

IUPAC Database Tree Structure  
Teleconference  
11:02am - 12:58pm EDST  
May 13, 2015

**Draft Minutes**

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**IUPAC Attendees:** Bonnie Lawlor, Chair, Committee on Publications and Cheminformatics Data Standards (CPCDS), Hugh Burrows, Robert Lancashire, James Liu, Bono Lučić, Dave Martinsen, Leah McEwen

**De Gruyter Attendees:** Katharina Butsch

The meeting opened at 11:02am EDST. The objective of today's meeting was to discuss the changes to the database tree structure that have been proposed by the freelancer doing the article tagging. The recommendations were circulated by Katharina Busch prior to today's meeting.

**Database Status**

The contract for the creation of the IUPAC Database on Standards and Recommendations has been signed. The freelancer has completed her first pass and has put forth recommendations for changes in the tree structure. De Gruyter's e-publication group will begin production in about two weeks' time (early June). Hence, the recommended changes must be agreed upon asap. Also, there are additional questions that will need to be answered by IUPAC and Katharina will submit them to CPCDS early next week. Katharina noted that she is working on the database with one of her colleagues who is also a chemist and she wanted to make it clear that both she and her colleague differed with some of the freelancer's suggestions and she will note those differences as the list is reviewed today. It was also noted that both IUPAC and De Gruyter agree that the tree structure may continue to evolve over time as new material is published and that is stated in the contract.

**Tree Structure**

The recommended changes were color coded: red, the freelancer recommended a general, more flat structure; blue, the freelancer said that it was difficult to assign entries to one specific subcategory; and green, the freelancer did not use the category (see pages 9-13 for the color coded tree structure). Katharina requested input on each of the suggested changes so that all present could agree on how to proceed. She also noted that if a category currently has no entries, the decision could be to not display it, rather than delete it. Robert Lancashire asked how difficult it would be to add a category later. Katharina said that the De Gruyter e-publications group said that it is better to keep a category that might be used and not display it rather than try to add it after the fact.

*Analytical section*

1. The freelancer did not use the subcategory "Nucleic Acid Sequencing" under "Biological Analysis." It was agreed to keep the subcategory and not display it until articles were added to it.
2. The freelancer said that the "Electrochemistry" subcategory overlapped with the "Electroanalysis" subcategory in the Physical Chemistry main section that appears later in the tree. Katharina and her colleague disagreed and felt that both the Analytical and Physical main sections should have the

subcategory, but asked if the subsections should be the same in each. Hugh Burrows suggested that the “electroanalysis” subcategory (not the entire subcategory on “electrochemistry”) in the Physical section be replicated in the Analytical section. James Liu agreed. At first Hugh suggested that the subcategories (Potentiometric measurement, Voltammetry, and Electrochemical Stripping Analysis) listed under “Electroanalysis” in the Physical main category be deleted, but it was later agreed to retain them until the final article count is made.

3. The freelancer found the subcategory “X-ray Fluorescence Analysis” under Radiochemistry too specific. Options are to delete it or not display it. Robert Lancashire thought it was a better fit in the Spectroscopy/Spectrometry” subsection and after some discussion it was agreed to move it there and not display it until articles are added. Katharina said that her colleague suggested that a new main section “Nuclear Chemistry” be added (not a necessity, but a nice-to-have) because there are some related articles that do not fit in the Analytical main section. Hugh Burrows agreed. When asked if there were subcategories that should be added under “Nuclear Chemistry” he said that there probably are, but that this was not his area of specialty. It was agreed that a new main section entitled “Nuclear Chemistry” will be added after the main section entitled “Nomenclature and Terminology.”

4. The freelancer found that the subcategories under “chemometrics” were too closely related to allow for differentiation so that articles would have to be added to both. She said that this will always be the case with full-text articles that touch on a variety of aspects. Hugh suggested that the subcategories be deleted rather than have articles appear in both subcategories. Dave Martinsen said that he understands the problem if the tags are added at the article level and asked if the tags could be added at the subdocument level so that the user could be directed to the section of the article that is appropriate to his/her query. Katharina said that she believes that the intention is to have the user enter at the full article level, but she will ask the e-publishing group if this can be done.

**ACTION:** *Katharina Butsch* will ask the De Gruyter e-publishing group if tagging can be done at the subdocument level.

If the subdocument tagging is not possible, the two subcategories under chemometrics will at the very least not be displayed, if not removed altogether.

