IUPAC Technical Report

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Supporting the Reviewing of Thermophysical and Thermochemical Research Publications (IUPAC Technical Report)[+]

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Abstract: In order to support scientific reviewing in the area of material property research and make the reviewing process easier and more efficient, checklists covering typical problems, lists of available resources, and computer-based tools to help compose reviewers' reports have been created. Our intention is to ensure that scientific communications show necessary and sufficient primary and supporting information about substances studied, conditions, properties, and techniques of interest with understandable terminology, in details assuring reproducibility of the obtained results. The principles and ideas of this project can be extended to other scientific areas.
Keywords: Checklists; Material properties; Publications; Reviewing; Thermophysical properties; Thermochemical properties

Introduction

IUPAC project #2019-013-1-100 "Good Reporting Practice for Thermophysical and Thermochemical Property Measurements" [1] coherent with the FAIR principles [2] articulated principles of reporting research results related to material properties. The following nine principles were formulated covering (I) essential aspects of data reporting, (II) data traceability and reliability, and (III) data reporting convenience:

I.1. Measured property data should be published in a numerical format (at least in a supplement).
I.2. Published data should be well defined (including system, state, property, and units).
II.1. All published data should be traceable to their origin.
II.2. Observations should be distinguished from interpretation.
II.3. Auxiliary (calibration) data should be identified and provided.
II.4. Necessary details of experimental methods or computation procedures should be given.
II.5. Uncertainty in each measured value should be reported and justified.
III.1. Importing reported data into analysis software should be easy and straightforward.
III.2. Complex mathematical equations should be provided in a machine-readable form.

The purpose of that project [1] was to guide authors of scientific publications to most effectively transmit their findings and avoid the loss of valuable information from their work. More than 40 various examples illustrating the above principles were described in the Technical Report [1]. Articles popularizing and detailing those principles also have been published [3, 4]. The participants of that project recognize, however, that even with their best efforts, the efficiency of just declaring good reporting practices may be insufficient (Dr. Alan Finkel once said: "More than anything, we must abandon the assumption that a passive apprentice system works." [5]). More effective mechanisms are to be found. We believe that peer review is a great opportunity to actively refine the communication process. We recognize that reviewing itself does not create additional information, but it is an essential part of the process of complete and unambiguous reporting of research results.

The goal of the current IUPAC project 2023-008-1-024 is to facilitate and organize the process of reviewing communications of experimental and modeling research by providing guidelines and tools for reviewers to detect typical reporting problems and, hence, help authors eliminate them. The focus of the project is on the following most common issues that appear in publications:

- insufficient identification of studied materials such as ambiguous isomeric or stereoisomeric composition of chemical substances;
- inadequate identification of the properties and physical states by giving incomplete or ambiguous definitions;
- not including primary measured properties with physical units and state variables in a numerical form;
- not providing essential supporting information, experimental details, and uncertainty budgets;
- not providing sufficient information allowing one to reproduce the obtained results.

This Technical Report presents reviewer guidelines supported by implementation examples of the guidelines via computer-assisted tools as well as a brief summarizing overview of related useful resources about experimental methods and data reporting. The guidelines are developed to provide a systematized (structured) approach for reviewers in their analysis of manuscripts. The computer-assisted tools navigate them (especially, new reviewers) through typical problems in the field of material property measurements, terminology, and data reporting.

1. Reviewing guidelines

Review reports for manuscripts can range in thoroughness from "I read and understood" to scrutinizing every detail of the report. We believe that the maximum impact on the quality and usefulness of publications with minimal labor and time is at an intermediate level between these two types of analysis. We tried to determine and enumerate the appropriate checks (listed in the Supporting materials) covering the description of the objects, properties and conditions, numeric data, and uncertainties. The goal is to uncover most errors and omissions efficiently. However, researchers and reviewers should use their own judgment about the level of effort to spend with the resources available.

