



(CPCDS) Committee on Publications and Cheminformatics Data Standards

IUPAC Database Proposal
Teleconference
10:05am - 11:10am EST
February 5, 2015

Draft Minutes

IUPAC Attendees: Bonnie Lawlor, Chair, Committee on Publications and Cheminformatics Data Standards (CPCDS), Hugh Burrows, Lene Hviid, Colin Humphries, Mark Kinnan, Robert Lancashire, James Liu, Bono Lučić, Leah McEwen

De Gruyter Attendees: Katharina Butsch

The meeting was opened at 10:05am EST. The objective of today's discussion was to finalize the tree structure. Suggested changes had been circulated prior to today's meeting. The group reviewed the document section-by-section, making adjustments as needed.

Analytical section

This section is as revised by Brynn Hibbert. The terms highlighted in yellow and orange were suggested by Leah McEwen. All present signed off on the section with no further changes being made. Bonnie Lawlor will contact Brynn who has been on vacation to see if he has any concerns with the suggested changes.

- > Analytical Chemistry
 - > Analysis using biological systems
 - > Characterization
 - > Properties
 - > Chemometrics
 - > Electrochemical methods of analysis
 - > General methods of analysis
 - > Titrimetry
 - > Gravimetry
 - > Instrumentation
 - > Mass spectrometry
 - > Metrology
 - > Calibration
 - > Standards
 - > Quality Assurance/Quality Control
 - > Microscopy
 - > Purification and Separation methods
 - > Gas chromatography
 - > Liquid chromatography
 - > Electrophoresis

- > Other principles of separation
- > Radiochemical method of analysis
- > Sampling
- > Spectrometry/Spectroscopy
 - > Atomic spectrometry
 - > Molecular spectrometry
- > Surface analysis
- > Thermal methods of analysis
- > Trace Analytics

Biochemistry section

The biochemistry section remains as originally drafted. All present signed off on the section.

- > Biochemistry
 - > Bioengineering and Biotechnology
 - > Biotransformation
 - > Enzymatic Processes
 - > Microbial Processes
 - > Biomolecules

Environmental section

After the last meeting, Bonnie Lawlor asked if the terms “fertilizers” and “soil” should be added under Agricultural Chemistry. After some discussion, it was agreed that a broader term, “Agricultural Chemicals” would replace both “pesticides” and “fertilizers” as there is a whole range of formulations used in this area. In addition, it was agreed to add “soil” under agriculture while also retaining it under Geochemistry. Hugh Burrows suggested adding “Energy” and “Green Chemistry” as subheadings in the Environmental section and all agreed. Katharina Butsch said she had not included those terms as she was unsure how much coverage IUPAC Standards and Recommendations has in those areas, but it was agreed that we will monitor the coverage as we move forward. She also asked Hugh if the new sub-heading should be “Alternative Energy,” but Hugh said that what is alternative today might not be alternative ten years from now so that we are better off with the broader term. Colin Humphries asked what was meant by “oils” under Geochemistry. Katharina said that she found about thirty-three articles (about four hundred pages) that were characterized as “oil sets and derivatives” and asked if Colin had another suggestion. Not having read the articles, he did not and it was agreed to leave the section as is and monitor the coverage as the tagging progresses. The Environmental section now reads as follows:

- > Environmental Chemistry
 - > Agricultural Chemistry
 - > Agricultural Chemicals
 - > Food Chemistry
 - > Additives
 - > Contaminants
 - > Fats
 - > Soil

- > Atmospheric Chemistry
 - > Pollution
- > Energy
- > Geo-Chemistry
 - > Soil
 - > Oils
- > Green Chemistry
- > Water Chemistry
 - > Concentrations
 - > Ground Water treatment
 - > Pollution

