

**Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on
Biochemical Nomenclature (JCBN)**

Minutes for the Annual NC-IUBMB and JCBN Nomenclature Meeting

Copenhagen, Denmark, May 27th 2016, 9:00

Present Members: Gerard Moss (GPM, Chairman); Ron Caspi (RC, Secretary); Kristian Axelsen (KA); Ture Damhus (TD); Marcus Ennis (ME); Karl-Heinz Hellwich (KHH); Masaaki Kotera (MK); Andrew McDonald (AGM); Amélia Rauter (AR); Ida Schomburg (IS); Hans Vliegthart (JFGV).

Observers: David C. Baker (DB); Thomas Lütteke (TL).

Apologies: Shuchismita Dutta (SD); Dietmar Schomburg (DS); Keith Tipton (KFT); Sameer Velankar (SV).

1) The chairman welcomed the participants.

2) Approval of the agenda.

IS requested that the BRENDA report (item 15 on the agenda) will be postponed to the following year. Other than that, the agenda was approved.

3) Approval of the minutes of the Braunschweig meeting, May 2015

The minutes from the 2015 meeting in Braunschweig were accepted in principle. KHH asked to add some information to item 15 of the minutes, regarding a link available on the ExplorEnz website to the paper described in that item, and GPM asked that the paper is described in standard citation format. RC will incorporate the requested changes and transfer the document to TD, who would transfer them to the IUPAC Secretariat on behalf of the Secretary of IUPAC Division VIII, Risto Laitinen, to be published on the IUPAC website.

4) Matters arising

There were no matters arising.

5) Reports

a) Chairman's Report

GPM reported that there had been progress with the different IUPAC projects over the past year. The throughput of the enzyme taskforce was somewhat lower in 2015 than in 2014, but still robust with about 200 new entries. He preferred not to elaborate since the assorted activities of the commission will be discussed in detail during the meeting.

b) Treasurer's Report

RC reported that this is the second year of the current triennium, which is funded by IUBMB at \$6000/year.

The IUBMB treasurer, Prof. Bonomi, has stated that he received reimbursement requests for only about \$1500 last year, leaving a surplus that should be sufficient to cover this year's expenses, which are predicted to be higher.

RC will prepare a short annual report following the meeting and submit it to the IUBMB General Secretary, Michael Walsh, as he has requested annual reports previously. These reports are presented to the IUBMB executive committee during their annual meetings during the International Conference of Biochemistry and Molecular Biology.

c) IUBMB Report

Since no IUBMB representative attended the meeting, no such report was presented. GPM has invited the IUBMB Member for Publications, Prof. Avadhesha Surolia, to attend the meeting, but has done so a rather short time prior to the meeting. As Prof. Surolia needs to arrange travel from India, it was agreed that in future years such invitations would be sent earlier.

d) IUPAC Division VIII Report

- i) TD described his involvement in two projects; the first project is "[Preferred IUPAC Names \(PINs\) for inorganic compounds](#)". The previous project leader, Richard Hartshorn, has been nominated IUPAC Secretary General, and TD replaced him as the project leader. A document that expands and delineates the grammar required for use of the kappa convention for describing coordination and specifying ligand-to-central atom bonds had not been finished because new difficulties kept arising, and progress had been very slow. The second project, originally named "[Nomenclature for polyhedral boranes and related compounds](#)", progresses well and should be finalized later this summer.
- ii) GPM and KHH discussed the extensive errata discovered in the new Blue Book, (Nomenclature of Organic Chemistry, IUPAC Recommendations and Preferred Names 2013). GPM stated that a total of 2398 errors have been discovered so far. 657 of those were reported recently by the Japanese translation team. A partial list of the errors is [available online](#). KHH pointed that he hopes that the PDF to be put online could already include some of the corrections.
- iii) KHH reported that at the end of 2015 a project proposal for additional improvements for the Blue Book, such as a new index, appendices for omitted material, a corrected PDF and, eventually, a completely revised new edition of the Blue Book, has been approved. The project is named "[Corrections, revisions and extension for the nomenclature of organic chemistry - IUPAC recommendations and preferred names 2013 \(the IUPAC Blue Book\)](#)". First drafts of appendices are already available.
- iv) KHH reported that the [Brief guide to the nomenclature of inorganic chemistry](#) has been published (Pure Appl. Chem. 2015; 87(9-10): 1039-1049). A [four-page version](#) of the document is available online as supplementary material. In addition, the guide

was reprinted as a four-page tear-off document in the centre of Chem. Int. 37(5-6) (2015). Translations into many languages are under way or already completed. A poster based on the guide may be prepared for presentation at conferences.

