

NOVEMBER 2014

REAXYS105

SEARCHING PROPERTIES

REAXYS R105

- ◆ Outlines techniques to find property information in **Reaxys** for the three common use cases:
 - ◆ To find property information on a single substance
 - ◆ To find property information on a group of substances
 - ◆ To find substances with specific property information
- ◆ Contains links to supplementary slides
 - ◆ Simply click the link for more information; when finished there is a link back to the referring slide

For an outline of other presentations in this series, go [here](#)

NOTES

- ◆ The properties of substances are of fundamental importance to the vast majority of the sciences and to many fields in industry
- ◆ Properties impact:
 - ◆ On studies in the medical sciences, on the environment, in the materials sciences and in engineering, and of course in the chemical sciences...
...even in astronomy, where the spectral properties of chemicals provide information on what is happening beyond our planet
- ◆ Reaxys R105 does not address chemical properties (the reactions of chemicals) which are discussed in Reaxys R104/R203), nor bioactivities of substances which are a key component of **Reaxys Medicinal Chemistry**
- ◆ Instead Reaxys R105 focuses on the vast array of other properties of substances, and gives examples in the broad area defined within physical and spectral properties

- ◆ A vast amount of literature in the sciences reports mainly on the properties of substances
- ◆ Reaxys contains information on properties in >500 fields, and has >>500 million property data values
- ◆ Reaxys has, by far, the world's largest database of experimental properties ...
... and has unique functions to search for them

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information

DISPLAY OF PROPERTY INFORMATION

BENZOIC ACID

- ◆ Property information varies with the property concerned
- ◆ To illustrate this, the initial display for the record for benzoic acid gives a summary of the **Available Data**, and further details are displayed after each of these is clicked

Structure



Synthesis | Show Data

Available Data

- Reactivity
- Identification
- Physical Data (2951)
- Spectra (421)
- Ecological Data (144)
- Use/Application (544)
- Natural Product (71)

- ◆ Note that some property fields have numeric data, and the value depends on the conditions under which the measurement is performed
 - ◆ Boiling point depends on pressure
 - ◆ Dipole moment depends on solvent
 - ◆ Solubility depends on solvent and temperature
 - ◆ Partition in octanol/water depends on temperature
 - ◆ Spectra may be run in solution, solid matrix or gas phases
- ◆ Other property fields have text information
- ◆ In **Reaxys** you may search:
 - ◆ The field (i.e., you search only for substances exists that have information in the field - check the box)
 - ◆ Text descriptors or numeric property values
 - ◆ Data in the sub-fields (e.g., the pressure at which the boiling point is measured)
- ◆ For some further details of the information available for benzoic acid, go [here](#)

Boiling Point (17)

| Boiling Point | Pressure | Comment | Reference |
|---------------|---------------|---------|--|
| 150 °C | 0.357788 Torr | | Earle, Martyn John; Katslars, Suhas Prabhakar Patent: US:2004/15:209 A1, 2004 Title/Abstract Full Text Show Details |

Exposure Assessment (10)

| Exposure | Reference |
|---|---|
| presence in PM _{2.5} , samples of emissions from prescribed burnings (Yosemite National Park's Mariposa Grove, CA and Toyahvale National Forest, NV), wildland fuel, simulated residential wood and agricultural combustions | |
| Reactions | Storage conditions; pyrolysis products arising from cellulose, lignin and waste |
| References | Mazzoleni, Lynn R.; Muesenmeyer, Hans; Zehnke, Barbara; Mazzoleni, Lynn R. Environmental Science and Technology, 2007, vol. 41, # 7, p. 2155 - 2122 Title/Abstract Full Text View citing articles Show Details |

Electrical Moment (28)

| Description | Moment | Temperature | Method | Solvent | Comment | Reference |
|---------------|--------|-------------|--------|---------|---------|---|
| Dipole moment | 1.29 D | | | benzene | | Srivastava, A. N.; Singh, Sukhvir; Kumar, Virendra Journal of the Indian Chemical Society, 1988, vol. 65, # 10, p. 720 - 731 Title/Abstract Full Text Show Details |

Partition octan-1-ol/water (MCS) (3)

| Partition Constant POW | log POW | Temperature | Reference |
|------------------------|---------|-------------|--|
| | 1.78 | | Bergo, Alessandro; Maggini, Michele; Martini, Maria Luisa; Scorrano, Gianfranco; Claesson, Sofia; Prato, Maurizio European Journal of Applied Chemistry, 2002, vol. 8, # 5, p. 1015 - 1023 Title/Abstract Full Text View citing articles Show Details |

Solubility (MCS) (497)

| Saturation | Temperature | Solvent | Comment | Reference |
|-----------------|-------------|-----------|--------------------------|---|
| in pure solvent | 17 °C | formamide | Solubility: 1.712 mol/kg | Gruchushnikova, Ivanov Russian Journal of Applied Chemistry, 2008, vol. 81, # 4, p. 597 - 622 Title/Abstract Full Text View citing articles Show Details |

Fluorescence Spectroscopy (16)

| Description | Solvent | Comment | Reference |
|-------------|----------------|--------------------|---|
| Spectrum | | 280.11 - 330.17 nm | Kamei, Shin-ichi; Abe, Haruo; Mikami, Naohiko; Ito, Mikasa Journal of Physical Chemistry, 1985, vol. 89, # 17, p. 3636 - 3641 Title/Abstract Full Text View citing articles Show Details |
| Spectrum | aqueous matrix | 270 - 304 nm | Poestl, David E.; McVey, Jeffrey K. Journal of Chemical Physics, 1964, vol. 40, # 5, p. 1901 - 1911 Title/Abstract Full Text Show Details |

Use/Application

Use (544)

| Use Pattern | Location | Reference |
|------------------------|-----------------------|--|
| Conversion to P.O. No. | Page/Page column 6, 7 | LOREN, S.A.; CSENYEK, Paula; WALK, Bob; WIGAN, Ann; LARIN, Patricia Patent: US:2003/027664 A1, 2003 Title/Abstract Full Text Show Details |

SEARCHING FOR PROPERTY INFORMATION IN REAXYS

SUMMARY

- Information on properties in **Reaxys** may be found:
 - In >48 million bibliographic records
 - In ~600 property fields that contain >500 million property values/data
 - Through records in >57 million unique substances
- Searches may be performed:
 - By natural language text queries through **Ask Reaxys**
 - By text queries and/or property values through **Search Forms**
 - Through property taxonomies in **ReaxysTree**
- In general, there are three use cases:

A SUBSTANCE => PROPERTIES
SUBSTANCES => PROPERTIES
PROPERTIES => SUBSTANCES

- Not only do you need functions to find properties, but you also need functions to find substances with specific properties

The screenshot shows the Reaxys search interface. At the top, there is a search bar labeled 'Ask Reaxys' with a 'BETA' badge and a placeholder 'Enter a keyword, structure or author'. Below the search bar are several navigation icons: Reactions, Substances, MedChemistry, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Physical' icon is highlighted with a red box. Below the icons is a 'Physical Data' section with various property fields: Melting Point (°C), Boiling Point (°C), Refractive Index, Density, Dissociation Exponent, Dynamic Viscosity (P), Optical Rotatory Power (deg), and log POW. Each field has a dropdown menu, a text input field, and a 'lookup' button. A red arrow labeled 'SEARCH FORMS' points to the 'lookup' buttons. At the bottom, there is a 'Show AND Buttons' section with 'Add to Query:' and buttons for 'Structure', 'Molecular Formula', 'Alloy', 'Add/Remove Fields...', and 'Search Substances'.

Q. And how do you find substances in **Reaxys**?

A. In fields available through:



Ask Reaxys **BETA**

Structure

Molecular Formula **BETA**

Alloy

and

Add/Remove Fields...

(i.e., in forms that search substance identification fields)

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FINDING PROPERTIES FOR A SINGLE SUBSTANCE

CIS-PLATIN

SUBSTANCE => PROPERTIES

- ◆ The general strategy is:
 1. Find the substance
 2. Click links through **Available Data**
- ◆ For example, if you want physical data on cis-platin you first find the substance and this may be done through:
 - ◆ Ask Reaxys
 - ◆ Substance identification querylets such as **Chemical Name**
 - ◆ Structure search (As drawn)
- ◆ Having found the substance, note the links through **Available Data**
- ◆ A summary of the spectral information is shown on the right, and a summary of the physical data is shown on the next slide

Ask Reaxys  CIS-PLATIN

| Structure | Structure/Compound Data | N° of preparations All Preps. All Reactors | Available Data |
|--|--|---|---|
|  Synthesis Show Details | Chemical Name: cis-[Pt(NH ₃) ₂ (Cl) ₂] Reaxys Registry Number: 11323862 CAS Registry Number: 15663-27-1 Type of Substance: Coordination compound/isotope or isotope containing compound Molecular Formula: Cl ₂ H ₄ N ₂ Pt Linear Structure Formula: Cl ₂ (NH ₃) ₂ Pt Molecular Weight: 306.047 InChI Key: LZZZYRPGZAFQLE-UHFFFAOYSA-L | 64 prep out of 667 reactions. | Bioactivity Identification Physical Data (59) Spectra (57) Uses/Applications (2971) Quantum Chemical Data (42) |

⚡ Spectra

- ▼ NMR Spectroscopy (20)
- ▼ IR Spectroscopy (11)
- ▼ Mass Spectrometry (1)
- ▼ UV/VIS Spectroscopy (19)
- ▼ NQR Spectroscopy (1)
- ▼ Raman Spectroscopy (1)
- ▼ Luminescence Spectroscopy (3)
- ▼ Other Spectroscopic Methods (1)

FINDING PROPERTIES FOR A SINGLE SUBSTANCE

PHYSICAL PROPERTY DATA FOR CIS-PLATIN

| | |
|--|--|
| <ul style="list-style-type: none"> ± Physical Data ▼ Refractive Index (3) ▼ Density (1) ▼ Conformation (1) ▼ Crystal Phase (2) ▼ Crystal Property Description (2) ▼ Decomposition (1) ▼ Dielectric Constant (1) ▼ Dissociation Energy (1) ▼ Electrochemical Characteristics (3) ▼ Electrolytic Conductivity (8) | <ul style="list-style-type: none"> ▼ Enthalpy of Formation (1) ▼ Further Information (19) ▼ Interatomic Distances and Angles (1) ▼ Ionization Potential (1) ▼ Magnetic Susceptibility (1) ▼ Molecular Deformation (1) ▼ Optics (1) ▼ Partition octan-1-ol/water (MCS) (1) ▼ Solubility (MCS) (8) ▼ Space Group (1) ▼ Transition Point(s) of Crystalline Modification(s) (1) |
|--|--|

± Electrolytic Conductivity (8)

| Electrolytic Conductivity | Temperature | Solvent | Kind of Conductivity | Comment | Reference |
|--|-------------|-----------------------------|-----------------------------------|--------------------------------------|--|
| 0.304 S*(cm ² /mol) | | N,N-dimethylformamide water | Conductivity at infinite dilution | | Hug, Fazlul; Mazumder, Mohammed Ehsanul Hoque; Yu, Jun Qing; Beale, Philip; Chan, Charles ChemMedChem, 2012 , vol. 7, # 10 p. 1840 - 1846 Title/Abstract Full Text View citing articles Show Details |
| 0.0019 S*(cm ² /mol) | 24 - 26 °C | DMSO | Molar conductivity | 1.9 mM | Benedetto, Luigina; Boccaleri, Enrico; Cavigliolo, Giorgio; Colangelo, Donato; Viano, Ilaris; Osella, Domenico Inorganica Chimica Acta, 2000 , vol. 305, # 1 p. 63 - 68 Title/Abstract Full Text View citing articles Show Details |
| 0.1077 S*(cm ² /mol) | 25 °C | H2O | Molar cationic conductivity | c = 1E-3 mol/l | Burglen; Heyn Zeitschrift für Chemie, 1984 , vol. 24, # 7 p. 264 - 265 Title/Abstract Full Text View citing articles Show Details |
| 0.031 S*(cm ² /mol) | 25 °C | DMSO | Molar cationic conductivity | c = 1E-3 mol/l | Burglen; Heyn Zeitschrift für Chemie, 1984 , vol. 24, # 7 p. 264 - 265 Title/Abstract Full Text View citing articles Show Details |
| 0.0107 - 0.1526 S*(cm ² /mol) | 35 °C | H2O | Molar conductivity | din.: 2000 l/mol; depending on time; | Chernyaev, I. I.; Yakshin, M. M. Inv. Plat., 1940 , vol. 17, p. 29 - 54 Full Text Show Details Gmelin Handbook: Pt: MVol.D, 104, page 243 - 245 Full Text Show Details |

