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The IUPAC Gold Book: A Compendium of Chemical Terminology

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NFDI₄Chem Ontology Workshop October 11th, 2023

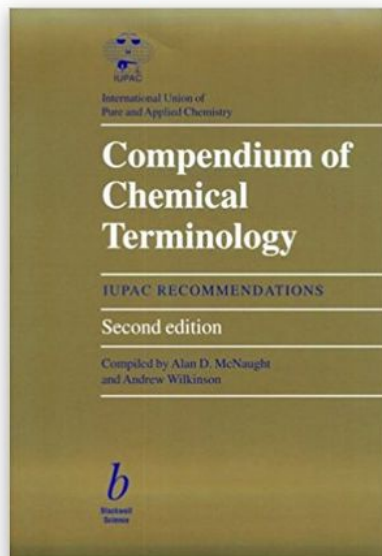
Alphabetical Index

A	B	C	D	E	F
G	H	I	J	K	L
M	N	O	P	Q	R
S	T	U	V	W	XYZ

Additional Indexes

Physical Constants
Units of Measure
Physical Quantities
SI Prefixes
Ring Index
General Formulae
Exact Formulae
Source Documents

Compendium of Chemical Terminology



Expanded Search!

New Download Page

Welcome to the
Chemical Terminology
these pages your
publication. Start

- browsing the
- using one of
- using the search

To learn more about
(Updated July 1st)

The Gold Book API

Alpha API v1.0 (5/31/19)

API

While we expect a lot of humans to stop by the Gold Book, it's about time that the vocabulary be friendly towards computers and have set up an application programming interface (API) so they may download a bunch of stuff. Here is the overview of the API and we are working on additional documentation. (click the headers below to toggle what's visible).

Terms

Endpoint/Notes

`/terms/index/[scope]/[format]/[download]`

List of terms in the Gold Book

[scope]: (all), A-W, XYZ (returns to referring page if no data)

[format]: (html), xml, json (rest are ignored)

[download]: (""), download (rest are ignored)

Example(s)

`/terms/index/all` (just "terms" works too)

`/terms/index/C/xml`

`/terms/index/XYZ/json/download`

`/terms/view/[identifier]/[format]/[download]`

A term from the Gold Book

[identifier]: term code or id

[format]: (html), xml, json (rest are ignored)

[download]: (""), download (rest are ignored)

`/terms/view/A00001`

`/terms/view/P04409/json`

`/terms/view/ZT07132/xml/download`

Sources (Click to show)

absorbance, A

Logarithm of the ratio of incident to transmitted radiant power through a sample the effective path length. The quantity is defined on the base of the logarithm a decadic and absorbance A , A_{10} , A_e . This quantity is sometimes called optical density, although the latter term called attenuation, is reserved for the quantity that takes into account the effects of luminescence and scattering as well.

Source:

Green Book, 2nd ed., p. 32 [Terms] [Book]

DOI

<https://doi.org/10.1351/goldbook>

Provenance

Currently developing the processes and practices needed to ensure definitions are born digital

<https://goldbook.iupac.org>



Gold Book: Sources & Scope

- Chemical concepts defined within IUPAC Recommendations
- Attributes, types, parameters, dependencies of chemical properties, measurements, etc.
- Published primarily in *Pure & Applied Chemistry* (authoritative source for scientific meaning)
- *Gold Book* aggregates with rich semantic metadata
- Does NOT include naming rules, quantity calculations, specific entities or instances

The screenshot displays four article entries from the IUPAC Gold Book. Each entry includes a thumbnail image, a title, the journal name, the date, and buttons for 'More', 'Cite', and 'Download PDF'. The articles are:

- Henry's law constants (IUPAC Recommendations 2021)**
Chemistry International
April 14, 2022
- Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021)**
Pure and Applied Chemistry
Charles L. Perrin, Israel Agranat, Alessandro Bagno, Silvia E. Braslavsky, Pedro Alexandrino Fernandes, Jean-François Gal, Guy C. Lloyd-Jones, Herbert Mayr, Joseph R. Murdoch, Norma Sbarbati Nudelman, Leo Radom, Zvi Rappoport, Marie-Françoise Ruasse, Hans-Ullrich Siehl, Yoshito Takeuchi, Thomas T. Tidwell, Einar Uggerud, Ian H. Williams May 23, 2022
- Glossary of terms relating to electronic, photonic and magnetic properties of polymers (IUPAC Recommendations 2021)**
Chemistry International
April 14, 2022
- Terminology and the naming of conjugates based on polymers or other substrates (IUPAC Recommendations 2021)**
Pure and Applied Chemistry
Michel Vert, Jiazhong Chen, Andrey Yerin, Karl-Heinz Hellwich, Roger C. Hiorns, Richard Jones, Graeme Moad, Gerard P. Moss
March 17, 2022



The Online *Gold Book*

- Early projects (1,2) to develop XML version of the *Gold Book* (released online 2006) enabled:
 - Basic search
 - DOI for each concept
- Technical update in 2019 added:
 - Comprehensive search
 - Device agnostic UI
 - REST API
- Updating content (ongoing)
 - ~24500 definitions, ~16000 unique
- License: CC BY-SA 4.0 per term

Gold Book Statistics

- 6463 concepts (Eight Divisions)
 - 1233 Div I (Physical)
 - 286 Div II (Inorganic)
 - 2204 Div III (Organic)
 - 644 Div IV (Polymer)
 - 1395 Div V (Analytical)
 - 597 Div VI (Environmental)
 - 493 Div VII (Health)
 - 127 Div VIII (Naming)
- 10K Wikipedia links (2,400 concepts)
- 1947 entries on Wikidata (P4732)
- 1K hits/day (since Jan 2021)

(1) Development “Standard XML data dictionaries for chemistry” <https://iupac.org/project/2002-022-1-024>

(2) Updating “Enhancement of the electronic version of the IUPAC Compendium of Chemical Terminology” <https://iupac.org/project/2007-016-1-024>

Example Concept Definitions

[Guidelines for Writing
a Concept Definition](#)

From: Perrin, Charles L., et al., "Glossary of terms used in physical organic chemistry (IUPAC Recommendations 2021)" *Pure Appl. Chem.*, vol. 94, no. 4, 2022, pp. 353-534. <https://doi.org/10.1515/pac-2018-1010>

α -effect

Positive deviation of an α nucleophile (one bearing an unshared pair of electrons on an atom adjacent to the nucleophilic site) from a Brønsted-type plot of $\lg \{k_{\text{nuc}}\}$ vs. $\text{p}K_{\text{a}}$. The argument in the \lg function should be of dimension 1. Thus, reduced *rate coefficients* should be used. Here $\{k_{\text{nuc}}\} = k_{\text{nuc}}/[k_{\text{nuc}}]$ is the reduced k_{nuc} .

Note 1: More generally, it is the influence on the reactivity at the site adjacent to the atom bearing a lone pair of electrons.

Note 2: The term has been extended to include the effect of any substituent on an adjacent reactive center, e.g., the α -silicon effect.

See [58–60].

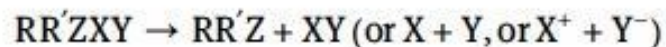
See also *Brønsted relation*.

rev[3]

α -elimination

1,1-elimination

Transformation of the general type



where the central atom Z is commonly carbon.

See also *elimination*.

rev[3]

Example Concept Page

The screenshot shows a web browser window displaying the IUPAC Gold Book page for 'absorbance, A'. The browser's address bar shows the URL <https://goldbook.iupac.org/terms/view/A00028>. The page features a yellow header with the IUPAC logo and the text 'Gold Book'. A search bar is located in the top right corner. On the left side, there is a navigation menu with an 'Alphabetical Index' section containing a grid of letters from A to XYZ, and an 'Additional Indexes' section with links to Physical Constants, Units of Measure, Physical Quantities, SI Prefixes, Ring Index, General Formulae, Exact Formulae, Source Documents, and Terms by IUPAC Div. Below the menu, it states 'Version 3.0.1 (6463 Terms)' and provides the DOI: [10.1351/goldbook](https://doi.org/10.1351/goldbook), along with the names of the content editor and technical editor.

