photoemission of electrons, photolytic oxidation/reduction of excited species and photosensitized electrolysis at semiconductor electrodes. Formation of solvated electrons when a metallic electrode/solution interface is irradiated, and redox properties of those species that scavenge the solvated electrodes. Theoretical modeling of the transient processes complements the experiments. Photoemission in a platinum half-cell with adsorbed chlorophyll aggregates. Role of oxygen as a super-sensitizer for photoreduction of excited dyes at p-type semiconductor electrodes.

298. A FUNDAMENTAL STUDY OF THE MECHANISM AND KINETICS OF CELLULOSE HYDROLYSIS BY ACIDS AND ENZYMES  
G. T. Tsao - School of Chemical Engineering

\$85,000

02-01

Utilization of cellulosic wastes as an alternative source of fuels and chemicals; conversion of cellulose into glucose and fermentable sugar by a two-stage process; acid pretreatment followed by enzymatic hydrolysis; isolation and purification of enzyme components for kinetic studies; activity of enzyme mixtures studied theoretically and experimentally. Studies on cellulose dissolution and separation from lignin.

## RICE UNIVERSITY

299. ENERGETICS OF ATOMIC AND MOLECULAR INTERACTIONS  
G. K. Walters, N. F. Lane - Department of Physics

\$200,000

01-03

Structure and interactions of excited atoms, molecules, electrons and ions in both gases and liquids, as well as properties of and atomic interactions with solid surfaces. Use of electron (e-beam) bombardment and time-resolved spectroscopy in the study of transient excited species in dense gases of laser importance; new approaches to the study of atomically clean crystalline surfaces, and their interaction with ambient gases; development of tuneable ultraviolet lasers; theoretical studies of collision processes involving electrons, ions, atoms and molecules.

## UNIVERSITY OF ROCHESTER

300. FUNDAMENTAL STUDIES IN ISOTOPE CHEMISTRY \$90,000 02-02  
 J. Bigeleisen - Department of Chemistry

Theoretical correlation of isotope effects with molecular and inter-molecular forces; experimental investigation of condensed media. Study of quantum effects via isotope effects. Isotope fractionation in two component mixtures. Isotopic chemistry of carbon and oxygen related to molecular potential functions. New class of sum rules for molecular vibrations.

## UNIVERSITY OF SOUTH CAROLINA

301. THE USE OF POLYETHERS IN THE TREATMENT OF ACIDIC HIGH ACTIVITY NUCLEAR WASTES \$25,141 02-02  
 M. W. Davis, Jr. - Department of Chemical Engineering

Search for crown ether able to extract Cs, Sr (to 99.9%) from nitric acid solution such as nuclear waste into kerosene or CCl<sub>4</sub> containing TBP. Modification of crown ether solubility by means of alkyl chains to reduce aqueous phase solubility.

## STANFORD UNIVERSITY

302. RESONANCE ABSORPTION SPECTROSCOPY OF COMBUSTION GASES USING DIODE LASERS \$46,800 01-02  
 R. K. Hanson, C. H. Kruger - Department of Chemical Engineering

A tunable infrared diode laser will be used to perform high resolution spectroscopy on combustion gases. Initially work will focus on measurement of NO and CO, species of interest in combustion research, using a flat flame burner.



## UNIVERSITY OF TENNESSEE

303. RESEARCH CONCERNING IONIC AND FREE RADICAL REACTIONS IN RADIATION CHEMISTRY \$63,000 01-01  
 T. F. Williams - Department of Chemistry

Radiation effects in liquids and solids, chemical reactions of highly reactive intermediates (ions and free radicals) generated by the passage of radiation. Paramagnetic intermediates possessing an unpaired electron, detection by electron spin resonance (ESR) spectroscopy; negative ions of fluorocarbons and other molecules formed by electron attachment to the parent molecule. Demonstration of electron attachment to many so-called saturated molecules; hypervalent radical ions, ionization and electron attachment processes as primary mechanisms of radiation damage. Ions discovered include  $(\text{MeO})_3\text{P}-\text{P}(\text{OMe})_3^+$ ,  $\text{Me}_2\text{Se}-\text{SeM}_2^+$ ,  $\text{F}_3\text{NO}^-$ ,  $\underline{\text{C}}-\text{C}_3\text{F}_6^-$ ,  $\underline{\text{C}}-\text{C}_4\text{F}_8^-$ ,  $\underline{\text{C}}-\text{C}_5\text{F}_{10}^-$ ,  $\text{CF}_3\text{X}^-$  (X = Cl, Br, I).

