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SUBCOMMITTEE ON
ENERGY-RELATED ATOMIC AND MOLECULAR SCIENCE

Committee on Atomic and Molecular Science
Assembly of Mathematical and Physical Sciences
National Research Council

NATIONAL ACADEMY OF SCIENCES
Washington, D.C.   1976 NAS-NAE

NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the Councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the Committee responsible for the report were chosen for their special competences and with regard for appropriate balance.

This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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Washington, D.C. 20418

PREFACE

This report has been prepared by an *ad hoc* subcommittee
of the Committee on Atomic and Molecular Science, Assembly
of Mathematical and Physical Sciences, National Research
Council. This group met in June 1975 to outline the con-
tent of this report and to define its general philosophy.
Members of the subcommittee then assumed responsibility
for the various sections of the report, and they in turn
called on other experts to help in the preparation of these
sections.

A final draft was then prepared and sent to members
of the subcommittee and several other experts in specific
areas for their comments, corrections, and revisions. The
full Committee on Atomic and Molecular Science received
this draft during its meeting in December 1975 at the
annual meeting of the Division of Electron and Atomic Phys-
ics of the American Physical Society in Tucson, Arizona,
and members' comments and corrections have been incorpor-
ated.

In addition to the subcommittee members, we acknowl-
edge significant contributions and suggestions from E. Beaty,
H. Bethe, R. Bullis, E. Hinnov, A. V. Phelps, F. E. Spencer,
Jr., R. H. Tourin, A. M. Weinberg, and J. Weymoth.

The final version of this report was prepared by
B. Bederson and S. Datz.

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CONTENTS

SUMMARY

All energy processes are eventually attributable to reac-
tions that occur on a molecular, atomic, or nuclear scale.
We can, and have been able to, exploit such processes even
though understanding of them has been incomplete, to say
the least. Thus, man has been making fires for over half
a million years without knowing much about the role of
excited-state energy transfer in wood combustion! Never-
theless, this empirical approach cannot be used as a basis
for the present quest for better, less ecologically damag-
ing, and more efficient, convenient, economic, and self-
sufficient energy sources. Instead, pure and applied science
has much to offer in the way of rational approaches to the
various aspects of the energy problem. In fact, in view
of the immense technological difficulties associated with
these problems, it is hardly likely that a purely empirical
approach has much, if any, hope of success.

One could define the main purpose of atomic and molec-
ular science in energy-related research to be the development
of an understanding of basic processes on a *microscopic*
level that govern such *macroscopic* phenomena as fossil-fuel
combustion and of essential processes in nuclear energy
utilization, that is, fission and fusion. This understand-
ing should result in improvements in energy-producing systems,
which presently suffer from serious external constraints.
These include the present limits on efficiency of combustion
devices, pollution products of combustion, and the need for
discoveries of substitutes for the diminishing sources of
historically well-known fuels.

Energy technologies involve the interconversion of
energy forms. The initiating event may be, as in combustion,
the release of energy stored in chemical bonds through chem-
ically reactive collisions or, as in fission or fusion, by
the release of potential energy stored in atomic nuclei.
Following the initial conversion event, energy is further

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redistributed by atomic and molecular collision processes until it is finally converted into the socially useful forms of electricity, heat, or propulsive power. Atomic and molecular collision physics, in addition to playing an important role in the conversion processes, has an impact on many aspects of fuel preparation, efficient energy utilization, and waste management.

To better understand the relation of atomic and molecular science to energy research, the Committee on Atomic and Molecular Science of the Assembly of Mathematical and Physical Sciences of the National Research Council recently undertook a study of various energy technologies and their connections to atomic and molecular science. A subcommittee on energy was formed and prepared the following report, of which this Section is a brief summary.

The reader is referred to the following sections for a more complete discussion of energy-related atomic and molecular science. It contains many details and examples of current needs and research interests.

We first discuss here the most ubiquitous energy conversion process of all--fossil-fuel combustion. Combustion experiments generally are concerned with flame composition and pollutant emission and involve the study of temperatures in different parts of a system, of the pathways followed by materials in the system, what happens when hot gases impinge on the combustion chamber walls, and how the effluent species interact with the ambient environment. In the study of these processes, the entire arsenal of diagnostic techniques developed in atomic and molecular science is employed. These include optical and mass spectrometers and lasers. Lasers are especially useful, because they permit measurements to be made with excellent spatial and temporal resolutions, so that accurate determinations of combustion parameters at different points in the system and at different times are possible. Here, we are referring to spatial dimensions as small as micrometers (one ten-thousandth of a centimeter) and times of nanoseconds (one billionth of a second) for such critical quantities as combustion temperature, species composition, electron density, and ion density.

Present methods used for coal hydrogenation to form liquid and gaseous fuels, for petroleum refining, and for treatment of automobile exhausts all use catalytic processes by which some agent in addition to the combustion materials themselves is introduced to speed up or to direct the transformation process. Yet the design of catalytic process systems is still largely semiempirical, lacking in the fundamental understanding that could result in important improve-

ments in more practical catalytic converters. Atomic and molecular science aspects involved here include the process of gas being absorbed or desorbed from container surfaces and the process by which energy is transferred from the gas mixture to the surface.

One of the most interesting goals of fossil-fuel combustion is the desire to eliminate the "middleman," namely, the engine-generator system, in the conversion of heat energy into electricity by means of direct conversion schemes.

The most promising of these is the magnetohydrodynam- ic (MHD) generator, which could be loosely described as a gas-phase analog of a mechanical turbine-generator combina- tion. For coal-fired MHD plants, atomic and molecular science contributes the basic data necessary to both under- stand and optimize the electric generation process. For example, the electrical conductivity of the conducting medium (i.e., the plasma) is a key element in determining the efficiency of MHD power generation. Atoms and molecules that have strong electron affinities will attach electrons and thereby rob the plasma of its ability to conduct elec- tricity efficiently. Studies of electron-molecule collision processes could help to control this difficult problem. More generally, large amounts of atomic and molecular col- lision and spectroscopic data are employed in constructing realistic theoretical combustion models. Such models are the basis for the fruitful comparison of theory and experi- ment, which is the hallmark of successful applied research.

The thermionic energy converter is another direct conversion device that employs a highly ionized gas exposed to a region that is hot at one end and cold at the other. It can be thought of as a gas-phase version of a thermo- couple, where a conducting gas is used instead of bimetallic strips. Optimizing the performance possibilities of such devices requires exhaustive examination of the basic micro- scopic processes, that is, the atomic and molecular physics of ionized gases.

The successful attainment of thermonuclear energy will probably represent the most direct application of knowledge obtained by atomic scientists. In the traditional thermonuclear plasma, we are dealing with a very dilute medium of electrons and ions at temperatures so high that no molecules can exist. The processes by which this plasma state is attained, starting from a simple gas mixture, are controlled by electron-atom collisions or by collisions of photons with ions and atoms. The way in which energy is lost from the plasma depends on similar fundamental processes.

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Although the ideal plasma would consist only of electrons and the simple hydrogen and helium nuclei, impurities in the form of heavier ions (iron, nickel, for example) introduced from the containing vessel inevitably enter as contaminants and introduce deleterious sources for radiating energy from the plasma. The fundamental processes by which these species gain and lose electrons and radiate energy are still imperfectly understood and need elucidation.

Also, as in the case of fission energy, we see the effects of radiation damage in the material components of the plasma container caused by collision cascades. These are initiated by the copious quantities of energetic neutrons emanating from the reacting plasma and could be better understood were a detailed knowledge of collision physics on hand.

In nuclear fission technology, ionic and molecular physics does not enter directly into the primary energy releasing event. Instead, its impact is felt in the processes of fuel preparation and the physical and biological consequences following the fission process itself.

Almost all existing and proposed methods for isotope separation depend heavily on input from atomic and molecular science. The established methods of gaseous diffusion, ultracentrifuges, and aerodynamic separation use information on gas transport properties that are closely linked to intermolecular scattering potentials. The newer and, as yet, undeveloped schemes of laser isotope separation demand highly detailed knowledge of photon-molecule and photon-atom interactions, as well as intermolecular energy transfer and chemically reactive collisions. Moreover, similar information bases are necessary for the development of the lasers (themselves a product of atomic and molecular science) that will be needed to carry out these processes on an industrial scale.

With regard to fission reactors, the role of atomic science has been and continues to be in the understanding of events following the nuclear fission event itself. Here, we are dealing with energetic heavy ions (fission fragments), neutrons, helium ions, electrons, and photons, which undergo a series of complex collision processes, giving rise ultimately to the heat used in power generation and to radiation damage. Similarly, the underlying science of the interaction of radiation from radioactive wastes with living systems and materials is appropriately within the scope of atomic collision physics.

Other interesting and important challenges for atomic and molecular science are offered by solar energy. For

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example, little practical use has been made thus far of
the possibilities offered by photochemical conversion by
simple, nonbiological systems in the gas phase.

The roles that atomic and molecular science is
likely to play in gas-phase solar energy conversion will
include supplying basic understanding of the photoexcita-
tion process and of excited-state collision processes, in-
cluding energy-transfer collisions, as well as generating
information concerning energy levels, transition probabil-
ities, branching ratios, and other molecular properties
related to photospectroscopy. The interactions of solar
radiation with all the constituents of the earth's atmo-
sphere, including pollutants, are also within the purview
of atomic and molecular science.

Finally, we consider the role played in the important
area of energy conservation. We have already alluded to
increased efficiency in the combustion process, where even
relatively small gains can have enormous economic effects,
and to more energy efficient (laser) methods of isotope
separation.

One area of atomic and molecular science that, his-
torically, has been built mainly on the need to conserve
electrical energy is gaseous electronics. This area can
be defined as the study of gaseous systems whose electrical
behavior can be varied by external means. Aspects that re-
late strongly to energy conservation include chemistry of
electrified species, lighting, and the design and operation
of switches. Examples of developments are fluorescent lamps,
which have a much higher efficiency than incandescent lamps,
mercury power switches, which eliminate the large power
losses through radiation and high resistance in metallic
switches, and the enhancement of chemical transformation,
which can be achieved by the passage of electrical current
through reacting gases. Appraisal of the future role of
basic research in gaseous electronics indicates that it will
continue to contribute to the more efficient utilization of
electrical power.

With regard to instrumentation, many of today's
arsenal of sophisticated testing and diagnostic scientific
tools, including all forms of particle and optical spectrom-
eters and lasers, were originally developed as by-products
of basic research in atomic and molecular science. This
is hardly an accident, since atomic and molecular science
deals with that region of the energy, or radiation, spectrum,
where most important energy-related processes of interest to
society actually take place. Also, traditionally, technology
amply repays its debt to basic research by adding the new
tools that are so essential in expanding the frontiers of

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fundamental knowledge. In no field has this fruitful inter-
play of pure and applied research been more dramatically
demonstrated in the past than in atomic and molecular
science; this mutually beneficial relation is still, to
this day, a basic feature of the field. A detailed dis-
cussion of this interaction is contained in Appendix A.
Appendix B discusses the problems of data acquisition,
evaluation, and dissemination, particularly as applied
to energy-related aspects of atomic and molecular science.

The nonscientist may wonder at the continuous ref-
erence in this report to such terms as collision cross
sections, excitation cross sections, lifetimes, and tran-
sition probabilities. The reason for their frequent oc-
currence is that they represent the fundamental processes
by which the scientist envisages transfer of energy to
occur on the atomic and molecular level. We include in
this report a brief glossary of the most important of these
terms, in the hope that this will make the report more com-
prehensible to the nonscientist.

1 INTRODUCTION

PURPOSE OF THE REPORT

The purpose of this report is to document the significance
of atomic and molecular science to energy-oriented research,
development, and technology. In approaching this difficult
task, one is first faced with the temptation to claim that
the connections are so deep and multifold that the task
need not even be attempted--that is, simply to state that
virtually all of atomic and molecular science is energy-
related. The nature of the field is such that a claim of
this sort is not unreasonable. Any energy process that
occurs in the gas phase necessarily involves properties of
individual atoms and molecules, for these govern the inter-
actions between atoms and molecules and of atoms and mole-
cules with radiation fields and with surfaces and solids.
*Such a general statement, however, is not particularly
helpful to those scientists and scientific administrators
who are trying to make judgments concerning areas of re-
search that could be of most value in the solution of en-
ergy problems.* Instead, we will here quantify this rela-
tionship.

Atomic and molecular science addresses the fundamen-
tal physical information on which energy-related research
employing phenomena in the gas phase and certain types of
surface phenomena is based. This information includes such
atomic and molecular properties and processes as ionization
and neutralization of ions; excitation and de-excitation
of atoms, molecules, and ions; scattering; energy loss;
charge transfer; ion-molecule reactions; certain neutral-
neutral chemical reactions in simple systems; thermionic
emission; surface ionization; absorption and desorption at
surfaces; and catalysis both in the gas phase and at sur-
faces.

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At the outset we note that the contribution of atomic and molecular science to the production of power through hydroelectric, geothermal, tidal, and wind-propelled means appears to be minimal. The areas on which atomic and molecular science bears most significantly are conventional combustion, nuclear fission, and controlled fusion, which are covered most thoroughly in this report.

At almost each stage in the preparation of this report, we were struck by the rich array of atomic and molecular processes that might be involved in some particular aspect of the energy problem. We were continually tempted to expand our descriptions to include more reactions and interactions in order to be as complete and accurate as possible. This would have led to the production of a document too cumbersome and detailed to have been of much use. Further, such a course would have led us in a direction that, we hope, has been avoided in this report, that is, the preparation of so-called "shopping lists" in the several energy-related areas that we discuss. Such shopping lists may be appropriate for specifically mission-oriented projects, and we do not disparage them. But our own purposes would not be well served by taking this approach. Such lists have a relatively short survival time, and often an important or even crucial cross section, reaction, or transition probability has not yet been recognized and is therefore omitted.

Our purposes are more general, and we prefer to leave to the individual scientist and science administrator the decisions on which particular quantities to study in detail.

As will be apparent from the organization of the report, we have chosen in most cases to discuss specific energy-relevant technologies and then to identify atomic and molecular science aspects of each of these. Instead, we could have started from the opposite direction, that is, specific scientific areas, e.g., photoionization or electron-atom excitation, and shown how each of these relates to various energy technologies. We preferred the former approach. Even so, it is not possible to be completely systematic in our approach, and where it appears sensible to be otherwise, we do not hesitate to depart from format, as in the discussion of laser research, lasers not being an area of energy technology *per se*.