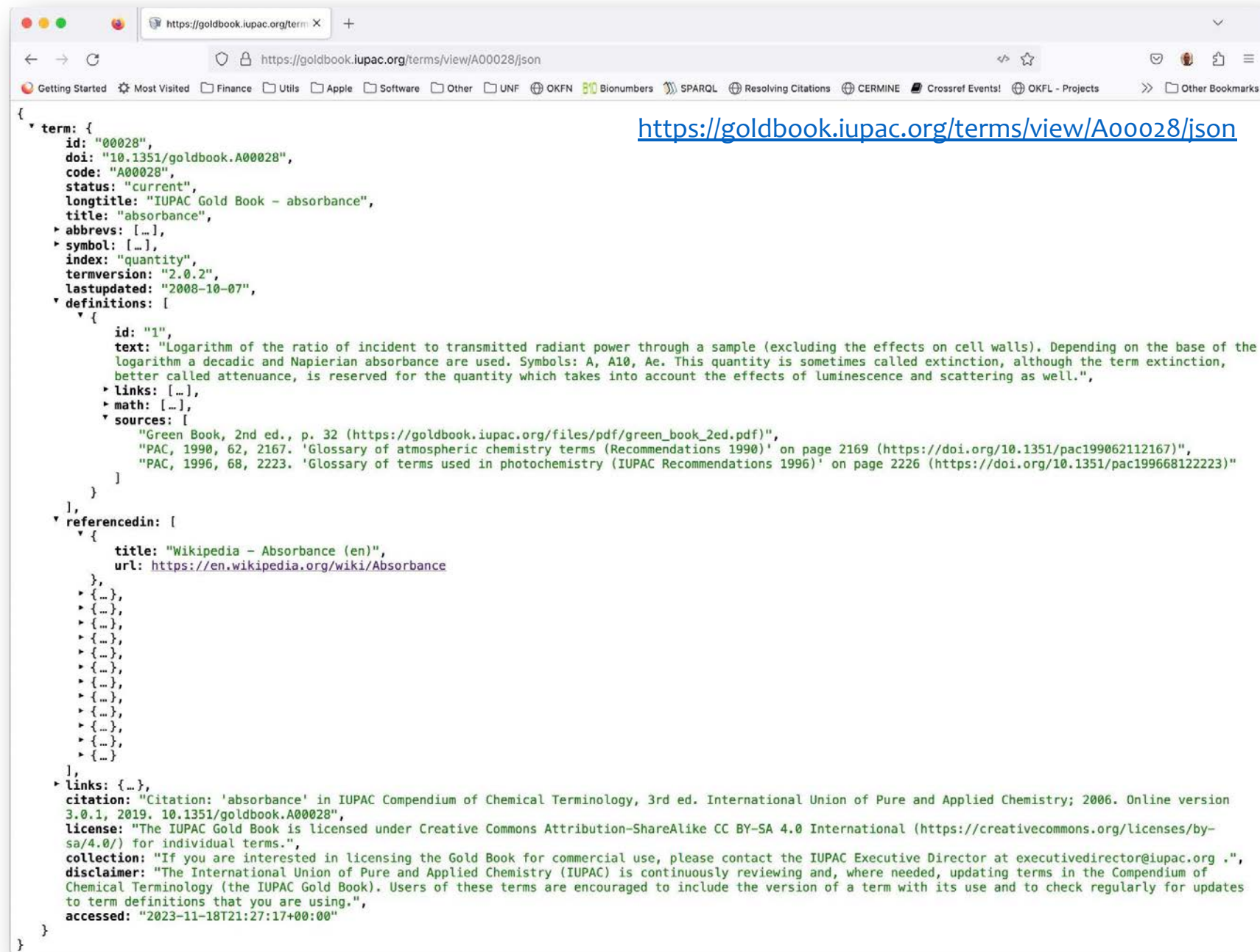
The main content area is titled 'absorbance, A' and includes a 'Copy' button for the DOI: <https://doi.org/10.1351/goldbook.A00028>. The definition states: 'Logarithm of the ratio of incident to transmitted radiant power through a sample (excluding the effects on cell walls). Depending on the base of the logarithm a decadic and Napierian absorbance are used. Symbols: A , A_{10} , A_e . This quantity is sometimes called extinction, although the term extinction, better called attenuance, is reserved for the quantity which takes into account the effects of luminescence and scattering as well.'

