

Renovating the IUPAC Gold Book for the Digital Era and the Next 100 Years

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Outline

- * IUPAC's Mission
- * IUPAC recommendations
- * Development of the IUPAC Gold Book
Compendium of Chemical Terminology
- * IUPAC Project 2016-046-1-024:
Backup, Maintenance, and Redevelopment of the IUPAC Gold Book website
- * Reimagining the IUPAC Gold Book
- * Conclusions

IUPAC's Mission

The International Union of Pure and Applied Chemistry is the global organization that provides objective scientific expertise and develops the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world.

IUPAC accomplishes its mission by fostering sustainable development, providing a common language for chemistry, and advocating the free exchange of scientific information.

In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of humankind.

IUPAC Recommendations


“IUPAC Recommendations are the output of IUPAC Projects or other studies on nomenclature, symbols, terminology, or conventions, and their purpose is to recommend unambiguous, uniform, and consistent nomenclature and terminology for specific scientific fields, usually presented as: glossaries of terms for specific chemical disciplines; definitions of terms relating to a group of properties; nomenclature of chemical compounds and their classes; terminology, symbols, and units in a specific field; classifications and uses of terms in a specific field; and conventions and standards of practice for presenting data in a specific field” – developed by chemical experts via consensus and through the formal IUPAC Inter-Divisional Committee on Terminology, Nomenclature and Symbols (ICTNS) process.

<https://iupac.org/what-we-do/recommendations/>


Development of the IUPAC Gold Book

- * Initiated by Victor Gold in the early 1980's
- * Digital (XML) version of IUPAC Gold Book started in 2002 (Project [2001-062-2-027](#))
- * First version of the website in 2006 by Miloslav Nic, Jiri Jirat and Bedrich Kosata
- * Last updated (before new project) in 2014

IUPAC Gold Book - absorbance, A
goldbook.iupac.org/html/A/A00028.html
90%
Search



IUPAC GOLD BOOK



Search...

Indexes

- alphabetical
- chemistry
- math/physics
- general
- source documents

Download

- Gold Book PDF

IUPAC > Gold Book > alphabetical index > A > **absorbance, A**

PREVIOUS

absorbance, A

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 attenuation, is reserved for the quantity which takes into account the effects of luminescence and scattering as well.


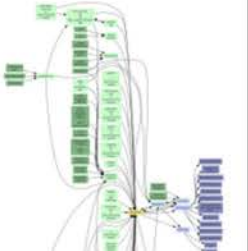
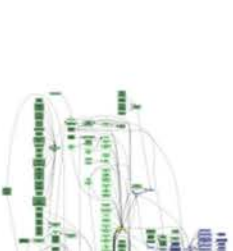
Source:
Green Book, p. 32

See also: PAC, 1996, 68, 2223 (*Glossary of terms used in photochemistry (IUPAC Recommendations 1996)*) on page 2226
PAC, 1990, 62, 2167 (*Glossary of atmospheric chemistry terms (Recommendations 1990)*) on page 2169

Related index:
IUPAC > Gold Book > math/physics > quantities

NEXT

Interactive Link Maps

First Level	Second Level	Third Level
		

IUPAC Project 2016-046-1-024:

Backup, Maintenance, and Redevelopment of the IUPAC Gold Book website

- * Missing 4000+ files in October 2016
- * Static website - 100k files in one folder
- * Missing files replaced Nov 2016
(from the [Wayback Machine](#) – see archived pages [here](#))
- * Migrated to new host (server) Nov 2016

<https://iupac.org/project/2016-046-1-024>

IUPAC Project 2016-046-1-024:

Backup, Maintenance, and Redevelopment of the IUPAC Gold Book website

- * Dedicated administrator
- * Backup of Gold Book website files
- * Cleanup pages (HTML 5)
- * Create a new version of the website
 - * Analyze the layout of a term page for content
 - * 'scrape' data out of HTML and XML files as appropriate
 - * Capture scraped data in a database (MySQL)
 - * Create new pages from database

IUPAC Project 2016-046-1-024:

Backup, Maintenance, and Redevelopment of the IUPAC Gold Book website

- * Additional features of the new website
 - * Application Programming Interface (API)
 - * REST Style URLs – E.g. /terms/view/A00028
 - * Responsive Interface – works on all devices
 - * Enhanced search – term, synonym, acronym
 - * Vocabulary downloads
 - * Project on GitHub (code/documentation repository)

IUPAC Project 2016-046-1-024:

Backup, Maintenance, and Redevelopment of the IUPAC Gold Book website

* REST API

- * /terms/index/[all|A-W|XYZ]/[json|xml]
- * /terms/view/[identifier]/[json/xml]/[download]
- * /sources/index/[all]/[json/xml]/[download]
- * /sources/view/[identifier]/[json/xml]/[download]
- * Additional API endpoints will be added to serve the needs of the community

Anatomy of an IUPAC Gold Book Term

- * From recommendations

- * Preferred term
- * Acronym/Symbol/Synonym
- * Deprecated/Obsolete/Superseded
- * Definition of term
- * Cross-referenced term
- * Reference (related to definition)
- * Notes/ExampleRelated term(s)
- * References (related to term)

- * From the IUPAC Gold Book

- * Contexts ('of' or 'in')
- * Also contains
- * Related index
- * Link map
- * Digital Object Identifier (DOI)
- * History of the term (online)
- * Version

<https://iupac.org/what-we-do/recommendations/guidelines-for-drafting-reports/>

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

- Physical Constants
- Units of Measure
- Physical Quantities
- SI Prefixes
- Ring Index
- General Formulae
- Exact Formulae
- Source Documents
- Terms by IUPAC Div

Download Vocabulary
PDF | JSON | XML

< >

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.

