

DEPARTMENT OF ENERGY
ENERGY-OPERATING EXPENSES AND CAPITAL ACQUISITION
FY 1979 CONGRESSIONAL BUDGET REQUEST BY ACTIVITY
(Tabular dollars in thousands. Narrative material in whole dollars.)

Energy Supply-Research and Technology Development
Basic Energy Sciences

	BA
Estimate, Basic Energy Sciences, FY 1979	\$211,500
Estimate, Basic Energy Sciences, FY 1978	177,359
Increase	\$ 34,141

The objective of the Basic Energy Sciences resource is to expand the knowledge base in science and engineering for all the energy production and conservation technologies. The program serves three general types of users: (1) scientists and engineers who will be involved in the next generation of energy development efforts; (2) scientists and engineers outside DOE interested in solving energy-related problems; and (3) scientists and engineers in current applied research and development programs of the Department. Direct commercialization of results from basic research has occurred fairly often; however, more often the benefits accrue as the accumulated knowledge and understanding of detailed processes become an integral part of the body of data on which applied technologies rest. Basic Energy Sciences comprises five activities: nuclear science; materials sciences; chemical sciences; engineering, mathematical and geosciences; and advanced energy projects.

Nuclear science includes research that expands the base of understanding of the behavior and properties of nuclei, nuclear matter, and individual isotopes, which can be applied in the development of fission and fusion energy as well as in biomedical and environmental research. It also contributes to understanding of the properties of the actinide elements and provides for production and distribution of isotopes internationally for research and industrial purposes. In FY 1979, nuclear data measurements important to the fission and fusion technologies will continue to be stressed, and increasing efforts will be applied to heavy element (actinide) research useful to radioactive waste management systems.

Materials problems are inherent in all energy technologies - either restricting economic viability or compromising technical feasibility. The materials sciences activity is directed toward providing a base for the relief of these roadblocks to success. New research projects planned or recently initiated include research on high temperature materials important to MID and other fossil technologies, black-chrome for solar heating and cooling technologies, radiation enhanced creep important to fission and fusion technologies, surfaces important to all technologies (catalysis and corrosion), polymers important to solar and conservation, and high voltage electron microscopy of across-the-board importance. The engineering materials and engineering physics areas initiated in FY 1978, which include research in such subjects as welding, materials processing and instrumentation, will assist in the application of basic materials sciences research to engineering systems. There will also be accelerated exploitations of new techniques using synchrotron light and low angle x-ray and neutron scattering in research involving, for example, catalytic processes and solar materials.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Research previously reported under the molecular, mathematical, and geosciences activity has recently been reorganized into two new activities (chemical sciences and engineering, mathematical and geosciences) in order to provide more focused attention to administering the widely important chemical sciences efforts and to encouraging hitherto neglected and important areas of engineering science. In FY 1979, the chemical sciences activity will expand efforts to seek new options in solar photo-conversion through research in photoelectrolysis, photogalvanics and photochemical reactions. Chemical phenomena important to fossil energy development, especially detailed organic characterization of coals, will be emphasized. Studies of cleaner and more efficient combustion systems will also be stressed using laser diagnostics and other advanced techniques. Some of the other research areas to be studied include thermochemical hydrogen production and storage, conversion of wastes to fuels and heterogeneous and homogeneous catalysis.

The engineering, mathematical and geosciences activity includes three disciplines which are very important across the entire spectrum of current and future energy systems. Engineering sciences is an area long neglected in which work is just now being initiated to provide understanding and data widely needed in energy systems development. Examples include studies of vibration damage to high-flow heat exchangers, aerodynamics of automobile undercarriages, remote thermometry to very high temperatures and energy process control. In the field of applied mathematical sciences, research will be pursued in applied analysis, statistics, numerical mathematics and related computer science and expanded into neglected areas including econometric modeling. In FY 1979, increasing emphasis will be placed on software engineering, advanced computation systems and data management. In the geosciences subactivity, existing programs will be expanded and three new interagency programs of potentially major significance to virtually all energy technologies will be initiated, as described below.

The advanced energy projects activity, which was initiated in FY 1978, provides support for novel energy concepts and energy-related inventions that appear theoretically sound but need additional study and experimental effort for verification of concept. The projects supported by this activity tend to be unconventional in nature and do not fit into the structure of any other established program area within DOE.

The FY 1979 request also includes certain charges involving the lease of a central computer system at Oak Ridge National Laboratory. This system, which has an estimated purchase value of \$10,000,000, is a general purpose computer which would serve a number of DOE program areas including, among others, nuclear research, biomedical and environmental research, fuel cycle research, the breeder reactor, basic energy sciences, and weapons activities. No single program user is expected to command more than fifteen percent of the computer's capacity. It is essential to the effective and efficient functioning of DOE programs at ORNL that a computer be obtained in FY 1979, since the capacity of the present ORNL computer system has reached the saturation point and demand is expected to expand dramatically. A thorough study of the computer workload documented the continued computational growth requirements through FY 1982. The computer will be utilized primarily for scientific purposes in support of the above mentioned programs. The new computer will replace the IBM 360/75 which will be made available for reutilization at another location. The total annual lease, operating, and maintenance costs for this computer are estimated at approximately \$3,600,000. However, these costs in FY 1979 are estimated between \$300,000 and \$900,000, dependent upon the time of installation and acceptance in the latter part of the fiscal year. In addition, the FY 1979 request includes funding for necessary inventory adjustments at the High Flux Beam Reactor and certain other facilities.

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The FY 1979 request includes an estimated \$40,300,000 in operating funds for direct university support, an increase of \$8,400,000 above the estimated FY 1978 level.

SUMMARY OF ESTIMATES BY ACTIVITY

Page No.	Activity	Actual FY 1977			Estimate FY 1978		Estimate FY 1979	
		BA	Obs.	BO	BA	BO	BA	BO
	Operating Expenses:							
RTBS-4	Nuclear Science	\$ 25,022	\$ 24,545	\$ 22,780	\$ 26,063	\$ 24,960	\$ 28,400	\$ 27,500
RTBS-7	Materials Sciences.....	57,941	58,354	54,951	65,709	61,407	72,000	68,900
RTBS-17	Chemical Sciences.....	35,265	35,777	33,386	43,285	40,325	48,200	46,700
RTBS-22	Engineering, Mathematical and Geosciences	10,311	10,379	9,923	11,480	10,737	23,200	22,800
RTBS-26	Advanced Energy Projects	0	0	0	3,187	3,000	3,800	3,600
	Subtotal, operating expenses	128,539	129,055	121,040	149,724	140,429	175,600	169,500
	Capital Acquisition:							
	Capital Equipment Not Related to Construction:							
RTBS-27	Nuclear Science	866	834	805	1,075	1,150	1,300	1,300
RTBS-28	Materials Sciences.....	5,100	5,091	3,400	5,400	5,050	5,900	5,600
RTBS-32	Chemical Sciences.....	2,685	2,659	2,336	2,700	2,300	3,300	3,100
RTBS-34	Engineering, Mathematical and Geosciences	615	609	597	900	500	800	700
RTBS-36	Advanced Energy Projects	0	0	0	0	0	200	100
RTBS-36	Other Capital Equipment	1,800	1,800	2,176	2,000	2,167	1,700	1,700
	Subtotal, capital equipment	11,066	10,993	9,314	12,075	11,167	13,200	12,500
	Construction Projects:							
RTBS-37	Materials Sciences.....	0	0	0	5,000	1,000	16,400	6,600
RTBS-43	Chemical Sciences.....	0	0	0	6,000	1,000	3,400	3,200
RTBS-46	General Plant Projects	3,115	3,115	434	2,560	530	2,900	800
	Prior Year Projects	12,495	12,711	4,392	2,000	9,987	0	8,500
	Subtotal, construction	15,610	15,826	4,826	15,560	12,517	22,700	19,100
	Subtotal, capital acquisition	26,676	26,819	14,140	27,635	23,684	35,900	31,600
	Total, Basic Energy Sciences	\$155,215	\$155,874	\$135,180	\$177,359	\$164,113	\$211,500	\$201,100

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

JUSTIFICATION OF ACTIVITY

Operating Expenses:

1. Nuclear science \$ 28,400

The nuclear science activity is centered around four major areas: 1) charged particle research; 2) neutron and fission research; 3) heavy element research; and 4) isotope preparations. Charged particle research is the study of nuclear interactions and nuclear structure based on the use of low energy (below the pi meson production threshold), light ion (nuclear mass of four-or-fewer units), accelerated particles. These studies include both fundamental and applied research problems. Neutron and fission research involves the study of nuclear reactions and structure using neutrons and the study of the nuclear fission process. In addition to supporting fundamental studies, this area funds the measurement, evaluation, and compilation of nuclear data in support of DOE's fission and fusion power development effort. Heavy element research is the fundamental and applied study of the chemical and physical properties of the heavy (actinide) elements. In addition to improving our understanding of this important series of elements, these studies provide the basis for the solution of the applied problems of actinides in the environment and waste management, to name two examples. The isotope preparation area provides isotopic samples for research and development purposes to an international community. The first three areas are discussed in greater detail below in the section entitled low energy nuclear science, which is followed by a discussion of isotope preparations.

The FY 1979 operating request of \$28,400,000 is an increase of \$2,337,000 over the FY 1978 level. This increase is required to fund the many research programs pursued in support of DOE's nuclear fission and fusion research and development efforts.

	Actual FY 1977			Estimate FY 1978		Estimate FY 1979	
	BA	Obs.	BO	BA	BO	BA	BO
a. Low energy nuclear science	\$ 17,611	\$ 17,275	\$ 16,030	\$ 18,363	\$ 17,590	\$ 20,100	\$ 19,500
b. Isotope Preparations	7,411	7,270	6,750	7,700	7,370	8,300	8,000
Subtotal, nuclear science	\$ 25,022	\$ 24,545	\$ 22,780	\$ 26,063	\$ 24,960	\$ 28,400	\$ 27,500

a. Low energy nuclear science \$ 20,100

Atomic nuclei are extremely complex quantum mechanical systems. Their structure, symmetries, normal modes of vibration and rotation, and their reactions are still understood only in terms of relatively crude, though complicated, models. Although the newer medium energy and heavy ion accelerators will certainly provide important new information about nuclei, they cannot replace the careful, precise study of nuclear structure and reactions which has been and continues to be obtained with low energy accelerators.

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The following examples of productive areas using low energy, light ion probes to study nuclei were given in an introductory talk at the recent international conference on nuclear structure in Tokyo: (1) Excited alpha particle vibration states in alpha pickup ($d, {}^6\text{Li}$) reactions may be able to clarify the question of the role of four-nucleon, alpha particle-like "pairing" in nuclear structure; (2) Other work using low energy alpha particles may have confirmed the existence of E-zero giant resonances in nuclei; (3) Back angle scattering measurements of protons and alpha's indicate that optical models may not vary smoothly with atomic number, but may be very sensitive to shell closures in nuclei.

An increase of \$752,000 is planned for charged particle research, which reverses the downward trend in recent years that resulted in the closing down of a number of the less-productive low energy accelerators. This increase permits the completion of an expansion of the BNL National Nuclear Data Center (NNDC) to manage the non-neutron nuclear data that is of importance to both applied and basic science research users. (The second half of the necessary upgrade of the computer facility at the NNDC is described under the Nuclear Science capital equipment request.) The increase also supports a program at LASL to measure at the lowest possible energies the cross sections for a number of light ion reactions, such as tritium-tritium and deuterium-deuterium. These cross section measurements are of general interest to fusion research, and possibly of specific use in the diagnostics of the performance of the Tokamak Fusion Test Reactor under construction at Princeton. Additional support is also being provided for the development of better polarized ion sources at the University of Wisconsin and at the University of North Carolina, the latter being a member of the Tri-University Laboratory at Duke.

The increase of \$510,000 planned for neutron and fission research includes funding for measurements at ANL of fission product yields for fissions induced by mono-energetic fast neutrons. Besides being of basic research interest, this data will be entered into the Evaluated Nuclear Data File B (ENDF/B) at Brookhaven for use in a variety of calculations that require the production rate of various fission products from fissionable materials exposed to fast neutron fluxes with varying energy spectra. The request includes funding for university nuclear physics groups to perform neutron nuclear data measurements of interest to the fission and fusion programs. It also would provide for initiation of a new research effort making use of the on-line isotope separator nuclear research facility (TRISTAN) that is being transferred to the Brookhaven National Laboratory (BNL) High Flux Beam Reactor after the closedown of the Ames Laboratory Research Reactor at the end of 1977. A new ion source developed at Ames will provide a great variety of very neutron-rich fission product nuclides for the study of their nuclear level structure and their decays, including the delayed neutron emission.

Heavy element research is centered around a study of the fundamental chemical and physical properties of the actinide elements - principally the transuranium elements. Detailed studies are pursued to determine the behavior of the elements in aqueous and non-aqueous solutions and molten salt media; their thermodynamic behavior in solution and in the gas phase; the crystal structures of the pure metallic elements and their chemical compounds; and the electronic, magnetic, and spectroscopic properties. These detailed studies of the individual elements are analyzed and correlated to derive a comprehensive understanding of the actinide series as a whole. It is this fundamental research program that constitutes the foundation for the more applied actinide-oriented studies in the nuclear fission fuel cycle. These include isotope separation; fuel form preparation; chemical reactivity of actinides with fission products and coolant and fuel element cladding components; fuel reprocessing; waste management; and the behavior of actinides in environmental and biological systems.

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Basic Energy Sciences - continued

An increase of \$475,000 in FY 1979 is requested for heavy element research. At Argonne National Laboratory (ANL), a major effort is devoted to a study of the spectroscopic properties of the actinides which should provide an improved understanding of the electronic energy levels in various host media. This information is showing promise for the development of new laser materials and analytical techniques using the lanthanides and possibly the actinides, and has resulted in the measurement of isotope shifts in the visible region, where excellent prospects for photochemically induced separations processes exist. The ANL group also works in collaboration with the laser fusion effort at Lawrence Livermore Laboratory (LLL). Another important study at Argonne is the investigation of the complex actinide oxide chemistry that takes place in long-burnup fission fuel elements. Chemical stability data has been derived for several fission product - actinide - oxygen compounds. At the Lawrence Berkeley Laboratory (LBL), a major effort continues in the study of actinide sequestering agents: the preparation of the compounds; measurement of their chemical stability; and molecular structure determinations. Preliminary testing in biological systems of prototype compounds in cooperation with the DBER - funded Donner Laboratory at Berkeley is underway. At Oak Ridge National Laboratory (ORNL), a study of the chemical properties of the transuranium elements (the very heavy actinides) is pursued. This includes element and compound preparations, determination of crystal structures, solution thermochemistry, photoelectron and x-ray spectroscopy, and fast-chemistry studies of short-lived, accelerator-produced heavy elements. A new research activity is the collaborative study of the ion exchange properties of geologic media with respect to actinides and fission products. This is in cooperation with the Assistant Secretary for Energy Technology's waste management program. This work is part of the new effort in the investigation of the general solution chemistry of the actinides. Several new programs are planned at Lawrence Livermore Laboratory and elsewhere in the study of einsteinium, fermium, and mendelevium chemistry and the investigation of magnetic and gas-phase thermodynamic properties.

b. Isotope preparations \$ 8,300

This subactivity supports at Oak Ridge National Laboratory a major effort in the production, separation, purification, and distribution of special elemental and isotopic samples for the research and development programs of an international community. The electromagnetic isotope separation (Calutron) facility separates stable isotopes for sale on a cost recovery basis to Federal and non-Federal domestic and foreign customers for a wide variety of studies. Annual sales have averaged approximately \$1,700,000. A loan pool of samples is maintained for non-destructive measurements of nuclear data of importance to DOE's fission and fusion energy development programs and for long range basic research problems. This facility also has a limited capability for the separation of certain actinide isotopes having long half-lives. This subactivity also supports the High Flux Isotope Reactor (HFIR) and the Transuranium Processing Plant (TRU). At HFIR, certain isotopes from plutonium to fermium (elements number 94 to 100) are produced by successive neutron capture. HFIR also provides irradiation services for non-routine isotope production as well as on-going user research programs on a "irradiation-unit recharge" basis. The TRU facility processes the isotope production targets from HFIR and separates and purifies the research samples for the scientific community studying the transuranium elements. The isotope preparations subactivity is the only source of supply in the western world for a number of the isotopes produced at the above-mentioned facilities. An increase of \$600,000 is requested for the services provided under this subactivity.

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Basic Energy Sciences - continued

2. Materials Sciences \$ 72,000

Materials sciences conducts basic research on materials properties and phenomena important to all energy systems. The aim is to provide the necessary base of materials knowledge required to advance the nation's energy programs. Materials often are the key limiting factor in the development of new systems, the performance of present systems, and the evolution of advanced concepts. In this activity, emphasis is placed in areas where problems are known to exist or are anticipated, and where significant improvements in performance must depend on the selection of materials (and engineering design) based on improved understanding of the underlying mechanisms. The activity includes a very broad spectrum of materials research from which: new solutions and new materials will emerge to apply to existing problems; insight will be provided to identify future materials trouble spots; and working models will be formulated to deal with unpredicted problems or phenomena when encountered.

During the past year, through interaction on the Energy Materials Coordinating Committee, program reviews, scientific symposia, and particularly the Materials Sciences Overview Workshops, the materials sciences staff and contractors have become more fully aware of the materials problems facing the Department of Energy, the research areas in need of emphasis, and the scientific opportunities ripe for exploitation. Because of the magnitude of the problems and the identified areas of opportunity, a more aggressive basic materials research program is required. Improved or new materials and expanded knowledge of the properties of conventional materials are required in all aspects of energy generation, conversion, transmission, storage, utilization and conservation. All too often, systems designers assume that materials with properties to meet requirements are available, discover that they are not, and then must make substitutions which compromise objectives in order to demonstrate feasibility of the concept. Developments in materials technology then become the pace setting factor in the maturing, or in some cases, the success of the concept. The full range of DOE's activities will require materials of almost every conceivable type to operate in environments from the mundane to the harshest imaginable. It takes a minimum of ten years for a new material to gain commercial acceptance. Most energy technologies have severe materials problems and new materials problems will emerge in these technologies. Also, new energy concepts will evolve in the years ahead with materials requirements not currently definable. Therefore, a strong, broad-based program of fundamental materials science is essential to assist the ongoing developmental programs and to provide the base for future programs.

In materials sciences, the disciplines of metallurgy, chemistry, engineering, ceramics, and solid state physics are brought to bear in an interdisciplinary manner on problems relevant to energy systems. A substantial fraction of the research supported is multi-directional. The need is to increase those materials research areas important to the non-nuclear and conservation technologies, while at the same time maintaining the high priority research important to the fission and fusion technologies. Even within these latter technologies there are new problem areas which require fundamental research. In particular, the requested increase will be devoted to areas related to solar energy, fossil energy, geothermal energy, and energy conservation. The new basic programs are being planned with recognition of the ongoing and planned applied materials efforts. This coordinated effort is facilitated by extensive communications among headquarters and field staff, for example, that occurring through the Energy Materials Coordinating Committee.

