

# Joint CCDC and FIZ Karlsruhe Webinar

Advancing our collaboration

27<sup>th</sup> August 2020



# Webinar overview

- An opportunity for you to learn about:
  - The Cambridge Structural Database (CSD)
  - The Inorganic Crystal Structure Database (ICSD)
  - The CCDC and FIZ Karlsruhe collaboration
- An opportunity for us to learn:
  - How you would like to see our joint services develop
  - User requirements for an advanced interface for searching all organic, metal-organic and inorganic structures

# The CCDC

International Data Repository  
Archive of crystal structure data  
High quality scientific database

Scientific Software Provider  
Search/analysis/visualisation tools  
Scientific applications

Collaborative Research Organisation  
New methodologies  
Fundamental research

Education and Outreach  
Conferences, Workshops,  
Bespoke Training, Teaching Materials

A UK registered charity

Originated in 1965

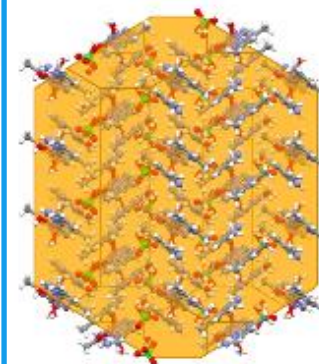
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 Facebook: ccdc.cambridge

[www.ccdc.cam.ac.uk](http://www.ccdc.cam.ac.uk)

*Dedicated to the advancement  
of chemistry and  
crystallography for the public  
benefit through providing high  
quality information services and  
software.*



CCDC

# FIZ Karlsruhe

Picture: Daniel Vieser . Architekturfotografie, Karlsruhe



One of the large non-academic information infrastructure institutions in Germany

Member of the Leibniz Association

Non-profit Institution

Main Shareholders:

German Federal Government

Federal State of Baden-Württemberg

We offer data, information and knowledge, software and services for research and innovation on open, law-compliant platforms. To this end we develop and operate both commercial and free products and services.

# Today's presenters



**Suzanna Ward**  
Head of Data  
CCDC



**Paul Raithby**  
University of  
Bath



**Matt Lightfoot**  
Editorial Team Lead  
CCDC



**Dejan Zagorac**  
Nuclear Sciences  
Vinča, Belgrade



**Stephan Rühl**  
Product Manager ICSD  
FIZ Karlsruhe

# Today's agenda

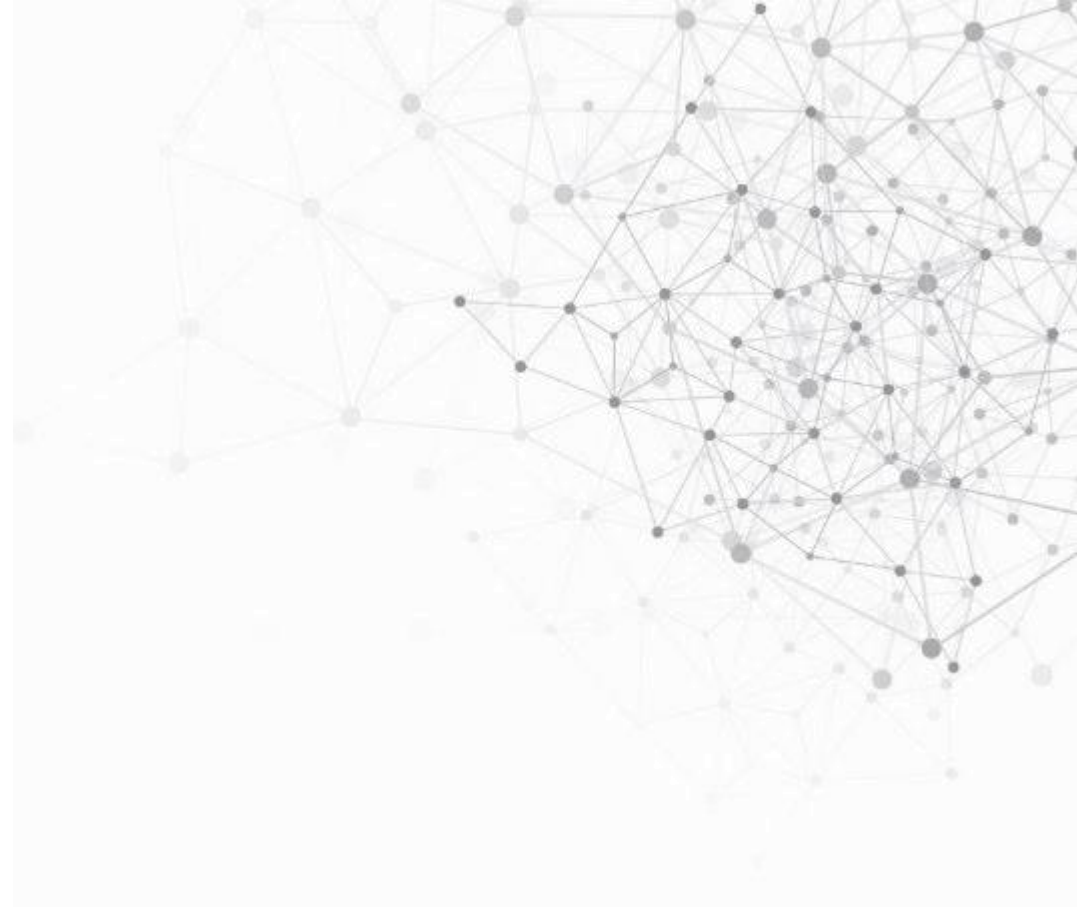
- Introduction
  - The CSD
  - The ICSD
- The CCDC and FIZ Karlsruhe collaboration
- User perspectives
  - Paul Raithby
  - Dejan Zagorac
- What's next?
- Q&A: the floor is yours



A screenshot of a GoToWebinar interface. The top part shows the 'Audio' settings window, which is currently muted. Below that, there is a 'Questions' section with a text input field containing the placeholder text '[Enter a question for staff]' and a 'Send' button. At the bottom, the interface displays 'Multi sessions different registrants', 'Webinar ID: 980-960-603', and the GoToWebinar logo.

# The CSD

Suzanna Ward



# The vision



- Established in 1965 by Olga Kennard
- She and J.D. Bernal had a vision that a collective use of data would lead to new knowledge and generate insights

J.D. Bernal and research group including Olga Kennard at Stonehenge in 1948



# The vision

## BERNAL'S VISION: FROM DATA TO INSIGHT

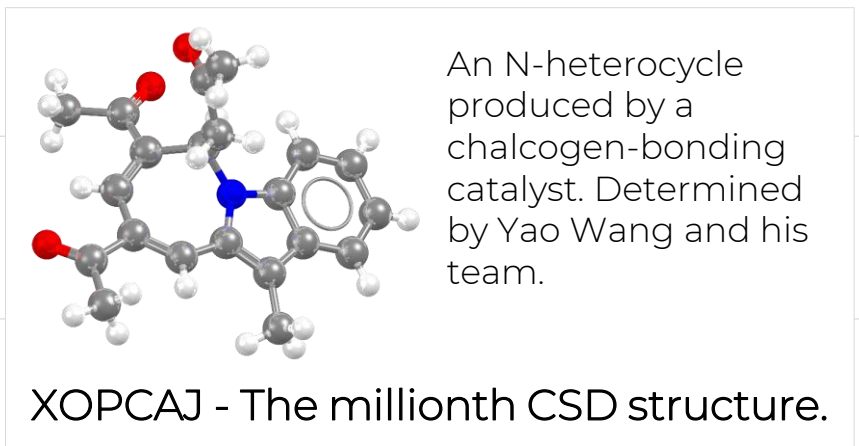
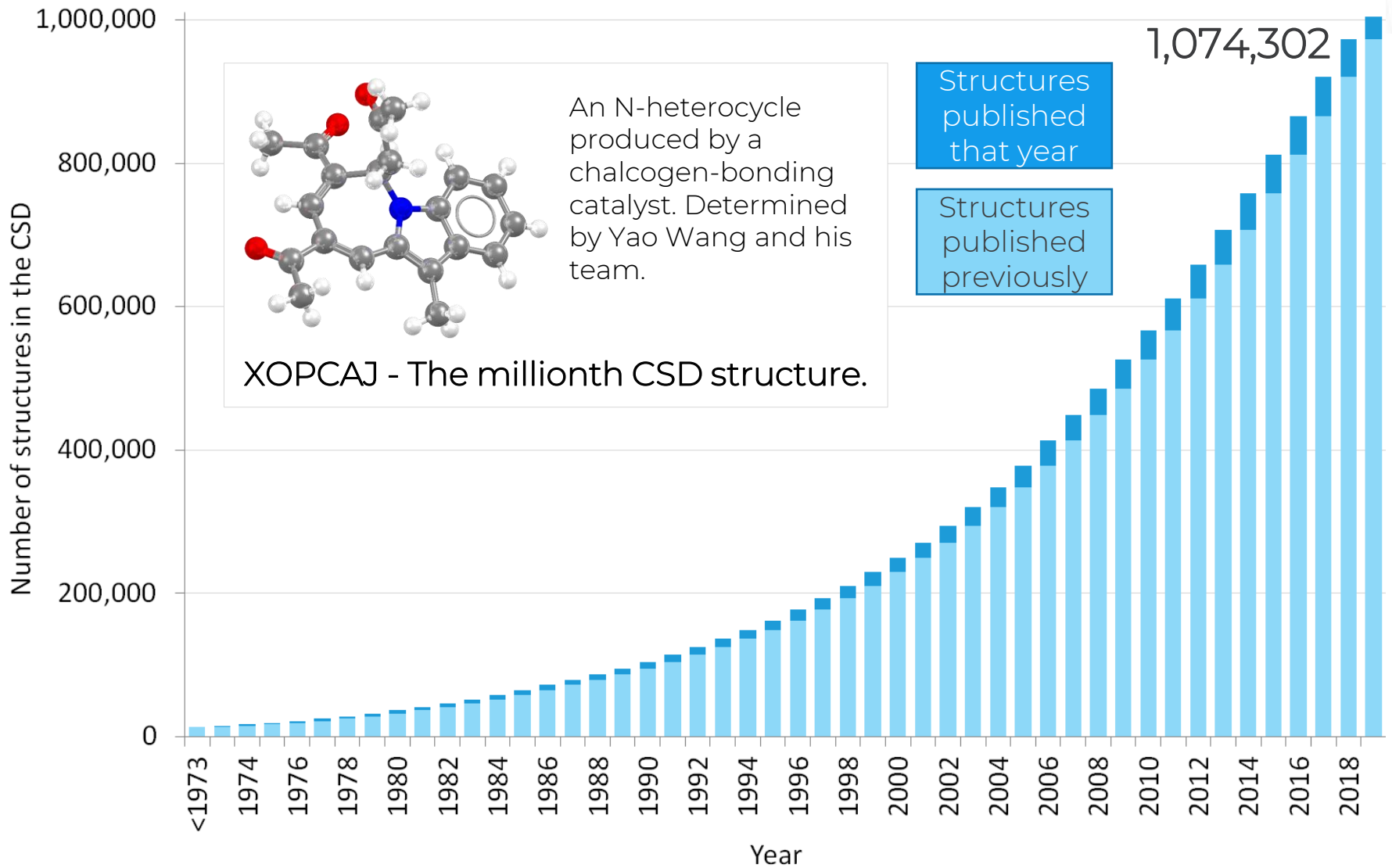
by Dr Olga Kennard OBE FRS

THE J D BERNAL LECTURE 1995  
delivered at  
BIRKBECK COLLEGE, LONDON



We clearly recognised even in those early days, that data banks have three principal functions. Firstly they must gather together existing knowledge and make it readily available to the scientific community. Secondly they can be used to reduce a large number of observations to a small set of constants and rules, and in this way transform a data base to a knowledge base. Such a knowledge base may obviate the need for further individual experiments in specific areas. Thirdly, they facilitate the comparison and collective analysis of individual results to gain insight into new or as yet unexplained phenomena. These ideas have been at the heart of the work of the Cambridge Crystallographic Data Centre and the driving force for improving methods of data collection, storage and dissemination. Most importantly they influenced development of computer programs and methodologies which are needed for the analysis and transformation of the accumulated information. (5)

# The Cambridge Structural Database (CSD)



- Every published structure
  - Inc. ASAP & early view
  - CSD Communications
  - Patents
  - University repositories
  - Thesis
- Discoverability of data and knowledge
- Sustainable for over 55 years

# Inside the CSD

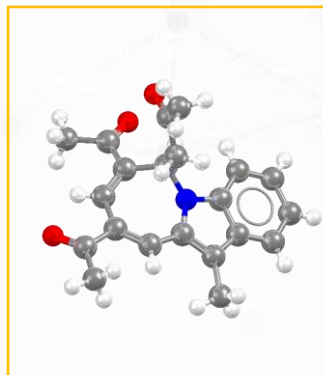
Organic  
43%

Metal-Organic  
57%

At least one transition metal,  
lanthanide, actinide or any of Al,  
Ga, In, Tl, Ge, Sn, Pb, Sb, Bi, Po

## Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



## Additional data

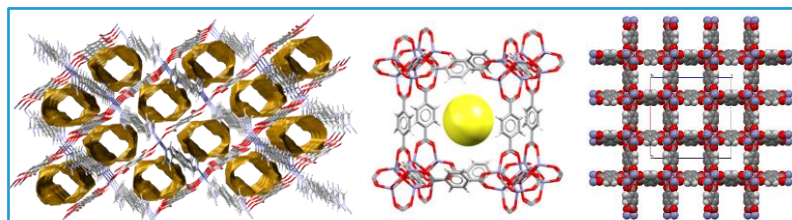
- 11,415 polymorph families
- 171,331 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,379 natural source data
- > 250,000 oxidation states

Not Polymeric  
89%

Polymeric: 11%

## Metal-Organic

- Metal Organic Frameworks
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding

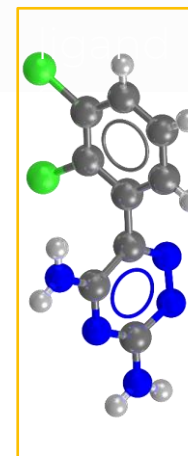


Single  
Component  
56%

Multi  
Component  
44%

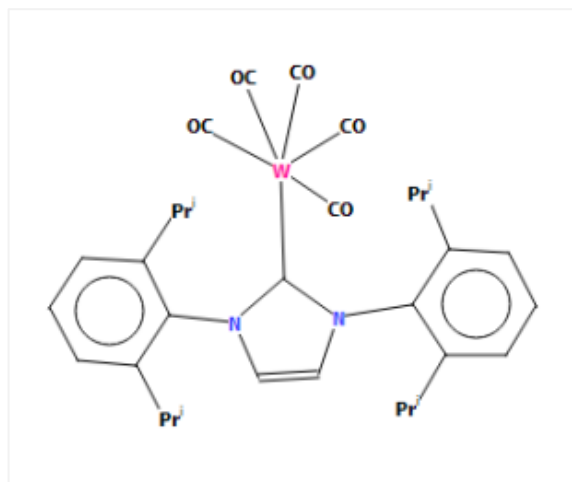
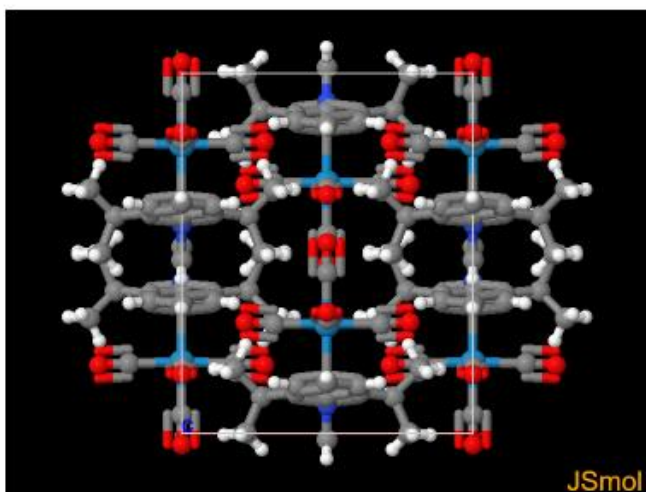
## Links/subsets

