

NOVEMBER 2014

# REAXYS101

## SEARCHING PROPERTIES

# NOTES ON REAXYS R101

## SEARCHING PROPERTIES

### REAXYS R101 SEARCHING PROPERTIES

- ◆ 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
- ◆ This presentation does not address chemical properties (the reactions of chemicals) which are discussed in Reaxys R101/R201), nor bioactivities of substances which are a key component of **Reaxys Medicinal Chemistry**
- ◆ Instead this presentation 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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Find properties for a group of substances

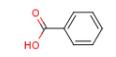
Find substances with specific property  
information

# 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



Synthesize | Show Details

Available Data

- Bioactivity Identification
- Physical Data (2931)
- 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        | 0.367788 Torr |         | <b>Earle, Martyn John; Katdare, Suhas Prabhakar</b><br>Patent: US2004/15009 A1, 2004 ;<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Show Details</a> |

▲ Exposure Assessment (10)

| Exposure  | Sources  | Reference   |
|---|--|---|
| presence in PM <sub>2.5</sub> samples of emissions from prescribed burnings (Yosemite National Park's Mariposa Grove, CA and Toiyabe National Forest, NV), wildland fuel, simulated residential wood and agricultural combustions | biomass combustion; pyrolysis products arising from cellulose, lignin and resins | <b>Mazzoleni, Lynn R.; Moosmueller, Hans; Zielinska, Barbara; Mazzoleni, Lynn R.</b><br>Environmental Science and Technology, 2007, vol. 41, # 7 p. 2115 - 2122<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |

▲ Electrical Moment (28)

| Description   | Moment | Temperature | Method | Solvent | Comment | Reference  |
|---------------|--------|-------------|--------|---------|---------|--|
| Dipole moment | 1.29 D |             |        | benzene |         | <b>Srivastava, A. N.; Singh, Sukhvir; Kumar, Virendra</b><br>Journal of the Indian Chemical Society, 1988, vol. 65, # 10 p. 729 - 731<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Show Details</a> |

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

| Partition Constant POW | log POW | Temperature | Reference   |
|------------------------|---------|-------------|---|
|                        | 1.78    |             | <b>Bagno, Alessandro; Maggini, Michele; Martini, Maria Luisa; Scorrano, Gianfranco; Claeson, Sofia; Prato, Maurizio</b><br>Chemistry - A European Journal, 2002, vol. 8, # 5 p. 1015 - 1023<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |

▲ Solubility (MCS) (497)

| Saturation      | Temperature | Solvent   | Comment                  | Reference   |
|-----------------|-------------|-----------|--------------------------|---|
| in pure solvent | 17 °C       | formamide | Solubility: 1.712 mol/kg | <b>Grechushnikov, Ivanov</b><br>Russian Journal of Applied Chemistry, 2008, vol. 81, # 4 p. 597 - 602<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |

▲ Fluorescence Spectroscopy (16)

| Description | Solvent        | Comment            | Reference  |
|-------------|----------------|--------------------|--|
| Spectrum    |                | 280.11 - 270.27 nm | <b>Kamei, Shin-ichi; Abe, Haruo; Mikami, Naohiko; Ito, Mitsuo</b><br>Journal of Physical Chemistry, 1985, vol. 89, # 17 p. 3636 - 3641<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |
| Spectrum    | gaseous matrix | 279 - 304 nm       | <b>Poeltl, David E.; McVey, Jeffrey K.</b><br>Journal of Chemical Physics, 1984, vol. 80, # 5 p. 1801 - 1811<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Show Details</a>  |

▲ Use/Application

▲ Use (544)

| Use Pattern             | Location              | Reference   |
|-------------------------|-----------------------|---|
| Cosmetics/dental/toilet | Page/Page column 6; 7 | <b>LOREAL S.A.; CZIRYAK, Paula; Shah, Anil; Kijacic, Ana; Laize, Fabrice</b><br>Patent: US2013/142740 A1, 2013 ;<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Show Details</a> |

# 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 displays the Reaxys search interface. At the top, there are two red boxes labeled 'NATURAL LANGUAGE' and 'TAXONOMIES' with arrows pointing to the search bar. The search bar contains the text 'Enter a keyword, compound or author'. Below the search bar is a navigation bar with icons for Reactions, Substances, MedChemistry, Literature, ReaxysTree, Physical, Spectra, Natural Product, and Advanced. The 'Physical' icon is highlighted with a red box. Below the navigation bar is the 'Physical Data' search form, which includes fields for 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 'Physical' icon. At the bottom of the search form, there is a 'Show AND Buttons' section with 'Add to Query:' and buttons for 'Structure', 'Molecular Formula', 'Alloy', and 'Add/Remove Fields...'. A 'Search Substances' button is located at the bottom right.

