NBSIR 75-944

NATIONAL MEASUREMENT SYSTEM FOR THE PHYSICAL PROPERTIES OF ATOMS AND MOLECULES

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U.S. DEPARTMENT OF COMMERCE, Elliot L. Richardson, Secretary
Edward O. Vetter, Under Secretary
Dr. Betsy Ancker-Johnson, Assistant Secretary for Science and Technology

NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Acting Director

Abstract

National activity in measurement, compilation, evaluation, and dissemination of atomic and molecular data, estimated at 20-25 million dollars annually, impacts directly upon applied research and development projects costing over one-third billion dollars annually. NBS atomic and molecular programs, costing about 3 million dollars annually, provide the basis for the accepted standards for length, time and frequency; provide advanced measurement techniques; set rigorous performance standards for generation of atomic and molecular data, and provide for the construction of a sound data base for the user community. The largest users are programs aimed at energy generation and conversion. Basic sciences of aerodynamics, astrophysics, atmospheric physics and plasma physics are important users. Benefits for a broad range of industrial research activities are potentially large. It is recommended that NBS undertake to ensure the reliability and adequacy of the data base needed for important national programs, expand its contacts with private industry, develop increased awareness of the methodology for applying atomic and molecular data to technological development, and encourage effective utilization of this sector of the measurement system for the benefit of the economy.

Key words: Atom; energy generation; industrial technology; molecule; primary standards; properties.

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THE NATIONAL MEASUREMENT SYSTEM FOR THE PHYSICAL PROPERTIES OF ATOMS AND MOLECULES

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EXECUTIVE SUMMARY

The national activity in the measurement, compilation, evaluation, and dissemination of atomic and molecular data is represented here as a component of the national measurement system. The significance and validity of this representation rests largely on the role of the National Bureau of Standards in the development of measurement techniques, the encouragement of standards of measurement performance and in efforts to generate an adequate and well-documented data base effectively constructed to meet the needs of the user community.

The level of national activity in this field is estimated to be in the range of 20-25 million dollars annually, and the NBS programs in atomic and molecular measurements and in data evaluation and dissemination are approximately 3 million dollars of the total. The output of this activity has a direct impact upon applied research and development projects currently funded at a level well in excess of a third of a billion dollars annually. The largest of these are ERDA-supported programs aimed at energy generation and conversion (conventional controlled thermonuclear research, laser fusion, laser isotope separation, coal-burning magnetohydrodynamic generators, etc). There are large potential benefits for a broad range of industrial research and development activities. Atomic and molecular measurements are also extremely important to basic research in astrophysics, atmospheric physics, plasma physics and aerodynamics.

Examples of recent and current contributions with large impact range from data on specific single processes which play a determining role in some development problems, such as the control of ion propulsion engines for NASA, to entire data sets with which the behavior of a laser plasma or an MHD generator may be programmed and studied with electronic computers. The maturing of this kind of computational capability is of the greatest significance for the advancement of the technology of plasma devices. This significance is well recognized by the atomic and molecular research community which sees it as the vehicle for meaningful contributions toward solution of urgent economic and social problems. It is increasingly recognized within ERDA energy source development programs as an essential tool for orderly progress in their projects. It is generally less widely recognized in the industrial development community.

Certain atomic and molecular properties are used at the limits of achievable accuracy as the basis of the accepted standards for length, time and frequency. An atomic standard for mass is foreseen. Precision measurement techniques developed by workers in the field of atomic and molecular physics have been incorporated in the development of standards for measurements of other quantities, for example, gas pressure and radiant flux.

It is recommended that the National Bureau of Standards undertake activities which involve direct participation and interaction with the major ERDA projects, that it use this experience to guide development of new measurement methodology in atomic and molecular physics, and that it undertake to ensure the reliability and adequacy of the data base needed for these projects. Furthermore, it is recommended that the NBS expand its contacts with private industry, develop increased awareness of the methodology for applying atomic and molecular data to technological development, and provide such advice and guidance as will assure the effective utilization of this sector of the measurement system for the benefit of the economy.

1. INTRODUCTION

Atoms and molecules are the basic building blocks of matter. Everything that we humans do is conditioned by their properties. Knowledge of the physical properties of atoms and molecules is important for such diverse purposes as understanding the beginnings of the universe and mastering new sources of light and energy.

Generation of data about the physical properties of atoms and molecules comprises a modest but extremely important portion of the National Measurement System. The resulting data are a significant subset in the National Standard Reference Data System for which NBS has prime responsibility. During the last decade needs have arisen in a number of applied areas for more precise and complete atomic and molecular data. For example, precise data on the detailed reactions involving constituents of the earth's atmosphere are needed to allow adequately detailed modeling studies of phenomena occurring at various altitudes. Such studies in turn are of extreme importance to problems of national interest such as missile detection and the possible destruction of the shielding ozone layer in the atmosphere. However, the major need for new atomic and molecular data arises from the sophisticated new devices that are fast becoming a part of our current technology and will become even more important in the future. Gas lasers, plasma devices of all kinds, and many instruments for chemical analysis all depend for some of their principal characteristics directly on specific properties of atoms and molecules; and therefore on a well-defined body of atomic and molecular data both for their design and development and for the detailed interpretation of their use. Industrial devices, such as industrial lighting systems and magnetohydrodynamic coal-fired electrical generators also require atomic and molecular data input for efficient design and operation.

Nationally and internationally the measurement of the physical properties of atoms and molecules has been carried out in colleges and universities, in NBS, in federally funded research and development centers administered by universities or by other non-profit corporations, and to a lesser extent in large industrial research laboratories. An estimated 20-25 million dollars is expended annually in the United States [1] on the measurement of basic properties of atoms and molecules, about half of this amount in colleges and universities. The NBS program in development of methods of measurement, data generation, data compilation and evaluation involving atomic and molecular properties costs about three million dollars annually (see table 3). The largest concentration of work at NBS is in two Divisions of the Institute for Basic Standards, the Optical Physics Division (232.00) in Gaithersburg, Maryland and the Laboratory Astrophysics Division (274.00) of the Joint Institute for Laboratory Astrophysics in Boulder. Other substantial NBS programs are supported in the Time and Frequency Division (277.00) in Boulder and the Physical Chemistry Division (316.00) of the Institute for Materials Research.

These basic programs have a direct impact on applied research and development programs in which federal funds estimated at a third of a billion dollars are committed annually (see table 4). These include most notably several major long-range energy conversion projects, but also important components of the space program, environmental projects, and certain areas of application of physical sciences such as aeronomy and astronomy.

Earlier attempts to characterize the national effort in atomic and molecular physics [1,2,3] were based primarily on statistical surveys of the academic community covering only the academic effort in this field, and on data collected from federal agencies regarding their funding of academic research. The present study of the national measurement system for the physical properties of atoms and molecules provides a different perspective from those earlier surveys. The interface with the user community is explored more extensively here, and questions are raised concerning the roles of the measurement of atomic and molecular properties as an element of the national measurement system. In this study important more recent changes in the technological and economic environment which effect all of atomic and molecular physics are recognized. The opportunities for major contributions to society have become more apparent in the light of current national needs; hence the user community is now more clearly perceived and appreciated by the atomic and molecular physics community--and vice versa. The focus is again on the interface. Finally this study concentrates on delineating the functions of NBS atomic and molecular physics programs, especially as they relate to this interfacing role and the uniqueness of the NBS fulfillment of that role. This question is appropriately considered within the framework of the National Measurement System study.

2. STRUCTURE OF MEASUREMENT SYSTEM

Since this impact study is concerned with the measurements needed to characterize a wide variety of properties and interactions of many different atoms and molecules and since attempts to critically evaluate and systematically improve measurement techniques and the resultant data for this field are rather recent, many of the structural elements found in other portions of the National Measurement System have not been formally established here. Formally recognized elements are the portions of National Standard Reference Data System (NSRDS) and the associated data centers which are concerned with the compilation, evaluation and dissemination of atomic and molecular data. The prime responsibility for the National Standard Reference Data System is assigned to NBS. Other elements of this sector of the measurement system, i.e., research laboratories, mission-oriented government agencies, developmental laboratories, etc., are less formally recognized as part of the system but are key elements because they carry out measurements, decide priorities, and apply the data.

2.1 Conceptual System

The term "measurement system" as applied to atomic and molecular data refers to the data themselves; to the processes by which the data are acquired, evaluated, reformulated, compiled, disseminated and applied; and to the factors that determine the priorities for the acquisition and use of the data. It is convenient to divide atomic and molecular data into those data that characterize the structure of isolated atoms and of molecules, and those data that describe the probabilities or rates of interactions of atoms and molecules with radiation, charged particles and other atoms or molecules.

The atomic and molecular data characteristic of *isolated* atoms and molecules include their energy levels, the data describing the perturbation of these levels by uniform electric and magnetic fields and the data characterizing the behavior of the atoms and molecules in non-uniform or slowly varying electric and magnetic fields. The energy level data are obtained by measurements of the characteristic frequencies at which electromagnetic energy is absorbed or emitted by the atoms or molecules using a wide variety of experimental arrangements or by theoretical calculations utilizing analytical and computational solutions to the appropriate quantum mechanical equations.

The atomic and molecular data that describe the probabilities or *rates* of interactions of atoms and molecules with electromagnetic radiation, with charged particles or with other atoms include: a) radiative transition probabilities and the associated cross sections for the absorption of photons resulting in excitation or ionization of an atom or molecule, or photodetachment of an electron from negative ion; b) cross sections for stimulated emission of radiation (as in a laser); c) cross sections for the elastic or inelastic scattering of a charged or neutral atom or molecule by a target atom or molecule; d) cross sections for the excitation, deexcitation, or ionization of an atom or molecule by electrons; and e) coefficients describing the simultaneous emission or absorption of a photon and the collision of two atoms or molecules or of a charged particle and an atom or molecule. In addition to these data, which describe the interactions under precisely specified conditions, it is often useful to express the atomic and molecular data in terms of rate coefficients representing averages of the cross sections over a range of particle collision energies and directions. These rate coefficients are particularly useful for characterization of the interactions of charged and neutral particles with atoms and molecules at the high gas densities used in energy generation and conversion devices, e.g., high power lasers and magnetohydrodynamic generators.

The atomic and molecular physics community is concerned with accurate quantitative characterization of the properties falling within the above classifications. These efforts include few strictly routine experimental and theoretical procedures. Even in relatively routine spectroscopic surveys considerable sophistication is required to avoid invalidation of results by subtle extraneous effects, and analysis of results is exceedingly complex. In theoretical work it has long been known that the simplest, least expensive procedures fail completely for just those processes which would be vital in most useful plasma devices. Highly trained, experienced and resourceful investigators are required. Since the field of investigators is not uniform in this respect, a range of quality and utility exists in the data found in the open unevaluated literature.

The *user* community is sometimes concerned with those principal characteristics of specific atoms or molecules which determine corresponding principal characteristics of some plasma device, such as the atomic transition probabilities that determine laser gain, or the specific momentum transfer cross sections that may determine conductivity in a magnetohydrodynamic (MHD) generator. More often the user finds that he must confront an array of competing processes, so that his model may consist of a system of equations with data input for each of the several processes. In either case the specification of accuracy requirements for data input to such a model must be met by reliable statements of the accuracy and applicability of the data available.

The user of atomic data is always faced with the problem of evaluation. For some processes, only a single measurement or theoretical calculation is available, so that the main task of evaluation is in determining the probable accuracy of the given measurement or calculation. However, there are often several independent and inconsistent determinations of the same set of data by alternative theoretical and experimental techniques; and the user is faced with the problem of selecting the best data in addition to estimating its probable accuracy.

The accuracy with which measurements of cross sections and rate coefficients for atomic and molecular processes can be made has improved slowly but steadily during the past thirty years. For example, as the result of the improvement in techniques for absolute radiant energy and gas pressure measurements and the development of improved electron guns, optical filters, etc. it is now possible to measure selected cross sections to an accuracy of better than 3%. Somewhat higher accuracies (<1%) are claimed for selected rate coefficients. However, according to studies sponsored by the National Standard Reference Data System most of the available cross section and rate coefficient data are much less accurate than these values. Furthermore, the effort currently devoted to the systematic measurement of cross sections and rate coefficients for a wide range of atoms and molecules is short of that required to meet the needs of, for example, the high power laser development programs for the generation of energy by laser induced fusion and for laser induced isotope separation (according to officials in charge of these programs).

