

International Union of Pure and Applied Chemistry

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Minutes of the ICTNS Meeting at the IUPAC GA 2011, San Juan, Puerto Rico, 31 July and 01 August 2011

1. Opening remarks and introduction of participants

Prof. Ron Weir called the meeting to order at 09:05, welcomed the participants and asked them to introduce themselves.

The following persons signed as present (acronyms used later in this report, as well as acronyms indicating their relation to ICTNS, are given in parenthesis):

Chair:

Prof. Ron D. Weir (RDW)

Secretary:

Prof. Bernardo J. Herold (BJH)

Titular members:

Prof. Jürgen Stohner (JS)

Dr. Gerry Moss (GM)

Associate members:

Prof. Amélia Pilar Rauter (AR)

Divisional representatives:

I. Physical and Biophysical Chemistry
Dr. John H. Dymond (JD)

II. Inorganic Chemistry
Dr. Norman E. Holden (NH)

III. Organic and Biomolecular Chemistry
Prof. Pietro Tundo (PT)

IV. Polymer
Prof. Richard G. Jones (RJ)

V. Analytical Chemistry
Prof. Brynn Hibbert [also representative of IUPAC
on BIPM¹-JCGM² Working Group 1 (GUM³)] (BH)

VI. Chemistry and the Environment
Dr. Petr S. Fedotov (PF)

VII. Chemistry and Human Health

¹ Bureau International des Poids et Mesures

² Joint Committee for Guides in Metrology

³ Guide to the Expression of Uncertainty in Measurement

Dr. Yvonne C. Martin	(YM)
VIII. Chemical Nomenclature and Structure Representation	
Prof. G. Jeffery Leigh	(JL)
Representatives of other organizations:	
BIPM ¹ Dr. Robert Wielgosz	(RW)
ISO/TC12 ⁴ Prof. Anders Thor	(AT)
The following remaining members of ICTNS had presented their regrets in writing:	
Prof. Monica Nordberg (Titular member)	
Prof. Jack Lorimer (Associate member)	
Prof. Hiroshi Ogino (Associate member)	
Also present were	
Prof. Kazuyuki Tatsumi, Vice-President IUPAC	(KT)
Prof. Paul De Bièvre, representative of IUPAC on BIPM-JCGM ² and its Working Group 2 (VIM ⁵)	(PB)
Dr. Ales Fajgelj, President of Division V and representative of IUPAC on BIPM-CCQM	(AF)
Dr. Zoltán Mester, Titular Member of Division V	(ZM)
Prof. Roberto Marquardt, Chair Commission I.1, Physicochemical Terminology, Symbols, and Units	(RM)
Prof. Robert J. Hinde, Member of Commission I.1,	(RH)
Dr. Fabienne Meyers, Associate Director IUPAC	(FM)

2. Approval of agenda

The Agenda had been made available to the members of ICTNS online previously to the meeting. *BH* suggested that there should be a standard format for files within IUPAC. *RW* asked for information on the terms of reference and membership of ICTNS. After *RDW* replying to these and other questions, and pointing out that item 12 “other business” allowed the introduction of sub-items and thus the discussion of subjects arising during the meeting, the Agenda was approved unanimously.

3. Minutes of Glasgow meeting, 02-03 August 2009

Attachment item 3

The minutes of the ICTNS meeting in Glasgow on 02-03-August 2009 had been made available online to the members of ICTNS as annex to the Agenda. *GM* asked to correct the typo *GP* to *GM* regarding the abbreviation of his name in item 1. The minutes were approved, with the condition that this correction is made.

4. Minutes of the Lisbon core members’ meeting, 09-10 April 2010

Attachment item 4

The minutes of the ICTNS core members’ meeting in Lisbon, 09-10 April 2010 had been made available online to the members of ICTNS as annex to the Agenda. The minutes were approved.

⁴ International Organisation for Standards, Technical Committee 12, Quantities and Units

⁵ International Vocabulary of Basic and General Terms in Metrology

5. Business arising from the Glasgow and Lisbon meetings

5.1 Glasgow minutes

RDW opened a discussion on the revision of IUPAC books.

BH, regarding the revision of the Green Book, appealed to those responsible to take into account GUM and VIM.

5.2 Lisbon minutes

Regarding item 4.2 IUBMB International Union of Biochemistry and Molecular Biology, *RDW* reported about the outcome of the controversy regarding the manuscript *Recommendations for Nomenclature and Databases for Biochemical Thermodynamics* by Alberty and Goldberg: The manuscript was published elsewhere in spite of all efforts for a conciliation. *JD* said he felt disappointed. *GM* explained the situation in more detail. *RDW* said he regrets what had happened.

Regarding item 4.3, International Vocabulary for Metrology (VIM), it was regretted that no action has been taken since the Lisbon meeting to implement the motion that had been approved. *RDW* promised to look to it. *BH* and *RW* wish all IUPAC publications to be in accordance with VIM.

Regarding item 6.1 PAC-REP-08-01-13 *Explanatory Glossary of Terms Used in Expression of Relatively Stable Isotope Ratios* by Coplen, *RDW* explained that the controversies reported in Lisbon were the reason for a joint meeting with Committee I.1 to be held later on the same afternoon.

Regarding item 6.2 PAC-REP-09-01-05 *Correction for the ^{17}O Interference in $\delta(^{13}\text{C})$ Measurements when Analyzing CO_2 with Stable Isotope Mass Spectrometry* by Brand, Assonov and Coplen, *RDW* reported that the authors accepted the objections of ICTNS review, and the manuscript will be published.