Q. And how do you find substances in Reaxys?  
A. In fields available through:

The diagram shows the search fields available for finding substances. It includes the 'Substances' icon, the 'Ask Reaxys' search bar, and buttons for 'Structure', 'Molecular Formula', and 'Alloy'. Below these buttons is the 'Add/Remove Fields...' button. The text '(i.e., in forms that search substance identification fields)' is shown below the 'Add/Remove Fields...' button. The word 'and' is placed between the 'Add/Remove Fields...' button and the text '(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 

| Structure   | Structure/Compound Data  | N° of preparations<br><a href="#">All Preps</a>   <a href="#">All Reactions</a> | Available Data   |
|---|--|---|--|
| <br> <br><a href="#">Synthesize</a>   <a href="#">Show Details</a> | <b>Chemical Name:</b><br>cis-[Pt(NH <sub>3</sub> ) <sub>2</sub> (Cl) <sub>2</sub> ]<br><b>Reaxys Registry Number:</b> <a href="#">11323862</a><br><b>CAS Registry Number:</b> 15663-27-1<br><b>Type of Substance:</b> Coordination compound isotope or isotope containing compound<br><b>Molecular Formula:</b> Cl <sub>2</sub> H <sub>6</sub> N <sub>2</sub> Pt<br><b>Linear Structure Formula:</b> Cl <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> Pt<br><b>Molecular Weight:</b> 300.047<br><b>InChI Key:</b> LXZZYRPGZAFOLE-UHFFFAOYSA-L | 64 prep out of 667 reactions.   | <a href="#">Bioactivity Identification</a><br><a href="#">Physical Data (59)</a><br><a href="#">Spectra (57)</a><br><a href="#">Use/Application (2971)</a><br><a href="#">Quantum Chemical Data (42)</a> |

### ▲ 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

|  |   |
|--|---|
| ⚡ <b>Physical Data</b>                       | ⚡ <b>Enthalpy of Formation (1)</b>                              |
| ⚡ <b>Refractive Index (3)</b>                | ⚡ <b>Further Information (19)</b>                               |
| ⚡ <b>Density (1)</b>                         | ⚡ <b>Interatomic Distances and Angles (1)</b>                   |
| ⚡ <b>Conformation (1)</b>                    | ⚡ <b>Ionization Potential (1)</b>                               |
| ⚡ <b>Crystal Phase (2)</b>                   | ⚡ <b>Magnetic Susceptibility (1)</b>                            |
| ⚡ <b>Crystal Property Description (2)</b>    | ⚡ <b>Molecular Deformation (1)</b>                              |
| ⚡ <b>Decomposition (1)</b>                   | ⚡ <b>Optics (1)</b>   |
| ⚡ <b>Dielectric Constant (1)</b>             | ⚡ <b>Partition octan-1-ol/water (MCS) (1)</b>                   |
| ⚡ <b>Dissociation Energy (1)</b>             | ⚡ <b>Solubility (MCS) (8)</b>                                   |
| ⚡ <b>Electrochemical Characteristics (3)</b> | ⚡ <b>Space Group (1)</b>  |
| ⚡ <b>Electrolytic Conductivity (8)</b>       | ⚡ <b>Transition Point(s) of Crystalline Modification(s) (1)</b> |