## UNIVERSITY OF TEXAS

304. PHOTOELECTROCHEMISTRY AND MOLECULAR STORAGE OF SOLAR ENERGY \$24,500 01-01  
 M. A. Fox - Department of Chemistry

Organic photoelectrochemistry. Identification of mechanisms in cells where an organic species photoemits electrons into an electrode and then accepts electrons from a second electrode. Measurement of potentials and quantum efficiencies. Study of photoejection mechanisms using flash photolysis and fast spectroscopic techniques. Mechanisms of subsequent reactions. Cyclooctatetraene and derivatives in various solvents. Micellar systems will be introduced to compare mechanisms and efficiencies of photoejection in these environments. In systems having low photoejection efficiencies, valence isomerizations will be studied mechanistically to determine optimum conditions for storing light energy chemically and releasing it as heat.

## TEXAS A&amp;M UNIVERSITY

305. HOT ATOM REACTIONS \$30,000 01-01  
 INVOLVING MULTIVALENT  
 AND UNIVALENT SPECIES  
 Y.-N. Tang - Chemistry Department

Reactions of high energy radioactive multivalent isotopes such as  $^{31}\text{Si}$ ,  $^{32}\text{P}$ , and  $^{11}\text{C}$  formed by nuclear transformations; abstraction, addition and insertion reactions of these hot atoms and their derived radicals in organic as well as inorganic systems; major controlling factors as well as the reaction mechanism for the hydrogen and halogen-abstraction processes; relative efficiencies of various olefin addition reactions involving  $^{31}\text{Si}$  or  $^{32}\text{P}$ , or their derived species, such as  $^{31}\text{SiH}_2$ ,  $^{31}\text{SiF}_2$  and  $^{32}\text{PH}$ . Irradiation either with a nuclear reactor or with a cyclotron, analysis by radio-gas chromatography.

306. THE APPLICATIONS OF \$25,714 02-01  
 FUNCTIONALIZED POLYMERS  
 IN CATALYSIS  
 D. E. Bergbreiter - Department  
 of Chemistry

This research is to demonstrate the value of polymeric reagents as mechanistic probes in heterogeneous catalysis. Catalytically active metal complexes bound to polymers are such polymeric reagents which are alternatives to conventional homogeneous catalysts. This research is concerned with the development of specific functionalized polymers as catalysts and the demonstration of the use of immobilized, phase-separated trapping agents to identify intermediates in heterogeneous processes. Such catalysts possess the activity and selectivity of homogeneous catalysts and the experimental simplicity of heterogeneous catalysts.

307. REACTIVE INTERMEDIATES \$37,500 02-01  
 IN CATALYTIC METHANATION  
 J. H. Lunsford - Department  
 of Chemistry

Determination of the surface complexes and intermediates responsible for the reaction of either carbon monoxide or carbon dioxide with hydrogen to form methane (the methanation reaction), active metal catalysts supported on surfaces of silica or zeolites, kinetic and spectroscopic data and model compounds employed to establish the nature of the important intermediates in the catalytic reactions. Study of the intermediates which are present on active ruthenium metal catalysts, selectivity of bimetallic clusters involving ruthenium, possibility of intermediates existing in the gas phase after being formed on the surface and the reactivity of model intermediates such as ruthenium carbonyl hydrides. Determination of the ruthenium metal in zeolites for the methanation reaction.

## TEXAS SOUTHERN UNIVERSITY

308. SOLVENT EXTRACTION \$28,580 02-02  
STUDIES USING HIGH-  
MOLECULAR-WEIGHT AMINES  
C. McDonald - Chemistry  
Department

Methods to remove metal ions, especially toxic metals such as lead, cadmium, mercury, and chromium, from aqueous solutions via amine liquid-liquid extraction or surfactant-foam separation. Methods to be conservative of energy and economic, and amenable to scale-up for industrial use with waste water. Elucidation of associated chemistry.

## UNIVERSITY OF UTAH

309. DYNAMICS AND MECHANISMS \$46,000 01-01  
OF HOT CHEMISTRY STIMULATED  
BY RECOIL METHODS  
L. D. Spicer - Chemistry Department

Reaction kinetics, atomic and molecular collision dynamics, and energy transfer in very high temperature systems, characterization of intramolecular and intermolecular flow of internal energy in hot molecules generated by recoil reactions. Decomposition kinetics of excited cyclobutane-t in the presence of selected bath gases, to explore intermolecular vibrational energy transfer from high levels of excitation and quantitatively characterize the kinetically controlled chemical activation technique. Chemical activation by recoil stimulated hot reaction at selected sites in haloalkyl cyclopropanes to study intramolecular energy transfer along the carbon backbone of alkane molecules, and to identify the time required for energy randomization in vibrationally excited hydrocarbons. Reactive deuterium isotope effects in molecular collisions at high relative, translational energies to elucidate dynamical factors in high energy collisions.

## VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY

310. REACTIONS OF CHARGED AND NEUTRAL RECOIL PARTICLES FOLLOWING NUCLEAR TRANSFORMATIONS  
H. J. Ache - Chemistry Department
- \$66,035
- 01-01

Kinetics of chemical reactions (in the gas, liquid and solid phase) occurring with nuclear-reaction-produced species not in thermal equilibrium with its surroundings. Reactions of nuclear-reaction-produced nuclides in solution, effect of the physical properties, such as dielectric constants, etc. of the solvent on the reaction pathways. Use of chemical effects of nuclear transformations to devise simple and direct methods to incorporate short-lived radio-nuclides into organic or biomolecules to prepare radiopharmaceuticals for diagnostic application in nuclear medicine. Reactions of "hot" tritium atoms generated in nuclear reactions with various reactor wall materials.

## WASHINGTON UNIVERSITY

311. REACTION STUDIES OF HOT SILICON AND GERMANIUM RADICALS  
P. P. Gaspar - Department of Chemistry
- \$55,000
- 01-01

The finding and understanding of new high energy reactions of silicon and germanium atoms and of molecules containing these elements are the goals of this study. Silicon and germanium resemble carbon in being able to form complex and useful molecules.

In this project high energy silicon and germanium atoms are generated and allowed to react with simple organic and inorganic compounds. The reactions are chosen so that the structures of the products help to reveal the details of the reaction sequence by which the free silicon and germanium atoms become incorporated in stable molecules. On their way toward becoming stable molecules silicon and germanium atoms are converted into short-lived species with one, two, and three bonds to the silicon and germanium atoms. These intermediates are very reactive and a major goal of this research is to determine the structures of these intermediates and to learn how the form and the amount of the energy carried by these intermediates influence their reactions.

In these studies silicon and germanium atoms are produced by nuclear recoil and by thermal evaporation. Divalent silicon and germanium radicals are produced by low pressure pyrolysis and by photolysis.

## WAYNE STATE UNIVERSITY

312. RADIOLYSIS STUDIES ON REACTIVE INTERMEDIATES \$90,000 01-01  
L. Kevan - Department of Chemistry

Reactive reaction intermediates in disordered systems; spin-lattice energy relaxation mechanisms of radiation-produced radicals in disordered systems studied by pulsed electron spin resonance; matrix dipolar interactions of trapped radicals studied by electron spin echo spectrometry; magnetic energy transfer and forbidden spin transitions by electron-electron double resonance; electron solvation in mixed solvents by laser photolysis; transport properties of electrons in condensed phase alkanes by conductivity and mobility methods; trapped radicals and ions produced by sub 4 K radiolysis by electron spin resonance and optical methods. Trapped electrons in alkane glasses; trapped radicals in glasses; electron-electron radical-radical correlation distances; electron localization in alkanes has been developed.

313. ELECTRONIC RELAXATION PROCESSES IN POLYATOMIC MOLECULES \$48,000 01-02  
E. C. Lim - Department of Chemistry

Radiationless transitions in polyatomic molecules; conversion of electronic energy into vibrational (heat) energy and factors which govern the efficiency of these processes. Excitation by light and heat energy detection directly by opto-acoustic signals or, indirectly, via molecular luminescence.

## COLLEGE OF WILLIAM AND MARY

314. THEORY OF PLASMA WAVES IN THE EARTH'S BOW SHOCK \$22,700 01-03  
S. P. Gary - Physics Department

Theoretical investigation of possible plasma instabilities in the earth's bow shock; solution of the complete electromagnetic, Vlasov, linear dispersion relation for conditions appropriate to perpendicular shocks, dominant instabilities, construction of appropriate nonlinear theories to determine saturation mechanisms and turbulent scattering frequencies. Structure of the earth's bow shock and how it heats the solar wind plasma. Dispersion relation for the case of unmagnetized ions and magnetized electrons undergoing an  $\vec{E} \times \vec{B}$  drift.

## UNIVERSITY OF WISCONSIN

315. STUDIES IN HOT ATOM CHEMISTRY AND RADIATION CHEMISTRY

\$60,000

01-01

J. E. Willard - Department  
of Chemistry

Nature and reactions of molecular fragments produced in organic solids by energy absorbed in the form of radiation, gamma rays, high speed electrons and ultraviolet light. Primary decomposition products are electrons, positive ions and free radicals. Solids at low temperatures (e.g., 4 K to 77 K); prolonged observation of fragments because diffusion is slowed and energy required for normal reactions is not available. Mechanisms of charge stabilization in relatively non-polar matrices and of its neutralization and reaction with additives; unexpected effects of substituting deuterated matrix molecules for protiated molecules; distinctive properties of radicals produced in close proximity; production of radicals in the solid state by mercury photosensitization; physical and chemical properties of the organic solid state. Evidence from visible, infrared, ultraviolet and electron spin resonance spectra and from luminescence, thermal effects and electrical conductivity.