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Basic Energy Sciences - continued

Much of this research is conducted at the multiprogram laboratories in close proximity to the applied programs. In this manner, the transfer of new information and techniques into technology is facilitated; at the same time, the needs of the applied programs are brought to the attention of the basic research community. The national laboratories have specialized and unique facilities capable of attacking highly complex materials problems involving unusual or extreme experimental conditions. The FY 1979 request includes new research programs both at DOE laboratories and other laboratories, private and governmental. The intention is to exploit the special capabilities of each type of research facility with special attention also being given to research capabilities at universities. The support of university-based research programs is desirable not only for the excellent work performed at the universities, but also for the development of manpower highly trained in the critical area of materials science and its application to energy technologies.

An increase of \$6,291,000 is requested for materials sciences. This will enable the program to continue the highest priority research underway. Some ongoing research will be terminated to enable support of research in new exciting areas important to energy as identified by the series of Materials Sciences Overview Workshops held in the spring of 1977. Of the increase requested, \$1,000,000 will be required for the decommissioning of the Ames Laboratory Research Reactor, which was begun in FY 1978. Increases will also be provided for pre-construction R&D costs associated with the National Synchrotron Light Source construction project at BNL, which was started in FY 1978, and the Intense Pulsed Neutron Source at ANL, which is being proposed as a construction project in FY 1979. In addition, there will be increased utilization of research reactors and new high voltage electron microscopes. Research areas to be emphasized include solar-related research, surfaces, theory and modeling, polymeric materials, and engineering materials science (ion implantation, SQUID instruments, welding, erosion, nondestructive testing, as examples). An aggressive research program will be maintained in fields important to fossil (stress corrosion cracking, catalysis, MHD electrodes and insulators, sulfidation, and alloy design), conservation (battery electrode reactions, high temperature materials, separator materials, and hydrogen embrittlement and storage materials), geothermal (corrosion and scaling), fission and fusion (radiation enhanced creep and neutron-ion correlation effects, ceramic materials, superconductivity, and fracture technology) and solar related materials research. Throughout, materials sciences program development will take place in those areas aimed toward increasing our understanding of materials properties and phenomena to enable the technology developers to more quickly establish the economic and technical feasibility of their technologies.

Materials sciences is divided into three major subactivities: (a) metallurgy and ceramics, (b) solid state physics, and (c) materials chemistry. These reflect both the technical content and the primary discipline employed, as shown below:

	Actual FY 1977			Estimate FY 1978		Estimate FY 1979	
	BA	Obs.	BO	BA	BO	BA	BO
a. Metallurgy and ceramics	\$ 24,500	\$ 24,707	\$ 22,763	\$ 27,500	\$ 25,625	\$ 29,900	\$ 29,000
b. Solid state physics	24,571	24,707	23,956	28,699	26,917	32,100	30,200
c. Materials chemistry	8,870	8,940	8,232	9,510	8,865	10,000	9,700
Subtotal, materials sciences	\$ 57,941	\$ 58,354	\$ 54,951	\$ 65,709	\$ 61,407	\$ 72,000	\$ 68,900

28.8
226.2
8.5
- 211.3

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

a. Metallurgy and Ceramics \$ 29,900

Under metallurgy and ceramics, research is conducted to better understand the relationship between materials properties and structure. Understanding this relationship is the key to improving present materials and creating new materials to meet the demanding needs of future energy systems. Important properties of materials such as fracture, plastic flow, superconductivity, corrosion resistance, radiation resistance, transport phenomena and others all depend on structure. As our understanding becomes more complete and our ability to create the beneficial structures increases, it will be possible to design materials to meet engineering requirements - a task not always possible at the present time. This research will ultimately enable designers to more accurately predict the behavior of materials and changes in material properties as a function of time, stress and a variety of environments. Although basic in nature, the program is centered around research areas deemed to be of greatest interest for energy systems. For example, there is within metallurgy and ceramics a strong emphasis on hydrogen effects, radiation effects, high temperature ceramics, erosion, corrosion, refractory metals and superconductivity, all important topics for energy systems.

An increase of \$2,400,000 is requested for metallurgy and ceramics. New research will be initiated in the areas of: environment accelerated fracture; solar energy; advanced techniques such as high voltage electron microscopy and ion channeling to investigate materials properties; radiation enhanced creep; small angle x-ray scattering; corrosion and sulfidation important to coal conversion processes; and high temperature strength and transport phenomena in ceramics and refractory alloys, among others. Research in engineering materials started in FY 1978 will focus attention on needs and research in the area of more complex phenomena and materials. Research in this area will provide the necessary transition between the relatively well understood simple materials systems and the complex materials systems utilized in energy conversion programs. Examples of work to be emphasized include: solidification and properties of weld metal, non-destructive evaluation and new processing techniques. The metallurgy and ceramics research reported here is closely coupled to the applied energy programs which are often supported within the same DOE laboratory division where both applied and basic research are conducted. This close coupling greatly benefits the nation's energy programs, as demonstrated by the large number of both scientific and technological accomplishments during the past year. Important new progress has been made in understanding the mechanical equation of state, fracture, erosion, diffusion in solids, stress corrosion cracking, superconductivity, and radiation enhanced creep, for example. The requested increase will permit a continuation of high priority programs in the base program and modest increases in the new areas cited below when coupled with selected decreases in other areas.

The structure of materials area supports research designed to enhance our understanding of the atomic, electronic, defect and microstructure of materials. Representative accomplishments during the past year include: understanding the atomic bonding in refractory metal carbides, determination of the electronic structure of binary and ternary oxides which are potential catalysts; and the development of a theory to explain composition inhomogeneities and structure of cast alloys. With the availability of several new experimental techniques to examine the structure of materials at all levels, this area is receiving special attention, and an increase of \$490,000 is requested. Highlighting the utilization of new techniques will be the completion of the installation and start of research at the high voltage electron microscope (HVEM) at ANL and

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the delivery and initial work on the 1.5 MeV HVEM at LBL. With these instruments, unique defect and microstructure studies will be possible in gaseous environments simulating those encountered in the actual use of a material. Phenomena such as oxidation, sulfidation or hydrogen attack can be studied for the first time as they actually occur. New initiatives during FY 1979 include both theoretical and experimental studies on materials with potential for energy storage, such as ceramics and hydrides. There will be an increase in effort to understand the physical and electronic structure of catalyst materials using new techniques such as x-ray photoelectron spectroscopy and small angle x-ray scattering. Programs to study the stability of the structure of high temperature alloys in the gaseous environment of coal utilization systems and the structure of coal using the new experimental techniques will be emphasized. In the area of solar energy, research will be conducted on the properties of photovoltaic materials prepared by unusual techniques such as sputtering. Also, new efforts to understand the basic electronic phenomena associated with impurities, defects, and surfaces in semiconductor photovoltaic materials will continue. Finally, research on understanding the structure and its development in high temperature materials will be emphasized.

Fundamental aspects related to structural integrity of all classes of materials are addressed in the mechanical properties area. Advances in alloy design and development are required for load-sustaining components of energy systems - ranging from cryogenic superconducting metals and intermetallic compounds to high temperature ceramics for energy conservation and coal conversion. Experimental and theoretical efforts are underway to investigate constitutive equations for creep and fatigue, deformation and fracture mechanisms, elastic behavior, and effects of corrosive gas and liquid environments, among others. Substantive progress was achieved last year in several areas: modelling fracture of fiber reinforced composites considered for flywheel energy storage, where high reliability is essential; correlating short time stress relaxation of steels and other metals with their long-term creep behavior, which offers possible reductions in the now-costly acceptance testing of alloys; measuring internal stresses generated in steels during tensile deformation and relating these to cyclic loading, as expected in turbines and pressure vessels; determining the influence of oxygen on hydrogen embrittlement of refractory metals and explaining the brittleness of their hydrides in terms of ordering of hydrogen atoms in the metal before its transition into a hydride, both effects being relevant to hydride storage technology; and establishing an analytical framework for surface film-induced softening of metals, as might be encountered in corrosive media. An increase of \$510,000 is requested to continue this important research and expand it selectively - in the areas of nonmetallic materials, theory, coatings and environmental interactions. Because of the need for refractory materials in both nuclear and non-nuclear energy concepts, new projects will be started on deformation mechanisms and crack initiation and growth in ceramics and intermetallic compounds. Structural degradation due to stress corrosion cracking, hydrogen embrittlement, and corrosion fatigue remain as major problems in energy plants. Therefore, cooperative mechanical-environmental phenomena warrant continued emphasis, as does the mechanical stability of coatings. High voltage electron microscopy will be developed and used for in-situ characterization of both structural and dislocation configurational changes associated with these phenomena. Increased theory is planned to evaluate the location of gas and other impurities in solids, grain boundary and interfacial structures, and their effect on resulting mechanical behavior.

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The physical properties area includes research aimed at increasing the understanding of fundamental phenomena controlling the thermal, optical, and electrical properties of materials. The effect of various heat treatments or other processing steps and external variables such as temperature and pressure on diffusion or superconductivity, for example, are being investigated. Representative examples of advances made this past year are: initiation of research at the new ANL positron annihilation apparatus to detect the presence of defects, voids, and crack nuclei which significantly affect materials behavior; an improved understanding of amorphous high temperature superconductors vital to the development of fusion power, MHD, and energy storage technologies; the pressure dependence of oxygen solubility in vanadium important for liquid metal utilization in breeder and fusion reactors; a new low temperature densification technique for ceramics which could provide significant energy savings in the electronic ceramics industry; an improved theoretical model of sulfur segregation in iron and nickel alloys important for fossil energy applications; and determination of the usefulness of sputtering as a technique to produce amorphous silicon for solar applications. An increase of \$410,000 is requested for this area. Research involving ceramics and superconductivity will expand utilizing new experimental techniques such as positron annihilation, EXAFS, and the HVEM. Several new efforts will be expanded on heat and mass transport in the steep thermal and composition gradients found in virtually all advanced energy systems. Other areas of increased emphasis will include surface effects, solute segregation and catalysis. A new surface properties program will be using ion implantation to control surface compositions. New studies on hydrogen effects and diffusion in intermetallic compounds, all critical to energy storage, will be continued. New efforts in solar thermal materials will be expanded, at the expense of decreases elsewhere in the program.

Research in radiation effects is directed toward understanding the interactions between radiation-induced defects and materials behavior needed for fission and fusion technologies. A broad theoretical and experimental program is supported on defect concentrations, their predominant transport mechanisms, structural and mechanical stability, and physical properties which are altered in radiation environments. Examples of recent accomplishments include: incorporating the binding energy between solutes and self-interstitials in void-swelling models; quantifying the lattice strain surrounding solute atoms and correlating this with swelling resistance of alloys; measuring, for the first time, the distance that metal atoms are displaced when impacted by energetic particles, which is a significant parameter determining cascade size; showing that transition metals can exist within discrete ionic groups rather than as part of the continuous network in glass and that these groups are readily leached out of the glass, which may limit its effectiveness as a host for radioactive nuclear waste. Important new particle accelerator facilities were brought on line for simulating radiation-enhanced creep of reactor fuel element cladding and for detecting near-surface segregation of solutes considered necessary for swelling resistance. Also noteworthy is the application of ion accelerators to non-nuclear needs, specifically to the study of planar defects in silicon being developed for photovoltaic solar energy conversion. The above capabilities will continue to receive emphasis in the future. In addition, support will increase for determining radiation effects in ceramics and glasses having potential for radioactive waste disposal. Substantial effort will be devoted to discerning events leading to clustering and dislocation loop formation and to the transition from these defects to void nucleation, using high voltage electron microscopy and combined gas-metal ion accelerators. An increase of \$350,000 is requested for this research.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Newly initiated engineering materials research supports basic studies aimed at understanding more fully the fundamental materials science on which engineering systems should be based. Some of the topics which are or will be studied include: friction and wear, mechanics, engineering corrosion and fracture studies, coupling of engineering design with materials sciences, joining and welding, nondestructive evaluation, extractive processes, and the forming and processing of materials. In general, this work will provide the link to engineering systems by studying more complex materials systems and phenomena. A modest start was undertaken in FY 1978 with new programs in weld pool solidification, nondestructive evaluation using ultrasonic techniques, processing of materials using sputtering techniques, brittle fracture and constitutive equations, fluid erosion, and engineering corrosion studies. The FY 1979 request will attempt to bring this program to a reasonable size with an increase of \$640,000. Programs on welding, nondestructive evaluation, and erosion will be strengthened. New efforts on ceramics processing and small angle neutron scattering as a nondestructive evaluation technique will be initiated.

b. Solid state physics \$ 32,100

Solid state physics is directed toward fundamental research on matter in the condensed state wherein the interactions and motions of electrons, atoms, and defects are analytically determined with the purpose of understanding the critical properties of solids and liquids, and their surfaces and interfaces. These interactions are the ultimate source of all materials properties. Research in solid state physics includes a broad spectrum of experimental and theoretical efforts which contribute basic solid state knowledge important to all energy technologies. Rapid advancements in unique experimental tools and the coupling of these tools with high speed computer systems have made important new advances possible. Through these efforts, fundamental understanding of matter in the condensed state contributes broadly to characterizing material properties and processes of basic interest covering many energy systems. In FY 1978, new engineering physics studies were begun on a small scale to fill a much needed gap between the current scientific efforts in solid state physics and the associated engineering needs. In addition, this area is designed to initiate new prototypic solid state concepts of an applied nature.

A few of the accomplishments during the past year include the following: (a) By a new field desorption, mass spectrometric technique, an organic structure has been imaged with a magnification of 2,000,000 times and a resolution of 8 angstroms. This achievement has great potential as a revolutionary development in microscopy. (b) A new laser glass material, BeF_2 , with the lowest nonlinear index of refraction coefficient ever reported, was fabricated successfully. This class of material has considerable potential for many laser system components. (c) A high temperature SQUID (15°K) was developed, and a SQUID magnetometer was successfully used in locating a geothermal anomaly deep in the earth without the necessity for drilling. (d) In the area of superconductivity, it was found that microwave radiation could enhance the critical temperature, and in the case of erbium-rhodium-boride, reentrant superconductivity, a new phenomena, was discovered. (e) Laser annealing of ion implanted solar grade silicon resulted in a composition distribution important to improved performance. This technique shows great promise for commercial application in manufacturing semiconductor devices. (f) The photoconducting threshold of germanium was increased from 100 microns to 200 microns by uniaxial crystallographic stress, thereby greatly increasing its capability as a detector in the infrared region, which is important in many scientific and technological areas.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

A central effort of this subactivity is directed toward accelerating progress in solid state physics research related to DOE programs in both the non-nuclear and nuclear areas. The FY 1979 request for solid state physics research is \$32,100,000, an increase of \$3,401,000 above FY 1978.

The neutron scattering task supports research of a unique kind, namely, the use of the neutron as an analytical probe of the properties of solids and liquids. With this probe, fundamental parameters of superconductors, hydrogenous materials, liquids and solid imperfections are determined in a manner that cannot be accomplished by any other technique. The exploitation of this probe is being advanced by recent development of more efficient monochromators, detectors, and by a small angle neutron scattering (SANS) facility for wider use of longer wavelength probes particularly important to molecular solids and polymers. The bulk of the nation's efforts in this important area has historically been supported at DOE laboratories where the advanced research reactors are in operation. However, rapidly escalating fuel costs are severely affecting the costs and operating efficiency of these facilities. The initial stages of the IPNS project will require operational funding of Booster II of the Zero Gradient Synchrotron complex, as well as the other R&D costs associated with design enhancement. In addition, funds are provided for the Ames Research Reactor decommissioning. To maintain a viable program for the use of neutron probes on hydrides, high temperature materials, surfaces, liquids, polymers and superconductors, an increase of \$1,560,000 is requested.

The experimental research task is very broad and includes all fundamental investigations, experimental in concept, on liquids and solids of metals, alloys, semiconductors, insulators, and compounds. The area of high temperature materials in both metals and non-metals, especially in relation to MHD electrodes and insulators as well as other high-temperature energy systems, will receive increased attention. Ion implantation and Rutherford backscattering research will be expanded to investigate surfaces, and to learn how to improve superconductor and photovoltaic performance. The studies of hydrogen and hydrides will be heavily pursued through ultra-high pressure and spectroscopic techniques. Superconductivity is a forefront area being given major attention through advanced techniques of fabricating composites and metastable materials of promise. Laser annealing of diffused species in solids will receive increased attention. Synchrotron light and low energy electron diffraction (LEED) will be more prominently utilized in characterizing surfaces with particular relation to catalytic response. Lifetime and recombination processes in important solar materials will be pursued, and a new search will be made for unusual thermal and electrical properties in new materials, including molecular solids and amorphous materials. The role of hydrogen siting and bonding in solids will be emphasized. With nearly all of these experimental areas, highly advanced theoretical research is closely coupled. A large part of the theoretical effort is directed toward dynamic processes in solids and liquids, and requires extensive use of DOE's most advanced computer complexes. Included in this research are theoretical predictions of LEED surface diffraction phenomena and modelling for predicting fracture propagation in solids. In advanced energy systems, material behavior is so unpredictable that a highly correlated experimental and theoretical effort is important. To support this experimental and theoretical research effort, an increase of \$1,491,000 is requested.

Under particle-solid interactions, a major effort will be given to correlating the complex effects of particles of different mass, energy, and charge not only on surfaces, but in bulk materials as well. Measurements of radiation damage in ultrathin metals have revealed results that are consistent with theory for the onset of damage in the early range of the damaging particle traverse. It is clear that correlation experiments are still of great importance even though synergistic effects make analysis very difficult.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Important experiments in the new area of low angle particle effects will be accelerated in sputtering processes. An increase of \$70,000 is requested for this area, which continues to be of considerable basic importance to fusion and fission systems.

A stronger effort is envisioned for engineering physics research in FY 1979. The purpose of this effort is to fulfill the much needed goal of utilizing solid state physics expertise in engineering physics research for which it has a unique capability, and in areas where it is now felt a gap exists. Typical of the work to be initiated are research laboratory investigations of novel processing mechanisms with mass spectrometer-computer control for complex material preparation (such as solar materials), and superconducting alloys, where large areas or very long lengths are required. SQUID improvements for mobile field instruments important to deep underground surveying will be pursued. Laser diagnostics of chemical vapor-deposition processes will be extended to improve material fabrication capabilities; ion implantation instrumentation will be studied as a continuous preparation process; and cryogenic and refrigeration techniques will be extended to new fluid systems which hold promise for the utilization of low grade heat. To accelerate this important new work, an increase of \$280,000 is requested in FY 1979.

c. Materials chemistry \$ 10,000

The materials chemistry subactivity embodies the application of chemical principles to attain an understanding of the interaction of large classes of condensed matter, with emphasis on the high temperature chemistry of molten salts and refractory oxides; the role of surface activity in corrosion, catalytic activity, and electrochemical phenomena; and the properties of molecular and polymeric materials. The principal contributions made by the program are generally the result of basic research performed by groups of scientists working in large team efforts. Examples of significant recent accomplishments include (1) the recovery of alumina from coal fly ash, (2) the structure correlation of composition of complex metallic hydrides with the vapor pressure of associated hydrogen, (3) the improved control of complex chemical equilibria governing the separation of plutonium from uranium in fuel processing, and (4) the adaptation of structural and phase relationships in metallic alloy systems leading to the fabrication of greatly improved electrodes for high performance batteries.

