Chemistry on the Internet: A Revolution In Chemical Information

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Member of the Wikipedia Chemistry Project
Overview

• Web 1.0 and Web 2.0
• Chemistry Web 1.0
• Chemistry Web 2.0
  – Wikipedia
  – ChemSpider and PubChem
  – Project Prospect
  – Open Access
• The future?
• Conclusion
WEB 1.0
The Web has already transformed chemical information.

[Image: Picture by azure elixir, on Flickr. CC license.]
• **Convenience** and **searchability**.
  • PDFs on your desktop vs. paper in the library.
  • SciFinder vs. paper Chem. Abs.
  • Browse amazon.com, instead of phoning up Wiley or the college bookstore.

**BUT....**
Web 1.0

The information is the same, just packaged differently.
• The Web becomes dynamic, interactive.
• You don't just spectate, you participate.
• The knowledge and resources of all humankind can now be made available – but how?
Logos are copyrighted by the organizations shown.
CHEMISTRY ON THE WEB
(VERSION 1.0)
Even Web 1.0 has transformed our work – now we can search for, find and read articles without leaving our desks!
We can search, find and read patents:

**Low temperature manufacturing process for nylon**

**Abstract**

This invention concerns a low temperature process for the manufacture of nylon.

**Inventors:** Lang, James Joseph (Wilmington, DE)

**Assignee:** E. I. du Pont de Nemours and Company (Wilmington, DE)

**Appl. No.:** 08/688,449

**Filed:** July 30, 1996

**Related U.S. Patent Documents**
• Google Scholar can also help us find recent articles by Lavoisier...

**ISCN (2005): An International System for Human Cytogenetic Nomenclature** - all 2 versions
... 1963. This publication also incorporates all previous human cytogenetic nomenclature recommendations. ... cytologie. © Lavoisier 2000-2008. ...
Cited by 68 - Related Articles - Cached - Web Search

**Before ‘modern’ chemistry: a stroll inside the French books from the Roy G. Neville Historical**
CLB Morveau, AF de Fourcroy, PJ Macquet, N Lemery... - Chemistry International, 2007 - search.informit.com.au
... of eight months of collaboration between its authors – Lavoisier, Guyton de Morveau, Berthollet and Fourcroy – Méthode de nomenclature chimique (Paris ...
Web Search - BL Direct

**Book Review: Chemistry, pharmacy and revolution in France, 1777–1809**
ODGilson, Modern History, 2007 - search.informit.com.au
Alkene and Alkyne Metathesis: Phaseolinic Acid (Selvakumar), Methyl 7-Dihydro-trioxacarcinoside B (Koert), Arglabin (Reiser) and Amphinolide V (Fürstner)

As N. Selvakumar of Dr. Reddy's Laboratories, Ltd., Hyderabad approached (Tetrahedron Lett. 2007, 48, 2021. DOI) the synthesis of phaseolinic acid (6), there was some concern about the projected cyclization of 2 to 3, as this would involve the coupling of two electron-deficient alkenes. In fact, the Ru-mediated ring-closing metathesis proceeded efficiently. The product unsaturated lactone 3 could be reduced selectively to either the trans product 4 or the cis product 5.
Who did that interesting work I read about?

However did we manage before the Web?
CHEMISTRY ON THE WEB
(VERSION 2.0)
Am I going to find improved methods for Suzuki couplings by contacting my “friends” on MySpace?

(picture removed)

What’s chemistry got to do with “social networks?”
• Scientists already depend on their own social networks to learn, share ideas.

• The Web offers us the chance to share the sum of human knowledge – including the deep knowledge of specialists such as scientists.

