Chemistry databases and alerting services for finding the best energy research content

Serin Dabb
Executive Editor, Data
Royal Society of Chemistry
Literature Updating Services

Databases

- Recently acquired *MarinLit*
- The Merck Index* Online

Other initiatives:
Energy Research Data

Materials

**Nanomaterials**: Inorganic and organic, rare-earth metals

**Carbonous materials**: Carbon fiber, graphene, graphite, diamond, nanotubes

**Polymers, Films**

**Ceramics**: Perovskites, zeolites

**Structural materials**, concrete, cement

**Porous materials**: Metal-organic-frameworks, Ceria

**Titanium dioxide, lithium salts, organic dyes, silicon**

Applications

<table>
<thead>
<tr>
<th>Catalysis for clean energy technologies:</th>
<th>biomass conversion; reduced emissions; electrocatalysts for batteries, fuel cells, and artificial photosynthesis</th>
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<tr>
<td>Harnessing the energy of the sun:</td>
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<td>Materials for extremes:</td>
<td>corrosion resistant materials; materials for high T/P; next generation lightweight materials for transportation and other applications</td>
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<td>Nuclear materials and fuels:</td>
<td>fuel cladding, fuel recycle, radiation resistant materials</td>
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<td>New materials and systems for the grid:</td>
<td>superconductivity; rare earths (substitutes, recovery); grid-scale storage; generation technologies</td>
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<td>Materials for energy efficiency:</td>
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<td>New technologies for enhanced recovery of fossil fuels</td>
<td>CO2 sequestration and conversion</td>
</tr>
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</table>
Finding information

Literature…. Data…
Linking all aspects of energy conversion and storage, alternative fuel technologies and global environmental science

An interdisciplinary journal, publishing work of international significance on all aspects of materials chemistry related to energy and sustainability

A premier journal publishing first reports of exceptional significance across the breadth of materials research
Topic Modelling

- Finding content related to energy research in general scope journals
  - Example: RSC Advances
- Uses Latent Semantic Analysis
  - Based on words, journals cited and pairs of words in same sentence (eg. “hydrogen…..storage”)

Each journal article is digested down to a bag of features - for example, which words the title and abstract contain - and then those bags of features are then digested down to an array of 300 numbers. These can be considered as vectors in 300-dimensional space, and by calculating the cosine of the angle between two vectors, you can work out how similar the vectors are.
Graphical representations of a subset of the topic vectors that underlie the topic modelling:
Electrochemical energy
Hydrogen

Specific material and application: Titanium dioxide as a photocatalyst
Specific type of device: Dye Sensitised Solar Cell

General: Solar Cell, photovoltaic, donor-acceptor
Topic Modelling

RSS feed of ‘Energy’ content, or even more specialised topics

Biofuels & Biomass (55)
Biotechnology (18)
Electrochemical energy (212)
Fossil fuels (104)
Hydrogen (53)
Materials & Nanotech (262)
Solar energy (127)
Literature Updating Services and Databases

- Monthly updates of the most relevant published work in your field:
  - Methods in Organic Synthesis
  - Catalysis and catalysed Reactions
  - Natural Product Updates

- And, highly bespoke searching of the analytical science literature:
  - *Analytical Abstracts*
Catalysts & Catalysed Reactions

- Visual graphical abstracts, allowing fast and effective access to new research
- Addition of around 150 new records every month, sourced from around 40 key journals
- Almost 25,000 records from January 2002 to present
- Searchable online database containing the entire backfile of records
- Indexing by Authors, Products, Reactants and Catalysts, Catalyst Type and Reaction Type
Searching

Catalysts & Catalysed Reactions

Most common method is to browse

Index terms

Further browsing
Search result

7468 Photochemical dechlorination of DDT catalyzed by a hydrophobic vitamin B<sub>2</sub> and a photosensitizer under irradiation with visible light

H. Shimakoshi; M. Tokunaga; T. Baha; Y. Hisaeda


\[
\begin{array}{c}
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\end{array}
\longrightarrow
\begin{array}{c}
\text{Cl} & \text{H} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\text{Cl} & \text{Cl} & \text{Cl} \\
\end{array}
\]