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PROPERTIES FOR A GROUP OF SUBSTANCES

ELECTROCHEMICAL CHARACTERISTICS (CYCLOVOLTAMMETRY) FOR FULLERENES

SUBSTANCES => PROPERTIES

- To find a property (e.g., cyclic voltammetry) for a group of substances (e.g., fullerenes), you may want to retrieve only those substances that have that property
 - There may be many substances in that group for which the specific property data is not yet available
- To achieve this, you need to search for the group of substances AND for the property field
- One way to search for “fullerenes” is to use operator “contains” in the Chemical Name Segment Querylet

Chemical Name Segment

contains

- Remember that in Reaxys, this operator automatically applies left- and right-hand truncation
- Add the querylet for Electrochemical Characteristics to your search box and check “exists” exists
- Finally, click **Search Substances**
- This search gives around 700 fullerenes for which cyclic voltammetry information is available
 - As an example (shown on the right), there are 29 reports (mainly in different solvents) of cyclic voltammetry for just one of them (fullerene C70)

Identification

Chemical Name: [Lookup](#) X

Chemical Name Segment: FULLER [Lookup](#) X

Molecular Formula: [Lookup](#) X


Show AND Buttons

Physical Data

Electrochemical Characteristics exists [X](#)

Show AND Buttons

Add to Query: [Structure](#) [Molecular Formula](#) [Alloy](#) [Add/Remove Fields...](#) [Search Substances](#)

 **Chemical Name:** C₇₀

Reaxys Registry Number: 6943004
CAS Registry Number: 741268-81-5, 741268-84-8, 133227-82-4, 133320-10-2, 133320-11-3, 133869-87-3, 134054-62-9, 134932-61-8, 149820-95-3, 149820-96-4, 157903-26-9, 175779-21-2, 115283-22-7, 958817-68-8, 958817-71-5, 958817-74-8, 958817-77-1, 958817-82-4, 140630-87-1, 140694-21-9, 151731-59-8, 157008-89-4, 220861-79-3, 220962-83-9

Type of Substance: isocyclic isotope or isotope containing compound/Coordination compound
Molecular Formula: C₇₀
Linear Structure Formula: C₇₀
Molecular Weight: 840.77
InChI Key: ATLUMFTEZPKKLC-LHFFFAQYSA-N

92 prop out of 504 reactions. [HI Data \(29\)](#) [Identification](#) [Physical Data \(626\)](#) [Spectra \(241\)](#) [Use/Application \(87\)](#) [Quantum Chemical Data \(102\)](#) [Show Targets](#) 773

Syntheses | **Hide Details**

Chemical Names and Synonyms
 C₇₀, [70]fullerene, fullerene C70, C70, fullerene C₇₀, [70]-fullerene, [5,6]fullerene-C70

Hit Data
 ± **Electrochemical Characteristics** (29 hits out of 29 view all)

| Description | Solvent | Temperature | Product XRM | Product | Comment | Reference |
|------------------|---------------------|-------------|-------------|---------|---|--|
| cyclovoltammetry | 1,2-dichlorobenzene | | | | transferred electrons 1; reduction potential: -1.09 V; Ferrrocene/ferrocenium; 0.1 M Bu ₄ NPF ₆ | Belov, Nikita M.; Brobman, Victor A.; Goryunov, Alexey A.; Ioffe, Ilya N.; Lukonina, Natalia S.; Magdesieva, Tatiana V.; Markov, Vitaly Yu.; Rybalchenko, Alexey V.; Samoylova, Nataliya A.; Semivashchaya, Olesya O.; Tretyakov, Sergey I.; Ruff, Adrian; Schuler, Paul; Speiser, Bernd; Ruff, Adrian <i>Chemistry - A European Journal</i> , 2013, vol. 18, # 52, p. 17968 - 17979 Title/Abstract Full Text Show Details |

[5,6]-Open and [6,6]-closed isomers of C₇₀(CF₂)₂: Synthesis, electrochemical and quantum chemical investigation
 Novel difluoromethylated [70]fullerene derivatives, C₇₀(CF₂)₂ (n = 1-3), were obtained by the reaction of C₇₀ with sodium difluorodichloroacetate. Two major products, isomeric C₇₀(CF₂)₂ (neno adducts with [5,6]-open and [6,6]-closed configurations, were isolated and their homofullerene and metafullerene structures were reliably determined by a variety of methods that included X-ray analysis and high-resolution spectroscopic techniques. The [6,6]-open isomer of C₇₀(CF₂)₂ constitutes the first homofullerene example of a non-nitro [70]fullerene derivative in which functionalization involves the most reactive bond in the polar region of the cage. Voltammetric estimation of the electron affinity of the C₇₀(CF₂)₂ isomers showed that it is substantially higher for the [6,6]-open isomer (the 70-electron π-conjugated system is retained) than the [5,6]-closed form, the latter being similar to the electron affinity of pristine C₇₀. In situ ESR spectroelectrochemical investigation of the C₇₀(CF₂)₂ radical anions and DFT calculations of the hyperfine coupling constants provide evidence for the first example of an inter-conversion between the [5,6]-closed and [6,6]-open forms of a cage-modified fullerene driven by an electrochemical one-electron transfer. Thus, [6,6]-closed C₇₀(CF₂)₂ constitutes an interesting example of a redox-switchable fullerene derivative. An open and shut case: Novel [6,6]-open and [6,6]-closed isomers of C₇₀(CF₂)₂ have been isolated and characterized (see figure). The 70-electron π system of the open isomer shows enhanced electron-withdrawing properties. Redox-controlled configurational switching is demonstrated for [6,6]-closed C₇₀(CF₂)₂. Copyright:

Keywords:
 Author: density functional calculations; fullerenes; molecular switches; spectroelectrochemistry; structure elucidation
Compendex Free Language: Fullerene derivative; Hyperfine coupling constants; Molecular switches; One-electron transfer; Quantum chemical investigation; Spectroelectrochemical investigations; Spectroscopic techniques; Structure elucidation
Compendex Descriptor: Density functional theory; Free radical reactions; Fullerenes; Quantum chemistry; Spectroelectrochemistry; Synthetic (chemical)
Compendex Headline: Isomers

| | | | | | | |
|------------------|--------------|--|--|--|--|--|
| cyclovoltammetry | benzonitrile | | | | transferred electrons 2; Half-wave potential: 0.45V; Saturated calomel electrode (SCE) | Gao, Xiang; Li, Zeng-Jun; Ni, Ling; Yang, Wei-Wei; Wu, Di <i>Journal of Organic Chemistry</i> , 2012, vol. 77, # 17, p. 7299 - 7306 Title/Abstract Full Text View citing articles Show Details |
|------------------|--------------|--|--|--|--|--|