Regarding item 7 Review of the New Blue Book, *BJH* expressed his disappointment by the delay in Division VIII submitting the manuscript to ICTNS. *GM* explained that there are still some substantial questions on which no agreement could be reached within Division VIII. *GL* alluded to other points that are still being discussed. *BH* drew a parallel to what was happening with the Orange Book.

RDW exemplified the kind of difficulties in obtaining a consensus between authors of recommendations and scientists working in a given area, by reporting on comments about the new definition of the year.

GM stressed the importance of the text by Ian Mills and Val Metanomski, on italicization⁶, written for authors who wished to submit manuscripts for publication in Pure & Applied Chemistry. He added however that it had to be updated, and asked whether there was a mechanism to do that. *BH* reminded that BIPM uses bold characters where IUPAC uses italics, and suggested that this circumstance should be taken into consideration.

⁶ I. M. Mills and W. V. Metanomski, On the use of italic and roman fonts for symbols in scientific text, Interdivisional Committee on Nomenclature and Symbols, IUPAC, December 1999. Web version under http://old.iupac.org/standing/idcns/italic_roman.html

6. Chairman's biennial report

Attachment item 6

The Chairman *RDW* was congratulated for the clear definition of the terms of reference of ICTNS in his report and that the Bureau has supported the reaffirmation of the role of ICTNS in their meeting 07 – 08 April 2010 in Sofia, regarding the reticence of some authors to follow IUPAC Recommendations. *BH* declared that Division V does also support ICTNS in the controversies at stake. *KT* expressed his hope that a compromise would be reached regarding the controversial manuscripts.

After discussion, the report was approved unanimously.

7. Reports from IUPAC Division Representatives

7.1. Division I Physical and Biophysical Chemistry

Attachment item 7.1

JD presented the report of Division I, which had been circulated together with the agenda. In the ensuing discussion *JD* mentioned a set of two unpublished manuscripts by Manuel Ribeiro da Silva on terminology and methods in Thermochemistry. *RDW* reminded that in the beginning there was only one manuscript, which had the characteristics of both a recommendation and a technical report. At the request of ICTNS the author divided the manuscript in two parts, one being a recommendation and the other one a technical report. These two manuscripts had still to be revised. The revised versions needed however previous review and approval by Division I. *RDW* recommended as a solution to the problem that an entirely new project should be proposed dependent, of course, on the wishes of professor Ribeiro da Silva.

The question whether the publication of the results of an IUPAC project in a journal other than IUPAC as “funded by IUPAC” need to conform to IUPAC rules on units, symbols, etc. was again discussed. *RDW* stressed that fact that some journals do not demand such conformity does not invalidate the decision of ICTNS that “Permission of any outcome of any IUPAC project elsewhere than in Pure & Applied Chemistry should be given on condition of conformity with IUPAC recommendations on terminology, nomenclature and symbols” (see Glasgow minutes item 5.2.1.). *AR* recommended that this requirement should be included in the information to submitters of project proposals.

The biennial report of Division I was approved.

7.2. Division II Inorganic Chemistry

Attachment item 7.2

NH introduced the report, which had been previously circulated together with the agenda and provided updated information on the Division II activities.⁷

During the ensuing discussion *RW* asked some questions about the publication on the definition of the year (within project 2006-016) and drew the attention of the meeting to the “BIPM Comments on the IUPAC-IUGS common definition and convention on the use of the year as a derived unit of time (IUPAC Recommendation 2011)”, (Appendix 7 of the report of BIPM to IUPAC to be presented and discussed under item 8.1 of the Agenda).

⁷ The oral update was followed by the remittance on 2011-09-08 of an updated, report, which is now added to the previous one in Attachment item 7.2

Regarding the same project 2006-016 “Recommendations for isotope data in geosciences” *RW* referred to Annex 8 of the same BIPM report, a draft with the title “The Selection of Values and Uncertainties for Atomic Weights in the Gas Metrology Community”.

BH mentioned that his report, as representative of IUPAC on GUM, of the meeting at the BIPM on 24-27 May 2011 (Attachment 2 to Agenda Item 8.1) also deals under section G1, page 6-7, with the problem of “Evaluation of uncertainty associated with atomic weights”. In spite of being the official IUPAC representative on BIPM¹-JCGM² Working Group 1 (GUM³) he was not informed by Division II.

GM questioned whether IUPAC should not have their own publication of isotope tables, instead of having them only in the CRC Handbook of Chemistry and Physics.

The biennial report of Division II was approved after the conclusion of the discussion.

7.3. Division III Organic and Biomolecular Chemistry

Attachment item 7.3

PT presented the biennial report of Division III and completed it with additional information.

In the discussion that followed *RW* mentioned that ISO standards on Biotechnology include terminology and that there will be a meeting on that subject that BIPM will attend. He asked if IUPAC would also attend the same meeting.

After discussion the report was approved.

7.4. Division IV Polymer

Attachment item 7.4

RJ introduced the report as made available to the participants prior to the meeting together with the Agenda and answered questions from the participants. The report was approved

7.5. Division V Analytical Chemistry

Attachment item 7.5

BH introduced the report as made available to the participants prior to the meeting, together with the Agenda and answered questions from the participants. The report was approved.

7.6. Division VI Chemistry and the Environment

Attachment item 7.6

PF introduced the report as made available to the participants prior to the meeting, together with the Agenda and answered questions from the participants.