The 'Source' is cited as: 'Green Book, 2nd ed., p. 32 [Terms] [Book]'. The 'See also' section lists two references: 'PAC, 1990, 62, 2167. (*Glossary of atmospheric chemistry terms (Recommendations 1990)*) on page 2169 [Terms] [Paper]' and 'PAC, 1996, 68, 2223. (*Glossary of terms used in photochemistry (IUPAC Recommendations 1996)*) on page 2226 [Terms] [Paper]'. A 'Citation' box at the bottom provides the full citation: 'absorbance' in *IUPAC Compendium of Chemical Terminology*, 3rd ed. International Union of Pure and Applied Chemistry; 2006. Online version 3.0.1, 2019. <https://doi.org/10.1351/goldbook.A00028>. It also includes buttons for RIS, BibTex, and EndNote.

At the bottom of the page, there are buttons for 'Div. I', 'PDF', 'Text', 'JSON', 'History', and 'Quantity', and a note that the page was 'Last revised: October 7, 2008'. The footer of the browser window shows the copyright notice: '© 2005–2023 International Union of Pure and Applied Chemistry'.

Example API Download

- API download as XML or JSON
- Crossref metadata also available via <https://api.crossref.org>



The screenshot shows a web browser window with the URL <https://goldbook.iupac.org/terms/view/A00028/json>. The browser's address bar and tabs are visible at the top. The main content area displays a JSON object representing the term 'absorbance'. The JSON structure includes fields for 'id', 'doi', 'code', 'status', 'longtitle', 'title', 'abbrevs', 'symbol', 'index', 'termversion', 'lastupdated', 'definitions', 'referencedin', 'links', 'citation', 'license', 'collection', 'disclaimer', and 'accessed'. The 'definitions' array contains a single definition with 'id', 'text', 'links', 'math', and 'sources' fields. The 'referencedin' array contains a reference to the Wikipedia page for 'Absorbance'. The 'links' field provides a citation for the term in the IUPAC Compendium of Chemical Terminology. The 'accessed' field shows the date and time the data was retrieved.

```
{
  "term": {
    "id": "A00028",
    "doi": "10.1351/goldbook.A00028",
    "code": "A00028",
    "status": "current",
    "longtitle": "IUPAC Gold Book - absorbance",
    "title": "absorbance",
    "abbrevs": [...],
    "symbol": [...],
    "index": "quantity",
    "termversion": "2.0.2",
    "lastupdated": "2008-10-07",
    "definitions": [
      {
        "id": "1",
        "text": "Logarithm of the ratio of incident to transmitted radiant power through a sample (excluding the effects on cell walls). Depending on the base of the logarithm a decadic and Napierian absorbance are used. Symbols: A, A10, Ae. This quantity is sometimes called extinction, although the term extinction, better called attenuation, is reserved for the quantity which takes into account the effects of luminescence and scattering as well.",
        "links": [...],
        "math": [...],
        "sources": [
          "Green Book, 2nd ed., p. 32 (https://goldbook.iupac.org/files/pdf/green_book_2ed.pdf)",
          "PAC, 1990, 62, 2167. 'Glossary of atmospheric chemistry terms (Recommendations 1990)' on page 2169 (https://doi.org/10.1351/pac199062112167)",
          "PAC, 1996, 68, 2223. 'Glossary of terms used in photochemistry (IUPAC Recommendations 1996)' on page 2226 (https://doi.org/10.1351/pac199668122223)"
        ]
      }
    ]
  },
  "referencedin": [
    {
      "title": "Wikipedia - Absorbance (en)",
      "url": "https://en.wikipedia.org/wiki/Absorbance"
    },
    { ... },
    { ... },
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    { ... },
    { ... },
    { ... },
    { ... }
  ],
  "links": { ... },
  "citation": "Citation: 'absorbance' in IUPAC Compendium of Chemical Terminology, 3rd ed. International Union of Pure and Applied Chemistry; 2006. Online version 3.0.1, 2019. 10.1351/goldbook.A00028",
  "license": "The IUPAC Gold Book is licensed under Creative Commons Attribution-ShareAlike CC BY-SA 4.0 International (https://creativecommons.org/licenses/by-sa/4.0/) for individual terms.",
  "collection": "If you are interested in licensing the Gold Book for commercial use, please contact the IUPAC Executive Director at executivedirector@iupac.org .",
  "disclaimer": "The International Union of Pure and Applied Chemistry (IUPAC) is continuously reviewing and, where needed, updating terms in the Compendium of Chemical Terminology (the IUPAC Gold Book). Users of these terms are encouraged to include the version of a term with its use and to check regularly for updates to term definitions that you are using.",
  "accessed": "2023-11-18T21:27:17+00:00"
}
```