Among the most important areas included within the scope of this program are fundamental studies of the properties of the fuels to be used in both fusion and fission reactors. Extensive studies are made of the equilibria governing the fixation and separation of tritium, its interaction with metallic and refractory oxides and the factors affecting its confinement in heat exchange systems. The need for fundamental data on the properties of actinide elements and their compounds serving as nuclear fuels is being addressed by programs that include studies for the preparation of advanced oxides and carbides, including physical processes for the homogenization of mixed (U, Pu)O₂, the development of methods for the precise control of particle size distribution in blended powders, and kinetic studies of the processes by which the various chemical forms of the fuels can be attained and transformed, either by decomposition or interaction at high temperatures with metallic elements. The chemical activity of precisely controlled surfaces is investigated with sophisticated LEED-AUGER mass spectrometer instrumentation.

A considerable effort is devoted to the study of the behavior of metallic and refractory oxide systems at high temperatures. These studies include phase equilibria studies of bimetallic systems and studies of ionic bonding in refractory oxides derived from ionization potentials. A critical assessment of the thermodynamic properties of a large body of materials including the actinide oxides is in progress.

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Basic Energy Sciences - continued

An effort will be made to continue the expansion of the off-site research program. It is recognized that the support of university research plays an important role in the attainment of long-range objectives.

Several programs are being carried out in continuous exchange with investigations in the applied or engineering programs. In several instances, the basic research programs provide the foundation for the engineering designs incorporated into large scale processes, and thus fulfill an essential role in the attainment of the goals of the applied programs.

To provide for the increased materials chemistry activities described in the following sections, an FY 1979 increase of \$490,000 is requested.

The structural chemistry area emphasizes the relationships between the configuration of atomic and molecular aggregates and the physical and chemical properties resulting from these configurations. The principal tools used in studies of these effects are nuclear magnetic resonance and x-ray and neutron diffraction, which (because of the unique capability of neutrons for locating hydrogen atoms) supplement each other as probes. These methods are being currently employed in the structural analysis of materials of potential use as energy storage media, as catalysts for the conversion of coal, and the analysis of "one-dimensional" (or "metallic") conductors, which because of their structural features, exhibit greatly enhanced electrical conductivity, approaching superconductivity in several cases. It is planned to emphasize research of polymeric materials, and to carry out structural analysis of these materials by the use of small angle neutron and x-ray diffraction. The relationships between structure and function of polymeric materials will be studied for (1) the potential synthesis of tailor-made polymers for enhanced oil recovery, (2) investigation of compositional factors that influence resistance to weathering effects, and (3) the search for improved fluorinated polymers for potential use as battery separators and inexpensive semi-permeable membranes. An increase of \$110,000 is requested for structural chemistry studies.

Engineering chemistry research includes a wide variety of programs related to the improvement of the efficiency of operation of energy sources, such as advanced batteries for energy storage and vehicle propulsion, fluidized beds related to the combustion of coal, as well as the improvement of other electrochemical processes such as metallurgical separations and the purification of process streams containing fine particulates. Studies of the removal of particulate matter employing vortex separators (hydroclones) have been applied successfully to viscous liquids simulating those resulting from coal treatment and conversion. It is planned to follow these studies with fundamental studies of the performance and the regeneration of deep-bed filters for the removal of extra-fine particulates that would increase the erosion of coal conversion equipment.

Calorimetric studies and heat transfer measurements will be carried out on selected polymers chosen to represent various categories of chemical compositions. They would be extensively characterized with respect to molecular weight, branching, cross-linking, etc. The study of heat transfer and critical state properties will be made on a variety of liquids ranging from organic liquids that associate in the vapor phase to the molten alkali metals that may be used as coolants or blankets in fission and fusion reactors. Research in the chemistry of molten salts will be continued in support of the advanced battery program. These have proven especially fruitful in the recent determination of the solubility of iron sulfide in the eutectic mixture employed in the lithium-sulfur battery. The distortion and swelling of the positive electrode upon repeated charge-discharge

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Basic Energy Sciences - continued

cycles is attributed to the formation of an insoluble phase in this material, and efforts to understand these effects have been advanced by these studies. Changes in the morphology of the negative electrode have also been examined, and experiments are currently underway that are expected to lead to the choice of new ternary alloys whose structural stability under charge-discharge cycles is much improved over the binary alloys now in use. These studies have recently been joined by an effort aimed at reducing the electrolytic degradation of ceramic conductors (e.g., beta-alumina) that are used in a different type of advanced battery employing the lithium-sulfur system.

Recent improvements in the recovery of alumina from coal fly ash have reached the 90 percent level. It is planned to carry out exploratory work on the conversion of the contained aluminum by chlorination of the fly ash, thus converting it to a form that would be directly matched to the new chloride process for the manufacture of aluminum. Comparisons of the chlorination process with the calcination process can then lead to a possible consideration of technical and economic factors influencing a potential choice of treatment.

Sulfur fixation studies on atmospheric oxidation of sulfur dioxide will emphasize the design of instrumentation providing finer resolution of particle size. The investigation of the role played by nitrates in the oxidation of atmospheric particulates continues to be an important part of this program. Control of sulfur emission from fluidized beds through dolomite scavenging will focus on the single stage regeneration reaction, and will emphasize the relationship between the micro-morphology of the half-calcined dolomite and the important kinetics of the chemical reactions.

An increase of \$200,000 is requested for the support of these important efforts in engineering chemistry.

Research in high temperature and surface chemistry will emphasize programs for the systematic collection and correlation of data for high temperature systems. Special attention will be directed to the assembly of phase rule relations for bimetallic systems of elements such as molybdenum, chromium, and nickel with other metals. Interest in these metals arises from their occurrence in a wide variety of high temperature systems important to the conversion and combustion of fossil fuels in units embodying advanced designs. The drive for higher thermodynamic efficiencies in energy converters places extreme requirements on turbines. Efforts will be made to contribute fundamental information affecting the synthesis of such materials as silicon nitride for the fabrication of turbine parts.

High temperature measurements of electromotive force in cells using solid electrolytes will be made as part of a program for the prediction of thermodynamic properties of metallic alloys. Interactions between metals with different numbers of electrons in their low-lying orbitals have been found to exert a profound effect on the thermodynamics of metal systems, and have been responsible for unexpected reactions between metals and refractories in automobile exhaust catalysts, nuclear power space capsules, and a variety of high-temperature systems in which platinum-group metals are in contact with compounds of metals of the more reactive transition metals. Matrix studies will be designed for a detailed examination of the interaction of atoms in pairs, triatomics, and larger clusters, using ultraviolet and infrared spectral studies to follow the diffusion and reactions of the atoms to form clusters and to characterize the properties of the products formed. The role of surface properties in affecting geothermal scaling and the effect of surface impurities is stress corrosion cracking will be studied. The synthesis of tailor-made catalysts for selected hydrocarbon conversions will be attempted by ion implantation methods.

An increase of \$180,000 is requested for research in high temperature and surface chemistry.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

3. Chemical sciences \$ 48,200

Research in the chemical sciences is carried out in order to generate the understanding and data which will serve as the basis for effective development of energy processes and lead to new options. Typical of the energy processes which need better understanding in order to reach better economics and lessened environmental effects, are fuel combustion, coal conversion, catalytic improvements of coal-derived liquids, nuclear fuel reprocessing and magnetohydrodynamic energy production. New ground must also be broken in solar-related chemical effects. Therefore, the chemical sciences activity supports forefront research in energy-related areas of chemistry and physics which bear on processes in liquids, gases and plasmas, as well as some solids like coal and chlorophyll. In other words, this is research on the chemical and physical properties of molecules, atoms, ions, electrons and plasmas. In order to cover importantly needed new work bearing on combustion, catalytic conversions, coal liquefaction, solar photochemical possibilities, fusion and magnetohydrodynamics, and in order to maintain the vigor of current work in basic energy-related chemistry, an increase of \$4,915,000 to a level of \$48,200,000 is requested.

The research in chemical sciences is administered in two subactivities, fundamental interactions and processes and techniques. These and the tasks which they comprise are described separately in the following pages.

	Actual FY 1977			Estimate FY 1978		Estimate FY 1979	
	BA	Obs.	B/O	BA	BO	BA	BO
a. Fundamental interactions	\$ 21,165	\$ 21,470	\$ 20,036	\$ 25,541	\$ 23,795	\$ 27,661	\$ 26,800
b. Processes and techniques	14,100	14,307	13,350	17,744	16,530	20,539	19,900
Subtotal, chemical sciences	\$ 35,265	\$ 35,777	\$ 33,386	\$ 43,285	\$ 40,325	\$ 48,200	\$ 46,700

a. Fundamental interactions \$ 27,661

The fundamental interactions subactivity supports research in the most basic aspects of chemical reactivity at the level of interactions of individual molecules, atoms and ions. It is concerned with the nature of the forces between these species, the means by which they absorb energy and redistribute it, and the nature of subsequent reactions. These phenomena are equally important in combusting fuels, in photochemical systems absorbing solar energy, in fusion and MHD plasmas, in catalytic fuel conversion systems and in energy storage systems. Research supported under fundamental interactions includes work in photochemical and radiation sciences, chemical physics, and atomic physics.

Among the outstanding recent achievements in this area, three examples demonstrate its breadth of science and of practical pertinence. Some of its researchers are seeking deeper understanding of photosynthesis, for the ultimate purpose of bending it to man's use for making clean fuels like hydrogen and sunlight. They have been measuring chlorophyll's fluorescent lifetimes to learn how long a sunbeam's energy is held ready by the chlorophyll before the energy is re-radiated and thus lost from usability. Recently they discovered that chlorophyll can act as a laser, which means that fluorescent lifetime measurements on chlorophyll in laboratories around the world must be re-examined, since laser action might masquerade as

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

fluorescence. In a related area, a whole new set of possibilities for solar photocells to generate electricity has been opened by the discovery that silicon photoelectrodes, which cannot function in water cells because they become coated with silicon dioxide, can function for long periods in other solvents like alcohol. Further research may bring their performance up to useful levels of electrical output. The third example is provided by researchers in the basics of combustion who are seeking the understanding needed to reach more efficient and cleaner use of current and future fuels. They have succeeded in measuring velocities of gas motions simultaneously in two different directions in an automobile's firing cylinder, which represents an important beginning toward analyzing the central but poorly understood role of turbulence in combustion.

Research in photochemical and radiation sciences was, at one time, narrowly confined to the study of the fundamentals of the interactions of light and radiation with matter. The increase of knowledge over the years and the changing, expanding mission of the Department has led to a considerable broadening of the scope of this research in at least two directions. The photochemical conversion of solar energy to a more useful form is a specific example of radiation chemistry that is being explored in a wide variety of ways. The other new aspect is the recognition that radiation can be used as a tool in the exploration of many phenomena where the radiation itself is not of primary interest. For example, laser spectroscopy and the entire study of fast reaction kinetics are direct outgrowths of radiation chemistry techniques and methods.

An increase of \$980,000 to a level of \$1,334,000 is requested for research in photochemical and radiation sciences. Most of this increase will be used to expand the search for new options in solar photoconversion. Among the approaches to be expanded are photoelectrolysis, photogalvanics, and photochemical reactions in homogeneous solution, in micelles, at membranes and in thin films on surfaces. Many classes of organic molecules are being considered as candidates for the molecular storage of solar energy by photochemical reactions creating strained, energetic molecules which can be made to release their energy as heat on demand. Some new funds will go to new photochemical and radiation induced studies designed to bring the techniques of fast kinetics and spectroscopy to bear on problems of combustion and environmental concern.

The second area of fundamental interactions is chemical physics, for which a \$1,275,000 increase to a FY 1979 level of \$10,682,000 is requested. This task accommodates a broad spectrum of studies in the fields of chemical dynamics, spectroscopy, structural chemistry and theoretical chemistry. Such studies have applicability to fields as diverse as combustion, plasmas, catalysis, isotope separation and the development and application of lasers.

In the realm of chemical dynamics strong support of molecular beam research will continue. The field will see an increased emphasis on experiments in which the laser is combined in the beam experiment giving rise to what is called state-to-state chemistry. Here one can begin to study elementary reactions in the absence of side effects. Elementary reactions involved in real combustion systems will be studied. In addition, some modest beginnings will be made in FY 1979 to support research in the new area of laser-induced chemistry.

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Basic Energy Sciences - continued

In the field of spectroscopy, there are two primary aspects that are of special interest. One is the use of spectroscopic information to deduce molecular structure. A second is the development and application of diagnostic tools for studying combustion systems. Ongoing research at the Sandia Livermore Laboratory will expand with the construction of the Combustion Research Facility. This facility, which was begun in FY 1978, will be completed in FY 1980 but will require operating funds in FY 1979 to continue to develop the instrumentation and techniques required when the doors open to outside users.

The final area of chemical physics research that requires expansion is theoretical chemistry. Theoretical studies play a role not only in predicting molecular structures but also in predicting chemical reactivity. New emphases in theory will be on the application of the methods of quantum chemistry to the calculation of information useful in the areas of combustion and magneto-hydrodynamics. In addition, a slight increase will be required for the jointly (DOE-NSF) funded National Resource for Computation in Chemistry at Lawrence Berkeley Laboratory. This Resource, which will greatly strengthen computational progress of academic and other chemical scientists in energy research, will be in the second year of a three year experiment.

Atomic physics research uses experiment and theory to obtain information on the nature, the energies, and the energy exchanges of atoms and simple molecules and their corresponding ions, all under a wide range of energetic conditions. This information is indispensable to the conception and design of new devices for energy generation. A decrease of \$135,000 to a level of \$4,645,000 will permit the continuation of the present most promising programs while providing funds for priority research elsewhere in the chemical sciences activity.

Continued support of long-range atomic physics research is necessary because it provides basic data for, among other developments, estimating the long-range prospects of all the various proposed approaches to controlled fusion energy. The work includes the theoretical calculation of a large variety of cross-sections (ion-atom collision, ion-ion collision, and charge transfer), as well as more efficient and accurate mathematical methods of making such calculations. These are very complicated calculations, and answers can be obtained only by making certain approximations. Such approximate calculations must be checked by experimental measurements, particularly since the numbers will be used to compute the conditions that must be met in the design of very costly equipment to demonstrate fusion. These experiments will be emphasized.

A similar state of affairs exists in the DOE's vigorous pursuit of methods of using the magnetohydrodynamic phenomenon to increase the electrical energy yield of coal-burning generators. Here, also, estimates of feasibility depend on a knowledge of cross-sections that can only be obtained by appropriate theoretical and experimental work. This research, too, will be expanded.

b. Processes and Techniques \$ 20,539

Understanding of the basic process by which matter and energy interact is fundamental to the advancement of the spectrum of energy technologies of current and future importance to DOE's mission. The increasing complexity of the systems involved

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Basic Energy Sciences - continued

requires added insight in order to measure their behavior under unusual process conditions and often at extreme levels of detection. Identification and development of new chemical process concepts are important needs, along with the needs for improvements of existing technologies, and for meeting goals of resource conservation and conversion, all while minimizing environmental insult with acceptable economics.

The processes and techniques subactivity includes four areas: chemical energy, separations research, analysis, and chemical engineering sciences. The emphasis is on obtaining fundamental understanding of energy-related chemical problems and high quality scientific data upon which the more applied research programs can draw, and which leads the way for new process concepts. Reliable techniques are developed for the measurement of chemical and physical changes; for modeling systems or subsystems of concern to such energy considerations as generation, conversion or storage of fuels; for carrying out energy and mass transfer; and for control of the processes which are vital to energy technological efforts. The most basic efforts involve experimental and theoretical studies of chemical reactions which are important to the improvement of DOE's technological areas of interest and to providing entirely new process insights.

Researchers funded by the processes and techniques subactivity also have many important achievements to their credit. Recent examples include pinning down for the first time the means by which nickel catalysts are poisoned by sulfur so that they cannot function to convert low grade gases to methane fuel. This research also revealed the means to regenerate these poisoned catalysts back to usability. Another advance has opened the door to measurement of certain details of the molecular structure of coal's constituents which bear on the efficiency of conversion to liquid fuels and, equally importantly, on minimizing the formation of cancer-causing substances during coal conversions. A third achievement is the discovery of a simple chemical method for stripping lignins from the cellulose in wood, thereby freeing the cellulose for conversion to glucose and then alcohol.

The requested increase of \$2,795,000 for processes and techniques will be used to maintain current high priority efforts, and allow selected new efforts, particularly in those areas of chemistry important to the utilization of fossil resources and the production of synthetic fuels. The four tasks of this category comprise a well integrated set having mutually beneficial interactions. The fundamental chemistry and process studies of the chemical energy task includes a broad spectrum of chemical disciplines, including organic and inorganic chemistry, which particularly focus on chemical reaction process mechanisms and catalysis. It utilizes developments in analytical chemistry for reactant and product characterization and on separations and engineering science concepts in the process studies related to fuel conversion and storage. In the separations research task, new concepts of separation are studied to evaluate mechanisms and chemical complexities, to synthesize and study new chemical separating agents and to attempt resolution of technical problems limiting technological separations. The development of analytical techniques in the analysis task often involves specialized separations to a) effect the removal of interfering impurities, b) provide pure species for standards, or c) make quantitative analytical results more readily available. New separation processes can and do arise from solutions to particular analytical problems, and analytical needs are frequently identified in separations research. In the chemical engineering sciences task, the scientific base of such phenomena as turbulence, gas-solid reactions, and heterophase catalysis are studied to develop the interrelated chemical and mathematical formalisms for more accurate process engineering. Engineering problems related to DOE technological efforts often are based on empiricism and, accordingly, the research in this task works to strengthen the scientific base of the chemical engineering discipline.

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Basic Energy Sciences - continued

An increase of \$1,746,000 in chemical energy to an FY 1979 level of \$10,940,000 is requested to allow essential strengthening of efforts related to fossil energy, hydrogen production and storage, conversion of wastes to fuels, and catalysis (homogeneous and heterogeneous). These efforts include, for example, basic organic chemistry of coal constituents for the characterization of the chemical linkages with heteroatoms (oxygen, nitrogen, sulfur) and hydrocarbon structures and the relationship of these linkages to thermal and chemical cleavage reactions, and work on the mechanisms of hydrogen transfer in organic systems, all of which are important to possible new concepts for efficient use of the various fossil resources. The newly started research efforts in homogeneous catalysts will be strengthened, emphasizing the synthesis of organometallic clusters and their relationship to heterogeneous catalytic systems, catalysts useful for coal conversion and hydrocarbon synthesis. Heterogeneous catalysis and reaction kinetics under vacuum and pressure conditions will also be strengthened, to continue building the bridge between the fundamental properties and reactions under practical conditions. Of particular interest are the factors which lead to deactivation of catalysts as well as subsequent regeneration.