In the ensuing discussion, regarding terminology it was recommended that, when IUPAC books were published, the authors should be asked to include glossaries. During the discussion of the report it became clear that none of the published books had been seen by ICTNS. This is in contradiction with the decision of ICTNS mentioned in the Glasgow minutes, items 5.2.1 and 5.2.2. The representative of Division VI was informed that, in future, the manuscripts had to be submitted to ICTNS prior to publication, in order to obtain the permission to publish.

The report was approved.

7.7. Division VII Chemistry and Human Health

Attachment item 7.7

YM introduced the report as made available to the participants prior to the meeting, together with the Agenda and answered questions from the participants. The report was approved.

7.8. Division VIII Chemical Nomenclature and Structure Representation

Attachment item 7.8

JL introduced the report as made available to the participants prior to the meeting, together with the Agenda, completed it with additional information and answered questions from the participants. The report was approved.

8 Reports from Representatives of Other International Organizations and from Delegates of IUPAC on the same organizations

8.1 BIPM (Bureau International des Poids et Mesures)

Attachments 1, 2.1 and 2.2, item 8.1

RW presented the report of BIPM made available to the participants as attachment to the Agenda (Attachment 1, item 8.1) and answered comments and questions.

During the ensuing discussion, the support of ICTNS for the proposals for the redefinition of SI units including the mole, decided in the Glasgow meeting (item 8.2.4 of the Glasgow minutes) was reiterated.

AF expressed his wish to propose an interdivisional project in order to evaluate the consequences of the new definition of the mole for the various branches of Chemistry. *RDW* informed that anyone might submit a project proposal. All relevant divisions can be included, but ICTNS would have to judge the output.

PB and *RM* made comments in support of the decisions of ICTNS at the Glasgow meeting 2009.

PB reported about his activities as representative of IUPAC on BIPM¹-CCGM² Working Group 1 (VIM⁵): VIM⁴ will not be published very soon, whereas VIM³ will be subject to approval in December 2011. It was released online on 15 June 2011 and is expected to be published soon in *Pure & Applied Chemistry*.

RDW confirmed that IUPAC supports VIM³.

PB informed that the question of including nominal properties in VIM⁴ is being considered. Documents on his contributions can be found in Attachment 2.1 item 8.1.

BH reported about his activities as representative of IUPAC on BIPM¹-CCGM² Working Group 2 (GUM³). For that effect he displayed on the screen his "Notes of the meeting held at BIPM on 24 – 27 May 2011" (see in Attachment 2.2 item 8.1). He asked what IUPAC would do in order to publicize VIM and GUM. The revision of GUM will come out in 3 or 4 years. At the above-mentioned meeting at BIPM he raised the problem of the evaluation of uncertainty associated with atomic weights (paragraph G1, page 6 of the same notes) at the request of IUPAC.

PB commented the appended paper by Antonio Possolo⁸ "Contribution to a JCGNM-WG1 Discussion of IUPAC's Definition of Atomic Weights" and drew the attention of the meeting to the fact that different groups are using the term 'distribution' with different meanings.

⁸ From the Statistical Engineering Division, Information Technology Laboratory, National Institute of Standards and Technology, United States Department of Commerce

RW added at the end of the discussion of these reports, that IUPAC has the right to publish JCGM documents with its own logo, as a consequence of an agreement among the six organizations involved.

8.2 ISO/TC12 International Organization for Standardization / Technical Committee 12 – Quantities and Units

Attachment item 8.2

The attached report was gratefully acknowledged, but due to the absence of the representative of ISO/TC12, the report was not subjected to any discussion.

8.3 IUBMB International Union of Biochemistry and Molecular Biology

Attachment item 8.3

GM added some information to the document provided, explaining the relation between IUPAC in IUBMB in JCBN Joint Committee on Biochemical Nomenclature, where *GM* represents IUPAC.

8.4 IUCr International Union of Crystallography

Attachment item 8.4

The attached report was gratefully acknowledged, but due to the absence of the representative of IUCr, the report was not subjected to any discussion.

8.5 IUNS International Union of Nutritional Sciences

No written report had been received.

8.6 IUPHAR International Union of Basic and Clinical Pharmacology

Attachment item 8.6

The attached report was gratefully acknowledged, but due to the absence of the representative of IUPHAR, the report was not subjected to any discussion.

8.7 IUPAP International Union of Pure and Applied Physics

Attachment item 8.7

The attached report was gratefully acknowledged, but due to the absence of the representative of IUPAP, the report was not subjected to any discussion.

9 Update on status of ‘colour’ books

9.1 Gold Book

There has been no substantial change in the status of the Gold Book since 2009. The conclusions of the discussion held at the Glasgow ICTNS meeting (see item 9 of the Glasgow minutes in attachment item 3 of the present minutes) still apply. It has to be admitted that in spite of the recommendations made in Glasgow, no action was taken by ICTNS.

FM confirmed that the questions raised in Glasgow are still open.

BH considers that the present situation is not tenable, but that rather than stop altogether the online version of the Gold Book it would be better to continue it as a mere collection of terms.

BJH suggested that the online version should have the possibility, like in Wikipedia, for users to make comments for improvement (dialogue boxes?).

RDW asked whether he should report the situation to CPEP.

JS asked if it would not be better to propose a task group for a preparing a database project for all divisions.

RDW reminded the meeting of the decision made in Glasgow (item 9.3 of the minutes).

FM said she would contact the Chair of CPEP.

PB asked whether the terms as defined in VIM3 would become part of the Gold Book. *BH* does support this proposal.

In *GM*'s opinion the Gold Book is 'invisible'. It should be more publicized.

It was concluded by the meeting that the solution of all the problems raised with respect to the Gold Book transcends the resources of ICTNS and that IUPAC should look at these problems at a higher level.