This report is intended as an overview of the subject. The Subcommittee on Energy-Related Atomic and Molecular Science plans to prepare more detailed presentations of individual subjects at appropriate times.
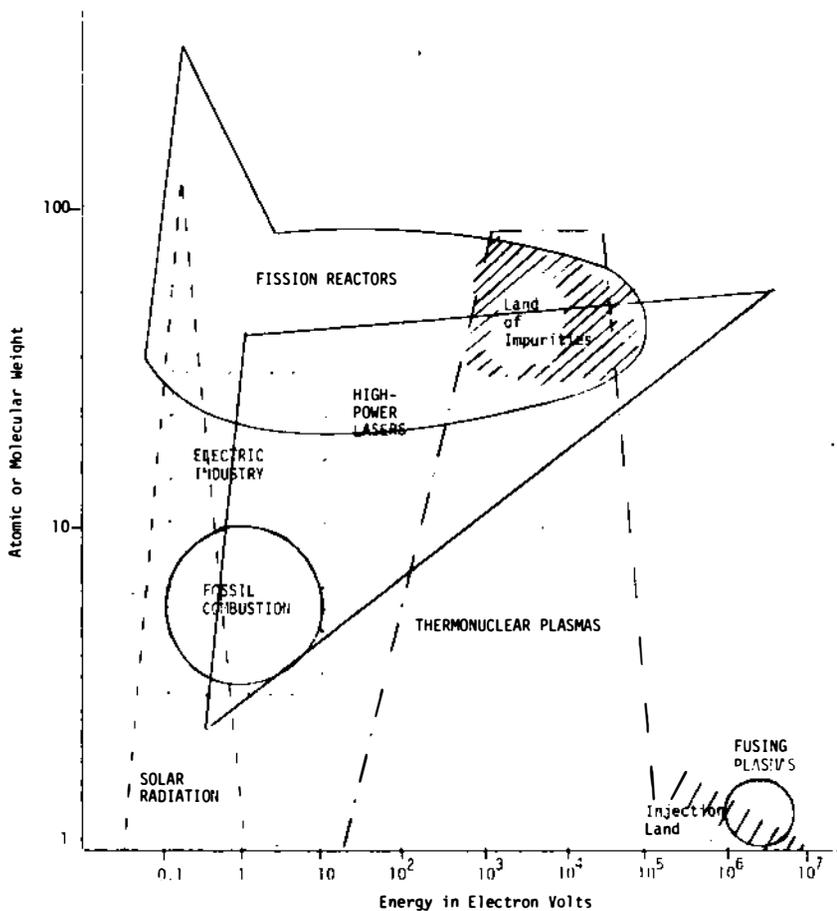
FIGURE 1 The relationship of atomic and molecular science to energy research.

In Figure 1, we chart the important areas of atomic and molecular science, insofar as energy research is concerned. In this two-dimensional map we plot energy as abscissa and atomic (or molecular) weight as ordinate. The energy in the chart refers to the atomic and molecular interaction energy rather than the energy of the relevant technology.

SOLAR ENERGY

Solar energy offers interesting and important challenges for atomic and molecular science. There are two fundamental ways of converting solar energy into useful energy. These are thermal conversion, in which the solar radiation is degraded to heat in the absorbing system, and quantum conversion, in which the solar radiation is used to cause some kind of photochemical or photoelectric process in the absorbing system. Existing "practical" solar conversion devices rely on thermal conversion almost exclusively, although, in some, use can be made by solar cells for direct conversion to electricity. Such conversion devices generally involve the interaction of radiation with surfaces and other condensed-matter systems. On the other hand, atomic and molecular physics processes play a major role in quantum conversion. Little if any practical use has been made of the potentially interesting possiblities offered by photochemical conversion by simple, nonbiological systems.

The roles that atomic and molecular science is likely to play in gas-phase solar-energy conversion will include supplying basic understanding of the photoexcitation process and of excited-state collision processes, including energy-transfer collisions, as well as generating information concerning energy levels, transition probabilities, branching ratios, and other molecular properties related to photospectroscopy. Atomic and molecular science also has an impact on solar-energy problems through atomic and molecular optical absorption and scattering in the atmosphere, involving both natural atmospheric constituents and pollutant additives.

Related to the terrestrial utilization of solar energy is the need to understand factors that govern the transmission of sunlight through the atmosphere. For the conversion of sunlight to energy, the efficiency of any solar device may be dependent upon its geographic location,

and the transmitivity of sunlight in any particular region
should be known. The interactions of solar radiation with
all the constituents of the earth's atmosphere, including
pollutants, constitutes an application of atomic and mo-
lecular science to the study of complex spectra. From the
viewpoint of this report, however, the role that atomic
and molecular science will play in solar-energy research
is as yet too indefinite to be included as a separate
chapter.

2   FUSION RESEARCH

Since the beginning of thermonuclear research in the United
States in the early 1950's, high-temperature plasma param-
eters have been dominated by atomic processes. Recently,
as plasma engineers have started conceptual designs of pro-
totype fusion reactors, the need for the solution of atomic-
physics problems occurring in high-temperature plasmas has
become urgent.

The importance of atomic-physics problems becomes
apparent if we compare typical atomic and nuclear cross
sections for particles in a thermonuclear reactor. Consider,
for example, the competition between the reaction rates for
a D-T reaction and charge exchange between a fast deuteron
and an impurity atom. The former reaction represents en-
ergy production; the latter represents energy loss since
the neutralized deuterium atom is no longer confined by
the plasma magnetic field and is thereby lost, along with
its kinetic energy. For a 10-keV ion temperature D-T plasma
the nuclear cross section to produce a neutron with 14-MeV
energy is 10^{-28} cm^2. The charge-exchange cross section for
a resonance collision is approximately 10^{-15} cm^2. Thus the
cross sections for charge exchange (as well as other loss-
producing atomic reactions) are as much as 10^{13} times larger
than nuclear cross sections. The relative energy gained in
a nuclear event is only perhaps 10^4-10^5 times greater than
the energy lost in atomic collisions. Thus *atomic reactions
can introduce extremely serious energy loss in thermonuclear
plasmas*, even at very low densities of the neutral impurities.

We will discuss here some atomic processes involved
in plasma heating, cooling, and diagnostics. Also of inter-
est are those atomic processes involved in the interaction
of a high-temperature plasma with the vacuum wall. In the
interest of brevity, remarks will be confined to Tokamak-
type plasmas, for which the present parameters are

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T_e (electron tempera-
   ture)   1-2 keV
T_i (ion temperature)   0.5-1.0 keV
n_e (electron density) 2.5×10^{13} electrons/cc
τ_E (energy containment
   time) 5×10^{-3} to 10×10^{-3} sec
T (pulse time) 50×10^{-3} to 300×10^{-3} sec
r (minor torus radius)   10-30 cm
R (major torus radius)   0.5-1.0 m
I_p (ohmic heating
   current)   100-300 kA

The corresponding parameters of planned prototype reactors
are

T_e 5-10 keV
T_i 10 keV
n_e 5×10^{13} to 5×10^{14} cm^{-3}
τ_E 1-4 sec
r 1 m
R 4 m
I_p 2-3 MA

Similar considerations apply to other types of confined
plasma systems.

PLASMA HEATING IN TOKAMAKS

In the past, the heating of toroidal plasmas has been ac-
complished by making the plasma the one-turn secondary of
a transformer and inducing a voltage of 2-5 V around the
torus. This induced voltage drives a current to heat the
electrons, which in turn transfer energy to the plasma ions.
After many cycles around the torus, the electrons approach
energies of several keV. At these energies, the plasma re-
sistivity, as well as the effective energy transfer through
Coulomb collisions from electrons to ions, becomes small,
and the heating may no longer keep up with the various
energy loss processes. Thus supplementary ways must be
found to heat the plasma.
       One approach to supplementary heating is to inject
large currents of fast neutral hydrogen atoms into the
plasma. Through resonant charge-exchange collisions with
plasma ions, the atoms become energetic protons, which are

captured by the confining magnetic field. These protons thermalize by energy transfer to both ions and electrons. In injection heating, it is necessary to have knowledge of the collisional processes in the atom beam source, which is basically an intense ion beam and a conversion cell where fast ions become fast neutrals.

For present injection heating experiments, pulsed ion sources have been developed for ion currents of up to 50 A and energies of 10-25 keV. The atomic and molecular ions are neutralized by charge exchange and dissociative collisions. As a result of space-charge effects, it is not practical to use magnetic analysis to preselect the beam current before neutralization, so that impurity ions from the source are injected along with the primary heating ions. To estimate the plasma losses caused by these impurities, it is necessary to know the electron capture cross sections of C^+, O^+, N^+, Pt^+, Fe^+, and Ta^+ in gases such as H_2, He, and N_2. Also, to predict the rate at which these impurity atoms enter the plasma one must know the electron-stripping cross sections for atomic species of these ions in the energy range 10-150 keV.

As experiments proceed to the prototype fusion reactor, it is necessary to increase the injected particle energy to the region of 150-200 keV. Two methods have been proposed and are being developed to obtain neutral hydrogen beams at these high energies: (a) negative D^- ions are obtained directly from an ion source, accelerated to the desired energy and stripped to the neutral state in a suitable gas target; (b) conventional positive ion sources are used from which hydrogen ion beams are extracted at 1-2 keV and passed through an alkaline vapor cell where 10-20 percent of the incident ions are converted to D^-, which is then stripped as in (a). Knowledge of the mechanisms producing D^- in the ion source is limited. Collision cross sections involving electrons on D_2 or D_2^+ in various states of vibrational excitation need to be known over the energy range from threshold to 500 eV. Current experiments indicate that tremendous gains in negative ion source output can be obtained by contaminating the walls and cathode of the ion source with alkaline vapors and other high-vapor pressure metals. The reaction kinetics involve deuterium atomic and molecular neutrals and ions interacting with surfaces contaminated with Cs, Mg, Na, and Li in the energy range 5-500 eV.

Conversion of atomic and molecular ions to D^- ions in an alkaline vapor cell involves a multiplicity of cross sections whose values are not presently available. Considerable work has been done for D^+ ions interacting with Cs,

Na, and Li vapor. Of more interest than cross sections
are the D^- equilibrium fractions formed in these vapor
cells. Discrepancies of a factor of three exist among
various determinations of the D equilibrium fraction from
Cs cells. Very little information is available for the
formation of D^- from collisions of D_2^+ and D_3^+. Also, the
differential scattering cross sections for D^- production
from both atomic and molecular species govern the accelera-
tion process for low-energy D^- ions.

Cross sections are available for the stripping of
D^- in many gases in the energy region 3–50 keV and about
300 keV, but the intermediate region needs to be filled in.
Of even more importance, the peak fraction of D^0 resulting
from D^- stripping needs to be measured. As the stripping
gas density is increased from 10^{13} cm^{-3} to 10^{16} cm^{-3}, the
D^0 fraction goes through a maximum and then decreases.
These maxima need to be identified for gases such as H_2,
He, N_2, O_2, Ne, Ar, and H_2O in the energy region 0.1–1 MeV.

In attempts to design and predict the behavior of
the next generation of plasma experiments, physicists must
understand the processes that result in trapping of the
injected beam. If only hydrogen ions occur in the plasma,
one can show that the injected neutrals will be trapped ap-
proximately uniformly across the magnetic field. However,
with impurity ions of even moderate densities present at
the plasma boundary, the incident neutral particles may be
ionized locally, setting up an instability. This instability
may occur in two ways: (a) by creating large pressure and
electric field gradients at the plasma boundary; (b) by
trapping at the plasma boundary, which may lead to increased
charge–exchange loss. These particles will bombard the
vacuum wall, giving more impurities, resulting in a cascade
process that will prevent any heating from the injected beam.
Charge–exchange cross sections for multiply charged atoms
of O, C, Fe, Au, and W with H and H_2 in the energy range
5–200 keV are needed to understand these losses.

PLASMA COOLING

Atomic-physics processes in a hot fully ionized plasma con-
tribute an important cooling mechanism that may limit the
obtainable temperature in an operating thermonuclear plasma.

Ideally, a thermonuclear plasma would consist of
deuterons and tritons. However, in existing plasmas, impurity

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ions and atoms are present in concentrations of up to sev-
eral percent. It has been shown that up to 40 percent of
the power loss in current plasma devices occurs through
line radiation from these impurities, which have been es-
timated to be up to 40 times ionized. These impurities
arise through particle and photon bombardment of the sur-
rounding surfaces and from charged-particle bombardment of
the "limiter." The limiter is an annular tungsten or
molybdenum ring placed at one point at the periphery of
the plasma, to prevent circulating particles from interact-
ing with the plasma vacuum container. Under fusion con-
ditions, the temperature will be sufficiently high that
these heavy impurities may be up to 70 times ionized. Thus,
in the presence of heavy ions such as tungsten, the power
loss may be so great that the temperature necessary for
fusion may not be obtainable.

Transitions between atomic-energy levels in the
reactor-type plasmas involve excitation and ionization by
electron collisions and de-excitation and recombination
through radiative processes, which remove particle energy
from the plasma. The appropriate excitation and ionization
cross sections are known adequately only in a few especial-
ly simple cases. Of particular interest are the strongest
resonance transitions of atoms stripped to the L-shell (Fe,
Cr, as well as O and C) and the M-shell (for heavier ele-
ments: Mo, W, Au, etc.), for the incident energy range
not far above the threshold energies (i.e., 1-10 times
threshold).

The states of ionization that an atom actually reach-
es in the plasma at a given temperature, density, and con-
finement time are important for both diagnostic purposes and
evaluation of radiation cooling processes. For example, a
completely stripped atom radiates much less efficiently than
one in helium-like or hydrogen-like excited states, and the
latter in turn much less than an atom retaining more than
two electrons. Therefore, quantitative understanding of the
recombination processes, which determine the state of ioni-
zation, are of critical importance, especially for the
heavier elements that are not completely stripped anywhere
in the plasma. The important recombination processes are
(a) radiative recombination, in which the incident electron
reaches a bound state by emission of continuum bremsstrahlung
(followed in general by radiative cascading to the ground
state of the ion), and (b) dielectronic recombination, in
which an intermediate unstable doubly excited state is sub-
sequently stabilized by emission of two or more photons.
Available estimates show that the dielectronic recombination

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is usually the dominant recombination process. Sufficiently quantitative information on the recombination processes is almost nonexistent for the important heavier elements (Mo, W, Au, etc.). For the lighter elements (Fe, Cr, O, C) a considerable amount of work also remains to be done. Because of experimental difficulties, most of this work will necessarily be theoretical. Thus any experiment capable of the reliable measurement of high-temperature recombination would be a particularly valuable "bench mark" for theory.

When a free electron is accelerated and deflected as it passes a positively charged particle, a photon is emitted. This process is referred to as free-free bremsstrahlung and is an important process in plasma cooling. Bremsstrahlung losses due to heavy charged impurities will be very harmful. If a plasma is heated by wave interactions such that the applied power is to the electrons, the bremsstrahlung loss can also be quite damaging. Experiments to measure bremsstrahlung in the keV energy range are virtually impossible to perform; accordingly, reliable computational techniques must be developed. Often the principles of detailed balancing can be employed to calculate equivalent cross sections. For example, elaborate close-coupling codes exist for the computation of photoionization cross sections, which can, by detailed balance, be identified with radiative recombination cross sections. In general, one could safely assume that the majority of atomic data for highly ionized elements will be generated by computation using reliable codes, rather than by systematic experimental determinations. As with recombination, experiments are particularly valuable when they can serve to check computational methods, since a general problem in the calculation of atomic cross sections is the lack of reliable theoretical estimates of computational error.