The development of procedures for insuring accurate measurements of the physical properties of atoms and molecules has often the form of extremely careful measurements (called *benchmark measurements*) of a small sample of the properties of a few atoms and molecules. In a few cases the results of these measurements have become the basis for the international standards, e.g., frequency and wavelength. In some cases professionally evaluated data compilations and critical reviews provide a basis for the individual researcher to select data for use as a standard with which to compare measurements of a given property for other species. However, in many cases carefully evaluated (or *standard reference*) data are not available. The researcher thus cannot make comparisons with reference data and so merely uses the latest published values.

The measurements system in atomic and molecular physics has a unique relationship to measurement systems described in other reports of this series. On the one hand, extremely precise measurements of radiant fluxes and energies, frequencies and gas pressures often at the limit of the state-of-the-art, are needed to perform benchmark measurements. The system thus relies upon the measurement systems for radiometry and photometry, vacuum-ultraviolet radiation, time and frequency and pressure. On the other hand, precise atomic and molecular data is often needed, either for instrumental calibrations or to provide a basic understanding of complicated measurements procedures which form a part of other measurement systems, in particular those concerned with laser parameters, spectrophotometry and surface physical measurements.

2.2 Basic Technical Infrastructure

2.2.1 Documentary System

The documentary aspects of the national measurement system for atomic and molecular data include the publication of bibliographies, data compilations, data evaluations, review papers, etc. by data centers associated with the (U.S.) National Standard Reference Data System (NSRDS); the Oak Ridge Atomic and Molecular Processes Information Center; journals devoted to data publication, data compilations by contractors to the Department of Defense, bibliographical data retrieval systems set up by universities and private companies (e.g., Lockheed); original research and review articles published in U.S. and foreign professional journals; and books printed by private publishers. Only the NSRDS and associated Data Center publications have an official role in the measurement system.

National Standard Reference Data System publications in the area of atomic and molecular data make up over half of the forty-seven NSRDS publications. See NSRDS publications list [4]. Journals publishing atomic and molecular data are the Journal of Physical and Chemical Reference Data (NSRDS) and Atomic and Nuclear Data Tables. Recent data compilations issued by DoD contractors include the Defense Nuclear Agency's Reaction Rate Handbook [5] and the Air Force sponsored Spectroscopic Constants for Selected Heteronuclear Diatomic Molecules [6]. One of the most readily available computer-based retrieval system for bibliographical data is the Lockheed Aircraft Corporation System.

Because of the limited fraction of the atomic and molecular species covered by compilations and reviews sponsored by NSRDS and associated data centers, the normal scientific literature forms a very important source of information on measurement techniques and data. The development engineer or scientist from another field is often unable to evaluate the relative merits of the published experimental techniques or data. Choices are often made on the basis of the scientific reputations of the institute at which the work was carried out. Among such institutions NBS is particularly noted for its precision measurements and for its collaboration with user groups.

Formal documentary standards, such as treaties and voluntary engineering standards, play only a minor direct role in this field, and vice versa. However, many of the documents described above, especially those of the National Standard Reference Data System, often function informally as such standards.

2.2.2 Instrumentation System

2.2.2.1 Measurement Tools and Techniques

The scientific and technological base for modern measurements in atomic and molecular physics includes a very broad range of sophisticated new techniques:

1) High vacuum technology and molecular beam techniques are basic to performing measurements on individual atoms and molecules including reactive species, effectively free of interactions with near neighbors and under controlled conditions of ambient fields, and/or incident flux of photons or other particles. Systems of advanced design can be built to reduce background populations to as low as $\sim 10^6$ atoms and molecules per cubic centimeter and to extend mean free-flight times to hours.

2) Particle mass and particle energy selectors based on a variety of physical principles are available to define the species content of beams as well as to define beam kinetic energy.

3) Monochromatic sources of electromagnetic radiation, notably those of the laser family, are revolutionizing modern spectroscopy. Tunable lasers in particular have greatly facilitated measurements of structure of molecules and are opening the way to investigation of interaction properties of short-lived excited states.

4) New detectors, based on photoelectric and photoconductive properties of solids recently discovered by solid state physicists, allow extremely sensitive measurements of photons, electrons and other particles. In many circumstances these are individually detected, counted and processed using

5) sophisticated digital electronic systems and compact laboratory minicomputers, which make it practical to handle large quantities of data automatically.

The accuracies required in measurements of atomic and molecular properties typically strain the measurement system in two areas:

1) Gas densities are exceedingly difficult to measure to accuracies of a few percent as sometimes required, especially for gases that are reactive to any degree, as in the low pressure regimes typical of atomic and molecular properties measurements. The most reliable measurements are accomplished at high pressures; and pressure divider techniques can be used to generate known density low pressure samples of non-reactive gases such as helium.

2) Radiant flux is difficult to measure in a laboratory situation, even using standard lamps supplied by NBS. In addition, interaction geometry is often a limiting factor.

Other quantities are measurable with quite sufficient accuracy using commercially calibrated instruments ultimately referred to the national standards. Wherever possible in the case of particle fluxes and photon fluxes, intensity measurements are reduced to counting procedures using single particle detectors and digital electronics, techniques borrowed from nuclear physics.

The concept of *benchmark measurements* has been applied by NBS as a technique for providing a convenient method of calibration and/or *measurement assurance* for several types of measurements. A well-defined property, such as the probability for electrons exciting principal radiations of the helium atom, may be measured with extraordinary care at NBS, utilizing the shortest possible chain to the primary standards. This carefully measured property may then be used to calibrate, in a relatively simple procedure, measurements of the corresponding properties of other atoms and molecules.

2.2.2.2 The Instrumentation Industry

Commercial optical spectroscopic and mass spectrographic instrumentation grew up in close association with atomic and molecular physics and has become a multimillion dollar industry. Atomic clocks are widely used in satellite tracking and timing, in connection with elaborate navigation systems, and in the television industry. Magnetometers based on properties of alkali vapors have been standard instrumentation in satellite and rocket measurements of magnetic fields in space. The continuous-wave gas laser is currently the basis for development of a multimillion dollar commercial laser metrology industry involving length measurement and control as well as holographic instrumentation. Some of these developments are treated in more detail in other measurement study reports.

The field of atomic and molecular physics is relatively small, specialized and varied, so that no distinctly identifiable measurement instrumentation industry exists to support it. A wide variety of commercial instrumentation and technology common to larger fields such as nuclear and solid state physics and space science, provide a base for this field. However, advanced work typically requires unique instrumentation, designed and built in-house.

2.2.3 Reference Data

Only a small subset of the available data on atomic and molecular properties has been critically evaluated either by NBS or by other leading authorities in particular subfields. This subset constitutes the reference data of this sector of the national measurement system. The atomic energy levels tables (NBS Circular 467) are an example of these types of data. It should be noted that the NSRDS-sponsored critical reviews and data evaluation publications exert an influence far beyond their immediate area of concern through the setting of criteria for reporting experimental conditions, of estimating errors, of critical evaluation and of making impartial choices among available data and experimental techniques.

Specific examples of measurements at NBS of data suitable for reference data are the wavelengths of selected atomic transitions used as standards in applied spectroscopy; the proposed international standards of wavelength utilizing lasers stabilized to spectral lines in the infrared and visible; the frequencies of various infrared molecular transitions being used in connection with the development of optical frequency standards; and cross sections for the electron excitation of selected spectral lines of helium. Examples of such measurements elsewhere are the very precise measurements of electron drift velocity and diffusion coefficients for selected gases made at the Australian National University and measurements of atomic hyperfine structure at various universities. One should note that there is a major requirement for additional reference data regarding rates of interactions with atoms or molecules. Chemical rate data are not included in this study.

The users of the reference data developed by the measurement system include scientists and engineers in industry- and government-supported R and D concerned with lasers [7-9], high efficiency illumination [10], electrical power generation and distribution [11,12], missile reentry [13], radio propagation [5], and chemistry [15].

The current methods of data acquisition for the properties of atoms and molecules generally involve design, construction and testing of specialized apparatus by individual scientists followed by computer controlled recording and computer analysis of data. The development of measurement techniques capable of yielding reference-data-quality results is particularly time consuming and is seldom undertaken outside laboratories such as NBS where there is an inherent appreciation of the desirability of extension of precision measurements.

One pattern of data use is for scientists and engineers engaged in invention and development to make computer models of their devices and systems using the most recently published data where available and educated guesses elsewhere. These models are used to understand the current devices and to predict the behavior of larger devices. Reference data on a particular species are also used to test similar measurements on other atoms and molecules.

2.2.4 Reference Materials

There are no examples of formally define-Standard Reference Materials in this field. See, however, discussions of benchmark measurements elsewhere in this document. Such benchmark data in combination with commonly available high-purity materials and well-defined experimental conditions fulfill a role comparable to the role of Standard Reference Materials. They are useful for the calibration of measurement systems in this and other fields. Examples are the intensity of radiation emitted from hydrogen atoms in a prescribed hydrogen arc, the frequency reference achieved by stabilizing lasers to certain infrared absorption lines of methane under prescribed conditions, and the radiation flux excited per incident electron in certain spectral lines of pure helium.

2.2.5 Science and People

Fields of science and technology supporting the national measurement system for the properties of atoms and molecules include computer science, laser technology, physical chemistry, surface science, high temperature technology, vacuum technology, electronic component and equipment technology. These fields support the measurement system by helping to make possible improved measurements over a wider range of experimental variables; improved analyses, storage and retrieval of data; more accurate calculations of individual atomic and molecular properties; and more realistic modeling of applications of the data.

Contributions of the national measurement system to science include new techniques for making and analyzing measurements, better understanding of correlation between experiment and theory, better calculational techniques for theory, and better ways of integrating individual measurements into models.

Professional societies relevant to this measurement system are the usual ones for physicists and physical chemists, i.e., American Physical Society, American Chemical Society, Optical Society of America, plus groups such as the Division of Electron and Atomic Physics of the American Physical Society, the International Conference on the Physics of Electronic and Atomic Collisions, and the Gaseous Electronics Conference.

Knowledge is disseminated by standard publications, e.g., Physical Review, Reviews of Modern Physics, Journal of Chemical Physics, and Reviews of Scientific Instruments. Data are also disseminated through preparation of articles for data journals, e.g., Atomic and Nuclear Data Tables and Journal of Physical and Chemical Reference Data, and for handbooks, such as the Defense Nuclear Agency's Reaction Rate Handbook.

The educational institutions and procedures for the scientists participating in this measurement system are those typical of physicists and chemical physicists. Relatively few people who are trained in other fields participate in this system. Important exceptions are the engineers who utilize much of the data generated by the system.

2.3 Realized Measurement Capabilities

Measurement range, accuracy and precision vary widely with effort devoted to and difficulty of measurement. Thus, for lifetime measurements of visible lines to determine oscillator strengths (a benchmark measurement) the highest attainable accuracy is $\sim\pm1\%$, while the current accuracy of measurement of the wavelength of the methane stabilized laser is about one part in 10^{14} when averaged over thirty seconds. Table 1 contains approximate values for the highest accuracy yet attained, representative applications for a few of the physical properties of atoms and molecules. This list of properties is only a small fraction of the list of importance to technology and science, e.g., ten categories compared to the over fifty categories in a recent report [16] to NSF on energy-related atomic and molecular physics. Similarly, only a fraction of the available experimental techniques and of the present and potential applications are cited. Note that in every case cited the accuracy required for applications equals or exceeds the accuracy generally available. Also, it should be noted that in cases in which very high accuracy has been achieved, technological advances have rapidly made use of the accuracy.