- v) KHH reported on the project "[Preferred names for polymers](#)". As reported last year, this long-term project has progressed following an agreement among the members that source-based polymer names must be based on IUPAC names for monomers, and that only a limited number of frequently encountered polymer names not based on IUPAC approved names should be retained. During the last year the document has been revised according to the comments received during internal review, and is now in second review.
- vi) KHH reported that the project "[Nomenclature of homodetic cyclic peptides produced from ribosomal precursors](#)", proposed by Martin Reaney, was accepted. More information is provided below (section 13) by GPM, who is a member of the team.
- vii) KHH reported on a newly approved project named "[End-of-line hyphenation of systematic chemical names](#)". The project aims to provide authors of chemical manuscripts with guidelines where systematic chemical names can be divided at the end of a line, to ensure that long names are not broken at illogical places (e.g. within locants). A draft for a document has been prepared by the task group's leader, Albert J. Dijkstra. However, KHH has stopped the review process after realizing that the document lacked some essential guidelines regarding breaking chemical names.
- viii) KHH also mentioned that the IUPAC Secretariat moved to a new office, and that the new website has been launched. While the new website is better structured and offers new features such as login accounts, it still suffers from shortcomings, errors and omissions. GPM pointed out that no projects are listed for JCBN. RC pointed out that the search function on the Project pages does not function.

6) Report from the Carbohydrate Nomenclature Group (JFGV)

JFGV described the progress made by members of the carbohydrate group regarding the project "[Carbohydrate nomenclature - revision and extension of IUPAC recommendations](#)".

- a) IUPAC has extended the project until the end of 2017.
- b) Regrettably, one of the team's key members, Derek Horton (DH), has passed away last year. David C. Baker (DB) from the University of Tennessee in Knoxville has been appointed member of the task group as successor of the late DH.
- c) DB has obtained access to the archives and e-mail correspondence of DH. He found that most of the proposals of DH were already incorporated in the draft document 3-Carb. Remaining material concerns mainly neo-glycoconjugates. This item has to be discussed further.

- d) For the items of 2-Carb 1 - 33, agreement in the group was obtained for nearly all items. A new draft for this part can be prepared.
- e) The items from 34 to the end of the 2-Carb document are more complicated. The first revisions were proposed and they will be the basis for renumbering and extension of the items to be covered.
- f) Significant progress was made with respect to glyco-informatics. Up to now all discussions were focused on the questions: What is a monosaccharide? Which chemical characteristics are needed to define a compound as a monosaccharide? Almost every proposed answer to these questions permitted the construction of a molecule that could fit the definition, yet would not be conceived as a monosaccharide by anyone. A pragmatic solution probably remains the best option. Martin Frank (MF) and TL made a proposal for the efficient encoding of carbohydrate building blocks for computer storage. This will be subjected to further discussion.
- g) It was decided that 3-Carb will comprise a series of subdocuments. A possible list of the subdocuments could be:
 - 3-Carb-I, covering most of the revised items of 2-Carb.
 - 3-Carb-II, dealing with neo-glycoconjugates.
 - 3-Carb-III, focused on glycoproteins.
 - 3-Carb-IV, focused of on glycolipids.
 - 3-Carb-V, dealing with glycoinformatics.
- h) The original document on branched sugars will be incorporated in 3-Carb-I.
- i) The document on "Symbols specifying the conformation of Polysaccharide Chains" was not discussed so far.
- j) A draft of the integral document should be ready before the next meeting in 2017.

7) Enzyme Nomenclature and Classification

- a) Report on enzymes classified during the past year (AGM)

AGM presented some statistics about the activity of the enzyme taskforce during the last year. This year the taskforce had only 3 batches, compared with 4 batches in the previous year, resulting in somewhat lower numbers. During 2015 199 new enzyme entries were created, 61 existing entries were modified, 27 were transferred, and 7 were deleted, for a total of 294 entries (compared to 337 in 2014). During the first 4 months of 2016 about 60 more new entries were created, 11 modified, and 13 transferred. In addition, there are currently more than 200 additional entries in the pipeline.

b) Report from the enzyme taskforce meeting (GPM)