- Drugbank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticides



# The CSD

BAXQAV : (1,3-bis(2,6-diisopropylphenyl)-2,3-dihydro-1H-imidazol-2-ylidene)-(pentacarbonyl)-tungsten  
**Space Group:** C m c m (63), **Cell:** a 11.250(2)Å b 13.869(2)Å c 19.759(3)Å,  $\alpha$  90°  $\beta$  90°  $\gamma$  90°



## Crystal details

<b>Habit</b>	lensoid
<b>Colour</b>	yellow

## Associated publications

Rajendra S. Ghadwal, Dennis Rottschäfer, Diego M. Andrada, Gernot Frenking, Christian J. Schürmann, Hans-Georg Stammer, *Dalton Transactions*, 2017, 46, 7791, DOI: [10.1039/C7DT01199G](https://doi.org/10.1039/C7DT01199G)

❑ Links to over 490,000 articles in over 1,500 journals from over 200 publishers

❑ Recognised data repository



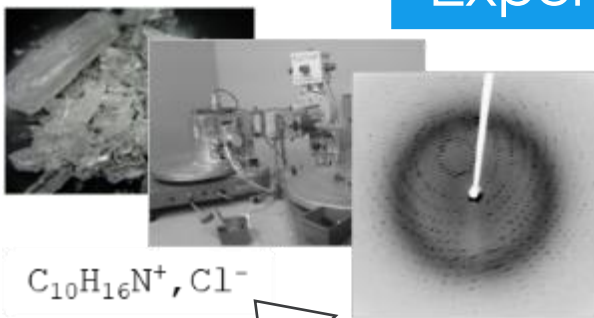
- CoreTrustSeal certification
- Clear Data Preservation Policy

❑ Datasets enriched and annotated by experts at the CCDC to enable:

- Generation of new knowledge
- Application of knowledge in digital platforms
- Support for scientific innovation across academia and industry

# From experiment to knowledge

Experiment



```

_diffn_ambient_temperature 90(2)
_diffn_radiation_type MoK $\alpha$ 
_diffn_radiation_wavelength 0.71073
_diffn_radiation_monochromator graphite
_diffn_measurement_device_type 'Bruker APEX CCD area-detector'
_diffn_measurement_method '\u03c9 and \u03c6'
_diffn_detector_area_resol_mean 512
_diffn_reflns_number 8892

loop_
_atom_site_type_symbol
_atom_site_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_occupancy
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_symmetry_multiplicity
_atom_site_disorder_assembly
_atom_site_disorder_group
Cl C11 0.23185(8) 0.78905(9) 0.55574(6) 0.02213(16) Uniq. d. 1 1 . . .
N N1 0.8031(3) 0.6811(3) 0.5363(2) 0.0172(4) Uniq. d. U 1 1 . . .
C C1 0.6996(4) 0.7867(6) 0.4367(2) 0.0224(5) Uniq. d. U 1 1 . . .
C C2 0.7510(5) 0.8922(5) 0.7089(3) 0.0256(6) Uniq. d. U 1 1 . . .
C C3 0.7409(4) 0.6944(4) 0.6644(3) 0.0187(5) Uniq. d. U 1 1 . . .
C C4 0.8700(4) 0.5637(4) 0.7481(3) 0.0236(6) Uniq. d. U 1 1 . . .

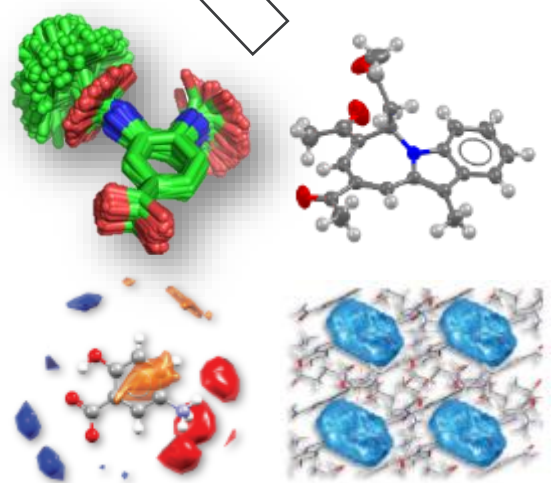
```

**Ritonavir: An Extraordinary Example of Conformational Polymorphism**

Authors: John Kester, Stephen Spornik, Wojciech Morys, John Quick, Walter Dalko, William Porter, John Merson

Abstract

**Purpose.** In the summer of 1998, Novartis semi-solid capsules supplied were threatened as a result of a new much less soluble crystal form of ritonavir. This report provides characterization of the two polymorphs and the structures and hydrogen bonding network for each form.



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Knowledge

Database	Database Number
# 103493	781070
# 103494	781071
# 103495	781072
# 103496	781073

Abstract of Entry

Database Number: 781070

Date Cleared: 2008-05-08

Keywords: Ritonavir; Hydrogen Bonding; Polymorphism



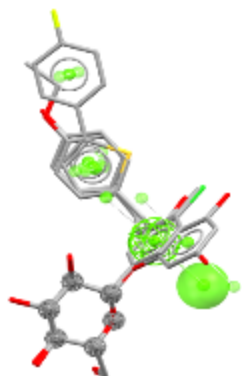
# The CSD software

Software enabling research across the breadth of structural science

## CSD-Enterprise

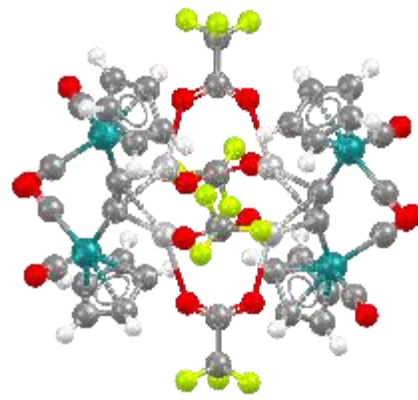
All CCDC application software (available to all Academics)

### CSD-Discovery



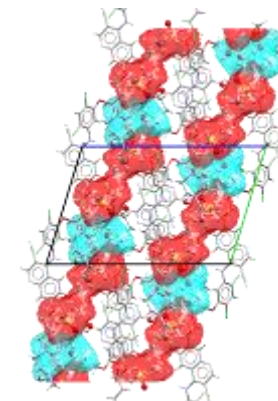
*To discover new molecules with pharmaceutical applications*

### CSD-System



*To search, visualise, analyse and communicate structural data*

### CSD-Materials



*To understand and predict solid form stability and properties*

The Cambridge Structural Database

# Recent developments and activities

- **Data**
  - New data releases
  - New data links and subsets
- **Software**
  - New CSD KNIME nodes
  - CSD Pipeline Pilot Component Collection
  - Aromatics Analyser in CSD-Materials
  - Descriptors Module in CSD Python API
- **Research**
  - Targeted classification of metal-organic frameworks
- **Education, Outreach and Events**
  - CCDC Home Learning
  - New workshops and How To videos
  - Global UGM – October
  - Crystal Conversations
- **Collaborations and initiatives**
  - ICDD collaboration
  - BioChemGRAPH collaboration between PDBe, ChEMBL and CCDC
  - New Hindawi workflow
  - CSP Consortium and CCDC Blind test



**FIZ Karlsruhe**

Leibniz Institute for Information Infrastructure

**ADVANCING SCIENCE**



# ICSD

## An Overview of Content and Recent Developments

August 28, 2020



# ICSD has a history of 40 years

- 1977 initiated by Prof. Bergerhoff, University of Bonn, Germany
- Crystal Structure Depot since 1980 (old paper version and electronic CIF archive)
- 1985 – 1989 joint venture University of Bonn and FIZ Karlsruhe
- 1989 – 1998 joint venture of the Gmelin Institute and FIZ Karlsruhe
- 1997 – 2017 joint venture FIZ Karlsruhe and NIST (National Institute of Standards and Technology)
- Since 2016 cooperation with Technicum Scientific Publishing in Stuttgart and Vinca Institute in Belgrad
- Since 2016 cooperation between FIZ Karlsruhe and CCDC (Cambridge Crystallographic Data Centre)



# ICSD contains records of inorganic crystal structures published since 1913

All crystal structures include atomic coordinates

Old definition:

no C-C- and C-H-bonds



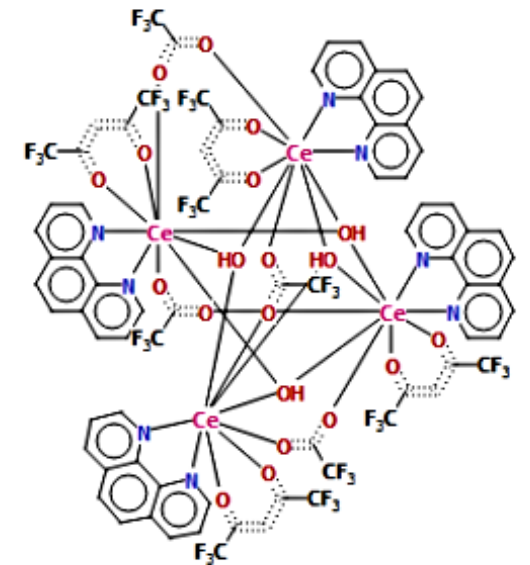
inorganic compounds, minerals, elements, metals and alloys

New definition:

all structures according to the old definition

plus organometallic structures with material properties relevant for inorganic applications and at least 3 metals/semi-metals

plus similar compounds with partly organic ligands



# ICSD contains records of inorganic crystal structures published since 1913

Added content:

- Wyckoff sequence, Pearson symbol → Structure Types
- standardized structures
- reduced cells
- mineral name/group
- special information for theoretical structures:
  - calculation methods
  - cutoff energy
  - K-point mesh

> 210,000 records

> 1,500  
journals

> 30,000 records  
(derived  
coordinates)

> 9,000  
structure types

> 80,000 authors

> 80,000 articles

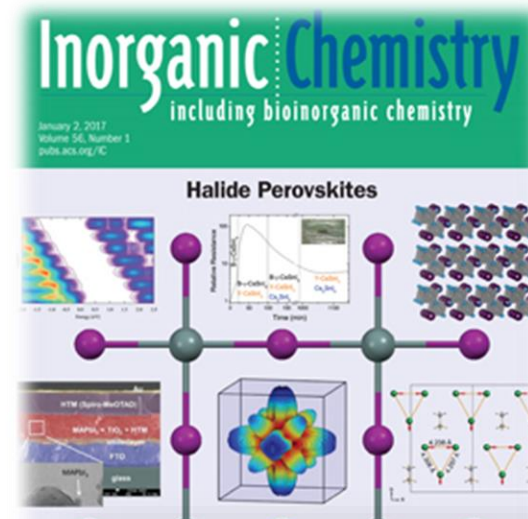
# Theoretical structures in ICSD

## Typical applications

- Prediction of new compounds
- Prediction of specific material properties
- Comparison of experimental and theoretical structures
- Optimization of experimental structures

## Main problem

- Large number of potential theoretical structures



Modification, Space group and Wyckoff position	Cell parameters (Å) and fractional coordinates	
	ICSD model	SPuDS model
CaMnO <sub>3</sub> -(1) <i>Pnma</i> (62) Ca 4c Mn 4b O1 4c O2 8d	(Bozin <i>et al.</i> , 2008) $a = 5.2790(2), b = 7.4438(3), c = 5.2583(2)$ 0.0344(1) 1/4 0.9931(1) 1/2 0 0 0.4877(1) 1/4 0.0671(1) 0.2873(1) 0.0346(1) 0.7109(1)	$a = 5.36, b = 7.54, c = 5.31$ 0.0123 1/4 0.0030 1/2 0 0 0.4955 1/4 -0.0479 0.2735 0.0240 0.7260
CaMnO <sub>3</sub> -(2) <i>R<math>\bar{3}</math>c</i> (167) Ca 6a Mn 6b O 18e	(Yanchevskii <i>et al.</i> , 2008) $a = 5.474(3), c = 13.376(7)$ 0 0 1/4 0 0 0 0.450(7) 0 1/4	$a = 5.31, c = 13.18$ 0 0 1/4 0 0 0 0.4529 0 1/4
CaMnO <sub>3</sub> -(3) <i>Imma</i> (74) Ca 4e Mn 4b	(Damay <i>et al.</i> , 1998) $a = 5.4312(2), b = 7.6250(3), c = 5.4729(2)$ 0 1/4 0.0011(3)	$a = 5.38, b = 7.51, c = 5.31$ 0 1/4 0.0030 0 0 1/2