316. INELASTIC MOLECULAR COLLISIONS- APPLICATIONS OF THEORETICAL METHODS TO PROBLEMS IN RELAXATION PHENOMENA AND LASER OPERATION

\$32,000

01-02

R. W. Conn - Nuclear Engineering  
Department

Studies of inelastic molecular collisions: development and implementation of new theoretical methods capable of handling realistic collision problems, mathematical methods and Hamiltonian-type techniques, vibrational relaxation of hydrogen fluoride (HF) and carbon monoxide (CO), modeling of HF lasing under various experimental conditions.

317. METAL CATALYZED HYDROGENATION OF CARBON MONOXIDE TO HYDROCARBONS

\$50,000

02-01

C. P. Casey - Department  
of Chemistry

This research involves the synthesis of new metal formyl complexes, a study of their thermodynamic and kinetic stability, and investigations of the further reduction of these complexes. Also of interest is the termination of hydrocarbon chain growth from a metal catalyst which is believed to involve the hydrogenation of a metal-carbene complex. This research relates to the eventual design of homogeneous catalysts for the reduction of carbon monoxide.

## WORCESTER POLYTECHNIC INSTITUTE

318. THE GAS PHASE RADIOLYSIS AND VACUUM ULTRAVIOLET PHOTOLYSIS OF HETEROCYCLIC ORGANIC COMPOUNDS \$32,000 01-01  
A. A. Scala - Chemistry Department

Interaction between high energy radiation and heterocyclic organic compounds; gas phase gamma-radiolysis and vacuum ultraviolet photolysis; primary and secondary modes of decomposition of complex organic molecules, factors which affect the reactions in these systems. Concern with ions as well as neutral excited molecules, deduce information concerning energy distribution in the decomposing molecules. Quasi-equilibrium situations, thermodynamic factors such as bond energies significant in determining reaction channels.

## WRIGHT STATE UNIVERSITY

319. THE DIRECT DETERMINATION OF ATOM AND RADICAL CONCENTRATIONS IN THERMAL REACTIONS OF HYDROCARBONS AND OTHER GASES \$43,420 01-02  
G. B. Skinner - Department of Chemistry

A program to measure concentrations of species such as H, O, OH and CH<sub>3</sub> in shock-heated mixtures of smaller hydrocarbons diluted with argon, sometimes in the presence of oxygen; atomic (or molecular) absorption spectroscopy; high temperature reactions of several hydrocarbons.

## YALE UNIVERSITY

320. RESEARCH ON HIGH-ENERGY CHEMICAL REACTIONS \$17,734 01-02  
R. J. Cross - Department of Chemistry

Chemical reaction rate dependence on the energy of the colliding molecules; one reacting species in a beam at a known and variable energy; amount of product formed measured as a function of beam energy. Theory to calculate the rate of energy loss of a fast atom as it collides with slow molecules.

## YALE UNIVERSITY (Continued)

<u>321.</u>	ENERGIES OF ORGANIC COMPOUNDS	\$60,000	02-01
	K. B. Wiberg - Department of Chemistry		

Experimental studies on the energies of molecules and development of methods for estimating the energies of molecules; development of automated systems for collecting calorimetric data; determination of the appropriate interaction parameters for the molecular mechanics method for estimating energies; ab initio molecular orbital calculations.



SECTION C

Summary of  
Funding Levels

SUMMARY OF  
FUNDING LEVELS

During the fiscal year ending September 30, 1977, the Chemical Sciences total support level amounted to about \$33.6 million in operating funds and \$2.6 million in equipment funds. The equipment funds are expended primarily at the Government-owned Laboratories and are not shown in this report. Equipment funds for the University and Corporate projects are included in the total contract dollars, being part of the operating budget. The following analysis of costs is concerned only with operating funds.

