Joint CCDC and FIZ Karlsruhe Webinar

Advancing our collaboration

27th August 2020

CCDC
advancing structural science

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

CCDC

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
Follow us on:
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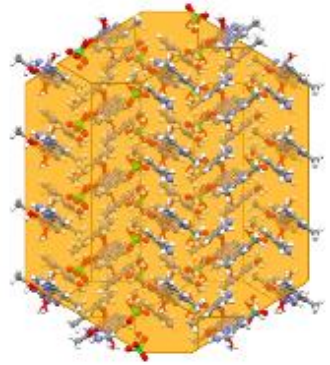
www.ccdc.cam.ac.uk

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



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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.

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

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

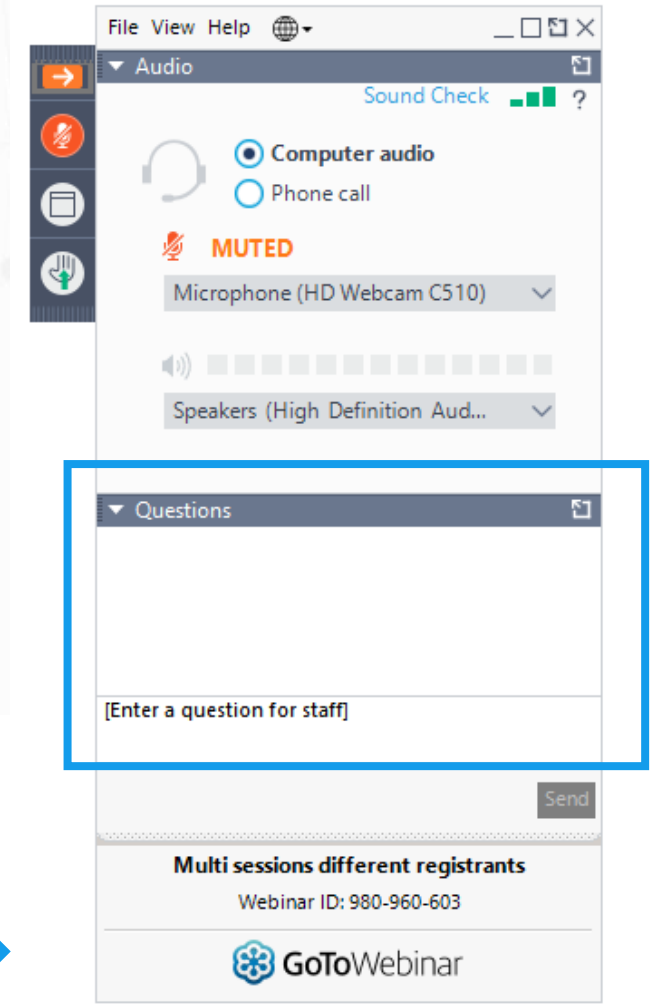
Product Manager ICSD

FIZ Karlsruhe

CCDC

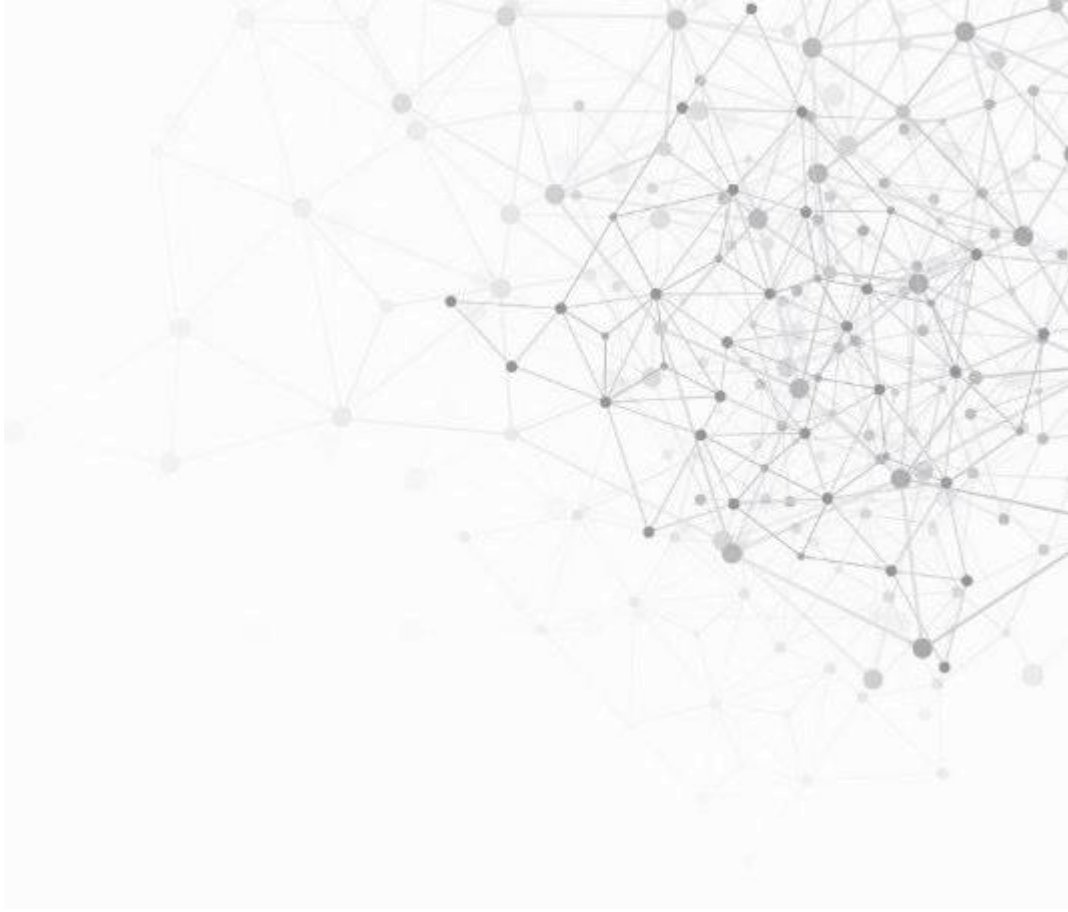
Today's agenda

- 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



The CSD

Suzanna Ward



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advancing structural science

The vision

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

- 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

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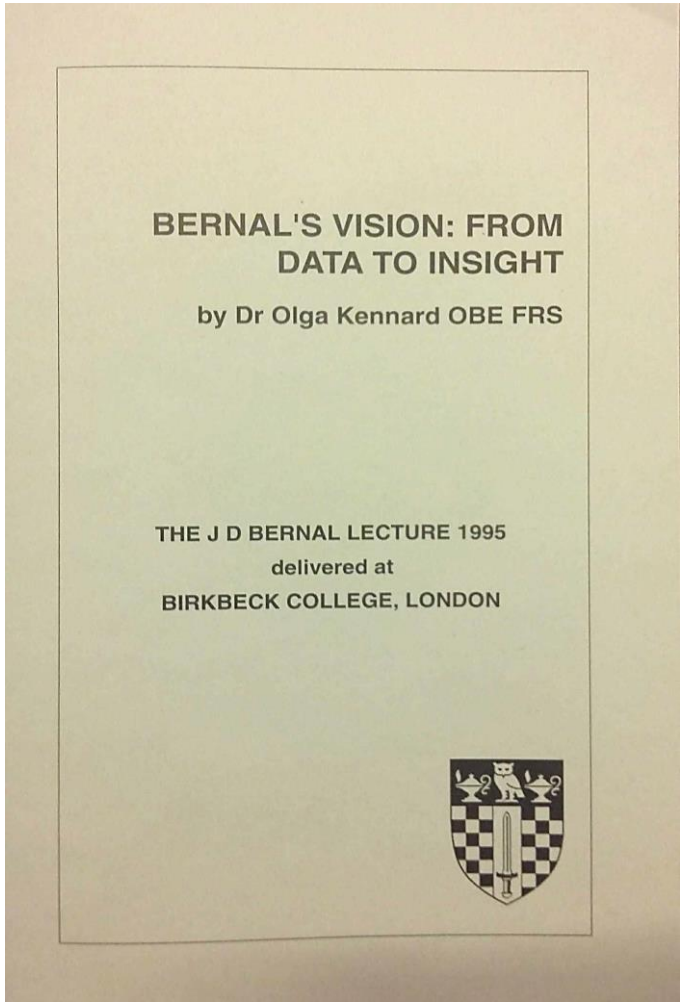
The vision



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)

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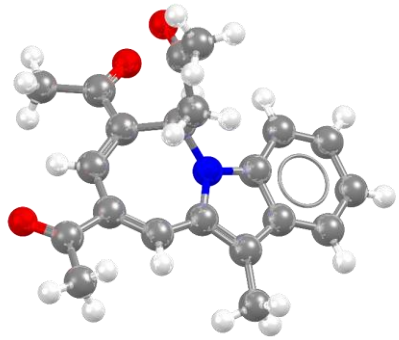
The Cambridge Structural Database (CSD)



An N-heterocycle produced by a chalcogen-bonding catalyst. Determined by Yao Wang and his team.

XOPCAJ - The millionth CSD structure.

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

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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

Not Polymeric
89%

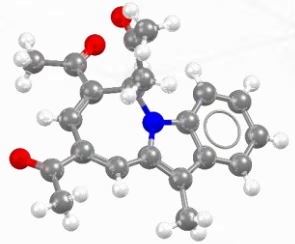
Polymeric: 11%

Single Component
56%

Multi Component
44%

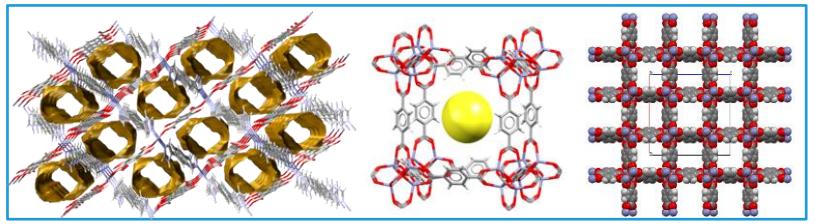
Organic

- Drugs
- Agrochemicals
- Pigments
- Explosives
- Protein ligands



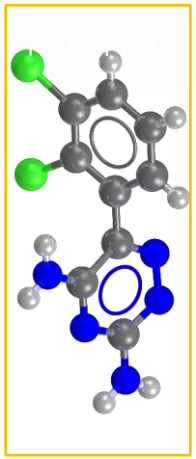
Metal-Organic

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



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



Links/subsets

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

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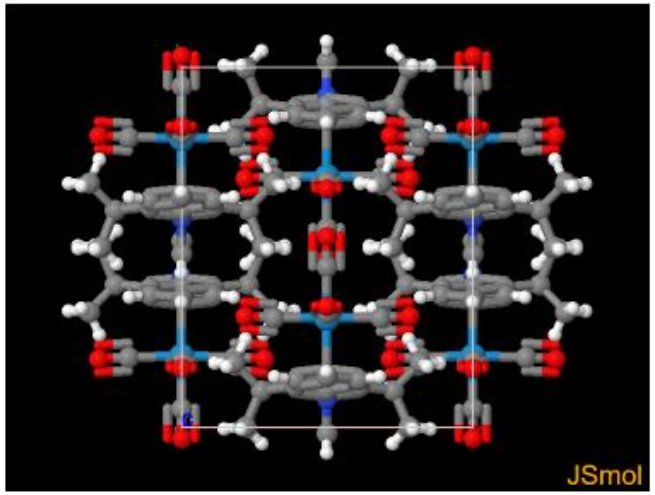
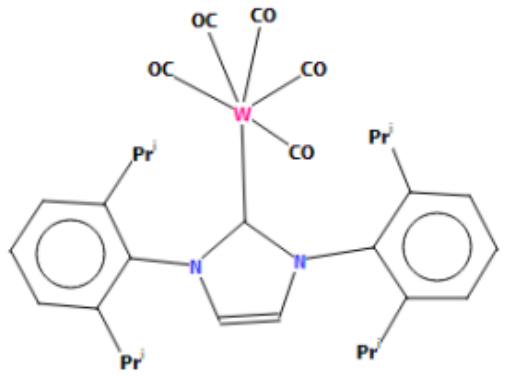
The CSD

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, *α* 90° *β* 90° *γ* 90°





Crystal details	
Habit	lensoid
Colour	yellow

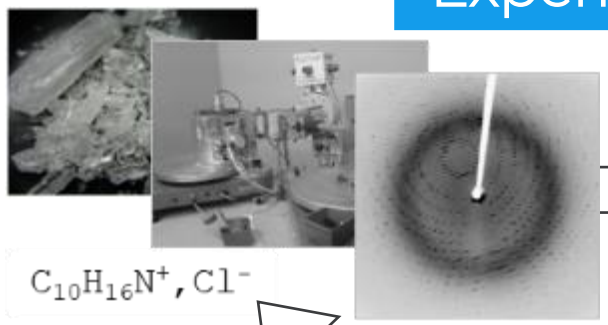
Associated publications

Rajendra S. Ghadwal, Dennis Rottschäfer, Diego M. Andrada, Gernot Frenking, Christian J. Schürmann, Hans-Georg Stammler, *Dalton Transactions*, 2017, 46, 7791, DOI: 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



$C_{10}H_{16}N^+,Cl^-$

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_diffrn_ambient_temperature      90(2)
_diffrn_radiation_type           MoK\a
_diffrn_radiation_wavelength     0.71073
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  'Bruker APEX CCD area-detector'
_diffrn_measurement_method       '\w and \o'
_diffrn_detector_area_resol_mean 512
_diffrn_refins_number            5892

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_adp_type
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_disorder_assembly
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Cl Cl1 0.23185(8) 0.78305(9) 0.55574(6) 0.02213(16) Uani d . 1 1 . .
N N1 0.8031(3) 0.6811(3) 0.5363(2) 0.0172(4) Uani d U 1 1 . .
C C1 0.6896(4) 0.7867(6) 0.4357(2) 0.0224(5) Uani d U 1 1 . .
C C2 0.7510(5) 0.8922(5) 0.7083(3) 0.0256(6) Uani d U 1 1 . .
C C3 0.7409(4) 0.6944(4) 0.6644(3) 0.0187(5) Uani d U 1 1 . .
C C4 0.8700(4) 0.5637(4) 0.7481(3) 0.0236(6) Uani d U 1 1 . .
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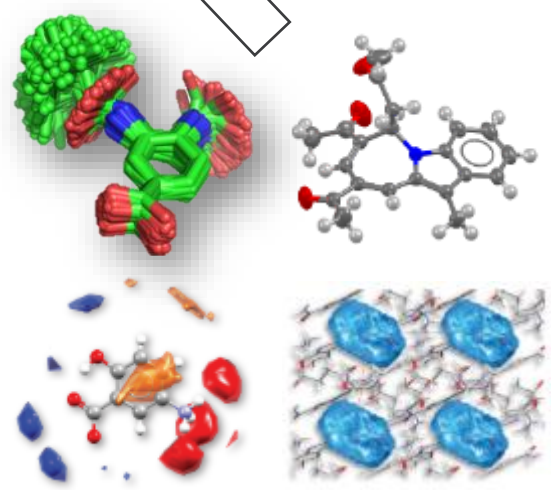
Ritonavir: An Extraordinary Example of Conformational Polymorphism

Abstract

Purpose. In the summer of 1998, Norvir semi-solid capsules supplies 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.