It is generally believed that the majority of atomic data for highly ionized elements will be produced by theoretical methods. Most prominent among them will be techniques that use in one way or another trends and regularities along isoelectronic sequences. However, a general shortcoming of theoretical data is that it is difficult to make an assessment of their accuracy. On the experimental side, work appears to be quite feasible in the areas of spectral-line identifications and atomic-energy-level analysis since suitable light sources are available, for example, vacuum sparks, with which spectra up to roughly 30 times ionized may be produced. For all other atomic quantities, that is, radiative transition probabilities, excitation cross sections, and collisional rate coefficients, including those for dielectronic recombination, no suitable experimental sources

appear to be available much beyond the fifteenth stage of
ionization. Most promising for experimental work (up to
these stages of ionization) is the theta-pinch; beam-foil
spectroscopy also has good potential for determinations of
selected oscillator strengths from atomic lifetimes again
up to about the fifteenth stage of ionization. Further
headway on the experimental side can only be made if a
really "high-energy," well-defined plasma research facility
becomes available.

DIAGNOSTICS

The two previous sections were directed toward understanding
the heating and cooling of a plasma. Diagnostics deals
with the experimental tools available to the plasma physicist
in quantitatively determining plasma parameters, such as
temperature, density, and local fields, as well as the prop-
erties of impurities present. A high degree of sophistica-
tion has been achieved in certain areas of plasma diagnostics,
such as the measurement of spatial electron temperature and
density by means of Thomson scattering of laser beams (wherein
the wavelength of the scattered laser beams is altered by
interaction with the swift-moving plasma electrons). However,
most important plasma parameters cannot yet be determined
with comparable accuracy.

For measurements of concentrations of heavy elements
in controlled thermonuclear fusion plasmas, one must know
the energy levels, wavelengths, and transition probabilities
of light elements, such as C^{n+} and O^{n+}, as well as of the
heavier impurities. Both resonant transitions, involving
zero change in principal quantum number n, and strong non-
resonant transitions with $\Delta n \neq 0$, are important. For
example, two specific problem areas of current interest are
(a) resonance lines of the copper and zinc isoelectronic
sequence, with particular attention to tungsten and gold,
to the upper end of the periodic table; (b) atomic structure
of the first 40 states of ionization of W and Au for simple
electronic configurations that lead to resonance lines.

Heavy-ion-beam probes have been developed in the past
few years to measure spatial plasma potential and densities.
In this method, a heavy ion beam with sufficient momentum
is projected across the plasma. At some point in the plasma
a fraction of the ions are converted to doubly charged ions
by electron or other types of ionization collisions. An

electrostatic analyzer placed external to the plasma can measure the change in particle energy of the doubly ionized component of the ion beam. The change in energy is proportional to the space potential at the point of ionization. The analyzer detector currents are proportional to the plasma density. These determinations can be made quantitative if the electron and deuteron ionization cross sections are known for singly charged ions of Li, Rb, K, and Ba. This information is needed in the energy range 0.05 to 1 MeV.

One technique useful for ion temperature measurements by Doppler broadening is to inject an impurity atom such as He, Ne, or Ar. The excitation of triplet states in He-like configurations and subsequent radiative decay is being used for high-temperature plasmas. A further and very attractive possibility is to use "forbidden" transitions, that is, magnetic dipole or electric quadrupole transitions, in various highly ionized heavier elements, particularly Fe, Cr, Kr, Mo, Xe, and perhaps W and Au.

Two additional techniques being developed using atomic physics to determine plasma parameters should be mentioned. In one, a lithium beam is projected across a toroidal plasma. An electron collision excites the atom, which radiates. By measuring the direction of polarization of this radiation, the magnetic-field direction at the point of ionization can be determined. By unfolding the magnetic-field direction, the plasma heating current distribution can be determined. Current distributions are important in theoretical calculations in Tokamak stability, and studies indicate that with fusion-type reactors the large heating currents will flow along the plasma skin leading to an unstable configuration. It is possible to conceive of even more sophisticated neutral beam probes for highly localized investigations of plasma properties.

Present laser scattering involves short-wavelength (8000 Å) lasers in which the scattered spectrum provides information about the electron temperature and density. For long-wavelengths (300–500 μm), the scattered spectrum arises principally from ions, and ion temperatures can be determined in this manner. Several laboratories are pumping CH_3F gas with CO_2 lasers to obtain coherent radiation at 496 μm. Radiation at this wavelength is also useful as a microwave interferometer and has possible use through photon echo techniques to study trapped electron lifetimes.

The National Bureau of Standards (NBS) is working to close the gap in radiometric standards that has existed in the 8–200 Å spectral region. Transfer standard detectors are now available covering the x-ray region and in the far

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uv down to 50 Å, where they can be overlapped with a new
extension of the NBS x-ray transfer standard detectors.
These standard detectors will allow the calibration of
diagnostic instruments at the individual CTR laboratories.
However, such a calibration requires that the diagnostic
groups themselves determine the transmission of their
spectrometers in order to complete the overall calibration
of the diagnostic tool.

A second approach, which would obviate the need for a
transmission measurement, is to develop a standard source for
this calibration. The only uv transfer standard source now
being developed at NBS is the wall-stabilized argon arc
for the spectral region above 1200 Å. The state of present
technology suggests that the best approach for a standard
source at shorter wavelengths is to develop a calibration
facility utilizing the Synchrotron Ultraviolet Radiation
Facility (SURF-II) at NBS. At this facility the capability
exists to provide a port where a diagnostic instrument can
be placed for calibration. The spectral content and ab-
solute intensity of the continuum radiation falling on this
instrument can be determined to better than 10 percent
throughout the spectrum down to about 50 Å.

This discussion has only presented some specific il-
lustrations of the role of atomic and molecular science in
CTR research. A more detailed and quantitative description
of specific areas where research is needed, together with
recommendations for manpower and cost allocations, is
contained in a number of other reports, but most particularly
in the Report of the Study Group on Atomic, Molecular, and
Nuclear Data Needs for CTR (Section 5, Part 6 of *The 1974
Review of the Research Program of the Division of CTR,*
ERDA-39, 1975).

In this section we have concentrated primarily on
atomic and molecular science related to magnetic confine-
ment. We have not discussed similar aspects related to
e-beam and laser fusion. These areas are relatively new,
and much of the effort to date has gone into development
of more powerful irradiation sources, that is, high-energy
pulsed laser and electron beams, and technology related to
pellet development, pulse shaping, plasma modeling, and the
like. As these fields mature, more attention will be paid
to atomic processes that occur in the imploding pellet. It
appears likely that problems similar to those encountered
in "conventional" fusion devices will be experienced, as
one learns more about these intriguing devices. In fact,
past experience in confinement plasmas should serve as a
warning that the present data base for atomic processes

that are important to implosion fusion devices is likely
to be inadequate.

We have also not discussed the extremely important
surface-physics aspects of confinement systems. Surface
phenomena that play important roles in existing devices
include sputtering, desorption, absorption, and secondary
emission. Other important surface effects include reactions
of gaseous constituents, particularly atomic hydrogen, with
insulators, surface reflection characteristics to synchro-
tron radiation, and neutron sputtering and damage.

In summary, one can conclude that atomic physics
plays a dominant role in the plasma scientist's quest for
thermonuclear power. Only through the solution of some of
the problems listed in the preceding pages can one offer the
hope that the temperature and confinement criteria demanded
of fusion plasmas will be met.

3 FISSION

Of all the technologies presently used in the generation
of significant amounts of electrical energy, fission is
the only one to emerge as a result of twentieth-century
science applied on a massive scale. Almost all of the
steps involved in the technology, from the introduction
of a new and useful fuel to the disposal of its waste pro-
ducts, have required the generation and exploitation of
concepts that did not exist 50 years ago. Moreover, be-
cause the industry resulted from the development of nuclear
weapons, and because of the lack of widespread knowledge
of the potential dangers of radioactive materials, the
development of nuclear power technology in all its aspects
has been closely controlled and managed by single govern-
ment agencies in the United States and elsewhere in the
world. This situation is unique in the history of tech-
nology. For example, environmental impact responsibilities
have had to be faced prior to, rather than after, the *de
facto* existence of a massive industry, and the agencies
involved have had as an important part of their mission the
responsibility for determining the effects of radiation
not only on materials but on living systems.

Clearly, there is a great deal more involved in
nuclear reactors than nuclear reactions. With this in mind,
let us briefly view fission technology as seen by an atomic
physicist. If we dispense with prospecting, mining, and
metallurgy, we come first on the problem of isotope enrich-
ment, an area almost exclusively in the domain of atomic
collision physics. Then, given the proper isotopic ratio,
we proceed to fabricate the fuel, reactors, and the like
and to arrange things so that the requisite number of neu-
trons cause the requisite number of fission events. Fol-
lowing the nuclear fission event, we are dealing with
energetic heavy ions (fission fragments), neutrons, helium

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ions, electrons, and photons, which undergo a series of complex collision processes giving rise ultimately to the heat used in power generation and to radiation damage. Similarly, the underlying science of the interaction of radiation from radioactive wastes with living systems and materials is properly in the area of atomic collision physics.

ISOTOPE SEPARATION

The primary market for isotopic enrichment processes has been, of course, for the preparation of uranium fuels. Although ~3 percent enriched material is generally used in most present reactors, higher enrichments may be desirable in high-temperature gas-cooled reactors, and, if efficient methods can be developed, isotopic cleanup may be desirable in future reactors fueled from plutonium breeders. Other possible applications exist in the treatment of radioactive wastes to reduce the storage capacity required.

Historically, the first method used for separation of uranium isotopes on a practical scale was the electromagnetic process, which relied heavily on atomic physics and gaseous electronics. This was later replaced by the more economic gaseous diffusion process. In this regard it should be realized that the efficiency of the gaseous diffusion process in terms of actual energy consumption, relative to the thermodynamic value necessary for obtaining 3 percent enriched material from the 0.7 percent naturally abundant material, is only 10^{-8} (that is, the ratio of the heat of mixing to the electric energy expended). The energy used in isotope separation corresponds to about 3 percent of the energy ultimately obtained from nuclear reaction using enriched uranium fuel, but in a nuclear-power-based economy this constitutes considerable energy consumption. The gas centrifuge method improves this power utilization figure by a factor of >10, but there is clearly still much room for improvement. The latter two methods and the aerodynamic jet approach utilize information on gas transport properties supplied by collision physics.

New techniques using laser excitation are currently under intensive investigation and require considerable and detailed input from collision physics. These methods generally rely on selective excitation of either the desired element in atomic or molecular form, followed by photoionization, or reaction of the excited particle.

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Using atomic species, the first step involves isotopically selective electronic excitation

$$X + h\nu \rightarrow X^* \tag{1a}$$

followed either by single or multiple photon excitation to ionization

$$X^* + h\nu' \rightarrow X^+ + e. \tag{1b}$$

Alternatively, associative ionization of the excited state atoms with a neutral atom or molecule R,

$$X^* + R \rightarrow XR^+ + e \tag{1c}$$

or by chemical reaction

$$X^* + RY \rightarrow XR + Y, \tag{1d}$$

might be possible.

For processes (1b) and (1c) the separation is simply accomplished by deflection in an electric field and collection on a surface. The photoionization process, (1b), has been investigated by a group at the Lawrence Livermore Laboratory,[1] which has demonstrated macroseparation of uranium isotopes.[2]

Process (1d), and perhaps (1a) as well, requires that the excited state undergo chemically reactive collisions while the ground state atom is nonreactive. This type of selective reactivity has been amply demonstrated, and an isotopic separation process based on this principle has been demonstrated in the case of mercury. The reaction is $Hg(6^3P_1) + H_2O \rightarrow HgO + H_2$, which is sensitive to the hydrogen isotopes involved.

Selective laser excitation of molecular species offers other possibilities for isotope separation schemes. Here the first step would be excitation either to higher vibrational or electronic levels

$$XY + h\nu \rightarrow XY_n^* \tag{2a}$$

followed by photodissociation

$$XY_n^* + h\nu' \rightarrow XY_{(n-m)} + Y_m \tag{2b}$$

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or by chemical reaction

$$XY_n^* + Z \rightarrow XY_{(n-m)} + ZY_m \tag{2c}$$
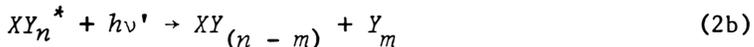
or by chemi-ionization

$$XY_n^* + Z \rightarrow XY_n^- + Z^+. \tag{2d}$$

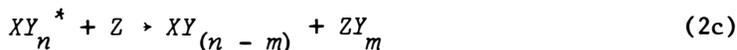An interesting example of processes (2a) and (2b) has been demonstrated recently in the Soviet Union[3] and at Los Alamos.[4] SF_6 is selectively photodissociated into $SF_5 + F$ under irradiation by the P-20 line of a CO_2 laser, which vibrationally excites the $^{32}SF_6$ molecule (the resultant fluorine is scavenged by H_2, which is added to the system). An interesting point here is that no other radiation source was used and multiphoton processes must be involved in the dissociation process. Although the exact mechanism has not been determined, it is known that the separation is sensitive to laser pulse intensity and duration.

Similar schemes for uranium isotope separation utilizing UF_6 are under investigation. However, the absorption spectrum of UF_6 vapor at room temperature is too complex to allow selective isotopic excitation. A Los Alamos group has recently disclosed that the internal temperature of UF_6 can be reduced to ~50K through nozzle expansion and that the resultant reduction in spectral complexity allows resolution of ^{235}U and ^{238}U components.

Clearly, numerous other schemes of the type described above could be devised, but all of these approaches need detailed information not only on the primary collision processes involved but also on those collision processes that could interfere with the separation. Excitation transfer from selectively excited states (1a) and (2a) to other isotopic species could be troublesome. Charge transfer prior to product collection in step (1b) or (2d) could decrease product selectivity. Chemical exchange reactions can reduce yields for processes such as (1d), (2b), and (2c).

The use of any of these processes on a commercial scale will require the development of high-efficiency, high-power lasers in the desired frequency range. This development also requires input from atomic and molecular science (see Chapter 5). Although the economic feasibility of any of these methods has yet to be demonstrated, none of these possibilities would exist without a strong foundation of knowledge in basic collision physics and chemistry. The opportunities for collision physics to contribute in

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these areas are broad and the possible payoffs are large, both in devising new reactions and in foreseeing contamination processes.

ATOMIC COLLISIONS IN SOLIDS: STOPPING POWER AND RADIATION DAMAGE

Radiation damage following a nuclear fission event is caused principally by the collisions of fast heavy ions in solids. The heavy ions in question are either fission fragments, which range in energy up to ~0.5 MeV/nucleon and are localized in the fuel region, or they arise from knock-on collisions of fast neutrons, which leave the fuel and collide in the containment material. These knock-ons can range in energy from 10 to 100 keV. In this latter regard the problem is similar in nuclear fusion reactors (CTR), where large fast-neutron fluxes will exist. In addition, the 14-MeV D-T neutrons can create knock-ons with energies up to ~500 keV.

Numerous experiments designed to simulate the effects of the enormous neutron fluxes that will be obtained in fast breeder reactors (and CTR reactors) are being carried out using accelerated heavy-ion beams. For example, 6-MeV Ni ions are injected into stainless steel, and in the region below the surface where they have slowed to ~0.5 MeV they simulate the effects caused by knock-on collisions of 14-MeV neutrons with Ni atoms. The initial high energy is necessary to penetrate below the surface region, where other effects may interfere. If accurate simulation can be achieved, the time scale for materials testing can be decreased by orders of magnitude. This, however, requires an understanding of the stopping over the entire range.

