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Guide for the presentation in the primary literature of numerical data derived from experiments

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ABSTRACT

This Guide contains general recommendations on the reporting of numerical data for the guidance of authors, editors and referees. It is not a style manual. The recommendations are intended to facilitate the use, evaluation and comparison of data. They cover description of experiments, the treatment of data derived from them and presentation of the final, numerical results. The emphasis is on data that may be verified by repetition, e.g., data on physical and chemical properties and processes.

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I. INTRODUCTION

This report is concerned with the presentation of numerical data that are capable of verification by repetition such as those on the physical and chemical properties and behaviour of material systems. The "properties" or "behaviour" may be microscopic (nuclear, atomic, or molecular) or macroscopic (e.g. density, crystal structure, transport properties, or energy transfer) or quantities associated with chemical transformations (equilibria, enthalpies of reaction, or rate constants). The "material systems" must be sufficiently well-defined to permit the measurements to be reproduced. Usually this means that the systems themselves must be of known purity and have a well-defined composition and state.

Recommendations are made concerning the information that should be reported so that the data may be compared and correlated with those obtained from other studies. These are general recommendations that apply to all branches of the physical sciences. Some existing specialized guides that expand upon these recommendations are listed in the bibliography; others are under preparation.

This is not a style manual for writing scientific papers. It is a statement of the minimum information that is needed to ensure that the reader can understand the quantitative data, can assess their precision and accuracy, and can recalculate the results when values for auxiliary data change.

The author of a paper has the primary responsibility for providing the reader with the type of information outlined in this Guide.

The Guide also provides journal editors and referees with a set of consistent, considered criteria for judging the completeness and acceptability of papers in so far as the reporting of numerical quantities are concerned. The recommendations reflect the experience of data evaluators; hence, adherence to them will permit evaluators to consolidate the author's results with existing data and facilitate their incorporation in critical compilations.

The word "data" has been used loosely above. Terms used in the later sections of the Guide are defined here. *Measurements* are made on material systems using suitable instruments and procedures. The instrument readings are the initial numerical *data*. The *results,* usually stated in terms of physical and chemical properties, may be the initial data. More frequently, however, they are derived from these data by a process called *reduction of the data.* Associated with the results are two numbers: the *imprecision* which records the reproducibility and the *inaccuracy* which estimates the overall reliability of the measurements.

Recommendations relating to these matters are considered below under three headings: description of experimental procedures, reduction of data, and presentation of results.

II. THE DESCRIPTION OF EXPERIMENTAL PROCEDURES

Provide an adequate description of the experimental procedures used to obtain the numerical data. The quality of the information about *how* measurements were made often determines the acceptability of the results. When it becomes necessary for a reader to compare the results of several studies, or to reinterpret data, he may need to know whether the author paid attention to details that have since been realized to be important or whether his technique could have revealed more recently reported phenomena. If these questions cannot be answered, later workers and evaluators may assign very little weight to the results.

The major points to be considered are:

1) *Definition of the system studied.* This must be defined as precisely as necessary to ensure the reproducibility of the investigated properties within the limits of experimental error. All relevant details about the physical state and the constraints on the system must be given, as well as information about the origin, treatment, history and chemical composition of the samples.
2) *Description or identification of (a) physical or chemical methods used in the measurements for analysis of composition or purity and (b) reference substances or methods used to test the reliability of the results obtained.* The results of the tests should be given.
3) *Brief qualitative description of the type of measurements made and apparatus used.*
4) *Description of apparatus.* Novel apparatus should be described in detail and the results of its testing given. In other cases the details may be given by reference to another publication. Where relevant, the author should indicate dimensions, constructional material, electrical and other components, major modifications in equipment, etc. For commercial apparatus and components the manufacturer and model number should be specified.
5) *Description of experimental procedures.* The quantities actually measured should be stated clearly since these may differ considerably from the derived results. If the procedures are novel, how they were tested must be explained. Standard procedures may be identified by reference to another publication. The laboratory environment (temperature, pressure, humidity, geographival location, etc.), should be stated if relevant.
6) *Performance of measurement system.* The sensitivity or resolution achieved in the measurements should be stated and proved. Methods of calibration and reference substances used, therefore, should be identified. International or national standards of scales that were used in the calibration should be cited.