Table 1. Accuracy of measurements of representative physical properties of atoms and molecules

Physical property measured	Experimental technique(s)	Highest accuracy	Typical accuracy of good data	Accuracy required for application	Representative application
I. Energy levels and structural properties*					
A. Visible spectra					
1. atoms	spectrometer, interferometer	$1:10^8$	$1:10^7$ well separated	$1:10^7$	isotope separation
2. molecules	stabilized laser	$2:10^{10}$ (iodine)	$1:10^8$ strong lines	$1:10^{13}$	"atomic" clock
B. Molecular infrared and					
1. rotational transitions	microwave absorption	$1:10^7$	$1:10^5$	$1:10^6$	
2. vibrational transitions	infrared spectrometer, stabilized laser	$1:10^7$ $5:10^{12}$ (methane)	$5:10^5$ ---	$1:10^6$ $<1:10^{13}$	laser induced chemistry, isotope separation, "atomic clock"
C. Ultraviolet and X-ray spectra	spectrometer crystal grating spectrometer	$1:10^6$ (copper K)	$1:10^6$ $1:10^5$	$1:10^7$	isotope separation fundamental constant determination
D. Atomic hyperfine separation	radiofrequency spectroscopy	$1:10^{13}$ (cesium)	$1:10^6$	$1:10^{13}$	"atomic" clock
E. Molecular quadrupole moment	microwave line broadening, high resolution Zeeman spectroscopy	10%	30%	10%	laser line width and energy transfer calculation
II. Kinetic properties					
A. Excitation cross sections by					
1. electrons	crossed beams, gas cell	3%	20%	10%	high power visible laser models
2. atoms and ions	crossed beams	20%	20%	10%	CTR plasma modeling
3. theory for electrons	numerical calculation	5%	factor of 2 (low energy)	10%	CTR plasma modeling and diagnostics
B. Vibrational excitation or deexcitation by					
1. electrons	crossed beams, gas cell drift tube	20% 5%	20% 10%	 10%	 high power laser modeling
2. atoms or molecules	laser induced fluorescence	10%	30%	10%	"chemical" reactors
C. Oscillator strengths, visible and ultraviolet	lifetime theory	1% $1:10^4$ (hydrogen)	25% 30%	 10%	laser development CTR plasma diagnostics
D. Oscillator strengths, infrared	absorption	5%		10% 10%	laser development atmospheric energy balance
E. Continuum absorption cross sections in gas mixtures	fluorescence	20%		20%	new visible laser development high power illumination development
F. Electron drift velocity	transit time	0.5%	5-20%	10% 10% 10%	high power laser development radar interference MHD generator development

*The accuracies given under items A-D for the highest accuracy and the required accuracy are only for orders of magnitude consideration and are subject to refinement and precise specification in the relevant publications, etc.

2.4 Dissemination and Enforcement Network

Since the national measurement system for the physical properties of atoms and molecules involves rapidly changing measurement techniques, a very large number of properties and species, and a user community with changing interests and accuracy requirements, it is very important that evaluated data be rapidly and widely disseminated. However, there is no mechanism for the enforcement of the use of recommended measurement techniques for obtaining atomic and molecular properties or for the use of recommended data. Peer evaluation and the need for more accurate data for specific applications are the main forces that promote the use of better available techniques and data.

Regulatory agencies, e.g., the Environmental Protection Agency, are ultimate users of the output of the atomic and molecular properties measurement system through their recommendation and enforcement of the use of techniques developed to measure the concentrations of, for example, pollutants. These agencies also participate in the measurement system through their encouragement and occasional support of the development of new measurement techniques.

The dissemination of the measurement techniques and properties of atoms and molecules has been discussed in Section 2.2.1.

2.5 Direct Measurements Transactions Matrix

2.5.1 Analysis of Supplier and User Interactions

The following "Direct Measurements Transactions" matrix, Table 2, is intended to show the principal interactions among and within the organizations associated with the national measurement system for the physical properties of atoms and molecules. The flow of data, measurement techniques, etc. is from the organization given in the left hand entry to the organization with the number given at the top of the column. Entries on the diagonal describe the flow within an organization. The code used within an entry is given at the bottom of the matrix table.

2.5.2 Identification of Major Users and User Needs

A very important aspect of the measurement system for the physical properties of atoms and molecules is the identification of the classes of users and the needs of these users for data and measurement techniques so as to enable an allocation of resources and to provide justifications for the measurement system. An example of an initial attempt to identify the user needs for those concerned with electrical power generation, transmission and utilization is given in Appendix C. A more detailed discussion of the needs of research on the magnetic confinement approach to controlled thermonuclear reactions is given in a report entitled "Atomic, Molecular and Nuclear Data Needs for CTR" [17] prepared for the Atomic Energy Commission. Of particular value at the present time would be an assessment of the current and future needs for measurements of the physical properties of atoms and molecules by the laser development programs of the Energy Research and Development Administration (ERDA) and of the Department of Defense.

While currently foreseen needs of technology should play an important role in the allocation of resources for measurements of atomic and molecular properties, it is essential that a significant fraction of the resources be devoted to the measurement of new properties and to the development of new measurement techniques. There are numerous recent examples in which the development of improved techniques for the measurement of properties of atoms and molecules has led to the proposal of a potentially important new laser mechanism. One example is the improved measurement of metal vapor-rare gas interactions in connection with excitation transfer measurements at NBS/JILA which led to the proposal of excimer lasers utilizing the radiation emitted by molecules formed from metal atoms and rare gas atoms [18,19]. A second example is the study of "inner shell" ionization and X-ray production which led to the proposal for the use of these processes for X-ray lasers [20].

Table 2

Direct measurements transactions matrix for physical properties of atoms and molecules

SUPPLIERS \ USERS	1	2	3	4	5	6	7	8	9
1 Knowledge Community & Publications	4 2 4 4	4 2 4 4	2 0 3 2	4 0 4 2	4 3 3 2	2 3 4 4	3 3 4 0	2 3 4 2	2 3 3 0
2 Data Processing Organizations: NSRD, Data Centers, etc.	3 0 3 2	X 0	2 0 3 2	3 0 4 2	3 0 4 2	3 0 3 2	3 0 4 2	3 0 3 2	3 0 3 2
3 Instrumentation Industry	2 0 4 2	2 0 1 0	?	2 0 3 2	2 2 3 2	3 2 3 2	3 2 3 0	3 0 3 2	2 3 2 2
4 NBS	3 0 4 2	3 0 4 3	2 1 2 2	3 0 0 4	2 0 4 2	3 0 4 3	3 0 4 2	3 0 4 2	3 0 3 2
5 Energy Res. and Dev. Admin. Mag. C.T.R.	3 3 2 2	4 2 3 3	?	4 2 3 2	X	X	X	2 1 2 2	2 3 2 2
6 ERDA: Laser Fusion & Laser Isotope	2 0 3 2	2 0 3 2	2 1 3 2	2 1 4 2	X	X	2 2 3 3	4 2 3 4	2 2 3 2
7 Dept. of Defense	2 3 2 0	2 3 2 0	2 3 3 0	2 3 3 0	X	2 2 3 2	2 2 0 2	2 2 3 0	1 2 2 0
8 Industry: Lasers	2 3 2 0	2 3 2 0	2 1 3 0	2 1 3 2	2 0 2 4	3 2 4 2	3 2 4 0	2 0 0 0	1 0 1 0
9 Industry Electrical Power Gen., Trans. & Use	2 3 2 0	2 3 2 0	2 1 3 0	2 0 2 2	3 0 4 2	2 1 2 2	2 0 2 0	2 2 3 2	2 0 0 2

KEY TO MATRIX ENTRIES

Each cell (USERS):

C		D
	A	
B		R

C - IMPORTANCE OF TRANSACTIONS

1 = Purely convenience
2 = Strongly desirable
3 = No real alternatives
4 = Essential

D - (IN)ADEQUACY OF SERVICES

0 = No improvements needed
1 = Could be improved
2 = Marginal
3 = Serious deficiencies
4 = Out of control

B - RATE OF CHANGE

N = Declining
0 = Stable
2 = Growing
4 = Growing explosively

A - MAGNITUDE OF TRANSACTIONS

0 = Trivial
1 = Minor
2 = Moderate
3 = Important
4 = Major

R = Flow of requirements info dominates

? = Unknown, X = Not studied, Blank = 0

3. IMPACT, STATUS AND TRENDS OF MEASUREMENT SYSTEM

3.1 Impact of Measurements

3.1.1 Functional, Technological and Scientific Applications

New methods of making and analyzing measurements of atomic and molecular properties and measurements of critical data are used to obtain data and understanding needed in the initial design, diagnostics, optimization and extrapolation of plasma devices. Atomic and molecular data are used in plasma models of varying degrees of complexity. In many cases the number of interactions which one can consider is limited by the size of available computers.

Technologies effected are lasers; electrical power generation and switching; commercial, highway and home illumination; isotope separation; information displays; thin film production; radio frequency, satellite and radar transmission; radiation detection; chemical processing; arc welding and metal processing; pollution monitoring; air cleaning; pyrotechnic flares; etc.

Scientific fields effected include molecular kinetics and structure, non-linear radiative processes, collision theory and experiment, radiation and charged particle transport, studies of spectral line shapes, gaseous electronics, astrophysics, aeronomy, and aerodynamics.

3.1.2 Economic Impacts--Costs and Benefits

The cost of all measurements in atomic and molecular physics carried out in the United States is estimated to be $20-25 million per year, based in 1968 data (approximately $15 million per year) for federal support of universities [1] adjusted for inflation, and a rough estimate as to other federal and non-federally supported programs.

The economic benefits of measurements of atomic and molecular properties cannot be precisely estimated, but one example can be given. Economic data available for one type of gas discharge lamp--the high pressure arc lamps for commercial and highway illumination--show annual sales of $60 million per year and a growth rate of ~20% per year [10]. The primary effect of an increase in efficiency or reduction of size of these lamps through the use of atomic and molecular data would be a reduction of sales of other types of lamps. Thus, the major impact would be energy conservation. Estimates of the portion of electrical energy used for all illumination purposes range from 8% to 20% [10].

A recent estimate [21] gives a 1975 budget of $55.5 million for laser research and development. Most of the effort will be directed toward laser fusion and isotope separation for use in the generation of energy.

3.1.3 Social, Human, Person-on-the-Street Impact

Although this portion of the measurement system has no immediate direct effect on everyday lives, its indirect effects are of great potential importance. For example, it provides the basis for future improvements in energy generation, distribution and utilization; improvements in reliability and ease of communications; more effective defense systems; more reliable fire detection, explosion prevention, and lightning protection; and more effective monitoring and alleviation of pollution. Social benefits of applications measurements of atomic and molecular properties ultimately will be determined in economic terms. Alternative benefits, such as energy conservation will be decided on an economic basis.

3.2 Status and Trends of the System

In selected areas of atomic and molecular physics NBS has very successful projects devoted to improving measurement and calculation techniques, collecting and evaluating critical data and improving techniques for data utilization. Areas that are well covered include electron-ion (positive and negative) collisions and excitation of neutral species by electron impact, radiative transport, atomic and molecular spectroscopy at all energies, and atomic transition probabilities. Some other areas, e.g., ion-molecule reactions and atom-molecule energy transfer measurements, are covered reasonably well by other laboratories (NOAA, U. of Pittsburgh, Stanford Research Institute). On the basis of requests for data [Appendix B] on the physical properties of atoms and molecules in systems of current technological interest, it appears that some very important areas to current technology, e.g., electron transport coefficients, are being ignored by the U.S. research community.

A factor which limits the effort devoted to the measurement of the physical properties of atoms and molecules by the major development laboratories--Energy Research and Development Administration, Department of Defense and industry--is that in most cases these laboratories [22] are being forced by current technical goals and market pressures to adopt very short-range time scales for their research programs. Most universities do not have the continuity of support or the incentive required for the development of new techniques needed to obtain the large amounts of accurate data on physical properties of atoms and molecules. Barring major changes in research management it will be up to laboratories such as NBS to provide the environment and support which will allow the long term, e.g., three years, investment in new measurement and theoretical techniques for data generation and, as well, the long-term investment in new data utilization techniques.

Examples of new and rapidly growing technologies that demand a broad range of data obtainable only by long-range research efforts are those which depend on the development of new classes of high power lasers for isotope separation and possibly for laser fusion, and also those directed to the development of controlled thermonculear power using plasma confinement techniques. Without improved data sets as the basis for more effective modeling and for more effective analytical and diagnostic measurements, development of these technologies will be handicapped [21].

4. SURVEY OF NBS SERVICES

4.1 Historical Background

NBS has been active in the measurement of the physical properties of atoms and molecules since the early 1920's. NBS work in this area has always consisted of three complementary steps, generally performed within the same laboratory as follows:

1. Development of new measurement techniques.
2. Data generation using these techniques and development of analysis techniques to interpret data thus obtained.
3. Compilation and critical review of all available data either within a particular category of atomic and molecular data or applicable to a particular perceived need.

The way in which these three aspects of atomic and molecular measurements have been pursued at NBS is aptly illustrated by the work in atomic spectroscopy, a field in which NBS has played a leading role over much of its history. Early work by Foote and Mohler was concerned mainly with development of techniques for measuring spectral wavelengths. Their work was continued and extended during the period of the 1930's-40's by Meggers and his associates and an attempt was made to provide as much information as possible on spectral line positions and the inferred energy levels. The motivation for these measurements was the need for these data in chemical analysis and for the analysis of astrophysical data. The compilation and systematic analysis of data of this type have been ongoing projects ever since, and NBS continues to maintain a current listing of all data in this well-defined area as a part of the National Standard Reference Data System. In this particular field a large part of the data available have been measured or analyzed by NBS staff workers either working in their own laboratories or in close collaboration with other workers in universities or other government laboratories.

