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Preparation, formatting and review of IUPAC Technical Reports and Recommendations, IUPAC-sponsored books, or other items carrying the IUPAC label

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IUPAC Task Groups or other IUPAC bodies may submit a Technical Report or a Recommendation for publication in *Pure and Applied Chemistry* (PAC), prepare a book draft, or produce other written or electronic documents. The content of the manuscript is the responsibility of the Division(s) sponsoring the document.

Books and other written or electronic documents that are not intended for PAC, but intended to carry the IUPAC label, are sent to the Chair of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) for review by ICTNS. The review focuses on terminology, nomenclature, symbols, and units; responsibility for the scientific content is with the editor(s) of the book or the author(s) of other items.

1 IUPAC Technical Reports and Recommendations in *Pure and Applied Chemistry*

PAC is the primary journal of IUPAC for all Recommendations and Technical Reports. Manuscripts intended for submission to PAC as IUPAC Technical Reports or Recommendations should be designated as such in their titles. The final decision, whether a submitted manuscript is accepted as a Technical Report or Recommendation, is with the Chair of ICTNS in their role as IUPAC Editor of PAC. The manuscript should be prepared following the guidelines in Section 4. The review process differs for Technical Reports and Recommendations because a Recommendation has a more authoritative standing due to its wider reach within IUPAC and across to other scientific bodies, engineering, trade, policy, and the public. Therefore, Recommendations mandate a particularly careful preparation and review process to ensure broad acceptance in the community. It is of utmost importance to maintain consistency with other existing Recommendations. Newer Recommendations in a specific field take precedence over previous ones in the same field.

A **Technical Report** is a report about a specific study, such as:

- compilations and critical evaluations of data
- critical assessments of methods and techniques
- guidelines for the presentation of methods of analysis
- quantitation of specific elements or compounds in selected samples in special environments
- studies of the interaction of materials with the environment
- aspects of quality assurance and chemical process control
- evaluations of properties of specific materials
- explorative studies or brief guides

A **Recommendation** results from studies on nomenclature, symbols, terminology, or conventions, and its purpose is to recommend:

- terminologies for specific fields, quantities, concepts, and groups of properties relevant to chemistry
- names of new elements
- nomenclature and structure representation of chemical compounds or classes of compounds
- conventions and standards of practice for presenting data in a specific field of chemistry

A Technical Report may warrant publication of a subsequent Recommendation. There is no requirement for a Recommendation to follow on from a Technical Report, but it may help identify those aspects that would benefit from the authority of a Recommendation.

2 Review workflow for Technical Reports and Recommendations

The manuscript review workflow is divided into four or five phases, depending on whether it is a draft Technical Report or a draft Recommendation:

Phase	1	2	3	4	5
Reviewers	Division	IUPAC Editor	External, ICTNS	Public, ICTNS, Division	IUPAC Editor
Technical Report	✓	✓	✓		✓
Recommendation	✓	✓	✓	✓	✓
Section below	2.1	2.2	2.3	2.4	2.5

In **phase 1 (Division review; Section 2.1)**, prior to submission, the manuscript must receive approval by the President(s) of the sponsoring Division(s), which should be given only after a careful Division review of the manuscript. Division reviews include dissemination of the manuscript among Division members and other relevant Divisions for discussion and comment. ICTNS participates indirectly in this process through the ICTNS Division Representatives. A thorough Division review will expedite the publication of the manuscript. The manuscript submission documents must include a written confirmation by the Division President(s) (DPs) that the Division review has been completed (DP approval). Otherwise, the manuscript will not enter the reviewing process.

To submit the DP-approved manuscript for **phase 2 (initial IUPAC Editor review; Section 2.2)**, the corresponding author should inform the IUPAC Secretariat that a manuscript is ready for submission (via email to secretariat@iupac.org). The Secretariat will provide access to ScholarOne Manuscripts. The IUPAC Editor then decides whether the manuscript is suitable for review.