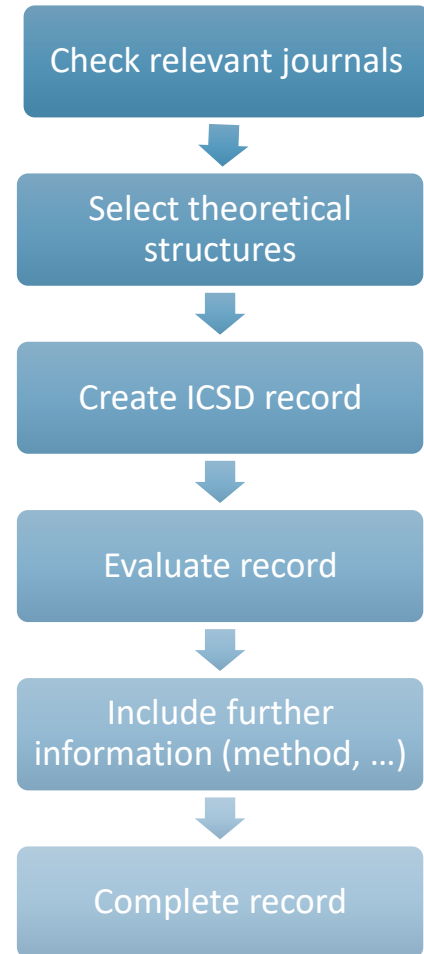
# Theoretical structures in ICSD

## Selection criteria

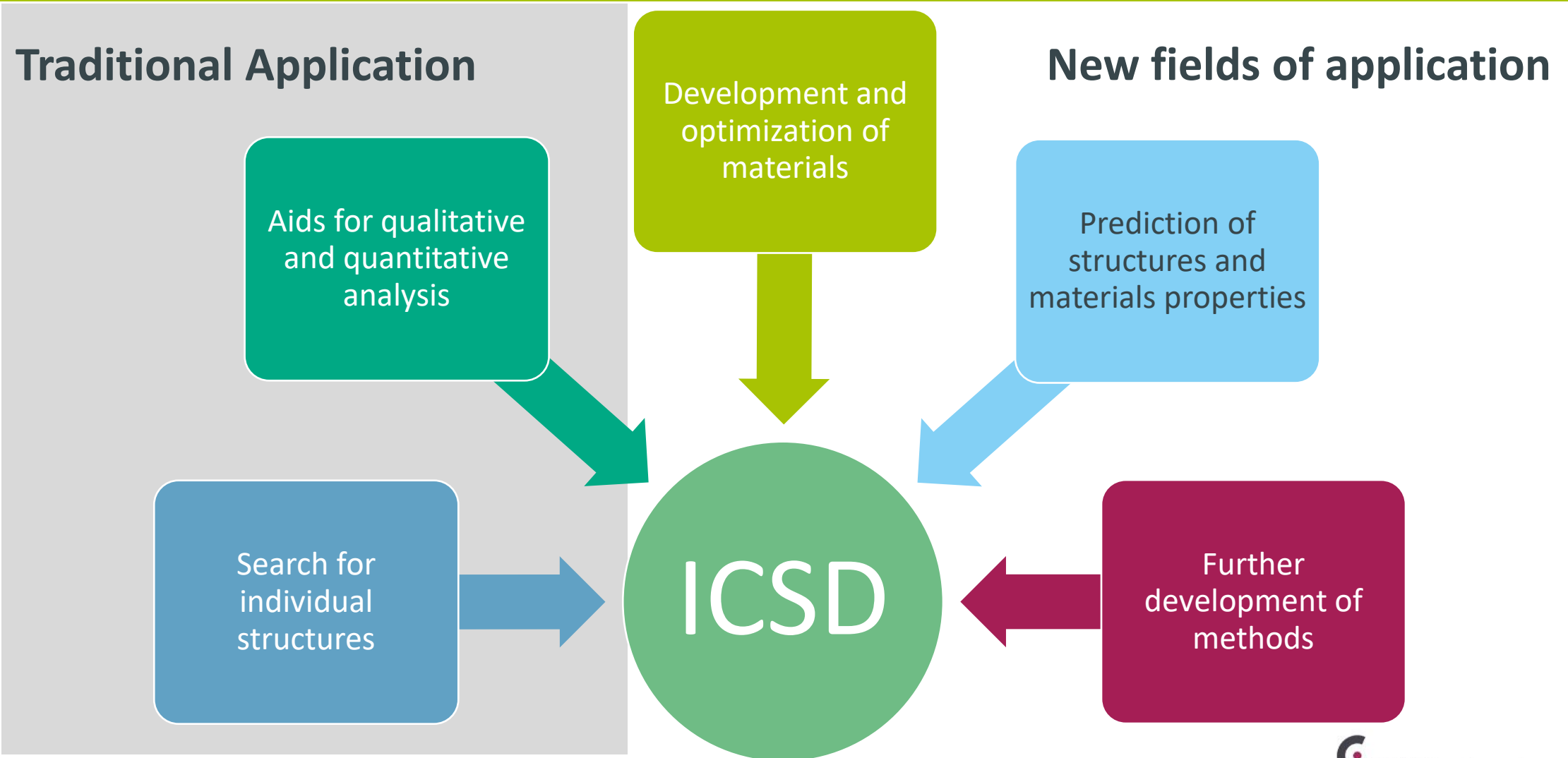
- Publication in a peer-review journal
- calculated minimum of total energy ( $E_{\text{tot}}$ )
- If more than one method is used (comparison), the one with results closest to experimental results is chosen

## Important information for theoretical structures

- Calculation method used and comparison with experimental structure, if applicable
- Keywords for material properties



# Typical applications of ICSD in crystallography and material science



# Recent developments

## Expert Search

Search Term	Description	Input Type
AUTHORS	BIBLIOGRAPHY: Authors name for the main (first) reference	Text
ARTICLE	BIBLIOGRAPHY: Title of article for the main (first) reference	Text
PUBLICATIONYEAR	BIBLIOGRAPHY: Year of publication of an article in the reference	Numerical, integer
PAGEFIRST	BIBLIOGRAPHY: First page number of an article in the reference	Numerical, integer
JOURNAL	BIBLIOGRAPHY: Title of journal for the reference	Text
VOLUME	BIBLIOGRAPHY: Volume of the journal in the reference	Numerical, integer
ABSTRACT	BIBLIOGRAPHY: Abstract for the main (first) reference	Text
KEYWORDS	BIBLIOGRAPHY: Keywords for the main (first) reference	Text
CELLVOLUME	CELL SEARCH: Cell volume	Numerical, floating point
CALCENSITY	CELL SEARCH: Calculated density	Numerical, floating point
CELLPARAMETERS	CELL SEARCH: Cell length a, b, c and angles alpha, beta, gamma separated by semicolon, i.e. 'a b c alpha beta gamma', if any value	Numerical, floating point
SEARCHCELLDATA	CELL SEARCH: Restriction of Cellparameters	experimental, deduced, standard
STRUCTUREFORMULA	CHEMISTRY SEARCH: Search for typical chemical groups	Text
CHEMICALNAME	CHEMISTRY SEARCH: Search for (parts of) the chemical name	Text
MINERALNAME	CHEMISTRY SEARCH: Search for the mineral name	Text
MINERALGROUP	CHEMISTRY SEARCH: Search for the mineral group	Text
ZVALUE	CHEMISTRY SEARCH: Number of formula units per unit cell	Integer
ANIONFORMULA	CHEMISTRY SEARCH: Search for the Anion formula	Text
CATIONFORMULA	CHEMISTRY SEARCH: Search for the Cation formula	Text

## ICSD Rest API

**authentication** methods to perform login or logout

- POST /auth/login Perform an authentication.
- GET /auth/ip Perform an IP-based authentication.
- GET /auth/logout Invalidates an authenticated session.

**search** search methods on ICSD database

- GET /search/simple Performs a simple search on any attributes of icad.
- POST /search/simple Performs a simple search on any attributes of icad.
- GET /search/expert Performs an 'expert' search for all icad attributes using search expressions.
- POST /search/expert Performs an 'expert' search for all icad attributes using search expressions.

**CIF** methods to get CIF content from database identifiers

- GET /cif/{idnum} Get crystallographic data in CIF format
- GET /cif/multiple Get crystallographic data in CIF format

**data** methods for data exports

- GET /csv Get crystallographic data in csv format
- GET /longview Get crystallographic data in long format

Set up complex search queries using:

- boolean operators (AND, OR, NOT)
- brackets

Use all ICSD functionality, including Expert Search to get specific data or programmatically download the whole database for data mining projects

## Our vision of ICSD

We want to support the community by further developing ICSD into an indispensable tool for materials science.

To achieve this, we will

- Expand the scope of the database and include as much „inorganic“ data as possible
- Offer scientists working at the interface between inorganic and organic chemistry an easier and faster way to find relevant structures
- Optimize access to ICSD data for data mining applications



# Thank you!

## Contact

**Dr. Stephan Rühl**

Product Manager ICSD

Content & Services

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Leibniz-Institut für Informationsinfrastruktur GmbH  
[www.fiz-karlsruhe.de](http://www.fiz-karlsruhe.de)



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 **FIZ Karlsruhe**  
Leibniz Institute for Information Infrastructure



*Leibniz*  
Leibniz  
Association

# The CCDC and FIZ Karlsruhe collaboration

Suzanna Ward and Matt Lightfoot



# Joint services - Access

CCDC FIZ Karlsruhe Leibniz Institute for Information Infrastructure Access Structures [Sign In](#)

Simple Search Structure Search Unit Cell Search Formula Search

Entry search

Welcome to Access Structures, the CCDC's and FIZ Karlsruhe's free service to view and retrieve structures. Please use one or more of the boxes to find entries. If you enter details in more than one field the search will try to find records containing all the terms entered. [More information and search help](#)

More advanced search functionality and additional curated data for the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD) is available through the CSD-System and ICSD, respectively. [Click here for more information.](#)

Identifier(s)	CCDC Number(s), CSD Number(s), CSD Refcode(s) or ICSD Number(s) ?	
Compound name	e.g. sulfadiazine ?	
DOI	A single publication DOI, CSD DOI or ICSD DOI ?	
Authors	e.g. F.H.Allen ?	
Journal	e.g. Journal of the American Chemical Society ?	
Publication details	Year ?	Volume ?
Database to search	<input checked="" type="radio"/> Entire published collection <input type="radio"/> CSD <input type="radio"/> ICSD <input type="radio"/> Teaching subs	

[Search](#)



**Database to search**

Entire published collection  CSD  ICSD

- Free to access
- Ability to search across the CSD and the ICSD

Simple Search   Structure Search   Unit Cell Search   Formula Search

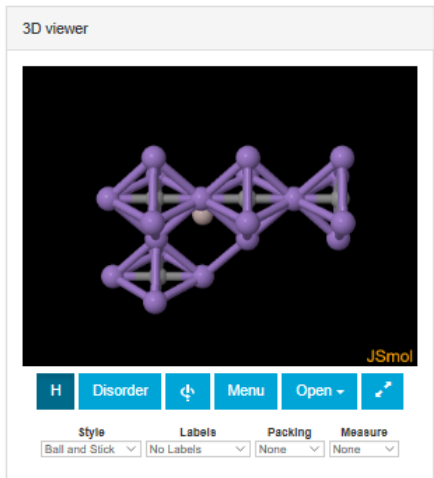
Your query was: Identifier(s): AHUDOZ AHUDIT, AHOQIA, 243366, 254369, 254371 and the search returned 10 records.

Back to Search List   Modify Search   New Search

Results	
<input checked="" type="checkbox"/> Database Identifier	Deposition Number
<input checked="" type="checkbox"/> ICSD 243366	1577704
<input checked="" type="checkbox"/> ICSD 254369	1565100
<input checked="" type="checkbox"/> ICSD 254371	1565103
<input checked="" type="checkbox"/> AHOQIA	1981609
<input checked="" type="checkbox"/> AHUDIT	1946311
<input checked="" type="checkbox"/> AHUDOZ	1946312
<input checked="" type="checkbox"/> BINJIS	243366
<input checked="" type="checkbox"/> FEDFEA	254369
<input checked="" type="checkbox"/> FEDFOK	254371
<input checked="" type="checkbox"/> ICSD 243366	1791301

Download -

ICSD 243366 : ICSD Structure : (C Mn)<sub>n</sub>0.3(AI)   
 Space Group: P m 3 m (221), Cell: a 3.875(2)Å b 3.875(2)Å c 3.875(2)Å, α 90° β 90° γ 90°



Chemical diagram

More information  
available from the ICSD

<https://icsd.products.fiz-karlsruhe.de/>

View group symbols key

Additional details	
Deposition Number	1577704
Data Citation	Hannes Dierkes, Jan van Leusen, Dimitri Bogdanovski, Richard Dronskowski CCDC 1577704: Experimental Crystal Structure Determination, 2017, DOI: 10.5517/ccdc.csd.cc1pyqp1
Deposited on	02/10/2017

Associated publications	
	Hannes Dierkes, Jan van Leusen, Dimitri Bogdanovski, Richard Dronskowski, <i>Inorganic Chemistry</i> , 2017, 56, 1045, DOI: 10.1021/acs.inorgchem.6b02816

CSD and ICSD entries

Download deposited CIF, hkl, checkCIF

Link to article

3D representation and link to ICSD

Data citation including Data DOI

# Links to and from publications

RETURN TO ISSUE | < PREV ARTICLE NEXT >

## Pressure-Dependent Crystallization Preference of Resorcinol Polymorphs

Fatemeh Safari, Anna Olejniczak and Andrzej Katrusiak\*

Cite this: *Cryst. Growth Des.* 2019, 19, 10, 5629-5635  
 Publication Date: August 14, 2019  
<https://doi.org/10.1021/acs.cgd.9b00610>  
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Article Views: 251 | Altmetric: 4 | Citations: -

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PDF (4 MB) Supporting Info (1) »

### Abstract

Polymorph  $\alpha$  of resorcinol, at ambient pressure stable to 365 K when it transforms to polymorph  $\beta$ , is exceptionally resistant to high pressure. The crystals of polymorph  $\alpha$  can be compressed to over 4 GPa without transforming to the  $\beta$  phase. We have performed high-pressure recrystallization of resorcinol aqueous and methanol solutions, and they yielded polymorph  $\alpha$  below 0.5 GPa and polymorph  $\beta$  above this pressure. Our single-crystal X-ray diffraction studies on resorcinol polymorphs in a diamond-anvil cell reveal the structural origins of the phase transition. The high pressure changes the angular dimensions of bistable hydrogen bonds OH...O, which destabilizes the H-atoms and the structure of polymorph  $\alpha$  above 0.5 GPa, consistent with the calorimetric and NMR results. The high-temperature, high-pressure polymorph  $\beta$  achieves the more dense packing through the changed conformation of one of the hydroxyl groups and the considerable twisting of the hydrogen bonds necessary for the formation of additional C-H... $\pi$  bonds. The large temperature and pressure hysteresis of the polymorphs  $\alpha$  and  $\beta$  are connected with the different topologies of their O-H...O networks.

### Synopsis

The pressure- and temperature-dependent transition between resorcinol polymorphs  $\alpha$  and  $\beta$  has been rationalized in terms of transforming H-bonds and their networks.

### Introduction

Resorcinol, an intermediate often used in chemical practice and a pharmaceutical agent, was one of the first organic compounds for which the phenomenon of polymorphism was described and the first organic compound for which the structures of both polymorphs were determined in 1938 by Robertson and Ubbelohde.<sup>(1,2)</sup> Until today, the resorcinol crystals belong to the best known examples of polymorphs.<sup>(3)</sup>

CCDC: 1913232  
 CCDC: 1913233  
 CCDC: 1913234  
 CCDC: 1913235  
 CCDC: 1913236  
 CCDC: 1913237  
 CCDC: 1913238  
 CCDC: 1913239  
 CCDC: 1913240  
 CCDC: 1913241  
 CCDC: 1913242

CCDC FIZ Karlsruhe  
 Leibniz Institute for Information Infrastructure

## CSD Entry: RESORA21

Sign In Licensed to: CCDC Main Site

Simple Search Structure Search Unit Cell Search Formula Search

Your query was: Identifier(s): 1913234, DOI: doi:10.1021/acs.cgd.9b00610 and the search returned 11 records. [Modify Search](#) [New Search](#)

Database Identifier	Deposition Number
<input checked="" type="checkbox"/>	RESORA16 1913235
<input checked="" type="checkbox"/>	RESORA17 1913236
<input checked="" type="checkbox"/>	RESORA18 1913237
<input checked="" type="checkbox"/>	RESORA19 1913232
<input checked="" type="checkbox"/>	RESORA20 1913233
<input checked="" type="checkbox"/>	<b>RESORA21 1913234</b>
<input checked="" type="checkbox"/>	RESORA22 1913238
<input checked="" type="checkbox"/>	RESORA23 1913239
<input checked="" type="checkbox"/>	RESORA24 1913240
<input checked="" type="checkbox"/>	RESORA25 1913241
<input checked="" type="checkbox"/>	RESORA26 1913242

RESORA21 - benzene-1,3-diol  
 Space Group: P n a 2<sub>1</sub> (33), Cell: a 10.3859(14) Å b 9.3317(5) Å c 5.6229(2) Å,  $\alpha$  90°  $\beta$  90°  $\gamma$  90°

3D viewer

Chemical diagram

View group symbols key

Download -

# Benefits of joint access

- Every published structure **free** to download
- Each new dataset assigned a **data citation** including **DOI**
- Ability to **search across** all organic, metal-organic and inorganic structures
- Increased **discoverability** of and linking of data
- Joint partnerships and workflows **increase efficiency and speed** data is available through databases

# Joint services - Deposition



### CIF deposition and validation service

First name(s)

Last name(s) \*

Your email address \*

Your ORCID ID  Create or Connect your ORCID ID

Additional email addresses

Institution (e.g. University/Company) \*

Deposition number(s) for revision

CIF/HKL/RES/FCF/Word/ZIP files   Done

YIGPIO03.cif  
4.42 KB

Details \*  Remember my details

Options \*  I wish to run the IUCr *checkCIF/PLATON* service on my data



# Joint services - Deposition

1 Login

2 Upload

3 Check Syntax

4 Validation

5 Add Publication

6 Enhance Data

7 Review

8 Submit

## CIF deposition Check Syntax

The files highlighted in red in the left-hand column contain errors that need fixing before proceeding.