In this report, we suggest a systematized (structured) approach. Our guidelines, or checklists, are collected in a spreadsheet in Supplement 1. Blocks of rows are related to particular objects, properties, or methods (Scopes). Based on the task group members' expertise, the following scope-specific review groups were identified:

0. Common (relevant for every review/scope)
1. Inorganic compounds
2. Organic compounds
3. Alloys
4. Polymers
5. Electrolytes
6. Ionic liquids
7. Mixtures/Solutions
8. Gas hydrates
9. Deep eutectic solvents
10. Phase equilibria
11. Reactions
12. Calorimetry and DSC
13. Computational methods

Each block contains the same set of sections covering the following aspects (Categories):

A. Research planning
B. Materials
C. Properties
D. Methods
E. Reporting
F. Uncertainties

Each row represents one issue and contains Observation, Suggestion, and Comments/Examples fields. The Observation field (*e.g.*, "Insufficient proof of synthesized compound identities", "Numerical values for all non-state variables are not given") encourages the user (reviewer) to check if the deficiency exists in the manuscript under review. The Suggestion field provides a tentative text to include in the review. The Comments/Examples field may provide additional information and references to examples with proper reporting.

It should be emphasized that reviewers make the ultimate decision on which comments apply to the manuscript they are reviewing. The reviewers can alter and amend the text because it is their ultimate authority and responsibility. The checklists do not cover all possible issues, but they include most frequent and problematic issues, based on our experience. If used by reviewers, they assure that such deficiencies in manuscripts are revealed and addressed.

The checklists can be supported by a computer program, Excel, Python, or a web service. To minimize the reviewer's efforts, only relevant blocks can be shown after the selection of the scope, and the logically grouped comments can be shown one block at a time. Such tools are expected to reduce human job by composing editable initial drafts of reviewers' reports. The reviewers can edit the report and indicate specific places in the manuscript where the comments apply. A web application supporting the checklists with easy-to-understood scope selection and display [6] and the corresponding demonstration video [7] have been created. Development of other similar applications by interested parties (publishers, funding agencies, educational institutions) is encouraged.

One may wonder whether the proposed checklists can be used in combination with artificial intelligence (AI) in order to figure out which comments are relevant and which parts of the reviewed document cause them. While this is possible, the use of AI is regulated by the owner of that document, or the publisher in the case of submitted manuscripts. Moreover, the reviewer is ultimately responsible for all the content of the review, including possible false positives and omissions.

2. Additional resources

2.1. Experimental method descriptions

While new experimental methods are being constantly developed, publications devoted to overview of techniques, such as those listed below, should provide full descriptions of common measurement methods, as described in the references. Reports on experiments should be made with methods adequate for the studied materials and conditions. Furthermore, sufficient method description information should be provided to prove the accuracy and reliability of their implementation and data treatment. Reviewers should either be familiar with the corresponding techniques used or consult references that describe the methods as given below. These are some essential sources for the corresponding areas:

- ✓ Reaction thermochemistry [8-10].
- ✓ Combustion calorimetry [8, 11] (Note: tools supporting processing of combustion calorimetry experimental data are becoming available, *e.g.*, Combustion Calorimetry Tool (CCTool) [12] developed by the Thermodynamics Research Center at NIST).
- ✓ Solubility measurements [13, 14].
- ✓ Phase equilibria at high pressures [15].
- ✓ Differential scanning calorimetry [10, 16].
- ✓ Dynamic light scattering [17, 18].
- ✓ Experimental thermodynamics and transport properties [19-28].
- ✓ Nuclear magnetic resonance (NMR) [29, 30] and its application to diffusion measurements [31].
- ✓ Mass spectrometry [32-34] and its application to thermophysical measurements [35].

2.2. Reference materials

Measurement equipment requires periodic validation of measurement quality and calibration for accurate recordings. Relevant materials having well-studied and accepted properties should be used. Reviewers should note if such calibration and validation have been included in the study under review.

