Chemical Abstracts Service

1907 As a division of the American Chemical Society. The first volume contained 11,847 abstracts. 865,066 abstracts in 2004. A total of 22,993,118 documents indexed.

Chemical Abstracts Service

CAS Registry Number (RN)

Originally just for CAS. Now standard method for uniquely identifying chemicals. Used by many chemical reference sources. All substances indexed by CAS get RN. Every chemically distinct substance gets its own RN, including stereoisomers, isotopically labeled substances, mixtures, polynucleotide and protein sequences, etc. Registry Numbers are of the form: xxxxx-xx-x. The number has no chemical meaning.

Chemical Abstracts Service

Importance of Chemical Abstracts

Scope
CA attempts to cover chemistry in the broad sense
Comprehensiveness
CA attempts to cover the literature of chemistry worldwide, in any language.
Chronological coverage
Print CA began in 1907; electronic CA in 1967

Chemical Abstracts Service

Contents of the Abstract Record

Title of the document
Author(s) or inventor(s) for patents (as in the original document)
Corporate source or patent assignee information
Source Information (journal, volume, issue number, and pages)
Language
Abstracts (usually)
Abstracts for journal articles usually written by the author. Patent abstracts fleshed out by the indexer. Dissertations and some other documents have no abstracts. Early abstracts much longer and more detailed.

Abstracts examples


Abbreviations

Journal names are listed using CASSI abbreviations.  
www.cas.org/sent.html

All abstracts use abbreviations for common chemical terms  
www.cas.org/ONLINE/standards.html

Author Index

First authors paper title and abstract number.  
Examples:

Ford, Peter Campbell  
Quantitative mechanistic studies of ... 148754a

Lange, Frederick Fouse  
See Miller, Kelly T.; Sudre, Olivier  
---; Lam, D.C.C.; Sudre, O.  
Powder processing and densification of ceramics 144196x

General Subject Index

Usually standard subject headings:

- classes of chemical substances
- physical and chemical phenomena
- types of reactions
- chemical technology
- industrial processes and equipment
- scientific names for living organisms
- biological and medical terminology

Indexing in Print CA

Volume & Collective Indexes  
www.cas.org/EO/collect.html

Author

General Subject

Chemical Substance

Molecular Formula

Patent

Alphabetizes by last name and initials.  Examples:

Ellis, A.  
Ellis, Arthur Baron  
Ellis, A. D.  
Ellis, Anthony Ewart

Names with "Mc", umlauted letters or transliteration from non-Roman alphabets can be tricky.  
Example:

Mössbauer is listed as Moessbauer

1. Author Index

Where an author is not the first author of an article, reference must be made to the first author to obtain abstract number.

Steele, G. Jr.  
See Kramer, R  
Steele, Glenn Jr.  
See Thomas, Peter  
Steele, Gregory Kent  
The prevalence of serum polychlorinated biphenyls and their association with blood pressure in a community environmentally exposed.  
120:142658r

Title of article by Steele.  Complete citation is found in volume 120 of CA, abstract number 142658r

1. Author Index
Subject Index

2. Subject Index

<table>
<thead>
<tr>
<th>Cross reference in the Index Guide; articles on “xylococcus bicolor” are indexed under “arthrospaphylus bicolor.”</th>
</tr>
</thead>
<tbody>
<tr>
<td>When a registry number [843329-47-5] appears in the index guide, this is an indication that the entry will be found in the Chemical Substances index.</td>
</tr>
</tbody>
</table>

Subject heading from 13th Collective Index

Abstract number; number preceding the colon is the volume number.

"R" indicates a review article.

Xylococcus bicolor

See Arctostaphylos bicolor

Xylofilcon

See 2-Propenoic acid, 2-methyl-, esters, 2-pyrrolidinone, 2-ethoxyethyl 2-methyl-2-propenoate, methyl 2-methyl-2-propenoate and 2-propenyl 2-methyl-2-propenoate [843329-47-5]

Pipes and Tubes

High-strength steel, crane booms made of; 121:39874w

High-strength steels for large pipes, 122: R 55686w

3. Chemical Substance Index

<table>
<thead>
<tr>
<th>Chemical substance index heading</th>
<th>Substance Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl- [58-08-2]</td>
<td>Old analysis biological studies occurrence preparations properties reactions uses and miscellaneous</td>
</tr>
</tbody>
</table>

New (additions to old headings)

formation (nonpreparative) processes separate uses and miscellaneous

The Challenge of Nomenclature

CA has their own system of nomenclature (not necessarily IUPAC). Unfortunately, this system can be complex.

For example: Dodecahedrane (C_{20}H_{20}) used to be listed as simply dodecahedrane. Then a systematic name was given:

5,2,1,6,3,4-[2,3]Butanylenedipentaleno [2,1,6-cde:2',1',6'-gha]pentalene, hexadecahydro-

Now it's treated as a member of the fullerene family:

[5]Fullerene-C20-Ih

Basic Rules of CAS Nomenclature

Part of the compound is selected as the heading parent. Substituents are listed after it. Name not always obvious.

Examples

- Toluene: Benzene, methyl-
- ortho-Xylene: Benzene, 1,2-dimethyl-
- Benzyl alcohol: Benzenemethanol

Multiple substituents listed in alphabetical order (with prefixes).

- carbon tetrachloride: Methane, tetrachloro-
- CCl_{2}F_{2}: Methane, dichlorodifluoro-
- CCl_{3}F: Methane, fluorotrichloro-

Compounds are listed first by parent compound (with any qualifiers and categories), then by substituted forms in alphabetical order. Substituents are read from left to right, ignoring numbers and punctuation.

Example: Benzene

- Benzene
- Benzene, analysis
- Benzene, uses and miscellaneous
- Benzene, compounds
- Benzene, polymers
- Benzene, azido-
- Benzene, chloro-
- Benzene, 1,2-dibutyl-
Much easier to find substances by molecular formula

**Hill order:**

- **Carbon** present: comes first, followed by hydrogen, then all other elements in alphabetical order.
- **No carbon**, then all (including H) in alphabetical order.

Benzene: C₆H₆
Teflon: (C₂F₄)ₓ
Ferrocene: C₁₀H₁₀Fe
Hydrochloric acid: HCl
Benzoic acid: C₇H₆O₂
Sodium benzoate: C₇H₆O₂, sodium salt... **NOT** C₇H₆NaO₂

### Molecular Formula Index

<table>
<thead>
<tr>
<th>Chemical formula &amp; chemical name</th>
<th>Registry number</th>
<th>Abstract number: the &quot;P&quot; indicates that this reference is to a patent.</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₅H₃CrNO₅</td>
<td></td>
<td>115: P 154913a; 116: 154901b, 158: 155213b, 160: 153304c; 120: 87416b, 123: 121855g</td>
</tr>
</tbody>
</table>