Please click on any red file names in the left-hand column, make the appropriate edits and then click the 'Save & Recheck File' button before proceeding to the next step.

For more information on how to fix errors please see our [correcting CIFs](#) page.

Pick file to edit

structure01.cif

structure02.cif

File contents structure01.cif

```
30 data_I
31 _audit_creation_method SHELXL-97
32 _chemical_name_systematic
33 ;
34 {5-[(7-chloroquinolinium-4-yl)amino]-2-hydroxybenzyl}diethylammonium dichloride
35 dihydrate
36 ;
37 _chemical_name_common Amodiaquine dihydrochloride dihydrate'
38 _chemical_formula_moiety 'C20 H24 Cl N3 O 2+, 2(Cl -), 2(H2 O)'
39 _chemical_formula_sum C20 H28 Cl3 N3 O3'
40 _chemical_formula_iupac 'C20 H24 Cl N3 O 2+, 2Cl -, 2H2 O'
41 _chemical_formula_weight 464.80
42 _chemical_melting_point ?
43 _symmetry_cell_setting monoclinic
44 _symmetry_space_group_name_H-M 'P 21/c'
45 _symmetry_space_group_name_Hall '-P 2ybc'
46 loop_
47 _symmetry_equiv_pos_as_xyz
48 'x, y, z'
49 '-x, y+1/2, -z+1/2'
50 '-x, -y, -z'
51 'x, -y+1/2, z+1/2'
52 _cell_length_a 7.76220(10)
53 _cell_length_b 26.8789(4)
54 _cell_length_c 10.7885(2)
55 _cell_angle_alpha 90.00
56 _cell_angle_beta 92.7840(10)
57 _cell_angle_gamma 90.00
58 _cell_volume 2230.91(6)
59 _cell_formula_units_Z 4
```

← Go Back

Save & Recheck File

Proceed to Next Step →

Error 44 No terminating () quote

# Joint services - Deposition

1 Login

2 Upload

3 Check Syntax

4 Validation

5 Add Publication

6 Enhance Data

7 Review

8 Submit

## CIF deposition Check Syntax

First name(s)

Last name(s)

Your email address

Your ORCID ID

Additional email addresses

Institution (e.g. University/Company)

Deposition number(s) for revision

CIF/HKL/RES/FCF/Word/ZIP files

Details

Options

## Check Syntax

The files highlighted in red

Please click on any red file before proceeding to the next step.

For more information, see the help page.

Pick file to edit

structure01.cif

structure02.cif

## Validation

View reports on the consistency and integrity of your structures

Structure	IUCr checkCIF	Unit cell check
<b>structure01.cif</b>		
data_I	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>
<b>structure02.cif</b>		
data_sa2906c	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>
data_sa2906a	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>
data_sa2906b	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>
data_sa2906g	<a href="#">View Report</a> <input type="text" value="No Response Required"/>	<a href="#">View Hits</a>

```
57 _cell_angle_gamma 90.00  
58 _cell_volume 2230.91(6)  
59 _cell_formula_units_Z 4
```

[Go Back](#)

[Save & Recheck File](#)

[Proceed to Next Step](#)

Error 44 No terminating () quote

# Joint services - Deposition

1 Login → 2 Upload → 3 Check Syntax → 4 Validation → 5 Add Publication → 6 Enhance Data → 7 Review → 8 Submit

## Validation

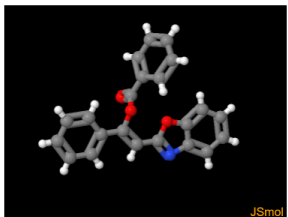
View reports on the consistency and integrity of your structures

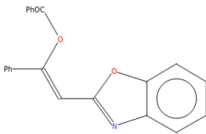
Structure	IUCr checkCIF	Unit cell check
structure01.cif	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>
structure02.cif	<a href="#">View Report</a> <input type="text" value="Enter Response"/>	<a href="#">View Hits</a>

**CheckCIF Responses:**

- Level A
  - PLAT027 \_diffn\_reflns\_theta\_full value (too) Low ..... 13.50 Degree
  - PLAT029 \_diffn\_measured\_fraction\_theta\_full value Low - 0.677 Note
- Level B
  - PLAT415 Short Inter D-H...H-X H1 ... H623 .. 2.00 Ang.
- Level C

**ABANEY01** : 2-(1,3-benzoxazol-2-yl)-1-phenylvinyl benzoate  
Space Group: P21/n, Cell: a 10.0298(8)Å b 13.2075(11)Å c 13.4578(11)Å, α 90° β 110.9676(11)° γ 90°

3D viewer:  JSmol

Chemical diagram: 

View group symbols key

<b>Level A</b>	Most likely a serious problem, resolve or explain
<b>Level B</b>	A potentially serious problem, consider carefully
<b>Level C</b>	Check. Ensure it is not caused by an omission or oversight
<b>Level G</b>	General information/check it is not something unexpected

# Joint services - Deposition

1 Login

2 Upload

3 Check Syntax

4 Validation

5 Add Publication

6 Enhance Data

7 Review

8 Submit

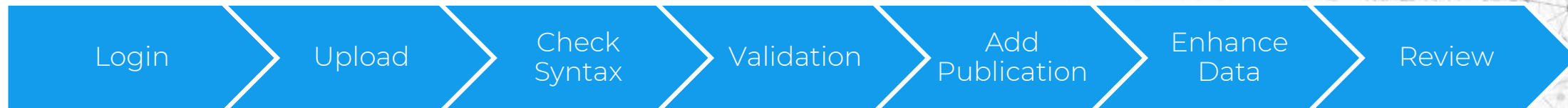
The image displays a sequence of overlapping screenshots from a web application, illustrating the workflow from step 3 to step 6:

- Step 3: Check Syntax** - Shows a form for user registration with fields for first name, last name, email, ORCID ID, and institution. A 'Pick file to edit' section contains two files: 'structure01.cif' and 'structure02.cif'.
- Step 4: Validation** - Shows a 'View reports' section with a list of files: 'structure01.cif', 'data\_1', 'structure02.cif', 'data\_sa2906c', 'data\_sa2906a', 'data\_sa2906b', and 'data\_sa2906g'. A table at the bottom shows CIF data: 

57	_cell_volume	2230.91
58	_cell_formula_units_Z	
59	_cell_formula_units_Z	
- Step 5: Add Publication** - Shows a form with the instruction 'Please check and add your publication details. If you don't know the details, click on the "Add Publication" button.' Fields for 'Journal', 'Publication', and 'Additional information' are visible.
- Step 6: Enhance Data** - Shows a detailed view for 'data\_YIGPIO3'. It includes:
  - 'Pick a structure to edit' section with 'YIGPIO3.cif' and 'data\_YIGPIO3' selected.
  - '3D viewer' showing a ball-and-stick model of the molecule.
  - 'Chemical diagram' showing a 2D chemical structure.
  - 'Associated DOIs' section with a 'Raw data DOI' field.
  - 'Data fields' section with input fields for 'Compound name', 'Synonyms/other names', and 'Crystal colour'.
  - A code editor showing CIF data for 'data\_YIGPIO3':

```
16 data_YIGPIO3
17 _symmetry_cell_setting orthorhombic
18 _symmetry_space_group_name_H-M 'P 21 21 21'
19 _symmetry_int_tables_number 19
20 _space_group_name_Hall 'P 2ac 2ab'
21 loop_
22 _symmetry_equiv_pos_site_id
23 _symmetry_equiv_pos_as_xyz
24 1 x,y,z
25 2 1/2-x,-y,1/2+z
26 3 -x,1/2+y,1/2-z
27 4 1/2+x,1/2-y,-z
28 _cell_length_a 9.831(6)
29 _cell_length_b 18.485(11)
30 _cell_length_c 20.261(12)
31 _cell_angle_alpha 90
32 _cell_angle_beta 90
33 _cell_angle_gamma 90
34 _cell_volume 3681.95
35 loop_
36 _atom_site_label
37 _atom_site_type_symbol
38 _atom_site_fract_x
```

# Deposition workflow



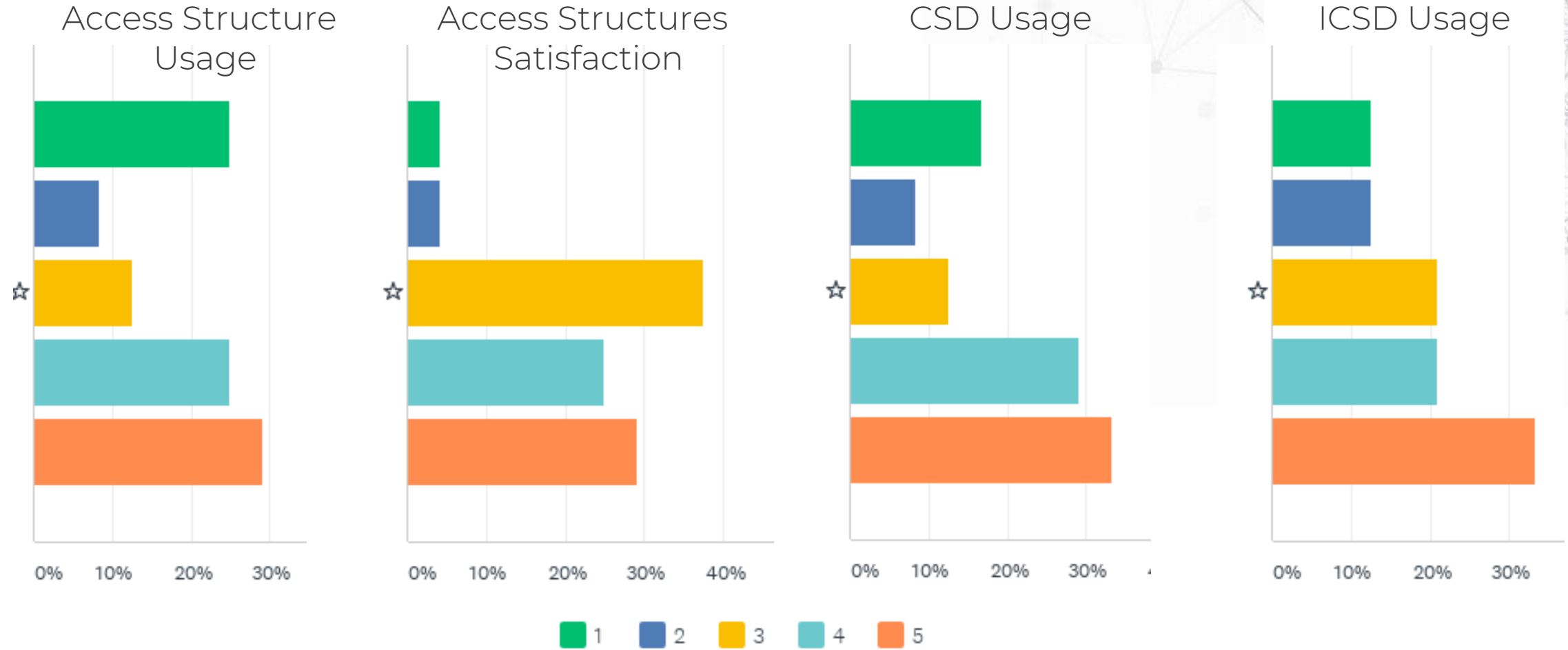
- Joint deposition service aim to make it easy for you to:
  - Follow community recommendations
  - Provide reliable data and metadata
  - Deposit all organic, inorganic and metal-organic data
- Components include:
  - Identification of contributors
  - Use of standard formats & syntax checking
  - Generation of validation report
  - Capture of publication, experimental and chemical metadata
  - Additional enrichment of data by CCDC and FIZ
  - Ability to publish directly in the CSD or ICSD as *Communications*

# Extending our partnership

Exploring the generation of a more advanced search interface across the CSD and the ICSD

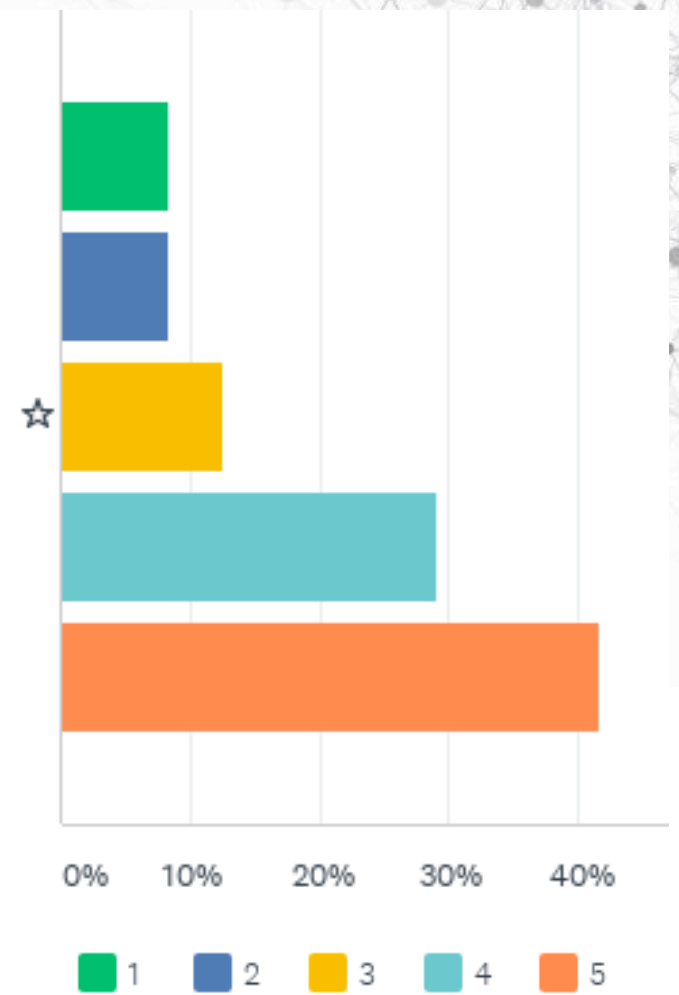
- Joint survey
  - Held in July/August
  - Designed to gauge interest in an advanced search interface
- Webinar today to gauge your interest
- Interactive discussion session planned for October to gather your requirements

# Survey results



# Survey conclusions

- All respondents were from academia
- Most popular sectors
  - Materials science
  - Catalysis
  - Education
  - Porous Frameworks
- >40% respondents interested in an advanced search interface







# Searching the CSD and ICSD

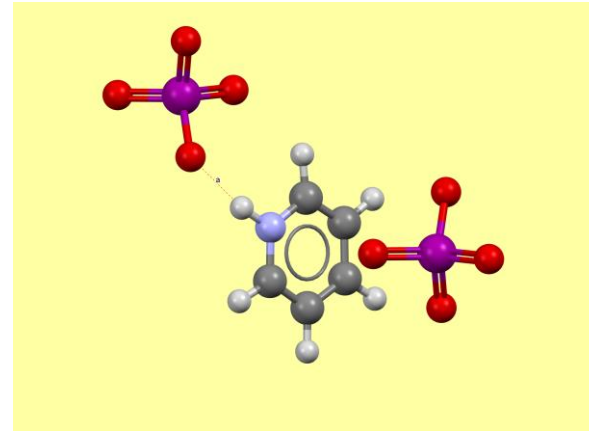
Paul Raithby

Department of Chemistry, University of Bath, UK

E-mail: [p.r.raithby@bath.ac.uk](mailto:p.r.raithby@bath.ac.uk)