- i) A significant backlog of more than 200 enzymes has accumulated. It has been decided to change the procedure in order to speed up the processing time and clear up the backlog. According to the new procedure, groups of 40 new and modified enzyme entries, as well as any transferred and deleted entries associated with them, would be transferred to internal review every month. Members will have one month to focus on those entries and prepare them for public review. After one month those entries would be moved to public review, and a new batch of 40 entries would enter internal review.
- ii) AGM and Keith Tipton (KFT) have previously written a manuscript named a 'brief guide' to enzyme nomenclature (as described in last year's minutes). KFT considers submitting the manuscript to Trends in Biochemical Sciences (TIBS). RC suggested considering the inclusion of a 2 page-formatted version as supplementary material, similar to what was done with the Brief Guide to the Nomenclature of Inorganic Chemistry (see item 5.d.iv). GPM raised the issue of copyrights.
- iii) Dr. Bernard Henrissat from Aix Marseille Université, an expert in carbohydrate enzymology who has created the carbohydrate-active enzyme database known as [CAZy](#), attended the enzyme meeting this year. In addition to promising to submit up to 200 suggestions for new enzyme entries, he has made several suggestions for potential new members of the enzyme taskforce, and expressed an interest in joining himself in a few years.
- iv) [Nomenclature of phosphorus-containing compounds of biochemical importance](#). Existing recommendations for the nomenclature of phosphorus-containing compounds have not been revised since 1976. A newer document, created in 2006 by Hal Dixon, has not been published, and is present in multiple parts in different formats, hindering efforts to finalize and publish it. It was decided that GPM will transfer the different parts to KA, who will format it into a single Microsoft Word document. KHH pointed out that he too has a version of the document, and that it is important to ensure that the latest version is used.
- v) Formate dehydrogenases: The enzyme list contains two groups of entries describing formate dehydrogenases. One group consists of older entries from the 1960's, which appear to have been misclassified under the 1.2 subclass, and the second group consists of more recent enzymes, which are classified properly under the 1.1 subclass. It was decided to move the former group to subclass 1.1, where they belong, despite the inconvenience caused by modifying EC numbers that have been established many years ago and have appeared in the literature.
- vi) Last year the taskforce decided to use the term HCO_3^- in reaction equations instead of the outdated and incorrect bicarbonate. Since KFT, who did not attend the meeting, objected to the decision, the matter was discussed again and it was decided to replace it with hydrogencarbonate. TD, who was nominated to analyse

the list for similar terms, found only a few other cases, including bisulfite, which will now be replaced with hydrogensulfite. He also mentioned the recurrent problem of 'nitric oxide', a name which is unacceptable to IUPAC because it signals oxidation state V rather than II (cf. nitric acid). While not endeavouring to eradicate 'nitric oxide' at this time, he thought one could mention acceptable alternative(s), e.g., nitrogen(II) oxide. He planned to circulate a written summary of his suggestions soon after the meeting.

- vii) News Items. Last year it was decided that short news items should be posted on the ExplorEnz website. However, this decision has not been implemented. This year several specific news items have been assigned to individual members of the taskforce, in the hope that personal assignments will result in a better outcome.
- viii) Classification rules. Last year it was decided that the classification rules document, which has become outdated, will be rewritten by DS and potentially KFT. Unfortunately DS was much too busy for this task, which has been reassigned to RC and IS.

8) Progress on the Small Molecule Glossary Project

ME has been assigned as the new leader of the project "[Glossary of small molecules of biological interest](#)". He has been communicating with the original leader, DC, but unfortunately DC is unable to continue the work. ME mentioned that a draft version of the introduction part for a Pure and Applied Chemistry publication has been completed by DC, and asked for help from the taskforce members in deciding which of the compounds should be included in the document. ME pointed to the fact that the database is rather small, with around 200 compounds, and that perhaps the size should be doubled. KHH suggested that it may be advantageous to keep the small number of compounds. GPM mentioned that this project is an update of a 1966 document, entitled [Trivial names of miscellaneous compounds of importance in biochemistry](#).

9) Progress on the Flavonoid Project (KHH)

AR reported on the progress of the project "[Recommendations on nomenclature of flavonoids](#)". The project was completed in 2013, and has been reviewed by ICTNS and ca. 25 reviewers. A second version that incorporates the comments made by the reviewers has been prepared and sent back to the taskforce members in the previous year. During the last year all members have sent their revisions to AR, with the exception of KHH, who committed to do so by the end of June.

10) Progress on the Phosphoryl Transferases Project (GPM)

GPM reported on progress in the project "[How to name atoms in phosphates, polyphosphates, their analogues, and transition state analogues for enzyme-catalysed phosphoryl transfer reactions](#)". The project has moved on to public review, and comments are expected by the end of June 2016.