The early work in spectroscopy at NBS showed a remarkable amount of foresight concerning atomic data and measurement calibration techniques that would be needed in the rapid expansion of technology that occurred in the period following the second world war. One of the crowning achievements of this work was the publication in 1949-52 of NBS Circular 467, a tabulation of most of the known atomic energy levels grouped by atom and charge state available at that time. This three-volume set compiled by Charlotte Moore-Sitterly using the extensive files of bibliographic and numerical data accumulated at NBS during the previous decades continues to serve as the prime reference source of atomic spectral data and as a model for further tabulations of this type.

The close relationship of work in atomic physics and basic standards of measurement is illustrated by the work on precise wavelength standards. In 1950 an electrodeless mercury vapor using Hg^{198} which had been obtained in pure form via transmutation of gold in a reactor was announced by Meggers and Westfall. This development and subsequent work on precise wavelength sources at NBS played an important role in the eventual adoption in 1960 of the krypton lamp which is the current international standard of length.

In addition to playing a leading role in the measurement of well-established physical properties of atoms and molecules, NBS has pioneered in the development and application of measurement techniques for properties previously unmeasured or poorly measured. For example, measurements by F. L. Mohler and associates of the absorption and emission of radiation by cesium vapor plasmas in the early 1930's provided the basis for testing newly developed theories of the emission of light by gases and, when chemically resistive ceramics became available after World War II, for the development of highly efficient metal vapor lamps. The work of Branscomb, et al. provided much of the data and methods of analysis of the interaction of photons and negatively charged particles in the ionosphere. The work of Broida, et al. provided the field of chemical physics with many of the measurement techniques now being used to study the ionospheric ozone problem and laser induced chemistry.

During the period from 1950 to 1962 the overall efforts in atomic and molecular physics were greatly expanded, chiefly in response to needs for atomic and molecular data from other government agencies (AEC, DoD and, after 1959, NASA). The efforts in atomic spectroscopy were extended to molecules by the formation of groups whose prime concern was the infrared and microwave spectroscopy of molecular systems. New programs in electron and far ultraviolet physics were added. In addition, NBS moved actively into the area of measuring rates for atomic processes, i.e., transition probabilities between atomic states and cross sections for photon induced processes.

The formation in 1962 of the Joint Institute for Laboratory Astrophysics (JILA), a cooperative effort between NBS and the University of Colorado, resulted in a further strengthening of NBS research in the area of the measurement of the physical properties of atoms and molecules. Since its formation JILA has become one of the leading laboratories for the measurement and calculation of atomic and molecular properties. Particularly significant activities of the past five years are the measurements of the properties of negative ions; development of the methane stabilized laser and its application to the precision measurement of wavelength; the measurement of electron excitation and recombination cross sections for neutral and ionized atoms and molecules; the measurement and interpretation of radiation emitted by metal vapor-rare gas molecules; the measurement of the distribution in energy of the products of electron-induced ionization of atoms and molecules; and the reviews, evaluations and compilations of the collision properties of atoms and molecules.

A theoretical program directed toward calculating atomic and molecular properties which cannot easily be measured or which provide a basis for understanding and evaluating measurements has developed. The theoretical program also provides accurate and efficient means for calculating the energy transport, degree of ionization, etc. in ionized gas systems. Recently, close ties have been established with scientists and engineers engaged in the development of devices utilizing the measurement techniques and data of this measurement system. This activity has resulted in a considerable increase in the JILA/NBS effort directed toward data utilization through the modeling of ionized gas devices and systems.

At NBS/Gaithersburg more recent program evolution includes the application of highly refined design techniques to the development of apparatus for measurement of electron collision cross sections and to the composition analysis of gas samples; the measurement of absolute spectral emissivity of plasmas and of spectral line shapes under plasma conditions for use as a radiation standard and as a plasma diagnostic; measurements of atomic transition probabilities; compilation and evaluation of atomic transition probabilities and compilation of references on spectral line shapes; the critical calculations of atomic transition probabilities; theoretical predictions and understanding of atomic structure, radiative absorption and collisions; applications of laser techniques to the measurement of frequencies of molecular transitions and to the enhancement of molecular interactions; the accurate measurement of the frequency of stabilized visible lasers; and the experimental and theoretical identification of interstellar and laser emission lines.

Other NBS programs concerned with the physical properties of atoms and molecules include the identification of and measurement of frequencies of molecular transitions; the development of heat pipe technology for spectroscopic studies of high temperature material such as metal vapors; the measurement of molecular energy relaxation rates; the prediction of molecular interactions and energy levels; and the development of accurate theories of spectral line shapes in plasmas.

The period since 1970 has resulted in a major shift in motivation for the measurement of the physical properties of atoms and molecules at NBS. Whereas during the 1960's atmospheric and astrophysical problems provided a focal point for major efforts, the major need for atomic and molecular data at present is in the detailed interpretation and prediction of the operation of devices or industrial processes involving interactions among radiation, electrons, atoms and molecules. Examples are gas lasers of all types, gas discharge lamps, magnetohydrodynamic generators and controlled thermonuclear fusion devices. Through its numerous contacts with user groups in government and industry NBS has responded rapidly and effectively to these changing needs.

4.2 The Present--Scope of NBS Services

4.2.1 Description of NBS Services

The major NBS organizational units participating in the measurement system for the physical properties of atoms and molecules are Divisions 232 (Gaithersburg) and 274 (part of JILA in Boulder). Approximately three-eighths of the Division 232 program and half of the Division 274 program fall in the sector of the measurement system included in the present study. The detailed division of this effort among projects is given in Table 3. As indicated above, other divisions of NBS contain projects which could properly be classified as part of the measurement system for atomic and molecular properties but which have somewhat closer ties to other parts of the national measurement system. A detailed description of the rationale for the choice of projects included is given in Section 4.2.4.

The scope of NBS services extends to all phases of the national measurement system for the physical properties of atoms and molecules as defined in Section 2.1. Thus, in addition to performing measurements and disseminating resulting data, NBS services include development of measurement methods of instruments for precise atomic and molecular measurements and of techniques for the analysis and orderly classification of atomic and molecular data. Detailed computational methods are also developed for use in the analysis and classification of data and for theoretical prediction of data that are not accessible to measurement. Other services provided are: preparation of critical reviews; consulting services as to sources of data, recommended data and the utilization of data; interpretation of user needs; participation on review committees of various government agencies to assess data needs; and recommendations to funding agencies as to data needed and the best people and places for getting work done. The NBS position of neutrality in these matters is crucial to the review and advisory services.

The technical base for these services includes the following components:

The atomic spectroscopy laboratory in Gaithersburg is well equipped with spectrographs covering the range 40-12,000 Å and data reduction procedures have been evolved utilizing present NBS computational facilities. An important part of the data analysis capability consists of a large set of theoretical computational programs which are used either to predict energy levels from theoretical parameters or alternatively to systematize available data by obtaining empirical parameters from measured spectra.

The technical base in molecular spectroscopy is similar to that in atomic spectroscopy. A number of high resolution instruments are used to obtain raw data in the microwave, infrared, visible, and ultraviolet spectral regions. Computerized data reduction is used here to systematize the data via the calculation of molecular constants which may in turn be compared with theoretical predictions.

Instrumentation for photoabsorption measurements of metallic vapors and gases is largely built about the NBS SURF-II facility, the principal source of high intensity ultraviolet radiation. This facility is complemented by several lower intensity laboratory sources. Several high resolution spectrometers, designed and constructed at NBS, are available. Absorption cells are provided by a number of heat pipe absorption furnaces which have been specifically designed and constructed at NBS for far ultraviolet absorption measurements. Design and testing of newer devices of this type is an ongoing effort.

Electron scattering and excitation cross sections are measured with high resolution electron spectrometers designed and constructed at NBS. These devices, which are continuously being modified and improved to meet the needs for new data, are operated under the control of a small computer and utilize computer techniques to identify and separate the contributions of up to four gas components.

Table 3. NBS projects in measurement system for physical properties of atoms and molecules

Project #		National Bureau of Standards	Sponsor National Standard Reference Data System	Other Agency
274012	1/2 of Visiting Scientists Program	140		
2740141	Energy Deposition in Gases	202		
2740158	Radiation and Energy Balance in Gas Discharge Lasers	93		20
2740180	Atomic Physics Cross Sections Information Center		149	
2740190	Transfer of Radiation Through Gaseous Media	60		
2740254	Low Temperature Plasma Collision Parameters	103		65
2740540	CTR and High Temperature Plasma Collision Parameters	73		40
		671	149	125
		(71%)	(16%)	(13%)
2320165	Electronic Spectra	62		
2320125	Laser Applications to Air Quality Analysis	50		
2320170	Transition Probabilities	327		
2320171	Transition Probabilities Data Center		50	
2320474	Data Center on Atomic Lines, Shapes and Shifts			5
2320477	Transition Rates			175
2320102	Consultants on Theory	64		
2320110	Rare Earth Atomic Spectra	151		
2320111	p & d Shell Atomic Spectra	143		
2320112	CTR Atomic Data	127		60
2320115	Atomic Energy Levels Data Center		70	40
2320120	Infrared Research	100		
2320121	Microwave Spectroscopy	171		
2320133	Infrared Reference Standards	53		
2320124	Application of IR Measurements to Air Pollution	65		
2320126	Laser Chemical Physics	34		
2320128	Molecular Electronic Spectroscopy	29		
2320129	Microwave Spectral Tables		42	
2320229	Diatomic Spectra Data		20	
2320426	Metal Oxide Molecular Spectroscopy			7
2320134	Refractometry			23
2320139	Refractive Index Evaluation and Compilation	5		
2320151	Electron Scattering in Gases	95		
2320155	Electron Spectroscopy for Gas Analysis	24		
		1500	182	310
		(75%)	(9%)	(16%)
	GRAND TOTALS - 2937	2171	331	435
	Exclude NSRDS	(74%)	(11%)	(15%)
		(83%)		(17%)

Unique measurement methods and instruments have recently been developed at JILA and applied to the determination of a number of accurate cross sections: for electron collisional excitation of radiating states of atomic ions including highly excited metal vapor atoms, degenerate states of neutral atoms, and metastable or slowly radiating states of molecules; for distributions in angle and energy of positive and negative ions produced by electron induced dissociative ionization and attachment; and for photodetachment thresholds and cross sections for a wide range of atomic and molecular and molecular negative ions. Other measurement techniques have been developed for the determination of molecular potential curves for ground and lower excited states of alkali atom-rare gas atom molecules.

Techniques have been developed for the calculation of cross sections and rate coefficients for the electron and photon excitation and ionization of light atoms and of ions; of the spectral distribution and intensity of radiation emitted by plasmas; of the electron scattering and electron induced radiation (bremstrahlung) emitted by a wide range of atoms; of the electron transport coefficients in a wide range of weakly ionized gas mixtures; and of the growth of current, temperature, etc. in a pulsed electrical discharge.

A primary function of the atomic and molecular research groups in NBS is to exploit the technical base described above to generate reference data in specific areas. These data may be obtained by experimental measurements or via theoretical computations. The primary modes of dissemination are via the NSRDS Data Centers or via publication in scientific journals, e.g., the Journals of the American Physical Society and American Chemical Society, the NBS Journal of Research, Atomic and Molecular Data and the Journal of Physical and Chemical Reference Data. Data often are distributed rapidly as NBS internal reports or are communicated via private communication to users by NBS scientists. Because of the close interactions of NSRDS Data Center personnel with those engaged in the measurement of atomic and molecular properties the data become available to the scientific and engineering community by becoming part of the data collections maintained by the various data centers supported by NSRDS in the two divisions.

The inputs received by the NBS atomic and molecular data groups are primarily requests for data from industry and other government agencies, but also include judgments of the principal NBS scientists as to what is needed to solve development problems. The other factors in determining the directions of programs are the state-of-the-art, opportunities for increasing physical understanding and for comparison of theory and experiment; and the scientist's perception of NBS goals as reflected in the availability of NBS and other agency funds. Outputs other than atomic and molecular data (i.e., measurement techniques, methods of data analysis, instrumentation, etc.) are generally disseminated as publications in scientific journals, either as parts of papers describing specific measurements or as papers devoted solely to descriptions of particular instruments or techniques. Critical reviews of given subfields, which describe the state-of-the-art of measurement in a particular area and assess the accuracy of the available data base are often produced by senior NBS staff workers or by visiting scientists at JILA, under NSRDS sponsorship.