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FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

1. PHOSPHORESCENCE QUANTUM CHEMICAL YIELD THROUGH SEARCH QUERYLET

PROPERTY => SUBSTANCES

- ◆ The general search strategy starts with finding records that contain the property of interest
- ◆ Depending on the type of search conducted, you may either browse records, or may use **Reaxys** post-processing tools, to identify **substances** of interest

- ◆ For example, if you were interested in substances for which PHOSPHORESCENCE QUANTUM CHEMICAL YIELD has been reported, you could *start* your search either:
 1. Through a Phosphorescence Spectroscopy Querylet
 2. Through ReaxysTree
 3. Through Ask Reaxys

◆ Steps for the Querylet search are:

1. Customize the Phosphorescence Spectroscopy Querylet (and its Description Querylet - we will use this soon) in your Search Form
2. Check exists then click **Search Substances**
 - ◆ **Reaxys** displays all substances that have information in the **Phosphorescence Spectroscopy** Field
3. Browse through the substances, or narrow them with options under **Analysis View** or under **Filter by:** (next slide)

The screenshot shows a search interface with a dropdown menu set to 'Phosphorescence Spectroscopy'. Below it is a search input field with a 'Description' label and a 'Lookup' button. At the bottom, there are several tabs: 'Structure', 'Molecular Formula', 'Alloy', 'Add/Remove Fields...', and a red 'Search Substances' button.

>10,000 substances have data in Phosphorescence Spectroscopy Field; the “Hit Data” Field is always shown for the Querylet searched

The screenshot displays a search results table. The first row shows a chemical structure and details for a substance with Reaxys Registry Number 2625119. Below the table, there is a section for 'Hit Data' showing 3 results for 'Phosphorescence Spectroscopy'. The table has columns for Description, Location, and Reference.


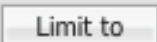
| Description | Location | Reference |
|-------------|------------------------|---|
| Spectro | Supporting Information | Arceval, Nicola; Yasari, Yasari; Zaki, Julian; Wieringarten, Jean-Francois; Albrecht-Gary, Anne-Marie; Heuck, Mohamed |
| | | Chemistry - A European Journal, 2014, vol 20, 4-5 p 223-230 |
| | | Title/Keyword: Full Text: Show Details |

FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

1. NARROWING SUBSTANCES THROUGH FILTER BY: SUBSTRUCTURE

PROPERTY => SUBSTANCES

- You may also choose options under **Filter by:** to narrow answers
- For example, if you were interested in Zn-containing substances for which there is information on phosphorescence spectra, from the querylet search (previous slide) follow the steps:

- Click 
- Draw the structure query (a Zn atom)
- Click Substructure
- Click 

- Reaxys displays >300 Zn-containing substances for which phosphorescence spectra are recorded



| Structure | Structure/Compound Data | N° of preparations All Pages All Reactions | Available Data | Target |
|-------------------------|---|---|--|--------------|
| <chem>H3C-Zn-CH3</chem> | Chemical Name: dimethyl zinc Reaxys Registry Number: 3587195 CAS Registry Number: 544-57-8 Type of Substance: acyclic Molecular Formula: C ₂ H ₄ Zn Linear Structure Formula: (H ₃ C)Zn Molecular Weight: 95.4596 InChI Key: AKAZHDGMAQTHQW-UHFFFAOYSA-N | 26 prep out of 3204 reactions. | HR Data (1) Druglikeness Identification Physical Data (114) Spectra (54) Uses/Application (8) Quantum Chemical Data (37) | Show Targets |

Chemical Names and Synonyms
dimethyl zinc, Me₂Zn, ZnMe₂, Zn(CH₃)₂, D32z, MeZn, ZnMe2

± Hit Data
± Phosphorescence Spectroscopy (1 Hits out of 1 view all)

| Description | Reference |
|-----------------|---|
| Phosphorescence | Bracken; Gurtler; McCaffrey Journal of Physical Chemistry A, 1997, vol. 101, # 51, p. 9854-5662 Title/Abstract Full Text View citing articles Show Details |

WHAT WE DID:

QUERYLET => SUBSTANCES => FILTER BY

WE ALSO NOTE...

Description
Phosphorescence

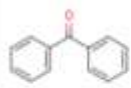
... and we wonder what terms are in this field (to see if this offers another way to narrow answers)

PROPERTY => SUBSTANCES

1. PHOSPHORESCENCE SPECTROSCOPY: DESCRIPTION QUERYLET




- ◆ Scientists are curious, right? We learn by observation, then in this case may wonder “What terms are in the Phosphorescence Spectroscopy => Description Field?”
- ◆ Simple..
Click **Lookup** in the **Description Querylet**, and note the drop-down text
- ◆ Click **phosphorescence quantum yield (767)** then click **Transfer**
- ◆ **Reaxys** transfers the information to the query box; click **Search Substances**
- ◆ **Reaxys** displays the specific data relating to phosphorescence quantum yield
- ◆ We have found another way to find substances with specific information on phosphorescence quantum yield!

The screenshot illustrates the workflow in the Reaxys interface. At the top, the 'Description' field contains the querylet 'IS'. A red box highlights the 'Lookup' button. Below this, a 'Select index items and click "Transfer"' dialog box is shown, listing various index items. 'phosphorescence quantum yield (767)' is selected, and the 'Transfer' button is highlighted. A red arrow points from this dialog to the 'Description' field, which now contains the full querylet 'IS : phosphorescence quantum yield'. The 'Lookup' button is again highlighted.