9.2 Green Book

BH mentioned the fact that the pdf version of the Green Book is not searchable. *JS* replied that he would look into this matter.

JS thinks that a general policy for the updating of colour books should be put in place, and not just for the Green Book.

9.3 Purple Book

The question was raised whether it would be possible to have an online version of the Purple Book, as is already the case for the Green and the Red Book. *RJ* alluded to the problem of having repaginated the Purple Book if updates were periodically included. *JS* explained that the possibility of online edition of the Purple Book would depend on the terms of the contract with RSC Royal Society of Chemistry. *BH* would prefer e-books instead of pdf files. *JS* is of the opinion that printed books should be always kept in parallel. *RDW* will ask CPEP whether there is general policy on colour books.

RDW raised the question whether IUPAC could not be its own publisher for the colour books.

9.4 Orange Book

BH informed that the Orange Book would be made accessible to Division V members through Wiki. He mentioned that in his opinion there should be a general policy on terms. New terms should be in conformity with VIM. *RW* stressed that VIM is however not a glossary.

9.5 Silver book

YM was asked to present to ICTND information about the Silver Book after the General Assembly.

9.6 Red Book

JL informed that the Red Book has been put online, but nothing that nothing else has been done about the Red Book.

9.7 Blue Book

The subject was considered as having been already treated in item 7.8. It was regretted that the approval of a final version by Division VIII has been a process extending now over 15 years

10 Update on status of ‘IUPAC’ approved books published outside IUPAC

The publications reviewed, edited and approved by ICTNS for publication elsewhere than by PAC in the last biennium consist of the three books already mentioned in the Chairman’s report (see item 6).

Four books are mentioned in the report Division 6 (see item 7.6), which were not submitted to ICTNS for review as required.

11 Memberships 2012-2013

The following members, whose term of office ends by 31 December 2011, cannot be re-elected, according to the IUPAC by-laws, because they have reached the maximum statutory limit of years in IUPAC bodies:

Bernardo Jerosch Herold (secretary)

John D. Lorimer (associated member, former chairman).

An associated member, whose mandate also finishes by 31 December 2011, remains however still eligible: Amélia Pilar Rauter (associated member).

The terms of all other titular and associated members continue until 2013.

This situation requires the appointment of a new titular member for the period 2012-2013 and of one of the titular members as secretary for the same period.

The terms of all division representatives terminate after each period of two years and have to be renewed. Regarding the representatives of other organizations, IUPAC accepts the appointments made by the same organizations.

12 Other business

GM considers that the recommendation “Use of Italic and Roman Fonts for Symbols and in Scientific Text by I. M. Mills and W.V. Metanomski, December 1999⁹ and its more recent version, slightly revised by ICTNS in 2007¹⁰, needs updating and intends to propose a project for that purpose.

BH expressed the opinion that *Pure & Applied Chemistry* should present definitions of terms according to standards of ISO, and advocated a debate on consistency of definitions.

AR announce that there will be proposed a project on abbreviations in nomenclature with a task group chaired by Margaret Bramble (Division III) and with Richard Hartshorne (Division VIII) and herself as members. It should also include a member from Division IV.

13 Adjournment

Before the meeting was adjourned the following two meetings had taken place: Joint meeting of ICTNS with Division I.1 and another joint meeting with Division II.1 on 31 July and 01 August respectively at 16:00.

⁹ World Wide Web version http://old.iupac.org/standing/idcns/italic_roman.html or download as pdf-file from the same address,

¹⁰ <http://old.iupac.org/reports/provisional/guidelines.html>

The meeting was adjourned on the afternoon of 01 August 2011.

Summary of the Joint Meeting of ICTNS and Division I.1 Commission on Physicochemical Symbols, Terminology, and Units, at 16:00 31 July 2011

RDW welcomed the participants from Commission I.1. who had not been present during the preceding session of the ICTNS meeting, namely its member Robert J. Hinde (*RH*), The chair and secretary respectively *RM* and *JS* were also present, as well as in the preceding session of ICTNS.

RDW opened the discussion by expressing his wish for more flexibility in the Green Book, which would allow smoother discussions with some certain authors of *Pure & Applied Chemistry*. The use of per mille and 'ppm' was quoted as an example.

JS perceives this comment as blaming Div. I.1 for not being sufficiently reactive to comments on the Green Book. He mentioned that one of the members of Di.I.1 is from ISO and that 'ppm' is deprecated by ISO, although SI accepts it.

RM stated that he does not want to make changes to the Green Book before the next printed edition.

JS asked if changes could be the object of a recommendation published in *Pure & Applied Chemistry*.

RDW suggested that an author who does not want to change a manuscript in order to conform to a given determination of the Green Book might petition Div.I.1. *RDW* asked also whether it would be possible to have the Green Book online, even at the cost of paying a royalty to RSC.

JS offered to contact RSC through IUPAC for specifying the time after which the Green Book can be openly accessible online. The 3d edition of the Green Book is presently online.

RDW expressed his opinion that an updated version of the Green Book is needed every year and hard copies every five years.

RM disagreed and suggested instead yearly articles in pdf on the web, pointing out the necessary updates.

RDW concludes that such a policy requires approval by senior IUPAC management.

AR criticized the citation of references without title and last page of a paper.

JS suggests the creation of a single page on the IUPAC website, where all typos of colour books would be recorded.

RM suggests a forum in *Chemistry International* showing examples of good use of symbols and units.

JS considers that the Green Book should be more advertised and to create a 'Green Brochure'.