[Co(II), C<sub>1</sub>ester]ClO<sub>4</sub> – [Ru(bipy)_{3}]Cl<sub>2</sub>

EtOH, hv; N<sub>2</sub>, 3 h

99% conversion, 71% selectivity

7255 Metolachlor photocatalytic degradation using TiO<sub>2</sub>, photocatalysts

V. A. Sakkas; I. M. Arabatzis; I. K. Konstantinou; A. D. Dimou; T. A. Albaris; P. Falaras


A number of organic transformation products are produced by the photocatalytic degradation of the herbicide Metolachlor

\[
\begin{array}{c}
\text{CH}_3 \\
\text{CH}_3 \\
\text{C} \\
\text{CH}_3 \\
\text{N} \\
\text{CH}_3 \\
\text{CH}_2\text{OCH}_3 \\
\text{CH}_3 \\
\text{H}_3\text{CH}_2\text{Cl} \\
\end{array}
\longrightarrow
\begin{array}{c}
\text{CH}_3 \\
\text{NH}_2 \\
\text{CH}_2\text{CH}_3 \\
\end{array}
\]

14 examples

7254 Homogeneous catalytic hydrodechlorination of CFC and HCFC compounds
To aid browsing the abstracts in Catalysts & Catalysed Reactions, pictorial representations are used. The graphical symbols represent:

- Assisted Catalysis (e.g. photocatalysis)
- Biocatalysis
- Chirality
- Environmental/Green Chemistry
- Kinetics
- Reaction Engineering
- Surface Science
- Theory

Assisted Catalysis:
- Photocatalysis
- Microwave
- Electrocatalysis
THE MERCK INDEX

NEW 15th Edition

• 500 new monographs
• 35% of existing entries updated
• Over 10,000 monographs
• Names, structures, physical and chemicals properties, key references
<table>
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<td>&quot;recovery AND fuel&quot;</td>
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<tr>
<td>CO2 sequestration and conversion</td>
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<td>&quot;CO2/carbon dioxide AND sequestration/conversion&quot;</td>
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<td>Carbon capture</td>
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</table>
For over 120 years The Merck Index has been regarded as the most authoritative and reliable source of information on chemicals, drugs and biologicals. Now this trusted resource is available online from RSC Publishing.
# Search Guidelines
You may use "=" prefix in text fields to specify exact query matching (e.g., "=acetic acid")
You can enter parameters in multiple fields to refine your searches.
Quick help can be accessed by clicking on the ? symbol next to any field, or See Help for further details.

## Text Search

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## Properties Search

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<td>Melting Point</td>
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<td>Log P</td>
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<td>Index of Refraction</td>
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<td>Optical Rotation</td>
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<td>Flash Point</td>
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<td>Absorption Max</td>
<td>nm</td>
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<tr>
<td>Toxicity</td>
<td>mg/kg</td>
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</table>

Search Clear
Foibles:
Fusion and Nuclear = biological processes
Solid-state = *Solid State Commun*.

No results for ‘modern’ expressions(?):
Carbon capture, fuel recovery
Gasoline

Properties


Use

As fuel in internal combustion engines of the spark-ignited, reciprocating type; diluent; finishing agent; industrial solvent.