CCDC

Knowledge

CCDC

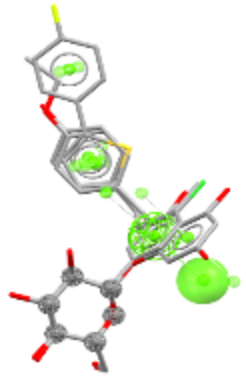
The CSD software

Software enabling research across the breadth of structural science

CSD-Enterprise

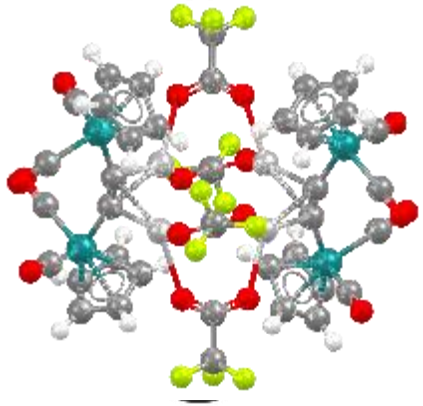
All CCDC application software (available to all Academics)

CSD-Discovery



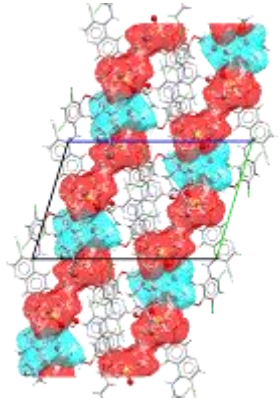
To discover new molecules with pharmaceutical applications

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

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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

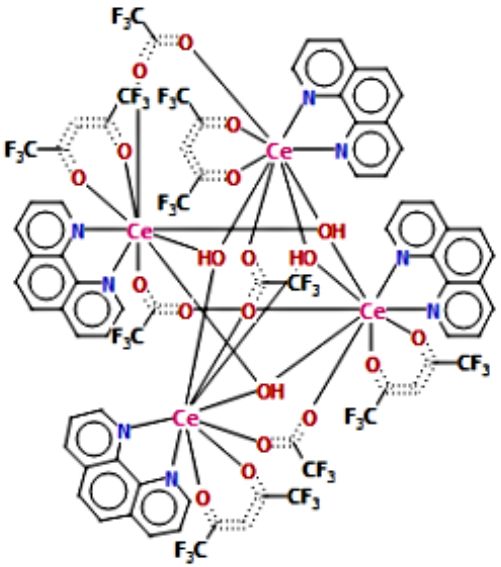
→ inorganic compounds, minerals, elements, metals and alloys

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

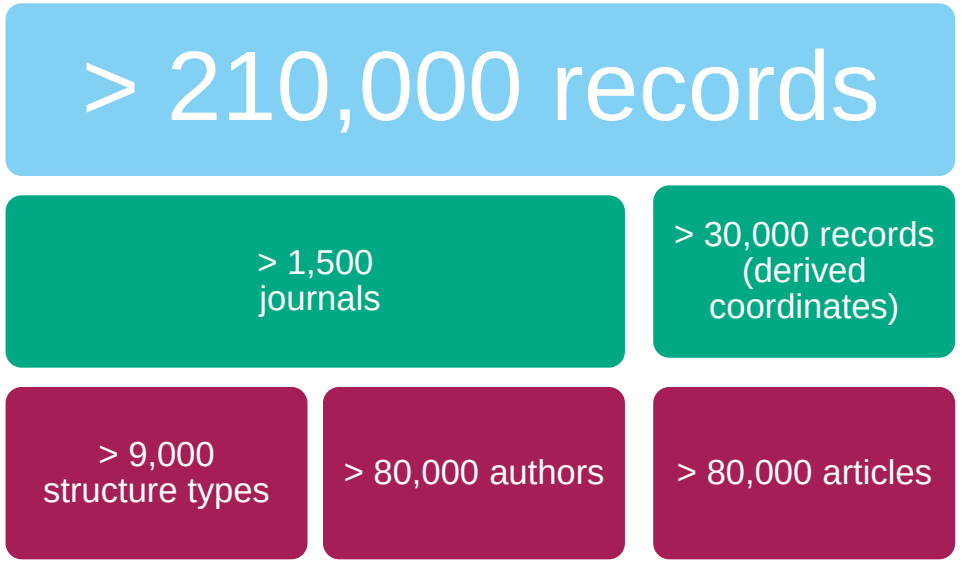
plus similar compounds with partly organic ligands



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 mash



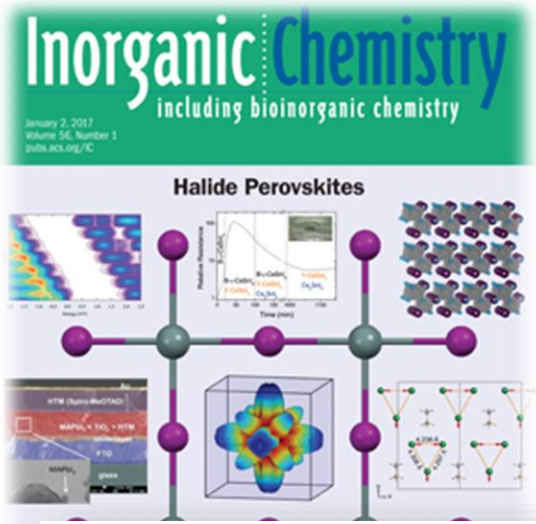
Theoretical structures in ICSD

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
$CaMnO_3$-(1) *Pnma* (62) Ca 4*c* Mn 4*b* O1 4*c* O2 8*d*	(Bozin *et al.*, 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
$CaMnO_3$-(2) $R\bar{3}c$ (167) Ca 6*a* Mn 6*b* O 18*e*	(Yanchevskii *et al.*, 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
$CaMnO_3$-(3) *Imma* (74) Ca 4*e* Mn 4*b*	(Damay *et al.*, 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

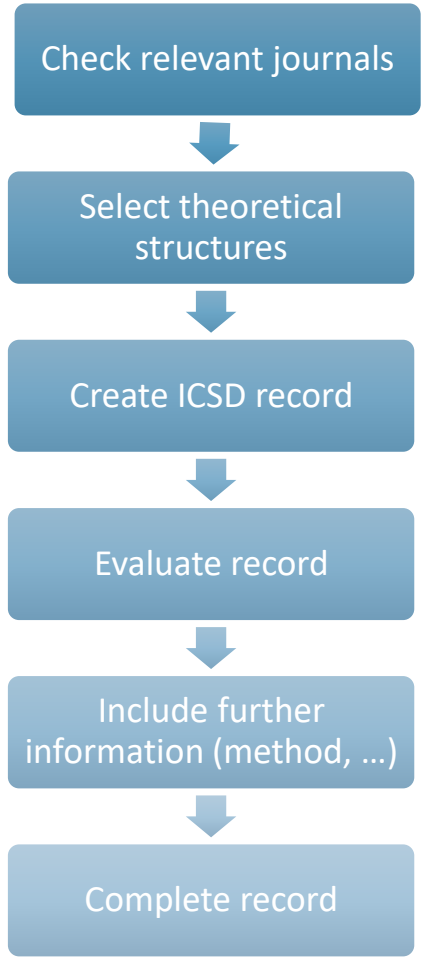
Theoretical structures in ICSD

Selection criteria

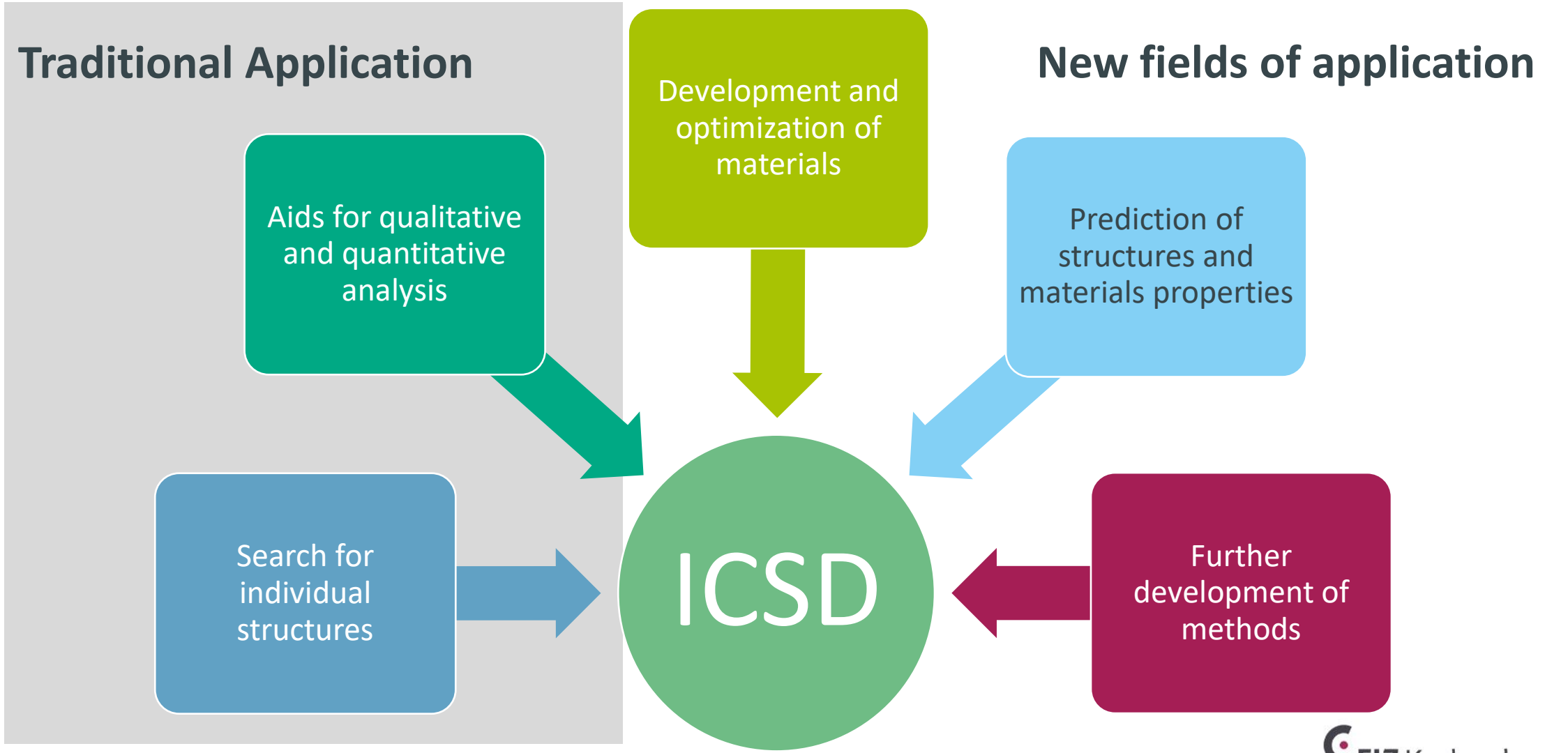
- Publication in a peer-review journal
- calculated minimum of total energy (E_{tot})
- If more than one method is used (comparison), the one with results closest to experimental results is chosen

Important information for theoretical structures

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



Typical applications of ICSD in crystallography and material science



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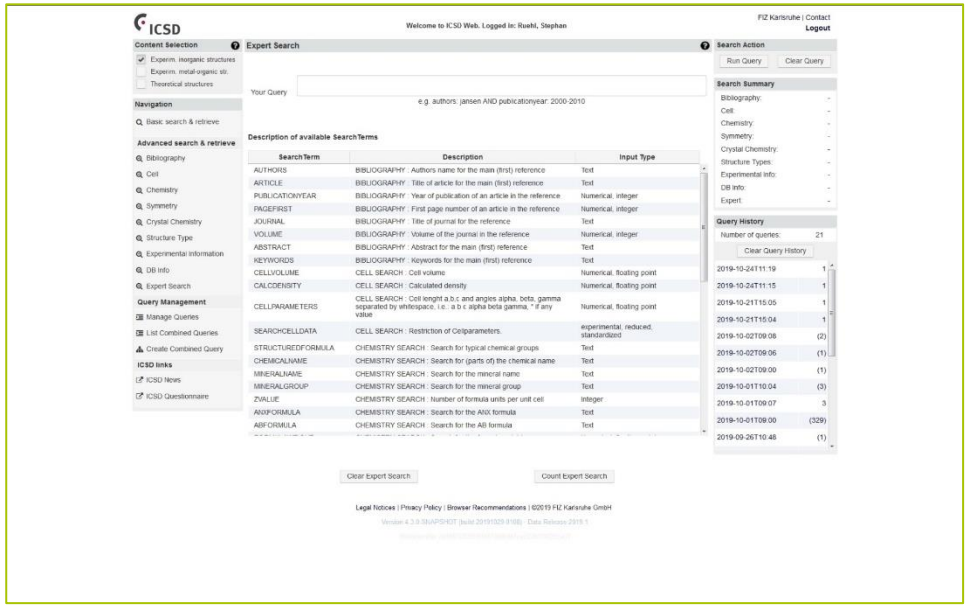
Recent developments

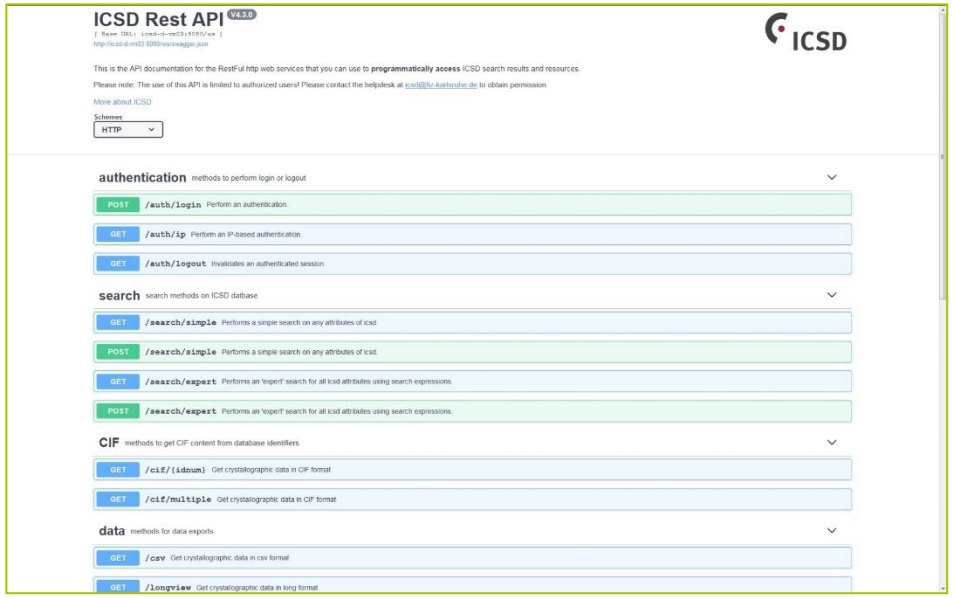
Expert Search



Set up complex search queries using:

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

ICSD Rest API



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

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

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

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

The CCDC and FIZ Karlsruhe collaboration

Suzanna Ward and Matt Lightfoot

CCDC

advancing structural science

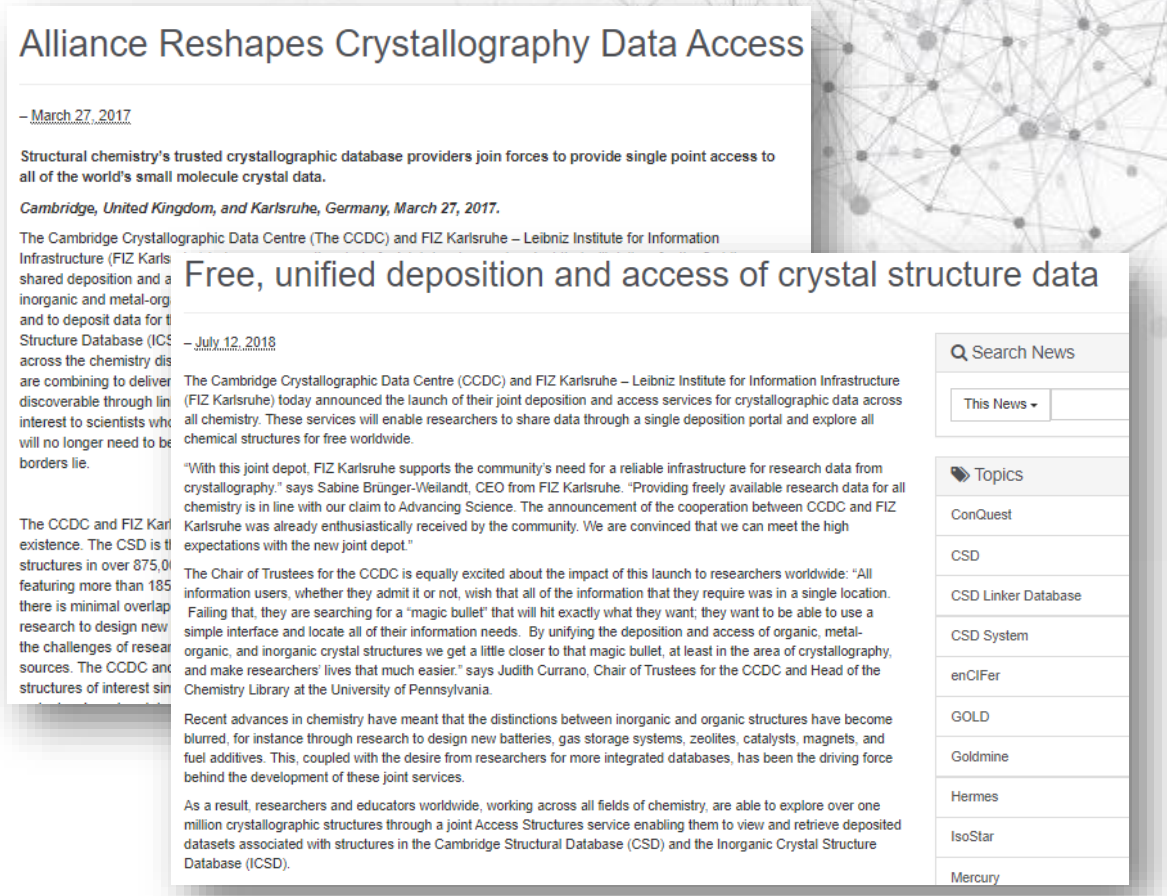
The CCDC and FIZ Karlsruhe

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure

Partnership goal: Connecting data resources, increase discoverability and simplify deposition of organic, metal-organic and inorganic structural data.