The processes attending the slowing of these ions in all cases are properly in the domain of atomic collision physics. The ions lose energy by inelastic loss caused by ionization and excitation of the electrons on the target atom and projectile ion (electronic stopping) and by "nuclear stopping," that is, elastic loss to the target atoms. At low velocities, elastic scattering causes collision cascades in the host and ends in an aggregate of point defects ("nascent" damage state). For the entire slowing-down process, the time scale is $\sim 10^{-13}$-10^{-12} sec. Following this, the processes of solid-state physics are dominant (diffusion, nucleation, precipitation, void formation, for example).

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The time scale here can be quite large. In metals, the nascent damage state is produced entirely by the atomic displacement, but in insulators and possibly in semiconductors, electron excitation can also lead to damage. For a detailed understanding of the elastic scattering cascade, a knowledge of the relevant interatomic scattering potentials is needed.

For the electronic stopping, a knowledge of inelastic events suffered by fast heavy ions is vital to understanding. The electronic stopping power (energy loss per atomic collision) initially rises with velocity, tops out, and then decreases. Most of the ions we are dealing with here have initial velocities in the lower region, where the stopping power curve is rising with velocity. This region has been handled theoretically by Lindhard *et al.*[5] in terms of electron gas interactions and by Firsov[6] in terms of charge exchange. Both lead to a linear dependence on velocity ($S = kv$) and to a monotonic dependence on the atomic number of the projectile in a given target. Both theories have been extremely valuable, but they were formulated before the recent burst of activity in heavy-ion collision physics and before the advent of "channeling" as a tool for understanding the motion of ions in solids.[7]

The study of atomic collisions in solids has been greatly aided by discovery and application of the channeling phenomenon. Channeling occurs when an ion enters a crystalline solid at a small angle with respect to atomic rows or planes. It undergoes a set of correlated small-angle scattering events with the closely spaced atoms, which tends to steer the ion's trajectory away from close collisions with a lattice atom. The potential that controls the motion of the ion can be viewed as a continuum potential made up of an orderly sum of the individual ion-atom potentials. Under these conditions, the ion is said to be "channeled" and, under easily achieved experimental conditions, more than 90 percent of ions entering a crystal can be channeled.

Ion-beam channeling experiments have helped to clarify the separate contributions of nuclear stopping and electronic stopping and to determine the effects of long-range and short-range electronic excitation.

For example, results obtained in the last few years have shown that the stopping powers are not monotonic with Z, the ionic charge, and that for heavy ions there is no truly linear region in the velocity dependence of stopping power. Periodic oscillations in the Z dependence of the electronic stopping (especially in large impact parameter collisions) have been shown to be related to electron mo-

mentum transfer minima encountered in the Ramsauer-Townsend effect. The nonlinearity of the velocity dependence may be related to an imperfect knowledge of the state of the ion as it penetrates the solid.

Inner-shell ionization caused by quasi-molecular electron promotion has been shown in numerous recent experiments to give rise to appreciable steady-state concentrations of inner-shell vacancies in ions penetrating condensed media. Similarly, inner-shell excitation of the target atoms by this process will contribute to the stopping and damage process in ways that have heretofore not been considered. Continuing investigations of charge-changing collisions in solids; comparison of x-ray yields and energies; and inner-shell processes in solid and gaseous media, such as charge-state dependence of Coulomb excitation and exit channel effects in quasi-molecular orbital promotion, will be required for a complete understanding of the atomic processes. There remains the application of this knowledge to the effects of radiation on materials.

HEALTH PHYSICS

The implementation of any technology demands a responsibility for the possible environmental effects on the personnel employed in the industry and the general population. In fission technology, these requirements are a considerable part of the capital and operating cost; and here atomic and molecular science plays an important role in the understanding of biological effects and in establishing a reliable dosimetry system.

The principal effects of ionizing radiation on living systems occur through the action of electrons generated along the track. Thus the consequences of many aspects of electron-molecule collisions are directly relevant. Fundamental studies of electron-induced dissociation, ion-molecule reactions, recombination reactions, intermolecular and intramolecular energy transfer are required as a base for the physical modeling of biological processes.

Ultimately the electrons are stopped and attach to form negative ions. Here electron attachment cross sections and molecular electron affinities are of importance. An example of the utility of this information is in the observation of a correlation of molecular electron affinity with carcinogenicity of certain classes of molecules.

Experimental studies on systems of complexity inter-
mediate between single scattering and living systems are
also required to establish similitude of simple systems
used in dosimetry to biological systems. These studies,
called "Energy Pathways," are used to establish final dis-
posal of the energy in a dense system. Studies usually
involve the measurement of the total degree of ionization
radiation emanating from an irradiated dense gas mixture.
In such dense systems, ionization occurs not only by direct
processes but also by transfer of electronic excitation
from atoms of high ionization potential to more easily
ionized species. This stored energy can come from meta-
stable states (Penning ionization) as in less-dense media
or from resonant states, which are populated in more dense
media as a result of trapping of resonance radiation. The
sum of these processes (Jesse effect) often enters strongly
into the total ionization effect. An additional high-
density feature is the formation of excited-state atomic
or molecular adducts ("eximers"), which themselves emit
relaxation radiation. Recently, time-dependent studies
with pulsed radiation sources have added much information
about the role of eximers in energy disposal processes.
Interestingly, the same methods yield information on the
mechanisms of e-pumped lasers, which may find use in future
isotope separation schemes.

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4 FOSSIL FUELS

The extraction of energy from fossil fuels by combustion
is perhaps the oldest industrial process. Under ordinary
conditions the process is a continuous one. The fuel is
burned essentially to completion, and the heat is extracted
and converted reasonably effectively to useful work or to
the generation of electric power, all without the necessity
for examining in detail the kinetics and energy-transfer
processes involved in the exceedingly complicated chemistry
of most fossil-fuel combustion systems. This is possible
because in most cases, especially for high-temperature com-
bustion, the rate processes are so fast that the control-
ling time intervals do not depend on them but on such
characteristics as gas flow, thermal conduction, and other
physical properties of the burning gas. Some reaction rates
and energy-transfer processes are, however, important in
connection with some of the spent products of combustion,
for the amount, therefore the environmental effects, of
these can be strongly dependent on the kinetics of their
production. For standard combustion processes, therefore,
the effort of atomic, molecular, and chemical kinetic sci-
ence will probably be directed largely toward the effluent
gases, their composition and control (e.g., the formation
of NO_x in combustion), and the instrumentation connnected
therewith.

     For specialized methods of combustion, such as the
internal combustion engine, or for extracting energy under
exceptional conditions, such as in MHD power sources, the
influence of reaction rates and energy-transfer processes
may be entirely different. For the conventional internal
combustion engine, for instance, smoothness of burning
during the cycle is of great importance and imposes strin-
gent conditions on the quality of fuel, mixture ratio, and
the like. When these are combined with other requirements,
such as efficiency of fuel utilization and limitations on

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environmental pollution, the requirements for optimum per-
formance become exceedingly severe, and the challenge to
seek new solutions by novel techniques becomes correspond-
ingly high.

All practical combustion systems share the feature
that the stored chemical energy is first released as heat,
and useful work is extracted by the use of some device
such as a piston or turbine engine or an MHD generator.
From general thermodynamic considerations, the efficiency
of conversion of such devices of the original chemical
energy cannot exceed $(1 - T_l/T_u)$, where T_l and T_u are the
lower and upper temperatures of the cycle. Much could be
gained if conversion of chemical to electrical (or mechan-
ical) energy could be achieved directly, without inter-
vention of an intermediary device. The existence of elec-
trical batteries, and the biological conversion of the
energy in sugars to mechanical (muscular) work or to elec-
trical discharges (viz. the eel) or to visible radiation
show that such conversion is sometimes possible. One of
the most interesting areas of basic research in energy-
related atomic and molecular science is this "direct con-
version" problem. In this chapter, however, we will dis-
cuss only heat-related primary energy sources and conversion
devices.

COMBUSTION

As we intensify our search for alternative energy sources,
we must nevertheless recognize that the combustion of fossil
fuels (oil, coal, and natural gas) probably will continue
to supply the bulk of our energy needs for the next 25 years.
At present, only about 3 percent of our primary energy
sources in the United States are *not* attributable to fossil
fuels! Even using optimistic predictions of the future
contributions from all other sources, as much as 80 percent
of our energy needs in 1990 will probably still come from
fossil fuels. A general discussion of basic combustion
processes, including such considerations as theoretical ef-
ficiency, portable energy sources, details of the combus-
tion process, diagnostics, and conservation problems, is
contained in the recent publication of the American Insti-
tute of Physics, *Efficient Uses of Energy.*[1] Commerical oil
and coal furnaces are relatively "efficient" devices, in
the sense that they do release most of the available energy
in the fuel, although the conversion to useful heat, which

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is governed by thermodynamic considerations, is not done efficiently in conventional heat-exchange furnaces. Conversion efficiency of coal gasifiers and of electrical power generation, via combustion, is even less efficient (50-70 percent and 30-40 percent, respectively).

The primary foreseeable improvement in coal combustion technology appears to be the fluidized bed burner, whose development will probably proceed without much help from the atomic and molecular community. Nevertheless, a better understanding of the atomic and molecular processes that occur during combustion could lead to improved direct combustion performance. One method of accomplishing this is by the use of sensing diagnostics to control mixing and other combustion parameters. Electrically aided combustion also appears to offer interesting possibilities. Such relatively sophisticated "on-line" combustion control can only be developed from a fundamental understanding of basic combustion processes, including the roles played by free radicals and excited states.

General rules for reactivity energy distributions and collisional energy transfer are just beginning to be developed. Many aspects of gas-phase reactions, such as intermolecular energy transfer, ion-forming and neutralization processes, associative detachment, and low-energy ion-molecule reactions have become far better understood in recent years than was previously the case. To a large measure, these aspects of collision physics were successfully attacked using such atomic-physics experimental techniques as afterglow measurements and crossed-beam technology. Now all of these processes must be studied in selected excited states; for this purpose, fortunately, the tunable laser has become an indispensable tool. Such studies are necessary if one is to establish a firm basis for a general-theory gas-phase chemical reactivity, which governs combustion processes. This might be described as the basic long-term goal of combustion chemistry.

In the shorter term, sophisticated methods such as crossed-molecular-beam experiments and laser fluorescence, which have been successfully used to study simple molecular systems (e.g., alkali atom and halogen atom reactions) must be applied to the more complex reactions involved in the combustion process. In this borderline area between atomic and molecular physics and physical chemistry it should be noted that many of the active workers in this field have been, and continue to be, trained in atomic and molecular science, and many of the techniques involved derive from this discipline.

Wall reactions, which deactivate molecules and which can contribute to chain-breaking by the removal of free radicals, can likewise be profitably studied using molecular-beam techniques.

In general, basic combustion experiments are concerned with flame composition and pollutant emissions and involve the study of temperatures, flow fields, and interactions with surfaces and the ambient environment, in addition to the reactant species themselves. Studying these *in situ* is not a simple matter, and techniques developed in atomic and molecular science, including optical and mass spectrometers and laser scattering and fluorescence, have yet to reach their full effectiveness as diagnostic tools, although in principle they permit spatially and temporally resolved measurements of combustion temperature, composition, electron and ion densities, and the like.

In addition, fundamental atomic and molecular data such as molecular constants, transition probabilities, lifetimes, collision cross sections, diffusion coefficients, and other transport parameters must be employed in any combustion models. Often uncertainty in knowledge of such basic parameters can lead to large errors in the calculation of combustion reactions. Matters relating to instrumentation and data accumulation and evaluation are discussed in more detail in Appendixes A and B.

Atomic and molecular science plays a basic role in problems relating to combustion-generated pollution and magnetohydrodynamic (MHD) power generation. For both of these, a greater understanding of basic atomic and molecular phenomena than currently exists is required to make significant progress. For example, in the combustion of fossil fuels one encounters the unpleasant generation of SO_2, SO_3, NO, and NO_2. The following sulfur- and nitrogen-bearing intermediate radicals have been identified:

$$S, S_2, SH, SO, CS$$
$$N, NH, NH_2, NH_3, HCN, CN$$

These species are trace constituents whose formation and subsequent reactions occur in a bath of the following species, which have been identified as intermediates in the combustion of the main body of the fuel:

$$O, O_2, OH, HO_2, H, H_2$$
$$C, C_2, CH, CH_2, CH_3, C_2H_2, C_2H_4, C_2H_6$$
$$CHO, CH_2O$$

The above lists are obviously only a partial description of the makeup of a coal or oil flame.

Perhaps the most inadequately understood aspect of combustion at present concerns the role of excited states, other than in their contributions to radiative outputs. It is likely that excited species play important roles in both energy-release and pollutant-formation chemistry, yet experimental studies of excited-state reactions are only in their infancy. For such studies, laser-induced fluorescence has become a powerful analytic tool. Conversely, fruitful exploitation of fluorescent analytic techniques requires a knowledge of excited-state-species energies, lifetimes, quenching, and reaction cross sections, along with absorption cross sections of the ground states. Laser-induced fluorescence can also be useful for the determination of the spatial distribution of temperature in flames, by monitoring the rotational distribution of some native or added diatomic molecule along the beam axis. For many of the species listed above, there is little documentation of excited-state properties. For some of them, even the ground states have not been fully characterized.

The single-mode tunable dye laser is also now being used to prepare atomic and molecular systems into specific excited states in crossed-beam experiments, for precision cross-section measurements. Experiments of this kind will doubtless play the role in excited-state collision physics that has been played by analogous experiments on ground states during the past decade.

More generally, the combustion process itself will continue to be employed under selected experimental conditions to measure most of the important molecular constants, reaction rates, and other parameters required for a better understanding of combustion systems, for these usually are not accessible by means of straightforward beam experiments. Phenomena such as ion-molecule reaction rates, recombination rates, and resonant and nonresonant energy transfer are among such processes.

In Figure 2, abstracted from Reference 1, we illustrate the areas of basic physics and chemistry that contribute significantly to the combustion process and indicate those specific areas that relate to atomic and molecular science. In the following subsections, we discuss atomic and molecular science aspects of combustion-related catalysis, MHD, and direct thermionic conversion. Although these also contain certain aspects that are relevant to other energy sources, they are particularly important at present in connection with fossil-fuel combustion problems.