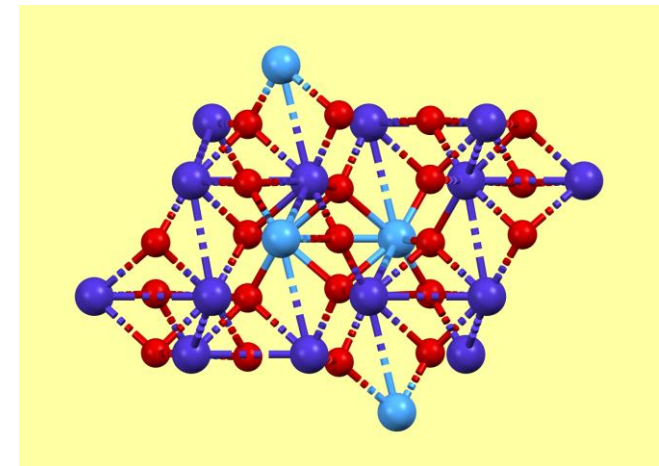
# Structural Science Areas where there are Advantages in Searching the CSD and ICSD

- Coordination and Materials Chemistry
- For example:
  - Functional coordination complexes
  - Ferroelectric materials
  - Perovskite and hybrid organic/inorganic materials
- To study structure/property correlations in the solid-state and solution
- Applications in catalysis, energy and electronic materials



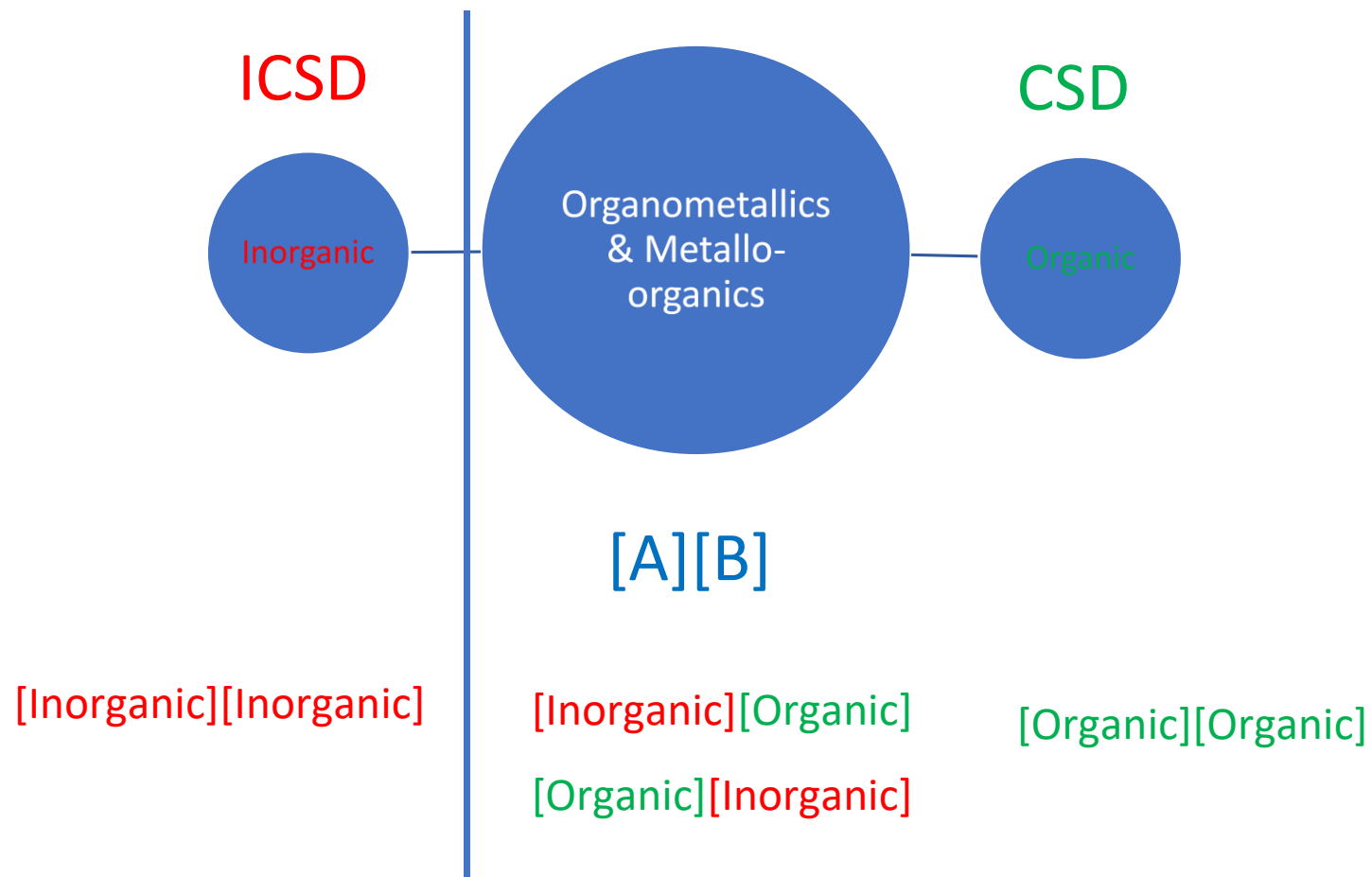
Pyridinium  
periodate

Co<sub>4</sub>(Nb<sub>2</sub>O<sub>9</sub>)



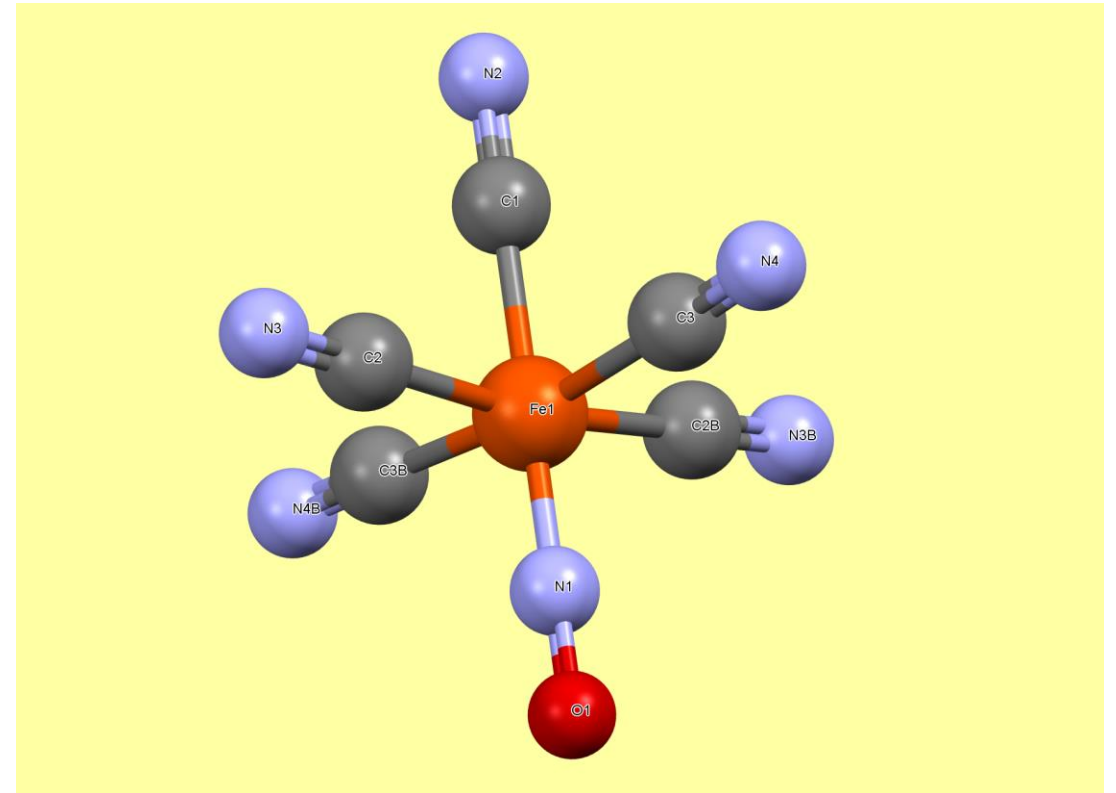
# Contents of the two Databases

## ORGANIC AND INORGANIC SALTS



# A Simple Example – the Nitroprusside Dianion

- CSD
  - 30 hits –with one or more organic or organometallic/metallo-organic cations
- ICSD
  - 42 hits – with inorganic cations such as  $\text{Na}^+$ ,  $\text{Ca}^{2+}$
- Some overlap between the two databases but two distinct sets that could be combined.

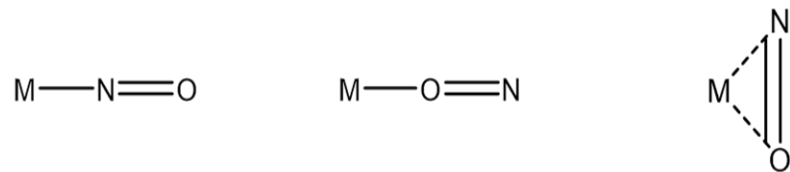


$[\text{Fe}(\text{CN})_5(\text{NO})]^{2-}$  dianion

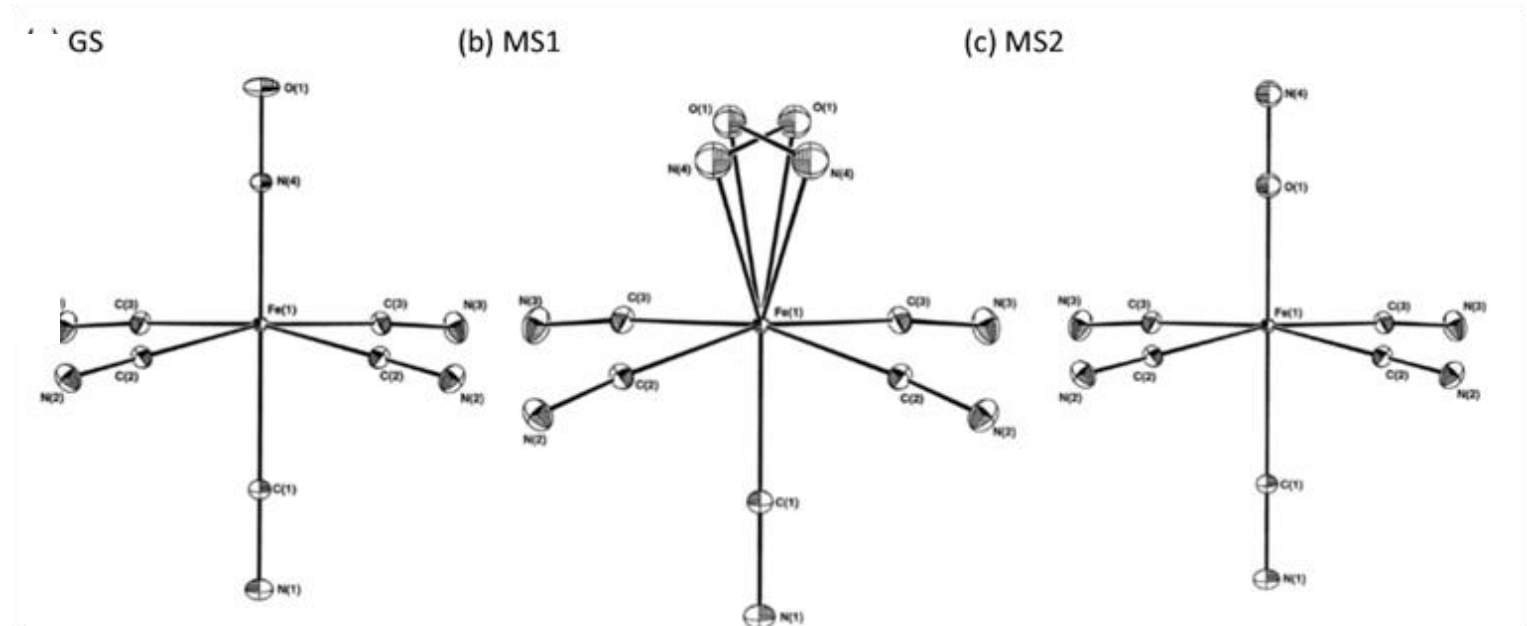
# Why the interest in Nitroprussides?

Within the nitroprusside complex the nitrosyl ligand (NO) can act as an ambidentate ligand. The different bonding modes are described as linkage isomers.

The nitrosyl group can undergo photoactivated switching between the M-NO form and the M-ON form, and also a side-bound form in the solid state, with changes in physical properties. Potential for molecular switches or as binary counting devices.

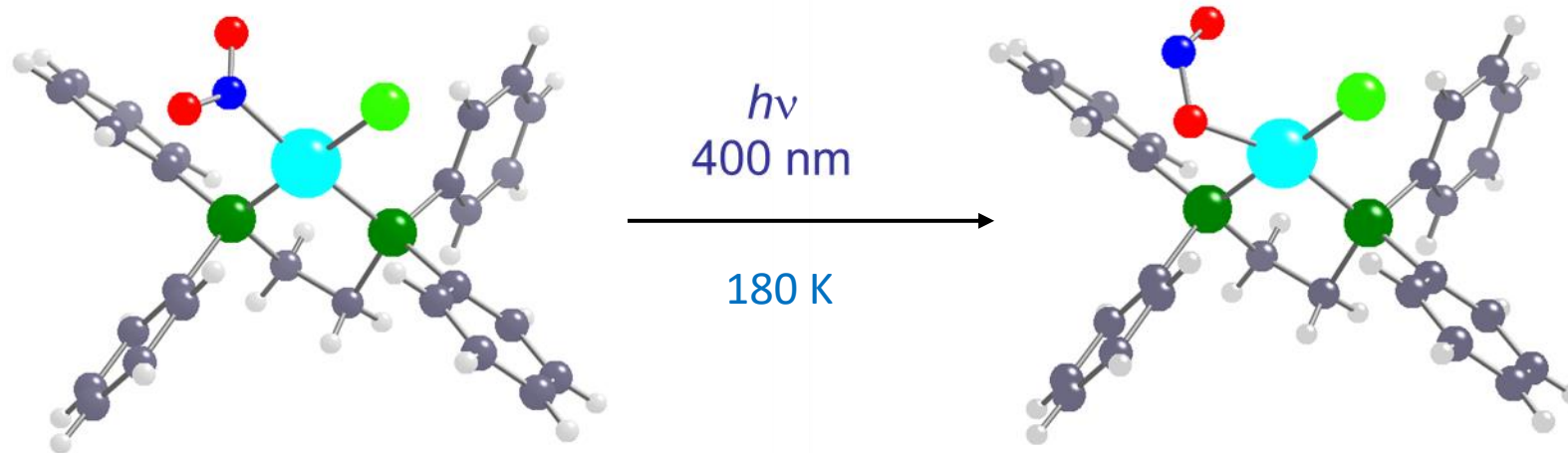
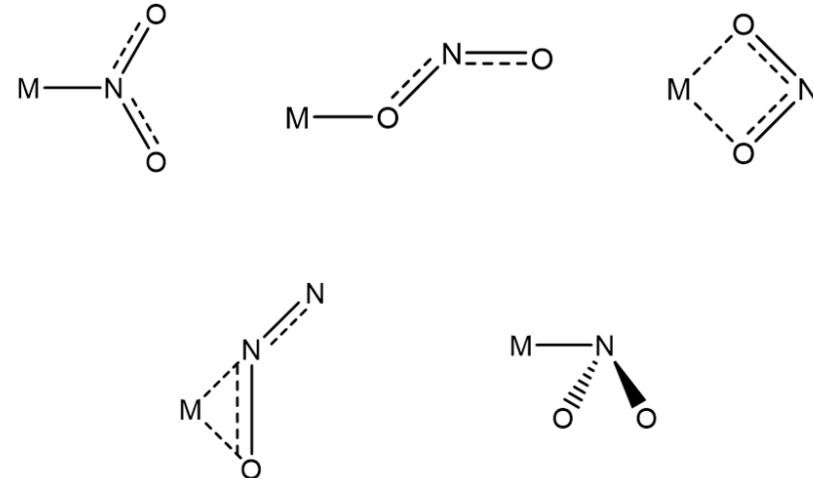


Analysis of bond parameters of a large number of nitrosyl-containing complexes, both inorganic and metallo-organic, helpful for reactivity studies.