⚡ **Electrolytic Conductivity (8)**

| Electrolytic Conductivity                             | Temperature | Solvent                     | Kind of Conductivity              | Comment                               | Reference  |
|---|-------------|-----------------------------|-----------------------------------|---------------------------------------|--|
| 0.304 S <sup>l</sup> /(cm <sup>3</sup> mol)           |             | N,N-dimethylformamide water | Conductivity at infinite dilution |                                       | <b>Huq, Fazlul; Mazumder, Mohammed Ehsanul Hoque; Yu, Jun Qing; Beale, Philip; Chan, Charles</b><br>ChemMedChem, <b>2012</b> , vol. 7, # 10 p. 1840 - 1846<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>                               |
| 0.0019 S <sup>l</sup> /(cm <sup>3</sup> mol)          | 24 - 26 °C  | DMSO                        | Molar conductivity                | 1.9 mM                                | <b>Benedetto, Luigina; Boccaleri, Enrico; Cavigliolo, Giorgio; Colangelo, Donato; Viano, Ilario; Osella, Domenico</b><br>Inorganica Chimica Acta, <b>2000</b> , vol. 305, # 1 p. 61 - 68<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |
| 0.1077 S <sup>l</sup> /(cm <sup>3</sup> mol)          | 25 °C       | H2O                         | Molar cationic conductivity       | c = 1E-3 mol/l                        | <b>Burglen; Heyn</b><br>Zeitschrift fur Chemie, <b>1984</b> , vol. 24, # 7 p. 264 - 265<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>  |
| 0.031 S <sup>l</sup> /(cm <sup>3</sup> mol)           | 25 °C       | DMSO                        | Molar cationic conductivity       | c = 1E-3 mol/l                        | <b>Burglen; Heyn</b><br>Zeitschrift fur Chemie, <b>1984</b> , vol. 24, # 7 p. 264 - 265<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a>  |
| 0.0107 - 0.1526 S <sup>l</sup> /(cm <sup>3</sup> mol) | 35 °C       | H2O                         | Molar conductivity                | diln.: 2000 l/mol; depending on time; | <b>Chernyaev, I. I.; Yakshin, M. M.</b><br>Izv. Plat., <b>1940</b> , vol. 17, p. 29 - 54<br><a href="#">Full Text</a> <a href="#">Show Details</a><br><b>Gmelin Handbook:</b> Pt: MVol.D, 104, page 243 - 245<br><a href="#">Full Text</a> <a href="#">Show Details</a>  |

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# PROPERTIES FOR A GROUP OF SUBSTANCES

## ELECTROCHEMICAL CHARACTERISTICS (CYCLOVOLTAMMETRY) FOR FULLERENES

### SUBSTANCES => PROPERTIES

- To find a property (e.g., cyclovoltammetry) 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”
- Finally, click **Search Substances**
- This search gives around 700 fullerenes for which cyclovoltammetry information is available
  - As an example (shown on the right), there are 29 reports (mainly in different solvents) of cyclovoltammetry for just one of them (fullerene C70)

**Identification**

Chemical Name: is  [Lookup](#) ×

Chemical Name Segment: contains  [Lookup](#) ×

Molecular Formula: is  [Lookup](#) ×

Show AND Buttons

---

**Physical Data**

Electrochemical Characteristics  exists ×

Show AND Buttons

---

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



**Chemical Name:**  
C<sub>70</sub>

**Reaxys Registry Number:** 6843004

**CAS Registry Number:** 741268-81-5, 741268-84-8, 133227-82-4, 133320-10-2, 133320-11-3, 133869-47-3, 134054-62-9, 134932-61-9, 149820-05-3, 149820-06-4, 157903-26-9, 175779-21-2, 115383-22-7, 958017-68-0, 958017-71-5, 958017-74-8, 958017-77-1, 958017-80-6, 140630-87-1, 140694-21-9, 151716-50-6, 157008-89-4, 220062-79-3, 220062-83-9

**Type of Substance:** isocyclic/isotope or isotope containing compound/Coordination compound

**Molecular Formula:** C<sub>70</sub>

**Linear Structure Formula:** C<sub>70</sub>

**Molecular Weight:** 840.77

**InChI Key:** ATLMTJZZPKLC-UHFFFAOYSA-N

[Synthesize](#) | [Hide Details](#)

92 prep out of 504 reactions.