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┌─────────────────────────────────────────────┐
│                                             │
│   Role of Fundamental Physics and Chemistry │
│                 in Combustion               │
│                                             │
│                                             │
│   Kinetic theory                            │
│       transport processes (A and M)         │
│       chemical equilibrium (A and M)        │
│   Equation of state (A and M)               │
│   Chemical thermodynamics                   │
│   Statistical mechanics                     │
│   Chemical kinetics (A and M)               │
│   Nonequilibrium kinetic theory (A and M)   │
│   Radiative transfer (A and M)              │
│   Thermochemical data (A and M)             │
│   Collision data (A and M)                  │
│   Spectroscopic data (A and M)              │
│   Turbulence, microscale processes          │
│                                             │
└─────────────────────────────────────────────┘
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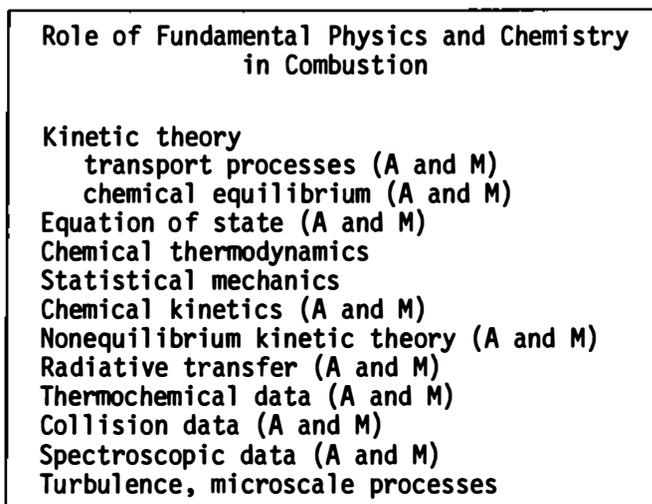
FIGURE 2 Important areas where fundamental physics and
chemistry relate to the combustion process. These are
all used to generate appropriate collective combustion
models and various conservation equation statements, as
well as in the establishment of appropriate boundary con-
ditions. Atomic and molecular areas are identified by
A and M. (From a complete combustion "flow chart," see
Reference 1, p. 164.)

CATALYSIS

Present methods used for coal hydrogenation (liquefaction
and gasification), petroleum refining, and automobile ex-
haust treatment all use heterogeneous catalysis (liquid-
solid, gas-solid) as an integral part of the process. Yet
the design of catalytic process systems is still largely
semiempirical, lacking in fundamental understanding that
could result in important improvements in practical cata-
lytic reactors. Atomic and molecular aspects involved
here include the processes of surface adsorption and de-
sorption, elastic and inelastic molecule-surface inter-
actions, and, most importantly, the vast array of atomic

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and molecular experimental techniques now being used to
study surface phenomena. These include:

> Low-energy ion backscattering (LIBS)
> Secondary ion mass spectroscopy (SIMS)
> Auger electron spectroscopy
> Electron spectroscopy for chemical analysis (ESCA)
> Auger electron appearance potential spectroscopy
> (AEPS)
> Characteristic energy-loss spectroscopy (CES)
> Soft x-ray appearance potential spectroscopy (SXAPS)
> Low-energy electron diffraction (LEED)
> Electron-stimulated desorption (ESD)
> Photon emission (characteristic radiation) from ion-
> bombarded surfaces
> Interaction of atomic and molecular beams with
> surfaces

With one, or a combination of several, of these
methods, the surface composition and structure of the sub-
strate and the bending vibration and stretching of the ad-
sorbed molecule can be studied. At present, there are
many uncertainties in these methods, which can be clarified
by further atomic and molecular science research. Two such
examples are the charge-capture cross sections of gas atoms
rebounding from a single collision with a surface atom (LIBS)
and the mechanism of excitation responsible for the photon
emission from sputtered atoms.

Molecular-beam experiments on surface reflection
have already contributed significantly to an understanding
of energy exchange and desorption, and beginnings have been
made using beam techniques for the study of catalytic re-
actions. Modulated molecular-beam experiments are unique
in their capability for measuring time-dependent surface
phenomena. A coupling of the sophisticated molecular-beam
techniques available to atomic and molecular science to
practical systems is now ripe for development.

DIRECT-CONVERSION MAGNETOHYDRODYNAMICS

The thermodynamic efficiency of present stationary power
plants based on steam as a working fluid is limited by the
practical upper limit on the steam temperature. This is
dictated by the maximum working pressure and temperature

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limits on heat-exchange tubes. One solution to higher
temperature operation with consequent gain in thermodynamic
efficiency in production of electricity is direct conversion
of heat energy through magnetohydrodynamic (MHD) generators.

MHD generators also represent a promising method for
direct conversion in nuclear reactor systems. For use in
combustion, "open-cycle" magnetogasdynamic (MGD) generators
are usually employed, for which the combustion reactants
are directly used in the MHD system. For use in nuclear
fission or fusion reactors, and other noncombustion MHD
generators, "closed-cycle" systems are more appropriate.
The characteristics and performance potential of such de-
vices are dominated by the properties of a partially ionized
plasma, which constitutes the working fluid. For this
reason a detailed understanding of the plasma is prerequi-
site to the design and successful operation of these energy
conversion devices.

Experience with closed-cycle MHD generators has
shown that these are nonequilibrium devices, for which
equilibrium thermodynamic models are inappropriate. On
the other hand, open-cycle devices seem to be fairly well
modeled using data computed for equilibrium conditions,
except possibly allowing for a moderate electron tempera-
ture elevation. In the case of combustion plasmas, un-
certainties in thermodynamic and transport data are so
large that it is not always clear that the discrepancies
with theory are attributable to nonequilibrium phenomena
or simply to inadequately modeled gas dynamics.

In closed-cycle systems, noble gases are generally
seeded with alkali metals and circulated in a closed loop.
For open-cycle systems, the hot combustion product gas
itself is seeded with alkali atoms in the working fluid.

The closed-cycle devices are intended to operate at
a temperature of about 2200 K and a pressure of 1-40 atm.
The fluid (He or Ar) is seeded with about 0.1 percent K
or Cs and the charged particles present are K^+ (or Cs^+)
and electrons. For this relatively simple system, many of
the required cross-section data are now fairly well known.
With availability of this fundamental information, the
transition rate equations for excited-state populations
for nonequilibrium alkali-noble gas plasmas are reasonably
well understood. Such analyses, which can be considered
as a simple prototype for the more complex open-cycle MHD
system, take into account the detailed mechanisms of charged-
particle production and loss, radiative energy loss and
transport processes, and the nonequilibrium nature of the
electron energy distribution.

This does not mean to imply that complicated systems are amenable to similar straightforward understanding. For a coal-fired MHD plant, the situation is considerably more complex. At projected temperatures of 2600 K, the gas would consist principally of N_2(~70 percent), CO_2(~10 percent), H_2O(~7 percent), and CO(~5 percent). (Some oxygen enrichment of the air could yield lower concentrations of N_2.) In addition, O_2, NO_x, OH, H_2, SO_x, and numerous free radicals would be present. Condensed species (fly ash) consisting of Al_2O_3, SiO_2, and Fe_2O_3 are also contained in the fluid, and at these temperatures certain metal oxides would be in the gas phase. Input from atomic and molecular science could contribute appreciably to an understanding of the process. For example, the formation of negative ions (OH^-, NO_x^-, SO_x^- . . .) is detrimental because of the attendant reduction of plasma conductivity. Electron affinities and attachment cross sections for the molecules of interest and electron emission and absorption at surfaces (especially of the particulates mixed in the gas phase) are important to a comprehensive modeling program. In addition, the presence of many polar and polarizable molecules that may have high momentum transfer cross sections with electrons will also significantly affect the conductivity, the electron energy distribution, and other properties of the plasma.

Recent concern over atmospheric pollution has added another important dimension to the analysis of MHD plasma characteristics on which basic electronic, atomic, and molecular data will exert an important bearing. Magneto-hydrodynamic generators used for electrical power production will be subject to the same constraints on emission and efficient fuel utilization as is the case with existing conventional generators. For this reason, future analysis of the working plasma medium in combustion-driven MHD generators must focus attention on minority species production and loss. This new need places demands for significantly improved cross-section and rate-coefficient data for the nitrogen oxides, sulfur oxides, carbon monoxide, and gaseous hydrocarbons. If MHD energy conversion is to play a role in the nation's electrical power production, a much better understanding of fundamental processes in MHD plasmas is required.

As an illustration of how atomic and molecular science relates to MHD, we will discuss the problem of electrical conductivity, which is one of the principal governing factors that determine the efficiency of MHD power generation.

The electrical conductivity is itself governed by a number of basic reaction mechanisms, particularly the momentum-transfer cross sections for electron-atom and electron-molecule collisions; electron-loss mechanisms, including recombination processes and negative ion formation; and Coulomb interactions, which determine the conductivity of the ionized portion of the combustion gas. The role of minority species, although not well understood, could be significant in determining conductivity. Thus, one can see that polar molecules, which offer extremely large cross sections for elastic scattering and rotational and vibrational excitation, even if representing a small fraction of the combustion products, could have an adverse effect on the electrical conductivity. Similar deleterious effects could result from minority species possessing large electron affinities. Affinity data and collision cross sections for a wide range of major and minor constituents would be helpful in assessing their role in determining conductivity. A partial list of important atoms and elements, in addition to those mentioned earlier in this section, would include Cl, SiO_2, Al_2O_3, Fe_2O_3, K_2O, Cao, K_2, TiO_2, MgO, P_2O_5, Na_2O, and B_2O_3. For cesiated systems, many of the very large polar molecules containing cesium could also be important in reducing conductivity.

THERMIONIC ENERGY CONVERTER

The thermionic energy converter (TEC) is a device in which heat energy is directly converted into electrical energy by employing nonequilibrium transport properties of the charged constituent of a partially ionized plasma, which is made to experience a temperature gradient. The TEC can be considered to be a gas-phase version of the thermocouple. For certain specialized applications, this type of device is already being used for direct conversion (specifically, in long-range spacecraft). Progress in this field is well documented in the series of conference proceedings on direct thermionic convergence.[2]
        As with the closed-cycle MHD generator, the characteristics and performance potential of such devices are dominated by the properties of a partially ionized plasma, which constitutes the working fluid. For this reason, a detailed understanding of the plasma is prerequisite to the design and successful operation of these energy conversion devices.

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2. See, for example, "Thermionic Electrical Power Genera-
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5 LASERS

The impact of lasers in the energy field is only begin-
ning to be realized, and it is likely to increase strongly
with time. Perhaps the most immediate and promising ap-
plication of lasers is in the isotope separation area,
where it appears that considerable economic savings can be
realized in both capital investment and operating cost of
future U and D_2O separation plants. The most direct and
efficient photochemical processes for such a plant have
not been determined as yet. Ongoing research concerns
various schemes involving lasers in the wavelength range
from the ultraviolet to the infrared. Lasers and isotope
separation are discussed more fully in Chapter 3.

The application of lasers to the initiation of fusion
reactions by the technique of pellet implosion is strongly
dependent on the development of new high-energy lasers.
Before this means of energy production becomes feasible,
lasers possessing considerably higher energy and better
efficiency will have to be developed in the visible to
near-uv range of wavelengths.

The use of lasers in energy-related research, however,
goes beyond their direct application to fusion and isotope
separation, since the laser is a basic tool for the study
of many atomic and molecular processes that directly or
indirectly relate to energy research. Some examples in-
clude Doppler-free spectroscopy and excited-state collision
physics and photochemistry, which play important roles in
some aspects of energy research and are described in ap-
propriate sections of this report. Thus it is difficult
to imagine any area in laser design that does not impact
in some way on the energy problem. With regard to atomic
and molecular science, of course, one is primarily concerned
with gas-phase lasers, and our discussion here is limited
to those.

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Since many high-energy lasers operate in the gas phase, atomic and molecular collisions in excited gases play a central role in determining the energy-transfer processes that control excited-state populations and ultimately determine the laser properties. A fairly detailed study published recently[1] resulted in a set of specific recommendations of areas of atomic and molecular science in which research is needed to speed the development of high-energy electronic lasers; the reader is referred to that study for detailed discussions of important reactions.

A large group of gas lasers relies on electron impact phenomena, and subsequent reactions, to achieve population inversion. The need to understand population inversion and laser action in gas discharges resulting from electron collisions and subsequent reactions puts enormous demands on our knowledge of pertinent cross sections. Ideally we would need to know a whole set of cross sections for elastic and inelastic electron collisions in the energy range from zero to about 20 eV for all the molecules or atoms of the gas mixture for gas-discharge lasers and to the kilovolt range for e-beam lasers. In addition, the cross sections for excited molecular species (vibrationally and electronically excited states) interacting with other molecular species are required. Negative and positive ions formed by electron impact also participate in reactions, forming new ionic and neutral species. Knowledge of all of these cross sections, combined with realistic models of the gas-discharge processes, including such phenomena as wall and radiation losses, instabilities, and other cooperative effects, would enable one to calculate electron energy distribution functions and population immersions and, in general, to characterize the medium accurately.[2]

In practice, of course, one must be somewhat selective in deciding which reactions need to be investigated in detail, since it is rather a tall order to expect that all of these processes can be adequately measured in a reasonable time. Detailed discussions of particularly relevant reactions are contained in References 1-3.

A most significant illustration of the relation of atomic and molecular collision physics to high-energy lasers is the development of the CO_2 electric-discharge laser. This was, to a large extent, the result of the ready availability of a relatively complete set of cross-section data.[3] The required data were generated in the late 1950's and early 1960's in connection with studies of upper atmospheric phenomena. Thus, when the potential for high power and

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efficiency from the CO_2 electric laser was demonstrated in the late 1960's, advances based on detailed modeling of laser characteristics proceeded rapidly.

No single development paced the advance in understanding high-power electric lasers more than the measurement and interpretation of low-energy electron-molecule cross sections for vibrational excitation.[2] Based on this information, electron energy distributions and pertinent electron-molecule excitation rates could be determined analytically for the species of importance in molecular laser discharges. In addition, coupling of this information with neutral-particle reaction rates permitted detailed modeling of electric laser characteristics.

Progress in laser development has led to the exploration of electric discharge configurations and operating conditions for which no prior experience exists. This is discussed further in Chapter 6. The required understanding of negative-ion processes and plasma stability accompanying these developments has been able, for the most part, to keep pace because of the availability of reliable electron cross-section data for the more common molecular species, for example, CO_2, CO, and N_2. Indeed, it can be stated with confidence that the present state of high-power electric-discharge laser technology reflects the successful combination of basic cross-section data and gas-discharge theory that existed prior to the catalyzing effect provided by the invention of the laser. However, the conditions under which high-power CO_2 and CO lasers operate have revealed a need for additional data. Specifically required are electron cross sections for collisions with vibrationally excited molecules, recombination and attachment rate coefficients at very low temperatures (~100 K), and a better understanding of charged-particle kinetic processes at high pressure ($\gtrsim 1$ atm).

The first generation of high-power electric-discharge lasers, such as those utilizing CO_2 and CO as the working medium, operate on vibrational transitions. Such "vibrational-transition" lasers generate radiation in the infrared portion of the spectrum. However, applications such as fusion and isotope separation require efficient high-power gas lasers with wavelengths in the visible and ultraviolet regions. Such lasers must operate on *electronic* transitions for which an entirely new set of cross-section data is required. In fact, the most promising short-wavelength laser candidates at present are the so-called eximer or ground-state dissociation lasers. Laser action in these systems depends on establishing conditions for the efficient

production of electronically excited molecules for which
the ground electronic state is repulsive. Promising laser
candidates are to be found among the rare-gas dimers,
alkali rare-gas molecules, and rare-gas halides, for ex-
ample, KrF. Charge exchange into excited states of multi-
ply charged ions is an example of a promising method for
the production of soft-x-ray lasers.

These are examples of systems that have not been
extensively studied; currently there are few basic cross-
section data on which to base appropriate macroscopic
models. Thus, the need for efficient laser systems opera-
ting at short wavelength has focused attention on a host
of atomic and molecular species for which cross-section
information is virtually nonexistent. Continued progess
in high-power laser technology will require the generation
of substantially more basic atomic and molecular data than
has been characteristic in recent years.