1. By Region of the Country:

	<u>Contract Research (%)</u>	<u>Total Program (%)</u>
(a) Northeast ..... (Conn., D.C., Del., Mass., Md., N.J., N.Y., Pa., R.I.)	35.7	25.8
(b) South ..... (Ala., Fla., Ga., Miss., S. C., Tenn., Va., W.Va.)	9.0	17.8
(c) Midwest ..... (Ill., Ind., Iowa, Kans., Mich., Minn., Mo., Nebr., Ohio, Wis.)	29.3	35.0
(d) West ..... (Ariz., Calif., Colo., Nev., N. Mex., Okla., Oreg., Tex., Utah, Wash.)	<u>26.0</u>	<u>21.4</u>
	100.0	100.0

2. By Laboratory and University Programs:

	<u>Total Program (%)</u>
(a) University Program (including laboratories where graduate students are involved in research to a large extent, e.g., Ames Laboratory, Lawrence Berkeley Laboratory, Notre Dame University (Radiation Laboratory) .....	38.4
(b) Laboratory Program .....	59.6
(c) Other .....	<u>2.0</u>
	100.0

3. By Laboratory:

	<u>Total Program (%)</u>
Ames Laboratory .....	5.9
Argonne National Laboratory .....	17.0
Atomics International .....	0.3
Bartlesville Energy Research Center .....	0.2
Brookhaven National Laboratory .....	18.6
Lawrence Berkeley Laboratory .....	10.0
Lawrence Livermore Laboratory .....	0.7
Los Alamos Scientific Laboratory .....	1.6
Morgantown Energy Research Center .....	0.2
Mound Laboratory .....	1.9
Notre Dame University (Radiation Laboratory) .....	4.4
Oak Ridge National Laboratory .....	15.7
Pacific Northwest Laboratory .....	2.8
Sandia Laboratory .....	0.6
Contract Research .....	<u>20.1</u>
	100.0

4. By Budget Number/Title

	<u>Contract Research (%)</u>	<u>Total Program (%)</u>
01-01 Radiation Sciences .....	35.5	28.5
01-02 Chemical Physics .....	15.9	20.5
01-03 Atomic Physics .....	19.2	10.8
02-01 Chemical Energy .....	14.5	19.9
02-02 Separations .....	10.6	10.6
02-03 Analysis .....	2.8	8.9
02-04 Engineering Sciences .....	<u>1.5</u>	<u>0.8</u>
	100.0	100.0

SECTION D  
Index of Investigators

The index refers to project numbers  
in Sections A and B.

Abell, G. C., 111  
Ache, H. J., 310  
Agron, P. A., 139  
Appelman, E. H., 40, 42, 45  
Aris, R., 271  
Arnold, W. D., 141  
Ashurst, W. T., 167  
Avona, V. L., 114

Baes, C. F., 137  
Bamberger, C. E., 136  
Barnes, R. M., 262  
Barnett, C. F., 133  
Bartlett, N., 97  
Bassham, J., 90  
Bayfield, J. E., 294  
Beauchamp, J., 235  
Begovich, J. M., 147  
Bell, A. T., 94  
Bell, J. T., 142  
Benjamin, B. M., 140  
Bergbreiter, D. E., 306  
Berkowitz, J., 34  
Bernstein, H., 56  
Berry, H. G., 38  
Berry, W. B., 125  
Beuhler, R., 58  
Bielski, B. H. J., 50  
Bigeleisen, J., 300  
Bowman, R. C., 111  
Brauer, F. P., 163, 166  
Brenner, D., 54  
Brink, G. O., 283  
Broida, H. P., 230  
Bryant, H. C., 280  
Brynstad, J., 144  
Burkhart, R. D., 279  
Burwell, R. L., 285  
Butt, J. B., 285

Cafasso, F. A., 47  
Callaway, J., 258  
Canada, D. C., 154  
Canon, R. M., 147  
Carlson, T. A., 132

Carr, R. W., Jr., 269, 271  
Carruthers, J. A., 272  
Casey, C. P., 317  
Cattolica, R. J., 167  
Chanin, L. M., 272  
Chen, T. C. S., 212  
Cheung, J. T. K., 129  
Childs, W. C., 36  
Chiu, L.-Y. C., 248  
Christie, W. H., 153  
Christoffersen, R. E., 255  
Clardy, J., 13  
Clarke, R. H., 215  
Clem, R., 100  
Clinton, S. D., 147, 148  
Cohen, J. B., 285  
Cohen, S. G., 219  
Coleman, C. F., 149  
Collins, C. J., 140  
Conn, R. W., 316  
Connick, R. E., 93  
Corliss, L., 60  
Cox, J. L., 157  
Cram, D. J., 227  
Crandall, D. H., 133  
Crawford, O. H., 131  
Creutz, C., 53  
Cross, R. J., 320  
Crosswhite, H. M., 30

Dale, J. M., 155  
Dalgarno, A., 247  
Davis, M. W., Jr., 301  
Demmitt, T. F., 158  
DeWitt, R., 114  
Dittner, P. F., 129  
Dodson, R. W., 50  
Dole, M., 214  
Donohue, D. L., 152  
Dorfman, L. M., 287  
Douslin, D. R., 49  
Dworkin, A. S., 144  
Dye, J. L., 267

