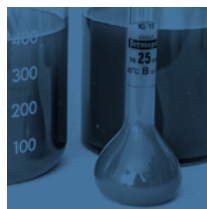


CHEMnetBASE

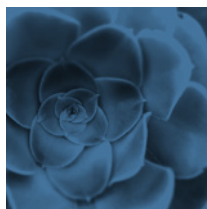
Chemical Databases Online



CRC Handbook of
Chemistry and Physics



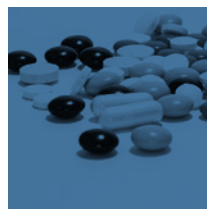
Combined Chemical
Dictionary



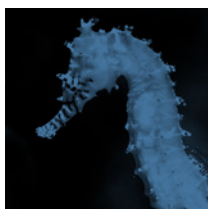
Dictionary of Natural
Products



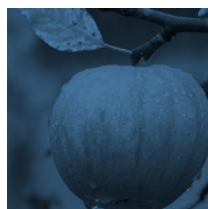
Dictionary of Organic
Compounds



Dictionary of Drugs



Dictionary of Marine
Natural Products



Dictionary of Food
Compounds



Polymers: A Property
Database



Properties of Organic
Compounds

NEW!

Cross Product Search Capabilities



One-Stop Search: Allows users to perform searches on chemical terms simultaneously across all databases within CHEMnetBASE.

- No need to run separate searches across different databases on CHEMnetBASE.
- Search results appear in tabbed format for easy identification across databases.

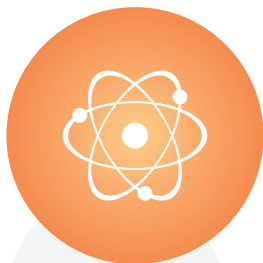


Chemical Structure Search: Enhanced multi-faceted research capabilities

- Users can draw a chemical structure using Marvin JS and then search by Exact Match or Substructure.
- Users can import a structure file or paste in a SMILES, SMARTS or InChI string into the search box.



Chemical Text Search: Enables users to search by Name, Synonym, Molecular Formula, CAS Registry Number, InChI, InChI key, and/or SMILES.



Improved transparency with interface redesign

- Easy to navigate and uncluttered home page, search tool and results page.
- Users can readily see which products they have access to, reducing queries to librarians.

Some Key Features of CHEMnetBASE include:

CHEMnetBASE is a collection of cutting-edge interactive chemistry databases that provides instant access to authoritative content and has 9 distinct products. Key elements of these products include:



MOBILE RESPONSIVE DESIGN

Allows users to use this web-based database on Tablets and mobile devices.



NEW CUSTOMIZATION

Enables users to set up search fields, hit list columns and save as their defaults.



SAVE SEARCHES

Improved functionality allows users to create and save their searches and columns in their hit list associated with them, which allows for easy reloading of previous results.



IMPROVED ENTRY DISPLAY

Allows users to expand and collapse compound sections within an entry for easy reading.



Combined Chemical Dictionary

Spanning the breadth of chemistry, The Combined Chemical Dictionary (CCD) provides access to chemical, physical, and structural data on chemicals. You can search content using the intuitive and powerful Marvin JS and JChem search engine from ChemAxon™, allowing you to draw your own structure queries. The CCD is updated twice a year.

A structured database, the CCD contains descriptive and numerical data, systematic and common names, and literature references as well as structural diagrams and their associated connection tables. With a listing for virtually every known natural product, including those of unknown structure, the CCD provides:

- Fundamental organic and inorganic compounds of simple structure
- Currently marketed drugs as well as those undergoing clinical trials
- Compounds with an established use such as catalysts, solvents, starting materials, synthetic reagents, and analytical reagents
- Co-ordination compounds such as amines, phosphines, alkoxy complexes, and major well-characterized bioinorganics
- Organometallic compounds representative of important structural types
- Important biochemicals, minerals, and newly synthesized compounds of active research interest

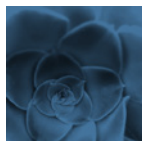
Given the vast range of data available, you will be able to conduct searches in a variety of ways, using single or multiple parameters, including structure searches.

**FREE
TRIAL**

**REQUEST
A FREE TRIAL:**

crystal@jaici.or.jp

The Combined Chemical Dictionary Plus consists of the following dictionaries:



DICTIONARY OF NATURAL PRODUCTS

A comprehensive structure database of natural products. Continually reviewed to keep pace with the current literature, this database is the most comprehensive source of natural product information available. Additionally, each natural product is linked, via the species name, to Catalog of Life (www.catalogueoflife.org), thereby providing authoritative taxonomic information.