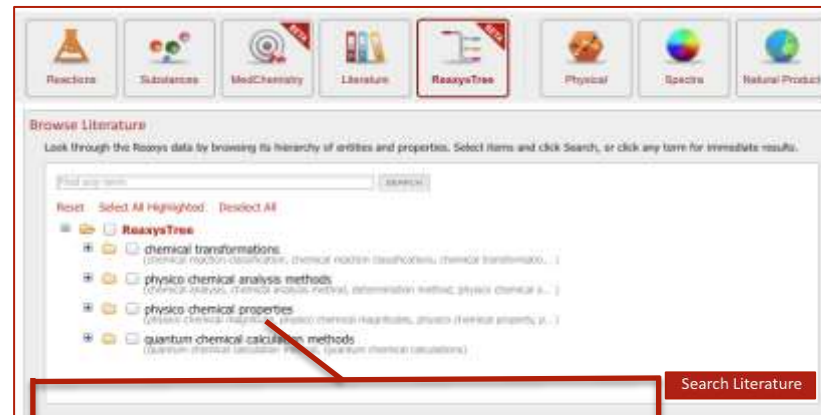
| Structure | Structure/Compound Data | N° of preparations All from All features | Available Data | Target | N° of refs |
|--|---|---|---|--------------|------------|
|  | Chemical Name: benzophenone Reaxys Registry Number: 1238185 CAS Registry Number: 119-61-9 Type of Substance: isocyclic Molecular Formula: C ₁₃ H ₁₀ O Linear Structure Formula: (C ₆ H ₅) ₂ C(=O)C ₆ H ₅ Molecular Weight: 182.222 InChI Key: RWCCWEUJRYNH-B-UHFFFAOYSA-N | 2799 prep out of 12364 reactions. | IR Data (1) Reactivity Identification Physical Data (1218) Spectra (882) Ecological Data (27) Use/Application (93) Quantum Chemical Data (1) | Show Targets | 10753 |
| Chemical Names and Synonyms benzophenone, carbonyl-bis-(phenylene), Benzophenon, o-oxodiphenylmethane, bis-(phenyl)-ketone, diphenylmethanone, o-oxoflavan | | | | | |
| IR Data | | | | | |
| Phosphorescence Spectroscopy (1 IRs out of 101 view all) | | | | | |
| Description | Temperature | Reference | | | |
| Phosphorescence quantum yield | -196.16 °C | Chen, Shun-Chi; Fang, Tai-Shan Chemical Physics Letters, 2007, vol. 450, # 1-3, p. 65-70 Title/Abstract Full Text View citing articles Show Details | | | |

FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

2. PHOSPHORESCENCE QUANTUM CHEMICAL YIELD THROUGH REAXYSTREE

- ◆ When using ReaxysTree you may either:
 - ◆ Scroll through the hierarchies to find fields of interest, or
 - ◆ Enter a property of interest in the Find any term box
- ◆ For example, one of the 4 headings in ReaxysTree is physicochemical properties
- ◆ **Click**  to see the next level in the hierarchy
 - ◆ There are 19 property fields at the next level
- ◆ **Click**  next to **magnetic property** to see the next level in the hierarchy
 - ◆ Further levels are available (click  next to the level of interest)

Perhaps there is something on phosphorescence spectroscopy in one of the hierarchies? ... (Let's try the Find any term box...)



Browse Literature

Look through the Reaxys data by browsing its hierarchy of entities and properties. Select items and click Search, or click any term for immediate results.

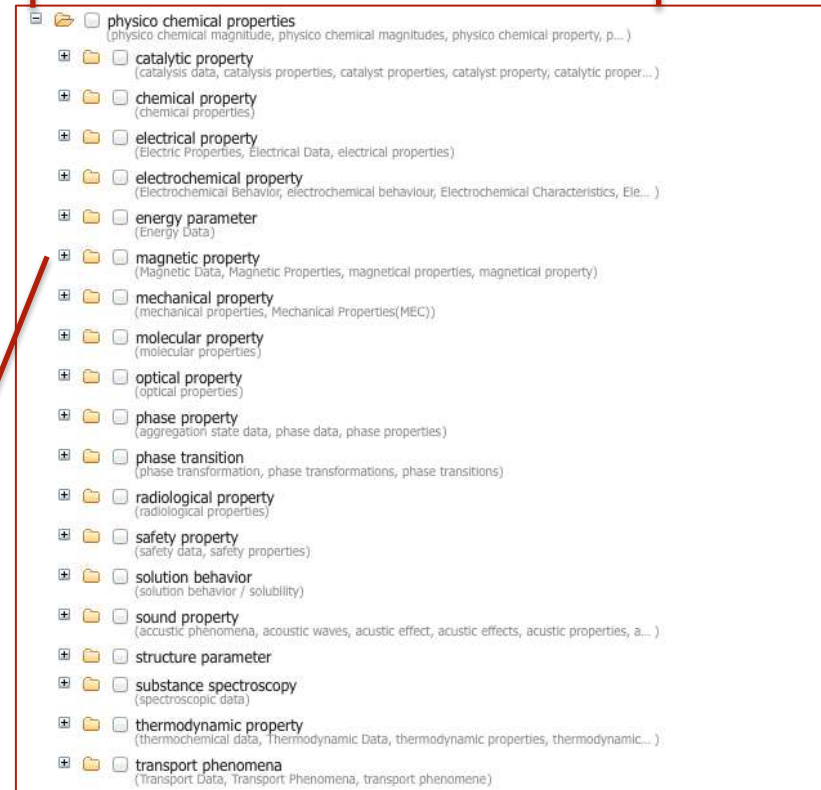
Find any term

Reset Select All Highlighted Deselect All

ReaxysTree

- chemical transformations
- physicochemical analysis methods
- physicochemical properties
- quantum chemical calculation methods

Search Literature



- physicochemical properties
- catalytic property
- chemical property
- electrical property
- electrochemical property
- energy parameter
- magnetic property
- mechanical property
- molecular property
- optical property
- phase property
- phase transition
- radiological property
- safety property
- solution behavior
- sound property
- structure parameter
- substance spectroscopy
- thermodynamic property
- transport phenomena

But where is
"phosphorescence"?



FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

2. PHOSPHORESCENCE QUANTUM CHEMICAL YIELD THROUGH REAXYSTREE

- ◆ Start typing in the Find any term box
- ◆ Click phosphorescence quantum yield
- ◆ Reaxys finds the term in the hierarchy
- ◆ Click **Search Literature**
- ◆ Reaxys gives citations
- ◆ Click **Show All Reactions (3)** **Show All Substances (9)** in the citations interest to see substances of possible interest


Search Literature

| Title of the Document | Authors | Year | Source | Times cited |
|--|--|------|---|-------------|
| Synthesis, characterization, luminescence properties, and DFT calculation of a cationic cyclometalated iridium(III) complex with fluorine-containing phenylquinolinyl and 2,2'-bipyridine ligands | Chen, Qun; Qiang, Jia-Yan; Xu, Ya-Qing; Zhang, Qian-Feng; Ma, Xiu-Fang; Qiang, Jia-Yan; Tong, Bihai; Xu, Ya-Qing; Zhang, Qian-Feng; Leung, Wa-Hung | 2013 | Inorganica Chimica Acta, 2013 , vol. 394, p. 184 - 189 Full Text View citing articles | |
| ± Title/Abstract Synthesis, characterization, luminescence properties, and DFT calculation of a cationic cyclometalated iridium(III) complex with fluorine-containing phenylquinolinyl and 2,2'-bipyridine ligands A cationic bis-cyclometalated iridium(III) complex, [Ir(hfppq) ₂ (bipy)] ⁺ [PF ₆] ⁻ ·0.5H ₂ O (hfppq = 1,1,1,3,3,3-hexafluoro-2-(2-phenylquinolin-4-yl)propan-2-ol, bipy = 2,2'-bipyridine, 1), was obtained from the reaction of the μ-chloro-bridged dimeric complex [Ir(hfppq) ₂ (μ-Cl)] ₂ and bipy in the presence of KPF ₆ . Complex 1 shows a strong emission both in the solid state (ca. 595 nm) and in CH ₂ Cl ₂ solution (ca. 585 nm) at room temperature with the phosphorescence quantum yield of ca. 0.698 and emission lifetime of 0.96 μs. Density functional theory (DFT) calculation was performed on the ground and excited states of complex 1 to provide insight into the structural, electronic, and optical properties of the cationic cyclometalated iridium(III) complex. Keywords: Author: Crystal structure; Cyclometalated; DFT calculation; Iridium(III) complex; Photoluminescence; Synthesis Reaxys Terms: 1,1,1,3,3,3-hexafluoro-2-(2-phenylquinolin-4-yl)propan-2-ol; 2,2'-bipyridine; CH ₂ Cl ₂ ; KPF ₆ ; bipy - ambient reaction temperature; density functional theory; luminescence type; optical property; phosphorescence quantum yield | | | | |
| Show All Reactions (3) Show All Substances (9) | | | | |

FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

3A. PHOSPHORESCENCE QUANTUM CHEMICAL YIELD THROUGH ASK REAXYS

- ◆ You may also Ask Reaxys in this case **Reaxys** gives citations directly
- ◆ Browse through records to look for substances of interest

Ask Reaxys 

| | | | | |
|--|-----------|------|--|---|
| Phosphorescence quantum yield determination with time-gated fluorimeter and Tb(III)-acetylacetonate as luminescence reference. | Perzkofer | 2013 | Chemical Physics, 2013 , vol. 415, p. 173 - 178 Full Text View citing articles | 1 |
|--|-----------|------|--|---|

◆ Title/Abstract
Phosphorescence quantum yield determination with time-gated fluorimeter and Tb(III)-acetylacetonate as luminescence reference
Phosphorescence quantum yield measurements of fluorescent and phosphorescent samples require the use of time-gated fluorimeters in order to discriminate against the fluorescence contribution. As reference standard a non-fluorescent luminescent compound is needed for absolute phosphorescence quantum yield determination. For this purpose the luminescence behavior of the rare earth chelate terbium(III)-acetylacetonate [Tb(acac)₃] was studied (determination of luminescence quantum yield and luminescence lifetime). The luminescence quantum yield of Tb(acac)₃ was determined by using an external light source and operating the fluorimeter in chemo/bioluminescence mode with a fluorescent dye (rhodamine 6G in methanol) as reference standard. A procedure is developed for absolute luminescence (phosphorescence) quantum yield determination of samples under investigation with a time-gated fluorimeter using a non-fluorescent luminescent compound of known luminescence quantum yield and luminescence lifetime.

Keywords:
Author: Luminescence lifetime; Luminescence quantum yield; Phosphorescence quantum yield calculation; Phosphorescence reference standard; Terbium(III)-acetylacetonate chelate; Time-gated fluorimeter
Reaxys Terms: rhodamine 6G - bioluminescence; fluorescent dye; luminescence lifetime; luminescence quantum yield; luminescence type; phosphorescence quantum yield; quantum yield

Show All Substances (2)

| | | | | |
|---|--------------------------|------|---|---|
| Room temperature phosphorescence lifetime and quantum yield of erythrosine B and rose bengal in aerobic alkaline aqueous solution | Perzkofer, Simmel, Riedl | 2012 | Journal of Luminescence, 2012 , vol. 132, # 4 p. 1055 - 1062 Full Text View citing articles | 5 |
|---|--------------------------|------|---|---|

◆ Title/Abstract
Room temperature phosphorescence lifetime and quantum yield of erythrosine B and rose bengal in aerobic alkaline aqueous solution
The room-temperature phosphorescence behavior of erythrosine B (ER) and rose bengal (RB) in aerobic aqueous solution at pH 10 (10⁻⁴ M NaOH) is investigated. The samples were excited with sliced second harmonic pulses of a Q-switched Nd:glass laser. A gated photomultiplier tube was used for instantaneous fluorescence signal discrimination and a digital oscilloscope was used for signal recording. For phosphorescence lifetime measurement the oscilloscope response time was adjusted to appropriate time resolution and sensitivity by the ohmic input resistance. In the case of phosphorescence quantum yield determination the gated photomultiplier oscilloscope arrangement was operated in integration mode using 10 MS input resistance. Phosphorescence quantum yield calibration was achieved with erythrosine B and rose bengal doped starch films of known quantum yields. The determined phosphorescence lifetimes (quantum yields) of ER and RB in 0.1 mM NaOH are $\tau_p = 1.92 \pm 0.1 \mu s$ ($\phi_p = (1.5 \pm 0.3) \times 10^{-5}$) and $2.40 \pm 0.1 \mu s$ ($(5.7 \pm 0.9) \times 10^{-5}$), respectively. The results are discussed in terms of triplet state deactivation by dissolved molecular oxygen.

