DATA IN THE APPLICATION OF NUCLEAR TECHNIQUES

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ABSTRACT

Beginning from the proposition that availability of reliable data is necessary to the application of nuclear techniques, we explore the questions of how such data are obtained and how the extent of their reliability is ascertained. These questions are considered first in general terms in relation to data types and organizational frameworks, then with particular reference to the journal *Atomic Data and Nuclear Data Tables*. The reliability issue is further discussed in terms of this journal's policies and unique presentation style.

Key words: Nuclear technique Atomic data Nuclear data

That the availability of reliable data is necessary to the application of nuclear techniques is readily illustrated in a few examples: to do ion implantation, we need data on stopping powers; to do neutron activation analysis, we need neutron capture cross sections; to do PIXE (particle-induced X-ray emission) analysis, we have to know ionization cross sections; and to perform Mossbauer studies, we require the values of the nuclear moments. this small list of examples of the data we need is of course not meant to be complete, but only to illustrate that in every case, we need the availability of a body of reliable data in order to develop and apply the various techniques.

The questions may be asked: how do we get these reliable data? and how reliable are they? we will examine these questions in two ways: first, in general; then, with particular reference to the data journal, the *Atomic Data and Nuclear Data Tables*.

To explore these questions, the different types of data may be considered: experimental, calculated, and semiempirical. In particular, we would consider these categories in relationship to their use in applications.

In the experimental data category, what is desired are data in organized collections. What should be collected and how they should be organized may depend on their intended uses. In general, the organizing frameworks for data collections are referred to as "vertical" and "horizontal". By vertical, it is meant that many data are collect about a particular physical species, as for example the compilations published in the *Nuclear Data Sheets*, where all the nuclear data are assembled according to the mass number *A*. Horizontal compilations, however, are often more useful in application areas. These are compilations of a specific physical quantity for a whole

class of elements or materials.An example is a compilation of all the measured nuclear moments, a new updated table of which will be published this summer in the *Atomic Data and Nuclear Data Tables.* This table, by P. Raghaven, is a comprehensive compilation of dipole and quadrupole moments up to 1988.

Calculated data may be used in applications for a variety of reasons. First, experimental data may not be available. Then, even if experimental values are available, the particular calculation may be capable of giving such accurate results that it is unnecessary to use the individual experimental data; it is of course convenient to be able to use an analytical expression if that expression is accurate enough for the purpose. In the semiempirical approach, by having an analytical expression whose adjustable parameters are able to take experimental results into account, it is often possible to achieve both convenience and good accuracy.

A paper where all three types of data are represented is: "X－ray attenuation cross sections for energies 100 eV to 100 keV and elements $Z=1$ to $Z=92$," by E. B. Saloman, J. H. Hubbell and J. H. Scofield [*Atomic Data and Nuclear Data Tables,* 38 (1988), 1]. The experimental data– base therein is that of the US National Bureau of Standards, the theoretical calculation uses a relativistic Hartree－Slater model by Scofield, and the semiempirical values are those from an earlier work by B.L.Henke and co－workers published in 1982 in this same journal [*ADNDT.,* **27** (1982), 1]. In this paper, one can, for example, observe the following in the cross section data for gold in the various energy ranges: In the 10 to 100 keV range, theory and experimental coincide essentially completely; in this range, therefore, there would seem to be no reason not to use the theoretical results in any application. In the 1 to 10 keV range, one begins to see some departure of the Scofield theory from the experimental data points. The semiempirical values, represented by the dotted line in the graphs, are giving a somewhat better fit. In the lowest energy range, 100 to 1000eV, the purely theoretical curve is now missing the experimental points rather systematically. In this case, if attenuation cross sections are needed in an application, the semiempirical values would probably be the most useful choice.

After the above general responses to the questions: how do we get reliable data? and how reliable are they? we now address these same questions with particular reference to the journal of the *Atomic Data and Nuclear Data Tables.*

The data in this journal are contributed from the international community of atomic and nuclear scientists. The data compilation or generation efforts are those of these individuals: unlike the *Nuclear Data Sheets,* this journal is not a sponsored project of any particular agency.