• Mashups can allow seamless sharing of data between sites.
“The free encyclopedia anyone can edit”
Free (GFDL) content supplied in many languages by volunteer writers from the public
2.4 million articles in English alone
Ranked #1 reference site, in top ten of all sites*
The Wikimedia Foundation oversees Wikipedia, as well as sister projects such as Wiktionary and Wikibooks and the Wikimedia software
Now a valuable source of chemical information

* Based on hits and reach, by Alexa
Welcome to the chemistry portal. Chemistry, from Arabic language khomeina meaning "alchemy", is a branch of science. Modern chemistry focuses on the study of elements of the world and the bonds between elements. Chemistry also deals with composition, structure, and properties of substances and the transformations that they undergo. In the study of matter, chemistry also investigates its interactions with energy and itself. Because of the diversity of matter, which is mostly in the form of compounds, chemists often study how atoms of different chemical elements interact to form molecules, and how molecules interact with each other.

In the news:

02-19: A new chapter in the history of quinine total synthesis: in an extensive Angewandte Chemie review, Jeffrey Seeman validates the 1944 quinine synthesis by Bob Woodward and William Doering. Read more...

02-07: University of Pennsylvania chemist Alan MacDiarmid died on February 7th at the age of 79. MacDiarmid is best known for the discovery and development of conductive polymers such as doped polyacetylene, work for which he shared the 2000 Nobel Prize for Chemistry. Read more...

01-23: Pharmaceutical giant Pfizer announced a
Wikipedia:WikiProject Chemistry

From Wikipedia, the free encyclopedia

WikiProject: Chemistry

Some *Wikipedians* have formed a *project* to better organize information in articles related to *chemistry*. This page and its subpages contain their suggestions; it is hoped that this project will help to focus the efforts of other Wikipedians. If you would like to help, please inquire on the *talk page* and see the *to-do list* there. Some Wikipedians maintain a chemistry portal at [Portal:Chemistry] too.

**Overview**

This Wikiproject strives to incorporate the collaborative efforts of those with interests within chemistry and related areas into the articles and thereby the overall quality of the wikipedia. In order to maintain a high-level of scientific and encyclopedic articles, and as members of this wikiproject, and even wiki itself, we have a duty to provide accurate verifiable information.

We allow anyone to participate within the wikiproject, collaborate, edit and participate in our article development drive, under the following conditions:

1. When new information is added, try to find *at least reference where you got it from*.
2. When you're adding new information...
   1. Make sure it's not already in the article or wikipedia.

**Things you can do**

Here are some things you can do:

- **Accuracy disputes:**
  *Uranium#Hazards* - *more*
- **Attention:** *List of important publications in chemistry* - *Standard molar entropy* - *more*
- **Update:** *Podophyllin* - *Santonin*
- **Articles needing an expert:** *lithium amide* - *Ethyl nitrate* - *iodobenzene* - *More*
- **Expand:** *Absorption (chemistry)* - *Johannes*
Wikipedia Chemicals Project

- ~60 members (~20 active)
- Collaborated on writing quality articles and standards for:
  - developing data boxes for articles
  - chemical naming, structure drawing
  - article assessment
- Data validation
- New collaboration with CAS

Wim Van Dorst, a Dutch member of WP:Chem since March 2005.
WikiProject Chemicals is a daughter WikiProject of the WikiProject on Chemistry. It concerns writing and improving articles about chemical compounds in Wikipedia. So far, more than fifty members of Wikipedia have signed up to participate in WikiProject Chemicals.

A worklist of representative chemical compounds have been finalized. Progress on the articles in this list is monitored by participants. Also, templates for Lists of Properties for the compounds have been standardized, as has formatting and naming articles on chemical compounds. Presentation of chemical structures should also be standardized (to some extent). This WikiProject also serves as a forum on how best to present chemicals information and proceed with work on chemicals in Wikipedia.

If you would like to help, please inquire on the talk page and look at the worklist. To join, simply list yourself at #Participating by adding * ~~~ to the section. If you would like to request a new chemistry-related article, please be referred to the WikiProject Chemistry requested articles list.

