Databáze chemických látek a jejich vlastností

E1020, 20.11.2018

Databáze chemických látek

- K čemu nám může sloužit databáze chemických látek a jejich vlastností ?

- Jak se budeme v takové databázi orientovat?

Kde najít běžná data?

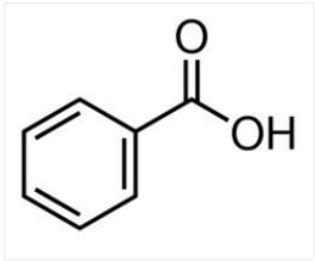
- U prodejců
- V encyklopediích
- V tabulkách

242381 Sigma-Aldrich

Benzoic acid

ACS reagent, ≥99.5%

CAS Number 65-85-0 | Linear Formula C_6H_5COOH | Molecular Weight 122.12 | Beilstein Registry Number 636131 | EC Number 200-618-2 | MDL number MFCD00002398 | eCl@ss 39023903 | PubChem Substance ID 24854555



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242381-3KG	Available to ship on 19.11.18 - FROM	8,590.00	0

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Properties

Related Categories	Acids, Acids & Bases, Benzoic Acid and Benzoic Acid Solutions, Building Blocks, C7, More...
grade	ACS reagent
vapor density	4.21 (vs air)
vapor pressure	10 mmHg (132 °C)
InChI Key	WPYMKLBDIGXBTP-UHFFFAOYSA-N
assay	≥99.5%
form	crystalline
autoignition temp.	1061 °F
packaging	poly bottle of 25, 100, 500 g
	poly drum of 3 kg
impurities	MnO_4^- reducers, passes test
	≤0.002% S compounds
	≤0.005% CH_3OH insol.
ign. residue	≤0.005%
bp	249 °C(lit.)
mp	121-125 °C (lit.)
solubility	water: soluble (2.9 g/l at 25 °C)
anion traces	chloride (Cl^-): ≤0.005%
cation traces	heavy metals (as Pb): ≤5 ppm

Show Fewer Properties

Description

Packaging
25, 100, 500 g in poly bottle

3 kg in poly drum

Application
Benzoic acid has been used in the preparation of vials for the HPLC analysis of various polyamines in biological fluids, tissues and isolated/cultured cells.[3]

It may be employed as an intermediate in the synthesis of the following:[1]
- paints
- pigments
- varnish
- wetting agents
- aroma compounds
- benzoyl chloride
- benzotrichloride

It may also be used to investigate the mechanism of complex addition reaction of hydroxyl radicals with various aromatic compounds.[2]

General description
Benzoic acid is an organic aromatic monocarboxylic acid. It can be synthesized by the cobalt or manganese catalyzed atmospheric oxidation of toluene. Recently, benzoic acid has been prepared from toluene by employing TiO_2 nanotubes electrode.[1]

Benzoic acid reacts with hydrogenating reagents to afford hexahydrobenzoic acid. The thermal decomposition of the product in the presence of lime or alkali produces benzene and carbon dioxide.[1]

Úloha 1: Kde získáte potřebná data? A co vlastně hledat?

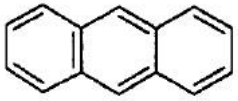
P 5.2 ***A Tricky Stock Solution***

You work in an analytical laboratory and you are asked to prepare 250 mL of a 0.5 M stock solution of anthracene in toluene (ρ^{20} (toluene) = [redacted]) as solvent. You look up the molar mass of anthracene, go to the balance, weigh out [redacted] of this compound, put it into a 250 mL volumetric flask, and then fill the flask with toluene. To your surprise, even after several hours of intensive shaking, there is still a substantial portion of undissolved anthracene present in the flask, although your **intuition tells you that these two aromatic compounds should form a near-ideal liquid mixture.**

(a) What is the problem?

(b) Give an estimate of how much anthracene has actually been dissolved (in grams).

(c) What is anthracene's concentration (in molar units) in the stock solution (at 20°C)? The necessary data can be found in Appendix C.



anthracene
T_m = 217.5 °C
T_b = 341.0 °C

(a) What is the problem?

(b) Give an estimate of how much anthracene has actually been dissolved (in

Schwarzenbach et al.: Environmemtal Oranic Chemistry, 2nd Ed., 2003, Wiley & Sons.

Identifikátory chemických látek

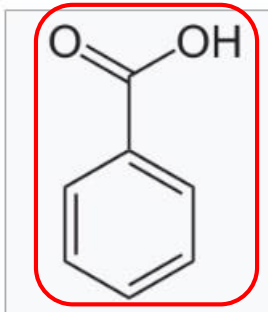
- Jednoznačné a čitelné

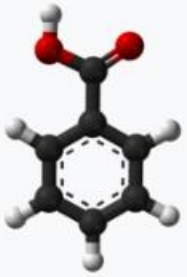
- Čitelnost je něco jiného pro člověka a pro počítač

Identifikátory chemických látek

- Které jsou pro člověka a které pro počítač?

