NOVEMBER 2014

REAXYS105

SEARCHING PROPERTIES

REAXYS®
HOW YOU THINK HOW YOU WORK

NOTES ON REAXYS R105

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**

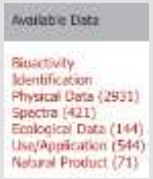
CONTENTS

REAXYS®
HOW YOU THINK HOW YOU WORK

DISPLAY OF PROPERTY INFORMATION

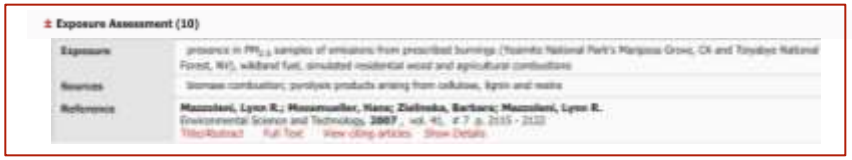
BENZOIC ACID

- 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



- 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 substa exists hat 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



REAXYS®
HOW YOU THINK HOW YOU WORK

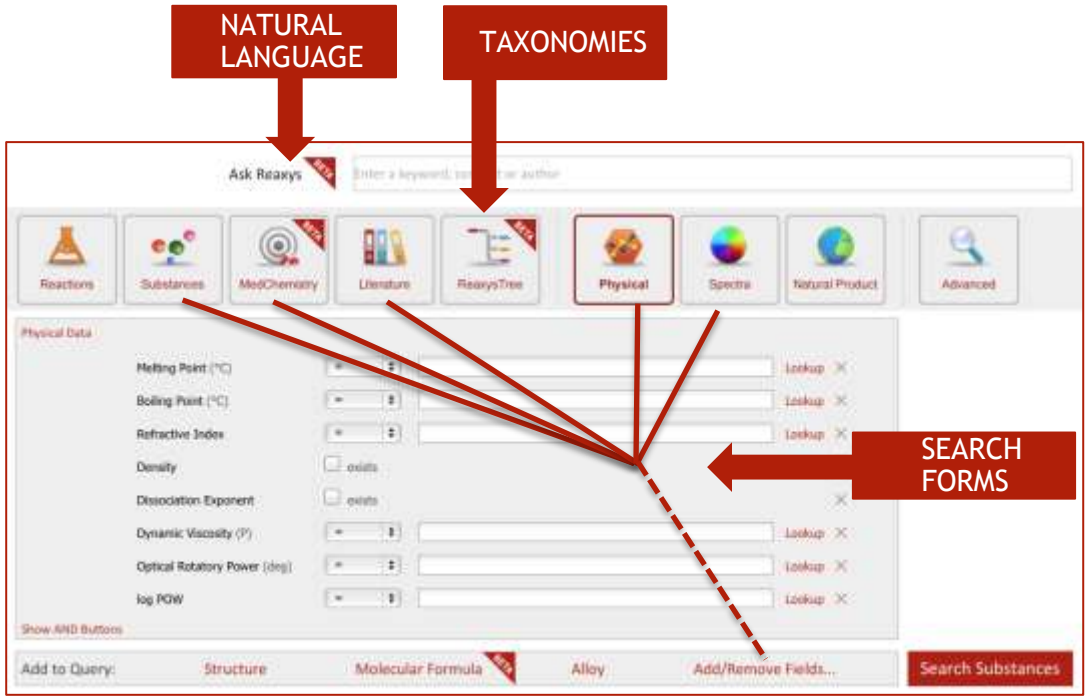
SEARCHING FOR PROPERTY INFORMATION IN REAXYS

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



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

Substances | Ask Reaxys BETA | Structure | Molecular Formula BETA | Alloy

and

Add/Remove Fields... (i.e., in forms that search substance identification fields)

