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Criteria for the Presentation in the Primary Literature of Scientific and Technical Information on Thermophysical Properties of Solids

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1. INTRODUCTION

The guidelines and criteria presented below concern numerical data that are capable of reproducibility by repetitive measurement of the bulk macroscopic properties of materials. The properties concerned are the bulk, macroscopic properties of materials that may undergo phase transformations or exhibit anisotropy. The materials must be sufficiently well defined or characterized 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 structure.

This is not an editorial 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, can remeasure the property, and can recalculate the results when values for auxiliary data change.

The author of a paper has the primary responsibility for providing the

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reader with the type of information outlined here. These guidelines also provide 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 is 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 critical evaluation.

When reporting numerical data, it is essential to specify two quantities: *imprecision,* which records the reproducibility of the observations, and *inaccuracy,* which estimates the overall reliability of the measurements. The specification of these two quantities is essential to the reporting of all numerical data.

The presentation below follows closely the recommendations in the International Council of Scientific Union's Committee on Data for Science and Technology Bulletin No. 9, December 1973 (available from the CODATA Secretariat, 51 Boulevard de Montmorency, 75016 Paris, France). The CODATA Task Group on Thermophysical Properties of Solids has made generous use of material presented therein, which also contains a bibliography of 35 references on the general subject covering: (a) symbols, units, and nomenclature; (b) physical constants and temperature scales; (c) precision and accuracy; and (d) available guides in various disciplines.

2. THE DESCRIPTION OF EXPERIMENTAL PROCEDURES

Authors should provide an adequate description of the experimental procedures used to obtain the numerical data. The major points to be considered are:

1. Definition of the system studied. 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. In other words, the material should be fully characterized.
2. Description or identification (a) of physical or chemical methods used in the measurements for analysis of composition or purity, and (b) of reference materials or methods used to test the reliability of the results obtained.
3. A brief qualitative description of the type of measurements made and apparatus used.
4. Description of apparatus. A novel apparatus should be described in detail and the results of its testing given. In other cases, the reporting of details may be satisfied by reference to an earlier publication. In general, all referenced publications should be readily available to

readers via the open literature. Where relevant, the author should indicate dimensions, constructional material, electrical and other components, major modifications in equipment, etc. The manufacturer and model number of commercial apparatus and components 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.
6. Performance of measurement system. The sensitivity or resolution achieved in the measurements should be stated and demonstrated. Methods of calibration and reference materials used should be identified. International or national standards of scales used in the calibration should be cited.

3. THE REDUCTION OF EXPERIMENTAL DATA

Authors should explain the conversion of the measurements to the reported results. This reduction of data is often 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. The boundary conditions maintained and corrections applied to certain observations should be clearly stated.
2. A complete description of physical models should be included (including relevant mathematical expressions) used to convert the observed data to results. Approximations should be explained.
3. Experimental results and physical constants taken from other sources should be identified.

4. PRESENTATION OF NUMERICAL RESULTS

As a general principle, authors should 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 or she can reanalyze them in terms of different hypotheses.

A. Citable Results

Authors should 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 experimental results.

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 the work in the manner described above, an author may include tables of smoothed numerical results such as, for example, electrical resistivity at selected temperatures, intended for use by the reader. In such cases, arrange the tables with values of the argument so spaced that no serious loss of accuracy will result during interpolation and give a sufficient number of digits to make such interpolation feasible. Alternatively, such smoothed data may be provided by empirical equations that 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 it is for imprecision. There are no clear rules; subjective judgment is involved. However, estimates of inaccuracies are important because unexplained differences between two sets of measurements may be significantly larger than 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 errors 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 measurement should be combined to give the total estimated inaccuracy.

E. Symbols, Units, and Nomenclature

Use symbols, units, and nomenclature recommended by the International Organization for Standardization and by the various international unions. In particular:

1. Use SI units and their accepted symbols [1–4] as far as possible.
2. Identify symbols used for all physical quantities and, where available, use those recognized internationally.
3. Use internationally accepted names for chemical compounds. Commercial and common (trivial) names and abbreviations should be defined.
4. Make figures and tables self-contained as far as possible.

5. CONCLUSIONS

We have attempted to set forth the important aspects of numerical data presentation so as to promote the usefulness of the quantitative results of scientific research. It may seem that there is an apparent conflict between these recommendations and the usual exhortations to authors by editors for brevity as well as clarity in their papers. Although these recommendations call for somewhat more detail than is commonly provided, they do not exceed what appears in the better papers today. The required statements may be terse and factual.

The ideal situation is to have all 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 placed in a suitable depository service such as the Center for Information and Numerical Data Analysis and Synthesis at Purdue University. 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.

REFERENCES

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