Benzoic acid





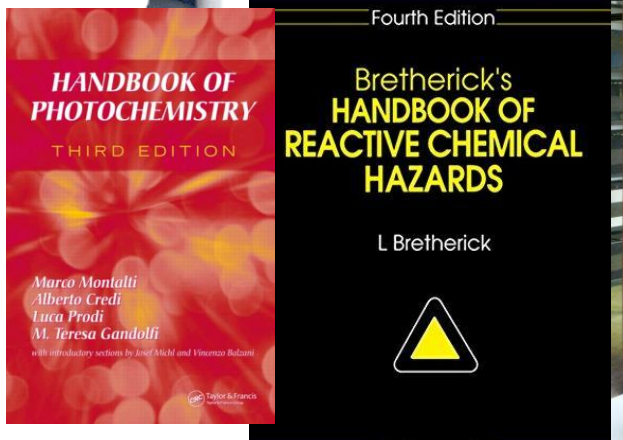
Names	
Preferred IUPAC name	Benzoic acid[1]
Systematic IUPAC name	Benzenecarboxylic acid
Other names	Carboxybenzene; E210; Dracylic acid; Phenylmethanoic acid

Identifiers	
CAS Number	65-85-0 ✓
3D model (JSmol)	Interactive image
3DMet	B00053
Beilstein Reference	636131
ChEBI	CHEBI:30746 ✓
ChEMBL	ChEMBL541 ✓
ChemSpider	238 ✓
DrugBank	DB03793 ✓
ECHA InfoCard	100.000.562
EC Number	200-618-2
E number	E210 (preservatives)
Gmelin Reference	2946
KEGG	D00038 ✓
MeSH	benzoic+acid
PubChem CID	243
RTECS number	DG0875000
UNII	8SKN0B0MIM ✓
InChI	[hide]
InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9) ✓	
Key: WPYMKLBDIGXBTP-UHFFFAOYSA-N ✓	
InChI=1/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H,8,9)	
Key: WPYMKLBDIGXBTP-UHFFFAOYAD	
SMILES	[hide]
O=C(O)c1ccccc1	

Properties	
Chemical formula	$C_7H_6O_2$
Molar mass	122.12 g·mol^{-1}
Appearance	Colorless crystalline solid
Odor	faint, pleasant odor
Density	1.2659 g/cm^3 (15 °C) 1.0749 g/cm^3 (130 °C)[2]
Melting point	122 °C (252 °F; 395 K)[6]
Boiling point	250 °C (482 °F; 523 K)[6] 370 °C (698 °F; 643 K) decomposes[2]
Solubility in water	1.7 g/L (0 °C) 2.7 g/L (18 °C) 3.44 g/L (25 °C) 5.51 g/L (40 °C) 21.45 g/L (75 °C) 56.31 g/L (100 °C)[2][3]
Solubility	soluble in acetone, benzene, CCl_4, $CHCl_3$, alcohol, ethyl ether, hexane, phenyls, liquid ammonia, acetates
Solubility in methanol	30 g/100 g (-18 °C) 32.1 g/100 g (-13 °C) 71.5 g/100 g (23 °C)[2]
Solubility in ethanol	25.4 g/100 g (-18 °C) 47.1 g/100 g (15 °C) 52.4 g/100 g (19.2 °C) 55.9 g/100 g (23 °C)[2]
Solubility in acetone	54.2 g/100 g (20 °C)[2]
Solubility in olive oil	4.22 g/100 g (25 °C)[2]
Solubility in 1,4-Dioxane	55.3 g/100 g (25 °C)[2]
log *P*	1.87
Vapor pressure	0.16 Pa (25 °C) 0.19 kPa (100 °C)

A kde najít specializovaná data?

- Databáze chemických látek: původně papírové, e.g.,
  - Gmelin: anorganické látky (Gmelins Handbuch der anorganischen Chemie, 1st Ed., 1817, Leopold Gmelin)
  - Beilstein: organické látky (Handbuch der organischen Chemie, 1st Ed., 1881, Friedrich K. Beilstein)
- Příručky: oborově specifické
- Dnes: elektronické, e.g.,
  - NIST, AIST, EChA, DDB
  - ChemSpider, Comptox EPA
  - Reaxys
  - a mnoho dalších…



List of academic databases and search engines

From Wikipedia, the free encyclopedia

This page contains a representative list of major databases and search engines useful in an academic setting for finding and accessing articles in academic journals, institutional repositories, archives, or other collections of scientific and other articles. As the distinction between a database and a search engine is unclear for these complex document retrieval systems, see:

- the general list of search engines for all-purpose search engines that can be used for academic purposes
- the article about bibliographic databases for information about databases giving bibliographic information about finding books and journal articles.

Note that "free" or "subscription" can refer both to the availability of the database or of the journal articles included. This has been indicated as precisely as possible in the lists below.

This is a dynamic list and may never be able to satisfy particular standards for completeness. You can help by expanding it with reliably sourced entries.

Name	Discipline(s)	Description	Access Cost	Provider(s)
Academic Search	Multidisciplinary	Several versions: Complete, Elite, Premier, and Alumni Edition[1]	Subscription	EBSCO Publishing[2]
Aerospace & High Technology Database	Aerospace, Aeronautics, Astronautics		Subscription	ProQuest[3]
African Journals OnLine (AJOL)	Multidisciplinary	Scholarly journals published in Africa[4]	Free abstracts; Subscription full-text	African Journals OnLine[5]
AgeLine	Sociology, Gerontology	Includes information on aging-related topics, including economics, public health and policy.	Subscription	EBSCO Publishing[6]
AGRICOLA: Agricultural Online Access	Agriculture		Free & Subscription	Produced by the United States National Agricultural Library. Free access provided by NAL.[7] Subscription access provided by ProQuest,[8] OVID.[9]
AGRIS: Agricultural database	Agriculture	Covers agriculture, forestry, animal husbandry, aquatic sciences and fisheries, human nutrition, extension literature from over 100 participating countries. Material includes unique grey literature such as unpublished scientific and technical reports, theses, conference papers, government publications, and more.	Free	Produced by the Food and Agriculture Organization of the United Nations. AGRIS
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Analytical Abstracts	Chemistry		Subscription	Royal Society of Chemistry[11]
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Anthropological Literature	Anthropology		Free to Harvard faculty, staff and students. Subscription for non-Harvard access.	Maintained by Harvard University. Non-Harvard access provided by OCLC[14]
Arachne	Archaeology, Art history	German language	Free	German Archaeological Institute & the University of Cologne[15]
Arnetminer	Computer Science	Online service used to index and search academic social networks	Free	Tsinghua University[16]
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Úloha 2: Jaká je rozpustnost antracenu?