REAXYS®
HOW YOU THINK HOW YOU WORK

CONTENTS

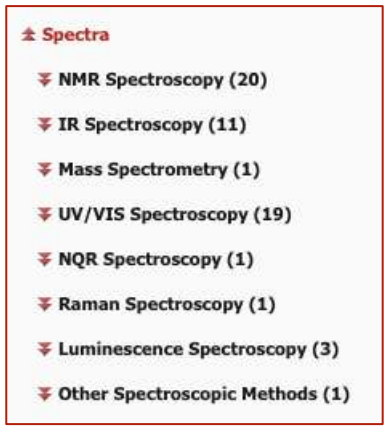
REAXYS®
HOW YOU THINK HOW YOU WORK

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



FINDING PROPERTIES FOR A SINGLE SUBSTANCE

PHYSICAL PROPERTY DATA FOR CIS-PLATIN

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)
- 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*l/(cm*mol)		N,N-dimethylformamide water	Conductivity at infinite dilution		**Huq, 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*l/(cm*mol)	24 - 26 °C	DMSO	Molar conductivity	1.9 mM	**Benedetto, Luigina; Boccaleri, Enrico; Cavigiolio, Giorgio; Colangelo, Donato; Viano, Ilario; Osella, Domenico** Inorganica Chimica Acta, **2000** , vol. 305, # 1 p. 61 - 68 Title/Abstract Full Text View citing articles Show Details
0.1077 S*l/(cm*mol)	25 °C	H2O	Molar cationic conductivity	c = 1E-3 mol/l	**Burglen; Heym** Zeitschrift fur Chemie, **1984** , vol. 24, # 7 p. 264 - 265 Title/Abstract Full Text View citing articles Show Details
0.031 S*l/(cm*mol)	25 °C	DMSO	Molar cationic conductivity	c = 1E-3 mol/l	**Burglen; Heym** Zeitschrift fur Chemie, **1984** , vol. 24, # 7 p. 264 - 265 Title/Abstract Full Text View citing articles Show Details
0.0107 - 0.1526 S*l/(cm*mol)	35 °C	H2O	Molar conductivity	dln.: 2000 l/mol; depending on time;	**Chernyaev, I. I.; Yakshin, M. M.** Izv. Plat., **1940** , vol. 17, p. 29 - 54 Full Text Show Details **Gmelin Handbook:** Pt: MVol.D, 104, page 243 - 245 Full Text Show Details

REAXYS®
HOW YOU THINK HOW YOU WORK

CONTENTS

REAXYS®
HOW YOU THINK HOW YOU WORK

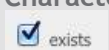
PROPERTIES FOR A GROUP OF SUBSTANCES

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**

  - 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)

REAXYS®
HOW YOU THINK HOW YOU WORK

CONTENTS

REAXYS®
HOW YOU THINK HOW YOU WORK

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**

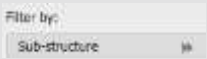
- Steps for the **Querylet** search are:
  1. Customize the **Phosphorescence Spectroscopy Querylet** (and its **Description Querylet** - we will use this soon) in your Search Form
  2. Check exists then click Search Substances
     - Reaxys displays all substances that have information in the **Phosphorescence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

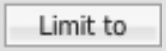
>10,000 substances have data in Phosphorescence Spectroscopy Field; the “Hit Data” Field is always shown for the Querylet searched

FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

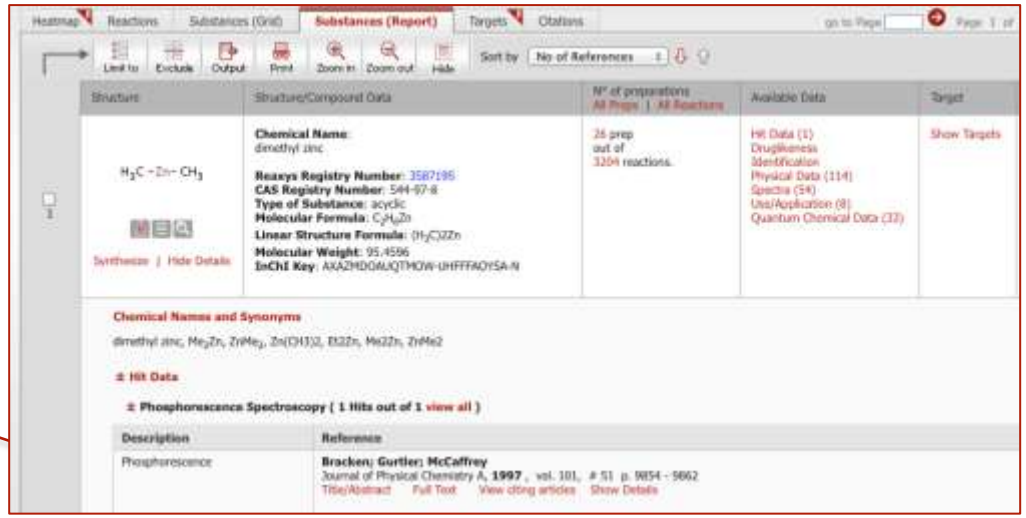
1. NARROWING SUBSTANCES THROUGH FILTER BY: SUBSTRUCTURE

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:
  1. Click 

  2. Draw the structure query (a Zn atom)
  3. Click Substructure
  4. Click 

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



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)