5. The freelancer found that the two subcategories under “Quality Assurance/Quality Control” were too specific to be differentiated. It was agreed that if subdocument tagging is not possible these two subcategories will at the very least not be displayed, if not removed altogether.

6. The freelancer found that the subcategory “Sampling” overlapped with a subcategory in the main section on “Measurement.” Katharina said that she and her colleague thought that it might be best to have the “Sampling” subsections in each of the aforementioned main sections be identical. It was agreed to move the more fine-tuned section that is in the “Analytical” main section for inclusion in the “Measurement” main section.

#### *Biochemistry section*

It was agreed to remove the “biomolecules” subcategory out of the “Biotransformation” subcategory and have it as a first-level subcategory on the same level as “Bioengineering and Biotechnology.”

*Environmental Chemistry section*

1. The freelancer had difficulty choosing the subcategories to which articles should be assigned. Katharina said that even with the difficulty, the freelancer was able to populate the subcategories and recommends that they remain. All agreed.
2. The subcategory “Oils” has no articles assigned to it. James Liu asked if “fuels” would be a better term. Katharina said that there have been no articles related to fuels so that changing the name of the subcategory would not help. It was agreed that the current subcategory will be retained, but not displayed until articles are added at which time the actual name may be reconsidered.
3. The subcategory “Greenchemistry” has no articles assigned to it, but it was agreed to retain it and not display until articles are added.
4. The freelancer found that the articles on water treatment were not related to ground water. It was agreed to change the subcategory to “Treatment” under the “Water Chemistry” subcategory. Hugh Burrows said that this change would be in alignment with the materials that he has seen.
5. James Liu had some suggestions related to the “Geo-chemistry” subsection. The first was to delete the hyphen and have appear as “Geochemistry” and this will be done. He then asked if there should be a subcategory on “isotopes.” Katharina noted that such a subcategory exists in the main section on Inorganic Chemistry (under “elements”). She will take a look at articles assigned to that subcategory to see if they are geochemistry-related. James asked if there were any articles related to ground water in the geochemistry subcategory and Katharina said “no.”

**ACTION:** *Katharina Butsch* will take a look at articles assigned to the “isotope” subcategory in the Inorganic Chemistry main section to see if they are geochemistry-related.

*Inorganic Chemistry section*

1. Robert Lancashire asked if having a subcategory “Boron Substances” was too specific. Katharina said she did not know how many articles have been assigned to it. Robert thought that it should be titled “Main Group Substances” rather than “Boron Substances.” Hugh Burrows agreed as he said that there are also articles on Silicon Substances. Katharina will make the change.

*Materials section*

1. The freelancer found overlap between the “coatings” subcategory and “Surface” and also between the Thin Films” subcategory and “Surface.” It was agreed that both the “Coatings” and “Thin Films” subcategories would be retained.
2. The freelancer found overlap between the “Colloids and Surfaces” subcategory in the Materials main section with the same subcategory in the main section on Physical Chemistry. Hugh Burrows suggested that the “Colloids and Surfaces” subcategory in the Materials main section be renamed “Soft Matter” and that the “Colloids and Surfaces” subcategory in the Physical Chemistry main section be retained. He also suggested that these two subcategories be linked. All agreed.
3. The freelancer found that articles on porous materials did not differentiate the pore sizes. Hugh Burrows did not see a need for the subcategories and it was agreed that they would be deleted.

4. The freelancer questioned the need for the “Stereochemistry” subcategory under “Structure” in the Polymer Chemistry subcategory in the Materials section, as there is a “stereochemistry” subcategory in the Organic Chemistry main section. There was discussion on whether or not it should be retained and not displayed or deleted altogether. Leah McEwen said that the literature on this topic is growing and she would prefer to see it retained. Hugh Burrows suggested that the subcategory be retained, but renamed “Stereoregularity” as this term is more common. It will not be displayed until it is populated. All agreed.

5. The freelancer has not used the “Amorphous Polymers” subcategory and questioned whether it should be retained. It was agreed to keep it, but not display it until it is used.

6. The freelancer found that any article with elastomers also fell into either the “Commercial Polymers” subcategory or the “Copolymers” subcategory. Katharina asked if the “Elastomers” subcategory is needed. Hugh Burrows said that users will look for elastomers as such and that the subcategory should be retained.