P 5.2 ***A Tricky Stock Solution***

You work in an analytical laboratory and you are asked to prepare 250 mL of a 0.5 M stock solution of anthracene in toluene (ρ^{20} (toluene) = 0.87 g·cm^{-3}) as solvent. You look up the molar mass of anthracene, go to the balance, weigh out 22.3 g of this compound, put it into a 250 mL volumetric flask, and then fill the flask with toluene. To your surprise, even after several hours of intensive shaking, there is still a substantial portion of undissolved anthracene present in the flask, although your **intuition tells you that these two aromatic compounds should form a near-ideal liquid mixture.**

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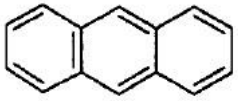

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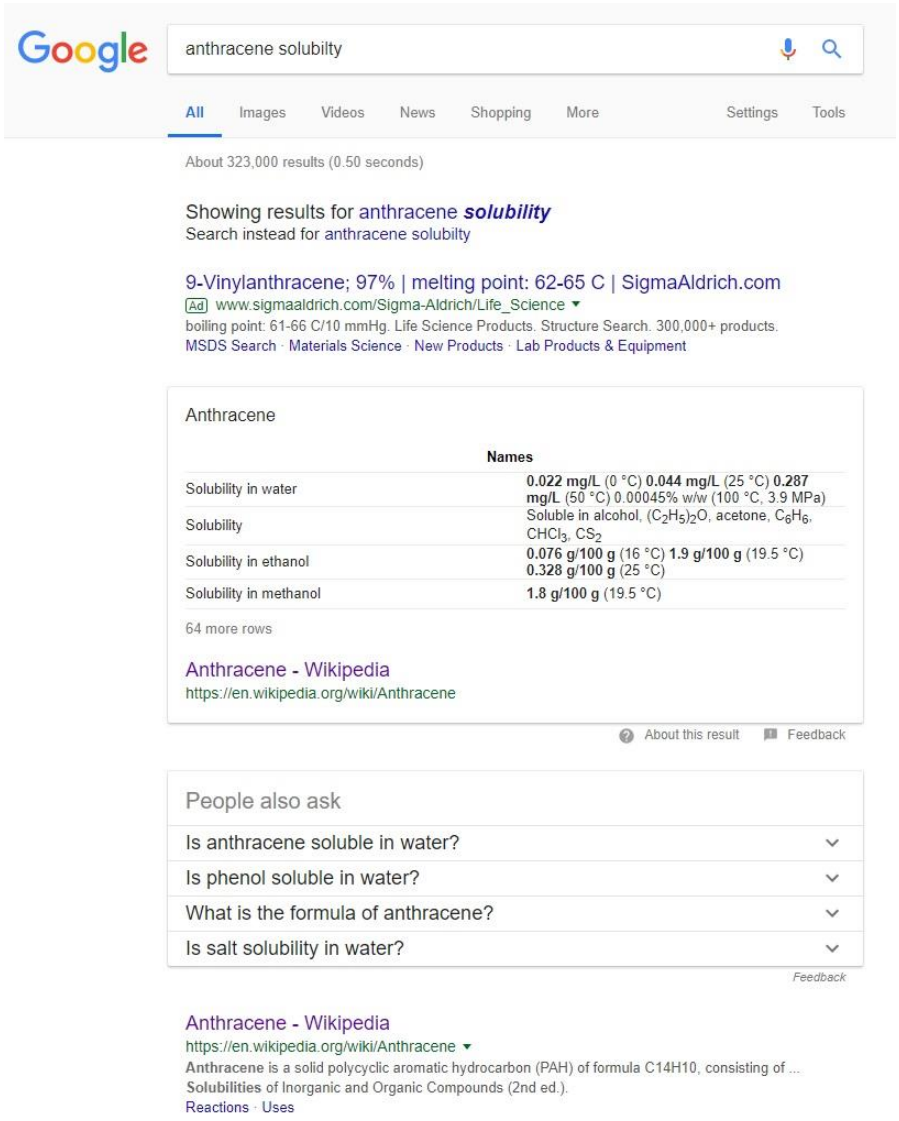
Schwarzenbach et al.: Environmemtal Oranic Chemistry, 2nd Ed., 2003, Wiley & Sons.