References

A mixture of C₄ to C₁₂ hydrocarbons. Natural gasoline, obtained by fractional distillation of petroleum, contains mostly saturated hydrocarbons; commercial grades of motor gasoline contain paraffins, olefins, naphthenes, and aromatics, all in substantial concns. Motor gasolines are made chiefly by cracking processes, in which heavier petr fractions are converted into more volatile fractions by thermal or catalytic decomp; have also been made commercially by catalytic high-pressure hydrogenation of soft coal and by catalytic synthesis of hydrocarbons from carbon monoxide and hydrogen. Some gasolines sold in the U.S. contain a minor proportion of tetraethyllead added to motor gasoline to increase the octane numbers and thereby prevent “knock” in engines in which the gasoline is used as fuel. Knock is the audible manifestation of an excessive rate of pressure rise when the gasoline vapor is ignited under compression in an engine. The relative knocking tendencies of gasolines are measured in terms of “Octane Number,” which is defined as the percentage of iso-octane, having “100 Octane No.,” to be blended with n-heptane, having “0 Octane No.” by definition, in order to obtain the same degree of knock as is obtained with the gasoline being rated, under standard conditions in a standardized test engine. Additives such as ethanol, methanol, benzene, toluene, MTBE and MMT, q.v., are replacing tetraethyllead, and only a small percentage of leaded gasoline is sold in the U.S. Review: J. C. Lane in Kirk-Othmer Encyclopedia of Chemical Technology vol. 11 (Wiley-Interscience, New York, 2nd ed., 1984) pp 652-695. Review of toxicity: N. K. Weaver, Ann. N.Y. Acad. Sci. 534, 441-451 (1988) [DOI: 10.1111/j.1749-6632.1988.tb0133.x PMID: 3291713]; of carcinogenicity: M. A. Mehlman, Toxicol. Ind. Health 7, 143-152 (1990); of toxicology and human exposure: Toxicological Profile for Gasoline (PB95-264206, 1995) 224 pp. Symposium on toxicology, exposure and health effects: Environ. Health Perspect. 101, Suppl. 6, 1-212 (1993).
Monograph ID: MONO1500009628
Title: Titanium Dioxide
CAS Registry Number: 13463-67-7
CAS Name: Titanium oxide (TiO₂)
Additional Names: unitane, C.I. Pigment White 6, C.I. 77891
Molecular Formula: O₂Ti
Molecular Weight: 79.87
Percent Composition: O 40.06%, Ti 59.93%

Properties

White powder, mp 1855°C. d (rutile): 4.23; (anatase): 3.90; (brookite): 4.13. Sol in hot concd H₂SO₄, HF. Insol in water, HCl, HNO₃, 2N H₂SO₄. The reactivity depends on a previous heat treatment; prolonged heating produces a less sol material. Also made sol by fusion with potassium bisulfate or with alkali hydroxides or carbonates to form alkali titanates. Possesses perhaps the greatest hiding power of all inorganic white pigments. Titania is a name applied to large TiO₂ crystals (translucent water-white or with yellowish cast) suitable for use in jewelry. These crystals have a refractive index (2.7) higher than diamonds (2.4), but lack the hardness of diamonds. When substantially pure, a massive single crystal (boule) of rutile has the properties of a precious gem with a very light straw color and with reflectance, refraction and brilliance measuring greater than those of a diamond.

Use

Airfloated ilmenite is used for titanium pigment manuf. Rutile sand is suitable for welding-rod-coating materials, as ceramic colorant, as source of titanium metal. As color in the food industry. Anatase titanium dioxide is used for welding-rod-coatings, acid resistant vitreous enamels, in specification paints, exterior white house paints, acetate rayon, white interior air-dry and baked enamels and lacquers, inks and plastics, for paper filling and coating, in water paints, tanners' leather finishes, shoe whiteners, and ceramics. High opacity and tinting values are claimed for rutile-like pigments. Pharmaceutic aid (coating agent).

References

Found in nature as the minerals rutile (tetragonal), anatase or octahedrite (tetragonal), brookite (orthorhombic), ilmenite (FeTiO₃),
**Monograph ID:** MONO1500008980  
**Title:** Strontium Titanate  
**CAS Registry Number:** 12060-59-2  
**CAS Name:** Strontium titanium oxide (SrTiO₃)  
**Molecular Formula:** O₃SrTi  
**Molecular Weight:** 183.48  
**Percent Composition:** O 26.16%, Sr 47.75%, Ti 26.09%

**Properties**

Density: $\rho = 2.409$. Hardness 5% on Moh's scale. Specific heat: $c = 10 \text{ J s}^{-1} \text{ K}^{-1} \text{ m}^{-1}$. Thermal conductivity: $\kappa = 52 \text{ mW cm}^{-1} \text{ K}^{-1}$.

**Use**

In electronics and electrochemical insulation; in photocatalysis; sputtering target for thin film capacitors; substrate for epitaxial growth of high temperature superconductor thin films. Diamond simulant gemstone.