A good fit:

- Established, trusted databases
- Value quality and high levels of curation
- Comprehensive
- Shared communities



Alliance Reshapes Crystallography Data Access

– March 27, 2017

Structural chemistry's trusted crystallographic database providers join forces to provide single point access to all of the world's small molecule crystal data.

Cambridge, United Kingdom, and Karlsruhe, Germany, March 27, 2017.

The Cambridge Crystallographic Data Centre (The CCDC) and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karls
shared deposition and a
inorganic and metal-org
and to deposit data for t
Structure Database (ICS
across the chemistry dis
are combining to deliver
discoverable through lin
interest to scientists who
will no longer need to be
borders lie.

The CCDC and FIZ Karl
existence. The CSD is t
structures in over 875,0
featuring more than 185
there is minimal overlap
research to design new
the challenges of resear
sources. The CCDC and
structures of interest sin

Free, unified deposition and access of crystal structure data

– July 12, 2018

The Cambridge Crystallographic Data Centre (CCDC) and FIZ Karlsruhe – Leibniz Institute for Information Infrastructure (FIZ Karlsruhe) today announced the launch of their joint deposition and access services for crystallographic data across all chemistry. These services will enable researchers to share data through a single deposition portal and explore all chemical structures for free worldwide.

"With this joint depot, FIZ Karlsruhe supports the community's need for a reliable infrastructure for research data from crystallography." says Sabine Brünger-Weilandt, CEO from FIZ Karlsruhe. "Providing freely available research data for all chemistry is in line with our claim to Advancing Science. The announcement of the cooperation between CCDC and FIZ Karlsruhe was already enthusiastically received by the community. We are convinced that we can meet the high expectations with the new joint depot."

The Chair of Trustees for the CCDC is equally excited about the impact of this launch to researchers worldwide: "All information users, whether they admit it or not, wish that all of the information that they require was in a single location. Failing that, they are searching for a "magic bullet" that will hit exactly what they want; they want to be able to use a simple interface and locate all of their information needs. By unifying the deposition and access of organic, metal-organic, and inorganic crystal structures we get a little closer to that magic bullet, at least in the area of crystallography, and make researchers' lives that much easier." says Judith Currano, Chair of Trustees for the CCDC and Head of the Chemistry Library at the University of Pennsylvania.

Recent advances in chemistry have meant that the distinctions between inorganic and organic structures have become blurred, for instance through research to design new batteries, gas storage systems, zeolites, catalysts, magnets, and fuel additives. This, coupled with the desire from researchers for more integrated databases, has been the driving force behind the development of these joint services.

As a result, researchers and educators worldwide, working across all fields of chemistry, are able to explore over one million crystallographic structures through a joint Access Structures service enabling them to view and retrieve deposited datasets associated with structures in the Cambridge Structural Database (CSD) and the Inorganic Crystal Structure Database (ICSD).

Search News

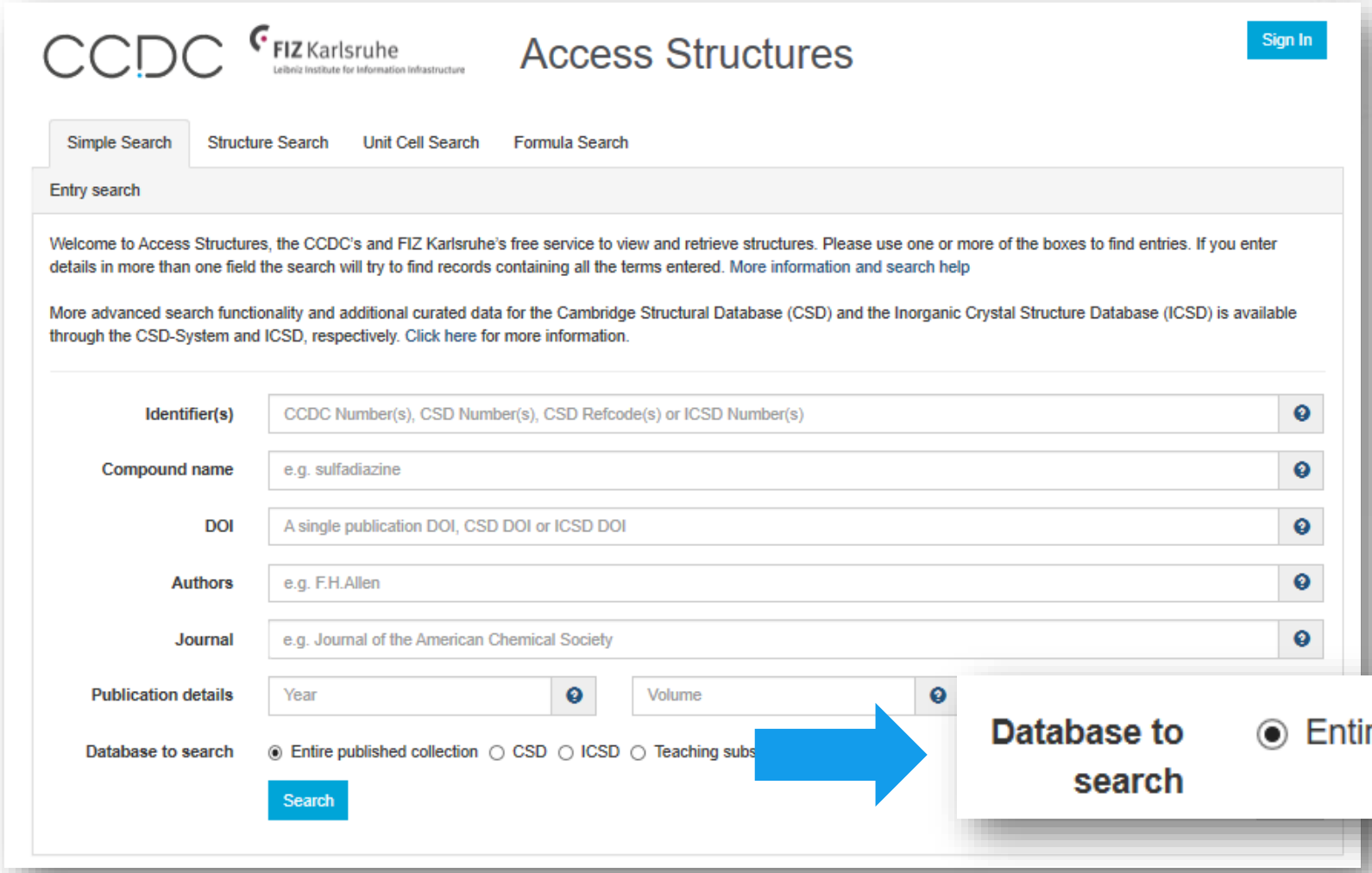
This News

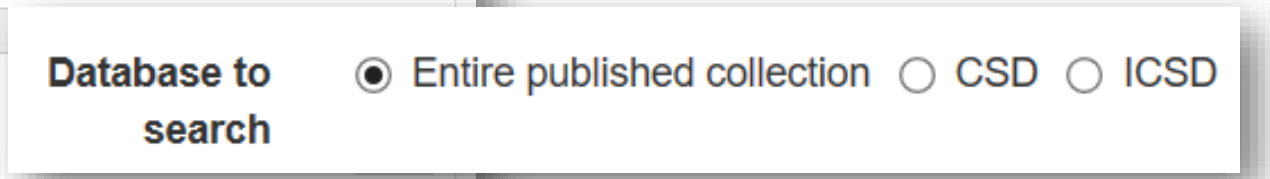
Topics

ConQuest
CSD
CSD Linker Database
CSD System
enCIFer
GOLD
Goldmine
Hermes
IsoStar
Mercury

CCDC

Joint services - Access





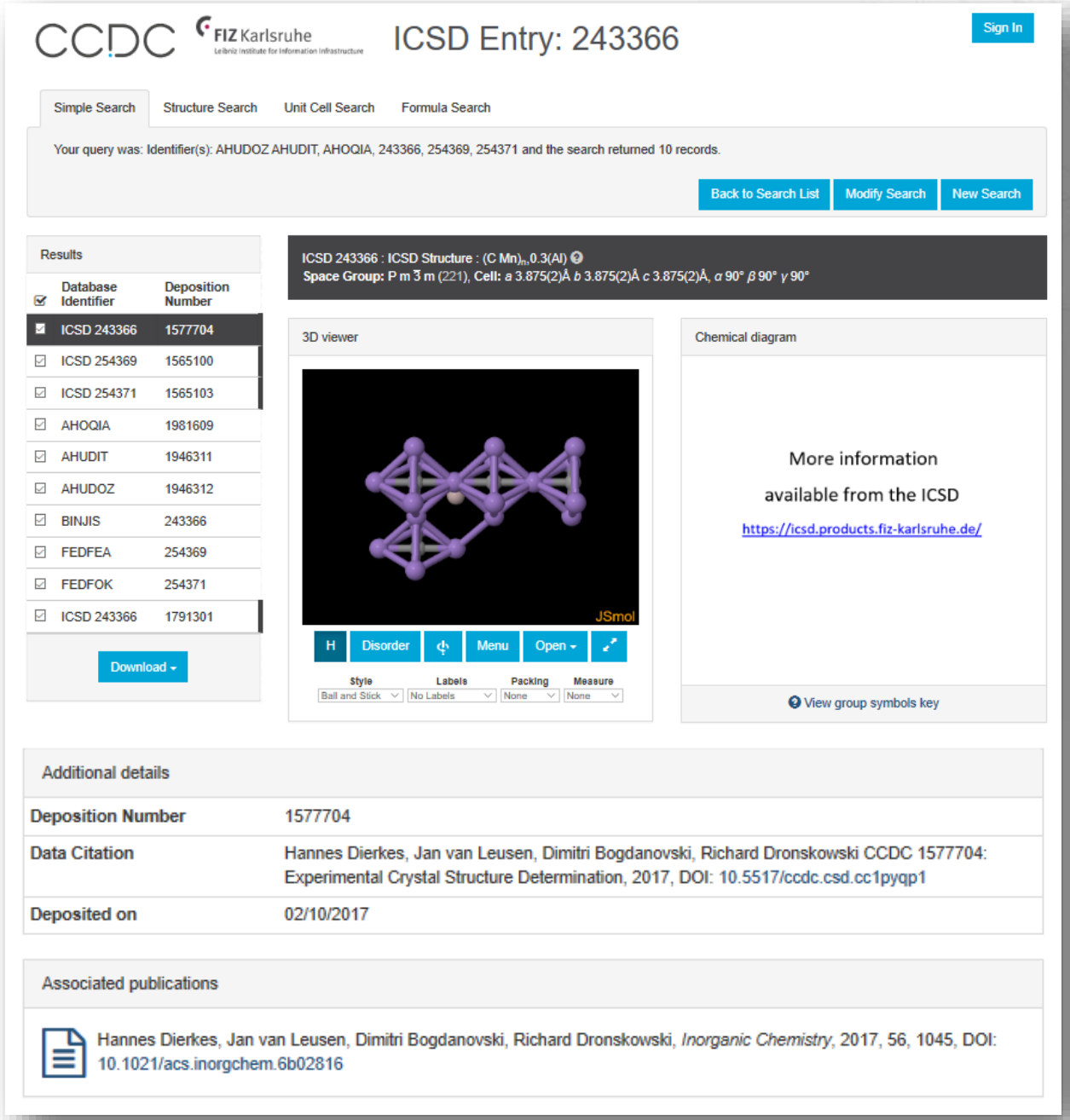
- Free to access
- Ability to search across the CSD and the ICSD