Keywords:
Author: Aerobic phosphorescence behavior; Erythrosine B; quenching phosphorescence quenching; Phosphorescence lifetime; Phosphorescence quantum yield; Rose bengal
Compendex Free Language: Aerobic phosphorescence behavior; Digital oscilloscope; Fluorescence signals; Input resistance; Nd-glass laser; Phosphorescence lifetime; m yield quantum yield; Photo multiplier tube; Q-switched; Room temperature phosphorescence; Rose Bengal; Second harmonic pulse; Signal recording; Starch films; Time resolution; Triplet state
Compendex Descriptor: Alkalinity; Cathode ray oscilloscopes; Dissolved oxygen; Doping (additives); Dyes; Electric resistance; Glass lasers; Light emission; Molecular oxygen; Neodymium lasers; Oscillographs; Photomultipliers; Quantum yield; Solutions
Compendex Mainhead: Phosphorescence
Reaxys Terms: erythrosine B; molecular oxygen; rose bengal - ambient reaction temperature; phosphorescence lifetime; phosphorescence quantum yield; triplet state

FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

3B. PHOSPHORESCENCE QUANTUM CHEMICAL YIELD THROUGH CITATION BASIC INDEX QUERYLET

- ◆ You may also try a search through the Citation Basic Index Querylet
- ◆ Here is one option - use
- ◆ From the records obtained you may display substances of possible interest
- ◆ From the answer on the right, note that:
 - ◆ terms from a variety of different keyword sources were retrieved
 - ◆ This is good! The point is that you have searched not only “free text” (terms the authors used in titles and abstracts) but also keywords that were considered important by both the authors and the producers of the databases in Reaxys
 - ◆ “contains” found electrophosphorescence

Bibliographic Data

Citation Basic Index

contains PHOSPHORESCENCE QUANTUM YIELD

Show AND Buttons

Add to Query: Structure Molecular Formula Alloy Add/Remove Fields...

1193 citations out of 3652 reactions and 16 bioactivities and 4707 substances and 1 targets

Heatmap Reactions Substances (Grid) Substances (Report) Targets Citations go to Page Page 1 of 133

Link to Exclude Output Print Zoom In Zoom Out Help Sort by Relevance

| Title of the Document | Authors | Year | Source | Times cited |
|---|--|------|--|-------------|
| Pure red electrophosphorescence from polymer light-emitting diodes doped with highly emissive bis-cyclometalated iridium(III) complexes | Asuka, Hitoko; Ikawa, Shigeru; Inai, Yuji; Neebe, Takeshi; Nakamura, Hiroyuki; Tsujimura, Hidetaka; Yagi, Shigeyuki; Sakurai, Yoshiaki | 2010 | Journal of Organometallic Chemistry, 2010, vol. 695, # 17 p. 1572 - 1578 Full text View citing articles | 12 |

Title/Abstract
Pure red electrophosphorescence from polymer light-emitting diodes doped with highly emissive bis-cyclometalated iridium(III) complexes
In order to develop highly emissive red phosphorescent materials for OLED application, novel bis-cyclometalated iridium(III) complexes were developed using the 1-(di-tert-butylamino)isoquinoline-N,C²(dtbq) cyclometalating ligand. When 1,3-bis(3,4-dibutylphenyl)propane-1,3-dionate (dbtp) is employed as an ancillary ligand, tris(dtbfq)₂(dbtp) 1 exhibits red photoluminescence (PL) at 640 nm with a quantum yield (Φ_{PL}) of 0.61 (in toluene, 298 K). Replacement of dbtp to dipivalylmethanate (dpm) and acetylacetonate (acac) [tris(dtbfq)₂(dpm) 2 and tris(dtbfq)₂(acac) 3, respectively] does not affect the PL spectrum, but reduces Φ_{PL} to 0.55 and 0.49 for 2 and 3, respectively. Similar tendency is also found in the doped poly(methyl methacrylate) (PMMA) film, and 1 is more emissive (Φ_{PL} = 0.17) than 2 and 3 (Φ_{PL} = 0.08 and 0.06, respectively). Using 1 as a phosphorescent dopant, polymer light-emitting diodes (PLEDs) were fabricated, of which structure was ITO/PEDOT:PSS (40 nm)/PVC:1-PBD (100 nm)/GF (1 nm)/AI (250 nm). Pure red electroluminescence (EL) is obtained from the fabricated PLEDs, affording a CIE chromaticity coordinate of (0.68, 0.31). When 0.51 molpercent of 1 is incorporated in the PVC-based emitting layer, the PLED shows maximum luminance of 7270 cd m⁻² at 16.5 V; power efficiency of 1.4 lm W⁻¹ at 7.5 V, and external quantum efficiency of 6.4percent at 9.0 V. PLEDs with the same structure and components were also fabricated using 2 and 3, and their device characteristics were investigated. In proportion to the PL quantum yields, 1 affords better device performance than 2 and 3. Owing to four butyl groups introduced to the dtbfq ligand, 1 exhibits high solubility in organic solvents such as chloroform and toluene, and thus, is an excellent red phosphorescent dopant for solution-processed OLEDs. A highly emissive red phosphorescent bis-cyclometalated iridium(III) complex, bis[1-(di-tert-butylamino)isoquinoline-N,C²]iridium(III) [1,3-bis(3,4-dibutylphenyl)propane-1,3-dionate-O,O] 1 was developed. It exhibits red photoluminescence with Φ_{PL} of 0.61 (toluene, 298 K). The electrophosphorescence from the polymer light-emitting diode containing 1 affords a CIE chromaticity coordinate of (0.68, 0.31) shifting to pure red over the NTSC standard.

Keywords:
Author: Bis-cyclometalated iridium(III) complex; Organic light-emitting diode; Photoluminescence quantum yield; Polymer light-emitting diode; Red phosphorescence
Compound Free Language: Acetylacetonate; Ancillary ligand; CIE chromaticity; Cyclometalating ligand; Device characteristics; Device performance; Electrophosphorescence; Emitting layer; Efficiency; quantum efficiency; High solubility; Iridium complex; Maximum luminance; Phosphorescent dopant; Photoluminescence quantum yield; PL quantum yield; PL spectra; Polymer light-emitting diodes; Power efficiency; Red electroluminescence; Red electrophosphorescence; Red phosphorescence; Red phosphorescent material; Red photoluminescence; Solution-processed
Compound Descriptor: Doped; Doping (additive); Electroluminescence; Esters; Fabrication; Iridium; Ligands; Light; Light emission; Light emitting diodes; Organic light emitting diodes (OLED); Organic solvents; Phosphorescence; Photoluminescence; Polymers; Propane; Quantum efficiency; Quantum yield; Quenching; Toluene
Compound Mainhead: Iridium compounds
Reaxys Terms: 1,3-bis(3,4-dibutylphenyl)propane-1,3-dionate; PLED; acac; acetylacetonate; bis[1-(di-tert-butylamino)isoquinoline-N,C²]iridium; dipivalylmethanate; poly(methyl methacrylate) - electroluminescence; organic solvent; photoluminescence; quantum yield; solubility

SEARCHING PROPERTIES

SUMMARY

- ◆ Information on properties in **Reaxys** may be found:
 - ◆ In >48 million bibliographic records
 - ◆ In ~600 property fields that contain >500 million property values/data
 - ◆ Through records in >57 million unique substances
- ◆ Searches may be performed:
 - ◆ By natural language text queries through **Ask Reaxys**
 - ◆ By text queries and/or property values through **Search Forms**
 - ◆ Through property taxonomies in **ReaxysTree**
- ◆ Often a combination of these search strategies may be used to maximize search precision/search comprehension

Reaxys R105 gives just samples of the techniques that may be used; discover other techniques yourself!