During **phase 3 (external expert and ICTNS review; Section 2.3)**, Technical Reports and Recommendations will be reviewed by both external experts from science and industry (up to 15 in case of Recommendations; about 5 for Technical Reports) and ICTNS. ICTNS members ensure consistency of the manuscript with IUPAC Recommendations and the IUPAC Green, Red, Blue and Purple Books [1–4]. They may also comment on any other aspects within their scientific expertise. Manuscripts may undergo several iterations and revisions during phase 3 before acceptance. The IUPAC Editor has the final responsibility for accepting or rejecting the manuscript.

Once phase 3 is complete for a draft Recommendation, the accepted manuscript is checked by the IUPAC Editor and the authors, and then enters **phase 4 (public review; Section 2.4)** as **Provisional Recommendation**. In contrast, an accepted Technical Report proceeds directly to phase 5. During phase 4, IUPAC will publish the Provisional Recommendation on a dedicated webpage for public review and comment. This public review allows the IUPAC National Adhering Organizations (NAOs), a wide range of other organizations, and individuals to comment on the Provisional Recommendation before it is finally revised for publication. The end date of the four months' public review is shown on the dedicated webpage. Provisional Recommendations should not be quoted publicly. The author(s) will revise the Provisional Recommendation in the light of the comments received during the public review phase and submit a revised manuscript via ScholarOne Manuscripts for final review by ICTNS members and the Division President.

Accepted Provisional Recommendations and Technical Reports enter **phase 5 (final editing and publication; Section 2.5)**. The publisher will edit the manuscript for language and publisher-specific issues. This copy-edited manuscript is checked by the IUPAC Editor and the authors. After typesetting by the publisher, proofs will be sent to the authors for final review. Before printing, the manuscript is cross-checked by the IUPAC Editor and released for publication. The additional phase 4 step required for Recommendations typically results in a longer average review time than for Technical Reports.

2.1 Phase 1 (division review)

Authors:

- prepare the manuscript according to the guidelines in Section 4
- submit the manuscript to the Division President of the lead Division

Division President of the lead Division (DP):

- disseminates the manuscript to Division members and other relevant Divisions for review
- when necessary following Division review, asks authors to revise the manuscript
- accepts the manuscript and sends a written approval email to authors

2.2 Phase 2 (initial IUPAC Editor review)

Authors:

- contact the IUPAC Secretariat to request access to ScholarOne Manuscripts
- once a submission point has been provided, submit the manuscript including written DP approval and external reviewer suggestions (15 for Recommendations; 5 for Technical Reports)

IUPAC:

- requests an online submission invite to be sent to the corresponding author

Publisher (De Gruyter)/ScholarOne Manuscripts:

- opens a submission point for the manuscript
- performs initial quality control (including a check for inclusion of the written DP approval)

IUPAC Editor of PAC (ICTNS Chair):

- verifies the written DP approval
- invites reviews by external experts from science and industry and ICTNS members

2.3 Phase 3 (external expert and ICTNS review)

Reviewers:

- are chosen as external experts from science and industry (up to 15 for Recommendations, about 5 for Technical Reports) and review the content of the manuscript
- are also all ICTNS members who are invited to review compliance of the manuscript with existing IUPAC-recommended terminology, nomenclature, and symbols, and manuscript content within their expertise

Publisher (De Gruyter)/ScholarOne Manuscripts:

- collates reviews via ScholarOne Manuscripts
- communicates with reviewers to ensure timely receipt of reviews
- communicates with the IUPAC Editor if insufficient reviews are received

IUPAC Editor of PAC (ICTNS Chair):

- determines the status of the manuscript once all reviews have been received:
- request for minor or major revisions from authors
-

- acceptance as is and entry to Phase 4 for Recommendations
- acceptance as is and entry to Phase 5 for Technical Reports
- rejection

Authors:

- prepare revised manuscript addressing reviewers' comments and resubmit to ScholarOne Manuscripts for further Phase 3 review (when minor or major revisions required)

2.4 Phase 4 (public review of Provisional Recommendations)

IUPAC Secretariat:

- creates a webpage with title, synopsis, linked manuscript (now termed “Provisional Recommendation”) and a form to gather feedback and comments (<https://iupac.org/what-we-do/recommendations/provisional-recommendations>)
- publishes the synopsis in *Chemistry International (CI)*
- informs National Adhering Organizations (NAOs) and other IUPAC-affiliated organizations of the new Provisional Recommendation, who in turn are encouraged to republish the title and synopsis in national chemistry journals, magazines, and newsletters