III. THE REDUCTION OF EXPERIMENTAL DATA

Explain the conversion of the measurements to the reported results. This reduction of data often is a long and complex process difficult for a reader to reconstruct. Inclusion of an example may be desirable. The procedures used for reduction of the data if adequately described in one publication may be given by reference in later publications.

Important components of this process are:

1) *Assumptions made about the experiments.* Usually some parameters are assumed to be unimportant, others are

assumed constant, and corrections are made for the variations in still others. These assumptions and procedures should be stated; if they are based upon auxiliary experiments, those should be described.

2) *Complete description of physical models (including relevant mathematical expressions) used to convert the data to results.* Approximations should be explained. References to important computer programmes employed should be given.
3) *Experimental results and physical constants taken from other sources.* These should be identified clearly as should their sources and their values stated.
4) *Identification of standards used to relate the measurements to the fundamental units of measure.* Examples are: a particular international temperature scale, a dated list of atomic weights, a national standard volt, etc.

IV. PRESENTATION OF NUMERICAL RESULTS

As a general principle, report results in a form as free from interpretation as possible (i.e. as closely as is practical to experimentally observed quantities). These results should be reported in such a manner that the degree of experimental randomness can be assessed. The reader should be able to recover enough of the experimental data so that he can reanalyse them in terms of different hypotheses.

A. **Citable Results. List important numerical results in explicitly titled tables.** These are the results that the author expects other workers to cite or use. Separate them from the discussion of the work. Results from other sources that are included in tables containing the new material should be clearly identified and referenced. Graphical and analytical representations of important results, although convenient for the reader, *are not acceptable substitutes* for tabular presentation of *accurate* experimental results. The author will, no doubt, interpret the primary results and present derived quantities. However, such secondary results should never be published at the cost of omitting the primary results upon which they are based.

B. **Compressed Presentation of Unsmoothed Data. An acceptable alternative to a complete table** (when there are many measurements) **is an easily used analytical expression supplemented by a deviation plot showing the individual points.** This procedure may save space and promote clarity, but must be sufficiently sensitive to permit full recovery of individual results.

C. **Presentation of Smoothed Data.** In addition to showing his work in the manner described above, an author may include tables of smoothed numerical results intended for use by the reader, for example, electrical resistivity at selected temperatures. In such cases, **arrange the tables with values of the argument so spaced that no serious loss of accuracy will result during interpolation (6) and give a sufficient number of digits to make such interpolation feasible.** Alternatively, such smoothed data may be provided by empirical equations which not only provide ready analytical interpolation, differentiation or integration, but can also save journal space. It is important that the deviation of the experimental values from the equation be within the imprecision of the experimental data.

D. **The "Imprecision" and "Inaccuracy" of the Results. Evaluate both in clearly defined terms.**

The various sources of uncertainty should be described rigorously, with clear separation between measurement imprecisions, numerical analysis limitations (or deviations from a model), and possible systematic biases.

Imprecision. The statistical or random uncertainty should be estimated using an appropriate standard statistical technique. It is only one component of the total error analysis and is not a sufficient statement of the reliability of the experiments.

Inaccuracy. Estimation of the other potential sources of error or limitations of the work is more difficult than is that for imprecision. There are no clear rules; subjective judgment is involved. However, these estimates of inaccuracies are more important than is that for imprecision because unexplained differences between two sets of measurements usually are larger than are the random errors.