Eby, R. E., 153  
 Egan, B. Z., 146  
 Egan, J. J., 73  
 Ehrenson, S., 57  
 Eland, J. H. D., 34  
 El-Sayed, M. A., 226  
 Erickson, N. E., 210  
 Espenson, J., 8, 10  
 Evans, W. J., 237

Fajer, J., 63  
 Fano, U., 236  
 Farr, J. D., 108  
 Fassel, V., 15  
 Feder, H. M., 47  
 Feldberg, S., 64  
 Feldman, C., 151  
 Feldman, W. C., 106  
 Ferraro, J., 33  
 Fessenden, R. W., 122  
 Filipescu, N., 243  
 Finston, H. L., 281  
 Firestone, R. F., 286  
 Fischer, C. F., 291  
 Fisher, P. W., 148  
 Fontijn, A., 201  
 Ford, P. C., 231  
 Fowler, J., 51  
 Fox, M. A., 304  
 Franklin, J. C., 154  
 Franz, J. A., 159  
 Freiser, H., 213  
 Friedman, A. M., 46  
 Friedman, L., 58  
 Fritz, J., 16  
 Fuller, E. L., 139  
 Funabashi, K. P., 116

Gaines, G. L., 204  
 Gallup, G., 278  
 Garrison, W. M., 79  
 Garvin, D., 208  
 Gary, S. P., 314  
 Gaspar, P. P., 311  
 Gemmell, D. S., 39  
 Gentry, W. R., 270  
 Gerstein, B., 12  
 Giaouque, R., 100

Gilpatrick, L. O., 144  
 Goles, R. W., 162  
 Good, W. D., 49  
 Goodman, L. S., 36  
 Gordon, G. E., 261  
 Gordon, R. J., 251  
 Gordon, R. L., 165  
 Gordon, S., 24, 25  
 Greene, E. F., 220  
 Grens, E. A., 98  
 Grover, J., 59

Hagaman, E. W., 140  
 Hambright, P., 250  
 Hamill, W. H., 125  
 Hammond, G. S., 233  
 Hampson, R. F., 208  
 Hanrahan, R. J., 241  
 Hanson, R. K., 302  
 Harbottle, G., 51, 71  
 Hardesty, D. R., 167  
 Harris, C. B., 80  
 Harris, L. A., 205  
 Hastings, J., 60  
 Headley, L. C., 110  
 Henry, R. J. W., 258  
 Hildenbrand, D. L., 206  
 Hill, F. B., 75  
 Hill, R. A., 167  
 Hillman, M., 61  
 Hochanadel, C. J., 126  
 Hoffman, D., 4  
 Hoffman, M. Z., 216  
 Holmes, H. F., 137  
 Holroyd, R. A., 50  
 Horowitz, E. P., 43  
 Hudis, J., 69  
 Hulett, L. D., 155  
 Hurst, F. J., 141

Ishida, T., 282  
 Ivey, J. L., 111

Jackson, W. M., 249  
 Jepson, B. E., 112  
 Johnsen, R. H., 242  
 Johnson, J. S., 143

- Johnston, H. S., 78  
Jolly, W. L., 95  
Jones, G., 217  
Jones, K. W., 67, 77  
Jones, L., 105
- Kaminsky, M., 35  
Kaplan, L., 25  
Karapinka, G. L., 109  
Katz, J. J., 26, 28, 29  
Katzner, J. R., 239  
Kaufman, J. J., 254  
Kaye, J. H., 161  
Kee, R. J., 167  
Kelley, J. M., 164  
Kelley, R. D., 210  
Kemme, J. E., 104  
Kessler, K. G., 209  
Kestner, N. R., 257  
Kevan, L., 312  
King, A. D., 244  
King, R. B., 244  
Kispert, L. D., 212  
Klatt, L., 155  
Klemm, R., 66  
Kleppner, D., 265  
Klingen, T. J., 273  
Knauer, J. B., 150  
Koetzle, T., 56  
Koski, W. S., 254  
Kozak, J. J., 117  
Kraner, H. W., 77  
Krause, H. F., 129  
Krikorian, O., 102  
Kruger, C. H., 302  
Kubas, G., 107  
Kuppermann, A., 234
- Lagergren, C. R., 165  
Lambrecht, R. M., 51  
Lampe, F. W., 290  
Lane, N. F., 299  
Law, C. K., 284  
Lawson, W. F., 110  
Lee, E. K. C., 222  
Lee, M. H., 246  
Lee, S. H., 49  
Lee, Y. T., 86
- Leventhal, J. J., 274  
Li, C. T., 160  
Lichtin, N. N., 216  
Lietzke, M. H., 137  
Lim, E. C., 313  
Linschitz, H., 218  
Lipsky, S., 268  
Livingston, R., 130  
Lloyd, M. H., 150  
Lonsdale, H. K., 203  
Love, C. M., 111  
Lunsford, J. H., 307
- MacDonald, J. R., 256  
Macek, J. H., 278  
Mackay, R. A., 240  
Mackenzie, D. R., 74  
Madey, T. E., 210  
Maggiora, G. M., 255  
Mahan, B. H., 83  
Mailen, J. C., 145  
Malm, J. G., 40  
Marrus, R., 89  
Marshall, W. L., 137  
Martin, D., 2, 11  
Martin, R. M., 229  
Matheson, M. S., 21, 23  
McDonald, C., 308  
McDowell, W. J., 149  
McLean, W. J., 238  
McMullan, R., 56  
Meisels, G. G., 276  
Michaels, E. D., 112  
Miller, J. A., 167  
Miller, J. R., 22  
Miller, P. D., 134  
Miller, W. H., 84  
Mitchell, R. E., 167  
Moak, C. D., 134  
Molton, P. M., 158, 159  
Morgan, H. W., 135  
Morrey, J. R., 156  
Mozumder, A., 116  
Muckerman, J., 57  
Mudge, L. K., 160  
Myers, A. L., 289  
Myers, R. J., 81