Research on thermochemical hydrogen cycles for dissociation of water molecules into hydrogen and oxygen will also be expanded with emphasis on the thermochemistry of difficult but promising reactions. The research efforts on conversion of cellulosic wastes to fuels will be maintained.

An increase of \$618,000 to a FY 1979 level of \$5,160,000 is requested for separations research. New efforts will be initiated in the radiation resistant processing of spent nuclear fuel to provide additional options for the treatment of waste streams. The increase will also allow strengthening of research on the use of energy-efficient cyclic absorption techniques for the removal of tritium, krypton and carbon-14 from spent fuel reprocessing effluents. Research will continue on new more selective extraction agents, the study of transfer mechanisms in contacting devices, and the recovery of uranium from both phosphate plants and fossil fuel fly ash. Research on separation methods is an integral part of the application of science to technology. The ability to separate different types of molecules, fundamental to a number of analytical techniques, is of relevance to such technological needs as isotopic separations, solid-liquid separations in viscous fluids, the energy-efficient concentration of ores, the winning of metals from the ores and their purification, and the preparation of standards.

An increase of \$312,000 to a FY 1979 level of \$3,923,000 is requested for the analysis task to allow the continuation of research on new absorption and emission spectroscopic techniques which have already been shown to provide quantitative analyses of multi-component mixtures of cations, even when their concentrations vary from trace to major components. Research will also be continued on the application of nuclear particle techniques to special problems and the application of the gas chromatograph-mass spectrometer combination, which is an extremely sensitive and quantitative tool, for detection of trace organic molecules. Chemical analysis is vital to the study of chemical processes since the study of a process depends upon the ability to identify and determine quantitatively the amounts of reactants and products at various concentration levels as a function of time, pressure, and temperature. The ability, therefore, to obtain precise kinetic and thermodynamic process data is dependent on forefront development of analytical techniques.

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Basic Energy Sciences - continued

An increase of \$119,000 to a FY 1979 level of \$516,000 is requested for the chemical engineering sciences task to address the difficult problems of turbulence modeling needed for combustion codes; development of thermodynamic models for establishing the properties of complex chemical substances including multicomponent systems; the development of advanced models for catalytic reactions using such new catalytic concepts as interfacial and fluid phase transfer catalysis; and gas-solid reaction modeling with the related mass, heat and momentum transport. Emphasis will be given to improving and/or developing the scientific basis for engineering generalizations, unifying theories and innovative processes. Such efforts are expected to advance work in fluid mechanics, particle dynamics, mass and energy transport (steady and unsteady state), engineering thermodynamics, and physical and chemical rate processes. The ongoing research on models for gas phase reactions in fluidized beds and entrained suspensions of importance to the scale-up of conversion units for synthetic fuel is being maintained.

4. Engineering, mathematical and geosciences \$ 23,200

Three important disciplines are grouped together under this activity and each has important goals underlying DOE's mission. A significant increase of \$11,720,000 to an FY 1979 funding level of \$23,200,000 is requested for this activity. The increase is necessary to initiate efforts in the long neglected area of engineering sciences and to expand to more credible levels research in applied mathematics and geosciences, all of which are directly intertwined with virtually every energy technology currently being developed or envisioned for the future.

	Actual FY 1977			Estimate FY 1978		Estimate FY 1979	
	BA	Obs.	BO	BA	BO	BA	BO
a. Engineering sciences	\$ 0	\$ 0	\$ 0	\$ 0	\$ 0	\$ 3,660	\$ 3,600
b. Applied mathematical sciences	6,800	6,839	6,539	7,420	6,947	11,810	11,600
c. Geosciences	3,511	3,540	3,384	4,060	3,790	7,730	7,600
Subtotal, engineering, mathematical and geosciences	\$ 10,311	\$ 10,379	\$ 9,923	\$ 11,480	\$ 10,737	\$ 23,200	\$ 22,800

a. Engineering sciences 3,660

This new subactivity is to be launched in recognition of very important gaps and needs for understanding and data in energy-related, broadly pertinent areas of engineering science. Progress in many kinds of energy systems will develop on sounder bases and with fewer costly delays as a result of the efforts supported in this subactivity. Five general areas have been identified which have needs for insights and hard data and in which new, advanced techniques will help to serve the needs. The work to be supported will therefore be selected from among these five and other important areas of energy related needs as they are identified by planned workshop activities.

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Basic Energy Sciences - continued

One of the five areas is applied mechanics, in which research is needed, for example, on the dynamics of submerged cylinders important in geothermal systems and underground fuel storage. Equally important is an ubiquitous problem of vibration damage to high-flow heat exchangers, causing costly overdesign. Automobile undercarriage aerodynamics and the more general subject of tribology (friction studies) are in need of attention.

A second area is advanced instrumentation, for example, optical remote thermometry to very high temperatures and studying the feasibility of underground radar to monitor in situ extraction processes or to select sites for nuclear waste storage. A third area is nondestructive testing where field units are needed for identifying parameters of dynamic behavior of structures which have nonlinear behavior characteristics threatening catastrophic failure. Similarly, means are needed for production-line spotting of cracks or voids in large wind turbine blades and similar components.

A fourth area needing attention is process control in energy systems, such as enzymatic conversion of wastes to fuels. Many process variables interact and have strong impact on efficiencies; these are to be analyzed, reduced to computer-amenable algorithms and optimized, for both specific systems and more general models. A fifth area of opportunity is applied electronics, aimed at higher temperature semiconductor devices, high voltage-high power semiconductor switches and improved energy storage capacitors.

For these initial efforts, FY 1979 funding of \$3,660,000 is requested in order to make viable starts in the areas described above. Emphases among them will be guided by planning workshops involving leading engineers and scientists. Because of the importance of this research, attempts are being made to identify within basic energy sciences funding for FY 1978 some resources to permit a very minor start on this work in FY 1978.

b. Applied mathematical sciences \$ 11,810

Applied mathematical sciences supports research in applied analysis, statistics and numerical mathematics, together with closely related topics in computer science. Emphasis is currently placed upon research underlying computational modeling: qualitative and quantitative analysis of very large, complex models arising from the technology of energy production, distribution and utilization, together with their environmental and health-related effects. Research efforts are directed toward: (a) analytical and numerical methods for formulating and solving large, complex models; (b) methodology for creating and evaluating efficient, reliable numerical software and (c) techniques for accessing and sharing computational resources via high-capacity computer networks.

It has become apparent that the current program is seriously inadequate for DOE's present and coming requirements. Therefore, an increase of \$4,390,000 to a level of \$11,810,000 is requested for bringing vitality to this research. Of this increase, \$685,000 is needed to initiate research in statistics and operations research underlying the exploratory analysis of very large data collections and the validation of large-scale socio-economic models. The basic characteristics of the large data set problem is a combination of two features: (1) the quantity of data taxes our technical ability to organize, display and analyze; and (2)

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

knowledge in the field of interest is insufficient to design a process which will summarize the information content of the data. Together, these features eliminate the possibility of adequate analysis by straightforward application of classical statistics. Such data collections exist in DOE today and, with the increasing focus on fossil and uranium resource data, environmental and health-related and energy supply-demand data, additional collections are continuously accumulated. Large econometric and environmental models are used to develop alternative strategies based on such data collections. There exists no accepted methodology for validating these models, for example, estimating sensitivity to errors in input data, estimating probability distributions of output data, sampling techniques for exercising large models and testing criteria.

An increase of \$470,000 is requested to expand research in software engineering to investigate impediments to lower cost development of reliable, efficient software for the classes of computational modeling and data management tasks prevalent in DOE. Software engineering research underpins the development of programming aids required to cope with the complexity of designing and developing the large programs typical in DOE applications. Areas of potential interest include: programming languages (e.g., languages which facilitate use of advanced architectures); program analysis; programming optimization; program transformation; and program validation. The cost of developing, using and maintaining software increasingly dominates the capital investment in computing equipment. Since this capital investment in DOE exceeds \$550,000,000, the impact of even small improvements through improved programming methodology will be great.

An increase of \$1,890,000 is requested to initiate a much-needed research program in advanced computation systems. Historically, computing requirements of the AEC, ERDA and now DOE have justified procurement of computers with the highest level of arithmetic performance. Recently, the requirements to manage very large collections of scientific, engineering, environmental and health-related, and socio-economic data have justified the procurement of the largest available storage devices. In both cases, the architecture of the available systems dictated their usage. But the magnitude of the problems facing DOE now requires a turn-around, such that future large-scale, high performance resources reflect the problem to be solved. Problem-oriented systems responsive to DOE requirements, requirements which do not match the mass market of the computing industry, can only be developed as we increase the communication between system architects and system users. Therefore, it is proposed to initiate ventures designed to identify features of major DOE problems, identify possible characteristics of future systems and compare the match between algorithmic and architectural features. It is particularly important to investigate the distribution of computational tasks across the power spectrum of future systems, systems ranging from special configurations of microprocessors to super computers.

An increase of \$945,000 is requested to initiate research in data management. Many DOE functions depend on the availability of information. Functions such as socio-economic impact studies, monitoring energy resources, policy analysis, resource allocation and the planning and siting of large-scale facilities require information extraction from multiple data sources. The need for proper tools to manage this information in DOE is complicated by the fact that data sources are numerous, heterogeneous and often geographically dispersed. Research issues in data management can be categorized into four general areas: user interfaces, system performance, distribution of the data base and data base transfer and conversion. For example, a performance issue is the study of access methods and storage structures to yield a specification of storage structures, both logical and physical, most suitable for very large data base applications.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

The balance of the requested increase, or \$400,000, will support development of numerical methods applicable to modeling of flows in three dimensions, e.g., methods applicable to combustion modeling, plasma simulation, and fossil resource recovery.

c. Geosciences \$ 7,730

The geosciences subactivity supports research in the earth and earth-related sciences with the principal goal of obtaining basic data and concepts which will further the Departmental objectives of (1) effective and efficient utilization of the nation's energy resources; (2) environmentally sound siting of large energy and energy-related facilities; and (3) maintaining and advancing the nuclear-based aspects of the national security and weapons programs. The research is focused on materials and processes of the earth with particular emphasis on the origin and space-time distribution of energy resources and on changes induced by energy-related resource extraction, conversion, consumption and waste by-product disposal activities. The long-term research objective of the program is the development of a physically sound and theoretically-based predictive capability regarding the formation and occurrence of energy and energy-related resources and the effects of energy-related actions on natural processes and materials. The currently supported research activities in the geosciences at universities, colleges and DOE national laboratories include:

- (1) geology and earth dynamics (large-scale earth movements, rock deformation and failure and properties of earth materials);
- (2) geochemistry (aqueous geochemistry, physics and chemistry of magmas, geochemistry of fossil fuels, rock-water interactions);
- (3) energy resource recognition and evaluation (information compilation, evaluation and dissemination, reservoir dynamics and modeling, exploration and analytical techniques); and
- (4) solar-terrestrial and solar-atmospheric interactions.

Research in these four broad areas is generic in nature and typically impacts on more than one energy resource technology (solar, fossil, geothermal and nuclear), conservation, national security or environmental aspects of the Departmental objectives. Four examples of the accomplishments in the basic geosciences during the past year are: determination of the temperature dependence of silica polymeric behavior in concentrated brines; development and use of quantitative method of analysis for both organic and inorganic sulfur in coal and coal constituents; determination of mode of fluid flow through crystalline rocks of low permeability at elevated pressure and temperature; and a successful multisensor approach developed and applied to determine size, shape and properties of a lava lake. In addition, the basic geoscience reservoir dynamics program at LBL has spun off applied research efforts which are now being supported by the radioactive waste disposal, geothermal energy and conservation programs in DOE.

The requested increase of \$3,670,000 to an FY 1979 level of \$7,730,000 will provide for a significant and necessary expansion of the geoscience base research program; initiation of an important new interagency (NSF, USGS, DoD) program of deep continental drilling; starting a long-term, interdisciplinary and coordinated multi-agency (USGS, NSF) program of fundamental studies related to chemical migration in the earth's crust; and initiation of an interagency (USGS, NSF) program designed to provide the

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

information necessary to evaluate the petroleum of marine sediments and rocks of the U.S. continental rise and slope. These activities are all supportive of the DOE technologies, or policy objectives, and are intensively coordinated at the inter- and intra-agency levels.

5. Advanced energy projects \$ 3,800

The advanced energy projects activity was initiated in FY 1978. Its objective is to seek out and support novel concepts related to energy research. These may involve new ideas, only recently proposed, or, in some cases, ideas which have been around for a while but, for one reason or other, were not actively pursued. A special category among projects supported by advanced energy projects includes concepts which are multidisciplinary by nature and therefore do not clearly fit into the existing DOE program structure.

Projects are selected from unsolicited proposals submitted by industrial concerns, universities and national laboratories. The preferred mode for proposal evaluation is peer review. Projects recommended for funding are normally supported at a level not exceeding \$200,000 per year, and usually for a period no longer than three years. It is assumed that successful concepts will eventually be transferred to the technologically appropriate DOE organizations, or else be picked up for funding by other organizations, private or public.

Examples of projects currently funded include a proof of concept study on a solid state heat engine with potential applications in the fields of solar energy and conservation, and basic studies on solar energy concentration. Proposals under active consideration include such topics as advanced concepts in electric power generation and storage, solar energy conversion, and hydrogen production.

The FY 1978 budget provides for support of about 20 projects. The proposed increase of \$613,000 in FY 1979 would allow continuation of promising work initiated in FY 1978, as well as the starting of a few new projects in FY 1979.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Capital Acquisition:

Capital Equipment:

1. Nuclear science \$ 1,300

The nuclear science research program is based at a number of accelerator and reactor facilities and has a continuing requirement for a variety of equipment items for research, facility operations, and isotope services. The following is a listing of examples of equipment items required in the nuclear sciences activity:

Argonne National Laboratory \$ 120

New items of equipment are needed to start up new weak interaction experiments and to provide instrumentation for the new photon detector system. Additional equipment is needed for accelerator and heavy element research projects. Items required include electronics (\$20,000); computer terminals (\$15,000); a gas jet source (\$15,000); a magnet power supply (\$10,000); a low-mass spark chamber (\$30,000); and a differentially pumped gas target (\$30,000).

Brookhaven National Laboratory 528

The National Nuclear Data Center (NNDC) compilation project requires \$505,000 in FY 1979 to complete the upgrade of the computer system based on the Central Data Processing Unit acquired in FY 1978. This consists principally of a high-density disk subsystem (\$160,000), a computer magnetic tape subsystem (\$155,000), a new core memory (\$140,000), a special line printer controller (\$40,000), and an upgrade of an existing disk controller (\$10,000). The total estimated cost of the NNDC computer system is \$900,000 including \$395,000 in FY 1978. The remaining \$23,000 is for miscellaneous equipment, including electronics for the neutron nuclear measurements program.

Lawrence Berkeley Laboratory 120

The heavy element research program at Berkeley requires a nuclear magnetic resonance (NMR) proton and carbon-13 spectrometer (\$120,000) for the structure studies of actinide-bearing organometallic compounds and plutonium sequestering agents.

Los Alamos Scientific Laboratory 70

Equipment is needed for high precision, low energy, charged particle cross section measurements in support of fusion energy studies. The major items are an energy analyzing and transport system (\$20,000); a regulated power supply (\$20,000); detectors (\$10,000); and electronics (\$20,000).

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Mound Facility \$ 40

Mound Laboratory requires equipment items such as chemical precipitation and evaporation components necessary for the production of special stable and heavy element isotopes for research purposes.

Oak Ridge National Laboratory 310

At ORNL, the nuclear sciences activity sponsors work at the Oak Ridge Electron Linear Accelerator, the High Flux Isotope Reactor, the Transuranium Processing Plant, the Transuranium Research Laboratory, and the Calutrons. Some of the most important equipment needs at these facilities include electronics and power supplies (\$50,000); actinide element fission chambers (\$16,000); a gas purification system (\$7,000); Calutron liners (\$30,000); a Californium irradiation facility (\$40,000); heavy element processing equipment racks (\$60,000); an ORELA klystron tube (\$60,000); and detectors (\$35,000).

Pacific Northwest Laboratory 10

Various items of equipment are needed in support of the fission product mass spectrometer system at PNL.

Offsite Research Contracts 102

The nuclear science activity supports three major university-based accelerator operations (at Duke University, the University of Colorado, and the University of Wisconsin) and in-house research programs. Diverse items of equipment, such as ion-source components, accelerator tubes, and data acquisition and computer components, are needed to keep these machines in proper operation and to support the research programs carried out at these locations.

2. Materials sciences \$ 5,900

The materials sciences activity has greatly expanded its research initiatives in non-nuclear energy fields related to solar, geothermal, conservation, and fossil energy while maintaining the important programs related to fission and fusion energy needs. Major new efforts have included corrosion research relevant to fossil and geothermal energy; electronic properties controlling photovoltaic and photothermal processes in solar energy utilization; and catalysis research needed for both coal conversion and fuel cells. This continuing reorientation and the need to maintain forefront research to understand materials behavior in these and other energy problem areas is dependent to a large degree on high quality equipment. Reflected in this equipment request, therefore, is the need both for providing new capabilities as well as for upgrading present instrumentation.

Major equipment needs are required for the following: engineering materials sciences - for research in welding, which is important for understanding the joining problems in pressure vessels for fossil and nuclear energy plants (\$170,000); computer control of evaporation of multicomponent thin-film superconductors, sputter-deposition of refractory ceramics, surface

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

science analysis of surface composition and structure and their effect on processes such as catalysis (\$390,000); advanced electron microscopes - one to study in-situ deformation and fracture and another to correlate surface and bulk structure (\$475,000); synchrotron radiation instrumentation - primarily for beam monochrometers and detectors and for a control system for simultaneous experiments planned on all classes of materials at the National Synchrotron Light Source being built at Brookhaven National Laboratory (\$520,000); studying environmental effects on gaseous and liquid corrosion and localized effects anticipated in nuclear, fossil, geothermal, corrosion and electrode reactions encountered in battery and fuel cell systems (\$280,000); mechanical properties - for cyclic loading in low cycle and corrosion fatigue (\$260,000); optical, electronic, and magnetic effects - for high critical temperature and field superconductors needed in fusion and magnetohydrodynamics, optical absorption and emission of photothermal solar materials, and characterization of photoelectrodes and metal-insulator-semiconductor photo-voltaics (\$430,000); neutron scattering - for emphasizing the uniqueness of the neutron probe of structural and hydrogen effects and providing beam analysis for the planned Intense Pulsed Neutron Source at Argonne National Laboratory (\$750,000); radiation effects - for exploiting the combined high voltage electron microscope and ion accelerator at Argonne National Laboratory (\$570,000); specimen preparation - for advanced casting and sputtering apparatus to be used in preparation of complex metallic, ceramic, and composite materials (\$250,000); and computerized data acquisition and processing - for efficient calculations needed for modeling and experimental data analysis (\$430,000).