Inorganic section

The term highlighted in yellow had been suggested by Leah McEwen. Bonnie Lawlor asked if we should include the term “Nomenclature” under “Inorganic Substances” since it was listed under “Elements” and under several other subheadings throughout the tree structure. High Burrows did not see any value in this. Leah McEwen noted that there are a lot of articles in *Pure and Applied Chemistry (PAC)* that deal with nomenclature and terminology. Katharina agreed with Hugh and suggested perhaps a totally separate section on this topic. Bonnie noted that Leah had also made this suggestion and drafted a section which was discussed later. All agreed not to add “Nomenclature” under “Inorganic Substances” and to delete it from under the subheading “Elements.” The agreed upon section on Inorganic Chemistry now reads as follows:

- > Inorganic Chemistry
 - > Elements
 - > Atomic Weights
 - > Isotopes
 - > Inorganic Substances
 - > Boron Substances
 - > Coordination Compounds
 - > Metals
 - > Processes **and inorganic reactions**
 - > Solid State
 - > High Temperature

Materials section

The term highlighted in yellow was suggested by Leah. Bonnie asked if there were any other changes being suggested. Katharina Butsch asked if the “Measurement” section was being suggested for inclusion under “Materials.” Bonnie said “No,” that it was being suggested as a standalone portion of the tree. Hugh suggested that “Biomaterials” be added as a subheading under “Materials” and all agreed. He then questioned whether or not the specific items listed under “substances” (PET, Polystyrene, PVC, Rotaxanes) should be included. Robert Lancashire asked how many articles were published on those topics. Katharina said that there were quite a lot of articles on polymers which was why she added the specific ones listed, but noted that they could be included under the subheading “Other.” Colin Humphries noted the absence of the term “polyolefins” and suggested that perhaps the specific polymers listed under substances could all be collapsed under the subheading

“Commercial Polymers.” All agreed. Colin suggested that the term “rubbers” be replaced by “elastomers” and that the term “Amorphous Polymers” be added since the term “Crystalline Polymers” was included. All agreed and the Materials section now reads as follows:

> **Materials**

- > Biomaterials
- > Ceramic Materials
- > Coatings
- > Colloids and Surfaces
- > Composites
- > Fullerenes
- > MOFs and Coordination Polymers
- > Porous Materials
 - > Macroporous Materials
 - > Microporous Materials
- > Thin Films
- > Polymer Chemistry
 - > Structure
 - > Stereochemistry
 - > Polymerization
 - > Properties
 - > Substances
 - > Amorphous Polymers
 - > Commercial Polymers
 - > Copolymers
 - > Crystalline Polymers
 - > Elastomers
 - > Ionic Polymers
 - > Membranes
 - > Nanotubes, Fibers
 - > Resins

Measurements section

Bonnie Lawlor noted that at the last several meetings on the tree structure measurements frequently came up in the discussions. She asked if this should be a section on its own and if so, what subheadings should be included. Leah McEwen thought that measurements should be a separate section and took the time to add subheadings. Her input was circulated prior to today’s meeting. Bonnie asked how the others felt about having this as a separate section. Hugh Burrows thought it was a good idea especially since there is a lot of material on calibration and reference standards. Leah asked if topical areas such as “analytical” and “physical” should be included as subheadings. Colin thought that searchers would go to those sections if that is what they were interested in. Leah agreed and added that she asked the question because she was thinking about how to crosslink the different tree sections. Bonnie noted that the analytical section did not have an explicit section or even subheadings on measurement. Hugh said that the subheading “Metrology” in the analytical section would provide a crosslink because it also focuses on calibration and standards. Later in the discussion

on the Physical Chemistry section it was agreed to add the term “pH Measurements” as a subheading here although we have to consider how it can be crosslinked to the Analytical Chemistry section. All agreed to add a standalone section on measurements that would read as follows:

Measurement

- > Calibration
 - > Reference Standards
- > Data Management
 - > Calculation
 - > Statistical Analysis
 - > Validation
- > pH Measurements
- > Sampling
- > Standards
 - > Data Standards
 - > Reference Standards
- > Units, Scales

