

IUPAC Database Meeting: December 8, 2014

The following is a summary of the key elements. Detailed minutes will follow.

Search Criteria

The agreed upon search criteria are as follows:

- Author names
- Full text search/ Key words
- Publication year/range of dates
- DOI of original publication
- Document type (e.g. definition, technical report, nomenclature ...)
- IUPAC's filing division
- IUPAC's project number
- Elements
- Substances (should be connected to InChi-Codes and is thus a long term option)
- Article titles
- Captions of figures and tables
- ORCID numbers

Sorting Criteria

The agreed upon sorting criteria are:

- Relevance (standards for all databases, based on statistics)
- Publication year
- Article type
- No. of citing references (to be determined)
- Alphabetic
- Name of first author

Search Functionalities

The agreed upon search functionalities are:

- Thesaurus (user searches for a term (s)he is used to & is redirected to the IUPAC term in the database, if necessary) – To come
- Cross linking between database entries
- Citation linking (CrossRef)
- Clickable browsing structure for each entry
- Element search by a clickable periodic table (wish list)

Working name of database: *IUPAC Standards Online*

Tree Structure

De Gruyter needs input on the tree structure and we agreed to give them a working document by January 5th (Katharina's draft follows on pages 2-6). Please review and edit as you see fit and send me any changes by January 1 at the latest. My sincere thanks for all that you are doing!!!!

- > **Analytical Chemistry**
 - > Actinometry
 - > Calibration
 - > Isotopic and Nuclear Techniques
 - > Microscopy
 - > Purification
 - > Quantitative Measurements
 - > Calorimetry
 - > Conductometry
 - > pH-Measurements
 - > Reagents
 - > Sensors
 - > Separation
 - > Adsorption
 - > Chromatography
 - > Spectroscopy
 - > Electron Spectroscopy
 - > EPR Spectroscopy
 - > Flame Spectroscopy
 - > Massspectroscopy
 - > Mössbauer Spectroscopy
 - > NMR Spectroscopy
 - > Optical Spectroscopy
 - > Absorption Spectroscopy
 - > Circular Dichroism Measurement
 - > Fluorescence Spectroscopy
 - > Interferrometry
 - > Spectroelectrochemistry
 - > Rheology
 - > Vibrational Spectroscopy
 - > IR-Spectroscopy
 - > Raman-Spectroscopy
 - > X-Ray Spectroscopy
 - > Stability Constant Measurements
 - > Standards
 - > Trace Analytics

Continued

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

- > **Environmental Chemistry**
 - > Atmospheric Chemistry
 - > Pollution
 - > Geo-Chemistry
 - > Soil
 - > Oils
 - > Water Chemistry
 - > Concentrations
 - > Ground Water treatment
 - > Pollution

Continued

> **Industrial Products and Materials**

- > Chemical Weapons
- > Food Chemistry
 - > Additives
 - > Contaminants
 - > Fats
- > Materials
 - > Ceramic Materials
 - > Coatings
 - > Colloids
 - > Composites
 - > Fullerenes
 - > MOFs and Coordination Polymers
 - > Porous Materials
 - > Macroporous Materials
 - > Microporous Materials
 - > Thin Films
- > Pesticides
- > Polymer Chemistry
 - > Nomenclature
 - > Structure
 - > Stereochemistry
 - > Polymerization
 - > Properties
 - > Substances
 - > Copolymers
 - > Crystalline Polymers
 - > Ionic Polymers
 - > Membranes
 - > Nanotubes, Fibers
 - > PET
 - > Polystyrene
 - > PVC
 - > Resines
 - > Rotaxanes
 - > Rubbers

> **Inorganic Chemistry**

- > Elements
 - > Atomic Weights
 - > Isotopes
 - > Nomenclature
- > Inorganic Substances
 - > Boron Substances
 - > Coordination Compounds
 - > Metals
- > Processes
 - > Solid State
 - > High Temperature

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

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

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

- > **Theoretical Chemistry**
 - > Force-Field Calculation
 - > Molecular Design
 - > Quantum Chemical Calculation
 - > Ground-State Structures
 - > Properties
 - > Quantum Mechanics

> **Toxicology**

- > Ecotoxicology
- > Exposure to Chemicals
- > Immunotoxicology
- > Metals
- > Toxicokinetics