CCDC

CSD and ICSD entries

Download deposited CIF, hkl, checkCIF

Link to article

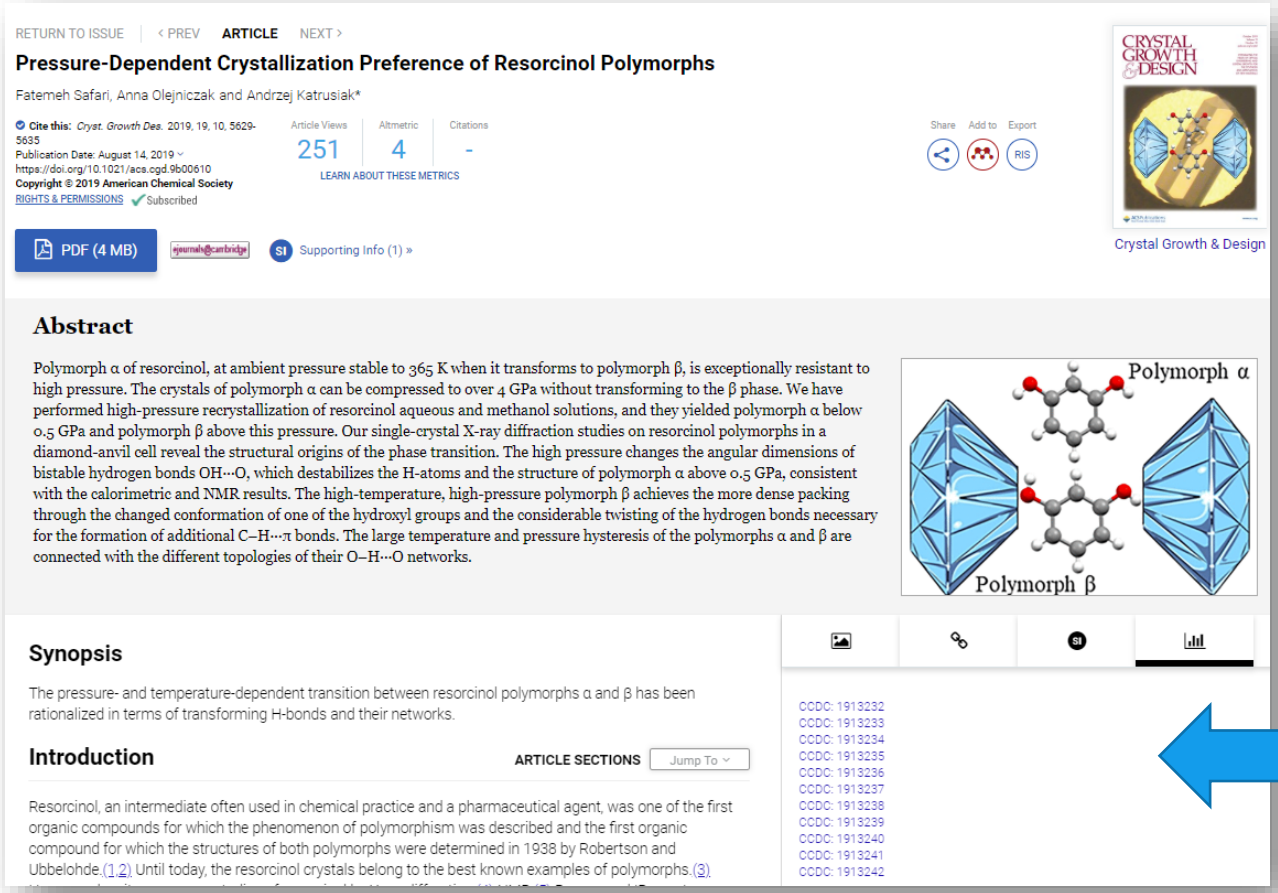


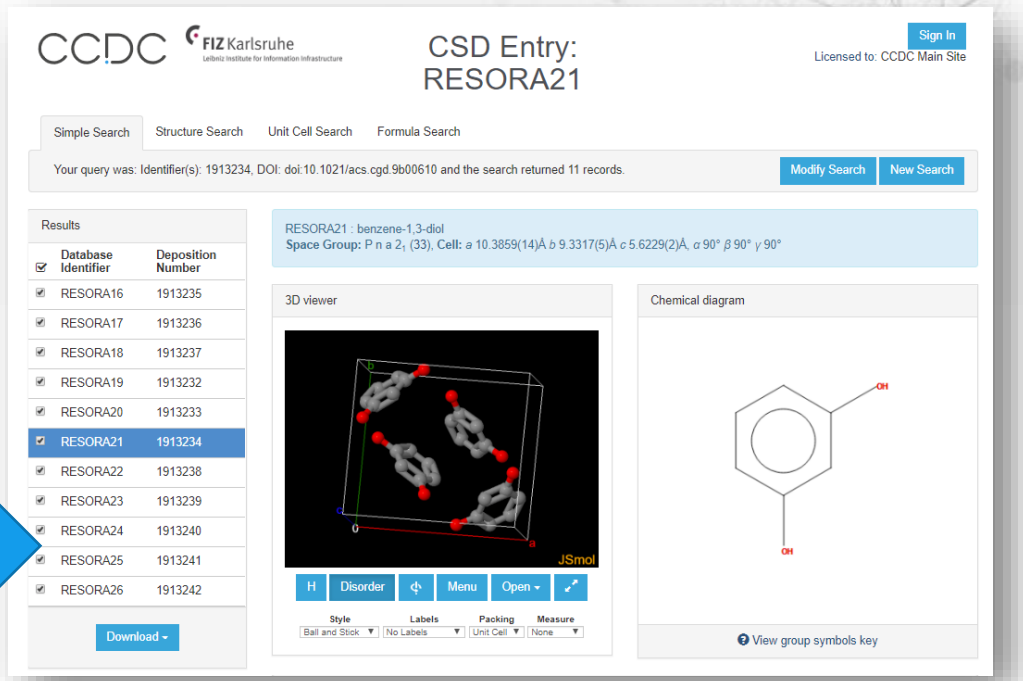
3D representation and link to ICSD

Data citation including Data DOI

CCDC

Links to and from publications





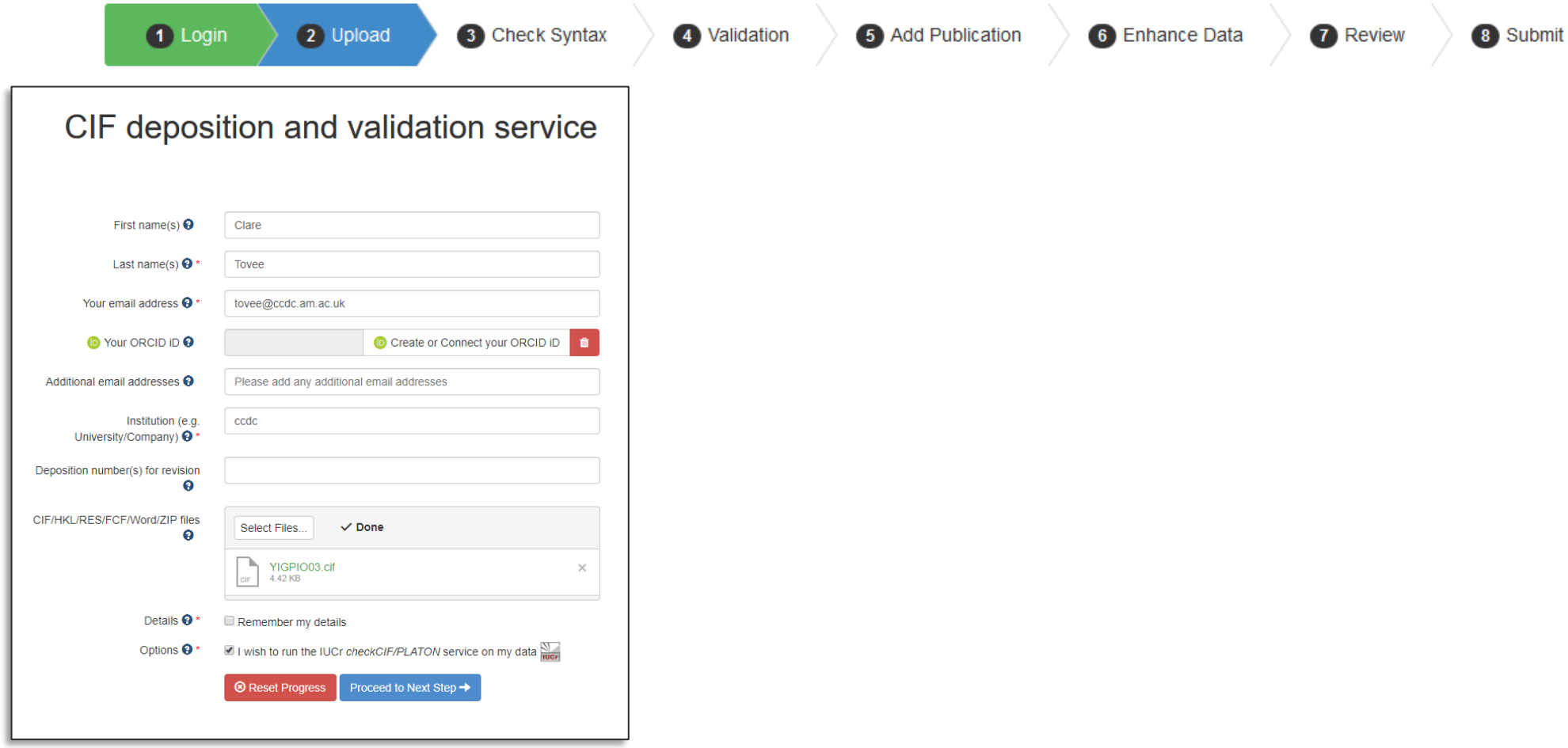
CCDC

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

CCDC

Joint services - Deposition



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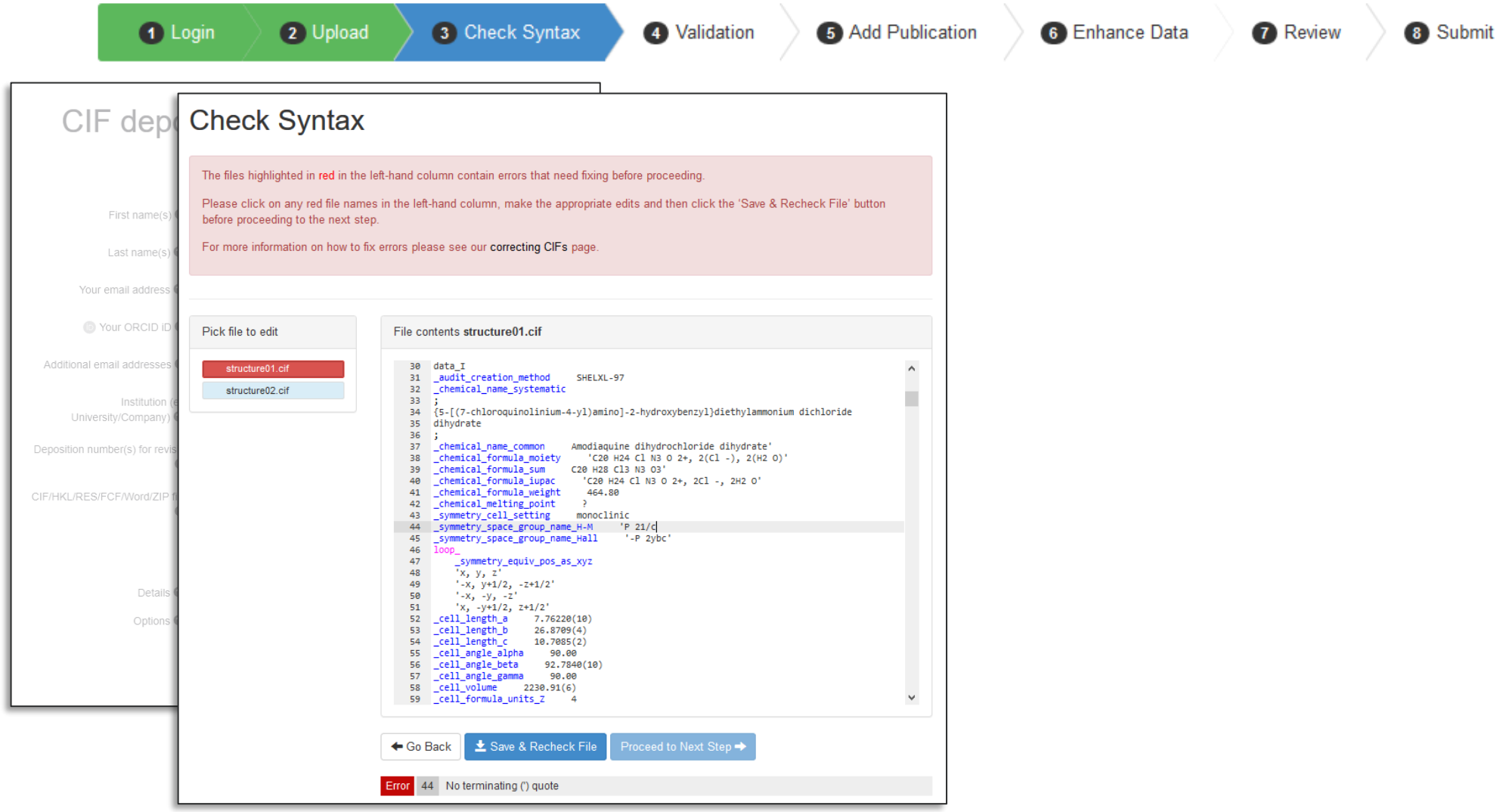
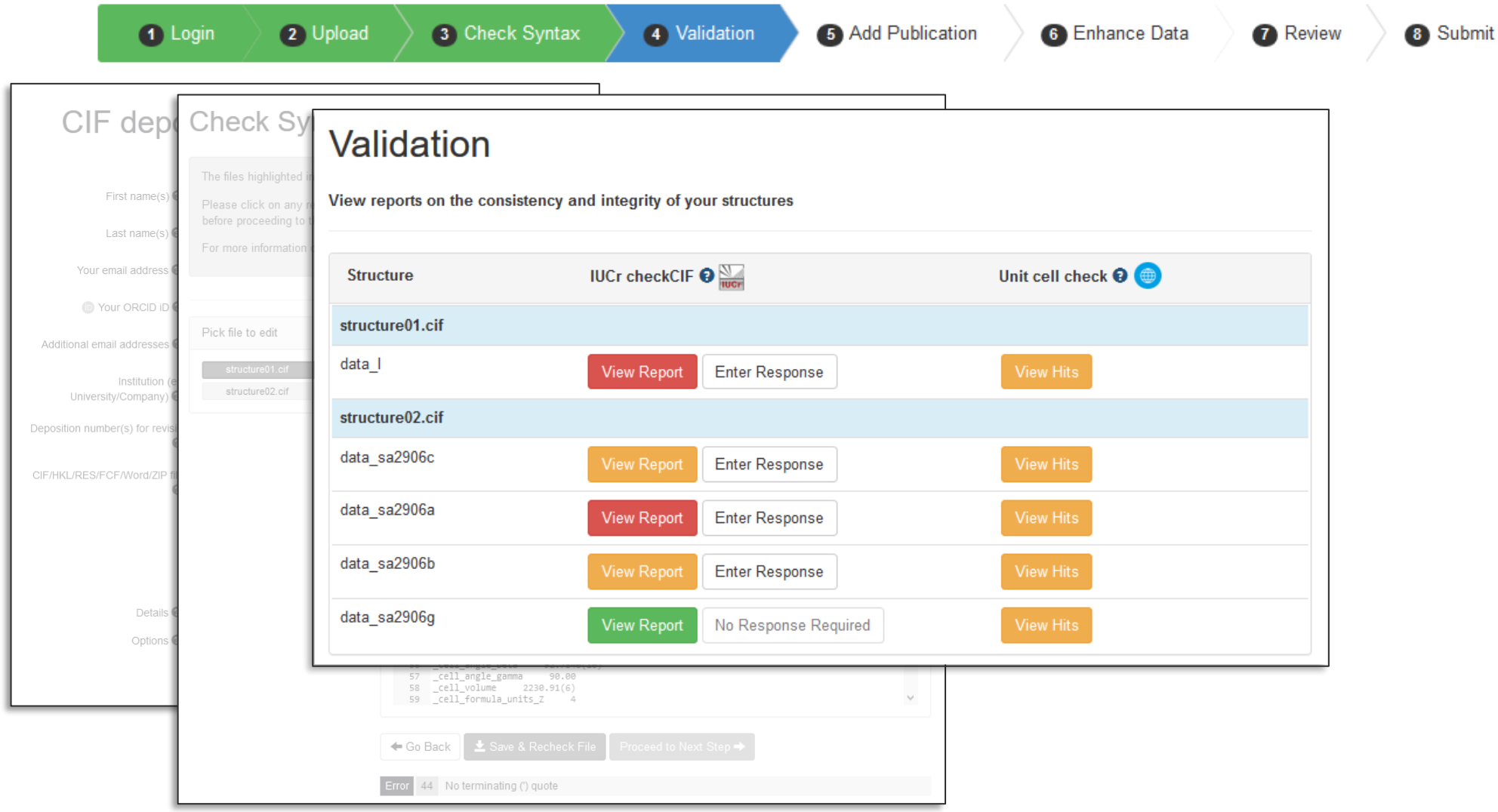