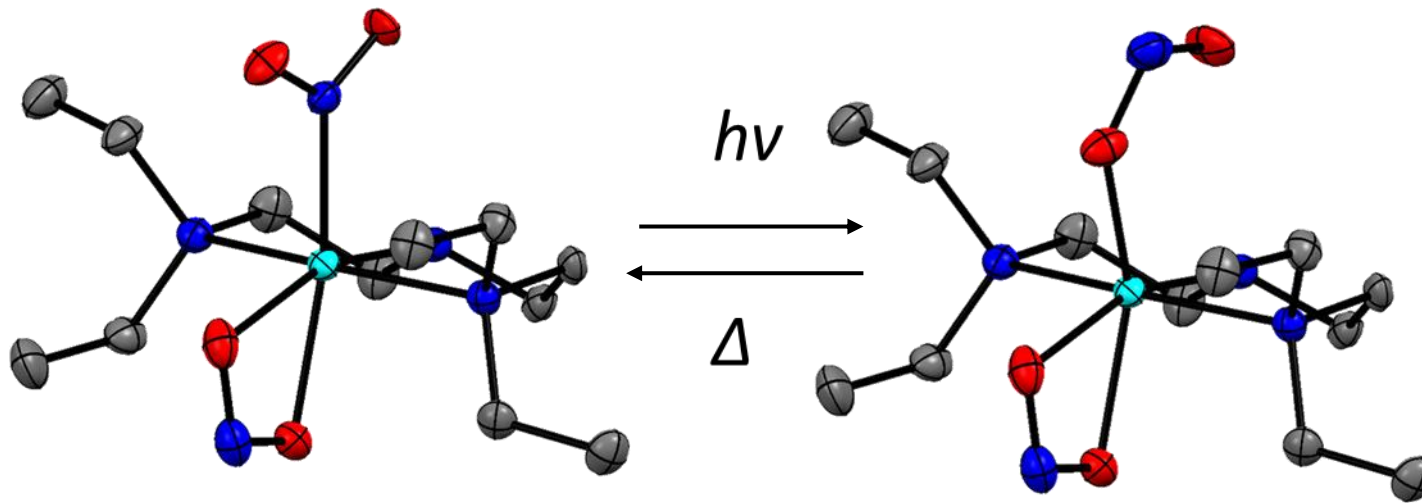


# Solid State Photoactivated Switching in Transition Metal Nitro to Nitrito Linkage Isomers

Transition metal complexes that contain nitro groups can also form linkage isomers



# Designing Effective Nitro-based Photoswitches



Require the photoactivated process to be:

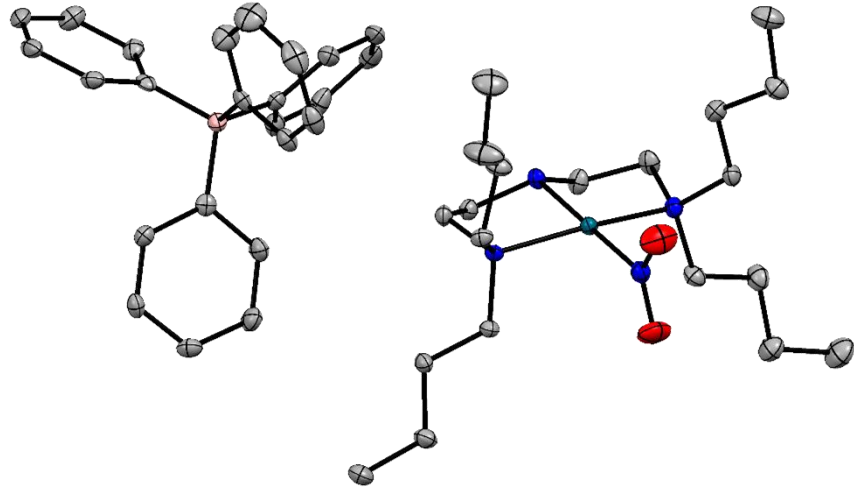
- Fast
- Fully reversible
- Occur near room temperature
- No significant degradation of the crystalline phase

Successful design requires:

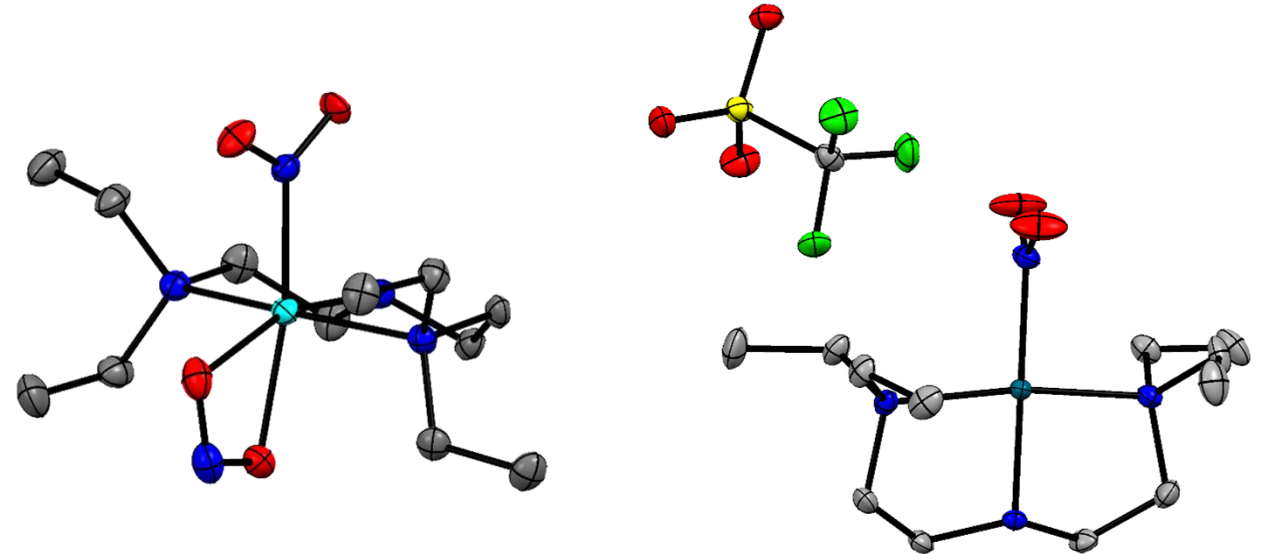
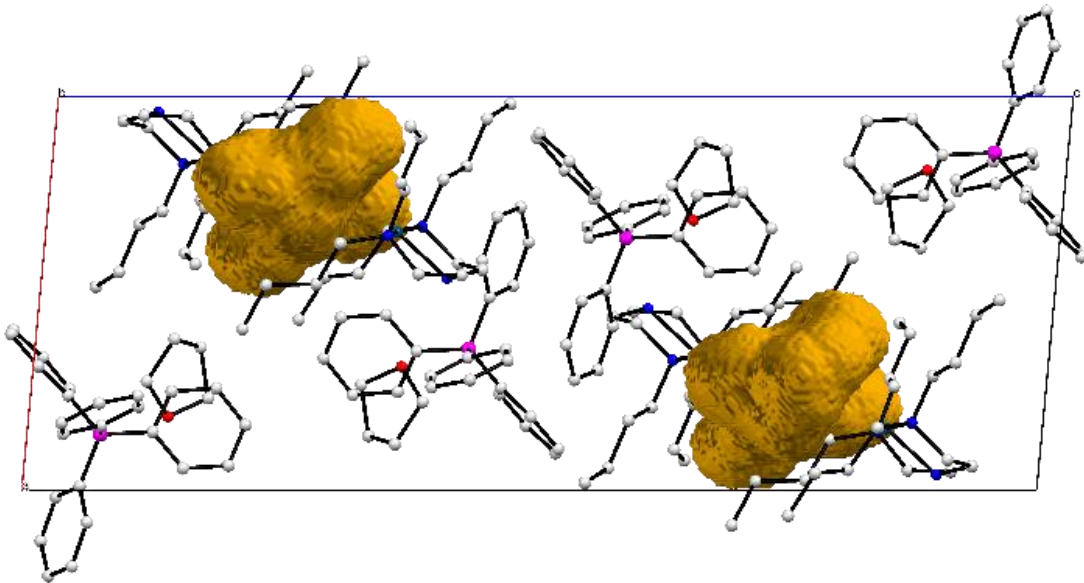
- 1) Control of kinetic factors
- 2) Control of crystalline environment around the photoactive species – control of intermolecular interactions and of the reaction cavity

Data from structural databases is very helpful in understanding (2)

# Engineering High Photoconversion - *sterics*



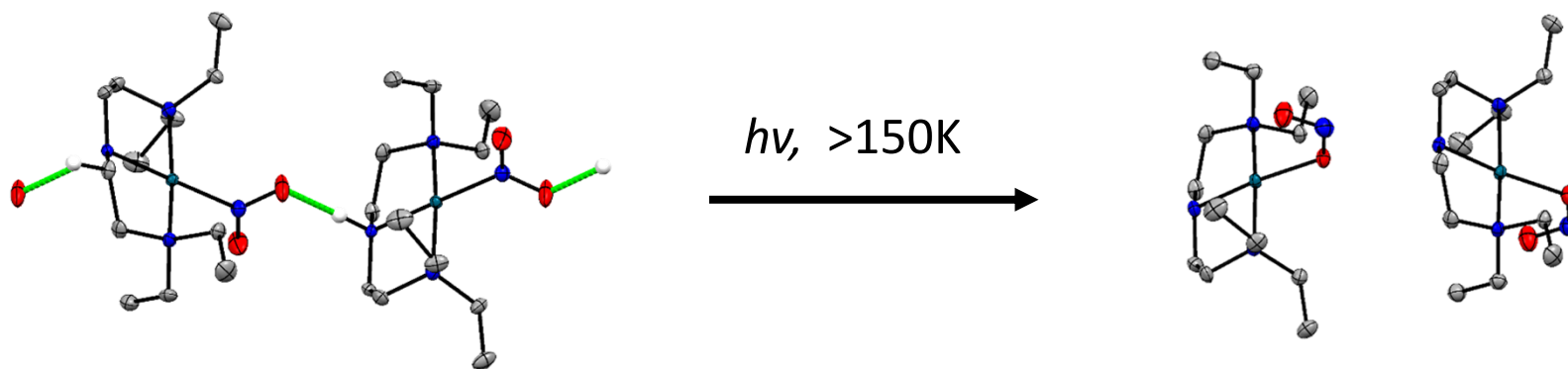
- Design of systems capable of very high photo-conversion levels (100%) using crystal engineering principles
- Use sterically-demanding, photo-inert ancillary fragments (co-ligands and/or counter-ions)
- Bulky inert fragments dominate crystal packing, generating a “reaction cavity” around the isomerising group
- Facilitates high photo-activation with minimal strain



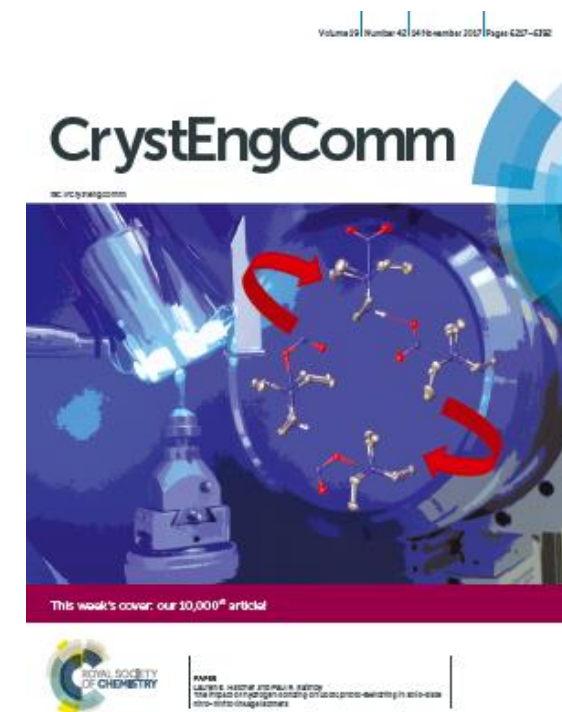


# Engineering High Photoconversion – *H-bonding*

- Avoiding H-bonding interactions all together is an unfortunate design limitation: *H-bonds are among the crystal engineers key tools*
- Two new crystal systems: [Pd(Et<sub>4</sub>dien)(NO<sub>2</sub>)]OTf and [Pt(Et<sub>4</sub>dien)(NO<sub>2</sub>)]OTf show that H-bonding limitations can be mitigated by careful temperature control



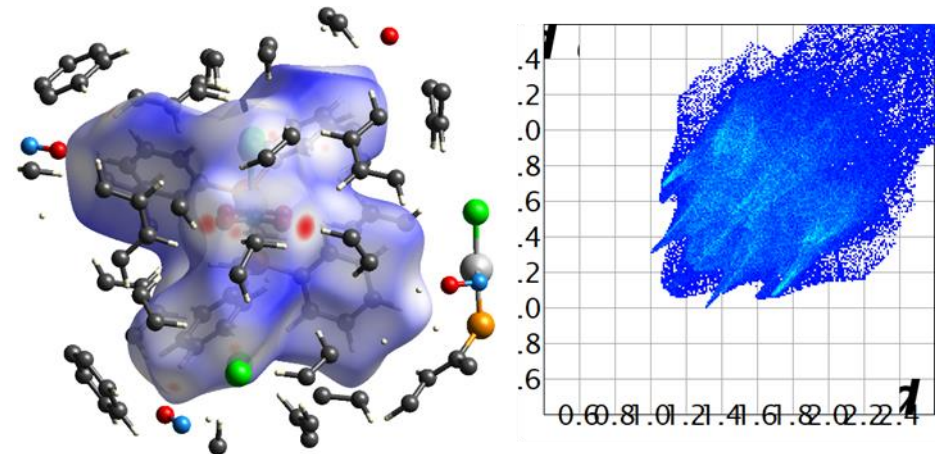
- Strong intermolecular H-bonds involving the GS NO<sub>2</sub> groups in both systems
- At low temp (100 K), only low photo-conversion achieved (*c.a.* 60 % max.)
- On warming to 150 K, 100% photo-conversion could be reached
- Raising the temperature weakens the H-bonding interactions and increases the reaction cavity volume – facilitating 100% activation



# Search the CSD and ICSD for Transition Metal Nitro Complexes

Look for patterns and trends:

- Extent of intermolecular interactions
  - Presence or absence of hydrogen bonding
  - Assess the available volume within the unit cell (reaction cavity)
- ICSD has 44 hits of inorganic nitro complexes
  - CSD has 829 hits for transition metal organometallic and coordination complexes



# Conclusions

- The combination of the CSD and ICSD offers new opportunities for knowledge mining that were not previously possible
- The comprehensive CSD software package makes searching for trends easier.
- I think that there are particular opportunities in the areas of
  - Materials chemistry
  - Coordination Chemistry
- Thanks go to the members of the CSD for providing insights into structural data and to my research group for carry out many of the studies.