**References**

Indigo

Monograph ID: MONO1500004981
Title: Indigo
CAS Registry Number: 54784-13-9 402-89-3
CAS Name: (2E)-2-(1,3-Dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one
Additional Names: Indigotin, Indigo blue, D & C Blue No. 5, C.I. Pigment Blue 56, C.I. Vat Blue 1, C.I. 73000
Molecular Formula: C_{10}H_{10}N_{2}O_{2}
Molecular Weight: 262.27
Percent Composition: C 73.27%, H 3.84%, N 10.68%, O 12.20%
Standard InChI: InChI=1S/C16H10N2O2/c19-15-9-5-1-3-7-11(9)17-13(15)14-16(20)10-6-2-4-8-12(10)18-14/h11-18-19-20, H2/qw-3
Standard InChIKey: COHYTHOBJLHDFUHFOGSPRA-N

Properties

Dark-blue powder with coppery luster. Sublimes at about 300°C, dec 390°C. d (cryst) 1.48. Practically insol in water, alcohol, ether, and dil acids. Dissolves in nonpolar solvents with red and in polar solvents with blue color. With fuming H_{2}SO_{4}, it forms a sol sulfonic acid.
The links below provide access to useful information relating to general chemical conventions and commonly used terms that are used in The Merck Index® Online database. They are based upon the appendices provided in the print edition but may differ from those as The Merck Index evolves and more data is added.

- Acronyms
- Alchemical Symbols Used in Biology and Botany
- Amino Acids Found in Proteins
- Atomic Weights Order of Atomic Number
- Chemical Terms Translator
- Common Heterocyclic Ring Systems
- Fundamental Physical and Mathematical Constants
- Glossary
- Greek Alphabet
- International Patent Country Codes
- International System of Units (SI)
- Latin Terms
- Nonproprietary Name Stems
- Numerical Prefixes Commonly Used in Forming Chemical Names
- Prescription Notation
- Radioactive Isotopes Used in Medical Diagnosis and Therapy
- Roman Numerals
- Russian Alphabet
- Selected Hexoses and Pentoses
- Table of Minerals
- Terms for Radicals and Groups Used for Nonproprietary Names
- Thermometric Equivalents
- Universal Conversion Factors
- Vaccines
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<th>Color</th>
<th>Streak</th>
<th>Crystal System</th>
<th>Hardness</th>
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<td>Acanthite</td>
<td>Ag₂S</td>
<td>gray-black</td>
<td>black</td>
<td>mono</td>
<td>2-2.5</td>
<td>-</td>
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<td>Actinolite</td>
<td>Ca₂(Mg₂Fe₅)Si₈O₂₂(OH)₂</td>
<td>green</td>
<td>white</td>
<td>mono</td>
<td>6</td>
<td>1.64</td>
<td>3.0-3.4</td>
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<td>Aegirine</td>
<td>NaFeSi₂O₆</td>
<td>dark green, brown, black</td>
<td>white</td>
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<td>6</td>
<td>1.82</td>
<td>3.6</td>
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<td>Allanite</td>
<td>(Ca,Ce)₃(Al,Fe)₂Si₃O₁₂(OH)</td>
<td>brown to pitch-black</td>
<td>colorless</td>
<td>mono</td>
<td>5.5-6</td>
<td>1.70-1.81</td>
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<td>Fe₃Al₂Si₃O₁₂</td>
<td>red to black</td>
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<td>iso</td>
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<td>1.83</td>
<td>4.0-4.3</td>
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<td>KAl₃(SO₄)₂(OH)₆</td>
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<td>LiAlFPO₄</td>
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<td>half-life</td>
<td>Heat of sublimation</td>
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<td>Standard electron potential</td>
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</tbody>
</table>
RSC’s ChemSpider

- 28 million structures
- Over 400 different data sources, including:
  - PubChem, ChEBI
  - NIST
  - Chemical Suppliers Catalogues
  - Patents
  - RSC journals
- Physical properties, spectra, safety information and much more
- Access it anywhere there’s internet

www.chemspider.com/
Search

Simple  Structure  Advanced  ▼ More searches...

dye

Systematic Name, Synonym, Trade Name, Registry Number, SMILES, InChI or CSID

▼ Options

Single/Multi-component
- Search Any
- Search Single-Component Structures Only
- Search Multi-Component Structures Only