7. Katharina said that she has found articles for the “Rubbers” subcategory so that is no longer an issue and she thinks that there will be some for the “Membranes” subcategory so both of these will be retained.

#### *Measurement section*

1. As agreed earlier, the “Calibration” subcategory will be retained. Katharina said that the “Reference Standards” subcategory has very few articles and questioned whether or not it should be retained. It was agreed to keep it for the time being and do an article count at a later date.

**ACTION:** Article count required for the “Reference Standards” subcategory.

2. The freelancer said that it is impossible to differentiate articles for categorization in any of the three subcategories (“Calculation,” “Statistical Analysis,” and “Validation”) under the “Data Management” subcategory. To date, everything has just been put under the broader heading of “Data Management.” Leah McEwen said that she agrees based on the literature that she has seen, but that perhaps differentiation will be easier as data management techniques are improved. After some discussion it was agreed that the subcategories would be deleted.

Dave Martinsen said that he is feeling a disconnect with having “Data Management” as a subheading under “Measurements.” It is a much broader topic today – metadata, software, and even publications are being discussed under this general topic. He questioned whether or not it should be a main heading that would touch on all of these things or is it broader only outside of the IUPAC context? Bonnie Lawlor said that “data management” means many things to many people, depending on the type of data with which they are concerned. Dave said he also notes that another broad category is missing and that is “Cheminformatics” which differs from “Chemometrics” (See the Analytical section). “Cheminformatics” would include InChI codes, software, etc. and perhaps “Data Management” would fit in here as well. Leah McEwen said that she believes “Data Management” should be a top level category because of the major focus that is being given to it. It was agreed that discussion of new top-level entries would be postponed until all of the proposed changes to the tree structure have been reviewed.

**ACTION:** Decision needed for “Data Management” as a top level entry in the tree structure. If, “yes,” what subcategories are needed?

3. As noted earlier, the freelancer found that the subcategory “Sampling” overlapped with a subcategory in the main section on “Analytical Chemistry.” Katharina said that she and her colleague thought that it might be best to have the “Sampling” subsections in each of these main sections be identical. It was agreed to move the more fine-tuned section that is in the “Analytical” main section for inclusion here in the “Measurement” main section.

4. Katharina noted that there are very few articles being put in the “Standards” subcategory, but there are some so she does believe it should be retained. However, the subcategory “Data Standards” under “Standards” has not been used. It is difficult to determine whether or not an article is referring to “standard data” or “standards for data.” The “Reference Standards” subcategory has been used. Leah McEwen said that when she had suggested the “Data Standards” subcategory she was thinking of file formats for data. It was ultimately agreed that the term refers to data presentation and that it will be retained as a subcategory pending an article count.

**ACTION:** Article count required for the “Data Standards” subcategory.

#### *Medicinal section*

1. The freelancer found that while there are medicinal chemistry articles for inclusion in the “Laboratory Technology” subcategory, there are also articles that discuss laboratory technology, but have nothing to do with Medicinal Chemistry. She suggested that perhaps a more general heading of “Chemical Laboratory” could be added as a main section for those articles. Katharina said that she and her colleague looked at the articles in question and found them to be more training-oriented and she suggested that a main section on “Education” be created. Bonnie Lawlor said that she can see a lot of articles falling under that category. Hugh Burrows said that “education” and “training” are not quite the same and that perhaps the main heading should be “Laboratory Training” rather than “Education.” Katharina said that the term “education” was put forth because of the IUPAC Division that focuses on education and she thought that perhaps there would be standards that would fall under that category. Hugh said in that case “Training” could be a subcategory under “Education.” Katharina suggested that she, her colleague, and the freelancer will review the articles that might fall under an education main section and make suggestions for subheadings. It was noted that the subcategory “Laboratory Technology” will be retained in the main section on Medicinal Chemistry.

**ACTION:** Decision needed for “Education” as a top level entry in the tree structure. If, “yes,” what subcategories are needed

#### *Nomenclature and Terminology section*

1. Katharina noted that the subcategory “Notations” has not been used and questioned whether it should be deleted. Bonnie Lawlor said that InChI codes are an IUPAC standard so there is at least one article that should be here and as the code is enhanced to handle more types of compounds there will be more articles published. It was agreed that this subcategory will be retained. InChI codes themselves may be added to the database as a future enhancement. In the interim, if an article includes them or talks about them the phrase “InChI Code” can be included as a keyword.