11) An extended appendix to the tetrapyrrole document (GPM)

Recent classification of enzymes involved in bacteriochlorophyllide biosynthesis has exposed some nomenclature deficiencies in this field that are not covered by the existing 1986 document, [Nomenclature of tetrapyrroles](#). GPM contacted Ray Bonnett (the convenor of the original document) regarding these deficiencies, and will continue contacting people in the field to see what should be done. IS recommended contacting [Dieter Jahn](#) from TU Braunschweig, who has written a chapter about tetrapyrroles in the 2nd edition of the book "[Biochemical pathways: an atlas of biochemistry and molecular biology](#)" Michal, G., Schomburg, D. (Eds.), John Wiley & Sons (2012). ME mentioned an upcoming [Gordon conference on tetrapyrroles](#), to take place in July.

12) Progress on the Conjugates Project (GPM)

GPM has described the progress on another project he participates in, "[Nomenclature for polymeric carriers bearing chemical entities with specific activities and names](#)". The project is usually referred to as the "conjugate project", and the name may be changed in the future to "Nomenclature and terminology of conjugates". An announcement of this project was published in Sep 2015. A draft composed of tentative names that allow easy recognition of the carrier, of the active substance and of the link between them has been prepared. A new mode of naming is proposed that includes a new prefix "conj" followed by the identification of the components that form a conjugate.

13) Update on Action Items from the Minutes of the 2014 Meeting

GPM is a member of the project "[Nomenclature of homodetic cyclic peptides produced from ribosomal precursors](#)", which he introduced to JCBN last year. The project leader is Martin J.T. Reaney. A work meeting has been scheduled, but as it is in Australia, GPM will not attend.

14) The use of outdated terms/chemical names in enzymes accepted names

KHH pointed out that the enzyme list contains names that are no longer recommended by IUPAC. GPM and RC explained that different fields on the EC entries have different requirements. For example, the "accepted name" field often reflects the name that has been in use by the scientists in the field and not a JCBN recommendation. In cases when scientists have not standardized on a name, or have been using a gene name, the enzyme taskforce suggests a new accepted name. Another field is the "other names" field, which simply chronicles names that have been used to refer to the enzyme, even if they do not conform to recommendations. When necessary an annotation such as "ambiguous", "misleading", or "incorrect" is added in parentheses.

In addition, reactions often contain trivial names, which are more likely to be recognized by the scientists in the field. When that is the case, the proper IUPAC name is provided in the glossary field.

KHH will compile a list of terms that are being used in EC entries but are not allowed according to the Blue Book, and the enzyme taskforce will analyse the list to see if any of these names should be replaced with proper names. In cases where the enzyme taskforce

feels that the current name should be retained, a list of these names would be provided to KHH, who will consider allowing their use.

15) Reports from Databases

This item has been postponed to next year.

16) Recent Biochemical Nomenclature Publications of Interest

GPM mentioned a recent paper discussing the relationship between EC numbers and enzymatic reactions. One of the findings is that almost one third of the EC numbers are associated with more than one reaction in the KEGG database. [Dönertaş H. M. et al, Characterising Complex Enzyme Reaction Data, PLoS One \(2016\) 11\(2\):e0147952](#). PMID 26840640.

17) Future projects

Two potential projects have been mentioned:

- a) If glycoproteins could not be dealt with properly within the carbohydrate project, they may merit a new project.
- b) There may be a need for a new document for the nomenclature of nucleic acids. Specific topics that need work include the naming of long acids (longer than oligonucleotides), and the treatment of modifications, including simple modifications such as methylation and more complex ones, such as those in morpholino oligomers (which contain methylenemorpholine rings and phosphorodiamidate linkages).

18) Membership of the Commission

Several changes in membership were discussed.

- a) During the 2012 meeting it was decided to establish the status of Emeritus members, to which Donald Nicholson and Minoru Kanehisa were nominated. However, that status does not appear in the website operated by GPM that lists [JCBN membership](#). GPM will update the website to include Emeritus members.
- b) The status of DC will change from a titular member to an Emeritus member.
- c) Since Dr A. Cornish-Bowden has not participated in the JCBN meetings or nomenclature work for many years, GPM will contact him to see if he is interested in being removed from the list of associate members.
- d) GPM reported that Dr. Janet Thornton has declined an offer to join the enzyme taskforce. He will approach two potential candidates recommended by Dr. Henrissat.

19) Any other business

No other topics were discussed.

20) Date and Place of the 2017 Meeting

- c) AM will investigate whether the next meeting could be arranged in Dublin or Killarney, Ireland. A majority of the commission members preferred Killarney to Dublin as the location of the meeting, and midweek rather than weekend scheduling.
- d) AR offered to host the 2018 meeting in Lisbon provided it could be scheduled in July instead of May.

GPM thanked TD and KA on behalf of the commission for their generous help in hosting and organizing the meeting.

The meeting was adjourned at 12:48.