Isotopically Labeled
- Search Any
- Search Isotopically Labeled Structures Only
- Disregard Isotopically Labeled Structures

Additional Filters
- Filter only those having analytical data

Search Hits Limit: 100

12 hits found.
Search terms: dye AND HaveSpectra
Indigo dye

ChemSpider ID: 4477009

- Type: Electron Impact
- Associated Hyperlink: http://www.nist.gov/srd/nist1a.cfm
- Comments: Provided with permission: March 12 2009. Owner NIST Mass Spectrometry Data Center Collection (C) 2007 copyright by the U.S. Secretary of Commerce on behalf of the United States of America. All rights reserved. Origin: NIST Mass Spectrometry Data Center, NIST Database mainlib; NIST MS number 341442
- Approved: No
- Submitted by: antony.williams

![Graph of Relative Abundance vs. Mass]
High efficiency and stable dye-sensitized solar cells with an organic chromophore featuring a binary π-conjugated spacer

Chem. Commun., 2009, 2198-2200

Donor group of dye
2. Edit molecule

- Exact
- Substructure
- Similarity

Search Options
- Match Tautomers

130 hits found.
Search terms: Substructure Search
Adding and curating data

*Adds quality and quantity*...
Users can comment for others to action

Registered users can:
- Curate names
- Add links, spectra, and multimedia resources

Depositors can add new compounds

Curators and Master Curators assess and approve additions
Materials Data

Chemical information underpinning research into energy generation and storage
Fact finding

- Survey at a UK materials conference (>100 participants)
- Market research (key external stakeholder conversations)
Which databases/resources do you currently use?

- Wikipedia
- Journals
- Sigma Aldrich
- Cambridge Structural...
- NIST Chemistry...
- ASM Handbook
- ICDD
- Polymer Handbook
- Web of Science
- SciFinder
- Google

- Other resources mentioned included ICSD, Scopus, ChemSpider and Reaxys

- Top 3 resources are Journals, Google and Web of Science
What data do you search for in articles?

- The majority of respondents used journals to search for property and structure data
Where do you share your research data?

- PC/Hard Drive storage was most commonly used. No respondent chose FigShare and many asked what it was. Some respondents were also unsure what an institutional repository was
Challenges with Materials

• Materials are incredibly diverse:
  • For examples: crystals vs polymers (Hard vs Soft)

• Data needed across research fields is very different

What IS a material property?
• For example: Efficiency of a solar cell – is this a property of the material or the device?

What IS the material?
• Materials are not discrete, and process/fabrication/synthesis can dictate the properties of the end product
  • For example: When reporting properties of a film, length of drying time affects properties (although the compound is the same)

http://en.wikipedia.org/wiki/Titanium_dioxide

https://www.rsc.org/Merck-Index/monograph/mono1500009628/
Royal Society of Chemistry announces a new repository for articles and data

We intend to develop a chemistry data repository for UK academia, and to build tools, models and services on this data store to increase the value and impact of researchers' funded work.

This repository extends the services the Royal Society of Chemistry already offers researchers. With this new service we are improving our ability to ensure that the outputs from research activity are made as widely available as possible - to meet the needs of the scientific community, funders and others interested in accessing our content in a more comprehensive, streamlined way.
Who would like to collaborate?

https://materialsproject.org/

A Materials Genome Approach

Accelerating materials discovery through advanced scientific computing and innovative design tools.

Database Statistics

49242 materials
1416 intercalation batteries
19650 bandstructures
16277 conversion batteries

Materials Explorer
Search for materials information by chemistry, composition, or property.

Lithium Battery Explorer
Find candidate materials for lithium batteries. Get voltage profiles and oxygen evolution data.

Crystal Toolkit
Convert between CIF and VASP input files. Generate new crystals by substituting or removing species.

Reaction Calculator
Calculate the enthalpy of thousands of reactions and compare with experimental values.

Pourbaix Diagrams
Generate Pourbaix Diagrams from experimental ion data

Find out more about our open Materials API and pymatgen library for querying large amounts of data.
Thank you

Peter Corbett
Colin Batchelor
Sandra Macaskill
Nicola Wise

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