- Neta, P., 123  
Netzel, T., 55  
Newman, J. S., 96  
Newman, L., 76  
Newton, M., 57  
Ng, C., 7  
Nicol, M. F., 225  
Norcross, D. W., 211  
Norris, J. R., 27  
Novakov, T., 92
- Oskam, H. J., 272  
Otvos, J., 90  
Overbury, S. H., 128
- Packer, L., 91  
Patterson, L. K., 123  
Pearlstein, R. M., 127  
Perlman, M. L., 69  
Perlmutter, D. D., 289  
Perlow, G., 37  
Perone, S. P., 297  
Pitzer, K. S., 82  
Poe, R. T., 228  
Powell, J., 14  
Pratt, D. W., 293
- Raaen, V. F., 140  
Rabitz, H., 295  
Rack, E. P., 275  
Rahn, L. A., 167  
Rainey, W. T., 154  
Regen, S. L., 259  
Reilly, J. J., 72  
Richard, P., 256  
Richardson, D. M., 136  
Rinker, R. G., 232  
Robben, F., 101  
Robertson, D. M., 164  
Robinson, D. W., 253  
Rodgers, B. R., 147  
Rogers, L. B., 245  
Rogers, M. T., 266  
Root, J. W., 221  
Ross, A., 121  
Ross, J., 264  
Routh, J. W., 103
- Rowland, F. S., 223  
Ruedenberg, K., 6  
Rutherford, W. M., 112
- Samson, J. A. R., 277  
Sauer, M. C., 22  
Sayre, E. V., 71  
Scala, A. A., 318  
Schaefer, H. F., 87  
Schreiner, F., 42  
Schuler, R. H., 118  
Schwartz, M. E., 117  
Schwarz, H. A., 50  
Seltzer, S., 68  
Setchell, R. E., 167  
Shaw, R. W., 155  
Sheng, S. J., 115  
Shirley, D. A., 85  
Shor, A. J., 143  
Shugart, H. A., 88  
Silverman, J., 260  
Simmons, W. H., 110  
Skinner, G. B., 319  
Small, G., 1  
Smith, D. H., 138, 152  
Smith, G. P., 144  
Smith, J. R., 167  
Somorjai, G. A., 94  
Spaulding, L., 65  
Spedding, F., 9  
Spicer, L. D., 309  
Starace, A. F., 277  
Stein, L., 40  
Stelzner, R. W., 151, 153  
Stevens, C. M., 45  
Stoenner, R. W., 71  
Strain, J. E., 151  
Strehlow, R. A., 139  
Struve, W., 3  
Studier, M. H., 41, 44  
Stwalley, W. C., 252  
Sutherland, J. W., 62  
Sutin, N., 53  
Svec, H., 5, 17  
Sworski, T. J., 126



Tang, Y.-N., 305  
Tanner, R., 76  
Taylor, W. L., 113  
Thomas, J. K., 119  
Thomas, R., 56  
Thomson, D. B., 105  
Tingey, G. L., 156  
Toth, L. M., 142  
Treat, R. P., 110  
Trozzolo, A. M., 120  
Tsao, G. T., 298  
Turkevich, J., 296

Ulrichson, D., 11

Valenty, S. J., 204  
Vannice, M. A., 292  
Vermeulen, T., 98  
Victor, G., 247  
Voigt, A., 18