Hit Data (29)  
Identification  
Physical Data (626)  
Spectra (241)  
Use/Application (87)  
Quantum Chemical Data (102)

Show Targets 773

---

**Chemical Names and Synonyms**

C<sub>70</sub>, [70]fullerene, fullerene C70, C70, fullerene C<sub>70</sub>, <70>-fullerene, [5,6]fullerene-C70

▲ **Hit Data**

▲ **Electrochemical Characteristics ( 29 Hits out of 29 view all )**

| Description      | Solvent             | Temperature | Product XRN | Product | Comment  | Reference  |
|------------------|---------------------|-------------|-------------|---------|--|--|
| cyclovoltammetry | 1,2-dichlorobenzene |             |             |         | transmitted electrons 1; reduction potential; -1.09 V; Ferrocene/ferrocenium; 0.1 M Bu <sub>4</sub> NBF <sub>4</sub> | <b>Below, Nikita M.; Brotsman, Victor A.; Goryunkov, Alexey A.; Ioffe, Ilya N.; Lukonina, Natalia S.; Magdesieva, Tatiana V.; Markov, Vitaliy Yu.; Rybalchenko, Alexey V.; Samoylova, Nataliya A.; Semivrazhskaya, Olesya O.; Troyanov, Sergey I.; Ruff, Adrian; Schuler, Paul; Speiser, Bernd; Ruff, Adrian</b><br>Chemistry - A European Journal, <b>2013</b> , vol. 19, # 52 p. 17969 - 17979<br><a href="#">Hide Title/Abstract</a> <a href="#">Full Text</a> <a href="#">Show Details</a> |

**[6,6]-Open and [6,6]-closed isomers of C<sub>70</sub>(CF<sub>2</sub>): Synthesis, electrochemical and quantum chemical investigation**

Novel difluoromethylenated [70]fullerene derivatives, C<sub>70</sub>(CF<sub>2</sub>)<sub>n</sub> (n=1-3), were obtained by the reaction of C<sub>70</sub> with sodium difluorochloroacetate. Two major products, isomeric C<sub>70</sub>(CF<sub>2</sub>) mono-adducts with [6,6]-open and [6,6]-closed configurations, were isolated and their homofullerene and methanofullerene structures were reliably determined by a variety of methods that included X-ray analysis and high-level spectroscopic techniques. The [6,6]-open isomer of C<sub>70</sub>(CF<sub>2</sub>) constitutes the first homofullerene example of a non-hetero [70]fullerene derivative in which functionalisation involves the most reactive bond in the polar region of the cage. Voltammetric estimation of the electron affinity of the C<sub>70</sub>(CF<sub>2</sub>) isomers showed that it is substantially higher for the [6,6]-open isomer (the 70-electron n-conjugated system is retained) than the [6,6]-closed form, the latter being similar to the electron affinity of pristine C<sub>70</sub>. In situ ESR spectroelectrochemical investigation of the C<sub>70</sub>(CF<sub>2</sub>) radical anions and DFT calculations of the hyperfine coupling constants provide evidence for the first example of an inter-conversion between the [6,6]-closed and [6,6]-open forms of a cage-modified fullerene driven by an electrochemical one-electron transfer. Thus, [6,6]-closed C<sub>70</sub>(CF<sub>2</sub>) 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 C<sub>70</sub>(CF<sub>2</sub>) have been isolated and characterised (see figure). The 70-electron n system of the open isomer shows enhanced electron-withdrawing properties. Redox-controlled configurational switching is demonstrated for [6,6]-closed C<sub>70</sub>(CF<sub>2</sub>). 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; Synthesis (chemical)  
**Compendex Mainhead:** Isomers

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

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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

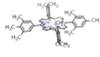
- ◆ For example, if you were interested in substances for which PHOSPHORESCENCE QUANTUM CHEMICAL YIELD has been reported, you could *start* your search either:
  1. Through a Phosphorescence Spectroscopy Querylet
  2. Through ReaxysTree
  3. Through Ask Reaxys

### ◆ 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)

Phosphorescence Spectroscopy  exists ×  
Description is  Lookup ×  
Structure Molecular Formula **BETA** Alloy Add/Remove Fields... **Search Substances**