Public (individuals and organizations):

- submit comments on a manuscript using the feedback form provided on the IUPAC website

Authors:

- revise the manuscript to address public comments and resubmit to ScholarOne Manuscripts

Division President of the lead Division (DP):

- approves the final revised manuscript

IUPAC Editor of PAC (ICTNS Chair):

- may invite additional reviews from previous reviewers and members of ICTNS
- approves the final revised manuscript

2.5 Phase 5 (final editing and publication)

IUPAC Secretariat:

- provides information on sponsoring bodies to be appended to the manuscript

Publisher (De Gruyter)/ScholarOne Manuscripts:

- performs copyediting and typesetting in consultation with the authors and the IUPAC Editor

Authors:

- perform proof-reading and make corrections if necessary

IUPAC Editor of PAC (ICTNS Chair):

- performs proof-reading
- gives final approval for publication

3 Republication/reproduction and translation of Recommendations, Technical Reports, IUPAC-sponsored books, or other items carrying the IUPAC label

IUPAC encourages dissemination of any Recommendations, Technical Reports, IUPAC-sponsored books, or other items carrying the IUPAC label by electronic or other means. No formal permission is needed on condition that an acknowledgment, with full reference to the source along with use of the copyright symbol ©, the name of IUPAC, and the year of publication are prominently visible.

Publication of a translation into another language of these documents is subject to prior written approval from IUPAC, its relevant Division(s), and National Adhering Organization(s) via the IUPAC Secretariat. Translations must stay as close as possible to the original version.

4 Guidelines for drafting IUPAC Technical Reports and Recommendations

The manuscript must be clear for its intended audience and consistent with the IUPAC Recommendations on terminology, nomenclature, symbols, and units in the Green, Red, Blue and Purple Books [1–4]. Terminology, nomenclature, symbols, and units in all areas of chemistry are continuously under development within IUPAC.

Authors should do their best to use correct spelling, grammar, and punctuation, and respect the publisher's guidelines.

IUPAC has agreed with BIPM that any PAC document concerned with terminology, nomenclature, symbols, and other conventions is consistent with the SI Brochure [5]. Documents should also be consistent with the "Guide to the expression of uncertainty in measurement (GUM)" [6] and the "International vocabulary of metrology (VIM)" [7] prepared by the Joint Committee for Guides in Metrology (JCGM) and published in the name of IUPAC and others.

Designations such as "(strongly) discouraged", "(strongly) deprecated", "not allowed" and "not recommended" should be avoided because they may leave the reader in doubt about the status of a name, term, or symbol. Instead, such names, terms and symbols should be described as "not acceptable". Technical Reports should avoid the verb "to recommend" or derivatives thereof.

4.1 Form of the manuscript

The title of the manuscript should reflect its contents to make the document easily findable and designate the manuscript as either a Technical Report or a Recommendation. The manuscript must include an abstract of up to 200 words and indicate the corresponding author.

The organization of the remainder of the manuscript is at the discretion of the authors except for Technical Reports and Recommendations that contain a list of terms (a "glossary"). Entries in such glossaries must follow a special layout (Section 4.7). In addition to "glossary", the list of terms may also be called "vocabulary", "dictionary" or "terminology", but this must be done consistently throughout the manuscript.

The document should include a list of all abbreviations (which includes acronyms, initialisms, codewords, or any other shortened form of a word or phrase) in alphabetical order, with their full meaning, just before the list of references.

Authors may decide to include a table of contents, in particular for longer manuscripts.

Manuscripts must be submitted in electronic form (Microsoft Word or LaTeX format). The submitted manuscript will be converted to portable document format that includes line numbering; this output needs to be checked carefully by the authors because it is the version sent out for review.

4.2 Nomenclature

Where several acceptable names for a substance exist, Recommendations may list them all and single out one as “preferred” (PIN: Preferred IUPAC Name) or may mention other names as “acceptable for use in general nomenclature”. Where IUPAC Recommendations allow several names for the same molecular entity, ICTNS may ask authors to use an alternative, according to the aims and context of the manuscript.