Important components in the evaluation of inaccuracy (i.e., of possible systematic errors) for which estimates should be made are:

1) *Sensitivity of measurement or resolution* possible in the experiments. This provides a lower bound for the inaccuracy.
2) *Effects of assumptions* made in processing the data. In particular, include uncertainties or defects in the physical model used.
3) *Possible sources and magnitudes of errors* due to limitations of the measurement system. These should be discussed both for those for which corrections were made and those for which this could not be done. Those inherent in the calibration procedures or standards used should be included.
4) *Uncertainties in auxiliary data* taken from other sources.

These estimates for the components of the measurements should be combined to give the total estimated inaccuracy. Statistical procedures used in the reduction and estimation of the imprecision and inaccuracy of the data should be cited. The inaccuracy estimate may be important in some applications of the results and not in others. A discussion of this point should be included.

E. **Symbols, Units and Nomenclature. Use symbols, units and nomenclature recommended by the International Standards Organization and by the various international unions.**

In particular:

1) *Use SI units* and their accepted symbols (1,2) as far as possible.
2) *Identify symbols* used for all physical quantities and, where available, use those recognized internationally (3-6).
3) *Use internationally accepted names* for chemical compounds. Commercial and common (trivial) names and abbreviations should be defined.
4) *Make figures and tables logically complete units,* independent of the main text. The caption should explain the table or figure. Particular care should be taken in labelling columns and rows of tables. The label must permit unambiguous recovery of the value for the physical quantity. Any label is acceptable as long as the meaning is clear.

Authors are reminded of the preferred convention: physical quantity = number x power of ten x units

e.g., $\lambda = 5.896 \times 10^{-7}$ m.

It is the *number* that is tabulated.

The preferred label, obtained by rearrangement of the equation above, is:

physical quantity divided by units.

That is, in the equation $\lambda/\mathrm{m} = 5.896 \times 10^{-7}$, the left hand side is the label and the right hand side is the number to be tabulated.

Other examples are: pressure as "P/MPa", temperature as "$T/10^5$ K" and a first order rate constant as "log (k/s^{-1})".

An alternative form, e.g. entropy as "S in JK^{-1} mol^{-1}" is acceptable.

The use of non-SI units and, even more, the use of non-metric units for reporting scientific data is discouraged. Occasionally there may be overriding reasons for using such units. In these cases the author should give factors for conversion to SI units. This may be done in a footnote : "Throughout this paper 1 torr = (101.325/760) kPa, 1 cal_{th} = 4.184 J, and 1 Å = 0.1 nm."

V. DISCUSSION

We have attempted to set forth the important aspects of numerical data presentation so as to save the data and to promote the usefulness of the quantitative results of scientific research.

There is an apparent conflict between these recommendations and the usual exhortations to authors for brevity as well as clarity in their papers. The needs of the general reader often can be met by a brief article not containing the detailed information we prescribe, but those of the specialist and of the evaluator cannot. Although these recommendations call for more (but not much more) detail than is commonly provided, they do not exceed what appears in the better papers today. The needed statements may be terse and factual.

The ideal situation is to have all of the relevant information in the published article. However, if this is not practical then the supplementary material should be put in an auxiliary publication (submitted together with the shorter manuscript) and either placed in a suitable depository service or published as microform together with the article. In any event, the details must be available to the public from some source other than the author. The means of obtaining such auxiliary information must be clearly stated in the publication.

In order to provide the author with more guidance these general recommendations have been supplemented by a bibliography. It includes a non-exhaustive list of useful reports on general topics (e.g., symbols, units, nomenclature, physical constants, temperature scales, precision and accuracy) that should be consulted (1-13).

For application to particular fields there is a need for interpretation and implementation of our recommendations. Some specialized guides already exist. They are noted in the bibliography (14-33). Specialists in the fields for which guides exist believe that these have improved the quality of data reporting.

This Task Group is endeavouring to promote the preparation by appropriate international scientific bodies of discipline-wide guides for important areas as well as more specialized guides for sub-disciplines. We will welcome suggestions concerning what should be done and by whom.

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