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

| Structure  | Structure/Compound Data  | N° of preparations<br>All Preps   All Reactions | Available Data                                | Target          | N° of ref. |
|--|--|---|---|-----------------|------------|
|  | <b>Reaxys Registry Number:</b> 26535115<br><b>Molecular Formula:</b> C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> Zn<br><b>Linear Structure Formula:</b> C <sub>22</sub> H <sub>22</sub> N <sub>2</sub> Zn<br><b>Molecular Weight:</b> 846.446 | no reactions.                                   | Hit Data (1)<br>Identification<br>Spectra (3) | Show<br>Targets | 1          |

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

| Description | Location               | Reference   |
|-------------|------------------------|---|
| Spectrum    | supporting information | <b>Armaroli, Nicola; Yoosaf; Yoosaf; Iehl, Julien; Nierengarten, Jean-Francois; Albrecht-Gary, Anne-Marie; Hmadeh, Mohamed; Nierengarten, Iwona</b><br>Chemistry - A European Journal, <b>2014</b> , vol. 20, # 1 p. 223 - 231<br>Title/Abstract 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

Filter by: Sub-structure

Search as / by

- As drawn
- Substructure: on heteroatoms, on all atoms
- Similarity

Options

- Include tautomers
- Ignore stereo
- No salts
- No mixtures
- No isotopes
- No charges
- No radicals
- No ring closures
- align results with query
- More options
- Include related Markush
- Keep Fragments ...
- separate together
- # of Atoms
- # of Fragments
- # of Ring Closures

Create Structure Template from Name

Copy Structure to Query Copy Structure from Query Limit to Exclude Close

### 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)

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

| Structure               | Structure/Compound Data  | N° of preparations<br>All Preps   All Reactions | Available Data   | Target       |
|-------------------------|--|---|--|--------------|
| <chem>H3C-Zn-CH3</chem> | <b>Chemical Name:</b> dimethyl zinc<br><b>Reaxys Registry Number:</b> 3587195<br><b>CAS Registry Number:</b> 544-97-8<br><b>Type of Substance:</b> acyclic<br><b>Molecular Formula:</b> C <sub>2</sub> H <sub>6</sub> Zn<br><b>Linear Structure Formula:</b> (H <sub>3</sub> C) <sub>2</sub> Zn<br><b>Molecular Weight:</b> 95.4596<br><b>InChI Key:</b> AXAZMDOAUQTMOW-UHFFFAOYSA-N | 26 prep out of 3204 reactions.                  | Hit Data (1)<br>Druglikeness<br>Identification<br>Physical Data (114)<br>Spectra (54)<br>Use/Application (8)<br>Quantum Chemical Data (33) | Show Targets |

**Chemical Names and Synonyms**  
dimethyl zinc, Me<sub>2</sub>Zn, ZnMe<sub>2</sub>, Zn(CH<sub>3</sub>)<sub>2</sub>, Et<sub>2</sub>Zn, Me<sub>2</sub>Zn, ZnMe<sub>2</sub>

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

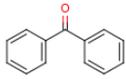
| Description     | Reference  |
|-----------------|--|
| Phosphorescence | <b>Bracken; Gurtler; McCaffrey</b><br>Journal of Physical Chemistry A, 1997, vol. 101, # 51 p. 9854 - 9862<br>Title/Abstract Full Text View citing articles Show Details |

# 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 search interface. At the top, a search box contains the text 'Phosphorescence Spectroscopy' and a dropdown menu set to 'is'. A 'Lookup' button is visible. Below this, a 'Select index items and click 'Transfer'' window is open, displaying a list of search terms with their respective hit counts. The term 'phosphorescence quantum yield (767)' is highlighted. A red arrow points from this term to the 'Transfer' button. Another red arrow points from the 'Transfer' button to the search box, where the text 'phosphorescence quantum yield' has been entered. The 'Search Substances' button is also visible in the top right of the interface.