### Contents

1. Scope
2. Assessment
3. Parentage
4. Descendant WikiProjects
5. Participants
6. Goals
7. Discussion forums
8. Activities in progress
   8.1 Worklist to ChemStart level as a minimum
   8.2 Worklist to A-Class level
   8.3 Style guide
9. Activities finalized
   9.1 Templates
   9.2 Chemical Infoboxes
Ammonium perrhenate

I don't have institutional access to journals anymore. There's an article in Inorg. Synth. which presumably describes the laboratory preparation of this compound:


Perhaps someone can read it and expand the article? --Rifleman82 (talk) 08:31, 2 June 2008 (UTC)

Hmm, what do you want adding? The article seems correct to me, and probably contains most of the verifiable data we're going to find on this compound. I am not sure that it is "the form in which rhenium is most commonly traded"—such an assertion should really have a reference, and I have almost always acquired my rhenium as the metallic powder—but otherwise I don't see great problems. Physchim82 (talk) 14:00, 2 June 2008 (UTC)

I agree about the "commonly traded" bit - I used to get it usually as the sodium salt.

With regard to the preparation section. The cited source doesn't suggest it is a lab scale process or not. If Inorg Synth says the same, then we can say that too: (I think this procedure is also usable in the laboratory[2]) I've come across some documents which suggest that any general rhenium-containing material may be dissolved in base piranha and precipitated the same way, but I can't remember the reference. Perhaps this ref will state that too?
--Rifleman82 (talk) 15:14, 2 June 2008 (UTC)

Niobium monoxide

Should this be Niobium(II) oxide?--Stone (talk) 17:36, 10 June 2008 (UTC)

Probably, yes, depending on whether it is appropriate to give it an exception for common use of the name (which I doubt). Physchim82 (talk) 17:43, 10 June 2008 (UTC)

My use of the stoichiometric name was deliberate, as I reckon that as a predominantly materials science related chemical, it is better known as that. I have also created a page niobium dioxide for NbO₂. If you want to change the titles go ahead as long as there are redirects it won't matter. Aploccuru (talk) 13:27, 18 June 2008 (UTC)

Template fixed

Hi all, I think I fixed the problems with Comments in the {{chemicals}} templates. They should now be editable, readable, visible, nestable, etc. If not completely
Wikipedia article traffic statistics

*hydrochloric_acid* has been viewed 100829 times in 200805

Enter another wikipedia article title

English ▼ 200805 ▼ hydrochloric_acid  Go

This is very much a beta service and may disappear or change at any time. Questions or comments should go to User:Henrik

(took 5.916778 sec)
Sodium sulfate - Wikipedia, the free encyclopedia

Sodium sulfate is an important... Bulk sodium sulfate is usually purified via the decahydrate form,...

SODIUM SULFATE

Not considered an explosion hazard, but violent explosions occur when potassium sulfate and sodium sulfate are melted with aluminum.

SGS Minerals Information: Sodium Sulfate

Statistics and information on the worldwide supply, demand, and flow of sodium sulfate.

Statistical Compendium - SODIUM SULFATE

Sodium sulfate is obtained from natural deposits and as a byproduct from... Less expensive imports and an abundance of byproduct sodium sulfate have...
Sodium sulfate

A B-class article from Wikipedia, the free encyclopedia

With an annual production of 4 million tonnes, sodium sulfate is one of the world's major commodity chemicals. The anhydrous sodium salt of sulfuric acid is a white crystalline solid Na₂SO₄. The dehydrate Na₂SO₄·10H₂O has been known as Glauber's salt or historically sal mirabilis since the 17th century.

Sodium sulfate is mainly used for the manufacture of detergents and in the Kraft process of paper pulping, although it has many other uses. About half of the world's production is from mirabilite, the natural mineral form of the dehydrate, and half from by-products of chemical processes.