Green Book, 2nd ed., p. 32 [\[Terms\]](#) [\[Book\]](#)

PAC, 1990, 62, 2167. (*Glossary of atmospheric chemistry terms (Recommendations 1990)*) on page 2169 [Terms] [Paper]

PAC, 1996, 68, 2223. (*Glossary of terms used in photochemistry (IUPAC Recommendations 1996)*) on page 2226 [Terms] [Paper]

Div. I PDF Text JSON History Quantity

Last updated: October 7, 2008 (v. 2.0.2)

REST API JSON

```
"term": {
  "metadata": {
    "id": "00028",
    "doi": "10.1351/goldbook.A00028",
    "code": "A00028",
    "status": "current",
    "longtitle": "IUPAC Gold Book - absorbance",
    "title": "absorbance",
    "abbrevs": ["abs"],
    "symbol": ["A"],
    "index": "quantity",
    "version": "2.0.2",
    "lastupdated": "2008-10-07"
  },
  "definitions": {
    "definition": [
      {
        "id": "1",
        "text": "Logarithm of the ratio of incident to transmitted radiant power through a sample (excl",
        "links": [ [21 lines]
        "math": [ [16 lines]
        "sources": [
          "Green Book, 2nd ed., p. 32 (https://dev.goldbook.iupac.org/files/pdf/green\_book\_2ed.pdf)",
          "PAC, 1990, 62, 2167. 'Glossary of atmospheric chemistry terms (Recommendations 1990)' on p",
          "PAC, 1996, 68, 2223. 'Glossary of terms used in photochemistry (IUPAC Recommendations 1996"
        ]
      ]
    ]
  },
  "links": { [7 lines]
  "citeas": "IUPAC. Compendium of Chemical Terminology, 2nd ed. (the \"Gold Book\"). Compiled by A. D. McNaugh",
  "license": "Licensed under Creative Commons Attribution-NoDerivatives (CC-BY-ND) 4.0 International (https://",
  "disclaimer": "The International Union of Pure and Applied Chemistry (IUPAC) is continuously reviewing and",
  "accessed": "2019-03-31T11:22:25-04:00"
}
```

Reimagining the IUPAC Gold Book

* ...for Semantic Chemical Annotation

- * Source IUPAC recommendations for the corpus of terms that the Divisions of IUPAC have published ...
- * ...and add them to Gold Book (make it a comprehensive compendium of chemical terminology)
- * Develop an IUPAC Chemical Ontology from the Gold Book terms
- * Publish the ontology to define chemical information in machines
- * Otherwise the community will do it anyway!

Reimagining the IUPAC Gold Book

Division	Terms
Analytical	2949
Biochemistry	895
Cheminformatics	645
Chemical Safety	1345
Data Management	244
Environmental Chemistry	2356
Inorganic Chemistry	675
Materials	2394
Measurement	181
Medicinal Chemistry	2111
Nuclear Chemistry	490
Organic Chemistry	2800
Physical Chemistry	2922
Theoretical/Computational Chemistry	3042
Toxicology	7064
TOTAL	30113

IUPAC Standards Online

<https://www.degruyter.com/view/db/iupac>

Semantic Examples of IUPAC Terms

- * REX – physico-chemical processes¹ [239]
- * ChemOnt – chemical classification² [86]
- * MOP – molecular processes³ [39]
- * CAO – chemical analysis⁴ [34]
- * CMO – chemical methods⁵ [10]
- * RXNO – reactions³ [3]

- * ChEBI – biologically related molecules⁶ [0]

- 1) <http://purl.obolibrary.org/obo/rex.obo>
- 2) http://classyfire.wishartlab.com/system/downloads/1_0/chemont/ChemOnt_2_1.obo.zip
- 3) <https://github.com/rsc-ontologies/rxno>
- 4) <http://champ-project.org/images/ontology/cao.owl>
- 5) <https://github.com/rsc-ontologies/rsc-cmo>
- 6) <http://www.ebi.ac.uk/chebi/>

Semantic Examples of IUPAC Terms: REX

electron transfer — REX:0000028 — http://purl.obolibrary.org/obo/REX_0000028

Annotations Usage

Annotations: electron transfer

Annotations +

rdfs:label [type: xsd:string]
electron transfer

id [type: xsd:string]
REX:0000028

has_obo_namespace [type: xsd:string]
rex.obo

definition [type: xsd:string]
The transfer of an electron from one molecular entity to another, or between two localized sites in the same molecular entity.

database_cross_reference [type: xsd:string]
<http://goldbook.iupac.org/E02011.html>

<http://purl.obolibrary.org/obo/rex.obo>

electron transfer

<https://doi.org/10.1351/goldbook.E02011>

The transfer of an electron from one molecular entity to another, or between two localized sites in the same molecular entity.