**FIZ Karlsruhe**

Leibniz Institute for Information Infrastructure

**ADVANCING SCIENCE**

# Webinar CCSD/ICSD

**ICSD examples and  
connections to CSD  
database**

**Dejan Zagorac**

**Senior Scientific Editor**

August 27, 2020

# 1. How to Search ICSD for experimentally observed (synthesized) inorganic structures

- Let's start with simple search perovskite. Perovskite is a calcium titanium oxide mineral composed of calcium titanate ( $\text{CaTiO}_3$ ). It is also applied to the class of compounds which have the same type of crystal structure as  $\text{CaTiO}_3$  ( $\text{ABX}_3$ ), known as the perovskite structure. Different cations can be embedded in this structure, allowing the development of diverse engineered materials .

The screenshot displays the ICSD search interface with several key elements highlighted in red and green circles:

- Content Selection:** The checkbox for "Experim. inorganic structures" is checked and circled in red.
- Chemistry:** The "Composition" filter is set to "Ca Ti O" and circled in green. The "Number of Elements" is set to "3" and also circled in green.
- Search Summary:** The result count "77" is circled in green.

The interface includes the following sections:

- Content Selection:** Includes checkboxes for "Experim. inorganic structures", "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** Lists search options like "Basic search & retrieve", "Bibliography", "Cell", "Chemistry", "Symmetry", "Crystal Chemistry", "Structure Type", "Experimental Information", "DB Info", and "Expert Search".
- Advanced search & retrieve:** Provides a list of search criteria.
- Basic Search & Retrieve:** Contains input fields for "Free Text Search", "Bibliography" (Authors, Title of Journal, Title of Article), "Chemistry" (Composition, Periodic Table, Number of Elements), "Cell" (Cell Parameters, Cell Volume, Tolerance), and "Symmetry" (Space Group Symbol, Space Group Number, Crystal System, Centering).
- Search Action:** Includes "Run Query" and "Clear Query" buttons.
- Search Summary:** Shows "Basic Search: 77".
- Query History:** Lists previous queries with their timestamps and result counts.

# 1. How to Search ICSD for experimentally observed (synthesized) inorganic structures

ICSD

Welcome to ICSD-Desktop.

FIZ Karlsruhe | Contact

**Content Selection**

- Experm. inorganic structures
- Experm. metal-organic str.
- Theoretical structures

**Navigation**

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info

**Chemistry Search**

**Composition**   **Number of Elements**

Structural Formula

Chemical Name

**Mineral Name**

Mineral Group

ANX Formula

AB Formula

Formula Weight

**Search Action**

**Search Summary**

Bibliography:	-
Cell:	-
Chemistry:	19
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
<b>Combined Results:</b>	<b>19</b>

**Query History**

Number of queries: 2

# 1. How to Search ICSD for experimentally observed (synthesized) inorganic structures

The screenshot displays the ICSD Desktop search interface. The top navigation bar includes the ICSD logo, a welcome message, and a contact link for FIZ Karlsruhe. The main search area is divided into several sections:

- Content Selection:** A sidebar with three options: "Experim. inorganic structures" (checked and circled in red), "Experim. metal-organic str.", and "Theoretical structures".
- Navigation:** A sidebar with search categories: "Basic search & retrieve" and "Advanced search & retrieve" (containing Bibliography, Cell, Chemistry, Symmetry, Crystal Chemistry, Structure Type, Experimental Information, and DB Info).
- Chemistry Search:** The central search area with fields for:
  - Composition (e.g. Na Cl) with a "Periodic Table" button.
  - Structural Formula (e.g. Pb (W O4)).
  - Chemical Name.
  - Mineral Name (circled in blue, containing "perovskite").
  - Mineral Group (e.g. Adamite).
  - ANX Formula.
  - AB Formula.
  - Formula Weight.
  - Number of Elements.
  - Number of Formula Units.
- Search Action:** Buttons for "Run Query" and "Clear Query".
- Search Summary:** A table showing search results across various categories:

Category	Count
Bibliography:	-
Cell:	-
Chemistry:	449 (circled in blue)
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
<b>Combined Results:</b>	<b>449</b>
- Query History:** Shows "Number of queries: 2" and a "Clear Query History" button.

Buttons at the bottom of the search area include "Clear Chemistry Search" and "Count Chemistry Search".

# 1. How to Search ICSD for experimentally observed (synthesized) inorganic structures: Example with Organic-Inorganic Hybrid Material

RETURN TO ISSUE | < PREV ARTICLE NEXT >

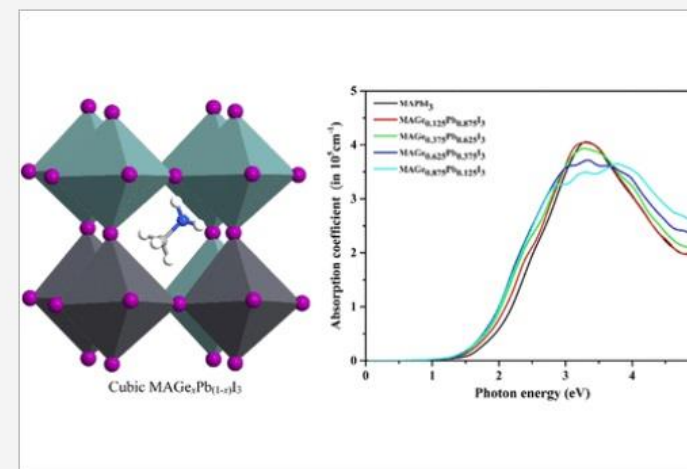
## First-Principle Insights of Electronic and Optical Properties of Cubic Organic–Inorganic $\text{MAGe}_x\text{Pb}_{(1-x)}\text{I}_3$ Perovskites for Photovoltaic Applications

Rishikanta Mayengbam, S. K. Tripathy\*, and G. Palai

✓ Cite this: *J. Phys. Chem. C* 2018, 122, 49, 28245–28255  
Publication Date: November 15, 2018  
<https://doi.org/10.1021/acs.jpcc.8b08436>  
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### Abstract

Owing to power conversion efficiencies of as high as 22.1%, hybrid organic–inorganic lead halide perovskites have become the fastest growing solar technology, competing with the conventional thin-film technology. Though unique and exceptional, long-term stability issue and toxic behavior caused by the lead content in the perovskites hamper large-scale commercial production. With this motivation toward achieving a stable and reduced toxic perovskite, we have investigated the structural, electronic, and optical properties of mixed  $\text{MAGe}_x\text{Pb}_{(1-x)}\text{I}_3$  perovskites with the generalized gradient approximation–Perdew, Burke, Ernzerhof exchange–correlation functional within the framework of density functional theory. Under structural properties, we have calculated the lattice constants, bond lengths, tolerance factors, enthalpies of formation, bulk moduli, and their derivatives for  $x = 0.0, 0.125, 0.375, 0.625,$  and  $0.875$ . We found that mixed  $\text{MAGe}_x\text{Pb}_{(1-x)}\text{I}_3$  perovskites are stable except at  $x = 0$ . The electronic properties such as band gaps, energy band level, and effective masses have been predicted for all combinations of  $x$ . We have also analyzed the projected and total density of states in detail. Optical properties like imaginary and real parts of dielectric function, refractive index, and extinction coefficient have been discussed. Further, to understand the light trapping capacity, we have examined the absorption coefficients for  $x = 0.0, 0.125, 0.375, 0.625,$  and  $0.875$ , and interband transitions are well estimated. The calculated values of all parameters were compared with the available experimental and theoretical values. A fairly good agreement has been obtained between them.





## 2. How to search for new (not-yet synthesized) structures or materials

- Maybe one of the most important examples for the experimental CSD/ICSD users is the use of the theoretical category: predicted (non-existing) crystal structure. As crystal structure predictions become more and more reliable, this category can be an excellent tool for synthesis planning.

The screenshot shows the ICSD-Desktop search interface. The 'Content Selection' menu on the left has 'Theoretical structures' selected. The 'Experimental Information Search' section has 'Calculation Methods' set to 'Predicted (non-existing) crystal structure'. The 'Search Action' section shows 'Run Query' and 'Clear Query' buttons. The 'Search Summary' table shows 3860 results for 'Experimental Info'. The 'Query History' table shows 7 queries, with the most recent one on 2020-04-03T23:24 resulting in 404 hits.

ICSD

Welcome to ICSD-Desktop.

FIZ Karlsruhe | Contact

**Content Selection**

- Experm. inorganic structures
- Experm. metal-organic str.
- Theoretical structures

**Experimental Information Search**

Temperature:  K

Pressure:  MPa

Comments:

Calculation Methods:

Clear Experimental Info Search    Count Experimental Info Search

**Search Action**

Run Query    Clear Query

**Search Summary**

Bibliography:	-
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	3860
DB Info:	-
Expert:	-
<b>Combined Results:</b>	<b>3860</b>

**Query History**

Number of queries:	7
Clear Query History	
2020-04-03T23:24	404

## 2. How to search for new (not-yet synthesized) structures or materials

- Obtaining information on predicted not-synthesized unknown compounds, or/and not-synthesized modifications of known compounds, could be an important advantage for CSD/ICSD users with numerous scientific, technological and industrial applications.
- Search for new predicted (non-existing) structures or materials can be more precise if the user combines search with standardized keywords in the ICSD.

<b>Theoretical category in the ICSD</b>	<b>No. of CIF files</b>
<b>Predicted (non-existing) crystal structure</b>	3860
<b>Optimized (existing) crystal structure</b>	2461
<b>Combination of theoretical and experimental structure</b>	1368

Table 1. Number of theoretical crystal structures (CIF files) in the ICSD Desktop (2019.2)

### 3. Search for parameters for method development and future calculations

- Optimized (or existing) crystal structures are theoretically calculated structures of existing experimental crystal structures in the ICSD until the year of publication.
- In experimental materials science and related sciences, they can be used as an excellent tool for industrial and technological applications where it is very important to fine-tune materials, because slight deviations between the calculation and experiment can lead to different properties of the material. [1]
- In computational materials science and related sciences, optimized structures can be used for method development and to generate parameters for future calculations.
- In the following text we show one such example.



[1] D. Zagorac, H. Müller, S. Ruehl, J. Zagorac and S. Rehme, J. Appl. Cryst. (2019) 52, 918-925.

### 3. Search for parameters for method development and future calculations

The screenshot displays the ICSD Desktop search interface. The top navigation bar includes the ICSD logo, a welcome message, and a contact link for FIZ Karlsruhe. The main search area is divided into three sections: Content Selection, Experimental Information Search, and Search Action.

**Content Selection:** This section allows users to filter search results by structure type. The options are:  Experm. inorganic structures,  Experm. metal-organic str., and  Theoretical structures. The 'Theoretical structures' option is highlighted with a red circle.

**Experimental Information Search:** This section provides advanced search filters. It includes:   
 - Temperature: A text input field followed by a dropdown menu set to 'K'.   
 - Pressure: A text input field followed by a dropdown menu set to 'MPa'.   
 - Comments: A text input field containing 'Cutoff energy 400 eV' and 'e.g. stable above'. This field is highlighted with a green circle.   
 - Calculation Methods: A dropdown menu set to 'Projector augmented wave method, Optimized existing crystal structure'. This dropdown is also highlighted with a green circle.   
 - Action buttons: 'Clear Experimental Info Search' and 'Count Experimental Info Search'.

**Search Action:** This section contains 'Run Query' and 'Clear Query' buttons.

**Search Summary:** This section provides a breakdown of search results across various categories. The 'Combined Results' row is highlighted with a black circle, showing a total of 182 results. Other categories include Bibliography, Cell, Chemistry, Symmetry, Crystal Chemistry, Structure Types, Experimental Info, DB Info, and Expert.

**Query History:** This section shows the number of queries performed, which is currently 0.

**Navigation:** A sidebar on the left provides quick access to different search and retrieval functions. The 'Experimental Information' option is highlighted with a green circle.

## 4. How to search ICSD for experimental and theoretical data on nanostructures

- Optimized structures are excellent tool for various applications, and maybe one of the most interesting is combination of optimized structures with standardized keywords.
- This searches can involve properties of materials (electronic, magnetic, optical, etc), or the use of keywords combined with, for example, chemical (elements) search, or structural (structure types) information easily enables searches for special materials like superconductors or piezoelectric materials, or technical applications like solar cells or solid electrolytes. [1,2]
- Search for nanostructures can be even further examined by including experimental nanostructures. This can be performed by using theoretical category: combination of theoretical and experimental structure (Table 1).
- If such data exist in the manuscript they are highly valuable to all materials scientists with a great variety of possible applications, owing to the high precision of the published data.
- In the following examples we will show how to search the ICSD for nanostructures.

[1] D. Zagorac, H. Müller, S. Ruehl, J. Zagorac and S. Rehme, J. Appl. Cryst. (2019) 52, 918-925.

[2] <https://icsd.products.fiz-karlsruhe.de/en/howuse/using-keywords-perform-very-specific-searches-icsd>

# 4. How to search ICSD for experimental and theoretical data on nanostructures

Welcome to ICSD-Desktop.