### Contents [hide]

1 History
2 Physical and chemical properties
3 Production
   3.1 Natural sources
   3.2 Chemical industry
4 Uses
   4.1 Commodity application
   4.2 Other applications
5 Precautions
6 References
7 External links

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<td>Appearance</td>
<td>White crystalline solid, hygroscopic</td>
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References

With an annual production of 4 million [[tonne]]s, "sodium sulfate" is one of the world's major [[commodity]] chemicals. The [[anhydrous]] [[sodium]] salt of [[sulfuric acid]] is a white crystalline solid of formula Na<sub>2</sub>SO<sub>4</sub>. The [[hydrate|decahydrate]] Na<sub>2</sub>SO<sub>4</sub>·10H<sub>2</sub>O has been known as "Glauber's salt" or historically "sal mirabilis" since the [[17th century]].

Sodium sulfate is mainly used for the manufacture of [[detergent]]s and in the [[Kraft process]] of paper [[pulping]], although it has many other...
Sodium sulfate

From Wikipedia, the free encyclopedia

Revision history
View logs for this page

(Latest | Earliest) View (previous 50) (next 50) (20 | 50 | 100 | 250 | 500).
For any version listed below, click on its date to view it.
For more help, see Help:Page history and Help:Edit summary.

(cur) = difference from current version, (last) = difference from preceding version,

b = bot edit, m = minor edit, → = section edit, ← = automatic edit summary

Compare selected versions

- (cur) (last): 04:22, 24 March 2007 Walkerma (Talk | contribs) (copyedit)
- (cur) (last): 00:24, 24 March 2007 Wimvandorst (Talk | contribs) (copy-edit lead)
- (cur) (last): 18:41, 18 March 2007 Wimvandorst (Talk | contribs) (→Other applications - adding late changes (after the unnoticed vandalism))
- (cur) (last): 10:38, 18 March 2007 Wimvandorst (Talk | contribs) (rv vandalism (I'll shoot him next time))
- (cur) (last): 17:29, 18 March 2007 Wimvandorst (Talk | contribs) (→Commodity application)
Image: Na$_2$SO$_4$ solubility.png

Solubility of Sodium Sulfate vs. Temperature

Grams Na$_2$SO$_4$, per 100 g water
• Aims to produce a CD/DVD/paper version of the “core” of Wikipedia.
• Activities are coordinated through the Wikipedia Version 1.0 Editorial Team.
• A “collaboration of collaborations.”
• Main subprojects:
  – Core topics
  – Work via WikiProjects
  – Version 0.7
So far only the German Wikipedia has produced WikiReaders – collections of articles printed as books.

The English Wikipedia hope to start producing WikiReaders as well as more CDs & DVDs.
• Wikipedia will continue to be an important (dominant?) information source for our students and faculty.
• Quality of articles patchy, but improving.
• Basic assessments on talk pages.
• The first validated information should be uploaded next month.
• Look for “flagged revisions”, structure searchability (via InChI Key), and offline releases.
One IUPAC workgroup recently used a wiki to reach consensus on Mass Spectrometry terms.
ChemSpider is a free access service providing a structure-centric community for chemists. Providing access to millions of chemical structures and integration to a multitude of other online services ChemSpider is the richest single source of structure-based chemistry information.
• Started by Antony Williams, March 2007.
• Now the world’s largest open chemical database (over 20 million substances).
• Open access, all content is free.
• Search for structural information, physical properties, predicted log P, spectral information.
• Most data pulled from databases, vendors and journals - now some are being updated by RSS feeds in real time.
• Data uploads and curation by volunteers.
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**SUPPLEMENTAL INFORMATION**

**Links & References**


[PubMed: 16562976] [DOI: 10.1021/ci050202s]

HPLC of Phenanthrene on Phenomenex Synergi 4u Max-RP 80A (EPA Method 550, PAH’s in drinking water)

**User Data**

- **Experimental Physchem Properties**
  - **Melting Point:** 99 - 101 C
  - **Boiling Point:** 336 C
  - **LogP:** 4.46
  - **Solubility:** -5.26

**NAMEs AND SYNONYMS**

**Validated by Experts**, **Validated by Users**, **Non-Validated**, **Removed by Users**, **Redirected by Users**, **Redirect Approved by Experts**

201-581-5 [*ETNecs/ELINCS*]

Phenantheren

Phenantherene, pure

85-01-8 [*RN*]

coal tar pitch volatiles
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**DATABASE ID(S)**

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• The goal of ChemSpider is to produce a “structure-centric community of chemists”

• Not trying to be “MySpace for chemists”, instead it offers useful chemical information, FREE.