See also: inner-sphere electron transfer, outer-sphere electron transfer, Marcus equation (for electron transfer)

Sources:
PAC, 1994, 66, 1077. (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1110 [Terms] [Paper]
PAC, 1996, 68, 2223. (*Glossary of terms used in photochemistry (IUPAC Recommendations 1996)*) on page 2239 [Terms] [Paper]

Cite as: IUPAC. *Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

Div. III PDF Text JSON History

Last updated: February 24, 2014 (v. 2.3.3)

Semantic Examples of IUPAC Terms: ChemOnt

[Term
id: CH
name:
def: "
an am
carbo
synon
synon
...
xref: I
(the 'C
Scient
is_a: C

amidines



<https://doi.org/10.1351/goldbook.A00267>

Derivatives of oxoacids $R_nE(=O)OH$ in which the hydroxy group is replaced by an amino group and the oxo group is replaced by $=NR$. Amidines include carboxamidines, sulfinamidines and phosphinamidines, $R_2P(=NR)NR_2$. In organic chemistry an unspecified amidine is commonly a carboxamidine.

See also: carboxamidines, sulfinamidines

Source:

PAC, 1995, 67, 1307. (*Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995)*) on page 1315 [Terms] [Paper]

Cite as: IUPAC. *Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

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by

Semantic Examples of IUPAC Terms: MOP

[Term]

id: MOP:0000656

name: elimination reaction

def: "A molecular process where two groups are lost with concomitant formation of an unsaturation in the molecule or formation of a new ring."

[doi:10.1351/goldbook.E02038]

is_a: MOP:0000543 ! molecular process

<https://github.com/rsc-ontologies/rxno>

elimination

<https://doi.org/10.1351/goldbook.E02038>

The reverse of an addition reaction or transformation. In an elimination two groups (called eliminands) are lost most often from two different centres (1/2/elimination or 1/3/elimination, etc.) with concomitant formation of an unsaturation in the molecule (double bond, triple bond) or formation of a new ring. If the groups are lost from a single centre (α -elimination, 1/1/elimination) the resulting product is a carbene or a 'carbene analogue'.

See also: α -elimination

Source:

PAC, 1994, 66, 1077. (*Glossary of terms used in physical organic chemistry (IUPAC Recommendations 1994)*) on page 1112 [Terms] [Paper]

Cite as: IUPAC. *Compendium of Chemical Terminology*, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

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Semantic Examples of IUPAC Terms: ChEBI

[Term]

id: CHEBI:33575

name: carboxylic acid

def: "A carbon oxoacid acid carrying at least one -C(=O)OH group and having the structure RC(=O)OH, where R is any any monovalent functional group. Carboxylic acids are the most common type of organic acid." []

synonym: "RC(=O)OH" |

...

property_value: http://p

...

xref: Wikipedia:Carboxy

carboxylic acids

<https://doi.org/10.1351/goldbook.C00852>

Oxoacids having the structure **RC(=O)OH**. The term is used as a suffix in systematic name formation to denote the **-C(=O)OH** group including its carbon atom.

Source:
PAC, 1995, 67, 1307. (*Glossary of class names of organic compounds and reactivity intermediates based on structure (IUPAC Recommendations 1995)*) on page 1326 [Terms] [Paper]

Cite as: IUPAC. Compendium of Chemical Terminology, 2nd ed. (the "Gold Book"). Compiled by A. D. McNaught and A. Wilkinson. Blackwell Scientific Publications, Oxford (1997). XML on-line corrected version: <http://goldbook.iupac.org> (2006-) created by M. Nic, J. Jirat, B. Kosata; updates compiled by A. Jenkins. ISBN 0-9678550-9-8. <https://doi.org/10.1351/goldbook>.

Div. III

PDF

Text

JSON

History

Last updated: February 24, 2014 (v. 2.3.3)

Conclusions

- * The expansion and ‘semanticization’ of IUPAC terms will leverage the significant time and effort IUPAC members have invested in creation of IUPAC recommendations and the IUPAC Gold Book
- * Renovating the IUPAC Gold Book for the digital era
 - * Opens chemical knowledge to digital applications
 - * Better supports the chemistry community
 - * Preserves chemical knowledge for the next 100 years (and beyond)
 - * Will make it easier to improve/expand maintenance
 - * Promotes the importance of IUPAC in digital science

Thanks to

- * IUPAC Gold Book Project Task Group
 - * Greg Banik*, Brynn Hibbert, Mark Kinnan, Bonnie Lawlor, Leah McEwen*, Ron Weir*
- * CPCDS Subcommittee on Cheminformatics Data Standards (SCDS)
 - * David Martinsen, Ian Bruno, Anthony Davies, Clàudio dos Santos, Chris Fellows, Jeremy Frey, Robert Lancashire, Andrey Yerin

* Also on the SCDS

Questions?

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