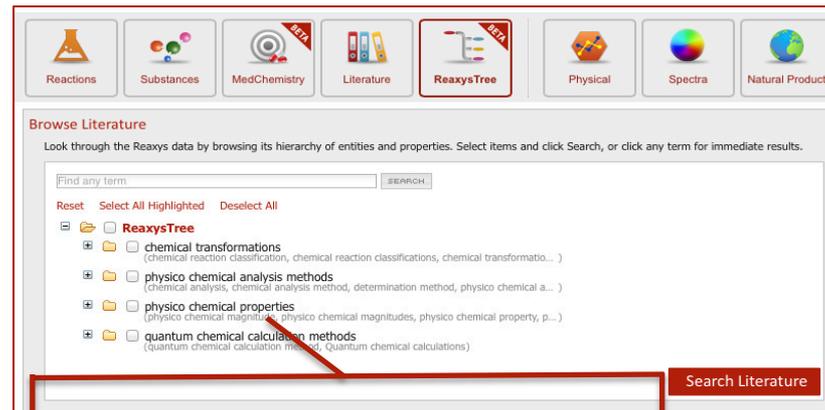
| Structure   | Structure/Compound Data   | N° of preparations<br>All Preps   All Reactions   | Available Data  | Target                       | N° of ref. |
|---|---|---|---|------------------------------|------------|
| <br><a href="#">Synthesize</a>   <a href="#">Hide Details</a>                      | <b>Chemical Name:</b><br>benzophenone<br><b>Reaxys Registry Number:</b> 1238185<br><b>CAS Registry Number:</b> 119-61-9<br><b>Type of Substance:</b> isocyclic<br><b>Molecular Formula:</b> C <sub>13</sub> H <sub>10</sub> O<br><b>Linear Structure Formula:</b> (C <sub>6</sub> H <sub>5</sub> )CO(C <sub>6</sub> H <sub>5</sub> )<br><b>Molecular Weight:</b> 182.222<br><b>InChI Key:</b> RWCCWEUUXYIKHB-UHFFFAOYSA-N | 2799 prep<br>out of<br>12464 reactions.   | <a href="#">Hit Data (1)</a><br><a href="#">Bioactivity</a><br><a href="#">Identification</a><br><a href="#">Physical Data (1219)</a><br><a href="#">Spectra (682)</a><br><a href="#">Ecological Data (27)</a><br><a href="#">Use/Application (93)</a><br><a href="#">Quantum Chemical Data (1)</a> | <a href="#">Show Targets</a> | 10753      |
| <b>Chemical Names and Synonyms</b><br>benzophenone, carbonyl-bis-(phenylene), Benzophenone, o-oxodiphenylmethane, bis-(phenyl)-ketone, diphenylmethanone, o-oxoditane |   |   |   |                              |            |
| <b>Hit Data</b><br><b>Phosphorescence Spectroscopy ( 1 Hits out of 101 view all )</b>   |   |   |   |                              |            |
| <b>Description</b>  | <b>Temperature</b>  | <b>Reference</b>  |   |                              |            |
| <a href="#">Phosphorescence quantum yield</a>   | -196.16 °C  | <b>Chen, Shun-Chi; Fang, Tai-Shan</b><br>Chemical Physics Letters, <b>2007</b> , vol. 450, # 1-3 p. 65 - 70<br><a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a> <a href="#">Show Details</a> |   |                              |            |