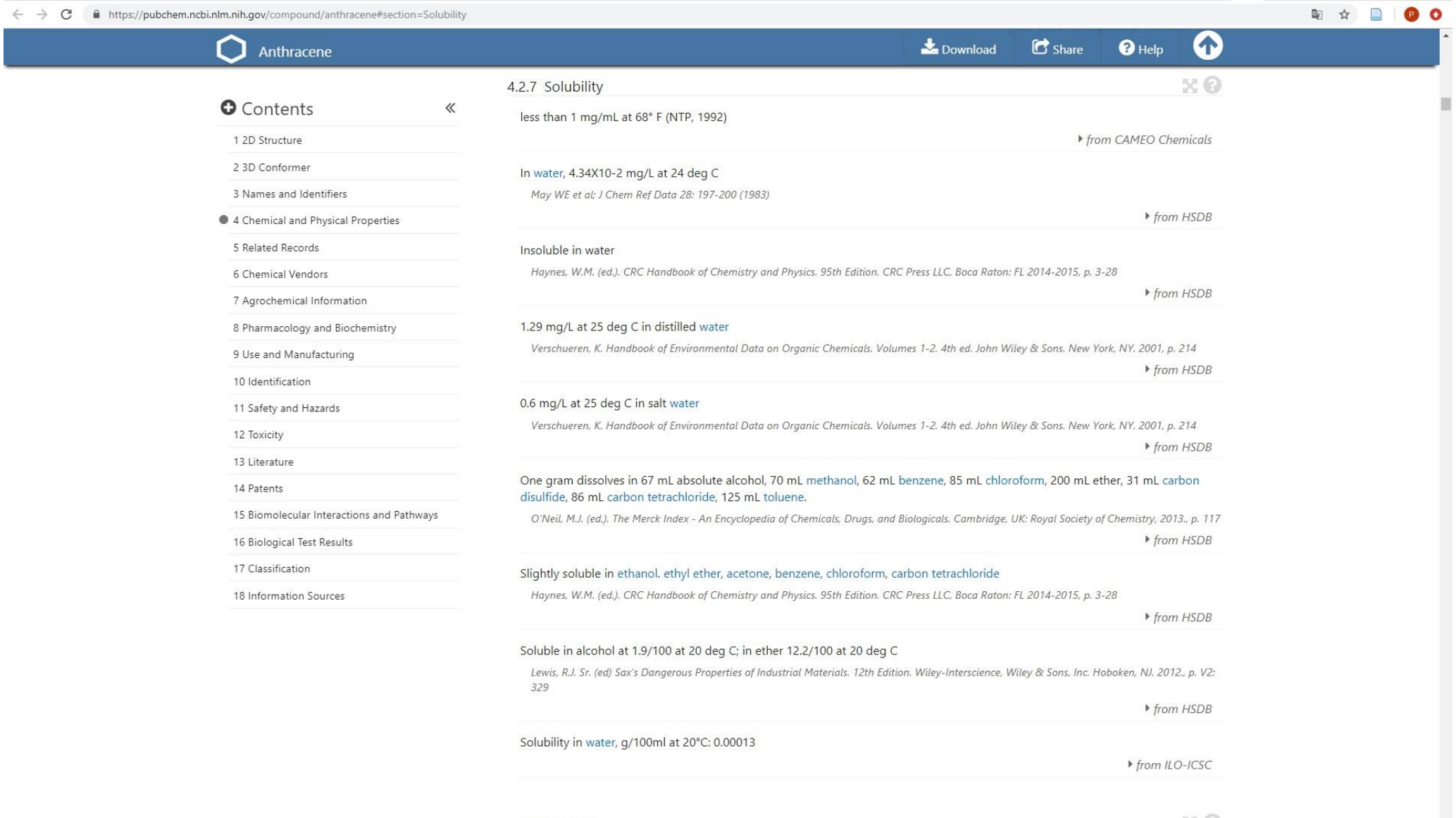
UTFG?



Properties	
Chemical formula	$C_{14}H_{10}$
Molar mass	178.23 g·mol^{-1}
Appearance	Colorless
Odor	Weak aromatic
Density	1.28 g/cm^3 (25 °C)[1] 0.969 g/cm^3 (220 °C)
Melting point	215.76 °C (420.37 °F; 488.91 K) at 760 mmHg[1]
Boiling point	339.9 °C (643.8 °F; 613.0 K) at 760 mmHg[1]
Solubility in water	0.022 mg/L (0 °C) 0.044 mg/L (25 °C) 0.287 mg/L (50 °C) 0.00045% w/w (100 °C, 3.9 MPa)[1]
Solubility	Soluble in alcohol, $(C_2H_5)_2O$, acetone, C_6H_6, $CHCl_3$,[1] CS_2[2]
Solubility in ethanol	0.076 g/100 g (16 °C) 1.9 g/100 g (19.5 °C) 0.328 g/100 g (25 °C)[2]
Solubility in methanol	1.8 g/100 g (19.5 °C)[2]
Solubility in hexane	0.37 g/100 g[2]
Solubility in toluene	0.92 g/100 g (16.5 °C) 12.94 g/100 g (100 °C)[2]
Solubility in carbon tetrachloride	0.732 g/100 g[2]
log *P*	4.56[1]
Vapor pressure	0.01 kPa (125.9 °C) 0.1 kPa (151.5 °C)[1] 13.4 kPa (250 °C)[3]
Henry's law constant (k_H)	0.039 L·atm/mol[1]
UV-vis (λ_{max})	345.6 nm, 363.2 nm[3]
Magnetic susceptibility (χ)	-130×10^{-6} cm^3/mol
Thermal conductivity	0.1416 W/(m·K) (240 °C) 0.1334 W/(m·K) (270 °C) 0.1259 W/(m·K) (300 °C)[4]
Viscosity	0.602 cP (240 °C) 0.498 cP (270 °C) 0.429 cP (300 °C)[4]