Joint services - Deposition



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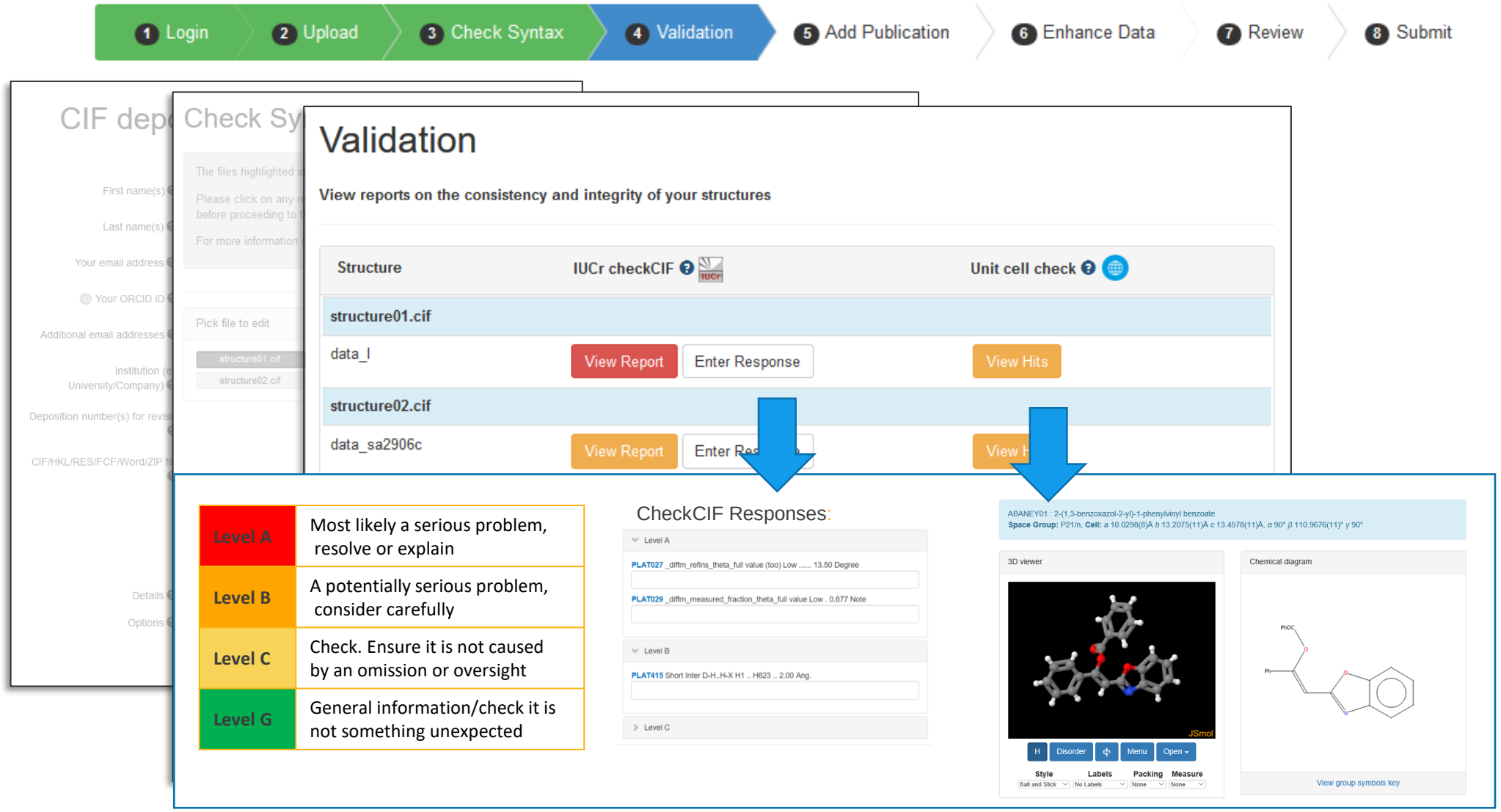
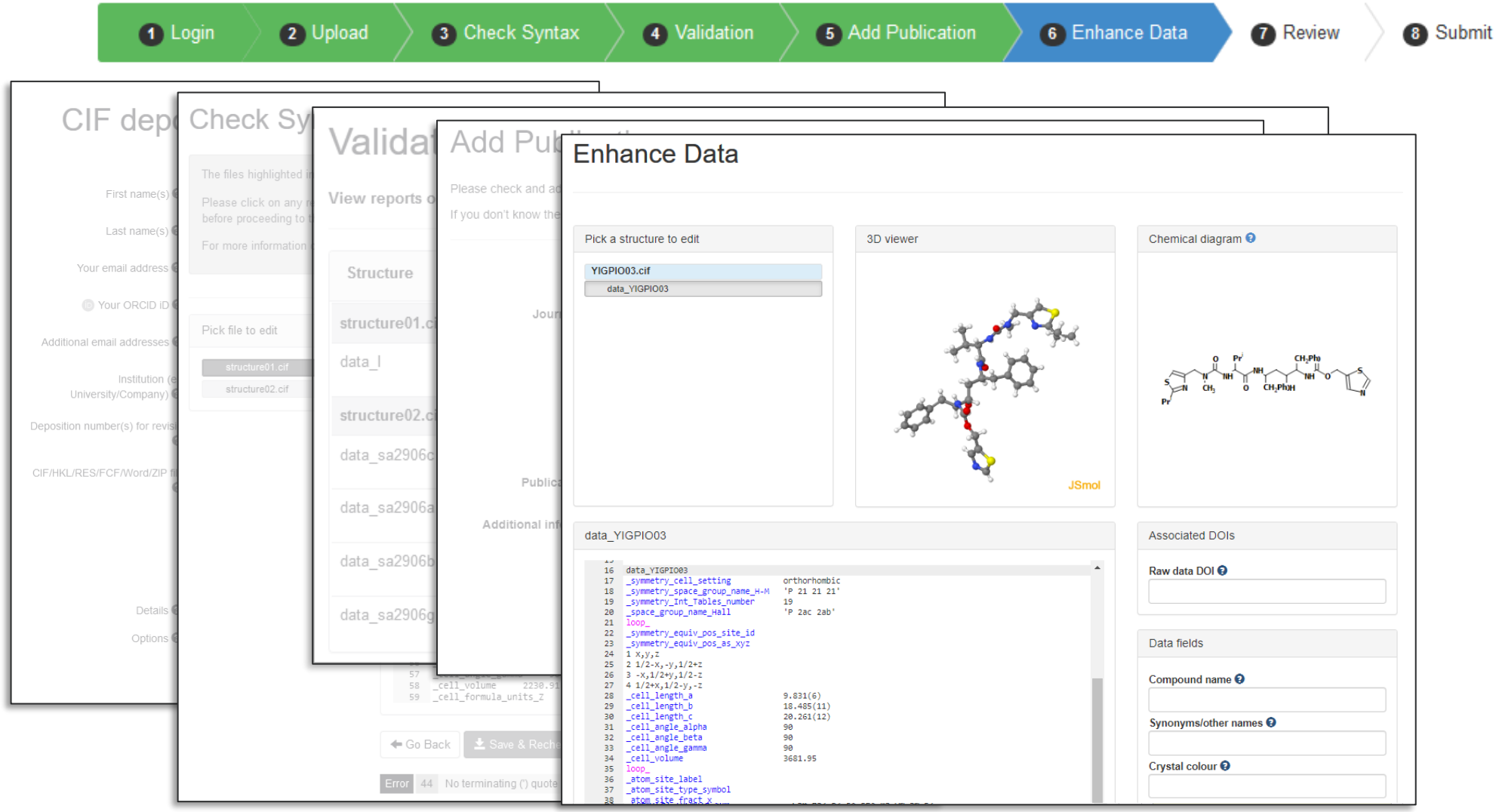
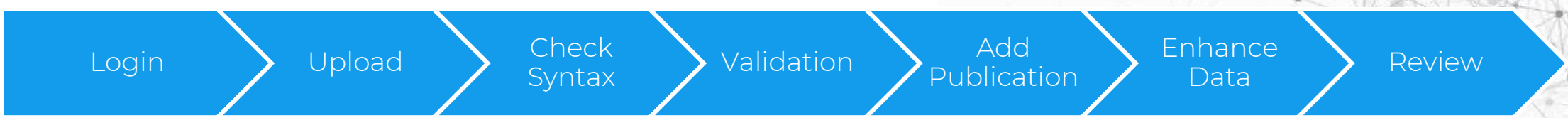


Joint services - Deposition



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*

CCDC

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

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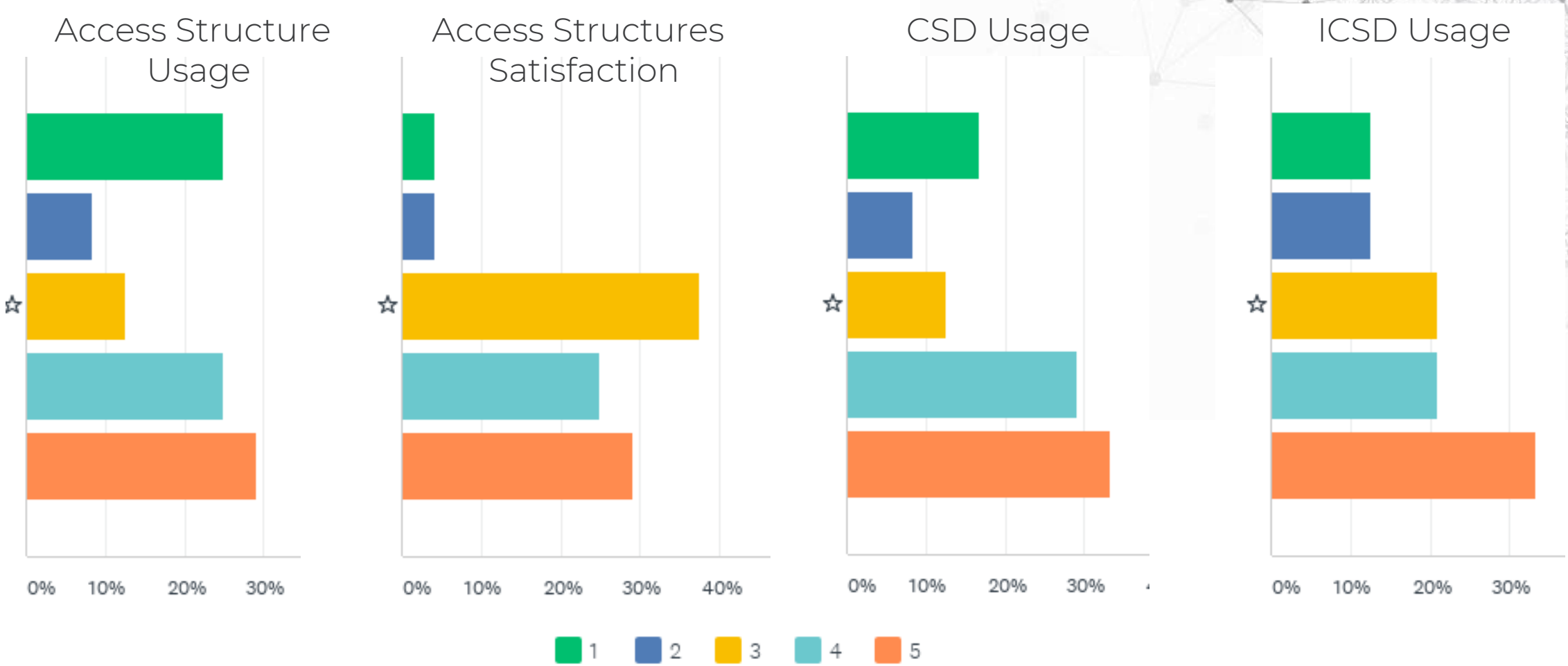
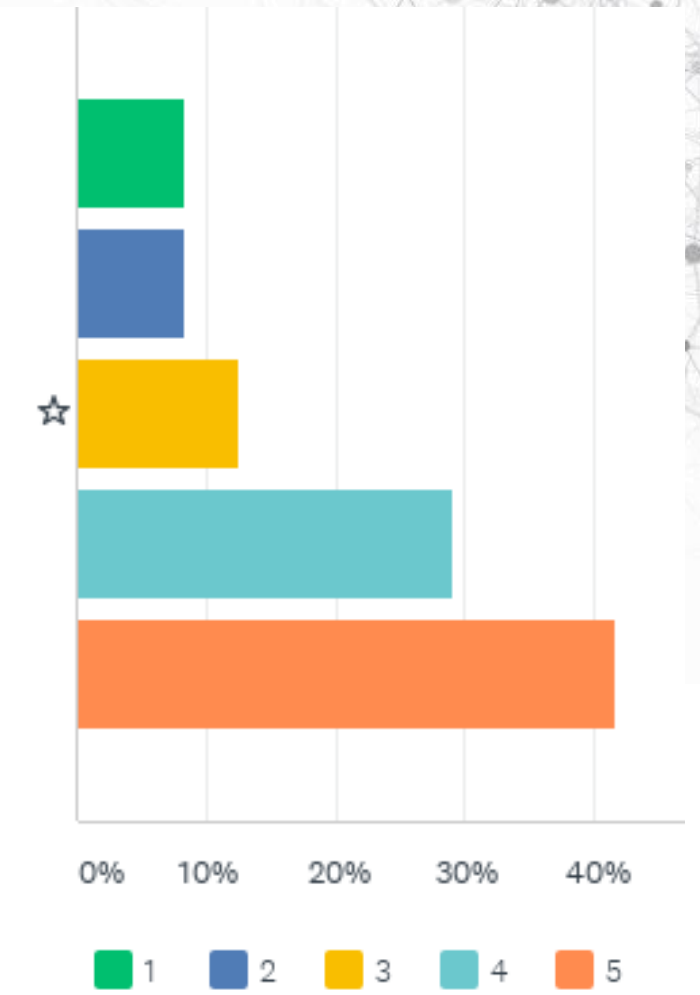
Survey results



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

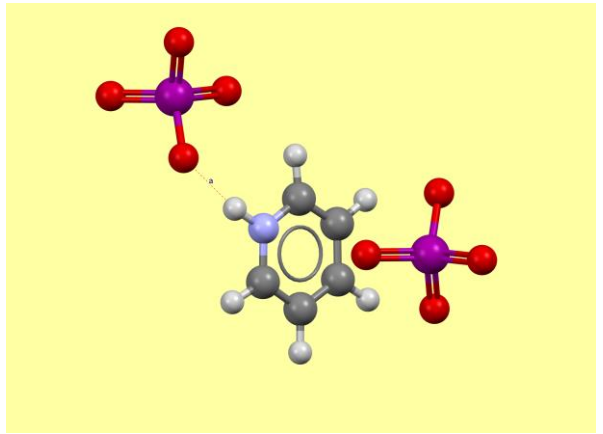
Paul Raithby

Department of Chemistry, University of Bath, UK

E-mail: p.r.raithby@bath.ac.uk

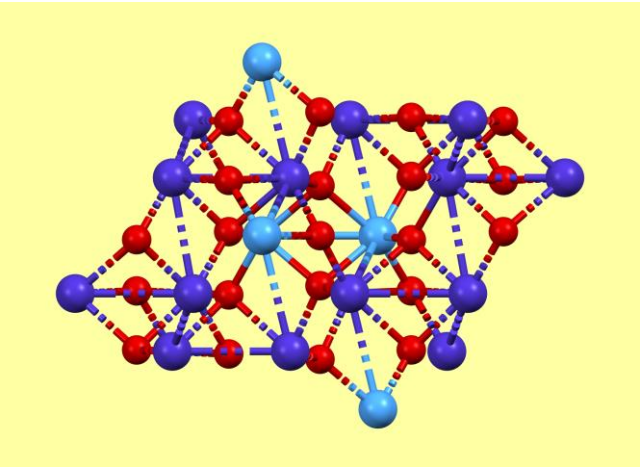
Structural Science Areas where there are Advantages in Searching the CSD and ICSD

- 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



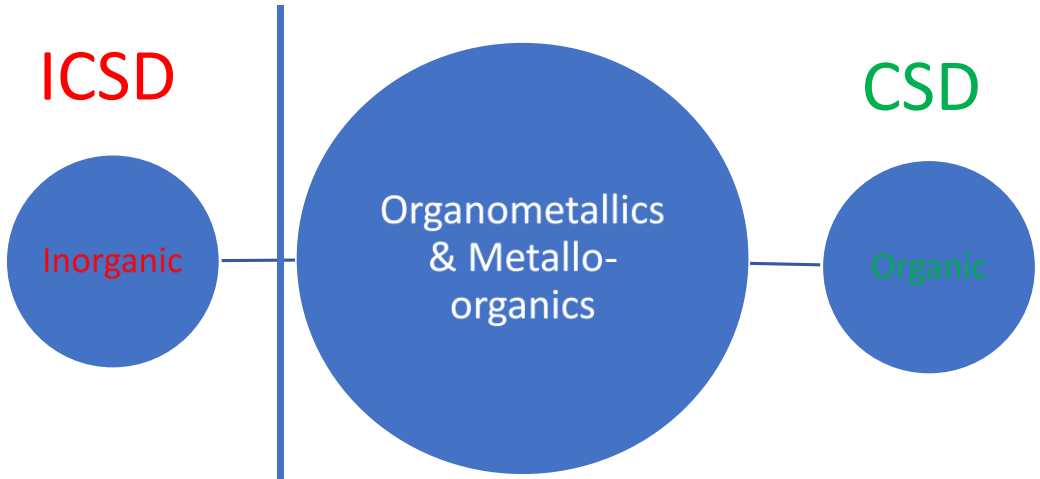
Pyridinium periodate

Co4(Nb2O9)