# 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...)



ReaxysTree

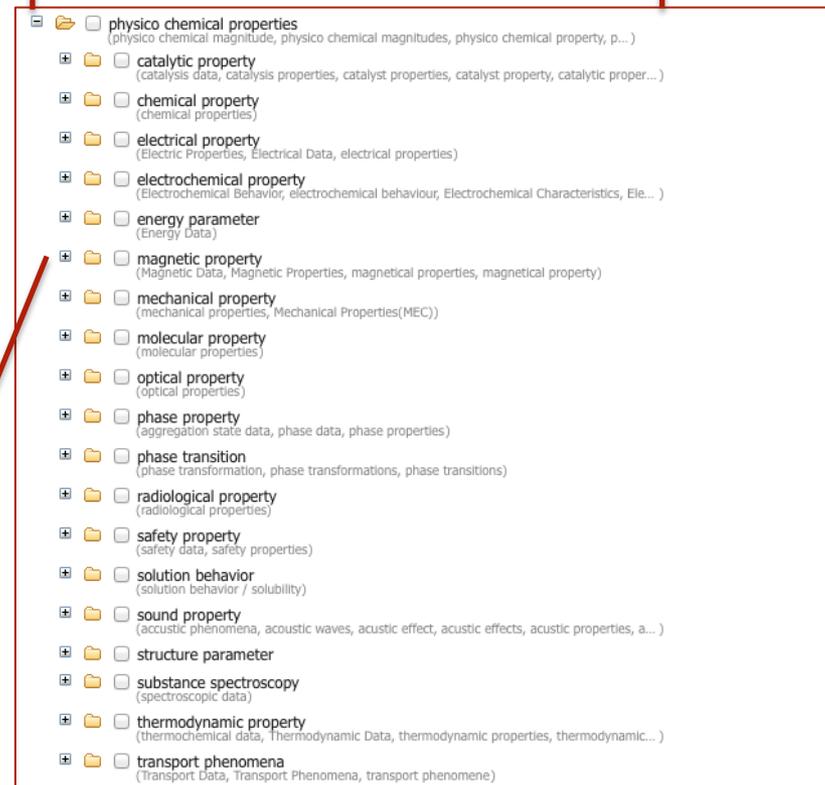
Browse Literature

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 (chemical reaction classification, chemical reaction classifications, chemical transformatio...)
  - physico chemical analysis methods (chemical analysis, chemical analysis method, determination method, physico chemical a...)
  - physico chemical properties (physico chemical magnitudes, physico chemical magnitudes, physico chemical property, p...)
  - quantum chemical calculation methods (quantum chemical calculation method, Quantum chemical calculations)



- physico chemical properties (physico chemical magnitude, physico chemical magnitudes, physico chemical property, p...)
  - catalytic property (catalysis data, catalysis properties, catalyst properties, catalyst property, catalytic proper...)
  - chemical property (chemical properties)
  - electrical property (Electric Properties, Electrical Data, electrical properties)
  - electrochemical property (Electrochemical Behavior, electrochemical behaviour, Electrochemical Characteristics, Ele...)
  - energy parameter (Energy Data)
  - magnetic property (Magnetic Data, Magnetic Properties, magnetical properties, magnetical property)
  - mechanical property (mechanical properties, Mechanical Properties(MEC))
  - molecular property (molecular properties)
  - optical property (optical properties)
  - phase property (aggregation state data, phase data, phase properties)
  - phase transition (phase transformation, phase transformations, phase transitions)
  - radiological property (radiological properties)
  - safety property (safety data, safety properties)
  - solution behavior (solution behavior / solubility)
  - sound property (acoustic phenomena, acoustic waves, acoustic effect, acoustic effects, acoustic properties, a...)
  - structure parameter
  - substance spectroscopy (spectroscopic data)
  - thermodynamic property (thermochemical data, Thermodynamic Data, thermodynamic properties, thermodynamic...)
  - transport phenomena (Transport Data, Transport Phenomena, transport phenomene)

But where is  
"phosphorescence"?

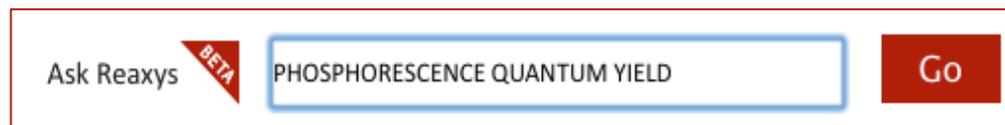




# FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

## 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



|   |           |      |  |   |
|---|-----------|------|--|---|
| <a href="#">Phosphorescence quantum yield determination with time-gated fluorimeter and Tb(III)-acetylacetonate as luminescence reference</a> | Penzkofer | 2013 | Chemical Physics, <b>2013</b> , vol. 415, p. 173 - 178<br><a href="#">Full Text</a> <a href="#">View citing articles</a> | 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 ( $\text{Tb}(\text{acac})_3$ ) was studied (determination of luminescence quantum yield and luminescence lifetime). The luminescence quantum yield of  $\text{Tb}(\text{acac})_3$  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)

|   |                          |      |   |   |
|---|--------------------------|------|---|---|
| <a href="#">Room temperature phosphorescence lifetime and quantum yield of erythrosine B and rose bengal in aerobic alkaline aqueous solution</a> | Penzkofer; Simmel; Riedl | 2012 | Journal of Luminescence, <b>2012</b> , vol. 132, # 4 p. 1055 - 1062<br><a href="#">Full Text</a> <a href="#">View citing articles</a> | 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 M $\Omega$  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  $\tau_p = 1.92 \pm 0.1 \mu\text{s}$  ( $\phi_p = (1.5 \pm 0.3) \times 10^{-5}$ ) and  $2.40 \pm 0.1 \mu\text{s}$  ( $(5.7 \pm 0.9) \times 10^{-5}$ ), respectively. The results are discussed in terms of triplet state deactivation by dissolved molecular oxygen.