Wahl, A. C., 32  
Walker, R. L., 152  
Walters, G. K., 299  
Walters, W. B., 261  
Wentorf, R. H., Jr., 205  
Weston, R. E., 52, 70  
Wexler, S., 31  
White, D., 288  
Wiberg, K. B., 321  
Wiese, W. L., 209  
Wilke, C. R., 99  
Willard, J. E., 315  
Williams, E. T., 281  
Williams, T. F., 303  
Wilson, R. H., 205  
Winicur, D. H., 124  
Wise, H., 207  
Wiswall, R., 72  
Wolf, A. P., 51  
Wolfsberg, M., 224  
Wrighton, M. S., 263

Yang, R. T., 74  
Yates, J. T., 210  
Yeung, E., 19, 20  
Yosim, S. J., 48

Young, J. P., 151

Zeldes, H., 130  
Zittel, P. F., 202  
Zoller, W. H., 261

SECTION E  
INDEX OF PROJECTS  
GROUPED BY  
PROGRAMMATIC AREA

01-01 RADIATION SCIENCES

Research involving the chemical reactions and species formed as the result of the introduction of radiation or high energy particles into chemical systems, including the chemical effects of radioactive decay and especially solar-induced photochemistry.

1, 2, 3, 21, 22, 23, 24, 25, 26, 27, 28, 29, 50, 51, 52, 53, 54, 55, 61, 62, 63, 78, 79, 90, 91, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 204, 205, 212, 214, 215, 216, 217, 218, 219, 221, 223, 233, 234, 235, 241, 242, 243, 252, 253, 254, 255, 257, 260, 263, 266, 268, 269, 273, 275, 276, 279, 286, 287, 290, 297, 303, 304, 305, 309, 310, 311, 312, 315, 318

01-02 CHEMICAL PHYSICS

Basic studies of gas phase ion and molecule interactions; optical, magnetic, particle, and mass spectroscopy as they relate to chemical reactivity; the determination of molecular structure and its relationship to molecular properties; and theoretical studies including quantum theory, kinetic theory, and statistical thermodynamics and their use for the prediction of chemical and physical properties.

4, 5, 6, 7, 30, 31, 32, 33, 56, 57, 58, 59, 60, 64, 65, 66, 80, 81, 82, 83, 84, 85, 86, 87, 92, 129, 130, 131, 167, 201, 208, 220, 222, 225, 226, 229, 230, 238, 248, 249, 251, 264, 267, 270, 274, 283, 284, 288, 293, 295, 302, 313, 316, 319, 320

01-03 ATOMIC PHYSICS

Research activities primarily related to the physics of matter in the gaseous, ionic and plasma states: spectroscopy, collision phenomena, atomic structure and dynamics.

34, 35, 36, 37, 38, 39, 67, 88, 89, 104, 105, 106, 132, 133, 134, 135, 209, 211, 228, 236, 247, 256, 258, 265, 277, 278, 280, 291, 294, 299, 314

02-01 CHEMICAL ENERGY

Research in thermodynamics, solution kinetics, electrochemistry, inorganic chemistry, the study of heterogeneous and homogeneous catalysts, energy conversion processes, and basics of the production and storage of chemical fuels such as liquefied coal and hydrogen.

8, 9, 10, 11, 12, 13, 40, 41, 42, 47, 48, 49, 68, 69, 72, 73, 74, 93, 94, 95, 96, 97, 98, 99, 102, 107, 108, 109, 111, 136, 137, 138, 139, 140, 144, 145, 146, 156, 157, 158, 159, 206, 207, 210, 231, 237, 239, 240, 244, 250, 259, 285, 292, 296, 298, 306, 307, 317, 321

02-02 SEPARATIONS RESEARCH

Research on the effects of isotopic substitution on the physical and chemical properties of atoms and molecules which can be used as either theoretical or experimental tools to effect isotope separation, as well as research on the separation methods themselves; research on methods of separating and purifying chemical species and research on the separation of materials in different physical states.

14, 43, 70, 75, 110, 112, 113, 114, 141, 142, 143, 147, 148, 149, 150, 202, 203, 213, 224, 227, 245, 246, 271, 272, 282, 300, 301, 308

02-03 ANALYSIS

Basic and developmental studies in laboratory analytical techniques and methods.

15, 16, 17, 18, 19, 20, 44, 45, 46, 71, 76, 77, 100, 151, 152, 153, 154, 155, 161, 162, 163, 164, 165, 166, 261, 262, 281

02-04 CHEMICAL ENGINEERING SCIENCES

Experimental and theoretical research involving mass, heat and momentum transport, and related chemical rate processes; engineering modeling, process control and engineering and chemical thermodynamic studies related to energy technologies.

101, 103, 160, 232, 289

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