• Chemists can share their own data
RSC Prospect

See science come alive - structured science within RSC journal articles

Search for structures within articles

02 April 2008

How can I find articles containing this compound?

What groups and relationships are there for this compound?

Is there any patent information?

Finding the answers to questions
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</table>

*a* FPU—filter paper cellulase units. *b* CMC-case—carboxymethylcellulase activity. BS—sugarcane bagasse cellulose sample.

The hydrolysis of bagasse cellulose sample with parent enzyme preparation resulted in production of glucose and further end product, probably due to the presence of very high amounts of β-glucosidase. On the other hand, the end products derived from the treatment of bagasse cellulose with mutant enzyme preparations contained both glucose and cellobiose (Table 2). The amount of xylose detected was insignificant, indicating a much lower amount of hemi-cellulose in the sugarcane bagasse cellulose. The mutants produced high levels of glucose because they are selected in the presence of 2-deoxyglucose. The presence of cellobioso in the mutant hydrolysate is due to a β-glucosidase in the crude enzyme mixture (Table 1). The presence of both glucose and cellobioso in the substrate is further hydrolysis to glucose because they are strong inhibitors of cellulases. However, this drawback of SSF methodology to produce lactic acid from bagasse cellulose sample using cellobioso utilizing microbial microorganisms. Considering the inexpensive nature of bagasse samples, there is no doubt about their high potential as substrates for production of glucose and further fermentation of glucose to other platform chemicals by SSF.

**Table 2** End product analysis of saccharification of Avicel and sugarcane bagasse cellulose sample using different enzyme preparations
Compound Information for 2-deoxyglucose

Synonyms:

- 2-deoxy-D-glucose
- 2-deoxy-D-arabino-hexopyranose
- 2-Deoxy-D-mannose
- D-2dGlc
- Deoxyglucose
- deoxyglucose
- 2-deoxyglucose

SMILES: [H]C(H)(C=O)[C@](H)(O)[C@](H)(O)[C@](H)(O)CO

InChI:
InChI=1/C6H12O5/c7-2-1-4(9)6(11)5(10)3-8/h2,4-6,8-11H,1,3H2/t4-,5-,6+/m1/s1

CML (Chemical Markup Language Representation)

2-D Image

Other articles referencing this compound:

- DOI:10.1039/b611326h

On the other hand, the SSF process resulted in production of the end products contained both glucose and cellobiose in a lower amount of hemi-cellulose hydrolysate due to an end-products inhibition, because they are selected as the strongest inhibitors of cellulases. However, this drawback can be overcome by using an inexpensive nature of bagasse samples, there is no doubt about their high potential as substrates for production of glucose and further fermentation of glucose to other platform chemicals by SSF.

Table 2: End product analysis of saccharification of Avicel and sugarcane bagasse cellulose sample using different enzyme prepreparations
• Web 2.0 methods depend on sharing data, to produce a network of information. The data need to be freely available and accessible.

• For information to be found (e.g., by Google), it needs to be open.

• “3Bs” (Budapest, Bethesda, Berlin) – agreements that define OA.