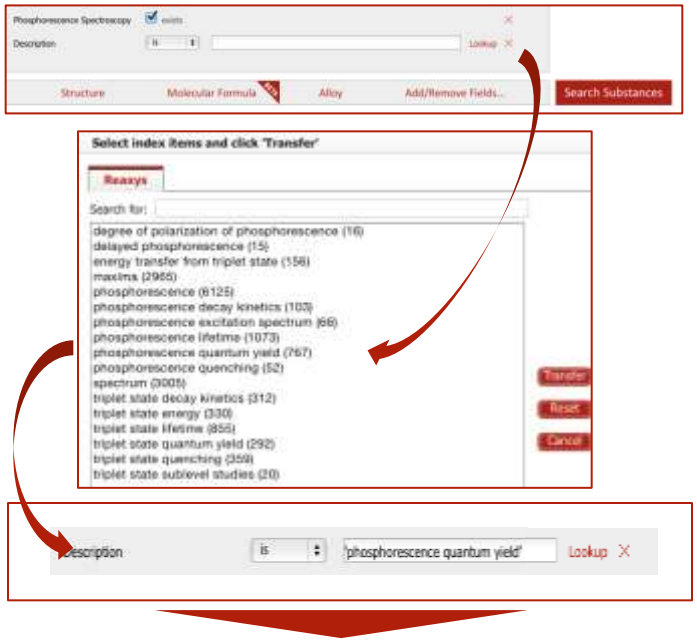
REAXYS®
HOW YOU THINK HOW YOU WORK

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!