The term “trivial name” may be used for names having no part used in a systematic sense. The term “semisystematic (or semitrivial) name” may be used for names in which at least one part is used in a systematic sense. Where such names are incorporated into systematic nomenclature, they may be called “retained names”.

Instead of IUPAC names, certain common names are acceptable in the following cases:

- for pharmaceutical substances, International Non-proprietary Names (INNs)
- for agricultural chemicals including pesticides, International Organization for Standardization (ISO) names
- for recently discovered natural products with complex structures, where systematic names would be too unwieldy and no IUPAC names exist yet, names derived from the biological materials in which they occur

4.3 Quantities, units, and symbols

The recommendations of the Green Book [1] and the SI Brochure [5] on notation and formatting of quantities, units and symbols must be followed, in particular:

- The symbols for quantities are generally single letters of the Latin or Greek alphabets, printed in an *italic* font, and are recommendations (for exceptions, see [1], Sections 1.3.1 and 2.15.1).
- The symbols for units and elements are mandatory and are printed in an upright font [5].
- Quantity calculus ([1], Section 1.1) is used for equations, graph axes and table headings.

All symbols used in equations must be defined.

When a document includes quantities, a summary table of relevant quantities can be included in the document, like the tables in the Green Book, with the headings: Name, Symbol, Definition, SI Unit, Notes. The definition may be an equation, verbal description, or both.

4.4 Use of terms from and transfer to the IUPAC Gold Book

In compiling a document, inspecting the IUPAC Compendium of Chemical Terminology (Gold Book) [8] is required to identify whether terms have been defined previously within IUPAC documents.

It is the intention that for all terms defined in future IUPAC Recommendations, corresponding entries are created in the online Gold Book or revised if they already exist. For this reason, the layout in Section 4.7 must be adhered to.

For Recommendations already published, a review/reconciliation process is underway to avoid duplications and inconsistencies when transferring terms from previous Recommendations into the Gold Book. The management and update of the Gold Book is under review by the Joint ICTNS–CPCDS Subcommittee on the IUPAC Gold Book (JSIGB, <https://iupac.org/body/039>). CPCDS (Committee on Publications and Cheminformatics Data Standards) has responsibility for the metadata management (i.e., digital expression) of terms. ICTNS has final authority over the terms transferred.

4.5 Formatting of citations and references

All references should be cited in the text or captions. They should be typed in brackets, e.g., [41], [42–44] or [41, 42, 45], in sequence, and numbered separately (i.e. [41], [42], ..., not [41(a), (b) ...]). Only primary and secondary references such as articles in journals, books, and issued patents should be used. Meeting abstracts and patent applications may not be quoted unless they are published in a form that is available for library reference.

References appear at the end of the manuscript in numerical order and should be accompanied by their digital object identifier (DOI), when available. Names of all authors should be used rather than “*et al.*” Abbreviations of journal titles should agree with usage by Chemical Abstracts (<https://cassi.cas.org>). For journal articles, only the first page is required, but for book chapters and sections, inclusive page numbers are desirable.

Examples:

- [40] J. P. Lee, G. C. Pimentel. *J. Chem. Phys.* **75**, 4241 (1981). <https://doi.org/10.1063/1.442652>.
- [41] S. Stoeva, G. Grübler, H. Echner, W. Rönspeck, W. Voelter. *Pure Appl. Chem.* **66**, 101 (1994). <https://doi.org/10.1351/pac199466010101>.
- [42] E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Tamaki, A. Thor. *Quantities, Units and Symbols in Physical Chemistry*. IUPAC Green Book, 3rd ed. RSC Publishing, Cambridge (2007).
- [43] ISO/IEC 17043:2010. *Conformity assessment – General requirements for proficiency testing*. International Organization for Standardization, Geneva (2010).
- [44] F. Bloch. US Patent 2960 649, Filed 18 June 1954, Issued 15 Nov 1960.
- [45] European Commission. *Commission Decision 2002/657/EC implementing Council Directive 96/23/EC concerning the performance of analytical methods and the interpretation of results*. European Union, Brussels (2002). <https://data.europa.eu/eli/dec/2002/657/oj>.