In terms of the question: "how reliable are the data published here?" the philosophical position of the journal is: as reliable as possible taking into account the status of the field and the intended use of the data. "As reliable as possible" of course

describes not an absolute outcome but a goal. To promote the achievement of that goal, two kinds of processes are relied upon: critical review of the scientific content, and rigorous implementation of requirements regarding presentation style. As a refereed journal, the articles are critically reviewed by experts in order to ascertain that the quality of the material meets the standards of the field in question. But, as a user-oriented data journal, the reliability issue is dealt with in a second, distinctive way, namely, by requiring a presentation style that is designed to communicate reliably. In the journal's "Information for Authors", the section describing what is expected to be given in the introductory material asks authors to organize their material as follows: Abstract, Table of contents, Explanation of tables, and Examples of use of the tables (if they are deemed helpful in clarifing how the data are to be used). The Introduction should include: for example, the precise scope, the compilation policies, treatment of errors, and so on. The Explanation of tables is a unique feature of this journal which, as much as possible, makes the tabulations userfriendly. The overall intent is to encourage authors to make what they have done very clear and very easily understood.

How these requirements are applied is best seen in some concrete examples. In a paper, "Energy dependence of the ion-induced sputtering yields of monatomic solids" by a group in the Institute of Plasma Physics in Nagoya [*ADNDT*, **31** (1984), 1], there are separate sections showing a sample calculation, an Explanation of tables and an Explanation of graphs, and then the data tables and graphs; the bulk of the data are shown as graphs. One of the Tables shows, at a glance by means of a matrix, what are the combinations of targets and ions for which data are displayed in the graphs. In making this compilation, the authors had also decided to exclude certain data which in their judgment do not meet the criteria they have imposed. Besides explaining these criteria in their introduction, they give in a separate Table a list of these excluded combinations, together with their reference. In this way, if a reader wishes to apply other criteria or to question the authors' judgment, the reader is provided with the information to pursue the matter. For the reader who would use the data provided, a sample calculation further makes explicit the correct application of the tabulated values.

While a sample calculation may not be suitable with every kind of data material, a section called Explanation of tables is required of every paper in this journal to ensure easy and correct usage of the tabulated data. Authors are informed that "the Explanation of tables should be arranged in a tabular style," with each symbol or term which appears in the data tables listed in the left-hand column. The explanation in the oposite right-hand column then defines that symbol or term, giving as well, where appropriate, the relevant equation number or units. An illustration may be seen in the paper: "Bremsstrahlung energy spectra from electrons with kinetic energy 1

keV to 10GeV. Incident on screened nuclei and orbital electrons of neutral atoms with $Z=1-100$," by S. M. Seltzer and M. J. Berger [*ADNDT.* **35** (1986), 345]. Here, the tables are computer printouts with column headings like T, K, PHIRAD, and so forth. These headings are explained, respectively, as follows: the incident electron kinetic energy, T, in MeV; photon energy in MeV, and the scaled total integrated radiative energy – loss cross section, ϕ_{rad}[Eq. (5)].

In addressing the reliability issue not only in the sense of the data being reliable in themselves but also in the sense of their being reliably communicated to the user, effort is made to ensure that the user has as clear and full a picture as possible. If, in some situations, the data available has limited or undetermined reliability, it is considered proper for authors to make that clear. Such an instance is illustrated in a paper by D.D.Cohen and M.Harrigan on "Calculated L–shell X–ray line intensities for proton and helium ion impact"[*ADNDT.*, **34** (1986). 393]. Here, the authors are providing data that are quite useful in some application areas. However, in discussing the Accuracy of the tables, they point out the many uncertainties on the question of reliability, making careful distinctions between the precision of their calculation and the actual accuracy of the values which is much more difficult to determine. These authors give the reader their best estimates; it is up to the reader to decide whether these are sufficiently reliable for the purposes for which he intends to use the data.

In summary, this discussion has attempted to answer the questions: how do we get those reliable data which are necessary to the application of nuclear techniques? and how reliable are they? These questions have been considered in a general sense, but also with particular reference to the *Atomic Data and Nuclear Data Tables*. This journal has provided atomic and nuclear data for basic and applied research for the past 20 years. The contributors to this journal have been researchers in many fields, who appreciate the importance of data, and who understand that data are an indispensable enabling factor in the advancement of both basic science and applied technology. Every effort is made to ensure that the data published are "as reliable as possible," and also that these data are presented in a full and reliable way.