

THE IAEA PROGRAM ON ATOMIC AND MOLECULAR DATA
FOR RADIOTHERAPY AND RELATED RESEARCHRECEIVED
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INTRODUCTION

Radiation measurements and dosimetry usually require reliable values of physical quantities that describe the interactions of radiation with matter. Examples of such quantities are the stopping power and the ionization yield (usually expressed in terms of the W value), as discussed by Grosswendt (1) in the present Symposium. Studies of the microscopic mechanism of radiation action or of advanced radiotherapy (using heavy ions, for instance) require even more detailed information, as described below.

In any material subjected to ionizing radiation, many energetic particles are present. These may be primary particles, charged or uncharged, or secondary particles, such as electrons ejected in ionizing processes. These particles deliver energy to molecules in the material in various collision processes, and energetic electrons are always the most numerous. Any serious analysis of the energy delivery processes requires knowledge about the collision processes, most importantly the cross sections for all major processes specified by energy transfer values.

Such an analysis may be carried out in many ways, depending on the specific purpose (2). Two major classes of approaches are readily recognized: the particle transport theory (3) and Monte Carlo simulations (4), as discussed by Bichsel (5) in the present Symposium. In either approach, it is important to use as input the cross section data that best represent elementary microscopic processes. An analysis based on unrealistic input data must be viewed with caution at best, because results might be misleading.

Cross section data found in the literature are often relative rather than absolute, discordant rather than unique, and fragmentary rather than comprehensive (i.e., covering the wide range of variables needed in radiation research and other applications). Therefore, it is highly desirable to compile cross section data in order to evaluate them for reliability and to recommend currently best sets of data to users.

Efforts toward this goal are being made by many workers in various ways. The purpose of this lecture is to survey major international efforts and activities.

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THE IAEA PROGRAM

Recognizing the need described above, the International Atomic Energy Agency (IAEA) more than a decade ago launched a proposal for an international collaboration. This effort was completed last year, and the final report (6) was recently published.

The final report consists of nine chapters, beginning with an introduction to charged-particle therapy. The following five chapters treat cross section data for ionization and excitation of atoms and molecules by charged particles (electrons and ions) and by photons. The final three chapters concern topics related to multiple collisions (i.e., stopping power, ranges, the yield of ions and excited states, and track structures). The participants in this international collaboration over the past decades are the following:

M. J. Berger, Bethesda, Maryland
 Hans Bichsel, Seattle, Washington
 D. T. Goodhead, Medical Research Council, Radiobiology Unit,
 Chilton
 Yoshihiko Hatano, Tokyo Institute of Technology
 Makoto Hayashi, Gaseous Electronics Institute, Nagoya
 Zdenek Herman, J. Heyrovsky Institute of Physical Chemistry and
 Electrochemistry
 Mitio Inokuti, Argonne National Laboratory (Chairman of the Program)
 I. G. Kaplan, Universidad Nacional Autonoma de Mexico
 N. P. Kocherov, International Atomic Energy Agency (Scientific
 Secretary of the Program)
 Ines Krajcar-Bronić, Ruder Bošković Institute, Zagreb
 Franz Linder, Universität Kaiserslautern
 Tilmann Märk, Universität Innsbruck
 Koichi Okamoto, Tokyo (former Scientific Secretary of the Program)
 H. G. Paretzke, GSF-Forschungszentrum für Strahlenschutz und
 Umweltforschung
 Helmut Paul, Johannes-Kepler Universität, Linz
 Pascal Pihet, Institut de Protection et Sûreté Nucleaires, Fontenay-aux-
 Roses
 Leon Sanche, Université de Sherbrook
 Dušan Srdoč, Brookhaven National Laboratory
 Michel Terrissol, Université Paul Sabatier, Toulouse
 L. H. Toburen, National Academy of Sciences
 Eberhard Waibel, Physikalisch-Technische Bundesanstalt,
 Braunschweig
 André Wambersie, Univiversité Catholique de Louvain, Brussels

A copy of the report is available upon written request to the IAEA, Vienna.

The IAEA now plans to launch a new program for preparing a computer-readable database of cross sections for use in track structure calculations (7). Current plans are for the database to concern five materials that are considered fundamental: H₂O vapor, H₂O liquid, carbon (in amorphous or microcrystalline phase), DNA (in a prototypical chemical

structure, without precise specification of the base sequence or conformation), and protein (in a prototypical chemical structure).

ACTIVITIES OF THE ICRU RELATED TO ATOMIC AND MOLECULAR DATA

The International Commission on Radiation Units and Measurements (ICRU), established in 1925, develops internationally acceptable recommendations concerning the quantities and units of radiation and radioactivity, the standard procedures for measurement of these quantities, and the standard physical data pertinent to radiation measurements and dosimetry. The ICRU has published over 50 reports presenting its recommendations and their scientific grounds. Among them, Report 31 on the total ionization yield (8), Report 37 on stopping powers for electrons and positrons (9), and Report 49 on stopping powers for protons and alpha particles (10) are most notable in the context of the present discussion. Work on stopping powers for heavier ions is in progress under the chairmanship of P. Sigmund.

A report on *Secondary Electron Spectra Resulting from Charged Particles*, prepared under the chairmanship of M. E. Rudd, will be issued by the ICRU next year.

A MONOGRAPH ON CROSS SECTION DATA

I edited a monograph entitled *Cross Section Data*, published as Volume 33 of *Advances in Atomic, Molecular, and Optical Physics* (11). This volume contains 11 articles on various efforts devoted to the determination of cross sections for electronic and atomic collisions, on needs for cross section data in selected applications, and on efforts toward the compilation and dissemination of these data.

The volume is intended to guide researchers in using cross section data with the best judgment and discretion and in producing better data through experiment or theory. Although the volume presents no large volume of data, it should convey a sense of the charm and challenge of what I call *data physics*, a field of research that fails to receive the appreciation that its importance to applications warrants.

CONCLUDING REMARKS

Although the results of the efforts described should be useful for many purposes, much remains to be done toward the establishment of a fully dependable set of atomic and molecular data as a basis of mechanistic studies in radiation chemistry and biology. In this report I point out three major issues.

First, cross sections for charged-particle collisions with molecules in the gas phase must be studied further, as must photoabsorption cross sections of molecules. Specifically, cross sections for polyatomic molecules, especially those for dissociation into neutral fragments, have been poorly characterized.

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Second, the dependence of cross sections on temperature (i.e., the rotational and vibrational excitation in the initial state of molecules) has just begun to be appreciated.

Third, cross sections of molecules in condensed matter differ appreciably from those of isolated molecules in certain respects (12), for instance, for collisions of electrons at low kinetic energies (i.e., tens of eV and below). Knowledge about this topic has been developed considerably, most notably through studies by Sanche (13); nevertheless, the current understanding remains limited in both scope and depth.

ACKNOWLEDGMENTS

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