The following is a listing of examples of equipment items required in the materials sciences activity:

Ames Laboratory \$ 550

Funding is required for equipment to support new and expanded projects on surface modification and characterization (\$90,000); for research on optical and solar materials (\$110,000); for apparatus for superconductor materials research (\$60,000); for coal characterization apparatus (\$80,000); for studies of transition metal clusters (\$60,000); for specimen transfer units and vacuum systems needed for hydrogen embrittlement (\$20,000); for corrosion studies (\$10,000); and for purification and casting of rare earth and refractory metals (\$30,000).

Argonne National Laboratory 1,600

The following equipment items are required at ANL: transmission electron microscope for analysis of defects in metals and ceramics controlling deformation and fracture, and structural stability of metals and ceramics (\$250,000); a transport system and target chamber to permit simultaneous ion and electron irradiation of specimens in the high voltage electron microscope (\$350,000); spectrometer control circuitry and a computerized system for time-of-flight and pulse height analysis for the Intense Pulsed Neutron Source (\$400,000); prototype SQUID field instrumentation (\$100,000); an electron diffraction unit for analyzing sulfur bonding in dolomite used in coal conversion (\$25,000); a spectrophotometer for measuring absorption in films for potential solar applications (\$35,000); a microcalorimeter for characterizing fission product compounds (\$50,000); surface characterization and property measurement equipment (\$100,000); and a superconducting magnet (\$120,000).

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Brookhaven National Laboratory \$ 910

The primary equipment needs are associated with the High Flux Beam Reactor and the National Synchrotron Light Source (NSLS). Equipment funds are needed for replacing crystal shielding at one reactor port (\$70,000); upgrading spectrometer motor control circuitry for all ports (\$150,000); apparatus to improve beam collimation (\$150,000); synchrotron vacuum lines for the design of the NSLS (\$100,000); x-ray and ultraviolet monochrometers and detectors (\$200,000); an experiment control system for the NSLS (\$150,000); and thin film apparatus for superconductivity and solar research (\$50,000).

Idaho National Engineering Laboratory 70

An environmental test chamber with atmospheric controls for geothermal scaling and corrosion studies (\$25,000) and specialized photographic equipment for welding research are required (\$30,000).

Lawrence Berkeley Laboratory 360

Equipment needs include updating of the mechanical test facility used to study plastic deformation of metals (\$60,000); a furnace and control system for hot corrosion studies (\$20,000); image analyzers for obtaining quantitative data from electron micrographs and interferometer photographs (\$50,000); an ellipsometer for investigating boundary layers formed in electrochemical processes (\$30,000); an electrochemical machining apparatus (\$40,000); and surface science equipment including a catalytic chamber (\$80,000).

Lawrence Livermore Laboratory 110

Equipment is required to measure dielectric losses and residual stresses in thin films (\$20,000). Other equipment requirements include a specialized camera to monitor laser pulses (\$50,000); a cryostat for deuterium-tritium studies (\$10,000); and a furnace for hot corrosion studies (\$10,000).

Los Alamos Scientific Laboratory 130

Major equipment requirements are related to: development of stations for proton irradiation (\$60,000); mass spectrometry (\$30,000); and multiaxial deformation in high temperature materials (\$30,000).

Mound Facility 20

A spectrophotometer is required to measure absorption of liquids at high temperatures.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Oak Ridge National Laboratory \$ 1,450

Equipment is needed for: research correlating performance of solar photovoltaics to defects in bulk and ion-implanted thin-film semiconductors (\$100,000); hydrogen-related studies such as neutron scattering measurements of hydrogen diffusion in metals and permeation of hydrogen isotopes through candidate fusion reactor blanket materials (\$250,000); analysis of chemical structures and reaction mechanisms in catalysts and energy-storage compounds (\$100,000); radiation effects studies, the major item being a scanning transmission electron microscope to evaluate microstructural stability of irradiated alloys (\$280,000); characterizing optical and physical properties such as absorptivity/emissivity of solar photothermal materials (\$160,000); infrared and ultra-violet spectroscopy of ceramics (\$60,000). Magnetic susceptibility equipment is also needed for superconductivity research (\$70,000).

Pacific Northwest Laboratory 160

Equipment is needed for surface temperature measurements during sputter deposition of refractory ceramics (\$50,000); laser control of surface contours of optical materials during grinding to extremely close tolerances (\$40,000); apparatus for load cycling as encountered in corrosion fatigue (\$20,000); and instrumentation for monitoring laser scattering from materials (\$25,000).

Sandia - Albuquerque 140

An apparatus for a field ion desorption microscope (\$60,000) and equipment associated with ion scattering experiments (\$50,000) are required.

Sandia - Livermore 30

Residual gas analyzer and glove box facilities are required for tritium gas desorption experiments.

Off-Site Program 370

Funding is requested for equipment for coatings and surface modification research (\$90,000); work on solar collector materials (\$50,000); mechanical properties and fracture analysis studies (\$80,000); and materials processing work including polymers (\$70,000).

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

3. Chemical sciences \$ 3,300

Ames Laboratory \$ 306

A new advanced effort in molecular beam research, of wide pertinence concerning energy processes, requires a scattering chamber, a mass spectrometer and related instrumentation (\$100,000). A rapid scan spectrometer is needed for homogeneous catalysis studies and other solution kinetics (\$28,000). Detection equipment is required for fast spectroscopy (\$12,000), and the photochemistry research is in need of a laser and spectrometer (\$18,000). Equipment is required for coal studies which are advancing the state of the art in nuclear magnetic resonance (NMR), for new analytical techniques and necessary replacements (\$148,000).

Argonne National Laboratory 445

A pulsed Fourier transform NMR spectrometer is required for studies of surfaces, catalysis, fuel chemistry and photochemistry (\$275,000). Laser diagnostic equipment is necessary for research in basics of magnetohydrodynamics and plasma torches (\$40,000). The Dynamitron accelerator, used for fusion-related research, needs improved control systems (\$60,000). A linear subharmonic prebuncher (\$40,000) will double the electron linac's current per pulse, which would improve the photochemical and radiation science effort significantly. The coal structure research requires a time-of-flight mass spectrometer to replace an outdated instrument (\$30,000).

Brookhaven National Laboratory 570

A gas-chromatograph mass spectrometer analytical system (\$120,000) is required for research in plasma and hot atom chemistry, fuel research and related studies. The porphyrin research, with its wide range of instrumentation, needs a minicomputer for experimental control and data acquisition (\$125,000). Upgrading the HFBR's neutron spectrometer will cost \$132,000. For laser equipment and spectrometers for new programs in picosecond spectroscopy and laser-induced chemistry, \$100,000 is required. A signal digitizer (\$22,000) will interface with an existing computer for rapid data acquisition in multiphoton isotope separation studies. Quantitative detection of fragile molecules by separation of their derived relatives requires a high pressure chromatograph (\$12,000). Other miscellaneous equipment requirements total \$59,000.

Lawrence Berkeley Laboratory 375

A pulsed laser, associated spectrographic equipment and electrochemical apparatus are needed for solar photochemistry (\$65,000). As part of the interagency agreement with the National Science Foundation, communication terminals are to be provided for service to users of the National Resource for Computation in Chemistry (\$100,000). The molecular beam program will require \$65,000 to modify equipment for combustion research. A gas phase x-ray photoelectron spectrometer (\$90,000) is needed for

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

studies of organometallic compounds, catalytic surfaces and energetic oxidizers, and other equipment is needed for the oxidizer studies (\$25,000). Raman apparatus and tunable dye laser for measurements of sulfur-oxygen substances will require \$30,000.

University of Notre Dame \$ 145

Principal equipment needs include components and electronic support items (\$35,000) for the Linac and Van de Graaff accelerators, key instruments in this Laboratory's photochemical and radiation science. Also included are computer peripherals for use with the chemical and physical experiments (\$33,000), an image intensifier for the laser Raman spectroscopy program (\$24,000), high pressure liquid chromatography equipment (\$14,000), tunable dye lasers for photochemistry research (\$25,000) and a subnanosecond transient recorder (\$12,000).

Oak Ridge National Laboratory 680

The artificial photosynthesis effort requires a tunable picosecond laser and related equipment (\$32,000). Equipment necessary to improved usefulness of the EN tandem Van de Graff accelerator will cost \$45,000. The fusion-related atomic physics program requires a scattering chamber and pumps (\$40,000), an x-ray spectrometer (\$25,000) and a fast oscilloscope (\$8,000). An angular distribution chamber (\$10,000) is needed for photoelectron spectroscopy. Photochemistry of uranium and plutonium will need a laser (\$25,000), and detection systems using the spark source mass spectrometer need \$30,000 for a microdensitometer. The ion microprobe mass analysis system requires a residual gas analyzer (\$20,000) for ambient background determination. A micro-processor-based quadrupole, gas chromatography-mass spectrometry system (\$65,000) is needed for forefront research, replacing an outdated system. The heavier workload and large sample, natural isotope work in fossil fuel chemistry require a high field NMR apparatus (\$300,000). Miscellaneous smaller items totalling \$80,000 are also needed to maintain forefront capabilities in these chemical science efforts.

Pacific Northwest Laboratory 100

An atomic absorption spectrophotometer (\$15,000) is needed to replace a far outdated instrument, enabling this laboratory to exploit its advanced analytical expertise. The coal chemistry model compound work needs a variety of minor items (\$30,000). Gas purification, NMR and gas chromatography detectors are needed for homogeneous catalysis research (\$25,000). Thermochemical studies of cellulosic waste conversion to fuels require a large stirred autoclave, a molecular still and a high-pressure liquid chromatograph (\$30,000).

Sandia Laboratories 301

At Sandia-Livermore, a pulsed neodymium-YAG laser (\$200,000) will be put into operation as a major part of the buildup for completion of the Combustion Research Facility (CRF). Laser and fluorescence detection equipment (\$40,000) is needed for the low pressure

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

flame facility. Continuous-wave laser equipment (\$50,000) will also be assembled as a central piece for the CRF. At Sandia-Albuquerque, equipment is necessary for new MHD research.

Other Miscellaneous Equipment \$ 378

The Bartlesville, Morgantown, and Pittsburgh Energy Research Centers require equipment funds (\$63,000) to enhance basic fossil chemistry research. These items include: advanced calorimetric instrumentation; platinum resistance thermometers; a diffusion battery; and a discharge tube for a spectrometer source laser. Equipment is required at Atomic International (\$13,000) for exploratory studies in coal conversion. At Los Alamos Scientific Laboratory, an x-ray diffractometer (\$40,000) is needed for structural studies bearing on sulfur chemistry. Lawrence Livermore Laboratory requires thermochemical equipment (\$15,000) for research in hydrogen-forming chemical cycles. Equipment needs at Mound Facility (\$47,000) include a data processing unit, molecular beam equipment, and other gas property-measuring instrumentation. Off-site research contracts involving new and strengthened efforts in the areas of coal chemistry, catalysts, combustion, laser induced chemistry, MHD and solar photochemistry will require advanced and novel instrumentation (\$200,000).

4. Engineering, Mathematical and Geosciences \$ 800

The following is a listing of examples of equipment items required for the Engineering, Mathematical and Geosciences activity.

Argonne National Laboratory 105

An additional attached processor, primary memory, secondary memory and terminals are required to use MATHNET to explore the use of minicomputers in optimization calculations (\$100,000). Temperature recording and indicating equipment and a pressure intensifier are needed for geoscience research (\$5,000).

Brookhaven National Laboratory 50

Terminals, including graphics capabilities, are required to utilize interactive systems. Developing a methodology for validating large-scale econometric models is an example of an application of these terminals.

Los Alamos Scientific Laboratory 100

For the research in rock mechanics, petrology and other geothermal-related geoscience research, the following items are required: seismometers (\$26,000), auxiliary motor generator (\$12,000), prototype instrumentation (\$25,000), pressure vessels and a furnace (\$13,000) and an energy dispersive analysis unit for an electron microprobe (\$24,000).

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Lawrence Berkeley Laboratory \$ 90

Microprocessor-based terminals with local computing capabilities are required to experiment with man-machine interfaces to very large distributed data bases, and also to analyze combustion modeling techniques (\$60,000). Rock permeability apparatus is needed for the geoscience research (\$30,000).

Lawrence Livermore Laboratory 40

The geothermal energy-related geoscience effort requires high precision and high strain apparatus for strain measurements, as well as hydro-test facilities.

Oak Ridge National Laboratory 65

A remote job entry capability (\$60,000) is required, since the Mathematics and Statistics Research Department is several miles away from the central computing facility. The geoscience effort requires a torsion balance for the isopiestic facility and a low pressure pump (\$5,000).

Pacific Northwest Laboratory 75

Mobile automatic scanning photometers (\$50,000) and high-precision multispectral image digitizing equipment (\$25,000) are required for the network to measure solar input.

Sandia - Albuquerque 100

The geoscience effort requires high pressure and high temperature capability for characterizing magnetic earth materials and sensing magma-related phenomena.

Off-Site Program 175

Engineering Sciences research will require specialized engineering equipment for studies involving applied mechanics, advanced electronics, energy process control, advanced instrumentation and nondestructive testing. Computer terminals and other peripheral devices will be required by participants in the applied mathematical sciences efforts to explore innovative uses of interactive computation systems.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

5. Advanced energy projects \$ 200

This activity supports novel energy-related concepts which do not clearly fit within existing DOE technology programs. \$200,000 is requested for equipment requirements for the projects to be supported, many of which will involve advanced instrumentation.

6. Other capital equipment 1,700

The Basic Energy Sciences resource supports other capital equipment requirements at Ames Laboratory and Oak Ridge National Laboratory. The general purpose items to be acquired consist of multipurpose equipment that is not identified with a specific DOE resource. In FY 1979, \$1,700,000 is required to properly equip laboratory-wide service and support functions at Ames and ORNL, such as health physics, plant engineering, medical services, machine shops, instrumentation, and central scientific computer systems. The request also provides for equipment required to meet Federal or DOE fire, safety and environmental standards. Thus, the productivity, efficiency, and safety of DOE's programs at these laboratories are directly related to the equipment items included under this activity.

Ames Laboratory \$ 100

General purpose equipment needs at Ames Laboratory include: safety devices for x-ray diffractometers (\$18,000); compressors for helium liquefiers (\$40,000); a programmable terminal (\$27,000); and a PDP-11/34 communications processor (\$15,000).

Oak Ridge National Laboratory 1,600

This large, multiprogram laboratory has many needs in the general purpose equipment area. Among these are: health physics survey meters/monitors (\$60,000); a PDP-11, T40 computer system (\$60,000); a high-speed photocomposer (\$120,000); a closed circuit television monitoring system (\$75,000); a drum scanner (\$65,000); a fire pumper for fire code required pumping tests (\$100,000); a 19 inch lathe for the fabrication shop (\$75,000); forklifts, heavy duty vehicles and other motor vehicles (\$280,000); an inductively coupled plasma emission spectrometer (\$100,000); an on-line mass storage device (\$195,000); graphical plotting devices (\$200,000); and a large number of replacement items of equipment ranging from maintenance tools such as water blasters and lathes to laboratory research tools such as smaller spectrometers and oscilloscopes, and other general miscellaneous laboratory equipment (\$270,000).

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Basic Energy Sciences - continued

		<u>TEC</u>	<u>Obligations Thru FY 1977</u>	<u>FY 1978 Estimate BA</u>	<u>FY 1979 Estimate BA</u>	<u>Future Funding Required to Complete Project BA</u>
Construction projects:						
<u>Project No.</u>	<u>Project Title</u>					
Materials Sciences						
79-1-k	Intense pulsed neutron source-I, Argonne National Laboratory, Argonne, Illinois	\$ 6,400	\$ 0	\$ 0	\$ 6,400	\$ 0
78-13-a	National synchrotron light source, Brookhaven National Laboratory, Upton, New York	24,000	0	5,000	10,000	9,000
Subtotal, materials sciences		\$30,400	\$ 0	\$ 5,000	\$16,400	\$ 9,000
Chemical Sciences						
78-13-b	Combustion research facility, Sandia Laboratories, Livermore, California	\$ 9,400	\$ 0	\$ 6,000	\$ 3,400	\$ 0
Subtotal, chemical sciences		\$ 9,400	\$ 0	\$ 6,000	\$ 3,400	\$ 0
General Plant Projects (GPP)						
79-6	General plant projects, various locations	\$ 2,900	\$ 0	\$ 0	\$ 2,900	\$ 0
Total, basic energy sciences construction projects		\$42,700	\$ 0	\$ 11,000	\$22,700	\$ 9,000

EXPLANATION OF PROJECTS

Materials Sciences

1. Project 79-1-k Intense pulsed neutron source, ANL, Argonne, Illinois \$ 6,400

The Intense Pulsed Neutron Source-I (IPNS-I) will be a dedicated, user-oriented national facility for the production of neutrons for condensed matter studies in the United States. IPNS-I will provide unique, new capabilities for fundamental condensed matter

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Basic Energy Sciences - continued

research and for materials research relevant to the national energy program. As a new generation neutron source, IPNS-I, at its completion, will provide a larger increase in epithermal neutron source strength than has been made available in more than twenty years. IPNS-I will utilize those facilities and components of the ZGS complex which may become available after ZGS shutdown.

The data sheet describes IPNS-I, in which the existing ZGS 500 MeV, 30 Hz Booster II accelerator will provide 5×10^{12} protons per pulse (12 kW beam power) to an experiment area in which facilities for neutron scattering and radiation damage measurements will be constructed. In IPNS-I, the peak thermal neutron flux is expected to be at least 10^{15} n/cm²-sec.

Studies are underway for IPNS-II, which will include a new 800 MeV, 60 Hz, High Intensity Synchrotron (HIS). HIS will be the central part of the IPNS-II and is expected to provide 5×10^{13} protons per pulse (400 kW beam power) for the IPNS-II neutron scattering and radiation damage facilities. In IPNS-II, the peak thermal neutron flux is expected to be at least 10^{16} n/cm²-sec. A recent NAS report has recommended an immediate commitment to construct a pulsed spallation neutron facility with a high flux peak of 10^{16} thermal n/cm²-sec.

The purpose of IPNS-I is to provide unique facilities for neutron scattering and radiation damage studies of condensed matter. These facilities will enhance the national capability of materials science to advance the understanding of matter in the condensed state, in order to provide a foundation for improving materials technology and for uncovering new materials options in areas associated with energy.

The power of the neutron scattering technique for studying the microscopic structure and dynamics of materials is now widely recognized, as exemplified by the vigorous programs at the Grenoble HFR, the Oak Ridge HFIR, the Brookhaven HFBR and many medium-flux reactors elsewhere. However, the thermal neutron fluxes available in research reactors have increased only from 0.4×10^{15} to 1.2×10^{15} n/cm²-sec over the past 20 years; and the epithermal neutron flux 2×10^{14} n/cm²-sec ($E < 0.5$ eV) in the 2000°C hot source at the ILL reactor in Grenoble represents about the highest level attained in research reactors. These limits are imposed by cost and engineering constraints. Application of neutron scattering methods in many classes of measurements has reached limits imposed by the intensity of existing neutron sources. In fact, many important classes of measurements have scarcely been attempted because of limitations in available fluxes. In order to realize the fullest potential of the neutron scattering technique to the extent made possible by present technology, a new intense neutron source is required.