Updating Gold Book Content: The Term Review System (TRS)

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Gold Book - Term Review System

Stuart
Dashboard
Logout

All Term Stats

Divisions

Recommendations

- Amplification Rxns. J
- Analytical Methods J
- Bioanalytical J
- Capillary Electromig. J
- Chemometrics J
- Chiral Separations J
- Chromatography J
- Electrochemistry (1985) J
- Electrochemistry (2018) J
- Enthalpimetry J
- Extraction (1993) J
- Extraction (2015) J
- Flow Methods J
- ISEs J
- Kinetic Anal. J
- Mechanised Anal. J
- Microanalysis J
- Non-Linear Chrom. J

Search

Open Tickets

Add ticket..

Checked?

DE GRUYTER
Pure Appl. Chem. 2016; 88(4): 407–443

IUPAC Recommendations

David B. Hibbert*

Vocabulary of concepts and terms in chemometrics (IUPAC Recommendations 2016)

DOI 10.1515/pac-2015-0605
Received June 20, 2015; accepted March 4, 2016

Abstract: Recommendations are given concerning the terminology relating to chemometrics. Building on ISO definitions of terms for basic concepts in statistics the vocabulary is concerned with mainstream chemometric methods. Where methods are used widely in science, definitions are given that are most useful to chemical applications. Vocabularies are given for general data processing, experimental design, classification, calibration and general multivariate methods.

Keywords: calibration; chemometrics; data analysis; design of experiments; experimental design; IUPAC Analytical Chemistry Division; multivariate analysis; pattern recognition; regression; terminology.

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1 Preface

The recommendations contained in this document concern the terminology relating to concepts in chemometrics. It recognises the existence of ISO Standards on terms used in statistics and probability [1] and applied statistics [2], and has not attempted to redefine basic concepts in statistics. See ISO 3454 [1, 2] and the IUPAC Green Book [3] for general rules on symbols and terminology in mathematics and statistics.

Generic quantities are denoted by upper-case letters, and individual values ('best estimates' in a mathematical framework) by the corresponding lower-case letter. In a measurement model, Y denotes the measurand, X_1, \dots, X_n the input quantities, and y, x_1, \dots, x_n the corresponding best estimates.

Article note: This work was started under project 2008-002-1-500: A glossary of concepts and terms in chemometrics, with membership D Brynn Hibbert, Pentti Minkkinen and Barry Wise. Public input was via an open wiki that was active from 2010 to 2012 [D. B. Hibbert, P. Minkkinen, N. M. Faber, B. M. Wise, *Anal. Chim. Acta* **642**, 3 (2009)].

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- ✓ alias structure PR
- ✓ aliased effects 1 PR
- ✓ alternating least squares regression PR
- ✓ artificial neural network 1 PR
- ✓ autocorrelation PR
- ✓ autoregression 1 PR
- ✓ autoscaling PR
- ✓ backward chaining PR
- ✓ backward propagation PR
- ✓ backward stepwise linear discriminant analysis PR
- ✓ Bayes classifier PR
- ✓ biplot PR
- ✓ bootstrapping 2 PR
- ✓ calibration 3 GB PR
- ✓ canonical variables PR
- ✓ canonical variate analysis 1 PR
- ✓ categorical data PR
- ✓ chemometrics 2 GB PR
- ✓ city-block distance PR
- ✓ classification 1 PR
- ✓ cluster GB PR
- ✓ coded experimental design 2 PR
- ✓ common factor analysis PR
- ✓ complete linkage PR
- ✓ contingency table PR
- ✓ core consistency diagnostic 1 PR
- ✓ correspondence factor analysis PR
- ✓ cross validation 3 PR