RW admitted that he did not know that the Green Book was online, and criticized that it is not very visible on the IUPAC website. *PB* confirmed that too many people do not know at all about the existence of the Green Book.

Before adjourning this joint meeting, the composition of Commission I.1 was discussed. It was recommended to include more titular members, in order to cover more fields of Chemistry and related sciences.

Summary of the Joint Meeting of ICTNS and Division II.1 Commission on Isotopic Abundances and Atomic Weights (CIAAW) at 16:00 01 August 2011

RDW welcomed the participants from Division II.1. Inorganic Chemistry, who had not been present during the preceding session of the ICTNS meeting, namely Robert Loss (*RL*), President of Division II.),

RL presented the regrets of the chair, secretary and remaining members proper of CIAAW, who had a meeting at this time elsewhere.

RDW reported on a manuscript submitted by CIAAW, which could not be published in Pure & Applied Chemistry, because of the refusal of one of the authors to introduce some minor changes necessary for conformity with the Green Book.

RL admitted that the Division II Committee had no control of the activities and the output of CIAAW and that probably a manuscript not approved by ICTNS would eventually be published elsewhere.

RS offered to send after the conclusion of the meeting a note with comments on the above mentioned manuscript. The notes which were received on 15 December 2011 are here reproduced and followed by the reproduction of a chapter of the "Handbook of High Resolution Spectroscopy" by Stohner and Quack, Wiley, 2011:

**Comment on the Topic of the Joint Meeting of ICTNS and Division II.1
Commission on Isotopic Abundances and Atomic Weights (CIAAW) at the IUPAC GA
2011, San Juan, Puerto Rico by JS and RM**

This written comment is intended to supplement and clarify the discussion concerning the Coplen Paper and difficulties associated with it and relates directly to the Comments by Bob Loss at the ICTNS Meeting. We take the liberty to this written comment because the Meeting was shifted without pre-announcement such that the Chairman of I.1 (RM) could not attend.

General Comments

We should first note that we agreed on including some information on the isotope delta in the next (4th) edition of the Green Book including an example. This has been communicated to Dr Coplen in emails dated 14 July 2007 and 17 July 2007.

A draft (2010/12/12) has been created to show as we think the isotope delta could be included in some forthcoming edition/printing of the Green Book. Therefore, Section 3.10.1 has been enlarged as much as possible keeping in mind that the layout of the book should not be affected too much. Due to limited space, we cannot make use of the full text mailed to us by Dr Brand in his letter dated 20 May 2010.

Dr Brand's letter collects various ways to write the "isotope delta". Each discipline has its own jargon and a tendency to stick with that. The wish or demand, however, that a notation or a symbol should be retained because it is frequently used in the published literature since decades does not at all justify its use. We would never get rid of pounds, miles, calories, angstrom, etc. if this would be a valid argument.

The Green Book presents a list of recommendations and it should help the general reader (not only a scientist working in his own particular field) in what is termed a good practice of scientific language. "If there are several well established uses or conventions, these have been mentioned, giving preference to one, when it is useful, but making allowance for variety, if such variety is not

harmful to clarity ... In cases where certain common uses are deprecated, there are very strong reasons for this and the reader should follow the corresponding advice."

Very many writings for the same quantity ("isotope delta") do exist in the literature or even in the same document; they are obtained by omitting qualifying information like sub- and superscripts. We believe that this is harmful for clarity to all scientists not working in the field of isotope research.

In a scientific paper, submitted to any publisher, an author is free to use his own jargon omitting or even changing definitions of certain quantities referred to in the paper. However, when IUPAC is involved, we are convinced that striving for highest possible clarity should not be a matter of discussion.

The two pages from section 3.10 of the Green Book, as mentioned above, show a good compromise how the "isotope delta" can be included in the text in a justifiable way especially in view of all our readers of the Green Book.

Comments on *Chemistry International*, July-August 2011 Issue, Supplement on "Isotopic Abundances and Standard Atomic Weights"

It is stated that "The atomic weight of an element is calculated from the sum of products of the atomic mass¹ and the isotopic abundance² of each stable isotope of that element." This is wrong. Reference ¹ (G. Audi et al., Nucl. Phys. A 729, 337 (2003) states on page 339 that "The atomic masses are given in mass units ... For the atomic mass unit we use the "unified atomic mass unit", symbol "u" ..."

Consequently, the products from the atomic masses and the abundances must be masses with unit "u". Therefore, all worked examples appearing in the second column of the supplement are wrong.

It should be noted that this supplement did not receive ICTNS approval as it was not submitted to ICTNS for reviewing.

Comments on *Chemistry International*, November-December 2011 Issue, page 32f

The guidelines (see Reference 1, Rapid Commun. Mass Spectrom. 25, 2538 (2011)) is not an IUPAC Recommendation nor is it approved by ICTNS. The authors recommend the use of "ppm" and "per meg" .

Comments of the letter of Bob Loss (dated 30 November 2010)

(1) The fact that the symbol is used for six decades seems not a valid argument to me. It can be used in the lab or any publication if the authors feel that way. However, in an IUPAC publication or recommendation, it must not be used in first place.

(2) A symbol should be explained/defined in the text where it is used for the first time and then a shorthand notion is acceptable, although probably not clear to a general reader. The final decision is with the Editor of the corresponding journal.

(3) The use of permille needs not to be discussed, see section 3.10.1 and shown examples in the printed hardcopy of the Green Book. ppt in place of permille, however, is deprecated (deprecating certain symbols, units etc. is not the business of the Green Book; it is rather an ISO decision). Note that percent and permille are not part of the SI and ISO recommends that they should never be used!