DICTIONARY OF ORGANIC COMPOUNDS



DOC has built a world-wide reputation as an indispensable reference work over its 80 years of publication, and covers a wide range of organic compounds – synthetic reagents, starting materials, fundamental compounds of simple structure, pesticides, and commonly used chemicals.



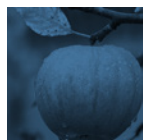
DICTIONARY OF DRUGS

Presenting accurate up to date and concise information on currently marketed drugs, those undergoing clinical trials, and pharmacological tools, this is a one-stop resource for the medicinal chemist.



DICTIONARY OF MARINE NATURAL PRODUCTS

A comprehensive resource for natural products isolated from marine organisms.



DICTIONARY OF FOOD COMPOUNDS

Comprehensive information on compounds found in food, including additives, flavors, natural food constituents, contaminants and nutraceuticals.



CRC Handbook of Chemistry and Physics Online

Save time and expand your resources with easy, flexible access to trusted chemical and physical data

The Online Handbook:

Interactive, Time-Saving Tools and More Data!

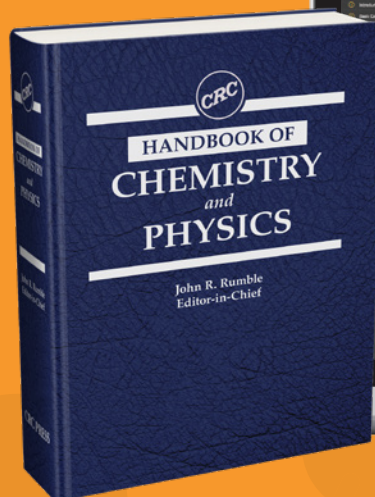
- Access expanded data and customize its display
- Search, sort, and merge data with ease and accuracy

EXTENSIVE SEARCH CAPABILITY

- **Searching by Various Fields**
Physical property, molecular formula, etc.
- **View Chemical Entry**
See core chemical properties and link to tables in handbook
- **Cross Table Searching**
Displays everything about a specific compound
- **Chemical Structure Searching**
Use the free Applet to draw a desired structure
- **Interactive Tables**
Customize the data in spreadsheet format

EXPANDED CONTENT & TABLES

- Create individual workspaces and customize your search screen
- Access from any device – mobile, tablets, etc.
- Graph search results and data tables
- Export chemical structures and images
- Expanded versions of print edition tables
- Access to tables archived from earlier editions
- Ability to export into Excel to print & filter



PROPERTIES OF GAS CLATHRATE HYDRATES

Carlton A. Koh, M. Rowed Phao, and E. Dewey Sloan

Gas clathrate hydrates (also known as gas hydrates) are crystalline inclusion compounds composed of hydrogen-bonded water cavities (hosts) which encage small gas (guest) molecules. Generally, a maximum of one guest molecule occupies each water cavity. Typical guest molecules that form gas hydrates are methane, ethane, carbon dioxide, and propane (see gas hydrate phase equilibria data in Table 18). The structural and physical properties of gas hydrates are given in Tables in this section. Data have been taken from the following references:

See the interactive table.

Table Ia. Gas Hydrate Structural Properties (All values are from Ref. 1 unless noted otherwise)

Structure	all Small	all Large	all Small	all Large	all Small	all Medium	all Large
Cubic systems	Cubic	Cubic	Cubic	Cubic	Hexagonal	Hexagonal	Hexagonal
Space group	Fm $\bar{3}$ m No. 223F	Fm $\bar{3}$ m No. 223F	Fm $\bar{3}$ m No. 223F	Fm $\bar{3}$ m No. 223F	Oh \bar{h} No. 192P	Oh \bar{h} No. 192P	Oh \bar{h} No. 192P
Lattice	Rhombohedral	Rhombohedral	Rhombohedral	Rhombohedral	Hexagonal	Hexagonal	Hexagonal
Lattice parameters ^a	a = 12.5 c = 3.1 × 10 ³	a = 12.5 c = 3.1 × 10 ³	a = 12.5 c = 3.1 × 10 ³	a = 12.5 c = 3.1 × 10 ³	a = 12.5, c = 101.8 a = 3 × 10 ³ , c = 120 ^b	a = 12.5, c = 101.8 a = 3 × 10 ³ , c = 120 ^b	a = 12.5, c = 101.8 a = 3 × 10 ³ , c = 120 ^b
Number of formula units	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)	36 ^c (16 ^d per 1/2 unit)
Cavity	Small	Large	Small	Large	Small	Medium	Large

Other Chemical Database Products

- Compendium Chemical Dictionary
- Dictionary of Organic and Organometallic Compounds
- Properties & Property Database
- Dictionary of Natural Products
- Dictionary of Chemical and Coal Compounds
- Properties of Organic Compounds
- Dictionary of Organic Compounds
- Dictionary of Marine Natural Products
- Dictionary of Drugs
- Dictionary of Food Compounds

About

One of the most practical benefits of this database system is that you can search by chemical structure.