Much research on radiation effects has been performed during the past twenty-five years. While the effects of fast neutron bombardment have been studied extensively in research directly related to reactor development, and very substantial fundamental research on neutron radiation effects has been done, a heavy emphasis has been placed on low energy electron bombardment studies. This work has been highly successful in the past few years, yielding information on the basic properties of an isolated interstitial atom and vacant lattice site which are the principal defects created by electron bombardment. In the case of energetic neutron bombardment, a large amount of energy is released locally causing a high density of interstitial atoms and lattice vacancies which strongly interact with each other. This complex, called displacement cascade, is primarily responsible for many of the property changes induced by the neutron bombardment of reactor materials. This important area of research is not well understood and requires extensive fundamental study.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Currently, the basic fast neutron damage research program in the U.S. is being conducted primarily at Argonne National Laboratory in the CP-5 reactor and at Oak Ridge National Laboratory in the Bulk Shielding Reactor. These facilities have usable fluxes of less than 2×10^{12} n/cm²-sec, $E > 0.1$ MeV/cm²-sec. Clearly, a new facility is required for advancement of these studies.

Details of Cost Estimate*

	<u>Item Cost</u>	<u>Total Cost</u>
a. Engineering, Design & Inspection at 15% of construction costs .		\$ 644
b. Construction Costs		4,398
(1) Land Improvements	\$ 12	
(2) Buildings	206	
(3) Special Components	4,098	
(a) Targets & Beam Lines	\$ 1,571	
(b) Experimental Instrumentation	2,507	
(4) Utilities	102	
c. Standard Equipment		<u>100</u>
Subtotal		5,142
d. Contingency at @ 24% of above costs		<u>1,258</u>
Total Project Cost		<u>\$ 6,400</u>

*Based on completed conceptual design.

Funding Schedule of Project Funding and Other Related Funding Requirements

	<u>Prior Years</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>Total</u>
a. Total project funding					
1. Total facility costs					
a. Construction line item	\$ 0	\$ 1,500	\$ 4,000	\$ 900	\$ 6,400
b. CP&D	400	0	0	0	400
c. Expense funded equipment	260	140	0	0	400
d. Inventories	0	150	200	400	750
Total facility costs	<u>\$ 660</u>	<u>\$ 1,790</u>	<u>\$ 4,200</u>	<u>\$ 1,300</u>	<u>\$ 7,950</u>
2. Other project funding					
a. R&D necessary to complete construction ...	\$ 1,676	\$ 649	\$ 700	\$ 350	\$ 3,375
b. Other project related costs	0	0	0	0	0
Total other project funding	<u>\$ 1,676</u>	<u>\$ 649</u>	<u>\$ 700</u>	<u>\$ 350</u>	<u>\$ 3,375</u>
Total project funding (Item 1 & Item 2)	\$ 2,336	\$ 2,439	\$ 4,900	\$ 1,650	\$ 11,325

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

b. Total related funding requirements (Estimated life of project: 20 years)	
1. Facility operating costs	\$ 1,815
2. Programmatic operating expenses directly related to the facility	2,777
3. Capital equipment not related to construction but related to the programmatic effort in the facility	300
4. GPP or other construction related to programmatic effort in the facility	50
5. Other costs	<u>0</u>
Total other related annual funding requirements	\$ 4,942
2. Project 78-13-a National synchrotron light source, BNL, Upton, New York	\$10,000

Financial Schedule

<u>Fiscal Year</u>	<u>Authorization</u>	<u>Appropriation</u>	<u>Obligations</u>	<u>Costs</u>
1978	\$ 24,000	\$ 5,000	\$ 5,000	\$ 1,000
1979	0	10,000	10,000	5,100
1980	0	9,000	9,000	10,500
1981	0	0	0	7,400

The basic approach of the complex is for two storage rings designed for flexible operation over electron energies extending up to 2.5 GeV for the x-ray ring, and up to 0.7 GeV for the ultraviolet ring. Each ring is designed for operation with circulating currents approaching 1 ampere, and the two rings will be served by a common injector, specially designed to accommodate the high current objectives.

As now conceived, the project includes a building of approximately 77,000 sq. ft. gross area, of insulated sandwich panel construction on steel frame with reinforced concrete slab and shielding. It will house the two storage rings, booster, linac and injector, experimental areas, and two adjunct wings supporting laboratories and mechanical and electrical equipment. The wings will house equipment necessary to building electrical needs, controlled environment air handling systems, standard laboratory service piping, and fire protection systems, as well as electric power and cryogenic equipment essential to operation of the storage rings and experimental apparatus. The building materials handling system will include four five-ton bridge cranes. Supporting utilities and drainage systems will be extended from existing plant distribution systems. Standard laboratory and office furniture will be provided in the laboratory wing.

The National Synchrotron Light Source is proposed as a national, user-oriented, dedicated facility for advanced multi-disciplinary research with synchrotron radiation, a powerful investigative tool which will be of major importance for the materials, chemical, and life sciences. Although the facility is proposed because of its value for fundamental research

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

in these broad areas, the work which would be done at such a facility is clearly relevant to the practical energy and environmental concerns of the Nation. Both in this country and abroad, researchers using synchrotron radiation have been limited by the characteristics of existing sources. The few facilities which are dedicated to this research are small and provide spectra extending from long wavelengths only to the far ultraviolet. Those sources which can furnish photons at x-ray wavelengths were designed for high energy physics, so that synchrotron radiation utilization is parasitic, with serious attendant shortcomings. Moreover, most of the latter sources are synchrotrons and do not have the beam stabilities provided by a storage ring. Thus, it has been recognized in the U.S. and elsewhere that there is a need for specially designed facilities intended exclusively for the production and utilization of synchrotron radiation in pure and applied research over the entire range of wavelengths starting from the infrared to the x-ray region.

It is evident from what has already been accomplished with the limited capabilities of existing facilities that a dedicated, specially designed facility for synchrotron radiation research would have a strong impact on a broad range of scientific and technical fields, because it would make feasible types of experiments otherwise impracticable. Among the many specific areas involved are: solid state, atomic and chemical spectroscopy over the entire spectrum; photo and radiation chemistry; crystal structure by diffraction; lattice defect structure studies, including microscopic strain field analysis of both intrinsic and extrinsic defects; the physics, chemistry, and structures of surfaces and thin films; amorphous and ordered structures by critical absorption; macro-biochemical structure, such as static and dynamic structure of muscle or membrane; x-ray microscopy; optics, including non-linear optics and holography; and a variety of possible technological applications, such as the wiring of compact integrated microelectronics and systematic investigation of processes related to solar energy applications.

Although innovative in design, the state-of-the-art presently available will permit an assured construction. The report of the National Academy of Sciences Panel entitled "An Assessment of the National Need for Facilities Dedicated to the Production of Synchrotron Radiation" makes a prime recommendation that: As a response to the national synchrotron radiation needs, the U.S. make an immediate commitment to construct a new dedicated national facility or facilities. The proposed construction project at BNL fulfills all of the technological requirements in that report.

Details of Cost Estimate*

	<u>Item Cost</u>	<u>Total Cost</u>
a. Engineering, design and inspection costs at approximately 26% of Construction costs, item b		\$ 4,100
b. Construction costs		15,730
(1) Improvements to Land: including site preparation, curbs, walks, paving, and special compaction	\$ 120	

*Based upon completed conceptual design.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

		<u>Item Cost</u>	<u>Total Cost</u>
(2) Buildings		\$ 3,900	
(a) Accelerator Building, approximately 62,000 sq. ft. @ about \$51/sq. ft.	\$ 3,180		
(b) Laboratory Wing, approximately 10,000 sq. ft. @ about \$48/sq. ft.	480		
(c) Mechanical Equipment Wing, approximately 5,000 sq. ft. @ about \$48/sq. ft.	240		
(3) Special Facilities		11,350	
(a) 2.5 GeV storage ring	4,510		
(b) 700 MeV storage ring	1,510		
(c) Injector system	1,260		
(d) Associated Apparatus	2,000		
(e) Experimental equipment	2,070		
(4) Utilities		360	
c. Standard Equipment			\$ 510
Subtotal			20,340
d. Contingency at 18% of above Costs			3,660
Total Construction Project Cost			<u>\$ 24,000</u>

Funding Schedule of Project Funding and Other Related Funding Requirements

	<u>Prior Yrs.</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>FY 1982</u>	<u>Total</u>
a. Total project funding						
1. Total facility costs						
(a) Construction line item	\$ 1,000	\$ 5,100	\$ 10,500	\$ 7,400	\$ 0	\$ 24,000
(b) CP&D	0	0	0	0	0	0
(c) Expense funded equipment	80	50	0	0	0	130
(d) Inventories	0	100	200	200	0	500
Total facility costs	<u>\$ 1,080</u>	<u>\$ 5,250</u>	<u>\$ 10,700</u>	<u>\$ 7,600</u>	<u>\$ 0</u>	<u>\$ 24,630</u>
2. Other project funding						
(a) R&D necessary to complete construction	\$ 2,030	\$ 1,090	\$ 1,230	\$ 1,260	\$ 100	\$ 5,710
(b) Other project related costs	0	0	0	0	0	0
Total other project funding	<u>\$ 2,030</u>	<u>\$ 1,090</u>	<u>\$ 1,230</u>	<u>\$ 1,260</u>	<u>\$ 100</u>	<u>\$ 5,710</u>
Total project funding	\$ 3,110	\$ 6,340	\$ 11,930	\$ 8,860	\$ 100	\$ 30,340

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

b. Total related funding requirement (Estimated life of project: 20 years)	
1. Facility operating costs	\$ 2,500
2. Programmatic operating expenses directly related to the facility	1,500
3. Capital equipment not related to construction but related to the programmatic effort in the facility	930
4. GPP or other construction related to programmatic effort in the facility	200
5. Other costs	<u>0</u>
Total other related annual funding requirements	\$ 5,130

Chemical Sciences

1. Project 78-13-b Combustion research facility, Sandia Laboratories	\$ 3,400
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Financial Schedule

<u>Fiscal Year</u>	<u>Authorization</u>	<u>Appropriation</u>	<u>Obligations</u>	<u>Costs</u>
1978	\$ 9,400	\$ 6,000	\$ 6,000	\$ 1,000
1979	0	3,400	3,400	3,200
1980	0	0	0	5,200

This project will provide a laboratory/office complex for necessary and planned expansion of combustion research and development programs which are currently underway. The facility will house new high-powered lasers that will be used for analyzing the combustion process.

The new facility will occupy 2 acres of the government-owned unimproved 60-acre site east of the present engineering and computer facility. Gross building area will be approximately 45,000 sq. ft. The complex will consist of concrete and steel structures with exterior insulated wall panels of concrete and masonry, with floor slabs on grade. Exterior windows will be double glazed for energy conservation and doors will be insulated hollow metal.

This project will establish a research laboratory at Sandia Laboratories, Livermore, which will house a national combustion research facility.

This facility will serve as a national center for combustion research with active participation by visiting scientists from academic and industrial laboratories. It is envisioned that up to two thirds of the staff will consist of outside users who come to take advantage of the state-of-the-art instrumentation and interaction with the resident specialists and with other visitors. For this reason, the new facility will be in an unclassified area of the laboratory site.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

The need for such a center has been supported by numerous national committees and studies. One such study took place at a 1974 National Science Foundation workshop "Energy Related to Combustion Research" held at Princeton University. The unique capabilities of this facility will center about high-powered and sophisticated lasers used for probing and analyzing combustion processes. This facility will also consolidate the combustion research programs currently underway at Sandia Laboratories, Livermore. The major research and development activities of the Combustion Research Facility respond to the need for concentrated programs in combustion technology which are currently not being pursued by any other Federal or industrial laboratory.

The expansion of the research programs for analyzing the combustion process requires specially designed combustion laboratories with access to the lasers and computer capability for combustion modeling. Activities include (1) basic combustion research, emphasizing turbulent reacting flows; (2) applied combustion research, emphasizing automotive propulsion, advanced coal-burning power cycles, and coal processing; and (3) diagnostics development, emphasizing new laser/optical techniques.

Details of Cost Estimate*

	<u>Item Cost</u>	<u>Total Cost</u>
a. Engineering, Design and Inspection @ approximately 15% of construction costs (item b)		\$ 950
b. Construction Costs		6,300
(1) Improvements to land	\$ 290	
(2) Building, approximately 45,000 sq. ft. @ about \$110/sq. ft.	4,950	
(3) Special facilities (fuel handling, load transfer and control systems, instrumentation, etc.)	360	
(4) Utilities	700	
c. Standard Equipment (includes pulsed lasers, gas analyzers, mini-computers, dynamometers and spectrometers)		650
Subtotal		7,900
d. Contingency at approximately 19% of above costs		1,500
Total Project Cost		<u>\$ 9,400</u>

*Based on completed conceptual design.

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

Funding Schedule of Project Funding and Other Related Funding Requirements:

	<u>Prior Yrs.</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>FY 1982</u>	<u>Total</u>
a. Total project funding						
1. Total facility costs						
a. Construction line item	\$ 1,000	\$ 3,200	\$ 5,200	\$ 0	\$ 0	\$ 9,400
b. CP&D	0	0	0	0	0	0
c. Expense funded equipment	350	1,300	650	0	0	2,300
d. Inventories	0	0	0	0	0	0
Total facility costs	<u>\$ 1,350</u>	<u>\$ 4,500</u>	<u>\$ 5,850</u>	<u>\$ 0</u>	<u>\$ 0</u>	<u>\$11,700</u>
2. Other Project funding						
a. R&D necessary to complete construction ..	\$ 0	\$ 0	\$ 0	\$ 0	\$ 0	\$ 0
b. Other project related costs	0	0	100	0	0	100
Total other project funding	<u>\$ 0</u>	<u>\$ 0</u>	<u>\$ 100</u>	<u>\$ 0</u>	<u>\$ 0</u>	<u>\$ 100</u>
Total project funding (Item 1 & Item 2) .	\$ 1,350	\$ 4,500	\$ 5,950	\$ 0	\$ 0	\$11,800
b. Total related funding requirements (Estimated life of project: 20 years)						
1. Facility operating costs						\$ 108
2. Programmatic operating expenses directly related to the facility						3,500
3. Capital equipment not related to construction but related to the programmatic effort in the facility						800
4. GPP or other construction related to programmatic effort in the facility						150
5. Other costs						0
Total other related annual funding requirements						<u>\$ 4,558</u>

Energy Supply-Research and Technology Development

Basic Energy Sciences - continued

General Plant Projects (GPP)

1. Project 79-6 General plant projects, various locations \$ 2,900

This project is required to provide for minor new construction, other capital alterations, and additions, and for retirements to land, buildings and utility systems. Where applicable, the request also includes the cost of installed capital equipment integral to a subproject. Funding of this type is essential for maintaining the productivity and usefulness of DOE-owned facilities. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may be expected to result in additions, deletions, and changes in the currently planned subprojects. In general, the estimated funding for each location is preliminary in nature, and is intended primarily to indicate the relative magnitude of the requirements. No significant R&D program is anticipated as a prerequisite for design and construction of the subprojects under consideration.

The funds requested for FY 1979 are estimated as follows:

Ames Laboratory	<u>FY 1979</u>
Notre Dame Radiation Laboratory	\$ 250
Oak Ridge National Laboratory	20
Total Project Cost	<u>2,630</u>
	\$ 2,900

DEPARTMENT OF ENERGY
ENERGY-OPERATING EXPENSES AND CAPITAL ACQUISITION
FY 1979 CONGRESSIONAL BUDGET REQUEST
(Tabular dollars in thousands. Narrative material in whole dollars.)

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

3. Date A-E Work Initiated: 1st Qtr. FY 1979

5. Previous Cost Estimate:
Date:

3a. Date physical construction starts: 3rd Qtr. FY 1979

6. Current Cost Estimates: \$ 6,800
Less CP&D 400

4. Date construction ends: 2nd Qtr. FY 1981

Date: 12/77 Net Cost \$ 6,400

7. Financial Schedule

<u>Fiscal Year</u>	<u>Authorization</u>	<u>Appropriations</u>	<u>Obligations</u>	<u>Costs</u>
1979	\$ 6,400	\$ 6,400	\$ 6,400	\$ 1,500
1980	0	0	0	4,000
1981	0	0	0	900

8. Brief physical description of project

The Intense Pulsed Neutron Source - I (IPNS-I) will be a dedicated, user-oriented national facility for the production of neutrons for condensed matter studies in the United States. IPNS-I will provide unique, new capabilities for fundamental condensed matter research and for materials research relevant to the national energy program. As a new generation neutron source, IPNS-I at its completion, will provide a larger increase in epithermal neutron source strength than has been made available in more than twenty years. IPNS-I will utilize those facilities and components of the ZGS complex which may become available after ZGS shutdown.

This data sheet describes IPNS-I in which the existing ZGS 500 MeV, 30 Hz Booster II accelerator will provide 5×10^{12} protons per pulse (12 kW beam power) to an experiment area in which facilities for neutron scattering and radiation damage measurements will be constructed. In IPNS-I, the peak thermal neutron flux is expected to be at least 10^{15} n/cm²-sec.

Studies are underway for IPNS-II, which will include a new 800 MeV, 60 Hz, High Intensity Synchrotron (HIS). HIS will be the central part of the IPNS-II and is expected to provide 5×10^{13} protons per pulse (400 kW beam power) for the IPNS-II neutron scattering and radiation damage facilities. In IPNS-II the peak thermal neutron flux is expected to be at least 10^{16} n/cm²-sec. A recent NAS report has recommended an immediate commitment to construct a pulsed spallation neutron facility with a high flux peak of 10^{16} thermal n/cm²-sec.

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1. Title and location of project: Intense pulsed neutron source - I,
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2. Project No. 79-1-k

Table I summarized the Argonne Pulsed Neutron Source Program.

Table I

Argonne Pulsed Neutron Source Program

Neutron Source	Proton Accelerator	Target Material	Frequency (c/sec)	Peak Thermal Flux (n/cm ² sec)	Operational Date
ZING-P'	ZGS Booster I	Pb	10	5 x 10 ¹¹	1974
ZING-P'	ZGS Booster II	W	30	10 ¹⁴	1977
IPNS-I	ZGS Booster II	238 _U	30	10 ¹⁵	1981

9. Purpose, justification of need for, and scope of project

The purpose of IPNS-I is to provide unique facilities for neutron scattering and radiation damage studies of condensed matter. These facilities will enhance the national capability of materials science to advance the understanding of matter in the condensed state, in order to provide a foundation for improving materials technology and for uncovering new materials options in areas associated with energy.