(4) Qualifying sub- or superscripts or both are perfectly accepted on an equal footing to, for example, giving the information in parentheses. The Green Book is full of examples where this can be seen.

Some historical Remarks from Email correspondence with TC

12 July 2007, JS to TC

Review period ended 31 March 2006; most comments, however, have been considered. To add an example for the delta terminology was too late at this stage of printing. Our answer was supported by ICTNS.

12 July 2007, TC to JS

"I am pleased that you and your colleagues have taken into account our comments and I appreciate your efforts."

14 July 2007, JS to TC

"We do not object to add it in the next edition."

Permille, percent, ppm, etc.

Still some dissatisfaction remains with the "replacement" column of Table 3.10.2. This section is concerned with deprecated usage. Various changes have been made to clarify the obvious misunderstanding raised by TC. See especially the last suggested changes published by Stohner and Quack in the "Handbook of High Resolution Spectroscopy", Wiley, 2011 (attached).

Furthermore, it is illustrative to look into some NIST documents:

NIST-sp811 Guide to the SI

A. Thompson, B.N. Taylor, Guide for the Use of the International System of Units (SI), 2008 Edition

1. Check list for reviewing manuscripts, Entry (3), Page v

"The combination of letters 'ppm', 'ppb', and 'ppt', and the terms part per million, parts per billion, and parts per trillion, and the like, are not used to express the values of quantities."

2. Section 7.10.3 **ppm, ppb, and ppt**, Page 20

"In keeping with Ref. [4: ISO 31-0], this Guide takes the position that the language-dependent terms part per million, part per billion, and part per trillion, and their respective abbreviations `ppm', `ppb', and `ppt' (and similar terms and abbreviations) are not acceptable for use with the SI to express the values of quantities. ... it is best that they be avoided entirely ...; the preferred way of expressing large numbers is to use powers of 10. This ambiguity in the names of numbers is one of the reasons why the use of ppm, ppb, and ppt, and the like are deprecated."

NIST-sp330

B.N. Taylor, A. Thompson, The International System of Units (SI), 2008 Edition

1. Section 5.3.7 **Stating values of dimensionless quantities, or quantities of dimension one**, Page 44

"... `ppb', `ppt', are also used, but their meanings are language dependent. For this reason the terms ppb and ppt are best avoided."

"* Editors' Note: The NIST policy on the proper way to employ the International System of Units to express the values of quantities does not allow the use of parts per million, parts per billion or parts per trillion and the like, nor the abbreviations ppm, ppb or ppt and the like. Further it only allows the use of the word `percent' and the symbol % to mean the number 0.01 in the expression of the value of a quantity..."

Conventions, Symbols, Quantities, Units and Constants for High Resolution Molecular Spectroscopy

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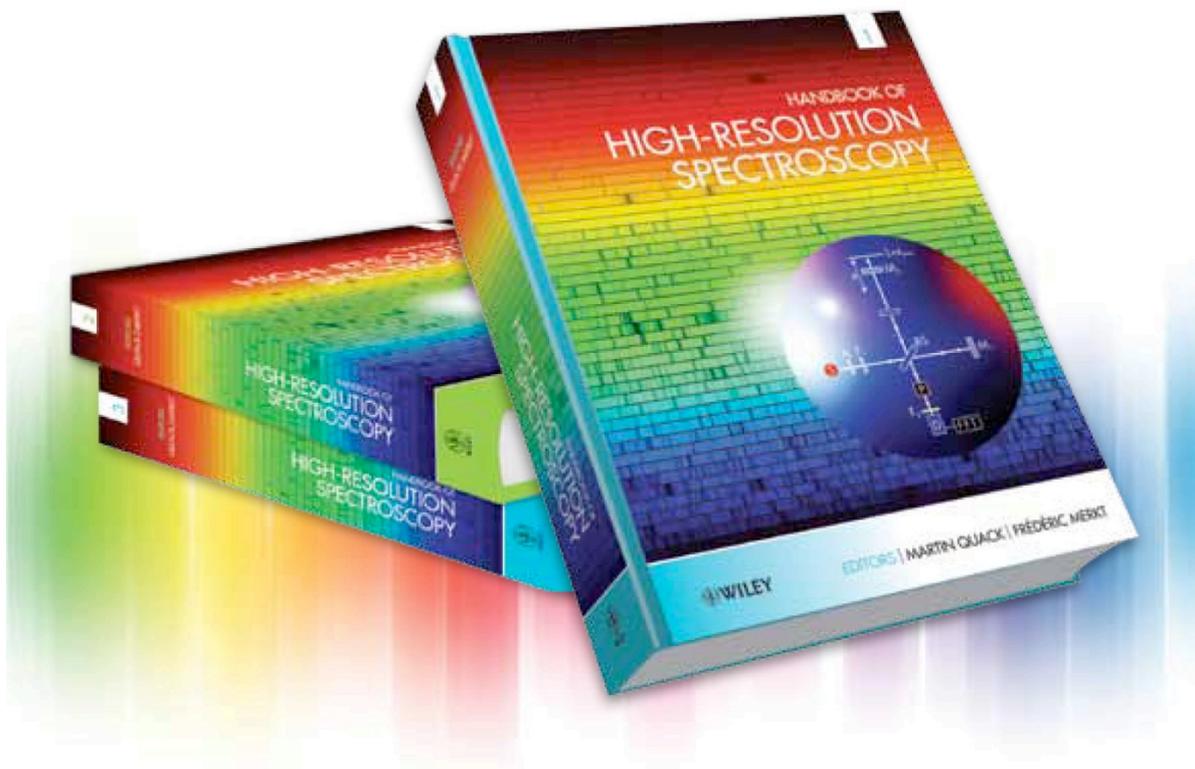
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1 INTRODUCTION

