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Guidelines for the Reporting of Numerical Data and Experimental Procedures

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General recommendations are made about the reporting of data and experimental procedures. These are intended as instructions to authors of papers in which quantitative physical and chemical data are reported. There is included a bibliography of standards documents and more detailed guidelines.

Key words: Chemistry; experimental procedures; numerical data; physics.

1. Introduction

Scientific journals give general guidance on the preparation of papers in editorial sections entitled "instructions to authors" and the like. Two guides of this type are presented here. They are concerned with numerical data and experimental procedures. They reflect the experience of data evaluators in decoding results reported in the primary literature. These guides indicate how numbers should be reported and what auxiliary information is needed if it is to be possible for a conscientious reader to reinterpret or repeat the measurements.

These guides are general. More specific directions have been written for particular types of experiments. A bibliography appended to this paper lists a number of these, together with some generally applicable documents that treat symbols, nomenclature and standards.

2. The Presentation of Numerical Data

Quantitative measurements of physical properties and molecular parameters have surprisingly long lives. They often survive several changes in interpretation. The author can enhance their survival value by presenting them in a form that will permit reinterpretation, permit comparison with other work and permit as assessment of both accuracy and precision.

A vital preliminary to the reporting of numerical results is an adequate description of the experimental procedures used to obtain them. What is needed is outlined in a separate section.

The suggestions below are guides to be used in planning the presentation of numerical data.

1. In the reporting of experimental measurements and of derived quantities, **use internationally approved nomenclature, symbols, units,** and **standards.** If there are over-riding reasons for using other symbols for units, identify these in terms of the internationally approved ones.

2. **Report data in a form as free from interpretation as possible.** The reader should be able to recover the measured quantities so that he may reanalyze them in terms of a different hypothesis. Often this means simply the addition of another column of data to a table. If there is a commonly accepted form for reporting the particular type of data, it should be used in addition to any form preferred by the author.

3. **Present quantitative data that still show the scatter in the measurements.** Whenever possible, publish experimental results in numerical form. If a choice must be made, plot or tabulate unsmoothed data instead of smoothed final results. Small, unexpected effects can be lost when data are smoothed or fit to a predetermined function.

4. **Put the final numerical results,** those the author wants accepted, **in a table.** Do not bury them in a discussion section—they will be lost.

5. **Report the "imprecision" of the measurements** (statistical or random uncertainty), **and define it unambiguously,** e.g. "twice the standard deviation of the mean" etc. Avoid qualitative estimates of this quantity.

6. **Estimate the "inaccuracy" of the measurements.** Quantitative data presented without an estimate of possible systematic errors deserves summary rejection. The components of this estimate include
   (a) the sensitivity or resolution possible in the measurements,

(b) the effect of assumptions made in processing the data,
(c) the effect of possible systematic trends, both those for which corrections were made and those for which this could not be done, and
(d) uncertainties in auxiliary data taken from other work.

If possible, state this estimate in the same terms as that used for imprecision. They should be comparable in meaning even though they may differ in magnitude. Experience has shown that systematic differences between two sets of data usually are more important than random errors. Attempts to estimate these possible effects usually lead to improved experimental design.

7. **Explain the method used to reduce the primary data.** This is the chain linking the measurements and the results. Often it is long and complex. Frequently, it is difficult for a reader to reconstruct it. An example is desirable. Important components of this chain are listed below. It is worthwhile to cover each point, but the detail depends upon the precision of the experiments.

(a) Mathematical expressions used to convert the data to results.
(b) Assumptions made about the experiments. Invariably some parameters are assumed to be unimportant, some are held constant and some are subject to substantial corrections. The treatment of all of these should be justified, preferably by experiment.
(c) Auxiliary data and constants taken from other sources. Both their values and imprecision should be stated.
(d) The use of standards in relating the measurements to the fundamental units of measure. The standards should be identified explicitly, particularly where changes have been made recently (as in the International Practical Temperature Scale, or atomic weights and masses).
(e) Cite the statistical procedures used.

3. The Reporting of Experimental Procedures

The quality of the information provided about how measurements were made often determines the acceptability of the results in the future. When it becomes necessary for a reader to compare the results of several studies, or to reinterpret data, he must ask, "Did the author pay attention to details that I now know to be important?" or "Could he have observed this (newly reported) effect?" If these questions cannot be answered, the work may be rejected.

The major topics that should be included in a description of the experimental procedures are listed below. Consideration of these points when planning the work will, inevitably, improve the experimental design and simplify the preparation of the final paper.

- Description of apparatus with dimensions (either directly or by reference to earlier work).
- Calibration of equipment, including a discussion of the magnitudes of possible systematic biases for which corrections were not made.
- Indication of whether and how the calibration is traceable to an established standard.
- Description of experimental procedure.
- Description of environmental conditions.
- Identification of analytical methods used (and proof of them if novel).
- Indication of the purity of materials and the evidence for it.
- Statement of sensitivity or resolution possible in the experiments and the proof thereof.
- Reporting on negative experiments.

4. Discussion

General directions for the preparation of a scientific paper serve several purposes. They set minimum standards for and promote uniformity of presentation of material. Also, they remind an author to tell his reader about what has been done as well as what has been deduced. But, in both cases such guides rely heavily upon the judgement of the author concerning what should be included.

More detailed guides are desirable when quantitative data are important *per se* as opposed to being aids in the development of concepts. These must summarize all the features of the work that should be recorded so that a step by step reanalysis can be made. Each such guide can only treat a specific type of work. Those few that have been written appear to have improved the quality of reporting of data. More are desirable.

5. Bibliography

5.1. Symbols, standards and basic quantities

SYMBOLS, UNITS, AND NOMENCLATURE

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American Soc. for Testing and Materials (New York, 1970)
(Includes factors for conversion of customary units to SI and procedures for rounding converted values)

American Chemical Society
"Handbook for Authors of papers in the journals of the American Chemical Society"
American Chem. Soc. Publications (Washington, 1967)
(This handbook includes a bibliography (pg. 49–53) on nomenclature of chemical compounds and, to a limited extent, on terminology and symbols.)

International Union of Pure and Applied Chemistry
"Information Bulletin"
(This series includes appendices on nomenclature, symbols, units and standards for specialized fields. Many of these are about the nomenclature of compounds, but some are on reporting of data. See "Guidelines")

CODATA Newsletters
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ATOMIC WEIGHTS

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