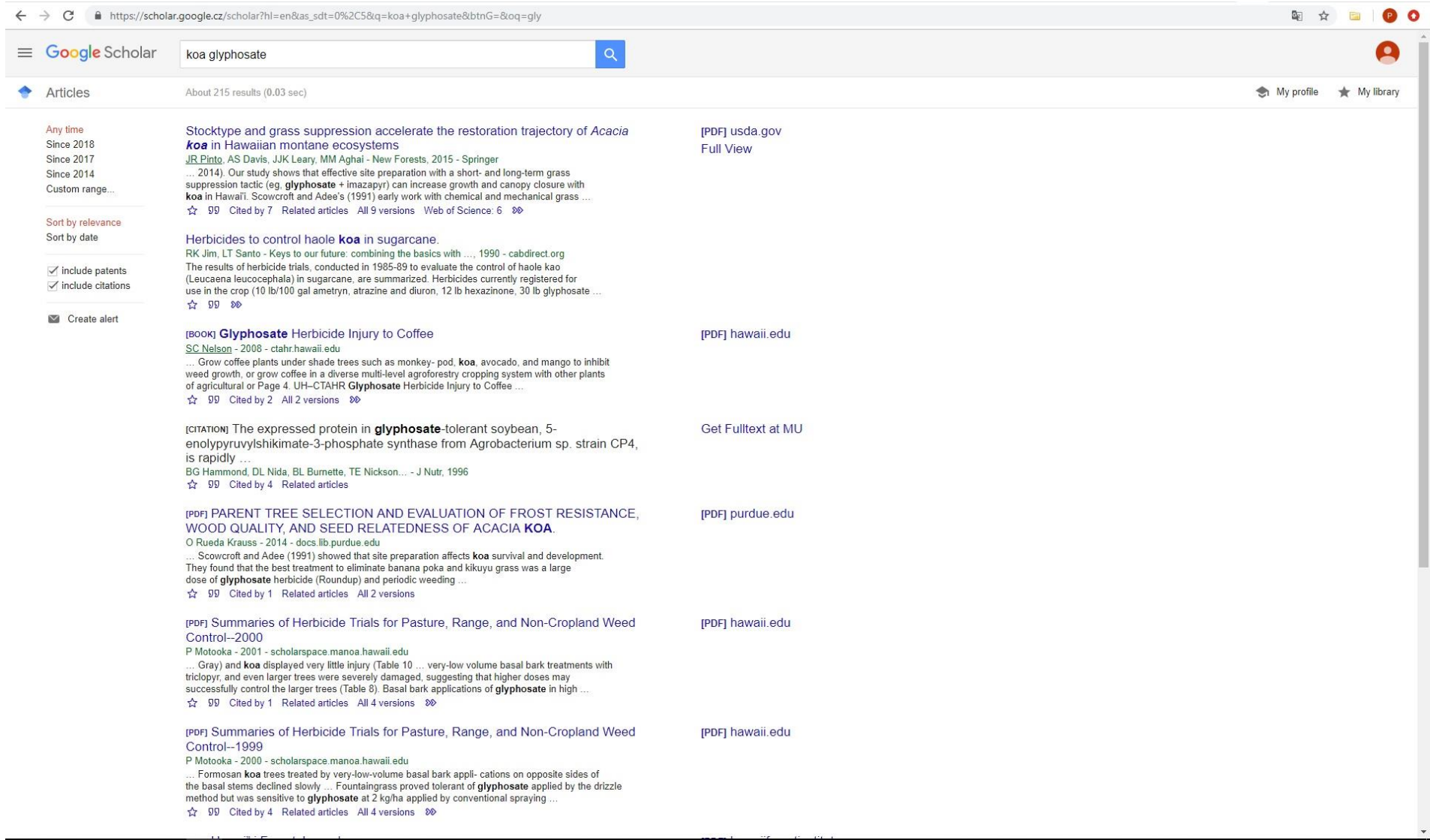
Use The Fabulous Google!

Other options: e.g., PubChem



Úloha 3: K_{OA} glyfosátu?

- UTFG?



Našli jste K_{OA} glyfosátu?

Environ. Sci. Technol. 2010, 44, 3041–3046

Determination of 1-Octanol-Air Partition Coefficient Using Gaseous Diffusion in the Air Boundary Layer

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Environmental Research Institute and Department of Environmental Engineering, Ajou University, Woncheon-dong, Yeongtong-gu, Suwon 443-749, Republic of Korea

Received November 30, 2009. Revised manuscript received February 28, 2010. Accepted March 1, 2010.

Exact determination of the partition coefficient between 1-octanol and air (K_{OA}) is very important because it is a key descriptor for describing the thermodynamic partitioning between the air and organic phases. In spite of its importance, the number and quality of experimental K_{OA} values for hydrophobic organic chemicals are limited because of experimental difficulties. Thus, to measure K_{OA} values, a high-throughput method was developed that used liquid-phase extraction with 1-octanol drop at the tip of a microsyringe needle. The concentration in the headspace surrounding the 1 μL octanol drop was equilibrated with liquid octanol containing polycyclic aromatic hydrocarbons (PAHs). The change in concentrations of PAHs in the octanol drop was measured to obtain mass transfer rate constants, and these rate constants were then converted into K_{OA} values using a film diffusion model. Thirteen polycyclic aromatic hydrocarbons with log K_{OA} between 5 and 12 were chosen for the proof of the principle. Experimental determination of log K_{OA} was accomplished in 30 h for PAHs with their log K_{OA} less than 11. The measured log K_{OA} values were very close to those obtained by various experimental and estimation methods in the literature, suggesting that this new method can provide a fast and easy determination of log K_{OA} values for many chemicals of environmental interests. In addition, the applicability of the method can be extended to determine Henry's law constant for compounds with low vapor pressure and to estimate gaseous transfer rate of semivolatile compounds for environmental fate modeling.