4.6 Data availability

IUPAC has endorsed the FAIR data principles (<https://iupac.org/iupac-endorses-the-chemistry-go-fair-manifesto>) to ensure that research findings are based on “findable, accessible, interoperable, and reusable” data, for both human readers and machine-processing (e.g., data-mining algorithms). The preferred means for providing access to data underpinning Technical Reports and Recommendations is through open data repositories, using DOI references and an IUPAC-approved reuse license. Where third-party data have been used, these need to be properly referenced as well. Data sets should be cited as: title, publisher/repository, identifier (publication year).

Where appropriate, software, algorithms or computer code used to produce the results should also be made available in FAIR-data compliant archives or repositories, as required by the open access policies of many institutions and funding agencies.

4.7 Construction of a glossary entry

A glossary entry for a term in an IUPAC Recommendation or Technical Report should give a concise and accurate definition, synonyms of the term, suggested symbols, and common abbreviations. Notes and examples should be added to give the appropriate context in chemistry. Relevant sources should be referenced.

4.7.1 Choosing a term

A glossary entry includes a term and its definition. Commonly used terms may be adopted without definition, but their usage must consider their specific technical definition, e.g., “quantity” ([7] entry 1.1) or different terms for

expressing abundance such as concentration, mass fraction, molality, which cannot be used synonymously. Alternatively, new specific terms may be coined. When choosing a term, possible ambiguities must be considered.

When an entry is transferred from an IUPAC Recommendation into the Gold Book, it loses the context of the original publication. Where this might lead to any confusion, a descriptive phrase should be added to the term. For example, “calibrator in activation analysis” should be defined separately from “calibrator” ([7] entry 5.1).

For a term with several meanings, an explanatory adjective should be added in parentheses, and each version of the term should be treated as a separate entry, e.g., “configuration (electronic)” and “configuration (stereochemical)”.

Noun-noun phrases (e.g., “laboratory bias”) should be listed alphabetically as if they were a single word. They can be listed under the headword as well (e.g., “bias, laboratory”) with a cross-reference to the main entry.

4.7.2 Definitions of terms

The definition should conform with the structure of a terminology entry (Section 4.7.6).

The Gold Book [8] should be inspected to ascertain if a particular term has been previously defined within IUPAC. If it has, but there is a need to repeat the definition, then the original wording should be retained, whenever possible. If the wording needs to be changed, e.g., if the original is too technical for a more general audience or if general terms need to be supplemented with more specific ones, then the changes should be kept to a minimum and justifying reasons given in an explanatory note, together with a reference to the original source.

To avoid confusion in the wider scientific community, definitions should consider and, if appropriate, reference recommendations by other authoritative bodies.

4.7.3 Referencing and sources

When a revised term has been defined previously in an IUPAC Recommendation, the original source should be cited with a note “Entry replaces IUPAC Recommendation [34] entry 1.23”. If the term has been defined by another authoritative body, the entry may be amended from the source, but the source should be referenced.

A reference should be styled as “Source: [7] p. 234”, “Source: [49] entry 3.123”, “Source: IUPAC Recommendation [34] entry 1.23”. Authors should bear in mind that Gold Book entries are not static and may change over time. Therefore, the original source should be cited, not the Gold Book entry.

4.7.4 Sorting and indexing of terms, abbreviations, and symbols

Glossary terms are sorted in alphabetical order. If the glossary contains more than one section, terms are arranged in alphabetical order within sections.

If a glossary is divided into two or more sections, an index is required to help the reader navigate to a particular entry. This should come after the main text and before the references. The index is a list of terms in alphabetical order with page numbers or other suitable cross-references. The index should include synonyms and can include terms that are not glossary entries. In these cases, the index should cross-reference the relevant main entry.

Abbreviations and symbols should be given as individual lists, separate from the main index.

4.7.5 Cross referencing within a glossary

A defined term mentioned outside its own glossary entry should be written in *italic* font. In the Gold Book, all cross references are hyperlinked to the appropriate entry.

4.7.6 Format of a glossary entry

The general outline of the structure of a terminology entry is given below. Carefully note the use of punctuation and different typefaces and the prescribed lines for an entry. Entries do not have to include all lines of entry shown in the outline.