Atomic and molecular data generation at NBS has always been closely connected with basic research in atomic and molecular physics. While most of the basic research in this area is carried out in colleges and universities either in the U.S. or abroad, NBS plays a key role in this area by providing new measurement techniques and methods of data analysis and by performing key measurements which may be used to compare with theoretical predictions.

4.2.2 Users of NBS Services

Users of NBS services in the area of atomic and molecular properties generation include:

1) Industrial and governmental energy generation groups concerned with the development of coal-fired and non-equilibrium magnetohydrodynamic generators.

2) Government, industrial and university groups engaged in the development of laser technology or in the use of lasers for various applications, e.g., national defense, energy generation, isotope separation, laser-induced chemical processes, etc.

3) National measurement systems at NBS and elsewhere concerned with the development of standards of length, frequency, etc., based on atomic and molecular properties.

4) Basic scientists engaged in aeronomy, e.g., those studying the problems of energy deposition, radio propagation through and light emitted by the earth's atmosphere, and the factors producing changes in the ozone layer.

5) Groups engaged in the study of energy deposition in matter caused by energy losses of incident electrons and photons, as in irradiation of biological materials.

6) Industrial and government groups designing and evaluating anti-ballistic missile systems, very low frequency communication systems and other defense systems operating in the earth's atmosphere.

7) Industrial groups engaged in the development of more efficient and more easily used gas discharge lamps for commercial, highway, and home use.

8) Astrophysicists and astronomers studying stellar atmospheres and interstellar media.

9) Basic research groups in atomic and molecular physics concerned with testing relationships between theory and experiment in the areas of atomic and molecular collisions and structure.

10) Spectrochemists concerned with the quantitative analysis of chemical reactions through spectroscopic observation.

11) Other NBS programs, particularly those concerned with measurements in such fields as air pollution, laser chemistry and fundamental physical constants and with precise measurement techniques of basic quantities such as length, frequency, pressure, and light intensity (radiometry).

4.2.3 Alternative Sources

Alternate sources for the atomic and molecular data generation services of NBS are universities, research foundations, industrial and other federally funded laboratories, e.g., Stanford Research Institute, General Electric Research Laboratories and Los Alamos Laboratories. Although university laboratories have made and are making extremely important contributions to the fundamentals of atomic and molecular physics, the measurement, calculation and interpretation of atomic and molecular data, such as cross sections and rate coefficients, are not favored areas in physics or engineering departments because of rapid turnover of workers (graduate students). Most of the university work in data generation has been by those interested in applications to astrophysics (Harvard) or to aeronomy (Pittsburgh). The research program in atomic and molecular data generation at one other institute, i.e., Stanford Research Institute (SRI), is much like that at NBS but has been concentrated on collisions among atoms and molecules rather than interactions of electrons and radiation with atoms and molecules. Also, SRI has concentrated relatively more effort on data production and less on inventing new methods of measurement, and has been less involved in the collection and evaluation of data through critical reviews. Research in industry leading to new measurement techniques and to new methods of analysis and calculation of atomic and molecular data has declined drastically in the past six years because of reduced government support and because of greatly increased emphasis by industrial research management and federal agency sponsors on short-term goals. The increased emphasis on short-term goals has seriously reduced the ability of governmental laboratories, e.g., the ERDA and DoD laboratories, to invest the development time and to make the careful measurements, accurate calculations and new interpretations required for the assessment and integration of the large number of individual collision processes that occur in plasma devices and systems.

The question of the degree to which the needs of users are now being met is best answered on the basis of the ability of the data centers concerned with the physical properties of atoms and molecules to supply reliable data requested by the users. Examples of contacts involving such requests in particular areas are given in Appendix B. A list of needs not now being met includes:

a) the needs of research programs in controlled thermonuclear fusion for information on the energy levels, cross sections for excitation, and transition probabilities of multiply ionized atoms 17 ;

b) the needs of the laser development groups for more extensive and more accurate data regarding electron transport, excitation, dissociation, attachment, and ionization coefficients in the less common gases and in mixtures of these gases with the more common gases see Appendix B ;

c) the needs of laser, isotope separation, gas discharge lamp and anti-ballistic missile development groups and of astrophysics, physical chemistry and aeronomy research groups for experimental or theoretical data for a large variety of molecular systems on the radiation emitted in collisions between excited atoms and molecules and other atoms and molecules see Appendix B ; and

d) the needs of laser development, isotope separation, and aeronomy research groups for accurate experimental data or theoretical prediction techniques for the transfer of energy among the excited states of atoms and molecules and for the collisional quenching of excited atoms and molecules [see Appendix B].

NBS has a number of unique advantages with regard to its services in the area of atomic and molecular physics properties measurement. They are:

1) Its recognized objective of making careful and controlled measurements leading to documented precision and accuracy. This emphasis on reliability and thorough investigation of sources often is incompatible with the developmental objectives of industry and the mission-oriented governmental agencies which generally take a short-range approach to supporting research in atomic and molecular physics. The projects selected for university research are generally chosen to allow completion in the two or three years available from a given graduate student's training, while NBS has the option of devoting longer periods to the development of apparatus and computational techniques. For example, the three years required for the development of the multi-stage interferometer for the study of the very weak, far-wing radiation emitted in collisions between excited alkali-atoms and rare gas atoms probably could not be quantitative explanation for long-standing anomalies but has opened the possibility of a new class of high power lasers. In principle, the non-profit institutes, e.g., SRI, could exercise the option of taking the time and spending the money required to improve the accuracy of measurements as distinguished from making new types of measurements. However, this has not been, and is not likely to become their usual approach, given the present attitude of most funding agencies, on which they depend for support.

2) An extremely capable and active atomic and molecular group is very closely associated with a very capable and active university astrophysical group. The advantage arises from the extensive needs of astrophysics for atomic and molecular data, from the extensive experience of astrophysicists in the modeling of the role of atomic and molecular processes in astrophysical plasmas and from the capable atomic and molecular scientists both in this country and abroad.

3) NBS is uniquely neutral in questions of industrial and governmental laboratory competition since most of its financial support does not depend upon contracts with other agencies. Thus, NBS personnel are asked to serve on advisory committees which judge proposals submitted by industry, universities, and non-profit organizations, and which advise mission-oriented agencies accordingly. The participation in such advanced planning by mission-oriented agencies allows NBS to adjust its data generation activities so as to better meet current and future needs, to alert users as to available resources and, in some cases, to lead the developmental programs into new areas.

4) Active collaboration with visiting domestic and foreign workers through guest worker and visiting scientists programs.

4.2.4 Funding Sources for NBS Services

In order to assess the funding sources of atomic and molecular data generation at NBS some judgments have to be made as to what specific projects are included in the program. These judgments are somewhat subjective for the following reasons. First, the dividing line between NBS projects which are specifically designed to generate atomic and molecular data or implement its use and those which provide other services is by no means clear. For example, studies of radiative transport carried out at JILA could alternatively be classified as a service intended to provide effective use of atomic and molecular data, or as an internal user of such data. Similarly, some of the projects concerned with laser chemistry in Division 232.00 are aimed at supplying needed atomic and molecular data, others are devoted to applications, and some to both.

Second, there are projects whose primary function is instrumentation that will eventually be used in both atomic and molecular data generation and in other activities. The recent conversion of the NBS synchrotron to a storage ring is an example of this type of instrumentation. It will be used both for atomic and molecular data generation and to provide precise vacuum-ultraviolet radiation standards.

Finally, the data centers, maintained by NSRDS, devoted to atomic and molecular data collection, compilation and dissemination play a special role. They can be classified as part of the NSRDS effort of data collection and dissemination but are also important to the program of atomic and molecular data generation since they provide a strong coupling between outside users and NBS services in their respective areas.

With the above points in mind we have identified a number of NBS projects in Divisions 274.00 and 232.00 which appear to be primarily concerned with atomic and molecular data generation services as defined in this report. Fiscal data for these projects are shown in Table 3 classified by division, project and source of funding. The special role of the NSRDS data centers is indicated by listing NSRDS support separately from other NBS funding. While these data centers should properly be considered as a part of the NSRDS program, the NSRDS support is included in the totals of Table 3 to give an estimate of the amount of effort devoted to related data center activity. Table 3 indicates that approximately 15% of the atomic and molecular data generation program (as defined by the projects included) is supported by other agency funds (NASA, AF, ARPA, ERDA). While the outside support is generally of limited duration and can only be used for the specific data needs of the sponsoring agencies, it plays an important role in defining the direction of atomic and molecular generation programs. Currently about 70% of the other agency funds are from ERDA and are used for projects which will supply data needed for controlled thermonuclear reactions.

4.2.5 Mechanism for Supplying Services

NBS supplies the services of its atomic and molecular data measurements program through a) direct consultation and correspondence with user groups, b) reports at user-producer workshops, c) speeches and papers at scientific meetings, d) reports to sponsors, e) publication in scientific journals, and through f) compilations and critical reviews including NSRDS publications.

4.3 Impact of NBS Services

The economic and technological impacts of atomic and molecular data generation are difficult to assess due to the rather complex way in which these services are propagated. The basic difficulties encountered in such an assessment spring from the following factors:

1) The services supplied consist of a number of indirect services such as the development of techniques and procedures for the analysis of atomic and molecular data or for their use in specific fields of application.

2) The users community as outlined in Section 4.2.2 is diverse. It ranges on the one hand from workers engaged in atomic and molecular data generation efforts very similar to those of NBS workers in the same field, to workers in specific applied fields (e.g., industrial lighting) with little interest or connection with NBS programs other than as a source of specific data.

3) The users of NSB data are, for the most part, engaged in what would normally be called research or development activities. Thus, the eventual economic or technological impact of NBS work on any broad area of activity (e.g., energy generation by controlled thermonuclear fusion, chemical separation or synthesis via lasers) can only be assessed relative to the subsequent impact of R & D effort in these areas.

4) The output of NBS services is difficult to trace to the eventual users. The impact of formal publication in the open scientific literature can only be gauged indirectly by analysis of reprint requests or citations by workers in allied fields.

4.3.1 Economic Impact of NBS Services

As stated above most of the users of NBS atomic and molecular data generation services are workers engaged in research and development in various technologies. One approach to assessing economic leverage is to compare the NBS effort with the total research and development efforts in various activities upon which this sector of the measurement system impacts. This kind of comparison is given in Table 4 which lists a number of areas of research and development funded by industry and government users of atomic and molecular data generation services. As seen from Table 4, NBS activities, at about three million dollars annually, are a small (less than 1%) part of the overall R & D activity in the areas listed. The potential economic leverage to be realized by essential current services in terms of atomic and molecular data generation can be as large as 100:1 in terms of current annual expenditures for national programs. Overlooked in this assessment is the permanent value of the data base being generated. A major NBS responsibility is to ensure that the data base is of high permanent value, i.e., is of adequate quality and scope to meet future needs and avoid high future costs of repeating and extending measurements as national programs evolve and as new needs arise.

4.3.2 Technological Impact of NBS Services

Since most of the output of the atomic and molecular data generation activity is via publication in the "open" literature, tracing the use of this information would be extremely difficult. In addition, the statistical information obtained from a survey may be misleading or possibly incorrect due to the difficulty of identifying the body of users. There is no basis for conducting a survey among a representative sample.

Table 4. Budgets for research and development areas utilizing measurement system for atomic and molecular properties

R & D Category	Major Sponsor	Funding M$	Problem Area
Controlled Thermonuclear Reactions	ERDA	100	Energy
High power lasers	ERDA, DoD and Industry	100	Energy, defense and materials processing
Laser induced chemistry (Isotope separation, etc.)	ERDA, DoD	15	Energy
Energy Generation by MHD	Office of Coal Research and Bureau of Mines	15	Energy
Atmospheric Science and Aeronomy	DoD, NASA	40	Defense, Air quality, communications
Commercial plasma devices	Industry	5	Illumination, electrical power dist., air cleaning, etc.
Astrophysics and astronomy	NSF, NASA, DoD	18	Space science
Research in atomic and molecular physics	NSF, ERDA, DoD	20	Basic research, measurement methods, etc.
Instrumentation	Industry	10	Chemical analyses
NBS (excluding other agency funding)		2.5	
		325.5	

The technological impact of NBS services may be illustrated by the direct day-to-day involvement (see Appendix B) that NBS staff members have with other research and development laboratories to which they supply atomic and molecular data and/or technical advice on the solution of specific problems. Several results of this type of activity at NBS are briefly described below:

1) Most laser development laboratories concerned with the CO_2 laser use the sets of electron excitation cross sections for CO_2, N_2 and He derived and recommended by NBS personnel.