Contents of the two Databases

ORGANIC AND INORGANIC SALTS



[A][B]

[Inorganic][Inorganic]

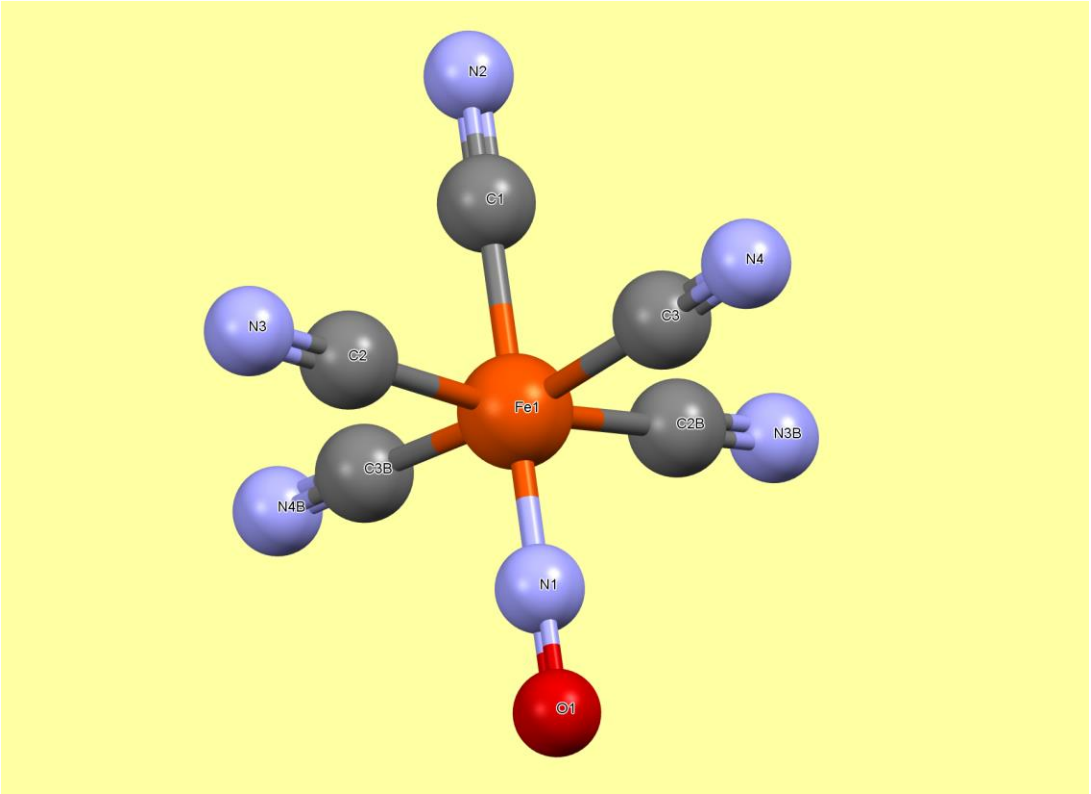
[Inorganic][Organic]

[Organic][Inorganic]

[Organic][Organic]

A Simple Example – the Nitroprusside Dianion

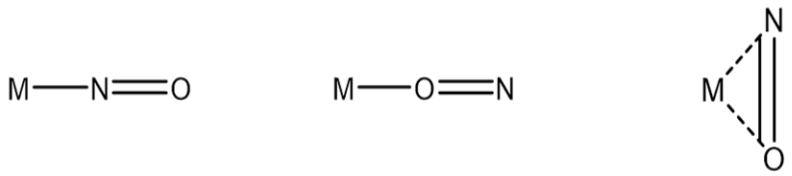
- CSD
  - 30 hits –with one or more organic or organometallic/metallo-organic cations
- ICSD
  - 42 hits – with inorganic cations such as Na^{+}, Ca^{2+}
- Some overlap between the two databases but two distinct sets that could be combined.



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

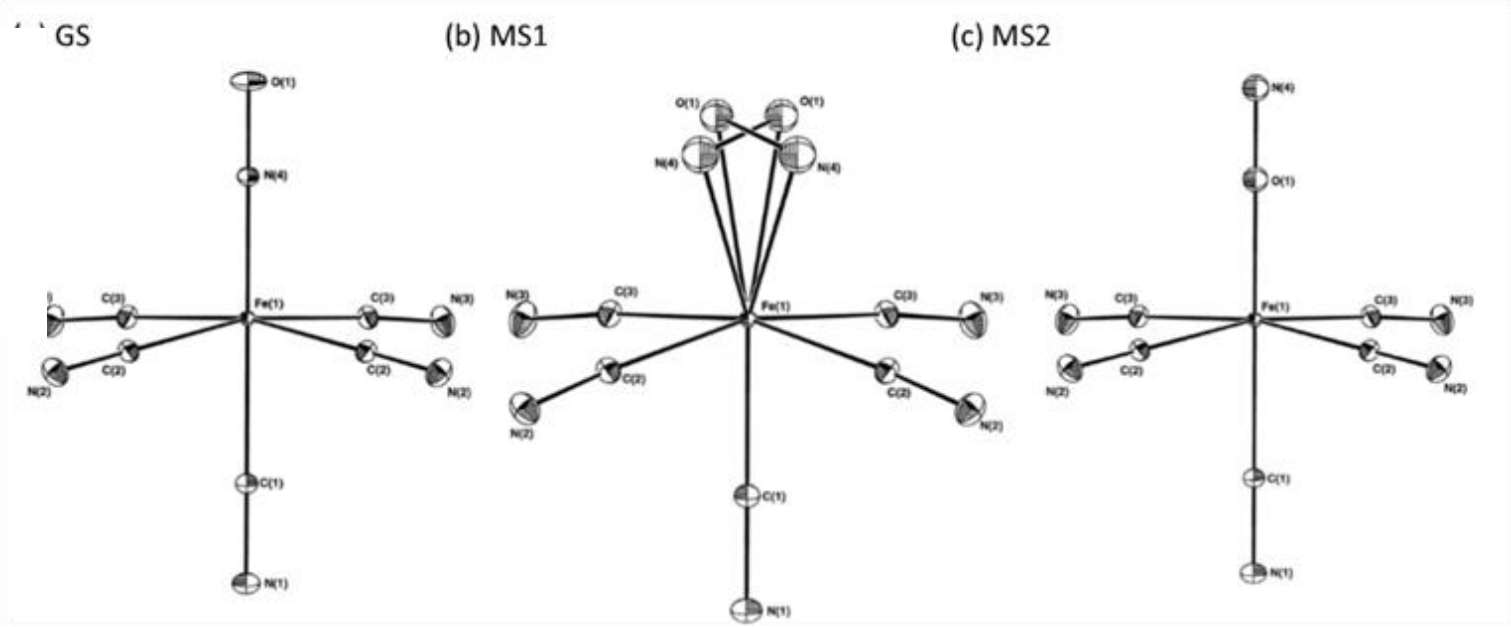
Why the interest in Nitroprussides?

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



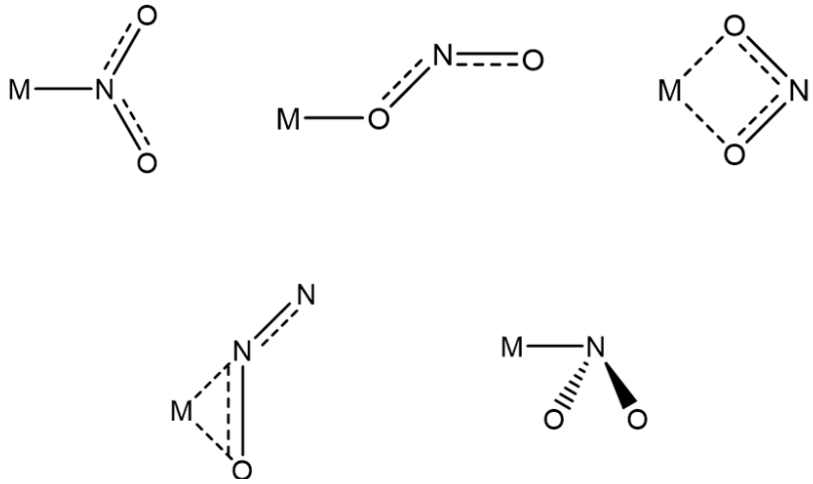
Analysis of bond parameters of a large number of nitrosyl-containing complexes, both inorganic and metallo-organic, helpful for reactivity studies.

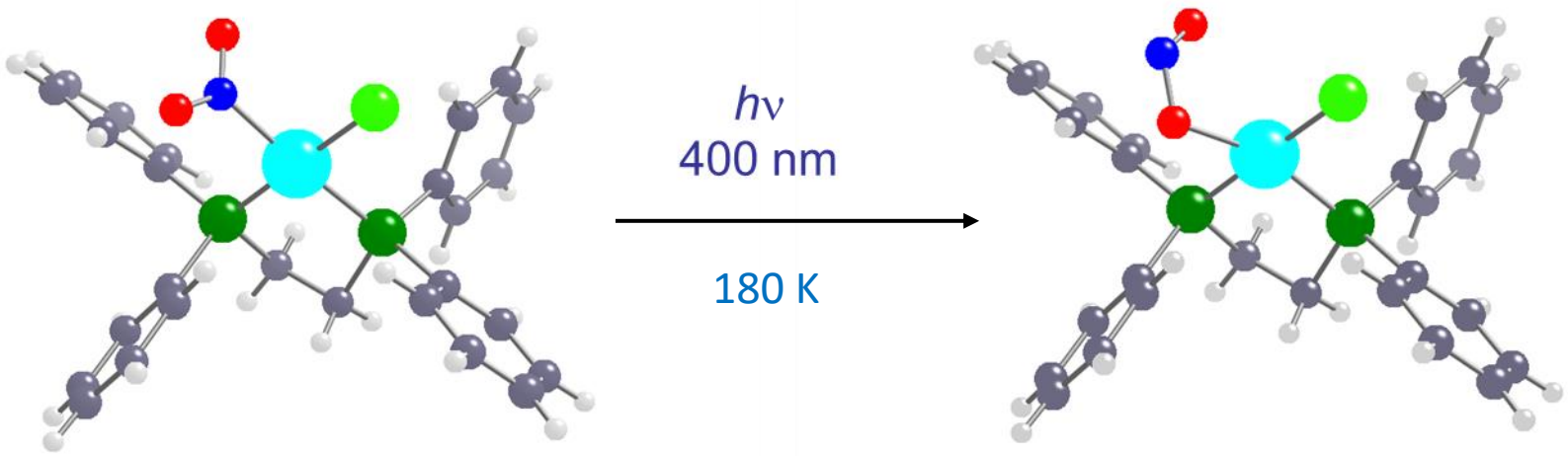
The nitrosyl group can undergo photoactivated switching between the M-NO form and the M-ON form, and also a side-bound form in the solid state, with changes in physical properties. Potential for molecular switches or as binary counting devices.



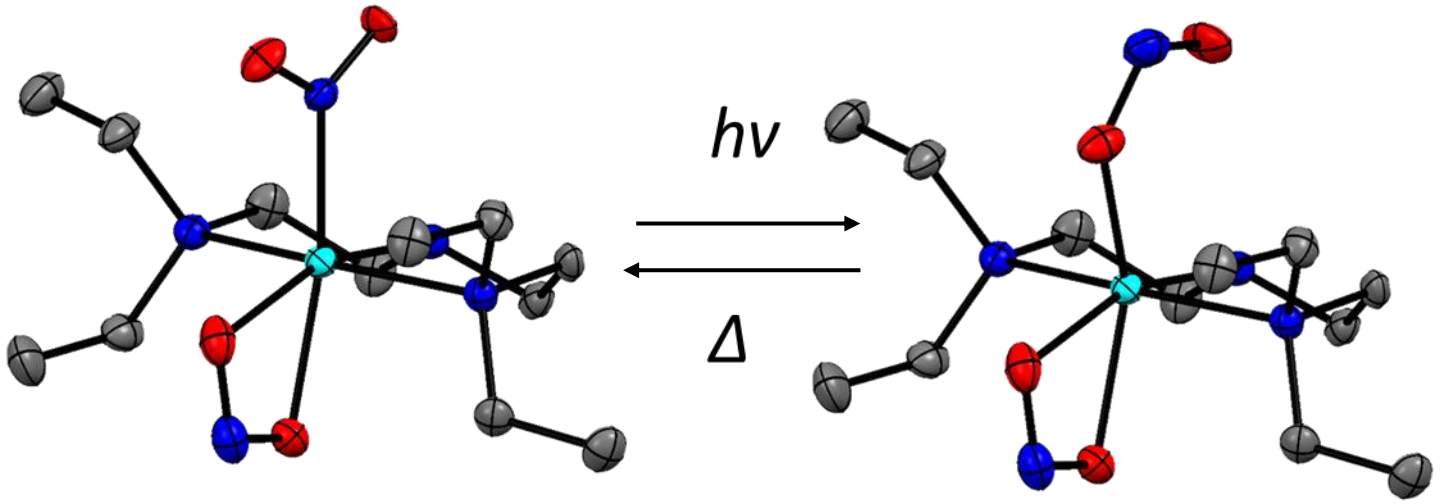
Solid State Photoactivated Switching in Transition Metal Nitro to Nitrito Linkage Isomers

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





Designing Effective Nitro-based Photoswitches



Require the photoactivated process to be:

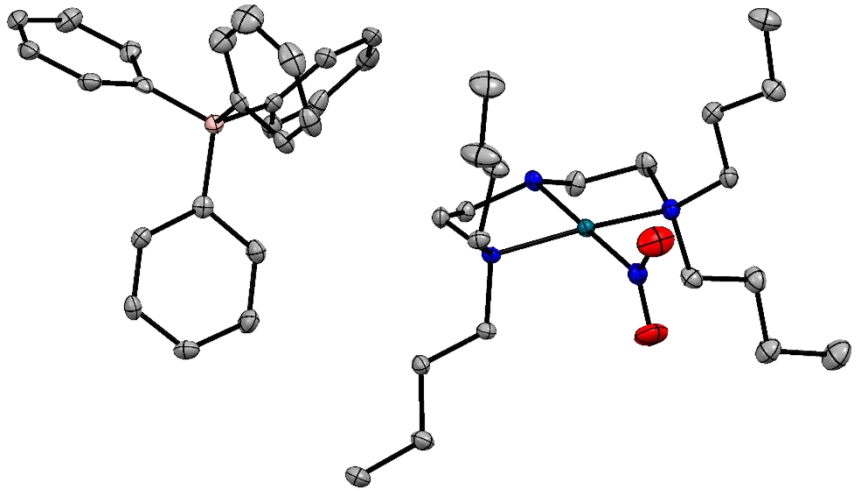
- Fast
- Fully reversible
- Occur near room temperature
- No significant degradation of the crystalline phase

Successful design requires:

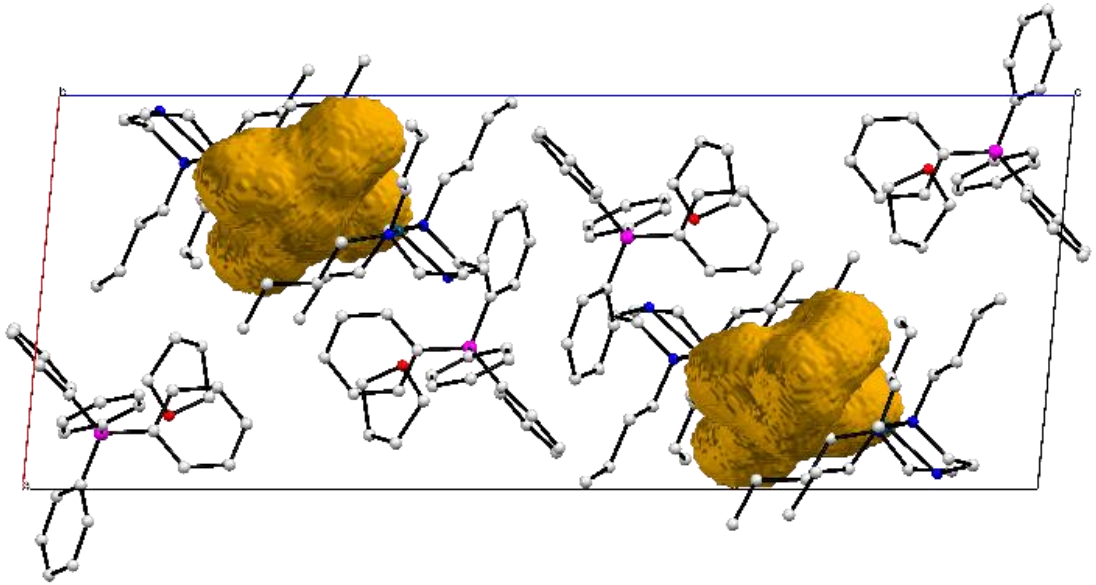
1) Control of kinetic factors
2) Control of crystalline environment around the photoactive species – control of intermolecular interactions and of the reaction cavity