More generally, a list of atomic and molecular
science processes that occur in gas-phase lasers could in-
clude essentially all important energy-transfer processes,
chemical reactions in ground and excited states, chemilum-
inescence and photochemistry, three-body processes, various
photon interactions, and electronic and ionic processes,
including various types of recombination, attachment, and
ionization. One of the great challenges of atomic and
molecular science is the development of reliable and ac-
curate computational techniques that have general applica-
bility to entire classes of specific reactions. It is
not the purpose of this report to summarize or evaluate
current progress toward this goal; instead, the reader is
referred to the vast literature of collision physics,
where theoretical work appears in abundance. The continu-
ing "ICPEAC" series (e.g., IXth International Conference
on the Physics of Electronic and Atomic Collisions, Abstracts
of Papers, J. S. Risely and R. Geballe, editors, University
of Washington Press, 1975), is particularly useful in in-
dicating the current status of such theoretical techniques
and their success in predicting experimental cross-section
values.

The basic atomic data discussed above serve as input
in suitably formulated models, based on the kinetic theory
of partially ionized gases, that is, plasmas. Momentum
and energy-flux equations and other relevant transport
equations are solved for the electron velocity distribution
function under suitable boundary conditions, using various
ground- and excited-state cross sections as parameters.
Such models are useful to optimize conditions for the

repression of instabilities and in predicting character-
istics of new molecular species and of novel laser tech-
niques. By these means, exploiting computational methods
that are now well developed, one can hope to achieve a
rational and systematic understanding of highly complex
systems.

We have not discussed some of the most dramatic
and significant aspects of laser physics, including the
recent revolutionary developments in single- and multiple-
mode tunable dye lasers, as well as progress in ultraviolet
lasers, chemical lasers, and optically pumped lasers, for
example, CH F, CH I, and alcohol.

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6 GASEOUS ELECTRONICS

Gaseous electronics can be defined as the study of the properties of a gas-phase system that is placed into a nonequilibrium state by some external means, generally by passing an electric current through it. As such, it is an outstanding example of a practical field whose foundation rests on atomic and molecular science. Although not in itself representing an energy field per se, it possesses many aspects that are directly relevant to the energy problem. Two specific applications of gaseous electronics, gas-phase lasers and controlled thermonuclear fusion, are discussed in this report within the context of the chapters devoted to those subjects. Here we will consider other aspects of the field, particularly involving illumination, switching, and plasma chemistry, as these relate to energy research.

LIGHTING

It can be estimated from lighting industry sales figures, together with estimated service life, that there are approximately 1.5 billion incandescent lamps in service in the Unites States, consuming an estimated 1.2×10^{11} kWh/year, approximately 6 percent of the nation's electric energy consumption (1.5 percent of the nation's total energy consumption). These lamps, which are predominantly used in residential lighting service, have an average efficacy of 15 lumens of light produced per watt of power consumed (1m/W) and produce an illumination of 1.8×10^{15} lumen-hours per year.

Discharge lamps produce light at substantially higher efficacy than incandescent lamps, typically five

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or more times as high.[1] Thus, if the *same* level of illumi-
nation now produced by incandescent lamps were to be pro-
duced by discharge lamps, the required energy consumption
could be reduced to 2.4×10^{10} kWh per year, a saving of
9.6×10^{10} kWh per year, approximately 5 percent of the
annual electric energy consumption or 1.25 percent of the
nation's annual total energy consumption. The annual
dollar value of such electric energy savings, at the con-
sumer level, is $3.8 billion.

Unfortunately, there are no wholly satisfactory
discharge lamps for residential lighting service, which
typically requires small lamps, 1000–2000-lumen rating
(for portable lighting fixtures) producing about 15,000
lumens/liter of lamp volume, retailing at 0.00003 cents
per rated lumen-hour and capable of instant-on, short-
term intermittent duty. Fluorescent lamps average 2000–
5000 lumens/liter of lamp volume, retail at about 0.000025
cents per rated lumen-hour but require an expensive and
heavy auxiliary ballast and perform poorly in short-term
intermittent duty. High-intensity discharge lamp types,
such as metal halide or high-pressure sodium lamps, achieve
30,000–50,000 lumens/liter. They are, however, not avail-
able in the 2000-lumen rating needed for portable fixture
service, retail at 0.000007 cents per rated lumen-hour
but require expensive and heavy auxiliary ballasts. They
are totally unsuitable for intermittent service, requiring
a 5-minute warmup time after switch-on and a 15-minute
cool-down after switch-off before relighting.

Thus, there is a need for new types of discharge
lamps to fit the requirements of residential lighting,
and investigation of means of meeting this need is cur-
rently in progress in all major electric lamp companies.

It is safe to say that the body of scientific in-
formation classified as atomic and molecular science,
including appropriate aspects of physical electronics and
plasma physics, will play as large a role in any such in-
vestigations as it has in the development of existing
discharge lamps. Examples of past contributions of atomic
and molecular science to the development, understanding,
and improvement of discharge lamps may be found in Refer-
ences 1 and 2. Also indicated in these references are
notable gaps in the atomic and molecular physics data base,
for example, reliable data on atomic transition probabili-
ties of rare-earth type atoms, most molecular transition
probabilities, excitation and ionization cross sections
for molecules and free radicals, and Townsend α-coefficients
for many gas mixtures, to name a few.

TABLE 1 Types and Characteristics of Gas Discharge Lamps

Type	Application	Gas	Discharge Characteristics	Problem Areas
Fluorescent	Commerical interior Highway Home	Hg in Ar, Ne, or Kr	Low pressure High average electron energy Uv photons converted by phosphor Negative V-I characteristic High efficiency at high frequency	Electrical ballast required Low brightness (large size) Flicker at low-frequency operation Noise at high-frequency operation Cathode lifetime Long starting time Striations and constriction failure Phosphor maintenance Efficient phosphors for proper color Control of metal vapor pressure Double-ended construction
High intensity discharge	High bay industrial areas Public buildings Streets and highway Parking lots Projection systems	Usually high- pressure Hg, with or without additive such as Na, Tl, InI, SnI, DyI	High-pressure arc Near LTE conditions Molecular continuum emission important (SnCl)	Vapor pressure of additive compounds Decrease in output with time Slow start Phosphors often required for good color Ballast required Long testing time requirements
Flash lamps	Laser pumping Airport and airplanes Stroboscopes Photography	Xe, etc.	High operating pressure Continuum emission important Near LTE conditions in arc	Fast and reproducible starting Gas cleanup Spectral matching Lifetime of envelope and electrodes
Cold cathode glow	Flat panel displays Digital readout	Ne	Low pressure Cathode regions dominant Uv resonance radiation often used with phosphor	Gas cleanup and impurity buildup Low brightness Reproduceable electrical switching High voltage requirements Limited frequency response

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Of course, the basic data discussed do not by them-
selves supply direct insight into problems relating to the
discharge lamp. Rather, the discharge lamp can be consid-
ered to be an application of gaseous electronics. The
connection between the illumination problem and atomic and
molecular science is a classic illustration of the depen-
dence of applications on applied science, which in turn
rests on basic science. We will here briefly discuss this
relationship.

From the viewpoint of illumination engineering, the
goals of gaseous electronics are to develop high-efficiency,
long-life, and inexpensive electrically excited, gas-
discharge lamps. Other characteristics of varying impor-
tance are color rendition, time delay for starting, elec-
trical impedance, physical size, operating temperature,
noise level, and temporal variation of light. Some types
of gas-discharge lamps and their applications are given
in Table 1. For the present discussion it is convenient
to divide the lamp characteristics into groups, such as
the radiative properties of the electrical discharge of
plasma and the electrical properties of the discharge,
and then to indicate how atomic and molecular science con-
tributes to one's ability to understand, predict, and im-
prove these characteristics. This is done in Table 2.
We do not discuss the important step in which the under-
standing and predictive ability of the various physical
characteristics of the discharge are used to attain the
desired economic and psychological characteristics.

SWITCHING OF ELECTRICAL CURRENT AND ENERGY CONSERVATION

The switching of electrical currents has long been an im-
portant application of gaseous electronics and the associ-
ated atomic and molecular science. Much of the early
interest in the cross sections for electron collisions with
mercury atoms was the result of the use of mercury vapor
in rectifiers and thyratrons. Similarly, the studies of
electron attachment and temporary negative ion formation
in SF_6 were originally motivated by the usefulness of SF_6
as an arc recovery medium and as an insulating gas in
electrical switchgear and the like. Recent progress in
the understanding and design of higher power circuit break-
ers has made extensive use of newly developed techniques
for predicting radiative energy loss and electrical and

TABLE 2 Lamp Characteristics and Atomic and Molecular Contributions

Problem Area	Atomic and Molecular Contributions	Characteristics (Energy, range, etc.)
Radiative properties of discharge	Spectra, strengths, and broadening of elements, e.g., Na and rare earths Molecular band and continuum intensities Free-free transition probabilities Radiative recombination and attachment probabilities Radiation transport Molecular kinetics and thermodynamics	Wavelength: 170 to 700 nm Gas pressure: 1 Torr to 10 atm
Electrical properties of discharge	Electron and ion transport Electron excitation efficiency Electron ionization and attachment Negative ion formation and destruction Discharge stability Electron emission from surfaces Collisional ionization by atoms Elastic scattering of electrons and ions Electron-electron and electron-ion collisions Excitation and ionization of excited states	Electron energy: 0.1 to 20 eV Electron-ion density: 10^{10} to 10^{17} cm^{-3}
Thermophysical properties of discharge	Thermal conductivity, specific heat, and viscosity of gaseous elements, molecules, and mixtures Vapor pressure of elements and compounds Separation (demixing) of gas mixtures Radiative, thermal, and convective transport, emission, and absorption	Gas temperature: 300 to 20,000 K Gas pressure: 1 Torr to 10 atm
Temporal properties of plasma	Electron-ion recombination Diffusion and mobility of ions Radiation transport Thermal transport	Times: 10 nsec to 1 sec

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thermal conductivity of gases at high temperatures. The
success of vacuum circuit breakers has resulted in the
need for much improved understanding of the interactions
between surfaces and plasmas, for example, vapor presssures,
electron emission, and surface erosion.

Table 3 lists some of the more important electrical
switching devices involving gas discharges and atomic and
molecular research.

ELECTRICAL BREAKDOWN AND ENERGY CONSERVATION

The role of basic atomic and molecular collision processes
that govern electrical breakdown in gases has been under
intensive investigation for over 50 years. Unfortunately,
there is probably only one experimental situation in which
one can properly say that all the essential collision pro-
cesses and their interactions are quantitatively understood.
This one case is microwave breakdown in helium, that is,
the growth of ionization up to discharge densities at which
collisions of electrons with other electrons and with ex-
cited atoms become important. At the other extreme is the
breakdown between clouds leading to cloud-to-cloud light-
ning, where the first conference paper purporting to explain
the fact that lightning channels are crooked appeared within
the last year. These and other electrical breakdown situ-
ations are listed in Table 4 along with some associated
problems and related areas of atomic and molecular science
research.

An important recent development in the investigation
of long-gap breakdown is the formation of a highly active
and capable European research group, with participation
from France, Italy, Great Britain, and Germany. This group
has brought together engineers, physicists, and others and
is making significant contributions to the understanding
of long-gap electrical breakdown. In the United States,
activity in this area is extremely low and shows no sign
of growth.

PLASMA CHEMISTRY AND ENERGY STORAGE

We will discuss here the role played by atomic and molecular
science in the rapidly burgeoning field of plasma chemistry.

TABLE 3 Electrical Switching Device

Type of Switch	Problem Areas	Related Atomic and Molecular Research
(1) High-power, circuit inter-rupter. Used to interrupt up to 40 kA or 200 kV. High-pressure air, SF_6, or oil forced into region between opening contacts	Breakdown after contact opening Decomposition of gas or vapor Electrode erosion Timing of contact opening Feedthrough insulation Gas dynamics during arc	Radiative absorption and emission coefficient for lines, bands, and continuums Thermophysical properties of molecules Electron scattering by atoms and molecules Radiation transport models
(2) Moderate power switchgear. Used for motor controls, local distribution, etc. Compact designs using SF_6 or air to fill arc gap and quench conductivity	Same as (1)	Same as (1)
(3) Rectifiers and inverters. Used for converting ac to dc for refining (Al), high torque motors, etc. Usually Hg pool cathode. May be replaced by semiconductor devices. Inverters for dc to ac conversion.	Arc back or breakdown between anodes Contamination buildup on Hg Electrode cooling Control of vapor pressure Anode erosion	Cross sections for excitation and ionization of ground and excited states Electron-ion recombination Electron emission from surfaces
(4) Triggered switches. Used for switching high-voltage energy storage systems, i.e., condenser banks, transmission lines. Gas is air, H_2, Hg, rare gas, etc. Triggered by high-voltage pulse or laser	Gas cleanup in sealed-off tubes Breakdown during reverse voltage Reproducibility of triggering delay Power required for trigger	Sputtering and electron yields Range of ions in solids Laser photon absorption process
(5) Low current contacts. Moderate- and low-current switching for appliances, signaling, ignition, etc. Arcing on making and/or breaking	Electrode erosion Electrode sticking Insulating layer formation Electrical noise from discharge Mechanical vibration	Sputtering and melting of electrodes Ionization attachment and detachment during breakdown

(6) Vacuum circuit interrupters. Vapor produced by arc during electrode opening	Electrode erosion at high currents Outgassing of metal electrodes Deposition of evaporated metal Vacuum tight container Electrode separator	Electron emission from surfaces Evaporation rates Ionization and excitation of metal vapor atoms Charge-transfer reactions
(7) Magnetically controlled arcs. A low-pressure, cold-cathode discharge switched by magnetic field (developmental)	Voltage drop at electrode Power requirements for switching	Same as (6)
(8) Voltage regulators. Cold-cathode discharges with variable active cathode to keep voltage fixed. May be replaced by semiconductor	Electrode stability	Electron yields from ion bombardment of surfaces Ionization and excitation of metastables and ground states

TABLE 4 Electrical Breakdown

Breakdown Situation	Problem Areas	Contributing Atomic and Molecular Areas
(1) High-voltage corona, "long-gap" breakdown, etc.	Variability of breakdown path Design of conductor surfaces Effect of mositure and fumes NO_x production Radio-frequency interference	Discharge propagation process Negative ion production and destruction Effect of excited states of ionization, etc. Photoionization in moist air
(2) Vacuum breakdown	Effect of surface irregularities Effects of electrode temperature Effect of gas leakage Discharges along surfaces	Electric-field-induced emission of electrons, ions, and fragments Evaporation, thermal conductivity, and melting point of metals and alloys
(3) High-pressure breakdown	Effects of surface irregularities Effects of loose particles Insulating layers Discharges along surfaces Decomposition, vapor pressure, etc. of insulating gases	Electron attachment, ionization, etc. to halogenated gases, etc. Field emission of electrons Decomposition products and rates
(4) Lightning	Effectiveness of lightning protection Prediction of critical periods for strikes Control of flow of current Recovery of electrical transmission systems from current surges, etc. Usefulness as violent storms indicator	Same as (1) Charging of water drops, ice, etc.
(5) Radio-frequency breakdown	Initial ionization in repetitive breakdown Effect of high pressure or low frequency Breakdown in poorly defined geometry, i.e., antennas	Ionization, attachment, and recombination Ambipolar diffusion Metastable de-excitation and ionization
(6) Laser-induced breakdown	Prediction of threshold intensity vs time Wavelength dependence Focal spot size dependence Target shielding by discharge	Laser absorption by free electrons Multiphoton photoionization Electron loss processes Radiation loss processes
(7) Breakdown from frictional charging ("static electricity") (airplanes, supertankers, hospitals, home, etc.)	Dependence on surface properties Prevention of charging or reduction of discharge energy Prevention of ignition of explosions	Frictional charging mechanism, including role of workfunction, etc. Discharge ionization, propagation, etc. Attachment and detachment Energy transfer by electrons Photoionization and absorption

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Plasma chemistry can be characterized as one method of producing chemical reactions between excited atomic or molecular states, which are in turn produced by excitation in a gaseous discharge. The impact of this research area goes well beyond energy-related research, for in principle, a wide variety of economically significant chemicals can be produced by this means. From the energy viewpoint, this field is important because plasma chemistry offers a novel and interesting means of producing energy-rich chemicals as either fuel source or for other energy-relevant processes, such as agriculture.