2) An intercomparison and analysis by NBS personnel of differing predictions of electrical conductivities and electron densities used by several federally funded and industrial MHD development projects showed that the size of the MHD generator proposed by one industrial laboratory was 30% to small to deliver the desired output. When electron collision cross sections suggested by NBS were used, the design discrepancy was reduced to within 10%.

3) The results of recent theoretical calculations of cross sections for rotational excitation of CO and N_2 were used to show that the predictions of gas heating being used in calculations of power output and efficiency in lasers were extremely optimistic. Gas heating effects are particularly important for CO lasers because of the requirement that they be operated at low temperatures, e.g., 77°K, in order to produce efficient energy extraction.

4) Techniques developed at NBS for explaining the continuum radiation emitted by excited alkali metal atoms in the presence of high densities of rare gases have been applied by two different industrial laboratories to the prediction of the radiation emitted by high intensity discharge (HID) lamps used for industrial and highway lighting. In one case NBS scientists were told that these analyses were considered to have resulted in very significant improvements in the commercial lamp. For proprietary reasons, details are not available from the company involved.

5) Measurements of the cross sections for the production of certain Hg II spectra lines made at NBS at NASA's request have shown that a scheme which they have been developing for monitoring the operation of mercury ion propulsion engines is likely to fail. Alternate schemes have been proposed to them.

6) Initial attempts by an industrial group to predict the usefulness of electron impact excitation of HCl for laser operation resulted in the prediction that most of the electron energy would be lost in rotational excitation because of the very large electric dipole moment of HCl. However, using improved methods of data analyses and very old data, NBS personnel showed that in spite of the large losses to rotational excitation there is a suitable range of mean electron energies where there is efficient excitation of vibrational levels of HCl. Very recent results by others using electron beam scattering confirm this result. Furthermore, a successful laser has subsequently been reported using electron excitation of the very similar molecule, HF.

7) Computer programs developed by NBS for radiation transport, which are normally applied by astrophysicists to stars, have been used to model pyrotechnic flares used for illumination by the Department of Defense.

8) The simple analytical and partially empirical approximations to the detailed computer results developed by NBS personnel have been applied by industrial development groups to the approximate prediction of the energy radiated and absorbed by elements with many-line spectra. These simplified treatments, when used with NBS tables of line positions and oscillator strengths, allow rapid screening of the periodic table for the gas mixtures with highest luminous efficiency and with satisfactory color.

9) The techniques described in 4) above have been the subject of two reports (JILA #110 and #114) which have been distributed to the laser community and have resulted in the initiation of several laser development programs (see Appendix B) based on the alkali-rare gas atom interaction and on alkali dimers as the active laser media.

4.3.3 Pay-off from Changes in NBS Services

One of the principal changes in NBS services in atomic and molecular data generation during the past few years has been the increased emphasis on visits to the industrial and government laboratories utilizing the technologies discussed above. This increased personal contact has made it possible for NBS to adjust its NBS funded and, especially, other agency funded programs to provide data measurement and analysis techniques that reflect the rapid changes in the active areas of technology and to provide a portion of the leadership in the choice of new areas of emphasis.

A second, and not unrelated change, is the increased emphasis of theory and experiment on obtaining data for more complicated highly ionized atoms, i.e., less emphasis on simple systems and more work on atoms with one or more electrons outside closed shells and on multiply-ionized atoms. This change has been in response to data needs of astrophysicists and of plasma physicists engaged in controlled thermonuclear research. These changes have been made possible by a significant increase in the sophistication of theoretical methods and computer codes used by and partially developed at NBS for calculating energy levels, electron scattering cross sections and radiative transition probabilities. These advances have resulted in the generation of much additional data required by astrophysicists for their models of stars and by plasma physicists interested in the properties of highly ionized atoms. These studies have also made possible a number of important tests of theory. The change in emphasis has also resulted in some decrease in activity in some more sophisticated areas of theory and experiment and their intercomparison, e.g., the recent measurements and theory of quantities such as alignment and orientation of electron excitation of atoms.

Some specific areas in which NBS might change its participation in the national measurement system for the physical properties of atoms and molecules are:

a) the generation, tabulation and dissemination of "best available" sets of data for atoms and molecules of high current technological interest. The objective of such a program would be to provide readily available and frequently updated cross sections, transition probabilities, etc. for species of interest in areas, such as laser, CTR, magnetohydrodynamic power generation research and development. This program would complement the more careful, long term critical reviews, such as have been carried out by NBS in the past, and so satisfy one of the more immediate needs, as well as the long term need of science and technology. Such a program has recently been initiated in connection with the CTR program.

b) the building up of data center activity in areas such as radiative transition probabilities and excitation transfer and quenching rate coefficients for molecules. These areas are of high current interest for laser development, isotope separation, gas phase chemistry, etc. Such a program should be of sufficient interest to the Energy Research and Development Administration for this agency to support the NBS effort. Their support of such a program would add to the official recognition of the NBS role already obtained in connection with the Controlled Thermonuclear Reactor program.

c) the deveopment and application of experimental techniques for the generation of large amounts of data in areas of special need and neglect. One example is the need for electron transport coefficients in gases, such as ionization rate coefficients, for designing high power electrical discharge lasers. Currently the U.S. has no effort in this area. An example of the successful development of such a program is the work at the National Oceanic and Atmospheric Administration on the measurement of ion-molecule reaction rate coefficients of atmospheric interest.

d) the development of a comprehensive program directed toward establishing standards, etc. for the measurement of the more important properties of ionized gas systems, such as electron density and energy. Except for the very successful work with the radiating properties of high current arcs, this topic has been one of considerable controversy and little progress at NBS. The fact remains that the measurement of these properties is important to the technology of ionized gas devices, including controlled thermonuclear reactors, electric discharges, lasers and electrical switchgear. As an example of the importance of such measurements, the recent near capture of the international market for small electrical circuit breakers by the Swiss has been attributed to the use of improved measurement techniques.

4.4 Evaluation of NBS Program

Strong points of the NBS program in atomic and molecular data generation

1) A strong research program in atomic and molecular physics with emphasis on the development of new and accurate measurement techniques, on the accurate measurement of data and on techniques of data application in the areas of the interactions of photons and electrons with atoms, ions, and molecules.

2) An active and successful visiting scientist program which attracts the world's leading atomic and molecular scientists to JILA/NBS for a year's association with the NBS programs.

3) An active program of visits by NBS scientists to industrial and governmental development to laboratories to allow NBS atomic and molecular data generation programs to respond to the changing needs of technology and to facilitate the transfer of and utilization of data.

NBS support coupled with other agency support, and at JILA, University of Colorado support of postdoctorates and graduate students, enables NBS to maintain an excellent program of atomic and molecular data generation in areas such as the development of measurement techniques and the measurement of the interaction of electrons and radiation with atoms and molecules. This does not mean that the NBS program is able to satisfy fully the rapidly growing and changing needs of technologies, such as high power lasers and isotope separation. Also, NBS has not attempted to support a comprehensive program in areas such as studies of collisions among atoms and molecules. The NBS program of evaluating existing data in several areas of atomic and molecular physics is at present not as user oriented as it might be. More emphasis needs to be given to selection of useful data from among the available experimental and theoretical data, analysis of these data to obtain the best available sets for a specific purpose and making the results available to the users rapidly and easily. Also, NBS should concern itself much more with the way the data it supplies are to be used in computer models, etc.

The needs for NBS services are determined by the NBS scientists through requests for data, the availability of funds, and the scientists' judgment as to the more productive and opportune areas of work. The Divisions 274.00 and 232.00 evaluation panels have played an important role in the general health of the atomic and molecular program through their recommendations.

Priorities among users are assigned on the basis of the individual judgment of the NBS scientist, influenced strongly by the users, and their willingness to support the work directly or indirectly. The programs are monitored by NBS management and by contract monitors of various government agencies.

There are important aspects of the NBS atomic and molecular measurement, data generation, and data review programs which are not fully duplicated in other types of laboratory operations. The question of whether these programs could be subcontracted would require a careful examination of those contributions which are unique to and characteristic of NBS and a judgment as to whether these could be preserved in the transfer of functions to industry, to universities, or to federally funded university (or non-profit) managed laboratories. In this field of atomic and molecular physics the NBS provdes leadership in the development and implementation of measurement capability as well as in the organization and utilization of data. In both areas the NBS sets standards of performance for the whole community. These functions rest on the existence of a highly competent career-professional staff oriented to public service; immediate access to a broad base of technical and scientific capability; a high degree of internal communication encompassing and interrelating the functions of measurement and data evaluation; and a base for access to both the academic-scientific community and to agencies and industries involved in the technological applications of atomic and molecular physics. *No plan for piecemeal contracting of NBS atomic and molecular programs to a number of scientific organizations of any type could preserve these aspects.*

Re-establishing a program of the same level of technical competence as the current NBS effort would require development of a single dedicated standards and measurements laboratory with initial funding at a very high level, and in any case would require many years of development. Such a program would have to duplicate in some way the rather sophisticated apparatus and data handling techniques currently available at NBS and would also have to attract a technical staff of roughly the same technical competence as the present staff.

4.5 The Future

Basically, the service provided by the NBS atomic and molecular portion of the measurements system is to focus the output of the atomic and molecular physics community into the generation of an adequate and reliable data base for mathematical representation of the principal properties of plasma devices and to permit mathematical analysis of factors that determine efficiency. Corresponding applications of the data base will occur in the sciences, notably plasma physics, aeronomy, astrophysics, and aerodynamics.

This will involve the invention of new methods of measurement to obtain properties of various species of atoms and molecules not measurable by traditional methods, and will be concentrated on the data needs of the following areas:

1) Controlled-Thermonuclear Research--Thermonuclear reactors are currently viewed as a very long-range solution of man's need for energy. Current research efforts in this field have a need for new data, particularly properties of multiply-ionized atoms, which are not currently available. A major effort to supply these types of data is now being carried out at NBS and is expected to continue in the near future.

2) Laser-Development and Applications--Atomic and Molecular data, particularly on molecular and atomic excitation cross sections by electron impact for various species, are currently needed. Future NBS work will be devoted to supplying these but will probably also make contributions to the overall understanding of how given devices or processes work, and will provide detailed models.

3) Industrial Processes Requiring Atomic Data--This is an area in which NBS has not been much involved in the past but to which it is currently making contributions (e.g., work on MHD coal-fired generators and commercial lighting). Applications of this type require close personal contact with industrial research and development efforts and NBS staff specialization in this type of problem. Work of this type probably will be expanded at NBS.

4) Commercial measuring devices which require atomic data for their design or interpretation--While there are a number of such devices currently in use (electron spectrometers for chemical analysis (ESCA), microprobes, commercial spectrometers of all types, etc.) very little has been said of their need for atomic and molecular data generation services simply because these needs have not been assessed in this report. Atomic and molecular data requirements for the calibration of such instruments has generally been left for the user to obtain by using secondary standards for pressure, radiant flux, electrical current, etc. It is expected that NBS will become increasingly involved in direct generation and compilation of atomic and molecular data for such purposes for the following reasons:

a) There is a need for a well-defined body of reference data relating to each instrument of this type. Presumably this data base will eventually become an integral part of the National Standard Reference Data System.

b) There are a number of such devices currently being used at NBS on other projects. See, for example, "The National Measurement System for the Measurement of Surface Properties" Vol. IV of this series.

5) Aeronomy and Atmospheric Science--Activity directed to these areas will probably decrease as a result of high priority of other areas.

5. SUMMARY AND CONCLUSIONS

The national activity in atomic and molecular properties measurements includes work carried out on a relatively small scale in a large number of different university departments, industrial laboratories, government laboratories and federally funded research centers. The objectives are diverse (pure basic research, product improvement, weapons design, astrophysical and atmospheric modeling, instruments and standards for measurement, and the development of new energy conversion systems) and the levels of sophistication and competence are not uniform. These activities are informally coupled through the recognized scientific literature, through the report literature and through the activities of the professional societies, all strongly academically oriented. Other types of coupling include the agency sponsored workshop designed to focus attention of a limited sector of the community on specific agency objectives, and the discipline or mission-oriented compilation of data (most mature for atomic and molecular data are those oriented toward aeronomy and astronomy).