Introduction

The fate and transport of hydrophobic organic chemicals are often characterized by thermodynamic partitioning processes. Among various partition coefficients used for describing the processes, the partition coefficient between 1-octanol and air (K_{OA}) is thought to be crucial for chemical transport through the atmosphere, either by gaseous form or sorbed to particulates (*1*, *2*). It has been widely used for the evaluation of long-range transport and deposition of persistent organic pollutants (*3*–*5*), screening persistence of new and existing chemicals (*6*), bioaccumulation in terrestrial organisms (*7*), and multimedia fate models for the terrestrial environment (*8*, *9*). The significance of K_{OA} has been highlighted by the fact that organic compounds with low K_{OW} but high K_{OA} can biomagnify to a high degree in terrestrial food webs emphasizing that K_{OA} is a better predictor of biomagnifications in air-breathing organisms than K_{OW}, conventional descriptor for hydrophobicity (*7*).

Although precise K_{OA} values are required in many related areas, there are high uncertainties in estimated or indirectly derived K_{OA} values, and experimental K_{OA} values are not easy to obtain. A generator column method is the conventional method for measuring K_{OA} values for various semivolatile organic compounds such as polycyclic aromatic hydrocarbons (PAHs) (*10*, *11*), chlorinated benzenes (*12*), polychlorinated biphenyls (*12*, *13*), polychlorinated naphthalenes (*11*), dibenzo-*p*-dioxins and dibenzofurans (*14*), polybrominated diphenyl ethers (*15*), organochlorine pesticides (*2*), and perfluorinated compounds (*16*, *17*). However, the generator column method is time-consuming, especially at low temperatures and for compounds with low volatility, and it needs many analytical steps which may result in experimental artifacts during the measurement of K_{OA} (*18*, *19*).

In order to simplify the measurement of K_{OA}, many researchers developed gas chromatographic methods using chromatographic retention time or gas chromatographic capacity factor in comparison with that of a standard chemical (*18*, *20*, *21*). Although these methods have been successfully applied to various types of semivolatile organic compounds, their success depends on the availability of reliable data that served as standard reference, and derived relations may not be applicable for different classes of chemicals. Therefore, there are still needs for high-throughput methods by which reliable K_{OA} can be measured.

Recent progress in solid-phase and liquid-phase microextraction showed that the extraction-time profile can be explained by a two-film model (*22*, *23*). Thus, the rate of extraction is related with diffusivities in both phases and the distribution coefficient between the extracting phase and the medium (*23*, *24*). For example, Jeannot and Cantwell (*22*) showed that solvent microextraction using a 1 μL octanol drop from the tip of a microsyringe needle in the aqueous solution is useful for the determination of mass transfer coefficient using a film theory of convective-diffusive mass transfer. Similarly, a dynamic permeation method was developed to determine high partition coefficients between poly(dimethylsiloxane) and water in a reasonably short experimental time using two parallel polymer disks separated by agitated deionized water (*25*). Thus, it would be possible to measure high K_{OA} in a reasonably short time with a simple experimental apparatus using mass transfer in the air boundary layer surrounding a liquid octanol drop if the phenomenon is well characterized by a film diffusion model.

Consequently, we developed a simple experimental device using liquid-phase microextraction by a microsyringe for measuring K_{OA} values of selected PAHs with log K_{OA} values ranging between 5 and 12 to provide proof of concept. The concentration in the headspace surrounding a 1 μL octanol drop at the tip of a microsyringe needle was equilibrated with liquid octanol containing PAHs. The change in concentration in the octanol drop was measured to obtain mass transfer rate constants, and these rate constants were then converted into K_{OA} values using a film diffusion model. The measured log K_{OA} values were compared with literature values determined by various experimental and estimation methods. Potential applications of this device are also suggested.