#### *Organic Chemistry section*

1. The freelancer has not used the two subcategories (Biocatalysis and Catalysts) under the first level subcategory “Catalysis” and suggested that perhaps the latter should be renamed “Catalysis and Catalysts.” Robert Lancashire said that most catalysts are inorganic. It was agreed that the two subcategories can be deleted and the first level subcategory will remain as “Catalysis.”

2. Katharina said that the subcategories under “Organic Molecules” are not used much. There are a few articles under “Carbenes,” but most articles are falling under “Cyclic Compounds.” She questioned whether or not it makes sense for a user to enter the Organic Chemistry section of the tree, to see only “Organic Molecules” then have to click on that to get to see only “Cyclic Compounds” and then click yet again to get to “Heterocycles.” She asked if the only entry should be “Organic Molecules” without further differentiation. Hugh Burrows said that there could be other classifications in addition to heterocyclics such as polycyclic aromatics and carbohydrates. He suggested that the articles be looked at and if nothing in addition to heterocycles is found, the subcategories under “Organic molecules” can be removed. It was agreed that Katharina will do an article count and this subsection will then be revisited.

**ACTION:** Article count required for the subcategories under “Organic Molecules.”

*Physical Chemistry section*

1. As noted earlier the “Colloids and Surfaces” subcategory will be retained and linked to the “Soft Matter” subcategory in the main section on Materials.

2. The “Electroanalysis” subcategory will be retained and replicated in the Analytical Chemistry main section as noted earlier. Katharina said that there are a few entries for the subcategories on “Potentiometric Measurements” and “Voltammetry,” but nothing for the subcategory on “Electrochemical Stripping Analysis.” It was agreed that a decision on deleting these subcategories will wait until the results of an article count.

**ACTION:** Article count required for the subcategories under “Electroanalysis” – applies to both the Physical and Analytical sections.

3. Katharina said that she had just found out that the articles being put in the “Transport Phenomena” subcategory in the “Magnetochemistry” main section were also going into the main section on “Phase Behavior.” Both Hugh Burrows and Robert Lancashire said that the subcategory “Transport Phenomena” has nothing to do with “Magnetochemistry” and should be moved under “Phase Behavior.” Katharina said that she will check to see if all of the subcategories currently listed under “Magnetochemistry” were meant to appear under “Phase Behavior.”

**ACTION:** *Katharina Butsch* will check to see if all of the subcategories currently listed under “Magnetochemistry” were meant to appear under “Phase Behavior.”

4. The freelancer has not used the subcategories (Luminescence and Quantum Yields) under “Photochemistry” for further differentiation and Katharina asked if they should be retained. Hugh Burrows said that they do need to be here and also asked the second subcategory be renamed “Quantum Yields and Lifetimes.” Robert Lancashire asked if “Luminescence” should also appear in the main section on Analytical Chemistry with the subcategory on “Molecular Spectroscopy.” It was agreed that the latter should read “Molecular Spectroscopy (IR, UV/Vis, Microwave, Fluorescence, Luminescence).”

5. Katharina said that the freelancer has assigned all the articles in the “Thermodynamics” main section to the “Equilibrium” subcategory as well and she question whether the subcategory is needed. All agreed that it can be deleted.

*Theoretical and Computational Chemistry section*

1. Katharina noted that the subcategories under “Quantum Chemistry” have not been used much. . It was agreed that a decision on deleting these subcategories will wait until the results of an article count.

**ACTION:** Article count required for the subcategories under “Quantum Chemistry.”

*Toxicology section*

1. Katharina said that all of the subcategories are good despite our original concern about this main section. However, she noted that the subcategory “Exposure” under “Metals” has not been used. After some discussion it was agreed that it should be deleted, but that “Metals” will be retained. Leah McEwen raised the question of whether or not a main section on “Safety” should be considered and if IUPAC plans to be part of the global discussion on that topic. Bonnie Lawlor said that she had the same question when the topic of laboratory technology was being discussed earlier. Chemical Safety is currently a major topic in academia and industry. Katharina said that every time a new main section is added, the articles must be reviewed again for possible inclusion.