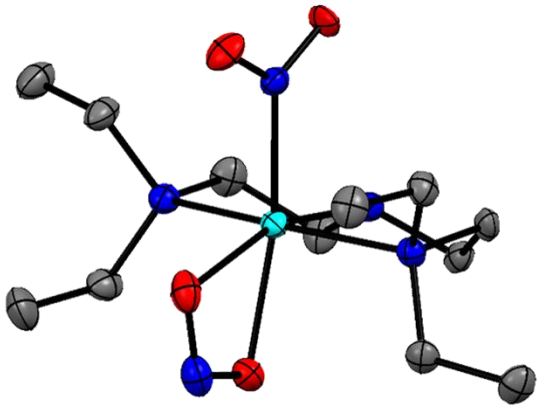
Data from structural databases is very helpful in understanding (2)

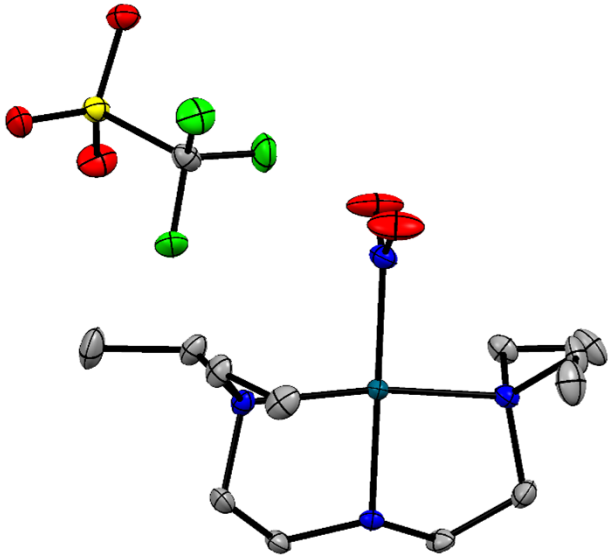
Engineering High Photoconversion - *sterics*



- 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

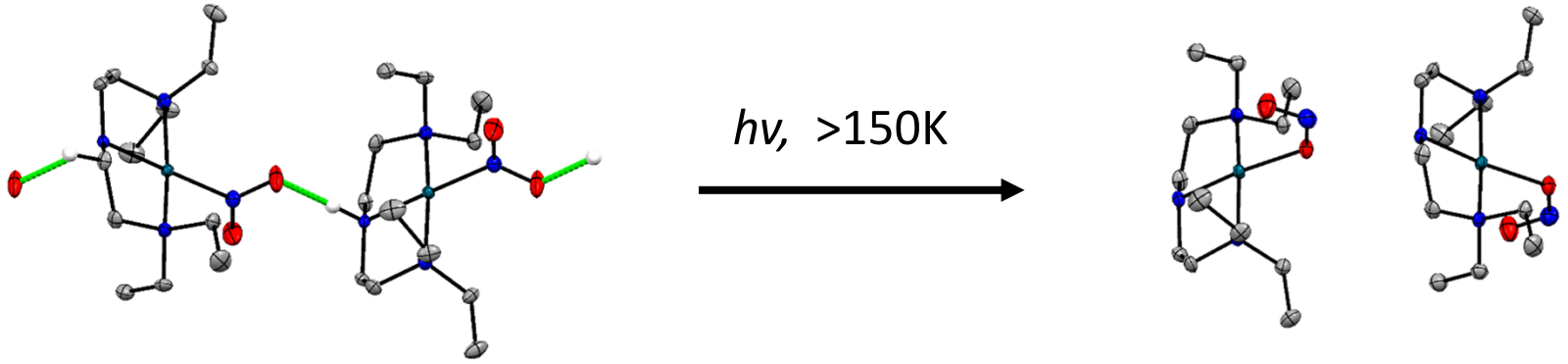






Engineering High Photoconversion – *H-bonding*

- 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_4dien)(NO_2)]OTf and [Pt(Et_4dien)(NO_2)]OTf show that H-bonding limitations can be mitigated by careful temperature control



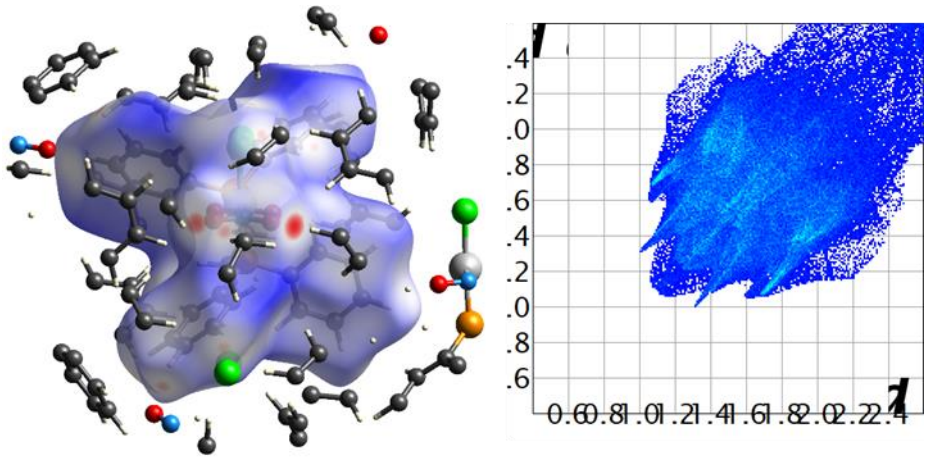
- Strong intermolecular H-bonds involving the GS NO_2 groups in both systems
- At low temp (100 K), only low photo-conversion achieved (*c.a.* 60 % max.)
- On warming to 150 K, 100% photo-conversion could be reached
- Raising the temperature weakens the H-bonding interactions and increases the reaction 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 fortransition 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.

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ADVANCING SCIENCE

Webinar CCSD/ICSD

ICSD examples and connections to CSD database

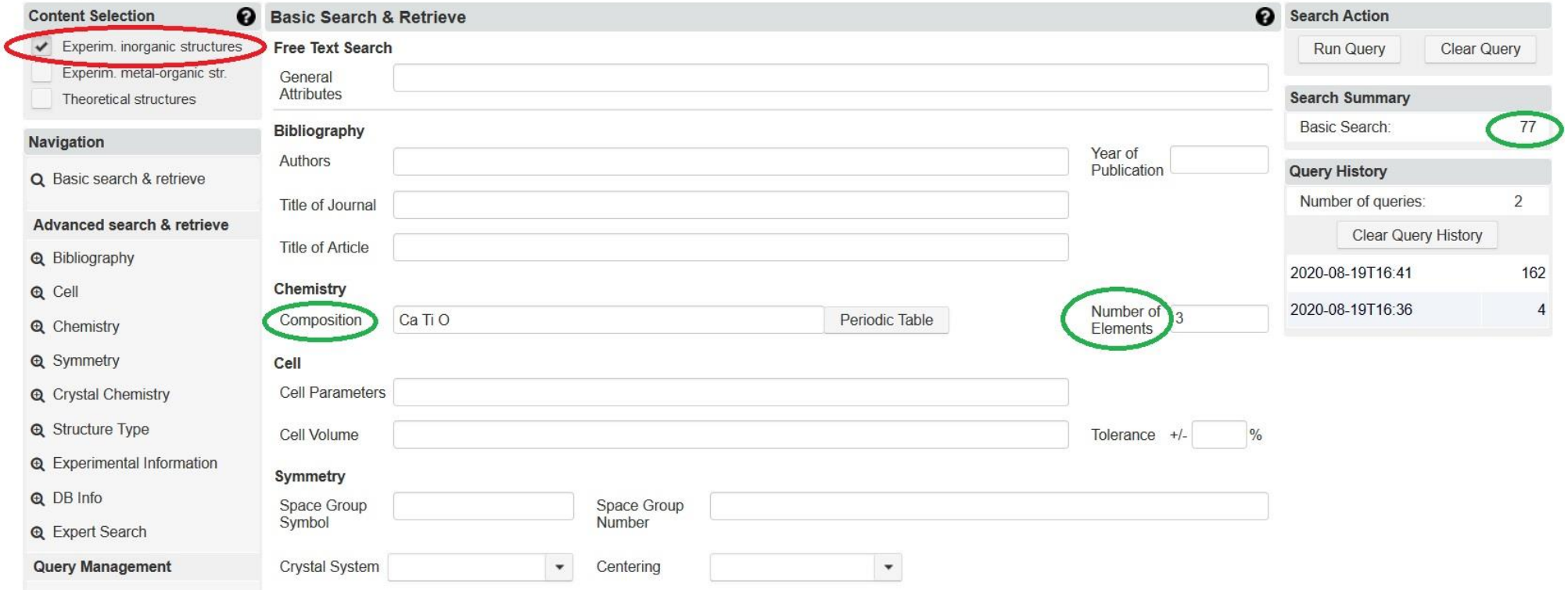
Dejan Zagorac

Senior Scientific Editor

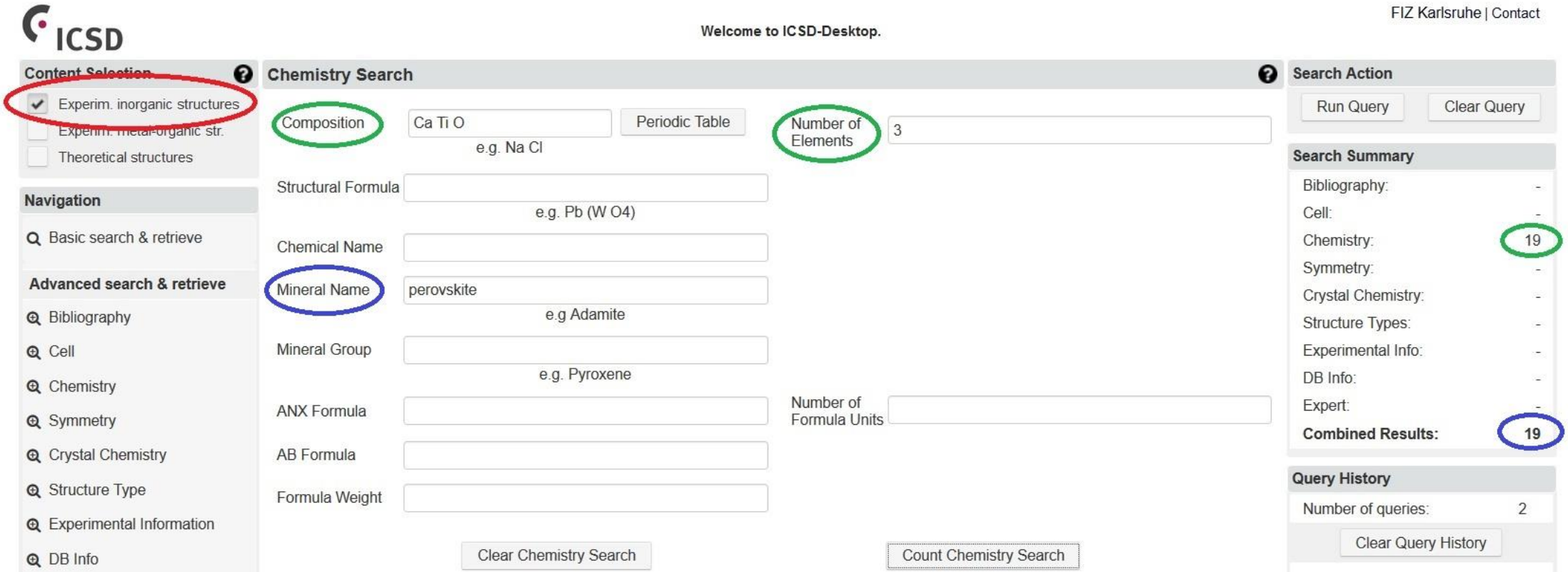
August 27, 2020

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 ($CaTiO_3$). It is also applied to the class of compounds which have the same type of crystal structure as CaTiO3 (ABX_3), known as the perovskite structure. Different cations can be embedded in this structure, allowing the development of diverse engineered materials .



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



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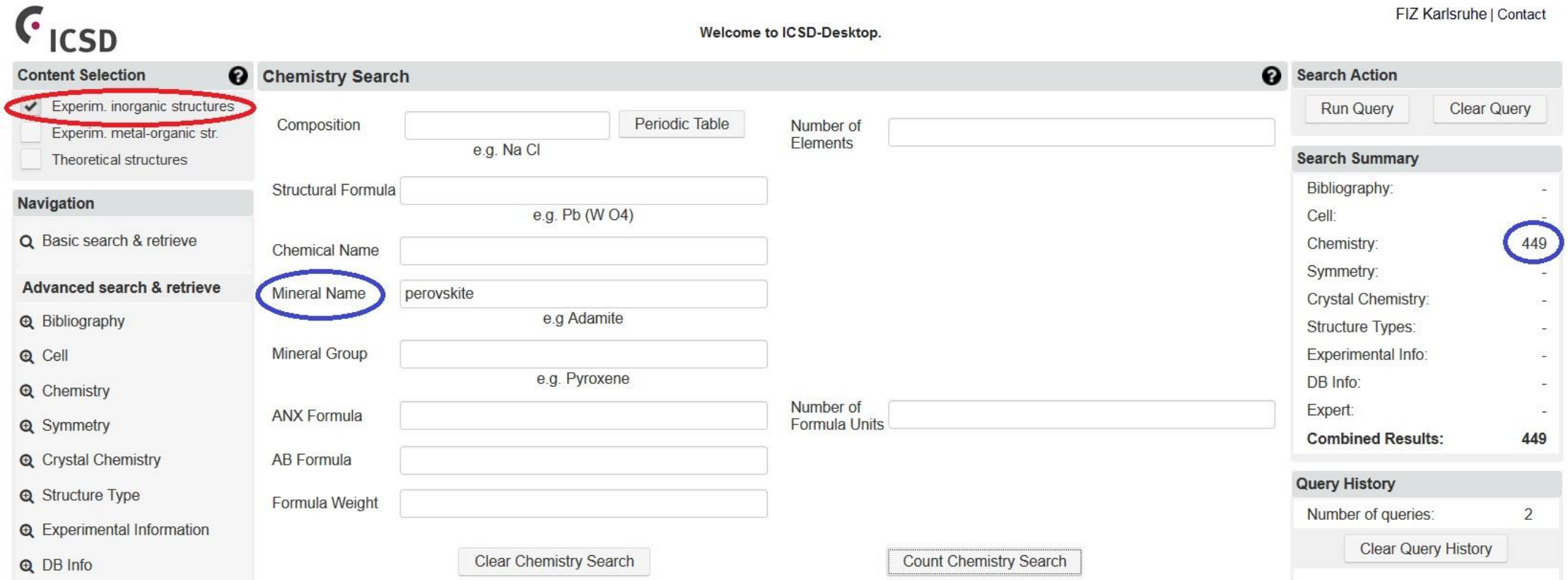
1. How to Search ICSD for experimentally observed (synthesized) inorganic structures



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

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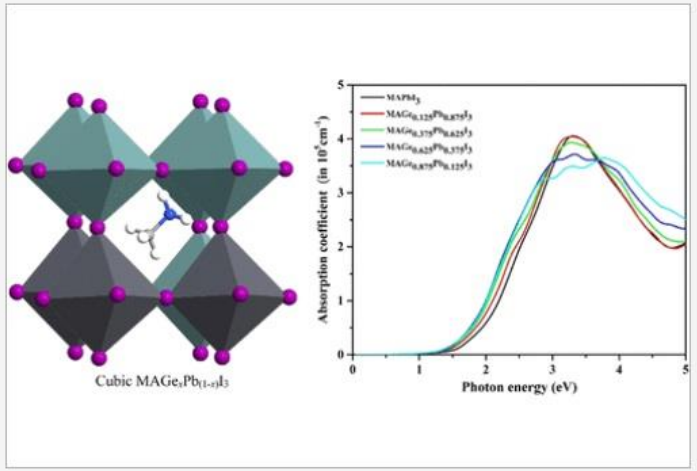
Publication Date: November 15, 2018
https://doi.org/10.1021/acs.jpcc.8b08436

First-Principle Insights of Electronic and Optical Properties of Cubic Organic–Inorganic $MAGe_xPb_{(1-x)}I_3$ Perovskites for Photovoltaic Applications

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

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 $MAGe_xPb_{(1-x)}I_3$ 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 $MAGe_xPb_{(1-x)}I_3$ 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.