References about materials and methods listed below have been made available under the auspices of IUPAC, ICTAC, PTB/GEFTA, NIST, and other national metrological agencies. The same materials can be used for either calibration or method verification. Many verification/calibration materials and methods are collected in a compilation [36], and many reference materials are available from NIST through the Standard Reference Materials program [37], German Federal Institute for Materials Research and Testing (BAM) [38], UK National Physical Laboratory (NPL) [39], National Metrology Institute of Japan (NMIJ) [40], Joint Research Centre (JRC) of the European Commission [41], French National Laboratory of Metrology and Testing (LNE) [42], National Research Council Canada (NRC) [43], Korea Research Institute of Standards and Science (KRISS) [44], *etc*. These are some essential sources about reference materials/systems for the corresponding areas:

- ✓ Calorimetry [45, 46].

- ✓ Differential scanning calorimetry (DSC) [45, 47-51]. (Note: adamantane should be used with caution because of possible kinetic effects).
- ✓ Density standards [52].
- ✓ Light scattering [53].
- ✓ Phase equilibria in mixtures [54-56].
- ✓ Thermal analysis [57].
- ✓ NMR [58].

Though not a formal recommendation of reference materials, the review [59] can be used as a source of the candidate substances for verification of methods and equipment for thermal conductivity and viscosity measurements. No formal recommendations on pure-compound vapor pressures are known to us, but several reliable correlations can be found in NIST REFPROP software [60, 61] supported by experimental data in [62-64].

2.3. Nomenclature, terminology, and reporting

Clear reporting requires commonly accepted terminology and nomenclature, unambiguous identification of the substances and materials, and detailed information about the objectives, properties, and methods. The IUPAC website [65] has links to recommendations for a broad range of organic and biochemical nomenclature, symbols, and terminology. There are resources for organic chemical nomenclature [66] (full version) and [67] (short version), for inorganic chemistry [68], for stereochemistry [69], for isotopes [70], and for polymers [71-73]. The most comprehensive resource on terminology is the IUPAC Gold Book –online version [74]. Terminology specific to physical organic chemistry is summarized in [75]. Specific terminologies are available for thermal analysis [76], mass spectrometry [77], and polymerization [78]. Reporting recommendations and standards exist for phase equilibria [79, 80], for chemical analysis [81], and for NMR [82]. Physical constants and atomic masses needed for property data can be found in [83-85]. Recommendations exist for reporting substance purity [86] and uncertainties [87-89].

Some journals have checklists to ensure that important aspects of those guidelines are covered [90-93].

Conclusions

To prevent typical deficiencies in communications on material property measurements and analysis, checklists have been composed, resources on methodology have been compiled, and a web-based service supporting scientific reviewing has been developed. We encourage publishers, funding agencies, and educators to not only make use of these guidelines, but also to disseminate them to members of their communities and support their implementation in their respective areas. We hope this effort will enhance the efficiency of reviewing, the reliability of published information, and the quality and usefulness of research reports.

Supporting materials

Supplement 1 (structured spreadsheet with checklists for reviewers) mentioned in the text can be found online as Supporting Information to this paper.

List of abbreviations and acronyms

BAM – Bundesanstalt für Materialforschung und -prüfung (Germany)

DSC – Differential Scanning Calorimetry
FAIR – Findability, Accessibility, Interoperability, and Reuse
GEFTA – Gesellschaft für Thermische Analyse e.V. (Germany)
ICTAC – International Confederation for Thermal Analysis and Calorimetry
IUPAC – International Union of Pure and Applied Chemistry
JRC – Joint Research Centre (Belgium)
KRISS – Korea Research Institute of Standards and Science (South Korea)
LNE – Laboratoire National de Métrologie et d'Essais (France)
NIST – National Institute of Standards and Technology (United States)
NMIJ – National Metrology Institute of Japan (Japan)
NMR – Nuclear Magnetic Resonance
NPL – National Physical Laboratory (United Kingdom)
NRC – National Research Council (Canada)
PTB – Physikalisch-Technische Bundesanstalt (Germany)

Membership of the sponsoring body

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