*Additional sections*

The freelancer had indicated that additional categories are needed for the following: Publication/Documentation/Bibliography; Education; and Chemical Weapons (there are articles that are on this topic, but IUPAC did not want it included). The freelancer has already tagged the relevant articles so that they can be put in those categories if they are created. Other topics identified during today’s discussion were Chemical Safety, Data Management, and Nuclear Chemistry. Topics such as metadata, software, and archiving/preservation were also raised. Katharina reminded everyone that for each new category that is added all of the articles must be reviewed again for possible inclusion.

**ACTION:** *Bonnie Lawlor* will discuss the need for a “Chemical Weapons” entry in the tree structure.

Bonnie Lawlor said that there really is insufficient time today to talk about the addition of new sections to the database tree structure, especially at the end of a lengthy (two-hour) teleconference. She asked that if possible, Katharina supply some details on the articles that the freelancer has identified as needing new categories; e.g. what were the topics discussed in the articles that she has identified as needing new categories? Hugh Burrows asked if there are any other articles that have not been assigned to main sections and if so, how would the freelancer categorize them?

**ACTION:** *Katharina Butsch* will supply some details on the articles that the freelancer has identified as needing new categories and will ask the freelancer if there are any other articles that have not been assigned to main sections and if so, how would she freelancer categorize them?

Katharina said that we will need to finalize the structure within the next two weeks. Also, next week she will be sending a list of questions that IUPAC will need to answer; e.g. when the articles are broken/cut into smaller pieces such as definitions, what article-related data stays with each piece.

**ACTION:** *Katharina Butsch* will forward a list of questions from the De Gruyter e-publishing group for which they want IUPAC advice on the database.



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

**ACTION:** *Bonnie Lawlor* will re-circulate Katharina Butsch's presentation on the database so that CPDS members can review the tree structure display.

**ACTION:** *Bonnie Lawlor* will draft minutes of today's meeting on the proposed tree structure changes.

**ACTION:** *Bonnie Lawlor* will survey the group in order to schedule a follow-up teleconference to discuss potential new top-level entries to the tree structure.

There being no further discussion, Bonnie thanked everyone for the input and for giving so much time out of their own schedules to participate in today's discussion. She said that she will schedule a follow-up teleconference and adjourned the meeting at 12:58pm EDST.

Respectfully Submitted,

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

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**Revised Tree Structure** (*Final for Agreement: February 11, 2015; Recommended revisions May 13, 2015*)

**Recommendations (color-coded)**

1. Color code: General more flat structure, more specific structure only for 10 or more articles.
2. Color Code: Difficulties to assign entries to one specific category
3. Color code: Not used by the freelancer

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> **Analytical Chemistry**

- > Analytical Methods Based on
  - > Biological Analysis
    - > -omics (Genomics, Metabolomics, Proteomics, etc.)
      - > Nucleic Acid Sequencing
  - > Biological Systems, Use of
    - > Enzymes
    - > Immunoanalysis
    - > Other
  - > Diffraction (X-ray, Electron)
    - > Electrochemistry ((Overlap with Physical Chemistry))
  - > Gravimetry and Titrimetry
  - > *In Situ* Analysis / Robotics / Lab-on-a-chip
  - > Microscopy
  - > Radiochemistry
    - > X-ray Fluorescence Analysis
  - > Spectroscopy/Spectrometry
    - > Atomic Spectroscopy
    - > Mass Spectrometry
    - > Molecular Spectroscopy (IR, UV/Vis, Microwave)
    - > Resonance Spectroscopy (NMR, ESR)
  - > Surface Analysis
  - > Thermal Measurements
  - > Trace Analysis
  - > Other
- > Metrology
  - > Chemometrics ((Subcategories can rarely be differentiated))
    - > Design of Experiments
    - > Calibration
  - > Reference Materials and Standards
  - > Quality Assurance/Quality Control ((Subcategories can rarely be differentiated))
    - > Method Validation
    - > Measurement Uncertainty
- > Sampling ((Overlap with Measurement))

- > Solid Phase
- > Liquid Phase
- > Gas Phase
- > Statistics of Sampling
- > Separation Methods
  - > Electrophoresis
  - > Gas Chromatography
  - > Liquid Chromatography
  - > Other
- > **Biochemistry**
  - > Bioengineering and Biotechnology
    - > Biotransformation
      - > Enzymatic Processes
      - > Microbial Processes
    - > <----- **Biomolecules**
- > **Environmental Chemistry** ((articles are often concerned with several aspects of Environmental Sciences, thus main categories seems best option))
  - > Agricultural Chemistry
    - > Agricultural Chemicals
    - > Food Chemistry
      - > Additives
      - > Contaminants
      - > Fats
    - > Soil
  - > Atmospheric Chemistry
    - > Pollution
  - > Energy
  - > Geo-Chemistry
    - > Soil
      - > „Oils“ ((working title - will be amended if needed))
  - > **Green Chemistry**
  - > Water Chemistry
    - > Concentrations
    - > **Ground Water** Treatment
    - > Pollution
- > **Inorganic Chemistry**
  - > Elements
    - > Atomic Weights
    - > Isotopes
  - > Inorganic Substances
    - > Boron Substances