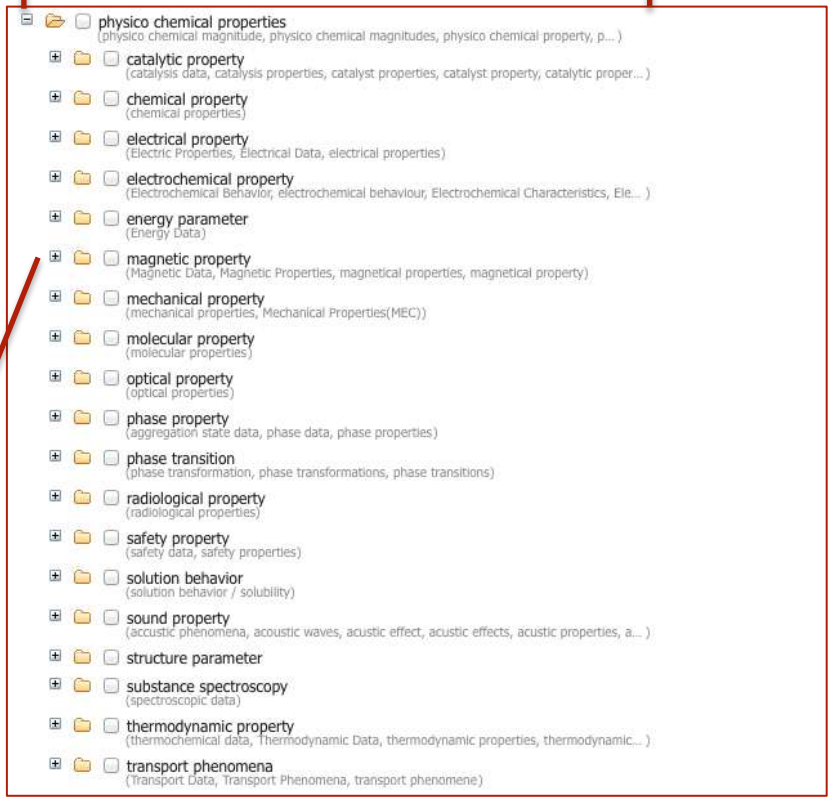
REAXYS®
HOW YOU THINK HOW YOU WORK

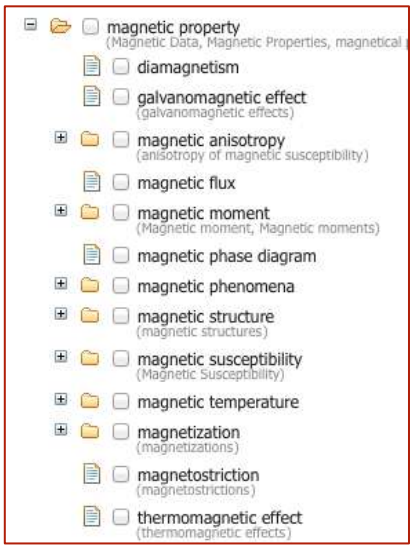
FINDING SUBSTANCES WITH SPECIFIC PROPERTIES

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…)



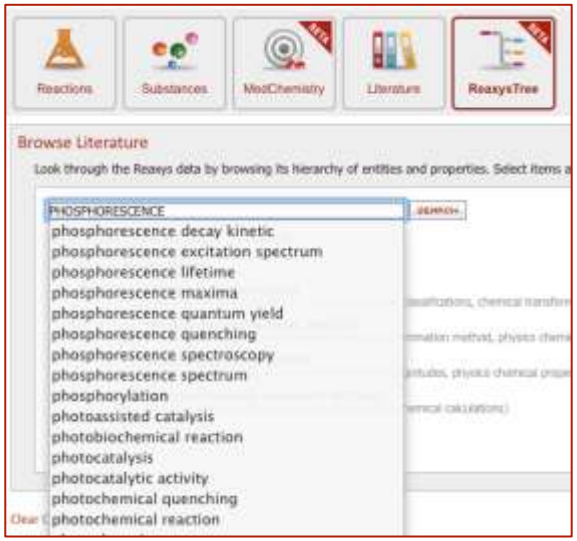


REAXYS®
HOW YOU THINK HOW YOU WORK

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



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, $[Ir(hfppq)_2(bipy)][PF_6]\cdot 0.5H_2O$ (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 $[Ir(hfppq)_2(\mu\text{-}Cl)]_2$ 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_2Cl_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_2Cl_2; KPF_6; bipy - ambient reaction temperature; density functional theory; luminiscence type; optical property; phosphorescence quantum yield

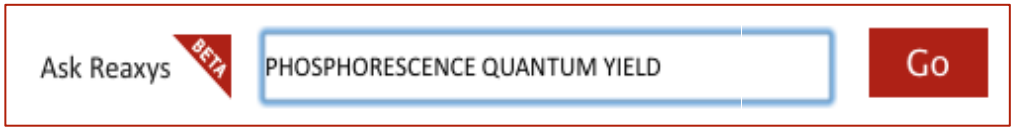
Show All Reactions (3)
Show All Substances (9)

REAXYS®
HOW YOU THINK HOW YOU WORK

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



Phosphorescence quantum yield determination with time-gated fluorimeter and Tb(III)-acetylacetonate as luminescence reference	Penzkofer	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; luminiscence 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	Penzkofer; 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 MΩ 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 τ_P=1.92±0.1 μs (ϕ_P=(1.5±0.3) ×10^{-5}) and 2.40±0.1 μs ((5.7±0.9) ×10^{-5}), respectively. The results are discussed in terms of triplet state deactivation by dissolved molecular oxygen.