At present, relatively few gaseous electronics processes are in current use, and these are for the production of relatively expensive products.[3] The most successful appears to be the Seimens process for the production of ozone, which makes use of a highly nonequilibrium corona-type discharge between ac excited electrodes coated with insulating material.[4] The high-pressure (~1 atm) arc has been used for the production of compounds such as C_2H_2 and HCN. We do not discuss the exciting new area of laser-induced chemistry, because most scientists do not believe that free electrons and ions play a significant role in such processes. Some of the chemical processes involving gaseous electronics in current use are listed in Table 5. A summary of research in this area is available in conference reports such as the *Advances in Chemistry* series.[5]

The use of nonequilibrium discharges is potentially a selective means of causing chemical reactions, because it is possible to arrange for a large fraction of the input energy to be deposited in either vibrational modes or in low-energy electronic states. The difficulties with chemical processes induced by nonequilibrium discharges are that (a) electron collisions in discharges usually produce reacting species by dissociation at a cost of roughly 1 kW-h/lb of reactant; (b) much of the electrical energy is used in vibrational excitation of the reactants and at reasonably high gas pressures, and all but the simplest molecules are quickly dissipated in heating the gas; (c) electrical discharges generally occur far from surfaces, making difficult the cooling of the products to stop reactions or the use of surface catalysts; and (d) the production of more complex species from readily available gases, for example, air, is made difficult by the relative instability of larger molecules against dissociation by electron impact.

The use of high-power electric arcs, usually in the form of dc plasma jets or radio-frequency induction plasmas, for chemical processing begins with the production of a

TABLE 5 Chemical Processes Involving Gaseous Electronics

Process	Discharge Characteristics	Problem Areas	Atomic and Molecular Contributions
Ozone production (major process)	Atmospheric pressure air High-frequency excitation "Corona"-type, intermittent	Poorly understood kinetics Low yield and efficiency Detrimental in home and office air cleaners	Ionization, attachment, and detachment data Photoionization data Rates of O_3 formation Collisional destruction of O_3
Oxide layer formation (commercial), and nitriding (experimental)	Low pressures Cold cathode	Poorly understood discharge Role of negative ions in O_2 Control of layer thickness Holes in layers Sputtering	Layer formation processes Electrode emission processes Ion and neutral formation
Production of HCN, C_2H_2 (one major installation), and NCN (experimental)	Atmospheric pressure Plasma (arc) jet Near LTE conditions except in critical "freezing"	Cooling (freezing) of plasma High capital investment Electrode lifetime	Kinetics of cooling Mechanisms of electrode emission Radiative properties of gases
Laser-induced chemistry using ions (experimental)	Very low gas density Very low currents Positive or negative ions	Back reactions Low photoionization cross sections Collection of products Efficient use of laser energy	Photoionization data for excited states Transition probabilities Excited state relaxation kinetics Charge-transfer cross sections
Electrically assisted combustion (experimental)	Atmospheric pressure High enough power to change flame temperature	Poorly understood discharge Poor understanding of flame processes Turbulence effects Changing gas composition Mixing of fuel and air near electrodes Contamination of electrodes	Electron and ion collision data on flame constituents Kinetics of processes in flames
Control of emission products in MHD systems (developmental)	Atmospheric pressure	Lack of high-temperature kinetic data Loss of energy by radiation	High-temperature reaction data Vibrational relaxation data Radiation loss data

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high-temperature (>4500 K) plasma in which the composition is usually close to statistical equilibrium and is followed by a rapid expansion, which cools the gas and "freezes" the gas composition to enhance a particular product. Thus, in the production of HCN from CH_4 the freezing is thought to occur at a temperature near 2000 K,[6] whereas the emission of N_xO_y compounds in the exhaust from MHD generators is reduced when "freezing" occurs slowly and at gas temperatures below 2000 K.[7] Thus, the electric arc uses very high temperatures to overcome the activation energy of chemical reactions and is a "brute-force" method as compared with the use of catalysts. On the other hand, there are no surfaces to "poison."

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APPENDIX A
INSTRUMENTATION

In this Appendix, we examine the role of instrumentation
arising from atomic and molecular science as applied to
the field of energy. The principal areas in which atomic
and molecular science bears most significantly on energy
research are conventional combustion, nuclear fission,
controlled fusion, and, to a lesser degree, solar energy.
Atomic and molecular instrumentation involves many aspects
of these areas, including exploration for resources, pro-
cessing of fuels, control of generating plants, utilization
(particularly of electrical power), and environmental ef-
fects.
 Many of our basic diagnostic tools, that is, instru-
ments, were developed in the first place from laboratory
studies of atomic and molecular science. Chief among these
is that class of devices called "spectrometers."

SPECTROMETERS

Spectrometers identify individual components and determine
their relative abundances, in a mixture of several species.
Different types of spectrometers accomplish these tasks
using different physical principles.

Electromagnetic (Photon) Spectrometers

The properties of electromagnetic spectrometers, particu-
larly in the infrared, visible, and near ultraviolet, do
not require elaborate discussion here. At least 10^{10} de-
cades of wavelength, from radio frequency up through the

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x-ray region, are relevant to energy studies, from rota-
tional spectra of heavy molecules to electronic transitions
in eximers.

Each region of the electromagnetic spectrum requires
its own characteristic group of spectrometers, depending
on details relating to detectors, sources, and method of
wavelength selection. Generally speaking, electromagnetic
spectrometers operate by spatially separating radiation
according to wavelength. In the near ultraviolet and near
infrared regions, this spatial separation can be accomplish-
ed by certain solid and liquid materials, usually in the
form of prisms, and by gratings, where constructive and
destructive interference of coherent radiation operates.
In the ultraviolet and x-ray regions, either man-made or
naturally occurring crystalline gratings are used. As one
approaches the microwave region, electromagnetic genera-
tors and receiver-amplifiers, tuned to a single frequency
(or wavelength), make unnecessary the step of spatial sep-
aration of radiation.

In *emission spectroscopy*, an atom or molecule is
excited by electron impact or other means, and the result-
ing radiation wavelengths and intensities are measured.
In *absorption spectroscopy*, radiation from a prepared source
is passed through a sample under test and then detected.
The difference in intensity with the sample in place and
removed is an indication of the abundance of the absorbing
material in the sample, and the wavelengths at which ab-
sorption occurs determine the chemical nature of the sample.
Fluorescence spectroscopy, or resonant scattering, is a
combination of the two. Absorption of a characteristic
spectral line excites the absorbing atom or molecule, which
then reradiates in a different direction from that of the
initial beam of radiation. In *Raman spectroscopy*, the
reradiated spectral lines are shifted to other than the
originally absorbed wavelength. Techniques in radio-fre-
quency spectroscopy include the various forms of magnetic
resonance, including nuclear magnetic resonance and elec-
tron spin resonance spectrometers. All of these have been
developed out of basic atomic and molecular science during
the past 30 years.*

A gigantic step in spectroscopy has been made over
the past decade through the advent of lasers, which are

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*The history of the development of these spectrometers,
particularly in their connection to atomic and molecular
physics, is described in the report *Atomic and Molecular
Physics* (National Academy of Sciences, Washington, D.C.,
1971).

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now available in the visible, infrared, and near-ultraviolet
spectral ranges. Lasers make enormously more satisfactory
light sources for absorption and fluorescence spectroscopy
because of their extremely high intensity, the intrinsic
coherence of their radiation output, and their extremely
narrow line widths, as compared with previously used light
sources. Operating as amplifiers, lasers also provide a
unique means of detecting very weak light signals produced
by emission.

In general, electromagnetic spectrometers operating
from the ultraviolet through the microwave ranges can de-
tect both atoms and molecules, the actual physical phenom-
ena involving only the outermost electrons. They function
optimally if the sample is in the gas phase, although many
liquid and solid samples are amenable to study. X-ray
spectrometry involves electrons that are deep within an
atom, that is, near the nucleus, so that the actual chem-
ical form in which an atom is held is of less consequence.
Solid samples are readily studied for their atomic abun-
dances using x-ray spectroscopy.

The principal limitation of photon spectrometers is
that by necessity they possess limited spectral ranges.
Some of the most important lines lie outside the operating
regions of commonly used instruments (particularly in the
far ultraviolet), and certain of the transitions of interest
are weak, and sensitivity of detection is less than satis-
factory. Finally, each atom or molecule emits and absorbs
many lines (or bands), and the spectrum of a complex mix-
ture of substances can be uninterpretable because of its
complexity. Nonetheless, photon spectrometers constitute
a major, perhaps, *the* major, class of instruments to have
emerged from atomic and molecular science.

Mass Spectrometers

Mass spectrometers have been used in atomic and molecular
science for over a half century. They were originally in-
vented for the purpose of determining the masses of individ-
ual atoms. Their greatest use, however, has been in the
area of chemical and isotopic analysis, and their greatest
virtue is their universality. If an atom or molecule can
be put into the vapor phase, then it is generally suscep-
tible to sensitive measurement by one of the several types
of mass spectrometers currently available. (Details of
operating characteristics of mass spectrometers are too
well known to warrant discussion here.) They all require

ionization and the action of dc and/or ac electric and/or magnetic fields to separate ions of different mass-to-charge ratios spatially or temporally.

Where a sample is not already ionized (a plasma of a CTR device is an example, where the plasma to be sampled is already ionized), it is necessary to convert the neutral atoms and molecules into ions, either by the addition or, more commonly, removal of one or more electrons. The usual method is by *electron-impact* ionization, wherein a beam of energetic electrons is fired into the sample, and a small fraction of the neutral atoms and molecules in the sample is converted into positively charged ions. That all atoms and molecules can be ionized by electron impact and that the cross section for ionization varies little between different atoms and molecules give mass spectrometry its universality as an analytical instrument.

Electron-impact ionization has the disadvantage that it produces many fragment ions as well as the parent ion from complex organic molecules, and the interpretation of mass spectra of mixtures of organic species can become exceedingly difficult. Two lines of activity have been pursued to overcome this problem. One is the use of a mass spectrometer in conjunction with a gas or liquid chromatograph. The gas or liquid chromatograph separates the components of a mixture into a series of peaks in time, and the mass spectrometer then makes positive chemical identification of each separated component and determines its relative abundance. The second is the use of an alternative ionization process. Such processes include photoionization, surface ionization, field ionization, field desorption ionization, and chemi-ionization. Other processes that can be used to obtain ions, particularly in cases where detection of small impurities with high selectivity and sensitivity is required, include associative ionization and, particularly, chemical ionization, wherein collisions between ions of one species and neutral molecules of a second species result in charge transfer, and ion-molecule reactions, which form ions of the second species. In favorable cases, levels of a few parts per trillion of biochemically important species present in another species are detectable.

Electron Spectrometers

This class of instruments uses the accurate knowledge of the energies of electrons liberated in interactions to determine the nature of the material from which the electrons

were emitted. Although the name *electron spectrometry for chemical analysis* (ESCA) is often applied to the entire field, increasingly this term is taken to mean the case for which excitation is produced by x rays

In a typical application, x rays are directed onto a solid sample and electrons are emitted. These electrons are then energy-analyzed, usually by electrostatic means. Discrete energies are found, and these can be associated with different types of atoms in the sample. Both outer- and inner-shell electrons are detected.

In *photoelectron spectroscopy* (PES) the incident radiation is ultraviolet light, so that only outer-shell electrons can be liberated.

The secondary electrons produced by an incident high-energy electron beam also show energy peaks characteristic of the atoms in the sample similar to those under x-ray irradiation. Since this analysis can be performed using an electron beam of the type used in electron microscopes, instruments that will give both a micrograph of a solid sample and simultaneous partial chemical analysis now exist.

With the discovery of resonances in electron-atom and electron-molecule collisions, a new method of observing molecular species *without* ionization has been developed. This method relies on the characteristic resonances in the scattering of slow electrons by molecules to identify them uniquely, while leaving them unaffected by the measurement process.

OTHER INSTRUMENTS

Beyond the "basic" instruments described above, there are a wide variety of instruments that operate in the gas phase and rely on atomic and molecular science principles. One such class uses gas discharges or electrical breakdown in gases as their physical basis for operation. Chief among such instruments, which are widely used in the energy field, are gas-phase detectors of nuclear radiation. These include Geiger-Müller counters, ionization chambers, and proportional counters. These instruments no longer monopolize the radiation field, as they once did, but they continue to be important.

For detection of specific vapors in the gas phase, certain specialized instruments of less complexity and cost

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than general-purpose spectrometers have been developed.
Such devices employing optical detection include chemi-
luminescence, laser fluorescence, and surface ionization.
In this latter instrument, a particulate is decomposed at
a hot surface and transfers its surface-ionizable constit-
uents and impurities to the surface. A burst of ions then
marks the arrival of the particle at the surface. The
electrical pulse height correlates with the particulate
size.

For the detection of small particulate matter pro-
duced in combustion, catalysis, and the like, optical
scattering is commonly employed, using either conventional
sources or lasers. These nephalometers are simple and re-
liable for detection of particulates whose dimensions are
not small compared to the wavelength of light. They de-
pend on the bulk properties of the particulate matter (e.g.,
index of refraction) and as such do not yield information
on the chemical nature of the particles. However, for
scattering by single particles, the strength of the signal
is a measure of the particulate size.

A type of particulate detector employing gaseous
electronics is a variant of the electrostatic precipitator.
A particulate is charged in a corona discharge, or other
charging means, with the amount of charge being related
to the particle size. An electrostatic field then draws
the charged particle out to a charge detector, the time
required depending on the charge on the particle and the
mobility of the particle through the air.

USES OF ATOMIC AND MOLECULAR INSTRUMENTATION IN ENERGY-RELATED ACTIVITIES

Energy Resources

EXPLORATION The use of Geiger-Müller counters in the search
for uranium is well known, with the gamma ray of either the
uranium itself and its nongaseous daughters or of the radon,
which diffuses up to the surface being detected.

FUEL ASSAY Almost all forms of optical and mass spectrom-
etry are used to assay both nuclear and fossil fuels and
to determine constituents and impurities (e.g., sulfur in
fossil fuels). Uses include assay of original ores, mine
tailings, outputs of processing plants (refineries, gasifi-
cation, and liquifaction plants), and used nuclear fuel
elements.