The project schedule has been arranged to make this unique facility available to a wide class of users in the shortest possible time. There is an urgent need for such a facility. The present DOE research reactors have been in operation for periods ranging from ten to twenty-two years. In contrast, the new High Flux Reactor in Grenoble, France, came into operation in 1972 and incorporates the most extensive neutron research facilities in the world. While scientific research is to a considerable degree a cooperative international activity, it is essential for the U.S. to maintain a leadership role to ensure that those problem areas of vital interest to the U.S. energy programs are fully addressed. To maintain this leadership, a major new facility must be constructed as soon as possible.

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
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Resource Name: Basic Energy Sciences

Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

Neutron Scattering

The power of the neutron scattering technique for studying the microscopic structure and dynamics of materials is now widely recognized, as exemplified by the vigorous programs at the Grenoble HFR, the Oak Ridge HFIR, the Brookhaven HFBR and many medium-flux reactors elsewhere. However, the thermal neutron fluxes available in research reactors have increased only from 0.4×10^{15} to 1.2×10^{15} n/cm²-sec over the past 20 years; and the epithermal neutron flux of 2×10^{14} n/cm²-sec ($E < 0.5$ eV) in the 2000°C hot source at the ILL reactor in Grenoble represents about the highest level attained in research reactors. These limits are imposed by cost and engineering constraints. Application of neutron scattering methods in many classes of measurements has reached limits imposed by the intensity of existing neutron sources. In fact, many important classes of measurements have scarcely been attempted because of limitations in available fluxes.

The highly instrumented IPNS-I pulsed neutron source will provide unique capabilities for scattering measurements in many areas of materials, chemical and biological sciences. Examples of some of these which are closely related to energy technology are studies of:

1. Proton binding and diffusion in metal hydrides related to hydrogen storage;
2. Surface-adsorbed and intercalated molecules in systems related to catalysis;
3. Structure of amorphous semiconductor materials and metallic glasses.

Examples of fundamental scientific studies are:

1. Structure of biological molecules and complexes, especially exploiting differential (deuterium vs. hydrogen) labeling;
2. High-frequency excitations in magnetic materials;
3. Structure and dynamics of molten salts, liquid metals and aqueous solutions.

In projecting the effect of having IPNS available for scientific studies, one must consider that the users will encounter a generation of pulsed sources more intense than any pulsed source that has so far been used for scattering measurements (such as the ZING prototype or the Harwell and Tohoku linacs). Thus, there is good expectation for breakthroughs with this radically new device that cannot now be predicted. This phenomenon is exemplified by the highly successful program at the Brookhaven HFBR which has revolutionized the field of structural phase transitions, but which could hardly have been predicted at the foundation of the HFBR project 15 years ago.

In addition to the qualitative effect of opening up areas which are not approachable with existing neutron facilities, there is

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an important quantitative effect expected from the emergence of a major new generation facility like IPNS. An illustration of this effect is given by the new European center for neutron scattering, the Institut Laue-Langevin in Grenoble, France. This is a cooperative French-German-British project which provides the three participating nations with neutron capabilities much more intense than their own national facilities (somewhat higher than the HFBR at Brookhaven). ILL involves scientists from over 130 European universities and research institutes, so that the neutron scattering technique is no longer the province of the experts at a few laboratories but an integral part of several hundred research programs.

Radiation Effects Research

Much research on radiation effects has been performed during the past twenty-five years. While the effects of fast neutron bombardment have been studied extensively in research directly related to reactor development, and very substantial fundamental research on neutron radiation effects has been done, a heavy emphasis has been placed on low energy electron bombardment studies. This work has been highly successful in the past few years, yielding information on the basic properties of an isolated interstitial atom and vacant lattice site which are the principal defects created by electron bombardment. In the case of energetic neutron bombardment, a large amount of energy is released locally causing a high density of interstitial atoms and lattice vacancies which strongly interact with each other. This complex, called a displacement cascade, is primarily responsible for many of the property changes induced by the neutron bombardment of reactor materials. This important area of research is not well understood and requires extensive fundamental study.

Currently, the basic fast neutron damage research program in the U.S. is being conducted primarily at Argonne National Laboratory in the CP-5 reactor and at Oak Ridge National Laboratory in the Bulk Shielding Reactor. These facilities have useable fluxes of less than 2×10^{12} n/cm²-sec, $E > 0.1$ MeV/cm²-sec. Clearly, a new facility is required for advancement of these studies.

The importance of having a dedicated device for radiation effects research cannot be overstated. The diversity of experiments requires that a high degree of operational control be possible with regard to bombardment. The degree of downtime and the consistency of flux levels should be placed in the hands of experimenters. Of equal importance is low nuclear heating. The interpretation of both basic and applied problems requires selectivity and consistency of bombardment temperature during the experiment. High nuclear heating makes it difficult if not impossible to maintain a constant selected temperature. Finally, a large fast neutron flux (free of thermal neutrons) compatible with a low nuclear heating rate is desired. The facilities provided by the IPNS program will have the above qualities.

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
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1. Title and location of project: Intense pulsed neutron source - I,
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2. Project No. 79-1-k

The IPNS-I radiation source will be equal in magnitude to existing damage research neutron sources. The separate target for neutron damage studies in IPNS-I provides a dedicated source with a high, fast neutron flux and with nuclear heating rates the order of 0.1 watt/gm or less.

10. Details of Cost Estimate*

a. Engineering design and inspection at 15% of construction costs			\$ 644
b. Construction costs			4,398
(1) Land improvements	\$ 12		
(2) Buildings	206		
(3) Special components	4,078		
(a) Targets & beam lines	\$ 1,571		
(b) Experimental instrumentation	<u>2,507</u>		
(4) Utilities		102	
c. Standard equipment			<u>100</u>
	Subtotal		5,142
d. Contingency @ 24% of above costs			<u>1,258</u>
	Total project cost		\$ 6,400

*Based on completed conceptual design

11. Method of Performance

Design of the following subprojects will be accomplished by the operating contractor due to the unique nature of the facilities required, due to the effects they exert on functioning of both accelerator and neutron source, and due to the specially-applicable knowledge and skills of laboratory staff:

1. Beam transport system.
2. Spallation targets, shield, and beam port arrangements.

Design specifications and much of the construction of the items of experimental apparatus will be performed by Argonne National Laboratory personnel.

Engineering, design and inspection of buildings and services will be on the basis of a negotiated architect-engineer contract. Construction will be accomplished by fixed-price contracts and subcontracts awarded on the basis of competitive bids.

Construction Project Data Sheet

Argonne National Laboratory

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Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	<u>Prior Years</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>Total</u>
a. Total project funding					
1. Total facility costs					
(a) Construction line item	\$ 0	\$ 1,500	\$ 4,000	\$ 900	\$ 6,400
(b) CP&D	400	0	0	0	400
(c) Expenses funded equipment	260	140	0	0	400
(d) Inventories	0	150	200	400	750
Total facility costs	660	1,790	4,200	1,300	7,950
2. Other project funding					
(a) R&D necessary to complete construction	1,676	649	700	350	3,375
(b) Other project related costs	0	0	0	0	0
Total other project funding	1,676	649	700	350	3,375
Total project funding (item 1 & item 2)	\$ 2,336	\$ 2,439	\$ 4,900	\$ 1,650	\$ 11,325
b. Total related funding requirement (estimated life of project: 20 years)					
1. Facility operating costs				\$ 1,815	
2. Programmatic operating expenses directly related to the facility				2,777	
3. Capital equipment not related to construction but related to the programmatic effort in the facility				300	
4. GPP or other construction related to programmatic effort in the facility				50	
5. Other costs				0	
Total other related annual funding requirements				\$ 4,942	

13. Narrative explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding
1. Total facility
 (a) Construction line item
 no narrative required

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
and Technology Development

Resource Name: Basic Energy Sciences

Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

(b.) CP&D

no narrative required

(c) Expense funded equipment

The equipment costs are for computer systems and data processing items required to support the neutron scattering work to be performed during the ZING-P' operation. The acquisition of these items precedes the funding of the Construction Line Item and therefore are not included in the TEC.

(d) Inventories

An inventory of critical spare parts is needed to insure replacement and repair capability in the event of failure of system components. Component failures could lead to shutdown of operations which would delay or possibly negate research programs. The optimization of operation would be enhanced by the immediate availability of parts so that repairs or replacement could be accomplished in as short a time as practicable.

2. Other project funding

(a) R&D necessary to complete construction

Experience with the accelerator system, neutron sources, moderators, and instrumentation is required as a prerequisite to design and construction of the IPNS-I sources. This experience will be gained using the ZING-P' prototype facility which was completed in the Fall of 1977. Work with ZING-P' will begin during Booster II accelerator tuneup and continue until the facility must be removed for the installation of the IPNS-I proton beam line.

(b) Other project related funding

no narrative required

b. Total related funding requirements

The potential lifetime of IPNS-I is estimated at 20 years.

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
and Technology Development

Resource Name: Basic Energy Sciences

Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

1. Facility Operating Costs

<u>Neutron Facilities</u>	<u>Dollars (\$1,000's)</u>
2 Staff	\$ 117
1 Technical	52
5 Hourly	227
Materials & Services	<u>110</u>
Subtotal	\$ 506
<u>Accelerator System</u>	<u>Dollars (\$1,000's)</u>
2 Staff	\$ 110
10 Technical	100
10 Hourly	454
Electricity	300
Materials & Services	<u>345</u>
Subtotal	<u>\$1,309</u>
Total Operating Costs	\$1,815

The effort related costs of the above and also section 2 below include General Laboratory Expense (indirect costs) as well as Program Direction and Direct Allocation Expense. These overhead costs are 40 to 45% of effort related costs.

2. Programmatic operating expenses directly related to the facility

Support of research performed for Neutron Scattering and Radiation Damage activities in the CHM, MSD and SSS Divisions of the Laboratory have been projected to the time of IPNS-I operation. These costs will remain essentially static throughout the life of IPNS-I. The costs are stated in 1979 dollars.

A group consisting of 18 staff and technical support personnel will be assigned to IPNS-I for effective use of instruments by experimenters outside the host laboratory, for maintenance and operation of instruments, instrument improvement, provision of special capabilities and instruction of users in measurement and data handling. This cost is therefore shown as a component of research costs.

Construction Project Data Sheet

Argonne National Laboratory

Mission Name: Energy Supply - Research
and Technology Development

Resource Name: Basic Energy Sciences

Activity Name: Materials Sciences

1. Title and location of project: Intense pulsed neutron source - I,
Argonne National Laboratory, Argonne, Illinois

2. Project No. 79-1-k

	Dollars (<u>\$1,000's</u>)	Manpower (<u>MY</u>)
Support of Research in Argonne User Divisions	2,148	31
Support of IPNS-I Technical Staff	<u>629</u>	<u>12</u>
Total Projected Research Costs	2,777	43

The planned operational mode for IPNS makes provision for a large outside user effort based on universities and other laboratories. This is expected to be larger than the ANL-based effort. The research costs associated with this outside user community are not listed here but are likely to amount to \$2,000,000 per year.

3. Capital equipment not related to construction but related to the programmatic effort in the facility

It is estimated that accelerator and facility modifications, provision of new research instrumentation and modification of installed research instrumentation will require equipment funding of approximately \$300,000/year.

4. GPP or other construction related to programmatic effort

The cost of additions to, and alterations of existing buildings and facilities, and of new buildings and facilities related to the research program is estimated to be \$50,000/year. These will be required to provide for needs which are reasonably expected to develop as the research program grows and changes direction. An example of such an addition is a second distant neutron scattering instrument building.

5. Other costs

no narrative required

DEPARTMENT OF ENERGY
ENERGY-OPERATING EXPENSES AND CAPITAL ACQUISITION
FY 1979 CONGRESSIONAL BUDGET REQUEST
(Tabular dollars in thousands. Narrative material in whole dollars.)

Construction Project Data Sheet

Division of Basic Energy Sciences

Mission Name: Energy Supply -
Research and Technology Development
Resource Name: Basic Energy Sciences

1. Title and location of project: General plant projects, various locations

2. Project No. 79-6

3. Date A-E Work Initiated: 1st Quarter FY 1979

5. Previous Cost Estimate:

3a. Date Physical Construction Starts: 2nd Quarter FY 1979

Date: \$ None

4. Date Construction Ends: 2nd Quarter FY 1981

6. Current Cost Estimate:

Date: 12/77 \$ 2,900

7. Financial Schedule

<u>Fiscal Year</u>	<u>Obligations</u>	<u>Costs</u>			<u>After</u>
		<u>FY 1977</u>	<u>FY 1978</u>	<u>FY 1979</u>	<u>FY 1979</u>
Prior Year Projects	\$ xxx	\$ 1,622	\$ 798	\$ 200	\$ 98
FY 1977 Projects	3,115	434	1,335	1,100	246
FY 1978 Projects	2,560	0	530	900	1,130
FY 1979 Projects	2,900	0	0	800	2,100
		\$ 2,056	\$ 2,663	\$ 3,000	\$ 3,918

8. Brief physical description of project

This project is required to provide for minor new construction, other capital alterations and additions, and for retirements to land, buildings and utility systems. Where applicable, the request also includes the cost of installed capital equipment integral to a subproject. Funding of this type is essential for maintaining the productivity and usefulness of DOE-owned facilities. Since it is difficult to detail this type of project in advance, a continuing evaluation of requirements and priorities may be expected to result in additions, deletions, and changes in the currently planned subprojects. In general, the estimated funding for each location is preliminary in nature, and is intended primarily to indicate the relative magnitude of the requirements. No significant R&D program is anticipated as a prerequisite for design and construction of the subprojects under consideration.

The funds requested for FY 1979 are estimated as follows:

Construction Project Data Sheet

Division of Basic Energy Sciences

Mission Name: Energy Supply -
 Research and Technology Development
 Resource Name: Basic Energy Sciences

1. Title and location of project: General plant projects, various locations	2. Project No. 79-6
	FY 1979
Ames Laboratory	\$ 250
Notre Dame Radiation Laboratory	20
Oak Ridge National Laboratory	2,630
Total Project Cost	\$ 2,900

9. Purpose, justification of need for, and scope of project

Following are examples of the major items of work to be performed at the various locations:

Ames Laboratory \$ 250
 Requirements include: upgrading the deionized water system (\$75,000); electrical system upgrades (\$60,000); equipment cooling systems (\$45,000); and other improvements (\$70,000).

Notre Dame Radiation Laboratory 20
 This project provides for modifications to the Radiation Research Building at the University of Notre Dame. Changes in the method of pursuing the research program necessitate some minor modifications and improvements for smooth and efficient operations.

Oak Ridge National Laboratory 2,630
 Requirements include: office additions to Engineering Building 9204-1 (\$200,000); office additions to Building 6000, related to heavy ion research (\$350,000); building 4508 ventilation system (\$95,000); office space for the Thorium-Uranium recycle facility (\$350,000); a manipulator repair facility (\$700,000); an 800 meter flight station for flight path #1 (\$500,000); lighting improvements (\$160,000); upgraded office areas (\$200,000); and safety improvements (\$75,000)

10. Details of Cost Estimate

See description, item 8. The estimated costs are preliminary and, in general, indicate the magnitude of each program. These include engineering, design, inspection, and contingency allowances.

11. Method of Performance

Design will be on the basis of negotiated architect-engineering contracts. To the extent feasible, construction and procurement will be accomplished by firm fixed-price contracts and subcontracts awarded on the basis of competitive bidding.

12. N/A

13. N/A

DEPARTMENT OF ENERGY
ENERGY-OPERATING EXPENSES AND CAPITAL ACQUISITION
FY 1979 CONGRESSIONAL BUDGET REQUEST
(Tabular dollars in thousands. Narrative material in whole dollars.)

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

3. Date A-E Work Initiated: 2nd Quarter FY 1978

5. Previous Cost Estimate:

3a. Date Physical Construction Starts: 3rd Quarter FY 1978

Date: \$ None

4. Date Construction Ends: 3rd Quarter FY 1981

6. Current Cost Estimate:

Date: 12/77 \$ 24,000

7. Financial Schedule

<u>Fiscal Year</u>	<u>Authorization</u>	<u>Appropriation</u>	<u>Obligations</u>	<u>Costs</u>
1978	\$ 24,000	\$ 5,000	\$ 5,000	\$ 1,000
1979	0	10,000	10,000	5,100
1980	0	9,000	9,000	10,500
1981	0	0	0	7,400

8. Brief physical description of project

This project provides for the design and construction of an electron storage ring complex for dedicated use as a high intensity synchrotron radiation source; for the design and construction of new building space to house the storage rings and associated experimental, laboratory and office areas; and for the design and fabrication or procurement of experimental equipment required to serve the basic initial needs of the scientific users.

The basic approach of the complex is for two storage rings designed for flexible operation over electron energies extending up to 2.5 GeV for the x-ray ring, and up to 0.7 GeV for the ultraviolet ring. Each ring is designed for operation with circulating currents approaching 1 ampere, and the two rings will be served by a common injector, specially designed to accommodate the high current objectives. Some of the large storage ring sectors will operate at moderate magnetic fields, primarily providing photon beams in the x-ray wavelength region. Other sectors will incorporate high magnetic field "wigglers" to simultaneously generate radiation at hard x-ray wavelengths. Each wiggler will consist of a triple superconducting dipole capable of attaining about 40 kilogauss at the center. This ring will be about 150 meters in circumference, and will provide as many as 40 photon source ports, some with small source size and exceptionally high brightness. Most of these ports

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

can be equipped to serve more than one experiment. The high current proposed will require an injection energy of about 650 MeV, obtainable from a ring booster equipped with either a linac or a 50 MeV microtron as its injector. A second smaller ring having a mean diameter of about 14m and a circumference of about 44m, will operate at 700 MeV with a circulating current of up to 1 ampere. It will be utilized in the long wavelength region and have 16 ports for experimental stations.

As now conceived, the project includes a building of approximately 77,000 sq. ft. gross area, of insulated sandwich panel construction on steel frame with reinforced concrete slab and shielding. It will house the two storage rings, booster, linac and injector, experimental areas, and two adjunct wings supporting laboratories and mechanical and electrical equipment. The wings will house equipment necessary to building electrical needs, controlled environment air handling systems, standard laboratory service piping, and fire protection systems, as well as electric power and cryogenic equipment essential to operation of the storage rings and experimental apparatus. The building materials handling system will include four five-ton bridge cranes. Supporting utilities and drainage systems will be extended from existing plant distribution systems. Standard laboratory and office furniture will be provided in the laboratory wing.

9. Purpose, justification of need for, and scope of project

The National Synchrotron Light Source is proposed as a national, user-oriented, dedicated facility for advanced multi-disciplinary research with synchrotron radiation, a powerful investigative tool which will be of major importance for the materials, chemical, and life sciences. Although the facility is proposed because of its value for fundamental research in these broad areas, the work which would be done at such a facility is clearly relevant to the practical energy and environmental concerns of the Nation. Both in this country and abroad, researchers using synchrotron radiation have been limited by the characteristics of existing sources. The few facilities which are dedicated to this research are small and provide spectra extending from long wavelengths only to the far ultraviolet. Those sources which can furnish photons at x-ray wavelengths were designed for high energy physics, so that synchrotron radiation utilization is parasitic, with serious attendant shortcomings. Moreover, most of the latter sources are synchrotrons and do not have the beam stabilities provided by a storage ring. Thus, it has been recognized in the U.S. and elsewhere that there is a need for specially designed facilities intended exclusively for the production and utilization of synchrotron radiation in pure and applied research over the entire range of wavelengths starting from the infrared to the x-ray region.