Line of entry	Comment
preferred term (abbreviation), word class, <i>symbol</i>	Use lower-case bold type for term, except when a proper name is part of the term. Abbreviations are optional and are printed in the same typeface as the preferred term. The word class is only necessary if the term can be used in different lexical classes and is given as an italicized abbreviation: <i>n.</i> (noun), <i>v.</i> (verb), <i>adj.</i> (adjective), <i>adv.</i> (adverb). If the term refers to a physical quantity, a symbol (in italics) should be chosen in line with recommendations in Ref. [1].
synonym(s)	Add if necessary and cross-reference the preferred entry as “See: <i>preferred term</i> ”.
obsolete term (obsolete)	Obsolete terms may be encountered in the literature, but are no longer in use, e.g., “gram-molecular weight”.
superseded term (superseded)	Superseded terms can still be found in the literature, but can be expressed in preferred terms, e.g., “relative density” rather than the less clear, superseded “specific gravity”.
not acceptable term (not acceptable)	Not acceptable terms are unsuitable synonyms, e.g., “optical density” or “extinction” are not acceptable as synonyms for “absorbance”; “number of moles” is not acceptable for “amount of substance”. A note should be added explaining why a term is not acceptable. The distinction between obsolete, superseded and not acceptable terms is somewhat arbitrary. The inclusion of obsolete, superseded or not acceptable terms may help readers find the recommended term.
definition of term	Use one or more complete sentences, i.e., starting with a capital letter and ending with a full stop. Avoid repeating the term or using phrases such as “Term describing ...”. A defining equation or an algorithm may be part of a definition. Mathematical equations should be written using quantity symbols, not quantity names. All quantity symbols in the equation must be identified. When defining terms involving a ratio of two quantities, use of a mathematical formula or the phrase “divided by” is recommended for clarity. Phrases like “x per unit y” should never be used, as they confuse physical quantities and units, and can be ambiguous.
Note 1, 2, 3, ...:	Explanatory notes can be added here, as many as necessary. Figures and tables are allowed in notes. The SI unit, if it exists, shall be given in a note, together with other units in common use. Reasons why a term is not acceptable can appear in a note. Notes may be referenced.
Example 1, 2, 3, ...:	Examples of the definition are added after notes, or after a note to which it pertains. Examples may be referenced in other entries.
Related terms:	Cross-reference related terms (see also Section 4.7.5).
Source:	See Section 4.7.3

5 Membership of the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS) for the period 2020–23

Chair: Jürgen Stohner (Switzerland); **Secretary:** D. Brynn Hibbert (Australia); **Titular Members:** Milan Drábik (Slovakia), Jan Kaiser (UK), Gerard P. Moss (UK); **Associate Members:** Linda Johnston (Canada, 2022–23), Juris Meija (Canada), Amelia P. Rauter (Portugal, 2022–23), Marcy Towns (USA, 2020–21); **Division Representatives:** Michael A. Beckett (UK, 2022–23), Jiazhong Chen (USA, 2022–23), Rita Cornelis (Belgium, 2020–21), Ture Damhus (Denmark, 2020–21), Petr S. Fedotov (Russia, 2020–21), Jeremy Frey (UK, 2022–23), Pavel Karen (Norway), M. Clara

F. Magalhães (Portugal), Graeme Moad (Australia, 2020–21), Amelia P. Rauter (Portugal, 2020–21), Ronald Weir (Canada, 2020–21), Irina Perminova (Russia, 2022–23).

References

- [1] Quantities, Units and Symbols in Physical Chemistry, 3rd ed. (IUPAC **Green Book**). Prepared for publication by E. R. Cohen, T. Cvitaš, J. G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H. L. Strauss, M. Takami, A. J. Thor, RSC Publishing, Cambridge, UK (2007), ISBN 978-0-85404-433-7 <https://iupac.org/what-we-do/books/greenbook>.
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- [6] Evaluation of measurement data – Guide to the expression of uncertainty in measurement (**GUM**). Joint Committee for Guides in Metrology JCGM 100:2008 <https://www.bipm.org/en/committees/jc/jcgm/wg/jcgm-wg1-gum>.
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- [8] Compendium of Chemical Terminology, 2nd ed. (IUPAC **Gold Book**). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997), ISBN 0-9678550-9-8 Online version 3.0.1 (2019–) created by S. J. Chalk. <https://doi.org/10.1351/goldbook>.