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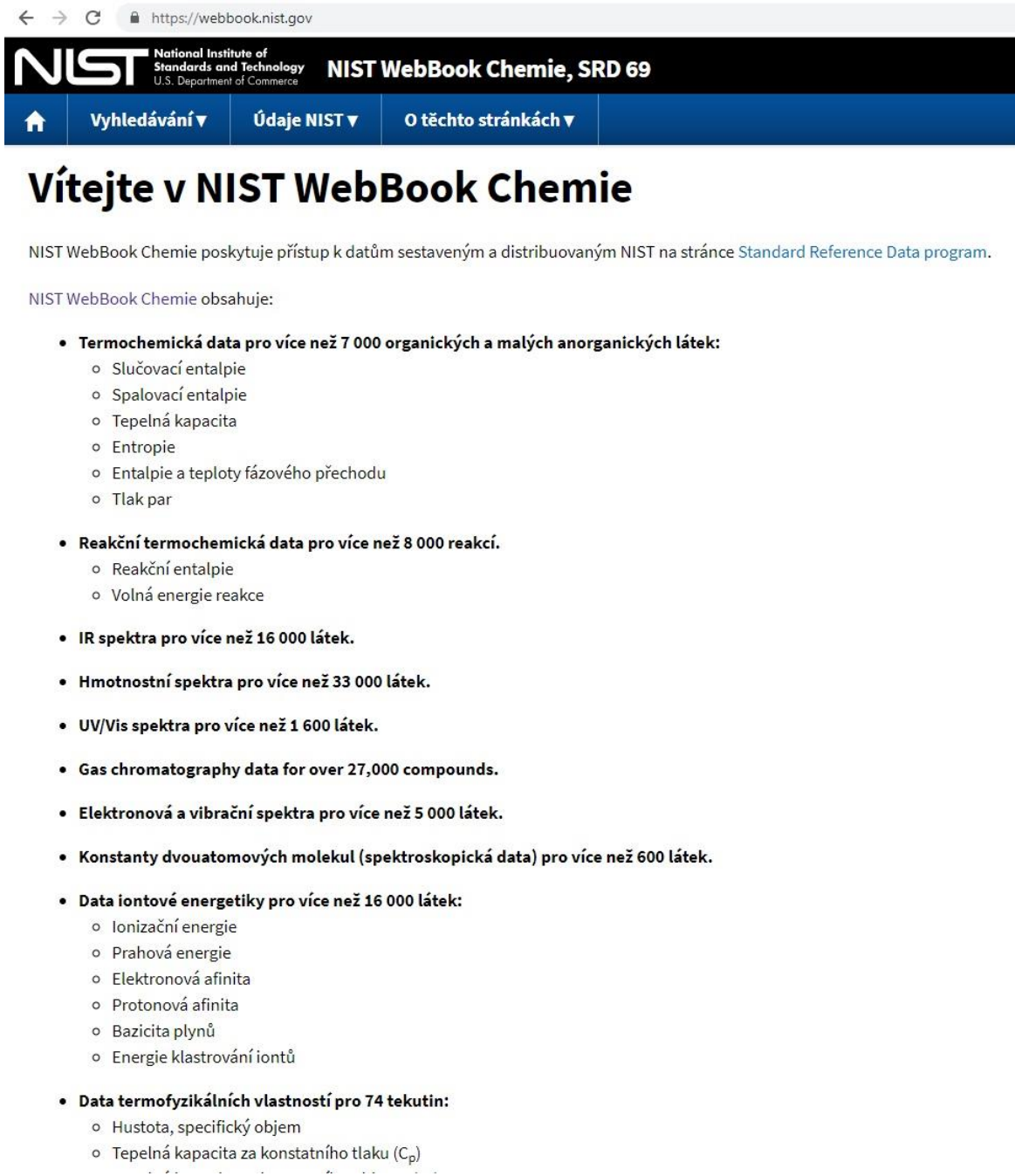
† Environmental Research Institute.
‡ Department of Environmental Engineering.

10.1021/es9035978
Published on Web 03/11/2010

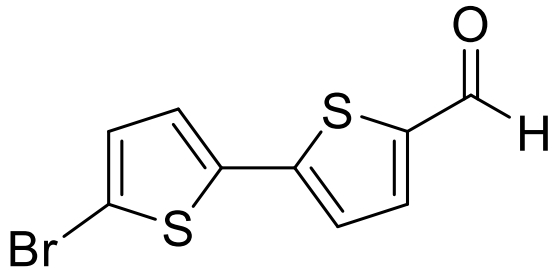
Databáze

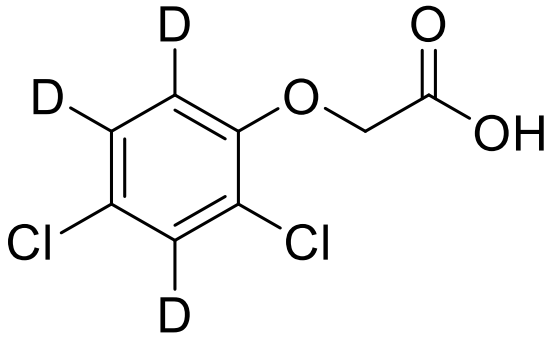
- NIST: webbook.nist.gov
- AIST: sdbs.db.aist.go.jp
- PubChem: pubchem.ncbi.nlm.nih.gov
- EChA: echa.europa.eu/information-on-chemicals/registered-substances
- ChemSpider: chemspider.com
- a mnoho dalších…



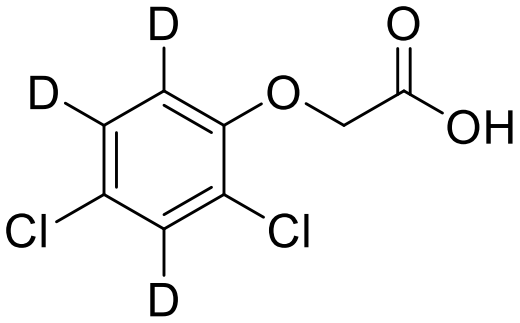
Úloha 4: Kde koupit?

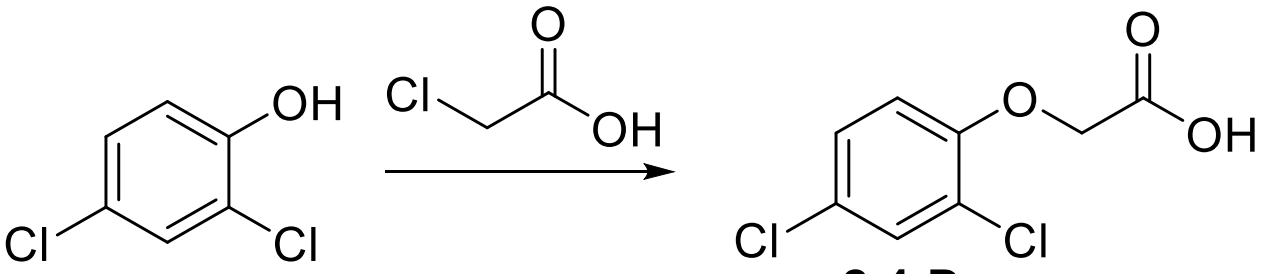
- A za kolik?