Conventions in spectroscopy, as conventions in science in general, are needed essentially for unambiguous use and exchange of scientific information and data. In essence, one has to define a consistent and correct usage of scientific language, similar to the usage of everyday language. At a first stage, every child learns language intuitively by taking over habits from parents. Similarly, scientists in a given field take over the habits and jargon of that field intuitively and requests for more precise definitions and rules are resisted frequently in both situations with comments of “triviality” on such efforts. However, for an unambiguous exchange of information between different groups of people, different fields of science and technology, a precise definition of language and, in particular, scientific language is primordial. The lack of a common, unambiguous scientific language can lead to enormous losses. A prominent example is the Mars Climate Orbiter story, which we may quote from the preface to Cohen *et al.* (2008):

A spectacular example of the consequences of confusion of units is provided by the loss of the United States NASA satellite, the “Mars Climate Orbiter” (MCO). The Mishap Investigation Board (Phase I Report, November 10, 1999)^a found that the root cause for the loss of the MCO was “the failure to use metric units in the coding of the ground (based) software file”. The impulse was reported in Imperial units of pounds (force)-seconds (lbf-s) rather than in the

metric units of Newton (force)-seconds (N-s). This caused an error of a factor of 4.45 and threw the satellite off course.^b

One can estimate that in the modern economic world, which is characterized by science and technology in most areas of everyday life, enormous economic losses still occur through inconsistencies in conventions and units. Indeed, such losses are expected to be quite gigantic on a worldwide scale compared to the example given above. Thus, there are great international efforts in providing conventions on symbols, quantities, and units in science and technology. The most prominent effort along those lines is clearly the development of the international system of units, the SI.

Turning specifically to the field of molecular spectroscopy, many of the habits and current language of this subfield of science can be found well represented in the famous set of books by Herzberg (1946, 1950, 1966). However, modern spectroscopy has many interactions with other branches of chemistry, physics, and engineering sciences.

A consistent summary of conventions in these areas closely related to spectroscopy can be found in the volume “Quantities, Units and Symbols in Physical Chemistry” (third edition, 2nd printing, Cohen *et al.* 2008) edited on behalf of IUPAC (third printing 2011).

In this article, we have drawn from this book those parts that are most relevant to spectroscopy and have supplemented them with a few examples referring specifically to spectroscopy. To avoid errors in transcription, many of the tables are taken over literally by permission in line with the general policy of IUPAC, favoring the widest possible dissemination of their publications.

Example

For the hydrogen molecule the equilibrium bond length r_e and the dissociation energy D_e are given by

$$r_e = 2.1 a_0 \quad \text{not} \quad r_e = 2.1 \text{ a.u.}$$

$$D_e = 0.16 E_h \quad \text{not} \quad D_e = 0.16 \text{ a.u.}$$

4.8 Quantities of Dimension One

Values of physical quantities of dimension one, frequently called *dimensionless quantities*, are often expressed in terms of mathematically exactly defined values denoted by special symbols or abbreviations, such as % (percent). These symbols are then treated as units and are used as such in calculations.

4.8.1 Fractions (Relative Values, Yields, and Efficiencies)

Fractions such as relative uncertainty, amount-of-substance fraction x (also called *amount fraction*), mass fraction w , and volume fraction φ are sometimes expressed in terms of the symbols in the table below.

Name	Symbol	Value	Example
percent	%	10^{-2}	The isotopic abundance of carbon-13 expressed as an amount-of-substance fraction is $x = 1.1\%$.
permille	‰	10^{-3}	The mass fraction of water in a sample is $w = 2.3\text{‰}$.

These multiples of the unit one are not part of the SI and ISO recommends that these symbols should never be used. They are also frequently used as units of “concentration” without a clear indication of the type of fraction implied, e.g., amount-of-substance fraction, mass fraction, or volume fraction. To avoid ambiguity, they should be used only in a context where the meaning of the quantity is carefully defined. Even then, the use of an appropriate SI unit ratio may be preferred.

Example

The mass fraction $w = 1.5 \times 10^{-6} = 1.5 \text{ mg kg}^{-1}$.
 The amount-of-substance fraction $x = 3.7 \times 10^{-2} = 3.7\%$
 or $x = 37 \text{ mmol mol}^{-1}$.
 Atomic absorption spectroscopy shows the aqueous solution to contain a mass concentration of nickel $\rho(\text{Ni}) = 2.6 \text{ mg dm}^{-3}$, which is approximately equivalent to a mass fraction $w(\text{Ni}) = 2.6 \times 10^{-6}$.

Note the importance of using the recommended name and symbol for the quantity in each of the above examples. Statements such as “the concentration of nickel was 2.6×10^{-6} ” are ambiguous and should be avoided.

The last example illustrates the approximate equivalence of $\rho/(\text{mg dm}^{-3})$ and $w/10^{-6}$ in aqueous solution, which follows from the fact that the mass density of a dilute aqueous solution is always approximately 1.0 g cm^{-3} . Dilute solutions are often measured or calibrated to a known mass concentration in mg dm^{-3} , and this unit is then to be preferred to using ppm (or other corresponding abbreviations, which are language dependent) to specify a mass fraction.

4.8.2 Deprecated Usage

Adding extra labels to % and similar symbols, such as % (V/V) (meaning % by volume), should be avoided. Qualifying labels may be added to symbols for physical quantities, but never to units.