• Groups that keep data behind a subscription firewall may lose market share.
BROWSE ARKIVOC

Previous Volume 

Volume List 

Next Volume

ARKIVOC Volume 2008

Part (i): Special Issue 'Reviews and Accounts'
Scientific Editor: Viktor Zhdankin

Part (ii): General Papers
(Issue completed with 30 papers and 293 pages)

Part (iii): Commemorative Issue in Honor of Prof. Csaba Szantay on the occasion of his 80th anniversary
Facilitator: Laszlo Hazai
Scientific Editor: Ramaiah Muthyala

Part (iv): Commemorative Issue in Honor of Prof. Irina P. Boletskaya on
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Now accepting submissions
Open-Source Science

Online research communities aim to unite scientists worldwide to find cures for neglected diseases

Sarah Everts

Scientists from Sydney to San Francisco have created an online research collaboration to develop cures for tropical diseases, using the "open source" programming model that produced freeware like Linux and Firefox, the award-winning Web browser.

The motivation is straightforward: Tropical diseases are low priority for big pharma because the return on drug development is so small. Patients in developing nations just don't have the financial ability to pay for patented drugs.

The structure is radical: Online discussions will prioritize a list of experiments that anyone can take on. Raw data will be posted online and discussed. Members of the consortium will solicit further ideas and expertise, hoping the greater research community steps up to the plate. The group, which operates under an umbrella website called Synaptic Leap, hopes that volunteered time, computer power, and resources
Objective
To convert adrenaline to DOPAL by acid catalysis

Procedure
A solution of adrenaline (1.0g 5.5mmoles) in 85% phosphoric acid was heated (116-118°C) in a round bottom flask (for 1 hour) in a heating mantle then removed from heat and allowed to cool. The solution was stirred for 90 min in distilled water and then saturated with NaCl. It was taken up in ethyl ether, and dried over anhydrous MgSO4. The ether extract was then evaporated to obtain DOPAL (80 mg 0.53mmol, 9.5% yield)

Characterization:

Results
1. TLC of 25A in 3:1 MeCl2:MeOH and in 6:1 MeCl2/MeOH, and stained with CAM
2. HNMR of 25A in acetone-d6, and the expansions of the prominent peak regions (one, three, four, five) (500MHz Varian inova). The integration is good enough to not require further purification.

Discussion
This is the first time that DOPAL was obtained pure (by NMR integration) immediately after extraction into...
GlaxoSmithKline Donates Cancer Genomics Dataset to Public Information Network

In a move likely to up the ante in the emerging Open Source Drug Discovery movement, GlaxoSmithKline have announced the donation of genomic profiling data for over 300 cancer cell lines to the National Cancer Institute's cancer Bioinformatics Grid (caBIG).

According to NCI's FAQ, caBIG is "an open-source, open-access information network..."
“I think that being able to walk around a molecule can add valuable new insight to thinking about and doing chemistry.” Jean-Claude Bradley, April 5, 2007.
THE FUTURE?
The Future?

• We will be able to find many more answers than before, even to “grey” questions.
• We will have a real web of information, where data are shared openly and seamlessly between sites.
• Free, fully open sites will thrive; closed sites may end up “closed” for good….
• Open sites that can get chemists to share their data will really thrive!
The future?

- One-click structure/substructure & reaction web searches from ChemDraw etc.
- All journals are open access, with complete data available at publication.
- Lab results directly uploaded to the web in real time?
- Academic collaborations by scientists via Web-based tools.
- A wiki for chemists, as an open repository for grey chemical information?
The future?

What if?
- You could upload your lab results directly onto the Web, for people to read immediately?

What if?
- You could perform “meta-searches,” such as, “Find me all of the rhenium-containing compounds that have a melting point below 200 °C and are soluble in pyridine.”

What if?
- The Web was truly “Semantic” – so web objects (structures, reactions, etc.) could be completely understood by search engines?
CONCLUSION
Conclusion

• The Web has already become the main provider of chemical information.

• Simply putting old media onto the Web is only a stopgap – we need new media that can take full advantage of the Web’s searchability.

• Data need to be open and free.

• We chemists will become more involved in real-time providing, as well as receiving, chemical information to the World.

• Sometimes revolutions take a little time!