The National Bureau of Standards has historically been very active in this field and today provides unique services which tend to tie this community more tightly into a measurement system for atomic and molecular data. These services include the setting of standards of performance in measurement; the development of measurement capability; the compilation, evaluation, and dissemination of data; and the establishment of benchmark data.

Essential to this role as a focus for this sector of the measurement system has been a high level of access to and communication with the user communities. Through the era of concentration on atomic and molecular structural information a principal interface was with the astrophysical community. The two decades just past have seen emergence of reliable measurements and calculations of the dynamic properties of atoms and molecules; and, in addition, a new preoccupation of the astrophysical community and the closely related controlled thermonuclear research community with the dynamics of stellar atmospheres, of interstellar media, and of plasma confinement efforts aimed at energy production. A major new user interface developed in the field of aeronomy, substantially motivated toward Department of Defense projects in ballistic missile detection, effects of severe man-made atmospheric disturbances, and in communications.

The further evolvement of measurement capability and of more complete and adequate data sets are now converging with advances in computer sciences and computational capability to provide an opportunity for a much broader and more direct technological impact. Urgent national requirements for advancements in industrial technology, the development of new energy sources, and the more efficient transmission and use of energy require that NBS should move rapidly to expand its interaction with the industrial community and with national laboratories where development projects depend on the ability to describe and predict properties of gases for absorbing, converting, or transmitting intense energy fluxes, as well as their aerodynamic and electrodynamic properties.

Specifically recommended are:

1) Expansion of coordination of NBS atomic and molecular programs with the search for new laser media and with the scaling refinement of existing types of high power lasers for the purpose of directing more effectively its own measurements of critical atomic and molecular data.

2) Improvement of the NBS coordination with groups developing and testing methods of using atomic and molecular data for industrial design of new plasma devices and for introducing improved efficiency factors in existing devices.

3) Expansion of the NBS role in the Controlled Thermonuclear Research (CTR) program, for the purpose of more effectively directing its own measurements of critically needed parameters, for supplying CTR fusion laboratories with the essential atomic and molecular data to permit more reliable diagnostics of high temperature plasma and to form the basis for better modeling calculations.

4) Re-examination and expansion of its atomic and molecular data compilation, evaluation, and dissemination activities to ensure that maximum effective utilization is made of the data output potential of the entire atomic and molecular community, the needs of the most urgent development projects are met by development and issuance of specialized data sets, and that the goal of realizing a generally accessible, generally useful and thoroughly reliable base of data and methodology directed to the needs of the industrial and scientific communities be kept in view.

5) Continuation of NBS support of measurement activities of the entire atomic and molecular physics community through development and testing of measurement techniques for properties needed by and not available to the user communities; execution of selected benchmark measurement programs; reexamination of transfer standards for measurement of gas density and radiant flux; and continuation and strengthening of NBS sponsorship of critical reviews and evaluated compilations with the objective of promoting quality output in areas of critical need.

Appendix A. Methodology of the Study

This study has been conducted 1) through a survey of literature relating to the scope of the field of atomic and molecular physics, relating to the activities and needs of many of the user groups, and where available relating to economic data and activity levels in principal areas of application; and 2) through extensive personal contacts with persons involved in pertinent research and development programs.

The literature has consisted of several types including surveys of levels of basic research activity conducted by the physics community, and studies and statistical surveys by organizations such as the National Science Board and the Electric Power Institute. There is a substantial body of literature directed at the research community which includes magazine articles and other reports intended to bring scientists up to date on areas of application of atomic and molecular physics. Finally the magazine Laser Focus is almost unique in its reporting on levels of activity in the laser industry.

Information and insight into the role of atomic and molecular data in other ongoing industrial programs are usually not spelled out in the literature. With some exceptions the atomic and molecular input is not represented by products identifiable with this field so thatproduct information is not very helpful. In this area heavy reliance has been placed on personal contacts with industrial scientists to obtain insights into current activities and needs for atomic and molecular data and measurement capability.

Appendix B. Examples of Interactions with Atomic and Molecular Data Users

A. Development of high power and ultraviolet lasers in industry and government.

INPUT--primarily requests for evaluated data on the interaction of electrons, ions and radiation with atoms and molecules of present or potential laser interest and requests for advice on interpretation of experiments, sources of data and areas of research to be investigated.

OUTPUT--tabulation of evaluated cross sections and rate coefficients for electron collision processes; measurement and calculation of radiative properties of potential laser molecules; development of new experimental techniques for the determination of atomic and molecular properties; and the development of new modeling techniques for the prediction of the electrical and radiative properties of lasers.

1) Industry

a) Airesearch Research Co. (Garret Corp.)

Principal contact: Dr. J. Kennedy

Interaction topics: supplied cross section sets for CO_2 and CO laser design; checked results of electron transport calculations in CO_2 mixtures.

b) Avco Everett Research Laboratories

Principal contacts: Drs. R. E. Center, D. H. Douglas-Hamilton, R. L. Taylor (formerly), and G. E. Caledonia (formerly).

Dates of interactions: vists to 1/72, 3/72 and 12/73 and from 2/72, 7/72 and 3/74; phone calls--numerous--three since 7/74; technical letters--6/73, 7/73 and 7/74.

Interaction topics: supplied electron collision cross section and transport coefficient data, negative ion-molecule reactions rates and rate coefficients for CO_2, CO and excimer laser processes; assisted in interpretation of electron loss data in CO.

c) Bell Telephone Laboratories

Principal contact: Dr. P. W. Smith

Interaction topic: discussions of possibilities for and data concerning electron transport and excitation in organic vapors, e.g., gas phase dye lasers.

d) Comarco Inc.

Principal contact: D. F. T. Wu

Interaction topic: supplied cross section set used in recently published analyses of CO lasers.

e) CALSPAN (Cornell Aeronautical Laboratories

Principal contact: DR. J. C. Rich

Interaction topics: supplied electron collision cross section sets for CO_2 and CO laser design; supplied theory and preliminary results on heating of CO in laser discharges.

f) Hughes Research Laboratories and Hughes Aircraft Co.--Laser Division

Principal contacts: Drs. R. Lind and J. Palmer

Dates of interactions: visit to 5/74; technical letters--6/74, 10/74; phone calls--5/73, 6/73, 9/73 plus several discussions at conferences.

Interaction topics: supplied cross section sets for CO_2 laser modeling and references on alkali-rare gas plasma processes; suggested technique being used for alkali density measurement; pointed out error in analyses of discharge instability growth; and supplied source of unpublished, foreign data on vibration relaxation at low temperatures. Note that their work on alkali-rare gas systems was initiated as the result of JILA Report #110.

g) Intercom Radiation Technology Inc.

Principal contact: Dr. J. T. Dowell

Interaction topics: supplied references on electron-positive ion recombination to alkali metal-rare gas plasmas.

h) International Business Machines Research Laboratories

Principal contact: Dr. R. T. Hodgson

Interaction topics: supplied NBS data on secondary electron energy distributions produced by ionizing collisions.

i) Mathematical Sciences Northwest
Principal contact: Dr. S. Byron
Dates of interactions: technical letters--3/74, 7/74, 10/74; phone calls--10/74.
Interaction topics: supplied electron collision cross section data for CO_2 and CO lasers; supplied references on electron attachment to carbonyl impurities in CO; discussed their evidence for role of metastable N_2 in N_2 and CO_2-N_2-He discharges; discussed operating conditions for electron beam sustained HF laser; discussed their evidence regarding rate of heating of gas in CO laser; supplied our revised cross sections for vibrational and electronic excitation of O_2.

j) Northrop Corp.
Principal contacts: Drs. M. L. Baumick and B. Lacina
Dates of interactions: visit from 7/72; technical letters 2/72; phone calls--3/73, 5/73 and 8/73.
Interaction topics: supplied electron excitation rate coefficients for HCl as determined from electron transport data; data and principles of excimer laser design; electron cross section data for CO_2 lasers; role of collisions of second kind in laser discharges.

k) Physical Sciences Inc.
Principal contacts: Drs. R. L. Taylor and G. E. Caledonia
Dates of interactions: phone calls 8/74; technical letters--7/74, 8/74, 9/74.
Interaction topics: supplied old electron cross section set and new references for H_2 and D_2 in connection with undisclosed laser scheme; supplied unpublished scheme for calculation of gas heating by rotational excitation near resonance; supplied revised electron excitation cross section set for O_2.

l) Science Applications Inc.
Principal contacts: Drs. R. E. Meredith and T. S. Chang
Interaction topics: discussion of the physics of excimer laser processes and a critical review of a contract report prepared by them on this subject.

m) United Aircraft Research Laboratories
Principal contacts: Drs. R. Bullis, W. L. Nighan and W. J. Wiegand
Dates of interactions: visit from 72; numerous phone calls and long discussions at technical committee meetings.
Interaction topics: supplied electron collision cross sections for CO_2, CO and HCl lasers and for impurities such as H_2 and H_2); compared in detail our calculations with their calculations of stability of laser discharges; supplied data on electron attachment and negative ion-molecule reactions in laser discharges, provided critical evaluation of processes in their MHD-laser scheme.

n) Westinghouse Research Laboratories
Principal contacts: Drs. J. J. Lowke, L. J. Denes, L. E. Kline and R. L. Humstad
Dates of interactions: visits to 6/72, 1/73, 8/73 and 8/74, from 4/72, 11/72, and 3/74; numerous phone calls. Joint paper with J. J. Lowke and B. W. Irwin, J. Appl. Phys. 44, 4664 (1973).
Interaction topics: developed and applied electron cross section set for analysis of CO_2 lasers and joint paper; discussed significance of NBS interpretation of their data showing extremely low electron-ion recombination coefficients in CO_2 laser discharges; found error in their calculation of gas heating in laser discharge; compared theories of growth of current leading to constriction and shorting of laser discharge.

2) Government
- a) Los Alamos Scientific Laboratory
  Drs. C. A. Fenstermacher, W. Leland, G. York and S. Rockwood
- b) Air Force Weapons Laboratory
  Drs. L. A. Schlie, D. Drummond, W. H. Proctor and Maj. R. Weber
- c) Lawrence Livermore Laboratories
  Drs. C. K. Rhodes and P. Hoff
- d) Naval Research Laboratories
  Dr. A. Ali
- e) Sandia Laboratories
  Dr. J. W. Gerado
- f) Office of Naval Research
  Dr. W. J. Condell, Jr. and Dr. J. G. Dardis (contract monitor)
- g) Naval Ammunition Depot
  Dr. B. E. Douda
- h) Naval Ordinance Lab
  Dr. M. Plummer

3) Other Governments
None
4) Journals
None recent
5) Other NBS
Division 271.00 (consulting and contract contacts)
Drs. E. W. Smith, M. M. Hessel, K. B. Persson, E. R. Mossburg, Jr., and D. L. Fransen
6) Educational Institutions
a) Wayne State University
Dr. E. Fisher
Exchange of results of modeling calculations; critical evaluation of modeling calculations at Wayne State.
b) University of Colorado
Dr. E. A. Crawford
Collaborative experimental study of the collapse of glow discharges in high pressure laser configurations. Published in Appl. Phys. Letters.
c) Stanford University
Prof. S. Harris
Discussions of excimers and molecular absorption in alkali rare gas systems.

B. Development of efficient, coal-burning energy conversion devices.

INPUT--primarily requests for evaluated data and new data for use in the design and evaluation of coal-fired magnetohydrodynamic generators.

OUTPUT--compilations and evaluation of collision cross sections, electron mobilities, and electron affinities of species of significance in MHD devices.

1) Industry
a) Avco-Everett Research Laboratories
Dr. R. L. Taylor
b) Westinghouse Research Laboratories
Dr. T. C. Tsu
2) Government
a) Bureau of Mines, Department of Interior
Dr. F. E. Spencer, Jr.

C. Prediction of disturbed ionospheric properties

INPUT--statement of data needs by DoD agencies and contractors and by NASA supported labortories.

OUTPUT--measured values of critical cross sections; reviews of available data relevant to ionospheric phenomena; calculations of cross sections not available from experiment.