Example

A mass fraction $w = 0.5\%$, but *not* $0.5\% (m/m)$.

The symbol % should not be used in combination with other units. In table headings and in labeling the axes of graphs, the use of % in the denominator is to be avoided. Although one would write $x(^{13}\text{C}) = 1.1\%$, the notation $100x$ is to be preferred to $x/\%$ in tables and graphs.

The further symbols listed in the table below are also found in the literature, but their use is not recommended. Note that the names and symbols for 10^{-9} and 10^{-12} in this table are here based on the American system of names. In other parts of the world, a billion often stands for 10^{12} and a trillion for 10^{18} . Note also that the symbol ppt is sometimes used for part per thousand, and sometimes for part per trillion. In 1948 the word billion had been proposed for 10^{12} and trillion for 10^{18} (Jerrard and McNeill 1980). Although ppm, ppb, ppt, and alike are widely used in various applications of analytical and environmental chemistry, it is suggested to abandon completely their use because of the ambiguities involved. These units are unnecessary and can be easily replaced by SI-compatible expressions such as pmol/mol (picomole per mole), which are unambiguous. The last column contains suggested replacements (similar replacements can be formulated as mg/g, $\mu\text{g/g}$, pg/g, etc., depending on the precise context). The advantage of these representations of the units (strictly speaking of dimension one) is to remind one of the definition of the quantity used in the equation (e.g., mass fraction), although that definition could be stated explicitly as well. While the mass fraction 5.65 ‰ in the example on the element Ti in the table below is replaced meaningfully by 5.65 mg/g, a replacement of the form 5.65 mA/A would not make much sense in connection

Name	Symbol	Value	Examples with a suggested replacement
part per hundred	pph ^(b) , ‰	10 ⁻²	The degree of dissociation is 1.5 ‰.
part per thousand, permille ^(a)	ppt ^(b) , ‰	10 ⁻³	A preindustrial value of the CO ₂ amount-of-substance content of the Earth's atmosphere was about 0.275 ‰ (0.275 ppt). The element Ti has a mass fraction 5.65‰ (5.65 × 10 ³ ppm) in the Earth's crust.
part per million	ppm ^(b)	10 ⁻⁶	The volume fraction of helium is 20 ppm. The proton chemical shift of chloroform is δ _H (CHCl ₃) = 7.27 ppm.
part per hundred million	pphm ^(b)	10 ⁻⁸	The mass fraction of impurity in the metal was less than 5 pphm.
part per billion	ppb ^(b)	10 ⁻⁹	The air quality standard for ozone is a volume fraction of φ = 120 ppb.
part per trillion	ppt ^(b)	10 ⁻¹²	The natural background volume fraction of NO in air was found to be φ = 140 ppt.
part per quadrillion	ppq ^(b)	10 ⁻¹⁵	

^(a)The permille is also spelled per mill, permill, per mil, permil, per mille, or promille.

^(b)Deprecated, see text.

with a mass fraction, although formally correct within the framework of quantity calculus.

4.8.3 Units for Logarithmic Quantities: neper, bel, and decibel

In some fields, especially in acoustics and telecommunications, special names are given to the number 1 when expressing physical quantities defined in terms of the logarithm of a ratio (Mills and Morfev 2005). For a damped linear oscillation, the amplitude of a quantity as a function of time is given by

$$F(t) = A e^{-\delta t} \cos \omega t = A \operatorname{Re}[e^{(-\delta+i\omega)t}]$$

From this relation it is clear that the coherent SI unit for the decay coefficient δ and the angular frequency ω is the second to the power of minus one, s⁻¹. However, the special names neper (Np) and radian (rad) (Sections 4.2 and 4.5) are used for the units of the dimensionless products δt and ωt , respectively. Thus the quantities δ and ω may be expressed in the units Np/s and rad/s, respectively. Used in this way, the neper (Np) and the radian (rad) may both be thought of as special names for the number 1.

In the fields of acoustics and signal transmission, signal power levels and signal amplitude levels (or field level) are usually expressed as the decadic or the napierian logarithm of the ratio of the power P to a reference power P_0 , or of the field F to a reference field F_0 . Since power is often proportional to the square of the field or

amplitude (when the field acts on equal impedances in linear systems), it is convenient to define the power level and the field level to be equal in such a case. This is done by defining the field level and the power level according to the relations

$$L_F = \ln(F/F_0) \quad \text{and} \quad L_P = (1/2) \ln(P/P_0)$$

so that if $(P/P_0) = (F/F_0)^2$, then $L_P = L_F$. The above equations may be written in the form

$$L_F = \ln(F/F_0) \text{ Np} \quad \text{and} \quad L_P = (1/2) \ln(P/P_0) \text{ Np}$$

The bel (B) and its more frequently used submultiple the decibel (dB) are used when the field and power levels are calculated using decadic logarithms according to the relations

$$L_P = \lg(P/P_0) \text{ B} = 10 \lg(P/P_0) \text{ dB} \quad \text{and}$$

$$L_F = 2 \lg(F/F_0) \text{ B} = 20 \lg(F/F_0) \text{ dB}$$

The relation between the bel and the neper follows from comparing these equations with the preceding equations. We obtain

$$L_F = \ln\left(\frac{F}{F_0}\right) \text{ Np} = 2 \lg\left(\frac{F}{F_0}\right) \text{ B} = \ln(10) \lg\left(\frac{F}{F_0}\right) \text{ Np}$$

giving

$$\text{B} = 10 \text{ dB} = (1/2) \ln(10) \text{ Np} \approx 1.151 \text{ 293 Np}$$