FIZ Karlsruhe | Contact

**Content Selection**

- Experm. inorganic structures
- Experm. metal-organic str.
- Theoretical structures

**Navigation**

- Basic search & retrieve
- Bibliography**
- Cell
- Chemistry
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

**Query Management**

**Bibliography Search**

Authors: e.g. Jansen

Title of Journal: e.g. Angewandte Chemie

Title of Article: e.g. Super conducting crystals

Year of Publication: e.g. >2008 or 2000-2006 or 2001

Volume: e.g. 10

Page first: e.g. 10

Abstract: e.g. hybrid cage clusters

Keywords: Nano e.g. Polymorphism

Clear Bibliography Search      Count Bibliography Search

**Search Action**

Run Query      Clear Query

**Search Summary**

Bibliography:	625
Cell:	-
Chemistry:	-
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	1368
DB Info:	-
Expert:	-
<b>Combined Results:</b>	<b>96</b>

**Query History**

Number of queries:	7
Clear Query History	
2020-04-03T23:24	404
2020-04-03T02:03	2

Figure 4a. Example on how to search the ICSD for theoretical nanostructures (ICSD Desktop 2019.2)

# 4. How to search ICSD for experimental and theoretical data on nanostructures: Example with Organic-Inorganic Hybrid Material

ICSD Welcome to ICSD-Desktop. FIZ Karlsruhe | Contact

Results: List View # of Hits: 96 (1 selected)

Back to Query Show Detailed View Export Data Print Visualize Structure Visualize Powder Pattern Column Selection Filter

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference	
<input checked="" type="checkbox"/> 670885	P 42/m n m	Ti O2	Rutile-TiO2	Density functional theory a	Zhang, Tianshi; Wojtal, Pa	RSC Advances (2015) 5, (	
<input type="checkbox"/> 670886	P 63 m c	Zn O	Wurtzite-ZnS(2H)	Density functional theory a	Zhang, Tianshi; Wojtal, Pa	RSC Advances (2015) 5, (	
<input type="checkbox"/> 671246	F m -3 m	Cd S	NaCl	Co effect on zinc blende-rc	Zhao, Rui; Wang, Pan; Yac	RSC Advances (2015) 5, (	
<input type="checkbox"/> 671247	F -4 3 m	Cd S	Sphalerite-ZnS(cF8)	Co effect on zinc blende-rc	Zhao, Rui; Wang, Pan; Yac	RSC Advances (2015) 5, (	
<input type="checkbox"/> 671334	F m -3 m	Ni3 Sn	Heusler-AlCu2Mn	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
<input type="checkbox"/> 671335	F m -3 m	Ni	fcc(ccp)-Cu	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
<input type="checkbox"/> 671336	I 41/a m d Z	Ni		Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
<input type="checkbox"/> 671337	P 63/m m c	Ni3 Sn2	Ni3SnP-Co1.75Ge	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
<input type="checkbox"/> 671338	F m -3 m	Sn	fcc(ccp)-Cu	Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	
<input type="checkbox"/> 671339	I 41/a m d Z	Sn		Modelling of phase diagra	Kroupa, A.; Kana, T.; Bursi	Physical Chemistry Chemi	

(1 of 10) 1 2 3 4 5 6 7 8 9 10

**Density functional theory and experimental studies of caffeic acid adsorption on zinc oxide and titanium dioxide nanoparticles**

Tianshi Zhang,<sup>a</sup> Patrick Wojtal,<sup>a</sup> Oleg Rubel<sup>a</sup> and Igor Zhitomirsky<sup>a,\*</sup>

<https://doi.org/10.1039/C5RA21511K>

**Abstract**

The outstanding adsorption properties of proteins, containing catecholic amino acid, L-3,4-dihydroxyphenylalanine (DOPA), and recent advances in nanoparticle functionalization using molecules from the catechol family have generated interest in the investigation of catechol adsorption and applications of catecholates in nanotechnology. Caffeic acid (CA) is the closest molecular analogue of DOPA. Density functional theory has been applied for the modelling of CA adsorption on the surface of ZnO and TiO<sub>2</sub>. Different adsorption modes have been investigated and corresponding adsorption energies were evaluated. According to the calculated energies, the adsorption of CA is energetically favourable at both surfaces with a stronger affinity to TiO<sub>2</sub>. The results of theoretical studies were supported by experimental investigations of CA adsorption. The use of CA as a dispersant for hydrothermal synthesis of ZnO allowed for the fabrication of ZnO nanorods with reduced size and increased aspect ratio. The CA, adsorbed during the hydrothermal synthesis on ZnO nanorods, allowed for their electrostatic dispersion and the electrophoretic deposition (EPD) of ZnO films from stable colloidal suspensions. In another strategy, CA was added as a dispersant for the dispersion of TiO<sub>2</sub> nanorods and the EPD of TiO<sub>2</sub> films. The advantages of catecholates for the synthesis of nanoparticles and fabrication of thin films are discussed.

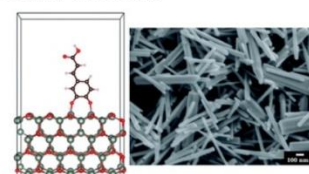
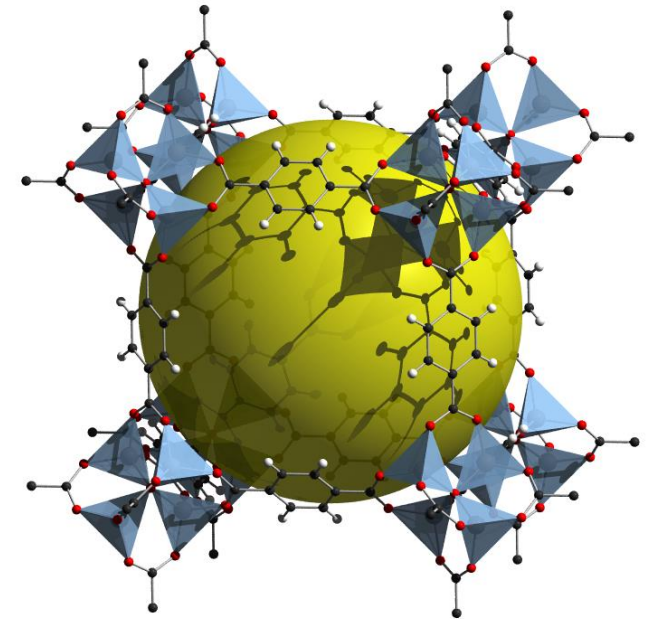


Figure 4b. Example on how to search the ICSD for combined theoretical and experimental nanostructures (ICSD Desktop 2019.2); Example with Organic-Inorganic Hybrid Material(Zhang et al.)

## 5. How to search for experimental metal-organic structures (MOFs)

- Recent advances in chemistry show that the distinction between inorganic and organic structures has become vague. This becomes more obvious in research areas on, for example, zeolites, catalysts, batteries, or gas storage systems.
- We now include pure inorganic structures plus organometallic structures where material properties are available or where inorganic applications are known.
- Biotechnological, medical or pharmaceutical contents are still not included.





# 5. How to search for experimental metal-organic structures (MOFs)

ICSD

Welcome to ICSD-Desktop.

FIZ Karlsruhe | Contact

**Content Selection**

- Experm. inorganic structures
- Experm. metal-organic str.
- Theoretical structures

**Navigation**

- Basic search & retrieve
- Advanced search & retrieve**
- Bibliography
- Cell
- Chemistry**
- Symmetry
- Crystal Chemistry
- Structure Type
- Experimental Information
- DB Info
- Expert Search

**Query Management**

**Chemistry Search**

**Composition**   Number of Elements

e.g. Na Cl

Structural Formula

e.g. Pb (W O4)

Chemical Name

Mineral Name

e.g. Adamite

Mineral Group

e.g. Pyroxene

ANX Formula  Number of Formula Units

AB Formula

Formula Weight

**Search Action**

**Search Summary**

Bibliography:	12312
Cell:	-
Chemistry:	167
Symmetry:	-
Crystal Chemistry:	-
Structure Types:	-
Experimental Info:	-
DB Info:	-
Expert:	-
<b>Combined Results:</b>	<b>167</b>

**Query History**

Number of queries:	3
<input type="button" value="Clear Query History"/>	
2020-08-20T14:08	167
2020-08-20T14:03	316

# 5. How to search for experimental metal-organic structures (MOFs)

ICSD Welcome to ICSD-Desktop. FIZ Karlsruhe | Contact

Results: List View # of Hits: 167 (1 selected)

Back to Query Show Detailed View Export Data Print Visualize Structure Visualize Powder Pattern Column Selection Filter

Coll. Code	HMS	Struct. Form.	Struct. Type	Title	Authors	Reference	Star	Download
<input type="checkbox"/> 2972	P 1 21/c 1	C12 H26 N2 Pb		Designing stability into the	Bacic, Goran; Zanders, Da	Inorganic Chemistry (2018)	☆	📄
<input checked="" type="checkbox"/> 3062	F d d Z	C105 H72 O33 Pb11		Syntheses, structures, lum	Xiao, Jun-Xia; Ma, De-Yun	Inorganica Chimica Acta (2018)	☆	📄
<input type="checkbox"/> 3211	P 21 21 21	C12 H10 N6 O9 Pb2		Six metal-organic framewo	Zhang, Qinke; Yue, Caiper	Inorganica Chimica Acta (2018)	☆	📄
<input type="checkbox"/> 3395	R -3 H	C168 H216 Br73 N24 Pb2		A nanowire array with two	Sun, Cai; Du, Ming-Xiu; Xu	Dalton Transactions (2018)	☆	📄
<input type="checkbox"/> 3529	C 1 2/c 1	C6 H2 O4 Pb S		Phosphorescence emissio	He, Jin-Yu; Deng, Zheng-F	Dalton Transactions (2018)	☆	📄
<input type="checkbox"/> 3604	P 1 21/n 1	C24 H26 N4 O4 Pb S2		Heterocyclic lead(II) thiou	Ketchemen, Kevin I.Y.; Mlc	Inorganica Chimica Acta (2018)	☆	📄
<input type="checkbox"/> 3716	P 1 21/c 1	C14 H8 N8 Pb1.90 S2		Four Zn/Pb complexes bas	Wang, Yu-Fei; Wang, Li-Pi	Zeitschrift fuer Anorganiscl	☆	📄
<input type="checkbox"/> 4562	P 1 21/c 1	Pb4 I4 (C2 H4 O2)2		Two new oxyiodoplumbate	Xiao, Hong; Zhou, Jian; Hu	Dalton Transactions (2018)	☆	📄
<input type="checkbox"/> 6334	P -1	C65 H143 Cl15 N8 Pb4		Blue emitting single crystal	Zhou, Chenkun; Lin, Haore	Journal of the American Cr	☆	📄
<input type="checkbox"/> 7068	C 1 2/c 1	C6 H12 I6 N6 Ni1 Pb2		Solvothermal synthesis, cr	Zhang, Limei; Tang, Chuny	European Journal of Inorg	☆	📄

(1 of 17) 1 2 3 4 5 6 7 8 9 10

Research paper

## Syntheses, structures, luminescent and catalytic properties of two 3D metal-organic frameworks

Jun-Xia Xiao<sup>a</sup>, De-Yun Ma<sup>b,✉</sup>

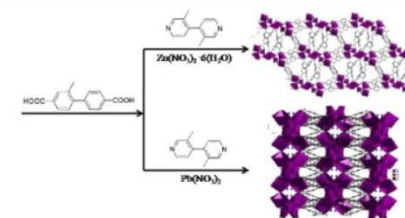
[Show more](#)

<https://doi.org/10.1016/j.ica.2018.07.054>

Inorganica Chimica Acta

Volume 483, 1 November 2018, Pages 6-11

Two new 3D metal-organic frameworks were obtained by reacting 2-methyl-4,4'-biphenyldicarboxylic acid and methyl-functionalized N-donor ligands with zinc(II) nitrate hexahydrate and/or lead(II) nitrate under hydrothermal condition. Furthermore, the luminescence of 1-2, and the catalytic activities of 1-2 for the degradation of methyl orange in a Fenton-like process have also investigated.



# Summary and Perspectives

- How to search for:
  - experimentally observed (synthesized) inorganic structures
  - new predicted (not-yet synthesized) structures or materials
  - parameters for method development and future calculations
  - experimental and theoretical data on nanostructures
  - experimental metal-organic structures (MOFs)
- Enables searches for group of structures/data with common descriptors (data mining, machine learning, etc.)



# Summary and Perspectives

- Reliable databases (such as CSD and ICSD), and crystal structure data of high quality can serve as an excellent tool in pandemic situation worldwide with less possibilities for performing experiments
- Border line between organic and inorganic materials is not strict
- Generation of a common search interface to provide researchers with easy access to the entire data set of inorganic and organic crystal structures (CSD&ICSD), trying to keep the content and increase the amount of data in the fields, especially with regard to data mining projects [1].



From the journal:  
**Dalton Transactions**

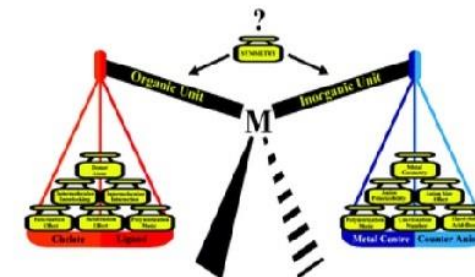
## Coordination chemistry of mercury(II) halide complexes: a combined experimental, theoretical and (ICSD & CSD) database study on the relationship between inorganic and organic units†

Ali Samie, <sup>a</sup> Alireza Salimi <sup>\*a</sup> and Jered C. Garrison <sup>b</sup>

### Article information

<https://doi.org/10.1039/D0DT01541E>

Submitted	27 Apr 2020
Accepted	31 Jul 2020
First published	01 Aug 2020



# Thank you for your attention and stay healthy!

## Your comments and suggestions are welcome as well as theoretical CIF files which you can send to: [crysddata@fiz-karlsruhe.de](mailto:crysddata@fiz-karlsruhe.de)

### Contact

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# Next steps

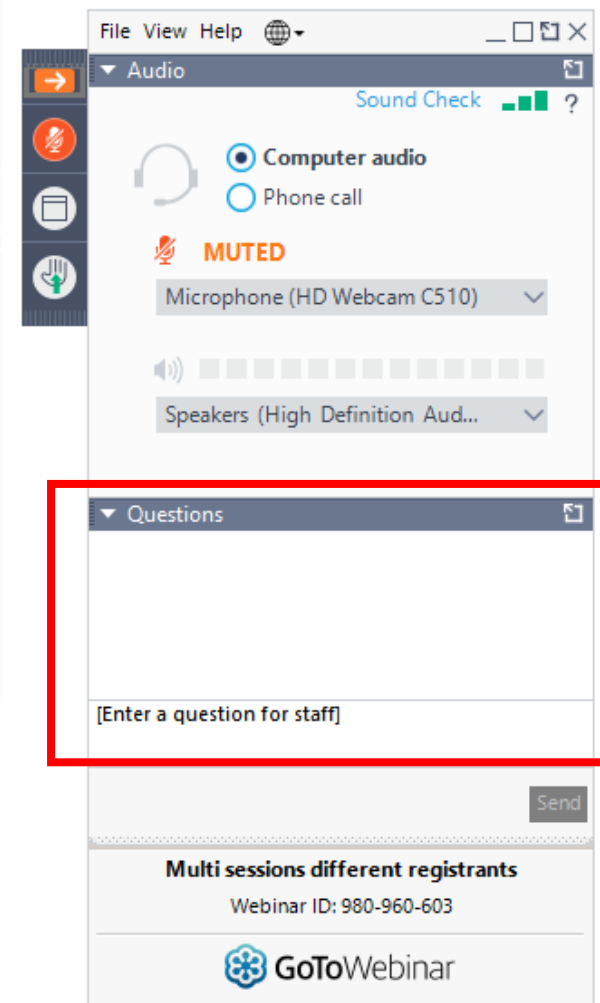
This webinar and our recent survey were designed to explore your need for a more advanced search interface across the CSD and the ICSD

## What next?

- Short Q&A session today
- Slides and recording available via CCDC and FIZ Karlsruhe websites
- We want to know more about your requirements and priorities
  - Interactive discussion session 7<sup>th</sup> October 2020

# Q&A

- Type your questions in the box as shown
- We will try to answer your questions and if we don't get time to answer them all we will get back to you after the webinar with a response



The screenshot displays the GoToWebinar interface. At the top, there is a menu bar with 'File', 'View', and 'Help'. Below it, the 'Audio' settings panel is visible, showing 'Computer audio' selected and 'Phone call' unselected. A 'MUTED' indicator is present, along with a 'Sound Check' button and a volume icon. The microphone is identified as 'Microphone (HD Webcam C510)' and the speakers as 'Speakers (High Definition Aud...'. A 'Questions' panel is highlighted with a red border, containing a text input field with the placeholder text '[Enter a question for staff]' and a 'Send' button. Below the input field, the text 'Multi sessions different registrants' and 'Webinar ID: 980-960-603' is displayed, followed by the GoToWebinar logo.

# Thank you

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