#### Keywords:

**Author:** Aerobic phosphorescence behavior; Erythrosine B; e quenching phosphorescence quenching; Phosphorescence lifetime; Phosphorescence quantum yield; Rose bengal

**Compindex 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

**Compindex 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

**Compindex 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  PHOSPHORESCENCE QUANTUM YIELD

Show AND Buttons

Add to Query:

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

Limit to Exclude Output Print Zoom in Zoom out Hide 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, Hotaka; Ikawa, Shigeru; Inui, Yuji; Maeda, Takeshi; Nakazumi, Hiroyuki; Tsujimoto, Hidetaka; Yagi, Shigeyuki; Sakurai, Yoshiaki | 2010 | Journal of Organometallic Chemistry, <b>2010</b> , vol. 695, # 17 p. 1972 - 1978<br><a href="#">Full Text</a> <a href="#">View citing articles</a> | 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-(dibenzo[b,d]furan-4-yl)isoquinolinato-N,C<sup>3</sup> (dbfiq) cyclometalating ligand. When 1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionate (bdbp) is employed as an ancillary ligand, Ir(dbfiq)<sub>2</sub>(bdbp) 1 exhibits red photoluminescence (PL) at 640 nm with a quantum yield (Φ<sub>PL</sub>) of 0.61 (in toluene, 298 K). Replacement of bdbp to dipivaloylmethanate (dpm) and acetylacetonate (acac) (Ir(dbfiq)<sub>2</sub>(dpm) 2 and Ir(dbfiq)<sub>2</sub>(acac) 3, respectively) does not affect the PL spectrum, but reduces Φ<sub>PL</sub> 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<sub>PL</sub> = 0.17) than 2 and 3 (Φ<sub>PL</sub> = 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)/PVCz:1-PBD (100 nm)/CsF (1 nm)/Al (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 PVCz-based emitting layer, the PLED shows maximum luminance of 7270 cd m<sup>-2</sup> at 16.5 V, power efficiency of 1.4 lm W<sup>-1</sup> at 7.5 V, and external quantum efficiency of 6.4 percent 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 butoxy groups introduced to the bdbp 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-(dibenzo[b,d]furan-4-yl)isoquinolinato-N,C<sup>3</sup>]iridium(III) [1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionate-O,O] 1 was developed. It exhibits red photoluminescence with Φ<sub>PL</sub> 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  
Compendex Free Language: Acetylacetonates; Ancillary ligands; 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  
Compendex Descriptor: Diodes; Doping (additives); 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  
Compendex Mainhead: Iridium compounds  
Reaxys Terms: 1,3-bis(3,4-dibutoxyphenyl)propane-1,3-dionate; PLED; acac; acetylacetonate; bis[1-(dibenzo[b,d]furan-4-yl)isoquinolinato-N,C<sup>3</sup>]iridium; dipivaloylmethanate; 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 R101** gives just samples of the techniques that may be used; discover other techniques yourself!

# SUPPLEMENTARY SLIDES

# FURTHER PRESENTATIONS IN THIS SERIES

## REAXYS R101

### A QUICK GUIDE

An overview of the functions of Reaxys 2014

## REAXYS R101

### TIPS FOR LITERATURE SEARCHING

A quick guide to searching literature

## REAXYS R101

### BASIC SUBSTANCE QUERIES

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

## REAXYS R101

### BASIC REACTION QUERIES

A quick guide to searching for chemical reactions

## REAXYS R101

### SEARCHING PROPERTIES

A quick guide to searching for properties

## REAXYS R201

### ADVANCED STRUCTURE QUERIES

Searching by substructure

## REAXYS R201

### ADVANCED NAME AND FORMULA SEARCHING

Searching for Substances by Names and Formulas

## REAXYS R201

### ADVANCED REACTION QUERIES

Additional ways to search for reactions

# EXAMPLES OF INFORMATION IN PROPERTY FIELDS

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