- > Coordination Compounds
- > Metals
- > Processes and Inorganic Reactions
  - > High Temperature
  - > Solid State
- > **Materials**
  - > Biomaterials
  - > Ceramic Materials
  - > Coatings ((partial overlap with "Surface" ))
  - > Colloids and Surfaces ((gibt es bei Physical Chemistry))
  - > Composites
  - > Fullerenes
  - > MOFs and Coordination Polymers
  - > Porous Materials
    - > Macroporous Materials
    - > Microporous Materials
  - > Thin Films ((partial overlap with "Surface"))
  - > Polymer Chemistry
    - > Structure
      - > Stereochemistry ((
    - > Polymerization
    - > Properties
    - > Substances
      - > Amorphous Polymers
      - > Commercial Polymers
      - > Copolymers
      - > Crystalline Polymers
      - > Elastomers
      - > Ionic Polymers
      - > Membranes
      - > Nanotubes, Fibers
      - > Rubbers
- > **Measurement**
  - > Calibration
    - > Reference Standards((see Metrology))
  - > Data Management
    - > Calculation
    - > Statistical Analysis
    - > Validation
  - > pH Measurements
  - > Sampling ((see Analytik))
  - > Standards((see Metrology; entries for Measurement/Calibration/Ref Standard are closely connected; differentiation is difficult))

- > **Data Standards**
- > **Reference Standards**
- > Units, Scales
  
- > **Medicinal Chemistry**
  - > Clinical Chemistry
  - > Diagnostics
  - > Laboratory Technology ((there are articles on general (chemical) laboratories as well, which would not be searched for in „Medicinal Chemistry“))
  - > Pharmaceuticals
  - > Properties and Units
  
- > **Nomenclature and Terminology**
  - > Nomenclature
    - > Elements
    - > Inorganic Chemistry
    - > Organic Chemistry
    - > Polymer Chemistry ((add others if needed))
  - > **Notations**
    - > **Chemical Identifiers**
  - > Terminology
    - > Abbreviations
    - > Definitions
  
- > **Organic Chemistry**
  - > **Catalysis** ((alternative: Catalysis and Catalysts))
    - > **Biocatalysis**
    - > **Catalysts**
  - > Molecular Structure
  - > Organic Molecules
    - > Carbenes
    - > Cyclic Compounds
      - > **Heterocycles**
    - > **Protecting Groups**
    - > **Radicals**
  - > Organic Reactions
  - > Physical Organic Chemistry
  - > Stereochemistry
  
- > **Physical Chemistry**
  - > **Colloids and Surfaces** ((see Materials; suggestion: if something is put in here it should also be put in Materials automatically))

- > Electrochemistry
  - > Corrosion
  - > Electroanalysis ((see Analytik))
    - > Potentiometric Measurements
    - > Voltammetry
    - > Electrochemical Stripping Analysis
  - > Electrodes
  - > Electrolytes
  - > Piezoelectricity
- > Kinetics
- > Magnetochemistry
  - > Processes
    - > Non-Aqueous Reactions
    - > Transport Phenomena
- > Phase Behavior
- > Photochemistry
  - > Luminescence
  - > Quantum Yields
- > Sensors and Activators
- > Solubility
- > Thermodynamics
  - >Equilibrium
- > **Theoretical and Computational Chemistry**
  - > Molecular Design
  - > Molecular Dynamics and Simulations
  - > Molecular Mechanics
  - > Quantum Chemistry
    - > Ground-State Structures
    - > Properties
- > **Toxicology**
  - > Ecotoxicology
  - > Immunotoxicology
  - > Metals
    - > Exposure
  - > Toxicokinetics

**Additional categories needed for:**

>Publication/Documentation/Bibliography

>Education

>Chemical Weapons ((examination of content strongly suggest to have a category with this name