INSTANT
access to your
specific search criteria
– Customized data
to suit your needs

ACCESS
archived PDF versions
of earlier editions
(back to 84th edition)

**MORE
DATA**
– more content and
faster access

The screenshot shows the 'Handbook of Chemistry and Physics' search interface. A central window displays a chemical structure drawing tool with a red circle highlighting a vertex. The interface includes a search bar, a list of search criteria (Exact Match, Substructure, Not Substructure), and a table of search results.

Draw a chemical structure or sub-structure in the illustration window. Search by either 'Exact Match', 'Substructure', or 'Not Substructure'.

The screenshot shows the search results for 'Acetone' in the 'Handbook of Chemistry and Physics'. The results are displayed in a table with columns for 'Molecular Weight', 'Boiling Point', 'Melting Point', 'Density', etc. The table is sorted by 'Molecular Weight'.

Custom sort results with editable navigation and filters. Comprehensive chemical quick facts.

The screenshot shows the 'STRUCTURES OF COMMON AMINO ACIDS' section of the 'Handbook of Chemistry and Physics'. It displays a grid of chemical structures for various amino acids, including Alanine, Arginine, Asparagine, Aspartic acid, Glutamic acid, Glutamine, Glycine, Isoleucine, Leucine, and Lysine.

View corresponding chemicals' structures of drawn structure and expansion of substructure.

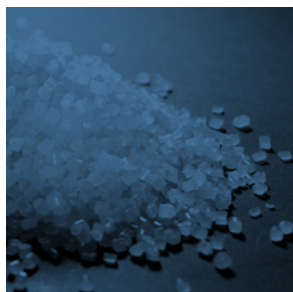
The screenshot shows the search results for 'acetone' in the 'Handbook of Chemistry and Physics'. The results are displayed in a table with columns for 'Physical Constants of Organic Compounds', 'Physical Constants of Inorganic Compounds', etc. The table is sorted by 'Physical Constants of Organic Compounds'.

Explore relevant chemical data in additional tables in the Handbook.



Properties of Organic Compounds

Now with a new interface, this is an easy-to-use tool for identifying unknown compounds, or for locating additional data for a known compound, **Properties of Organic Compounds** contains entries on the most commonly sought organic compounds, featuring physical data and spectral data (UV, IR, MS, ^1H NMR and ^{13}C NMR). With the database's high-quality display and powerful search capabilities, you can search in a variety of different ways. These are just a few of the features that make the database a useful and time-saving resource.



Polymers: A Property Database

With scientific and commercial information on polymers and monomers, this database provides a single, first-stop reference invaluable to anyone involved in polymer science and technology. Each entry includes trade names, properties, constituent monomers, commercial applications, manufacturing processes, and references.

INTERACTIVE FEATURES

Powerful retrieval software

Structure searchable monomers database

Cross-referencing and browsable indexes

Each section of the database, Polymers and Monomers, can be searched independently. You may use the monomers you have identified to cross-reference to polymer entries, or you may use the extensive property search capabilities on the polymers data directly. The polymers section of the database can be searched using 92 possible properties combined in any way you choose. These are grouped into the following sections:

- General Description
- Volumetric and Calorimetric Properties
- Surface Properties and Solubility
- Transport Properties
- Mechanical Properties
- Electrical Properties
- Optical Properties
- Polymer Stability
- Applications and Commercial Products

CHEMnetBASE Database Packages

PRODUCT	CHEMNETBASE*	COMBINED CHEMICAL DICTIONARY (Commonly referred to as CCD)	COMBINED CHEMICAL DICTIONARY PLUS (Commonly referred to as CCD Plus)
CRC Handbook of Chemistry and Physics Online Version	✓		
Dictionary of Natural Products	✓	✓	✓
Dictionary of Organic Compounds	✓	✓	✓
Dictionary of Drugs	✓	✓	✓
Dictionary of Marine Natural Products	✓		✓
Dictionary of Food Compounds	✓		✓
Polymers: A Property Database	✓		
Properties of Organic Compounds	✓		

*You can subscribe to CHEMnetBASE in its entirety or subscribe to individual products within CHEMnetBASE.