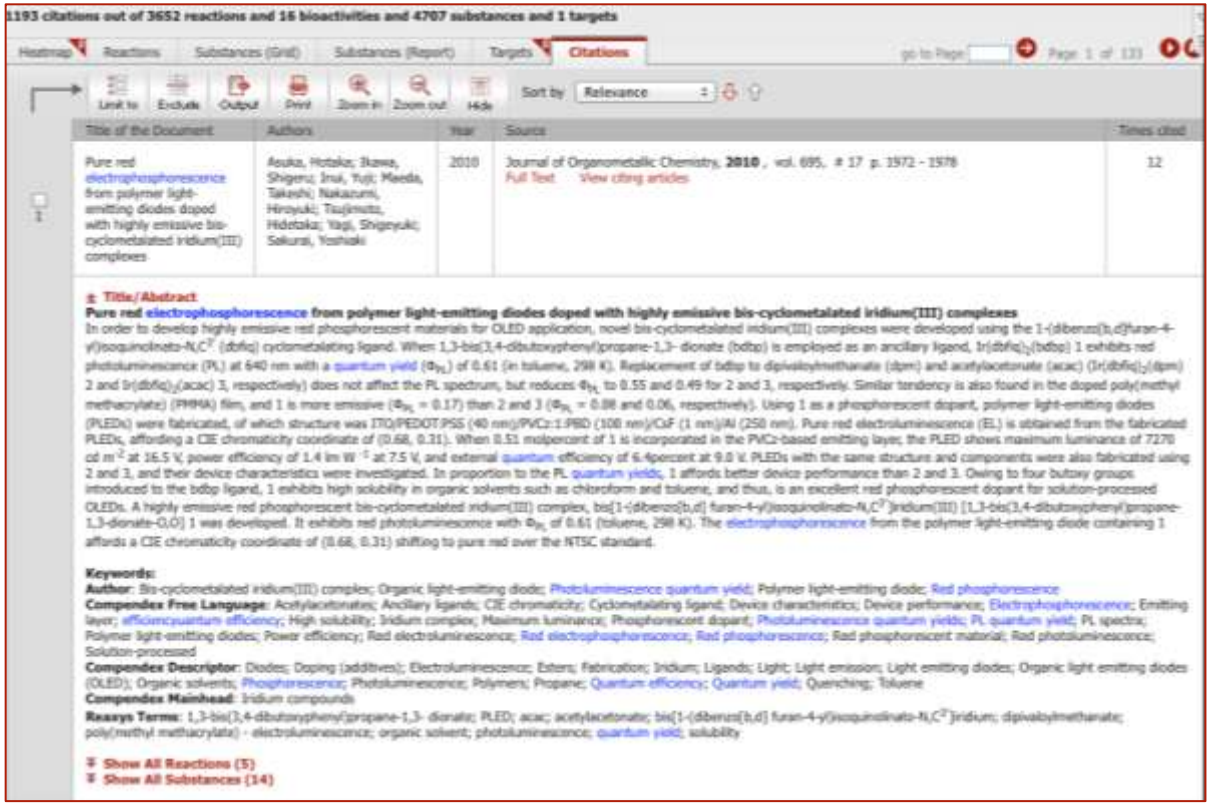
Keywords:
Author: Aerobe phosphorescence behavior; Erythrosine B; e quenchingphorescence quenching; Phosphorescence lifetime; Phosphorescence quantum yield; Rose bengal
Compendex Free Language: Aerobe phosphorescence behavior; Digital oscilloscope; Fluorescence signals; Input resistance; Nd:glass laser; Phosphorescence lifetime; m yieldantum yieldantum 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

REAXYS®
HOW YOU THINK HOW YOU WORK

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 contains
- 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



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

REAXYS R101

A QUICK GUIDE

An overview of the functions of Reaxys 2014

REAXYS R102

TIPS FOR LITERATURE SEARCHING

A quick guide to searching literature

REAXYS R103

BASIC SUBSTANCE QUERIES

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

REAXYS R104

BASIC REACTION QUERIES

A quick guide to searching for chemical reactions

REAXYS R105

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

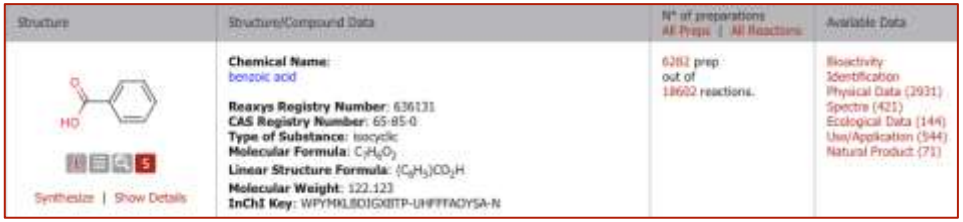
ADVANCED REACTION QUERIES

Additional ways to search for reactions

REAXYS®
HOW YOU THINK HOW YOU WORK

Back to referring Slide

EXAMPLES OF INFORMATION IN PROPERTY FIELDS



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)