Úloha 5: A





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Filters and Analysis

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- Solvent
- Catalyst Classes
- Solvent Classes
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- Reactant Availability
- Reaction Classes
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27 Reactions out of 46 Documents containing 23 Substances

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24 Conditions | Find Similar

Yield	Conditions	Reference
99.6%	Stage #1: chloroacetic acid With sodium hydroxide In water for 1h; Stage #2: 2,4-dichlorophenol With potassium hydroxide In water for 1h; Stage #3: With tetrabutylammomium bromide; potassium bromide In water at 130°C; for 2h; Reagent/catalyst; Temperature; Experimental Procedure	Shandong Runbo Biological Technology Co., Ltd.; Sun Guoqing; Hou Yongsheng; Zhang Guozhong; Zhao Guangli; Chen Guiyuan - CN108503536, 2018, A Location in patent: Paragraph 0029; 0030; 0031; 0032; 0033; 0034; 0035-0046 Full Text Details Abstract
99.7%	Stage #1: chloroacetic acid Green chemistry; Stage #2: 2,4-dichlorophe for 6h; Green chemistry; Stage #3: With hydrogenc 2h; Reagent/catalyst; Tem Experimental Procedure	
95%	With sodium hydroxide	
95%	With sodium hydroxide;	
94%	Stage #1: chloroacetic aci carbonate; potassium iod Substitution; Stage #2: With hydrogenc	

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2,4-DICHLOROPHENOL (RING-D3, 98%)

Item Number	DLM-1359-0.1
Chemical Formula	Cl2C6D3OH
Unlabeled CAS#	120-83-2
Labeled CAS#	93951-74-7
Molecular Weight*	166.02
Chemical Purity	98%

* For isotopically labeled compounds, MW listed is for the fully enriched product.

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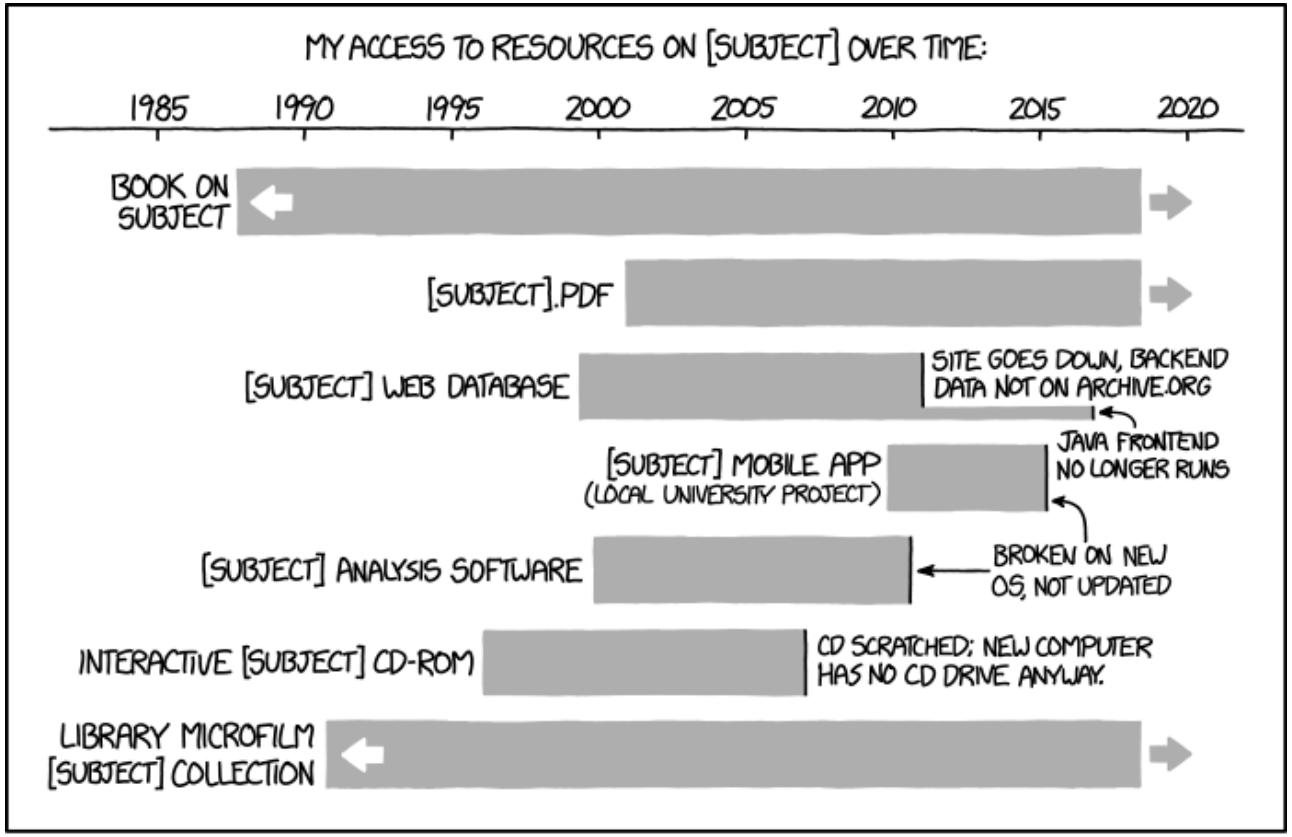
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