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Energy Production

COMBUSTION   Both optical and mass spectrometry are used in basic research on combustion, flame inhibition, and explosion limit determination and to monitor practical devices for completion of combustion, production of undesired gaseous pollutants, and efficiency of catalytic conversion.

MAGNETOHYDRODYNAMIC POWER PRODUCTION   Optical and mass spectrometry are used to determine the nature of the ions and production and loss of ions in MHD generators. Mobilities, processes for formation, and destruction of ions are types of basic atomic and molecular research related to MHD power production.

CONTROLLED FUSION RESEARCH   Optical and mass spectrometry constitute the principal diagnostic means in CTR work of all kinds. Optical spectrometry is used to determine temperatures or plasmas and levels of deleterious impurities. It is to be noted, however, that the absence of some fundamental cross-section information, and even of spectral lines of some of the more highly charged ions, limits the quantitativeness of such diagnostics.

FISSION REACTORS   A variety of instruments are used to monitor the operation of nuclear reactors. Mass spectrometry, particularly with chemical ionization, provides an extremely sensitive method for detection of fission product leakage into cooling lines and the air. Surface ionization monitors for detection of sodium coolant leakage will likely be incorporated into all liquid-sodium-cooled reactors.

Energy Utilization

Widespread use of atomic and molecular instrumentation is made in energy utilization efficiency; this could become the area in which atomic and molecular instrumentation makes its strongest contribution. Starting from efficiency of combustion, discussed above, we can enumerate other areas: (1) assay of ores and mine tailings for materials whose processing will require energy; (2) process control in refineries, chemical plants, synthetic fiber production, electronics components manufacturing, steelmaking (basic oxygen process), and other basic metal production; (3) improvement of efficiency of lamps and other light sources.

Environmental Effects

Atomic and molecular instrumentation is currently used ex-
tensively in evaluating the impact on the environment of
energy production and use. Gaseous, liquid, and solid pol-
lutants are subjected to both electromagnetic and mass
spectrometry for chemical analysis, and aerosols are moni-
tored using the particulate detectors described earlier.
Particularly of interest at present are the monitoring of
pollutants from fossil-fueled power stations; industrial
processing plants; automobile, aircraft, and rocket exhausts;
and nuclear reactors. Of particular importance in the near
future will be the determination of pollutants from pro-
cesses for gasification and liquifaction of coal.

APPENDIX B
SCIENTIFIC DATA:
EVALUATION AND DISSEMINATION

We address here the tactical problems of making an effec-
tive connection between scientific research effort and
technological application in energy-related atomic and mo-
lecular science. Although the general issues are not pe-
culiar to this field, its multiple connections to many
different areas of energy technology can introduce compli-
cations into the process of developing appropriate and
effective communications channels between the scientific
efforts and the technological problems to which they are
potentially applicable.

We first summarize the various types of information
resources available to the researcher, and then briefly
discuss the role played by Data Centers in evaluating and
disseminating information.

Ordinarily, data tabulation and evaluation have
received scant attention and support as compared with orig-
inal scientific research. Among scientists, the greatest
honor and personal gratification comes from making new
discoveries and producing fundamentally new results. Among
many funding agencies whose function is to support long-
range and basic research, the same value system applies.
Agencies whose mission is highly applied typically view
their mission as limited, at most, to the production of
the specific items of information for which they can see
an immediate and pressing need. Seldom do their needs
obviously extend to the tabulation, evaluation, and publi-
cation of a broad pattern of data.

There have been, of course, important exceptions
to this generalization. The need for extensive tabulations
of nuclear data, for both reactors and weapons, has led to
a major investment in nuclear data tabulations, supported
formerly by the Atomic Energy Commission and now by the
Energy Research and Development Administration. This

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development was no doubt facilitated by the fact that a single agency had the entire responsibility for both the science and technology in the whole nuclear area. Consequently, it could take a long-range view encompassing the whole broad picture. Where the missions have been divided among agencies, there has been much less effective action.

Other important data compilations are those on chemical reactions of atmospheric species, notably the compilations supported by the Department of Transporation's Climatic Impact Assessment Program, motivated by the SST problem. Tabulations of thermodynamic data have long been broadly used in chemical computations, and their general importance has led to a continuing program for evaluation and publication of important data in this area by the National Bureau of Standards. Also, the importance of such information for rocket propellant and thrust calculations led to the compilation known as the JANAF (Joint Army, Navy, Air Force) tables. The American Petroleum Institute has been a major source of support for tabulations needed in that industry. The coming importance of coal chemistry turns the spotlight on a great current deficit in tabulated data applicable to that whole domain of chemistry and technology.

At present, it seems that the level of effort nationally devoted to data evaluation and publication is not more than a few tenths of a percent of the total dollars spent for basic research. In atomic and molecular science, this effort is much smaller than it is in either chemistry or nuclear science. The largest compilations in this science have probably been those devoted to atomic spectra and energy levels, together with similar information for diatomic and other small molecules. Tabulations of radiative transition probabilities are also available. For collision processes in atomic and molecular science, systematic data compilation exists only in certain selected areas (this is discussed in more detail below under Data Centers). Part of the reason lies in the diverse nature of the market for this information, which makes it difficult to find one agency that has sufficiently compelling motivation to provide the support needed.

Apart from the data compilations discussed above, the following are briefly summarized normal methods of obtaining needed data, physical constants, and the like.

Formulas, Rules, and Generalizations: Either handbooks applicable to a broad field of science or engineering or handbooks of information especially applicable to a particular technological problem area, for example, a DNA reaction-rate handbook.

TABLE 6   Summary of Data Centers in Atomic and Molecular Science

Data Center for Atomic Transition Probabilities and Atomic Line Shapes and Shifts

W. L. Wiese
NBS, Washington, D.C.
Scope: Radiative transition probabilities of atoms and atomic ions in
       the gas phase

Atomic Energy Level Data Center

W. C. Martin
NBS, Washington, D.C.
Scope: Atomic energy levels and spectra

Data Center for Atomic and Molecular Ionization Process

H. M. Rosenstock
NBS, Washington, D.C.
Scope: Attenuation coefficients for high—energy photons

X-Ray and Ionizing Radiation Data Center

J. H. Hubbell
NBS, Washington, D.C.
Scope: Attenuation coefficients for high—energy photons

Controlled Fusion Atomic Data Center

C. F. Barnett
ORNL, Oak Ridge, Tenn.
Scope: Heavy ion collision, electron and photon collisions, particle
       interaction with surfaces, particle transport, particle inter-
       action with macroscopic matter

Gaphor Data Center

J. L. Delcroix
Orsay, France
Scope: Atomic and molecular properties, interaction between particles,
       and macroscopic properties basic to gas and plasma dynamics

Atomic Data Center

K. Takayanagi
Tokyo, Japan
Scope: Atomic collisions

Atomic Data Study Group

H. Suzuki
Nagoya, Japan
Scope: Atomic collisions, atomic and molecular spectroscopic data

Atomic Collision Cross Section Information Center

E. C. Beaty
JILA, Boulder, Colorado
Scope: Low-energy atomic collisions, cross-section data, particularly
    electron and photon interaction with atoms and simple molecules

Chemical Kinetics Information Center

D. Garvin
NBS, Washington, D.C.
Scope: Rates of homogeneous chemical reactions in gaseous, liquids,
    and solid phases; photochemistry; inelastic scattering

Diatomic Molecular Spectra and Energy

P. H. Krupnie
NBS, Washington, D.C.
Scope: Optical spectroscopic data and constants for diatomic molecules;
    molecular parameters derived from spectroscopic measurements

Treatises, Systematic Reviews, and Textbooks: Usual-
ly appearing as scientific monographs, "Advances" series,
and review journals.

Computer Techniques for Data Production: Program
exchanges; program libraries; networks and other communi-
cation devices to access computer resources; computer
centers for specialized purposes, for example, the proposed
National Resource for Computation in Chemistry.

Computer Codes and Modeling of Complex Phenomena:
This developing technique is becoming increasingly impor-
tant; it shortcuts expensive and lengthy experimental
prototype development and requires reliable input data.
It also requires "bench-mark" experiments to check the
models--a model will not tell you if some process has been
left out, nature will.

Data Centers: In the President's Science Advisory
Committee report, *The Responsibilities of the Technical
Community and Government in the Transfer of Information,*
1963, the need was emphasized for specialized centers to
process information or data appearing in the archival
journals.

During the past 12 years, specialized information
institutes have been founded in the physical, natural,
and social sciences. The latest *Directory of Federally
Supported Information Analysis Centers* describes the ac-
tivities and scope of 108 data centers. These data centers
have as their primary function the following: (a) the
analysis, evaluation, and condensing or compiling of in-
formation for the expressed purpose of helping the user
to better assimilate it; (b) the presentation of data in
the form of compilations, critical reviews, or state-of-
the-art reports; (c) the provision of evaluated responses
for information for the entire technical community in a
given discipline.

At present, there are 11 atomic or molecular data
centers located worldwide that serve the physics and chem-
istry community, with possible application to energy re-
search. Table 6 lists the centers, their locations, direc-
tors, and scope. In addition to these centers there are
others supported by private industry whose holdings and
services are not available to the technical community. For
example, many chemical companies have exhaustive files of
infrared spectroscopic molecular data.

Of utmost importance to the operation or establish-
ment of a data center is the justification of the expendi-
ture involved in the operation from the viewpoint of the
sponsor(s). This is a most difficult question to address

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in a general sense; each case must be treated in the con-
text of specific goals and needs. Quantitative evaluations
of data centers themselves is a difficult undertaking and
has not been exhaustively studied.

Probably the best justification for the establish-
ment of data centers is the success of existing data centers.
Three such centers could be singled out in connection with
this report for mention here: the Atomic Energy Level Data
Center at the National Bureau of Standards; the Controlled
Fusion Atomic Data Center at Oak Ridge National Laboratory,
established in 1961 to provide evaluated data to the fusion
community; the Data Center at the Joint Institute for Lab-
oratory Astrophysics, Boulder, Colorado, which for the past
ten years has accumulated and evaluated data and has spon-
sored critical reviews, particularly in the area of elec-
tron and photon interactions with atoms and simple molecules.

One of the more complicated aspects of the applica-
tion of atomic physics or chemistry to research in the
field of energy is the diversity and the magnitude of the
various programs. A partial listing of the energy research
programs in which atomic or molecular data are needed would
include all the areas discussed in this report. Established
data centers are in a position to supply most of the atomic
needs of these various programs. The chief need for an
additional data center is probably for molecular data; a
"Data Center Steering Committee" could provide a valuable
focus for establishing national data accumulation and eval-
uation policies in atomic and molecular science and for
serving as a clearinghouse for channeling data requests by
users.

APPENDIX C
SELECTED GLOSSARY
OF TERMS EMPLOYED IN THE TEXT

Angstrom unit ($\overset{o}{A}$): A convenient unit of length in atomic
physics, equal to 10^{-8} cm. Visible light possesses
wavelengths in the range 4500–7500 Å; atomic dimen-
sions are normally of the order of several angstroms.
The radius of the ground-state orbit of atomic hydro-
gen is about 1/2 Å.

Bremsstrahlung: The radiation emitted by a charged particle
when it undergoes rapid acceleration of some kind.
This is a particularly effective means of producing
electron energy loss in high-temperature magnetically
confined plasmas.

Charge exchange: The process whereby an atomic or molecular
ion in collision with a second neutral or charged
atom or molecule interchanges charge states, e.g.,
$X + Y^+ \rightarrow X^+ + Y$.

Cross section: The "effective area" presented by an atomic
or molecular target to a colliding particle. This
area will generally depend on energy and the nature
of the interaction. Atomic cross sections can vary
over an enormous range but usually possess values
between 10^{-14} and 10^{-18} cm^2. In describing specific
reactions, one refers to elastic cross sections, in-
elastic cross sections, ionization cross sections,
etc.

Diffusion coefficient: A measure of the ability of a par-
ticular species to transport itself through a bulk
medium, such as a dense gas or liquid.

Dimer, trimer, etc.: The two-, three-, etc. atom system
formed from atomic species that normally occur as
single atoms, e.g., Na_2, Na_3, etc.

Doppler broadening: The widening of spectral lines result-
ing from the motions of the radiating atoms or
molecules.

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Elastic cross section: An atomic or molecular collisional process in which two particles scatter without change in their internal energy states.

Electron affinity: The energy required to remove the excess electron from a negative ion. Electron affinities are generally considerably less than ionization energies, usually being in the range of 0.1-1 electron volt.

Electron volt (eV): A convenient unit of energy for atomic reactions, equal to 1.6×10^{-19} joule (J).

Excitation: The placing of an atom or molecule into an energy state that possesses a higher energy than the ground state. Usually the atom or molecule will then spontaneously undergo a transition to the ground state, either by emitting electromagnetic radiation or by transfer of its excess energy to another particle.

Fluorescence: The radiation in a gas or other transparent medium resulting from prior excitation of atoms or molecules by electrons, photons, or other means.

Ionization: The process of removal of one or more electrons from an atom or molecule. The remaining atomic system is referred to as a "positive ion."

Isoelectronic sequence: A series of atomic ions all possessing similar valence electron configurations, obtained by moving across the periodic table and removing a single electron in each step, e.g., H, He^+, Li^{++}, B^{+++}.

Metastable state: The state of an excited atom or molecule in which the normal process of radiative decay to a lower energy state cannot occur. An atom or molecule in such a state therefore acts as an effective carrier of excess energy.

Negative ion: An atom or molecule that possesses an excess number of electrons.

Photodetachment: The removal of an electron from a negative ion resulting from the interaction of the ion with a photon, e.g., $X^- + h\nu \rightarrow X + e$, where $h\nu$ represents the photon.

Photoionization: The removal of an electron from a neutral atom or molecule, or a positive ion, resulting from the interaction of the particle with a photon, e.g., $X + h\nu \rightarrow X^+ + e$, where $h\nu$ represents the photon.

Polarizability: The atomic or molecular property that is characterized by its ability to be distorted by an externally imposed electric field.

Recombination: The process whereby two charged particles
unite to form a single atom or molecule, e.g.,
$X^+ + Y^- \rightarrow XY$.

Resonance: In atomic physics, usually refers to a narrow
energy region in which two colliding particles form
a temporary combined "compound state," before flying
apart again. Resonances often result in the appear-
ance of anomalous narrow structure in the magnitude
of the cross section.

Rotational excitation: A molecular excitation process
wherein the rotational energy, referred to some
internuclear axis of the molecule, is changed in a
collision.

Singlet state: The state of an atom or molecule in which
the intrinsic angular momenta, i.e., the spins, of
the electrons cancel each other out in pairs, so
that the net spin of the system is zero.

Transition probability: The relative chance that an ex-
cited atom or molecule will spontaneously undergo
a radiative transition to a lower state. Inversely
related to "radiative lifetime," since the greater
the transition probabilities the shorter the life-
time.

Triplet state: The state of an atom or molecule in which
the intrinsic angular momenta, i.e., the "spins"
of two of their electrons are oriented along the
same direction.

Vibrational excitation: A molecular excitation process
wherein the vibrational energy of the molecule
about an equilibrium internuclear position is
changed in a collision.