Medicinal Chemistry section

There were no changes to the original section on Medicinal Chemistry and Bonnie Lawlor asked if the group was content with it as it stands. Before the meeting closed, James Liu noted the absence of anything on pharmaceuticals and it was agreed to add it as a subheading here. There were no additional comments so the section stands as follows:

- > Medicinal Chemistry
 - > Clinical Chemistry
 - > Diagnostics
 - > Laboratory Technology
 - > Pharmaceuticals
 - > Properties and Units

Organic Chemistry section

Bonnie Lawlor noted that the term highlighted in yellow was suggested by Leah McEwen and asked if there were any additional suggestions (Bonnie’s questions regarding the addition of the term “nomenclature” was resolved earlier in the discussion when it was agreed to have a standalone section on this topic). Hugh Burrows noted that there is a lot of material on physical organic chemistry and suggested that it be a separate subheading. Katharina Butsch said that she saw about four hundred and eighty pages of material on the physics of organic chemistry so she agreed. Hugh suggested two wordings for the addition – “Physical Organic Chemistry” or adding the term “and Mechanisms” to the already existing subheading “Organic Reactions.” The former was chosen. Katharina asked if the subheading of “Molecular Structure” should stay since the term “nomenclature” was not being added. Hugh said it should be retained because the topic is approached from different angles. The Organic Chemistry section now reads as follows:

- > Organic Chemistry
 - > Catalysis

- > Biocatalysis
- > Catalysts
- > **Molecular Structure**
- > Organic Molecules
 - > Carbenes
 - > Cyclic Compounds
 - > Heterocycles
 - > Protecting Groups
 - > Radicals
- > Organic Reactions
- > Physical Organic Chemistry
- > Stereochemistry

Physical Chemistry section

Bonnie Lawlor noted that the terms highlighted in yellow were suggested by Leah McEwen and asked if there were any additional suggestions. Hugh Burrows noted the misspelling of “voltammetry.” Robert Lancashire asked if “equilibrium” should be moved under “thermodynamics.” Katherina Butsch said that originally she had included the term “Phase Equilibrium,” but changed it to the broader term “equilibrium” based upon Leah’s suggestion. Hugh said that he thought the term “Phase Behavior” might be better and agreed with Robert to put “equilibrium” under “thermodynamics.” Colin said that he saw a question from Robert about the absence of a subheading on pH. Katharina said that it was originally under “Analytical Chemistry.” It was agreed to add pH as a subheading in the Measurements section. Hugh Burrows suggested adding the term “sensors” read “Sensors and Activators. The section on Physical Chemistry now reads as follows:

- > Physical Chemistry
 - > Colloids and Surfaces
 - > Electrochemistry
 - > Corrosion
 - > Electrodes
 - > Electrolytes
 - > Electroanalysis
 - > Potentiometric Measurements
 - > Voltammetry
 - > Electrochemical Stripping Analysis
 - > Piezoelectricity
 - > Magnetochemistry
 - > Processes
 - > Non-Aqueous Reactions
 - > Transport Phenomena
 - > Phase Behavior
 - > Photochemistry
 - > Luminescence
 - > Quantum Yields
 - > **Sensors** and Activators

> Solubility

- > Thermodynamics
 - > Equilibrium
- > Kinetics

Nomenclature and Terminology

As discussed earlier Leah McEwen had suggested the inclusion of a standalone section entitled “Terminology and Nomenclature” (it was agreed to reverse the terms and begin with “Nomenclature”). If so, the subheading “nomenclature” will be removed from the sections in which it currently appears. Katharina Butsch said that she believes a separate section on this topic is important Bonnie asked if the separate topical areas (elements, organic, inorganic, polymers, etc.) should be included. Hugh Burrows suggested that perhaps we should not be too specific and see how it evolves. Bonnie suggested that we include at least subheadings for the sections in which the term “nomenclature” originally appeared and give the freelancer guidelines to add additional subheadings as needed. The section on Nomenclature and Terminology now reads as follows:

- > Nomenclature and Terminology
 - > Nomenclature
 - > Elements
 - > Inorganic Chemistry
 - > Organic Chemistry
 - > Polymer Chemistry
 - > Notations
 - > Chemical Identifiers
 - > Terminology
 - Abbreviations
 - Definitions

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Theoretical Chemistry section

Bonnie Lawlor noted that the terms highlighted in yellow were suggested by Leah McEwen and asked if there were any additional suggestions. Hugh Burrows suggested that the main heading be modified to read “Theoretical and Computational Chemistry,” and that a new subheading, “Molecular Dynamics and Simulations” be added. Katharina Busch noted that the term “simulation” does not appear anywhere else so that this would be good. Bonnie asked Hugh if any additional subheadings are needed and he said “No.” There were no additional suggestions. All agreed to the changes and the section now reads as follows:

- > Theoretical and Computational Chemistry
 - > Force-Field Calculation
 - > Molecular Design
 - > Molecular Dynamics and Simulations
 - > Quantum Chemistry and Molecular Mechanics
 - > Quantum Chemical Calculation
 - > Ground-State Structures
 - > Properties

Toxicology section

There were no changes to this section as originally drafted. Bonnie Lawlor asked if there were any final suggestions. Colin Humphries asked if there was a better heading as he thinks the section looks asymmetric. He also reacted to the subheading "Exposure to Chemicals" which he interpreted to mean exposure to synthetic chemicals. Hugh Burrows said that most of the technical articles in *PAC* that deal with exposure are dealing with the environment. Katharina Butsh noted that the Chemistry and Health Division had about four hundred and fifty pages on exposure but the material appears to be related to health. Robert Lancashire suggested changing "Exposure to Chemicals" to "Occupational Health," but Colin then thought it would not belong in this section. He suggested changing the term to "Exposure Science" or simply "Exposure." Leah McEwen suggested "Environmental Health and Safety." Katharina said that most of the articles related to exposure deal with metals so perhaps "exposure" could be a subheading under metals. After some additional discussion it was agreed to leave the section as is with the exception of deleting the subheading "Exposure to Chemicals" and adding the term "exposure" under metals. It was agreed that the freelancer would be given the flexibility to add additional subheadings as deemed needed. The section on Toxicology now reads as follows:

- > Toxicology
 - > Ecotoxicology
 - > Immunotoxicology
 - > Metals
 - > Exposure
 - > Toxicokinetics

Other discussion

Robert Lancashire asked what will happen if there is no place in the tree for an article to be placed. Bonnie Lawlor said that the freelancer will flag it and make a suggestion to which we can react. The freelancer will also have the flexibility to put articles under more than one heading and to suggest additional subheadings that we may have overlooked.

James Liu noted the lack of anything related to pharmaceuticals. He was not necessarily suggesting that it be added, but wanted to note its exclusion. After some discussion it was agreed to add it as a standalone subheading under Medicinal Chemistry.

Bonnie and Katharina agreed to compare notes within the next twenty four hours so that an agreed-upon tree structure is available to the freelancer on Monday, February 9th. Bonnie will also provide a summary of guidelines for use by the freelancer. Another meeting of the group will be scheduled after the freelancer has provided some material for review.

There being no further discussion, the meeting was adjourned at 11:10am EST.

Respectfully submitted,

Bonnie Lawlor, Chair
IUPAC Committee on Publications and Cheminformatics Data Standards (CPCDS)
February 6, 2015



**(CPCDS) Committee on Publications and
Cheminformatics Data Standards**

General Guidelines:

1. Each article can be classified under more than one heading as needed.
2. If appropriate main heading(s) or subheading(s) do not exist for an article please let us know and make suggestions as to what should be added.
3. Monitor the amount of material that is being added to each section of the tree. Are there any sections for which there is very little?
4. Are there any sections of the tree for which additional subheadings are required and if so, make suggestions. (e.g. Some sections (e.g. Toxicology) need careful scrutiny with regard to subheadings)
4. Are there any subheadings that seem inappropriate and need to be replaced and if so, please make suggestions.