It is evident from what has already been accomplished with the limited capabilities of existing facilities that a dedicated, specially designed facility for synchrotron radiation research would have a strong impact on a broad range of scientific and technical fields, because it would make feasible types of experiments otherwise impracticable. Among the many specific

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

-
1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York
2. Project No. 78-13-a
-

areas involved are: solid state, atomic and chemical spectroscopy over the entire spectrum; photo and radiation chemistry; crystal structure by diffraction; lattice defect structure studies, including microscopic strain field analysis of both intrinsic and extrinsic defects; the physics, chemistry, and structures of surfaces and thin films; amorphous and ordered structures by critical absorption; macro-biochemical structure, such as static and dynamic structure of muscle or membrane; x-ray microscopy; optics, including non-linear optics and holography; and a variety of possible technological applications, such as the wiring of compact integrated microelectronics and systematic investigation of processes related to solar energy applications.

Although innovative in design, the state-of-the-art presently available will permit an assured construction. The draft report of the National Academy of Sciences Panel entitled "An Assessment of the National Need for Facilities Dedicated to the Production of Synchrotron Radiation" makes a prime recommendation that: As a response to the national synchrotron radiation needs, the U.S. make an immediate commitment to construct a new dedicated national facility or facilities. The proposed construction project at BNL fulfills all of the technological requirements in that report.

Preconstruction R&D costs associated with this facility are estimated at \$900,000 in FY 1978. Annual facility operating costs are estimated at \$2,500,000 and associated research costs at \$1,500,000, in FY 1978 dollars. The \$10,000,000 requested for appropriation in FY 1979 will provide for continuation of the engineering and design effort, procurement and construction. The request includes funds required for improvements to land and for the laboratory-office building.

10. Details of Cost Estimate*

	<u>Item Cost</u>	<u>Total Cost</u>
a. Engineering, design and inspection costs at approximately 26% of Construction costs, item b		\$ 4,100
b. Construction costs		15,730
(1) Improvements to Land: including site preparation, curbs, walks, paving, and special compaction	\$ 120	
(2) Buildings	3,900	
(a) Accelerator Building, approximately 62,000 sq. ft. @ about \$51/sq. ft.	\$ 3,180	
(b) Laboratory Wing, approximately 10,000 sq. ft. @ about \$48/sq. ft.	480	

*Based upon completed conceptual design.

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York

2. Project No. 7R-13-a

	<u>Item Cost</u>	<u>Total Cost</u>
(c) Mechanical Equipment Wing, approximately 5,000 sq. ft. @ about \$48/sq. ft.	\$ 240	
(3) Special Facilities	\$ 11,350	
(a) 2.5 GeV storage ring	4,510	
(b) 700 MeV storage ring	1,510	
(c) Injector system	1,260	
(d) Associated Apparatus	2,000	
(e) Experimental equipment	2,070	
(4) Utilities	360	
c. Standard Equipment		\$ 510
Subtotal		20,340
d. Contingency at 18% of above Costs		3,660
Total Construction Project Cost		<u>\$24,000</u>

11. Method of Performance

Design of the conventional facilities will be on the basis of a negotiated fixed price architect-engineer contract, with design of the special facilities (magnet sectors, main vacuum chamber, rf cavities, etc.) by Brookhaven National Laboratory. Conventional construction will be accomplished by fixed price contracts awarded on the basis of competitive bid. Fabrication of special facilities, as well as the provision of magnet and rf power supplies, cryogenics, control equipment, etc., where possible will be by commercial vendors on the basis of fixed price contracts awarded on the basis of competitive bidding. Assembly and testing will be performed by Brookhaven.

12. Funding Schedule of Project Funding and Other Related Funding Requirements

	<u>Prior Yrs.</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>FY 1982</u>	<u>Total</u>
a. Total project funding						
1. Total facility costs						
(a) Construction line item	\$ 1,000	\$ 5,100	\$ 10,500	\$ 7,400	\$ 0	\$24,000
(b) CP&D	0	0	0	0	0	0
(c) Expense funded equipment	80	50	0	0	0	130
(d) Inventories	0	100	200	200	0	500
Total facility costs	\$ 1,080	\$ 5,250	\$ 10,700	\$ 7,600	\$ 0	\$24,630

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

	<u>Prior Yrs.</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>FY 1982</u>	<u>Total</u>
2. Other project funding						
(a) R&D necessary to complete construction .	\$ 2,030	\$ 1,090	\$ 1,230	\$ 1,260	\$ 100	\$ 5,710
(b) Other project related costs	0	0	0	0	0	0
Total other project funding	<u>2,030</u>	<u>1,090</u>	<u>1,230</u>	<u>1,260</u>	<u>100</u>	<u>5,710</u>
Total project funding	\$ 3,110	\$ 6,340	\$ 11,930	\$ 8,860	\$ 100	\$ 30,340
b. Total related funding requirement (estimated life of project: 20 years)						
1. Facility operating costs						\$ 2,500
2. Programmatic operating expenses directly related to the facility						1,500
3. Capital equipment not related to construction but related to the programmatic effort in the facility						930
4. GPP or other construction related to programmatic effort in the facility						200
5. Other costs						<u>0</u>
Total other related annual funding requirements						\$ 5,130

13. Narrative explanation of Total Project Funding and Other Related Funding Requirements

a. Total project funding

1. Total facility

- a) Construction line item - no narrative required
- b) CP&D - no narrative required
- c) Expense funded equipment - This includes linac, ultravacuum systems, and fast valve safety systems for beam lines
- d) Inventories - This includes high voltage capacitor systems and RF cavity models

2. Other project funding

- a) R&D necessary to complete the project totals \$5,710,000 including \$2,030,000 expended in prior years. This R&D is related to computer calculation of electron orbits, magnet configurations, injector upgrading, preliminary beam line and wiggler design, vacuum systems, interim building, machine cooling and power criteria, RF systems, and RF cavity model work.
- b) Other project related funding - no narrative required.

Construction Project Data Sheet

Brookhaven National Laboratory

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Materials Sciences

1. Title and location of project: National synchrotron light source,
Brookhaven National Laboratory, Upton, New York

2. Project No. 78-13-a

b. Total related funding requirements

It is anticipated that the facility will be utilized for research for at least twenty years beyond its completion in 1982.

1. Facility operating costs

The major operating costs include power, water, and facility operational maintenance.

2. Programmatic operating expenses directly related to the facility

The programmatic operating expenses, \$1,500,000 in FY 1983, are associated with the (a) scientific manpower, (b) material handling and preparation, (c) data acquisition and analysis, and (d) experimental beam line preparation.

3. Capital equipment not related to construction but related to the programmatic effort in the facility

The annual requirement for equipment for the period FY 1979-FY 1983 is \$930,000 and presently is scheduled to be reduced to \$600,000 thereafter.

4. GPP or other construction related to programmatic effort

This includes refurbishing the laboratory housing for investigating linac alignments, magnet models, and wiggler preparation.

5. Other costs - no narrative required

DEPARTMENT OF ENERGY
ENERGY-OPERATING EXPENSES AND CAPITAL ACQUISITION
FY 1979 CONGRESSIONAL BUDGET REQUEST
(Tabular dollars in thousands. Narrative material in whole dollars.)

Construction Project Data Sheet

Sandia Laboratories

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Chemical Sciences

1. Title and location of project: Combustion research facility, Sandia Laboratories,
Livermore, California (SLL) 2. Project No. 78-13-b

3. Date A-E Work Initiated: 2nd Qtr. FY 1978 5. Previous Cost Estimate:
Date: \$ None
3a. Date Physical Construction Starts: 1st Qtr. FY 1979
4. Date Construction Ends: 2nd Qtr. FY 1980 6. Current Cost Estimates:
Date: 12/77 \$9,400

7. Financial Schedule

<u>Fiscal Year</u>	<u>Authorization</u>	<u>Appropriation</u>	<u>Obligations</u>	<u>Costs</u>
1978	\$ 9,400	\$ 6,000	\$ 6,000	\$ 1,000
1979	0	3,400	3,400	3,200
1980	0	0	0	5,200

8. Brief physical description of project:

This project will provide a laboratory/office complex for necessary and planned expansion of combustion research and development programs which are currently underway. The facility will house new high-powered lasers that will be used for analyzing the combustion process.

The new facility will occupy 2 acres of the government-owned unimproved 60-acre site east of the present engineering and computer facility. Gross building area will be approximately 45,000 sq. ft. The complex will consist of concrete and steel structures with exterior insulated wall panels of concrete and masonry, with floor slabs on grade. Exterior windows will be double glazed for energy conservation and doors will be insulated hollow metal.

Each heavy laboratory interior will be designed for sound attenuation and vibration damping. Ventilation will be arranged to carry off potential fuel and combustion gases; systems will be included for capturing or separating combustible or contaminating products. A Halon system for extinguishing fuel fires will be installed.

Heating and air conditioning for the remainder of the complex will be provided by units with chilled and hot water coils.

Construction Project Data Sheet

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Chemical Sciences
2. Project No. 78-13-b

Sandia Laboratories

1. Title and location of project: Combustion research facility, Sandia Laboratories
Livermore, California (SLL)

The air handlers will be provided with enthalpy control units to give maximum savings with an economizer system. Interior plumbing will include hot and cold water, drains, natural gas, compressed air, process water for laser and equipment cooling, and cylinder gases. Restroom and janitorial facilities will be provided. Wet-type automatic systems will be located throughout with alarm provisions to the LLL fire department and SLL communication center.

An 8-inch water main will be extended to the complex from a nearby supply main. Steam, natural gas, and sanitary sewer will also be extended from existing facilities. Capacity of the SLL central steam plant is adequate for this proposed facility. A 13.8 KV, 3-phase feeder in underground duct will be installed from an existing main substation. Perimeter lighting will be extended around the fenced area of the new site.

9. Purpose, justification of need for, and scope of project

This project will establish a research laboratory at Sandia Laboratories, Livermore, which will house a national Combustion Research Facility.

This facility will serve as a national center for combustion research with active participation by visiting scientists from academic and industrial laboratories. It is envisioned that up to two thirds of the staff will consist of outside users who come to take advantage of the state-of-the-art instrumentation and interaction with the resident specialists and with other visitors. For this reason, the new facility will be in an unclassified area of the laboratory site.

The need for such a center has been supported by numerous national committees and studies. One such study took place at a 1974 National Science Foundation workshop "Energy Related to Combustion Research" held at Princeton University. The unique capabilities of this facility will center about high-powered and sophisticated lasers used for probing and analyzing combustion processes. This facility will also consolidate the combustion research programs currently underway at Sandia Laboratories, Livermore. The major research and development activities of the Combustion Research Facility respond to the need for concentrated programs in combustion technology which are currently not being pursued by any other Federal or industrial laboratory.

The expansion of the research programs for analyzing the combustion process requires specially designed combustion laboratories with access to the lasers and computer capability for combustion modeling. Activities include (1) basic combustion research, emphasizing turbulent reacting flows; (2) applied combustion research, emphasizing automotive propulsion, advanced coal-burning power cycles, and coal processing; and (3) diagnostics development, emphasizing new laser/optical techniques.

Recent studies have shown that application of advanced technology to combustion systems can result in significant increases in fuel economy. Design improvements in practical combustion systems are severely restricted, however, by current limitations in the understanding of the fundamental combustion processes involved. The attainment of such knowledge is, in turn, currently restricted by the inability of established experimental techniques to obtain basic data on gas composition and temperature in combustion environments. Within the past few years, however, new experimental techniques utilizing the unique characteristics

Construction Project Data Sheet

Sandia Laboratories

Mission Name: Energy Supply - Research
and Technology Development

Resource Name: Basic Energy Sciences

Activity Name: Chemical Sciences

1. Title and location of project: Combustion research facility, Sandia Laboratories,
Livermore, California (SLL)

2. Project No. 78-13-b

of lasers have been demonstrated to be capable of such measurements. For example, optical scattering experiments using high power continuous and pulsed lasers for Raman and Raleigh scattering, and using sophisticated tunable dye lasers for fluorescence scattering, have enabled detailed studies of flame combustion processes that have not previously been possible. Unfortunately, the laser systems required for the application of these new techniques to practical combustion problems are very complex and expensive, and widespread development and application of the new techniques have not been possible. The proposed Combustion Research Facility will include a central laser bank and data acquisition electronics to enable the new techniques to be used for a variety of basic and applied combustion experiments and serve as a unique and valuable national resource.

Sandia Laboratories has initiated programs in fundamental and applied combustion science. These programs include the development and application of new experimental techniques, the analysis and numerical modeling of combustion processes, and the development of a variable-displacement engine. These Sandia activities require new laboratory space and facilities. The required access to high power lasers is not possible in existing facilities, and no laboratory is available which can accommodate the growing combustion research activities and staff.

Several other energy and DOD related combustion problems would receive direct analytical support or indirect benefit from the fundamental research programs. These include chemical laser combustion for DOD, gaseous target intense neutron source chemistry for DOE's fusion program, and isotope separation diagnostics. Sandia Laboratories has a degree of involvement in each of these programs.

The Combustion Research Facility will also assimilate and disseminate combustion research literature, conduct national meetings and workshops in combustion science, initiate cooperative programs with industry and universities, and foster communication among combustion scientists. Although combustion science is central to energy research, no organization exists which performs all of these functions in the United States. Briefing and conference rooms will be required at the facility to accomplish this function. The facility, including laboratories, offices, and meeting rooms, will be located outside the classified areas at Sandia Laboratories to simplify the involvement of the outside user community.

Annual operating costs at facility completion for maintenance, utilities, salaries and wages, and programmatic costs are estimated at \$3,600,000 per year.

Construction Project Data Sheet

Sandia Laboratories

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Chemical Sciences

1. Title and location of project: Combustion research facility, Sandia Laboratories,
Livermore, California (SLL)

2. Project No. 78-13-b

10. Details of Cost Estimate*	Item Cost	Total Cost
a. Engineering, Design and Inspection @ approximately 15% of construction costs (item b)		\$ 950
b. Construction Costs		6,300
(1) Improvements to land	\$ 290	
(2) Building, approximately 45,000 sq. ft. @ about \$110/sq. ft.	4,950	
(3) Special facilities (fuel handling, load transfer and control systems, instrumentation, etc.)	360	
(4) Utilities	700	
c. Standard Equipment (includes pulsed lasers, gas analyzers, mini-computers, dynamometers and spectrometers)		650
Subtotal		7,900
d. Contingency at approximately 19% of above costs		1,500
Total Project Cost		<u>\$ 9,400</u>

*Based on completed conceptual design.

11. Method of Performance

Facility design and construction management will be on the basis of a negotiated fixed-fee contract with a design-construction management firm to maintain control of time and cost. Construction, to the extent feasible, will be accomplished by a series of staged lump-sum, fixed-price contracts awarded on the basis of competitive bids.

12. Funding Schedule of Project Funding and Other Related Funding Requirements:

	Prior Yrs.	FY 1979	FY 1980	FY 1981	FY 1982	Total
a. Total project funding						
1. Total facility costs						
a. Construction line item	\$ 1,000	\$ 3,200	\$ 5,200	\$ 0	\$ 0	\$ 9,400
b. CP&D	0	0	0	0	0	0
c. Expense funded equipment	350	1,300	650	0	0	2,300
d. Inventories	0	0	0	0	0	0
Total facility costs	<u>\$ 1,350</u>	<u>\$ 4,500</u>	<u>\$ 5,850</u>	<u>\$ 0</u>	<u>\$ 0</u>	<u>\$11,700</u>

Construction Project Data Sheet

Sandia Laboratories

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Chemical Sciences

1. Title and location of project: Combustion research facility, Sandia Laboratories
Livermore, California (SLI)

2. Project No. 78-13-b

	<u>Prior Yrs.</u>	<u>FY 1979</u>	<u>FY 1980</u>	<u>FY 1981</u>	<u>FY 1982</u>	<u>Total</u>
2. Other Project Funding						
a. R&D necessary to complete construction	0	0	0	0	0	0
b. Other project related costs	<u>0</u>	<u>0</u>	<u>100</u>	<u>0</u>	<u>0</u>	<u>100</u>
Total other project funding	0	0	100	0	0	100
Total project funding (item 1 & item 2)	<u>1,350</u>	<u>4,500</u>	<u>5,950</u>	<u>0</u>	<u>0</u>	<u>11,800</u>

	<u>Annual Estimates</u>
b. Total related funding requirement (estimated life of project: 20 years)	
1. Facility operating costs	\$ 108
2. Programmatic operating expenses directly related to the facility	3,500
3. Capital equipment not related to construction but related to the programmatic effort in the facility	800
4. GPP or other construction related to programmatic effort in the facility ..	150
5. Other costs	0
Total other related annual funding requirements	<u>\$ 4,558</u>

13. Narrative explanation of Total Project Funding and Other Related Funding Requirements

- a. Total project funding
 - 1. Total facility
 - (a) Construction line item
no narrative required
 - (b) CP&D
no narrative required
 - (c) Expense funded equipment

Increased recognition of the urgency of conservation-related combustion research makes it important to avoid any delay in full utilization of the Facility's capability. Therefore, intensified development of some of the necessary sophisticated instrumentation must proceed during the construction period in order that it be available as soon as the Facility begins operation. The figures in this line are the operating costs required to accomplish this research and development.

Sandia Laboratories

Construction Project Data Sheet

Mission Name: Energy Supply - Research
and Technology Development
Resource Name: Basic Energy Sciences
Activity Name: Chemical Sciences

1. Title and location of project: Combustion research facility, Sandia Laboratories,
Livermore, California (SLL)

2. Project No. 78-13-b

(d) Inventories

No narrative required

2. Other project funding

(a) R&D necessary to complete construction

No narrative required

(b) Other project related funding

Moving of equipment purchased prior to completion of construction from temporary space to the facility.

b. Total related funding requirements

1. Facility operating costs

These operating costs cover utilities, janitorial and maintenance for 45,000 sq.ft. at \$2.40/sq.ft. This level is the average cost of operating and maintaining the other facilities at Sandia Laboratories at Livermore which totals some 400,000 ft² of floor space.

2. Programmatic operating expenses directly related to the facility

These operating expenses include support for the Facility operators and scientific staff conducting R&D at the Facility. Programs support the needs of the Division of Basic Energy Sciences, and the Division of Power Systems.

3. Capital equipment not related to construction but related to the programmatic effort in the facility.

The annual capital equipment needs will average \$800,000. The R&D programs at the Facility are capital intensive and, because of the frequency of new starts from visiting scientists from universities and industry, will require continuing investment in new and improved electro-optical and minicomputer data analysis equipment.

4. G.P.P. or other related construction.

Funds will be required to modify the facility as requirements change for experiments.

5. Other costs

No narrative required