1) Industry
a) General Electric Company
G. E. Tempo: Mr. A. Feryok
G. E. Valley Forge: Drs. T. Baurer and M. H. Bortner
Writing of two chapters for DNA handbook.
b) R & D Associates
Dr. F. R. Gilmore
c) Mission Research Corp.
Drs. M. Schiebe and P. G. Fisher
2) Government
a) NASA supported laboratories:
i) LASP--University of Colorado
Dr. M. Rees (secondary electron energy data)
ii) University of Florida
Dr. A. E. Green (secondary electron energy data)
b) Defense Atomic Support Agency
i) Dr. R. Huffman (ARCRL contract monitor)
(Measurement of rates of excitation of infrared emitting levels of molecules and advice on ionospheric heating model)
ii) Dr. R. Mace (ARO(D) contract monitor)
(Measurement of photodetachment cross sections for complex negative ions of ionospheric interest)
iii) Dr. E. Bauer (IDA)
(Calculations of infrared emissivity of ionospheric plasmas at moderate temperatures)
iv) Served on DNA committee to evaluate their program.

D. Development of higher-efficiency, good-color, more easily used lighting.

INPUT--statements of needs and discussions of problems by industrial development groups for data required for the prediction of the electrical and radiative properties of electric discharge lamps.

OUTPUT--measurements of radiative properties of molecules obtained by the use of experiment and theory developed at LAD; compilations and evaluations of published experimental data.

1) Industry
a) Sylvania Electric Company
Dr. J. F. Waymouth
b) Westinghouse Research Laboratories
Drs. R. J. Zollweg and J. J. Lowke

E. Development of miscellaneous industrial devices such as ozonizers, information displays.

INPUT--needs of industrial and university groups as determined by discussion and by study of publications.

OUTPUT--recommendations of data and calculation techniques; development of new techniques for modeling of electrical discharges in gases.

1) Industry
a) Avco-Everett Research Laboratories
Dr. D. H. Douglas-Hamilton
Collision processes of importance in chemical production by electrical discharge devices.

Appendix C. Atomic and Molecular Physics and Energy Research

This appendix summarizes some of the areas in which research in atomic and molecular physics can be expected to contribute significantly to increasing our ability to generate, distribute and utilize electrical energy in an efficient and environmentally acceptable manner. The various areas of research are categorized by the area of application rather than by the scientific specialty in order to make the material more readily understood by those primarily concerned with energy problems. It will be noted that since the topics discussed are concerned with the generation, distribution and use of electrical energy, we omit most of the research concerned with other energy forms and the closely related branch of chemical physics. Also, we have attempted not to include areas normally considered as plasma physics, i.e., the collective phenomena occurring in essentially fully ionized gases.

I. Electrical Power Generation

A. Controlled thermonuclear reactions

1. Magnetically confined plasmas

Research in atomic and molecular physics provides data required for measurement of the properties (diagnostics) of CTR plasmas; the development of neutral beams for fuel injection and plasma heating; the prediction of plasma cooling due to impurities; and the understanding and optimization of the interaction of the plasma and radiation with surfaces. As indicated in the Liess Report of March 1974 [17] these requirements show the need for extensive research in areas such as atomic radiative transition probabilities; collisions of ions with gases, surfaces and electrons; and the collisions of charged particles and radiation with bulk solids.

2. Laser induced, controlled thermonuclear reactions

Laser induced fusion is a much newer area of energy research than that of magnetic confinement and is much more in need of supporting research from fields such as atomic and molecular physics. This is particularly true for the problems of high power laser development and the propagation of laser energy. The needs for atomic and molecular data in the area of the properties of the very high temperature (~10^7K) fuel pellet are similar to those of the magnetic confinement approach. In the search for a laser medium capable of generating the extremely short pulses and high powers needed for laser induced fusion much use has been made of atomic and molecular collision cross section and radiative property data which have been generated with support from DoD programs concerned with the modeling of high altitude nuclear explosions and with missile reentry into the earth's atmosphere. Unfortunately such data are not available for the more exotic molecules now under consideration as laser media and neither the DoD nor the AEC has been supporting the research required to develop the new techniques required to handle these gases and to obtain the data.

B. Isotope separation for conventional nuclear power fuel

Recent research appears to have shown that the highly monochromatic, high intensity radiation from lasers can be used to prepare atoms and molecules of different isotopes in different states so as to allow significant separation of the isotopes. Effective exploitation of this technique will require extensive research in the areas of variable wavelength, highly stable, high power lasers and of the effects of differing isotopes on atomic and molecular structure and collision cross sections for ground and excited (or ionic) states of these atoms or molecules.

C. Magneto-hydrodynamic power generation

Although the primary research needs in the area of MHD are concerned with erosion, conductivity and electron emission of impacted wall materials, seed recovery, and pollution by combustion products, there is a serious lack of reliable data which would allow prediction of the electrical conductivity of the thermal and non-equilibrium plasmas. In particular, there are the needs from A & M research for electron affinity data, electron transport (collision) data, and for the development of reliable diagnostic techniques for plasma composition, temperature, etc. The understanding and control of the products of high temperature combustion will eventually require measurements of the individual collision processes which determine the chemical species present, the temperature at which energy relaxation is incomplete, etc. Similarly, surface erosion depends upon rate of collisional energy and momentum transfer, rates of evaporation and nucleation, etc.

D. Thermionic converters for power generation

Thermionic converters make use of ionized metal vapors to neutralize space charge and so make possible the flow of usefully large electron currents between mechanically realizable surfaces of widely different temperatures. In addition to solutions to the severe fabrication and materials compatability problems there is a need for better understanding of the properties of electron emitting surfaces, the collisions among the electron and the charged and neutral atoms, and of radiation transport.

E. Conventional power generation

Areas of conventional combustion driven steam and gas turbine generators in which atomic and molecular physics may make significant contributions are: the more efficient and/or environmentally acceptable burning of fuel through the sensing and control of flame condition, electric discharge aiding of combustion, and the measurement, understanding and prediction of the role of flame additives. As in the MHD systems there is a need for better understanding of the processes of turbine blade erosion by collisions of molecules, droplets and unburned fuel, and the factors determining the end products of combustion. Finally, there is the control of pollutants through devices, such as electrostatic air cleaners with their numerous gas discharges, surface conductivity, and other similar problems.

II. Electrical Power Transmission and Switching

A. High voltage systems

The desire to reduce losses in the transmission of electrical energy has led to the use of high voltages with a resultant increase in insulation problems and in corona loss and interference. Although significant progress has been made in obtaining engineering data, we are a long way from being able to predict or understand the path of a long electrical spark in air or along a surface or to describe or predict quantitatively the variations in corona discharges which occur with changes in geometry, moisture concentration, etc. Although we believe that data describing the most relevant collision processes are available, a few have not been studied quantitatively and, most importantly, only in the simplest geometries and gas mixtures can we synthesize these processes so as to make predictions and provide understanding. As examples, we still do not know the role of electron detachment from negative ions in air at atmospheric pressure nor can we describe quantitatively the reasons for the crooked path or the step-like propagation of the current in a long spark.

B. Lightning protection

The high probability that electrical transmission systems will be struck by lightning has led to significant investments in protective switching, etc. As for the long sparks discussed above our predictive ability for lightning is almost entirely empirical largely because of our limited ability to synthesize the large number of atomic and molecular processes with realistic geometries, etc.

C. Electrical switchgear

The understanding of electrical switchgear requires that one bring together the results of research in mechanics, fluid dynamics, metallurgy, and atomic and molecular processes. An example is the crucial role of molecular dissociation in causing a sharp peak in the temperature dependence of the specific heat with the resultant large temperature gradients in the arc temperature profile and the rapid diffusion of heat when an attempt is made to interrupt the arc current. A second example is the important role of radiative energy dissipation in the higher current, higher pressure arcs used at high power levels.

III. Electrical Energy Utilization

A. Illumination

The application of atomic and molecular radiative processes is the basis for recent improvements in the efficiency of sources of illumination which range from fluorescent lamps to high intensity sodium lamps. Through improved understanding of the individual collision processes and improved ability to describe the relations among large numbers of important processes one expects to develop illumination sources of higher efficiency, better color rendition and longer life. As an example, techniques are just beginning to be developed for predicting quantitatively the intensity of the broad-band radiation which dominates the output of many high pressure lamps.

B. Material processing

The use of electrical arc furnaces for the melting and processing of steel has become a large consumer of electrical energy and often taxes the ability of regional distribution and generation systems to supply a constant voltage. Although it is not clear at this time what atomic and molecular physics studies would be of help in optimizing the use of electrical energy in these systems, the success of arc symposia held at conferences sponsored by the professional societies shows that arc physicists can make use of the results of atomic and molecular data and techniques. Thus, the studies of the welding arc have included an accounting for energy flow by conduction, convection and radiation, the processes leading to electron production at the cathode and ion production near the anode, and the effects of various gas or vapor additives or shields. Another type of arc which has been investigated in terms of atomic and molecular processes is the plasma jet used for crystal growth and metal shaping. Low pressure electrical discharges are used for growth of oxide surfaces on semiconductors, sputtering thin films onto surfaces, etc.

C. Chemical processing

Although the use of electrical energy for chemical processing is expensive compared to more conventional chemical processing, there are a number of commercially important processes. One of these is the production of ozone in the ozonizer discharge, i.e., a series of short high voltage discharges. It has been suggested that ozone should replace chlorine for water purification. Unfortunately, we understand very little about the electrical discharge and chemical processes occurring in these devices. A second example is the use of plasma jets, with or without magnetically induced rotation, to produce acetylene. As yet unsuccessful attempts have been made to use electrical discharges to produce hydrazine and other high energy content fuels.

Appendix D. Atomic and molecular physics and energy research matrix

	Mag. CTR	Laser CTR	Isotope Sep.	MHD	Therm. Conv.	Conv. Pwr. Gen.	High Voltage	Lighting	Switch.	Illum.	Mat'l. Process	Chem. Process
Elec.-collisions	✓	✓		✓	✓		✓	✓	✓	✓	✓	✓
Ion-collisions	✓	✓	✓				✓	✓				
Neut.-collisions		✓				✓	✓		✓			✓
Atomic spectra	✓	✓	✓	✓	✓					✓	✓	
Molecular spectra		✓	✓			✓				✓		✓
Transition prob.	✓	✓	✓	✓		✓			✓	✓	✓	
Line shapes	✓	✓	✓	✓					✓	✓		
hν transport	✓	✓			✓				✓	✓	✓	
Elect. transport		✓		✓	✓		✓	✓	✓	✓	✓	✓
Neutral transport		✓				✓		✓	✓			
Neut. thermo. prop.			✓	✓		✓		✓	✓	✓	✓	✓
Elect. surface	✓				✓							✓
Ion-surface	✓				✓		✓					✓
hν-surface	✓						✓					
Neut.-surface	✓											✓
Elect. affinity				✓			✓	✓				✓
Electrical breakdown	✓	✓		✓	✓		✓	✓	✓	✓	✓	✓
Molecular association			✓			✓			✓	✓	✓	✓

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NBS-114A (REV. 7-73)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBSIR 75-944	2. Gov't Accession No.	3. Recipient's Accession No.

4. TITLE AND SUBTITLE

National Measurement System for the Physical Properties of Atoms and Molecules

5. Publication Date September 1976

6. Performing Organization Code 274.00

7. AUTHOR(S)

J. W. Cooper, A. V. Phelps and S. J. Smith

8. Performing Organ. Report No.

9. PERFORMING ORGANIZATION NAME AND ADDRESS

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

10. Project/Task/Work Unit No. 2741900

11. Contract/Grant No.

12. Sponsoring Organization Name and Complete Address *(Street, City, State, ZIP)*

Same as Item 9.

13. Type of Report & Period Covered

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

National activity in measurement, compilation, evaluation, and dissemination of atomic and molecular data, estimated at 20-25 million dollars annually, impacts directly upon applied research and development projects costing over one-third billion dollars annually. NBS atomic and molecular programs, costing about 3 million dollars annually, provide the basis for the accepted standards for length, time and frequency; provide advanced measurement techniques; set rigorous performance standards for generation of atomic and molecular data, and provide for the construction of a sound data base for the user community. The largest users are programs aimed at energy generation and conversion. Basic sciences of aerodynamics, astrophysics, atmospheric physics and plasma physics are important users. Benefits for a broad range of industrial research activities are potentially large. It is recommended that NBS undertake to ensure the reliability and adequacy of the data base needed for important national programs, expand its contacts with private industry, develop increased awareness of the methodology for applying atomic and molecular data to technological development, and encourage effective utilization of this sector of the measurement system for the benefit of the economy.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

Atom; energy generation; industrial technology; molecule; primary standards; properties.

18. AVAILABILITY	19. SECURITY CLASS (THIS REPORT)	21. NO. OF PAGES
[XX] Unlimited [ ] For Official Distribution. Do Not Release to NTIS	UNCLASSIFIED	38
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USCOMM-DC 29042-P74

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