FLEXIBILITY

to subscribe to CHEMnetBASE
in its entirety or to its individual
databases and dictionaries

SUBSCRIPTION-
BASED PRICING
MODEL

Interactive databases in CHEMnetBASE include:

- CRC Handbook of Chemistry and Physics
- Combined Chemical Dictionary
- Polymers: A Property Database
- Properties of Organic Compounds

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AVAILABLE ON A SUBSCRIPTION BASIS ONLY.

Explore New Search Functionalities

CHEMnetBASE introduces cross product search functionality. One central portal searches across all dictionaries and databases in the collection for a comprehensive record of quality results.



Ability to search by Name, Synonym, Molecular Formula, CAS Registry Number, InChI, InChI key, and/or SMILES.

The screenshot shows the CHEMnetBASE search results page. The table displays the following entries:

Name	Synonyms	Molecular Formula	SMILES	CAS Registry No.
Acetamide	Methyl cyanide	C ₂ H ₅ N	CC(=O)N	75-06-6
Acetamide, N-methyl		C ₃ H ₇ NO	CC(=O)N(C)C	1363-95-8
2-Acetylphenacetamide	Lactamide, acetate	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C(=O)O	1363-95-2
N-Acetylphenacetamide		C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	1443-88-7
N-Acetylphenacetamide		C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	1363-95-4
Acetamide	Propionamide	C ₃ H ₇ NO	CCC(=O)N	122-13-3
Acetamide, N-methyl		C ₃ H ₇ NO	CC(=O)N(C)C	1463-87-6
N-methylacetamide, N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C(C)C	6811-34-8
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	3345-37-5
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	1363-95-6
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	2332-40-1
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	873-74-5
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	2332-40-8
N-methylacetamide	3-Ethoxy-1-propanamine	C ₇ H ₁₅ NO	CCOCCCN(C)C	15019-66-9
N-methylacetamide		C ₄ H ₉ NO	CC(=O)N(C)C	

Search results are organized by database, and the ones that you subscribe to appear at the front and will display a green 'Subscribed' tick.

The screenshot shows the CHEMnetBASE search results page. The table displays the following entries:

Name	Synonyms	Molecular Formula	SMILES	CAS Registry No.
1-Acetylphenacetamide, N-methyl	1-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	120051-43-0
5-Acetylphenacetamide, N-methyl	5-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	
1,2-Acetylphenacetamide, N-methyl	1,5-Dicapronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	86038-79-2
Acetylphenacetamide, N-methyl	N-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	23657-68-5
1-Acetylphenacetamide, N-methyl	1-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	39653-27-0
5-Acetylphenacetamide, N-methyl	5-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	69796-03-6
1,2-Acetylphenacetamide, N-methyl	1,2-Dicapronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	89330-43-3
Acetic acid, Methyl				
Acetamide	Methyl cyanide, Cyanoethane, Methylacetamide, Ethanimide	C ₂ H ₅ N	CC(=O)N	75-06-6
Acetamide, N-methyl		C ₃ H ₇ NO	CC(=O)N(C)C	1363-95-8
2-Acetylphenacetamide	2-Acetylpropyl-2-propionamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	1443-88-7
2-Acetylphenacetamide, N-methyl	n-Capronamide	C ₁₁ H ₁₃ NO	CC(=O)N(Cc1ccc(C)cc1)C	1363-95-4
2-Acetylphenacetamide, N-methyl, phenylacetamide				


Click on a tab to take you to your chosen database.

The screenshot shows the CHEMnetBASE search results page. The detailed entry for Acetamide is as follows:

Acetamide
CAS Registry Number: 75-06-6
Molecular Formula: C₂H₅N
SMILES: CC(=O)N
CAS Number: 75-06-6
General Statement: Smiles is a freely generated and used in only the open source (Creative Commons) license to allow for free distribution of data.
Physical Description: No data provided.
InChI Key: FCC(=O)N(C)C(=O)O
MOLINFO: CONSIDER

References:
Meyers, R. et al. J. Org. Chem. 1978, 43, 3481-3488 (abstract).
Meyers, R. et al. J. Org. Chem. 1980, 45, 8750-8775 (abstract).
Meyers, R. et al. J. Org. Chem. 1981, 46, 1023-1048 (abstract).
Meyers, R. et al. J. Org. Chem. 1984, 49, 1044-1048 (abstract).
Meyers, R. et al. J. Org. Chem. 1985, 50, 1044-1048 (abstract).
Encyclopedia of Reagents for Organic Synthesis and Reagents, L. J. Wiley, 1955, 1, 48-49.

Click the details button in the search results list to view a typical entry.



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E-mail: crystal@jaici.or.jp