SUPPLEMENTARY SLIDES

FURTHER PRESENTATIONS IN THIS SERIES

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An overview of the functions of Reaxys 2014

REAXYS R102

TIPS FOR LITERATURE SEARCHING

A quick guide to searching literature

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BASIC SUBSTANCE QUERIES

A quick guide to searching for specific substances by name, formula and structure

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BASIC REACTION QUERIES

A quick guide to searching for chemical reactions

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SEARCHING PROPERTIES

A quick guide to searching for properties

REAXYS R201

ADVANCED STRUCTURE QUERIES

Searching by substructure

REAXYS R202

ADVANCED NAME AND FORMULA SEARCHING




Searching for Substances by Names and Formulas

REAXYS R203

ADVANCED REACTION QUERIES

Additional ways to search for reactions

EXAMPLES OF INFORMATION IN PROPERTY FIELDS

| Structure | Structure/Compound Data | N° of preparations All Phys All Reactions | Available Data |
|---|---|--|--|
|    Synthesize Show Details | Chemical Name: benzoic acid Reaxys Registry Number: 636131 CAS Registry Number: 65-85-0 Type of Substance: isocyclic Molecular Formula: C ₇ H ₆ O ₂ Linear Structure Formula: (C ₆ H ₅)CO ₂ H Molecular Weight: 122.123 InChI Key: WPYMKLBDIGXITP-UHFFFAOYSA-N | 6282 prep out of 18602 reactions. | Bioactivity Identification Physical Data (2931) Spectra (421) Ecological Data (144) Use/Application (544) Natural Product (71) |

Available Data in the Physical Data, Spectra and Ecological Data Fields for benzoic acid

Physical Data

- ▼ Melting Point (97)
- ▼ Boiling Point (17)
- ▼ Sublimation (4)
- ▼ Refractive Index (10)
- ▼ Density (33)
- ▼ Adsorption (MCS) (127)
- ▼ Association (MCS) (271)
- ▼ Azeotropes (MCS) (21)
- ▼ Boundary Surface Phenomena (MCS) (9)
- ▼ Chromatographic Data (6)
- ▼ Circular Dichroism (3)
- ▼ Complex Phase Equilibria (MCS) (1)
- ▼ Compressibility (3)
- ▼ Conformation (2)
- ▼ Critical Pressure (1)
- ▼ Critical Temperature (1)
- ▼ Crystal Phase (29)
- ▼ Crystal Property Description (8)
- ▼ Crystal System (1)
- ▼ Decomposition (1)
- ▼ Dielectric Constant (1)
- ▼ Dissociation Energy (2)

Dissociation Exponent (657)

- ▼ Dynamic Viscosity (8)
- ▼ Electrical Data (32)
- ▼ Electrical Moment (28)
- ▼ Electrical Polarizability (2)
- ▼ Electrochemical Behaviour (60)
- ▼ Electrochemical Characteristics (7)
- ▼ Energy Data (MCS) (49)
- ▼ Enthalpies of Other Phase Transitions (1)
- ▼ Enthalpy of Combustion (15)
- ▼ Enthalpy of Formation (3)
- ▼ Enthalpy of Fusion (11)
- ▼ Enthalpy of Sublimation (23)
- ▼ Enthalpy of Vaporization (3)
- ▼ Further Information (378)
- ▼ Gas Phase (1)
- ▼ Heat Capacity Cp (13)
- ▼ Heat Capacity Cp0 (3)
- ▼ Henry Constant (MCS) (1)
- ▼ Interatomic Distances and Angles (2)
- ▼ Ionization Potential (3)
- ▼ Liquid Phase (14)
- ▼ Liquid/Liquid Systems (MCS) (118)

Liquid/Solid Systems (MCS) (146)

- ▼ Liquid/Vapour Systems (MCS) (32)
- ▼ Magnetic Susceptibility (4)
- ▼ Mechanical & Physical Properties (MCS) (8)
- ▼ Mechanical Properties (4)
- ▼ Molecular Deformation (3)
- ▼ Optics (16)
- ▼ Other Thermochemical Data (15)
- ▼ Partition octan-1-ol/water (MCS) (3)
- ▼ Self-diffusion (1)
- ▼ Solubility (MCS) (497)
- ▼ Solubility Product (MCS) (1)
- ▼ Solution Behaviour (MCS) (33)
- ▼ Sound Properties (3)
- ▼ Space Group (2)
- ▼ Static Dielectric Constant (1)
- ▼ Surface Tension (3)
- ▼ Transition Point(s) of Crystalline Modification(s) (3)
- ▼ Transport Data (1)
- ▼ Transport Phenomena (MCS) (60)
- ▼ Triple Point (2)
- ▼ Vapour Pressure (13)

Spectra

- ▼ NMR Spectroscopy (147)
- ▼ IR Spectroscopy (91)
- ▼ Mass Spectrometry (29)
- ▼ UV/VIS Spectroscopy (75)
- ▼ ESR Spectroscopy (3)
- ▼ Rotational Spectroscopy (1)
- ▼ Raman Spectroscopy (26)
- ▼ Luminescence Spectroscopy (8)
- ▼ Fluorescence Spectroscopy (16)
- ▼ Phosphorescence Spectroscopy (23)
- ▼ Other Spectroscopic Methods (2)

Ecological Data

- ▼ Exposure Assessment (10)
- ▼ Concentration in the Environment (43)
- ▼ Transport and Distribution (8)
- ▼ Bioaccumulation, Biomagnification and Biomonitoring (1)
- ▼ Biodegradation (43)
- ▼ Abiotic Degradation, Hydrolysis (31)
- ▼ Abiotic Degradation, Photolysis (6)
- ▼ Oxygen Demand (2)