Proposed Changes to Definitions

Review Terms for Approval

Concept Updates - Revised Schedule



- Ingestion of content for all source IUPAC Recommendations into the TRS by the Summer 2024
- By January 2024
 - Nine Recommendations from 2021 onwards (~2000 terms)
 - “Glossary of Physical Organic Chemistry” - 618 terms
 - “Glossary of Methods/Terms used in Analytical Spectroscopy” - 586 terms
- Divisional review and approval of older recommendations 2024
 - Linking is only ‘within’ recommendations - across?
 - Analysis of same terms across multiple IUPAC Divisions
 - One definition with notes OR multiple definitions w/context
- Updated Goal - to be completed by July of 2025 at the IUPAC GA
- *Reminder: IUPAC is a volunteer organization...*

GOAL: Enable Semantic Chemistry



- Enable the Gold Book to support chemistry related ontologies
 - Expose appropriate metadata to derive machine-processable meaning and allow reference to source scientific definitions (DOI trace)
 - Develop mechanisms by which Gold Book concepts can be utilized in ontologies, and expose that reuse back through the Gold Book
 - Identify gaps in concepts/terminology and pipeline into the formal IUPAC Recommendation process
 - Contribute to IUPAC-community projects on concept definitions and semantic mapping
- IUPAC concepts need to be reusable across a broad and diverse community (academic, industrial, interdisciplinary, international, etc.)
 - What are your needs for chemical concepts, what is missing?
 - Are there classification schemes that support a range of reuse applications?

Reuse of IUPAC Defined Terms in Ontologies



- NFDI4Chem and IUPAC have been working on guidance document on how to incorporate terms into ontologies
- This includes:
 - Citation - DOI of Gold Book term
 - Abstracting relevant metadata - concept, genus, and differentia
 - Alignment with an upper level ontology (if appropriate)
- Examples follow
 - How transferable would these constructs be for different use cases?
 - What needs more chemistry context? classification?
 - How do we handle dependencies (e.g., other concepts, other sources)?

Reuse of IUPAC Defined Terms in Ontologies



- Example 1:
 - IUPAC Term: 3.5 additive matrix effect
 - Source: “[Metrological and analytical concepts in analytical chemistry](#)”
 - Definition: *Matrix effect that is independent of the measured quantity value [VIM 2.10] of the measurand*
 - Metadata
 - Concept: [additive matrix effect](#)
 - Genus: [matrix effect](#)
 - Differentia: [independent of the measured quantity value of the measurand](#)
 - Outcome: Good
 - Comment: Definition is aligned with this analysis

Reuse of IUPAC Defined Terms in Ontologies



- Example 2:
 - IUPAC Term: 3.1.15 sorbent trap
 - Source: “[Glossary of terms used in extraction](#)”
 - Definition: *Tube filled with porous sorbent typically used to extract analytes from the gas phase*
 - Metadata
 - Concept: [sorbent trap](#)
 - Genus: [extraction device](#)
 - Differentia: [sorbent packed into a tube such that analytes may be extracted from a gas phase](#)
 - Outcome: Ambiguity in definition - “typically”
 - Comment: Needs more context, section 3.1 is “Gas-phase extraction”

Reuse of IUPAC Defined Terms in Ontologies



- Example 3:
 - IUPAC Term: chemical species
 - Source: "[Glossary of terms used in physical organic chemistry](#)"
 - Definition: *Ensemble of chemically identical molecular entities that can explore the same set of molecular energy levels on the time scale of an experiment. The term is applied equally to a set of chemically identical atomic or molecular structural units in a solid array.*
 - Metadata
 - Concept: [chemical species](#)
 - Genus: [molecular entities](#)
 - Differentia: [chemically identical molecular entities that can explore the same set of molecular energy levels on the time scale of an experiment](#)
 - Outcome: Incomplete...how to represent at different levels?
 - Comment: Complicated...



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