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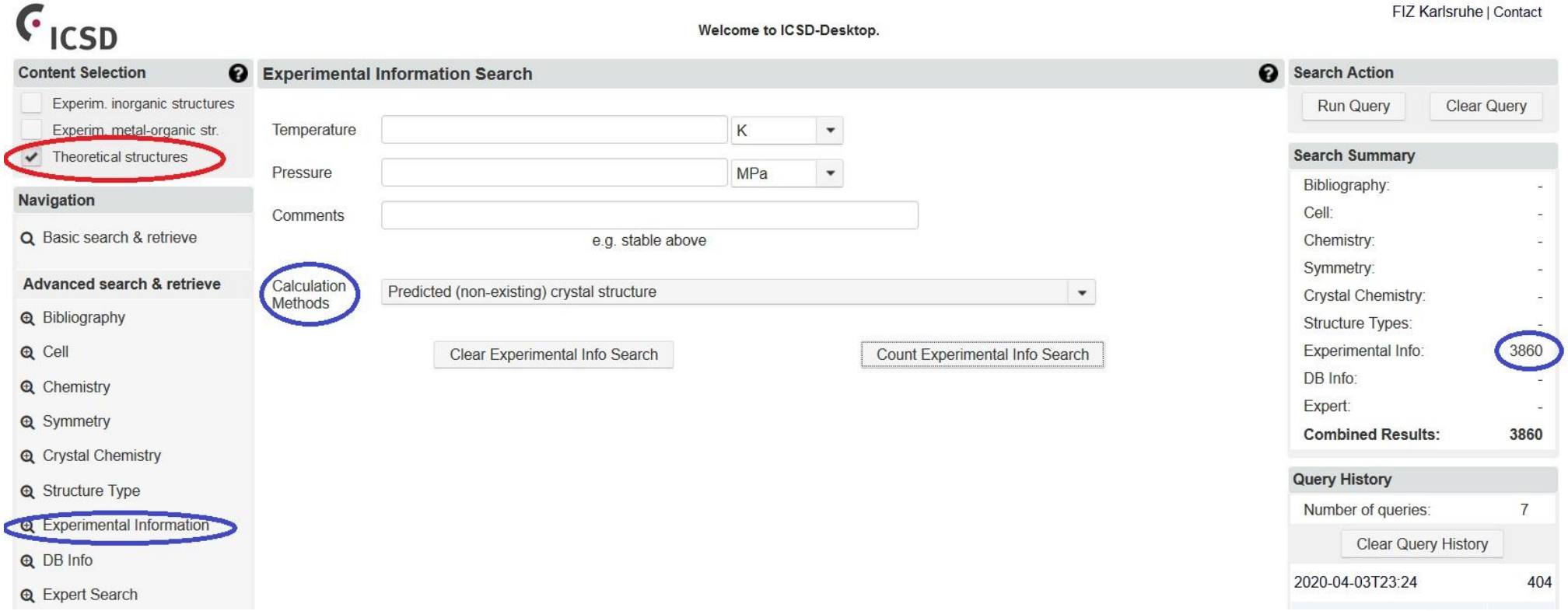
2. How to search for new (not-yet synthesized) structures or materials

- 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.



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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.

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

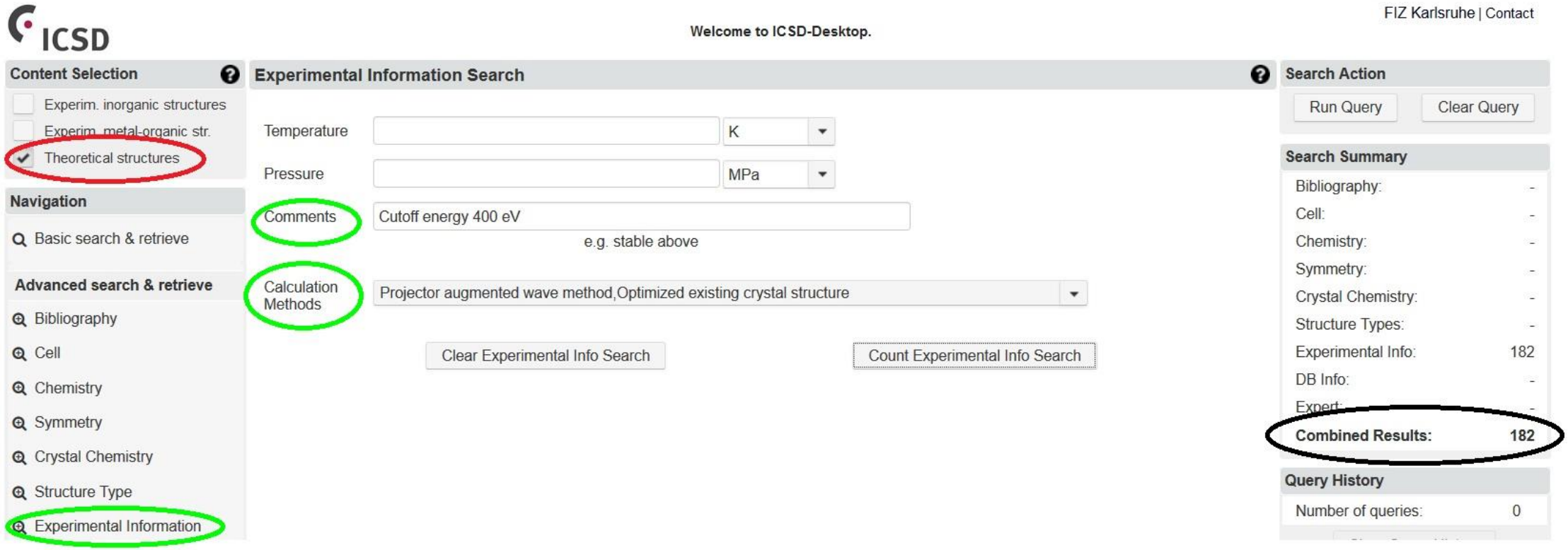
Table 1. Number of theoretical crystal structures (CIF files) in the ICSD Desktop (2019.2)

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



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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

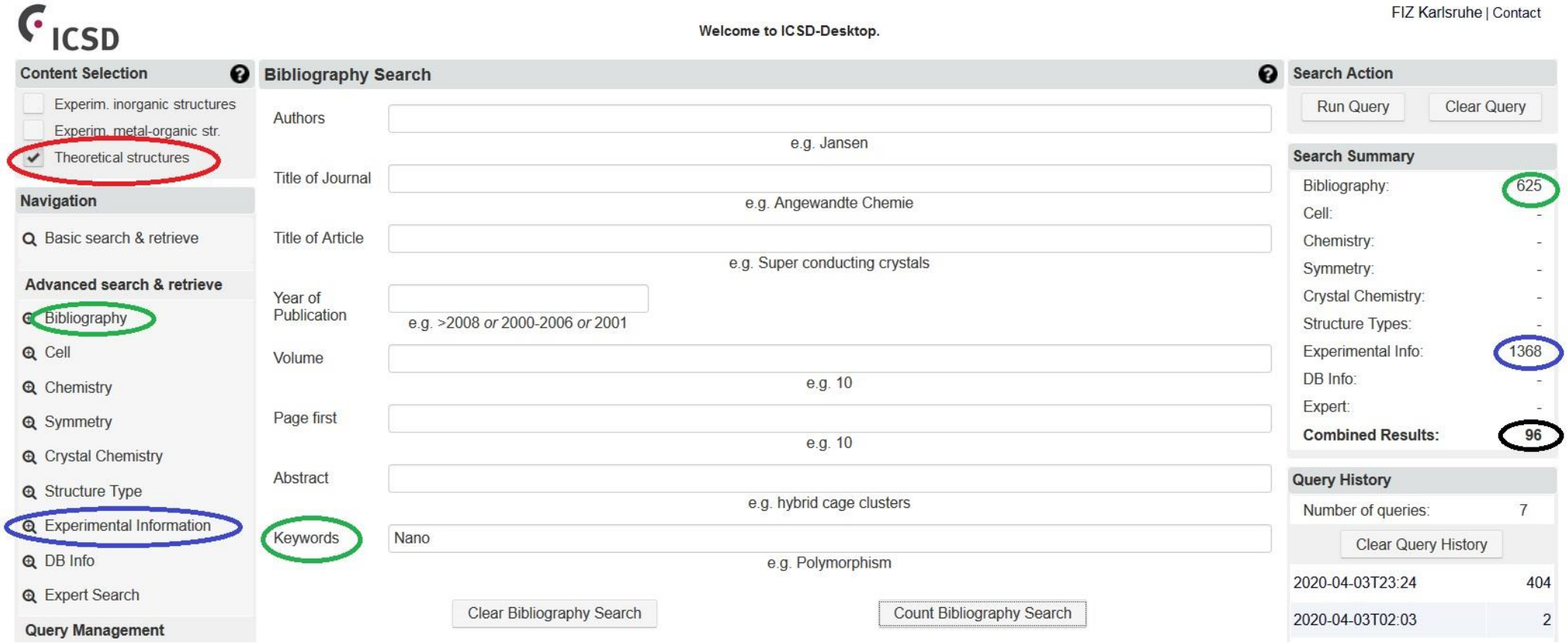

Figure 4a. Example on how to search the ICSD for theoretical nanostructures (ICSD Desktop 2019.2)

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

ICSD

Welcome to ICSD-Desktop.

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Results: List View

# of Hits: 96 (1 selected)

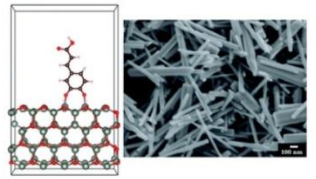
Back to Query | Show Detailed View | Export Data | Print | Visualize Structure | Visualize Powder Pattern | Column Selection | Filter

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

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

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

Check for updates



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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_2. 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_2. 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 electrosteric 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_2 nanorods and the EPD of TiO_2 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.)

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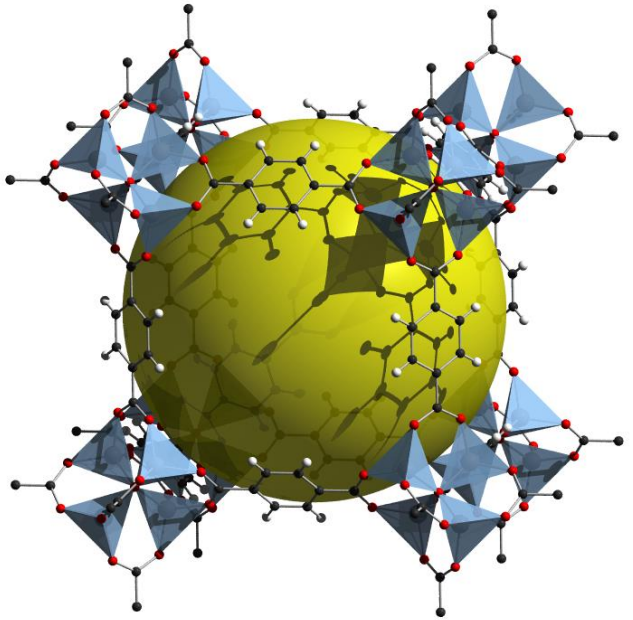
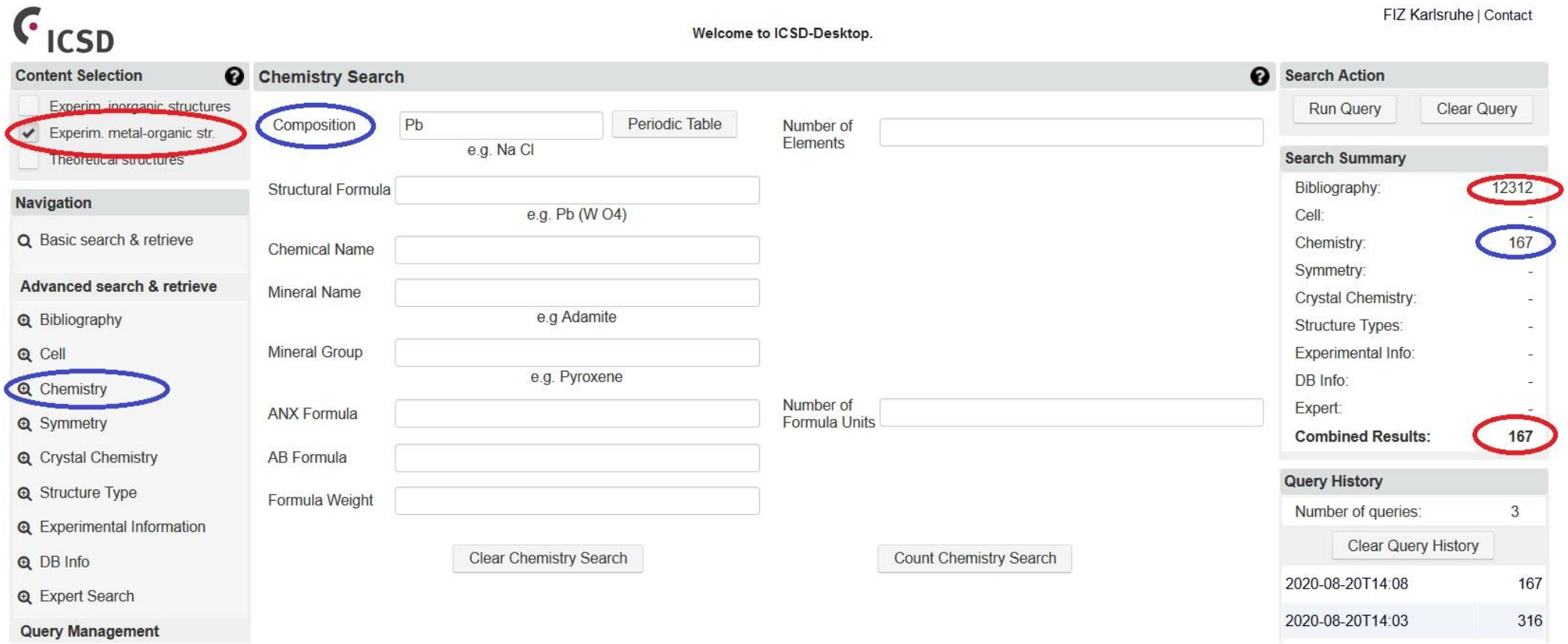
5. How to search for experimental metal-organic structures (MOFs)

- 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)



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

ICSD

Welcome to ICSD-Desktop.

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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
2972	P 1 21/c 1	C12 H26 N2 Pb		Designing stability into ther	Bacic, Goran; Zanders, Da	Inorganic Chemistry (2018
3062	F d d d Z	C105 H72 O33 Pb11		Syntheses, structures, lum	Xiao, Jun-Xia; Ma, De-Yun	Inorganica Chimica Acta (2
3211	P 21 21 21	C12 H10 N6 O9 Pb2		Six metal-organic framewo	Zhang, Qinke; Yue, Caiper	Inorganica Chimica Acta (2
3395	R -3 H	C168 H216 Br73 N24 Pb2		A nanowire array with two	Sun, Cai; Du, Ming-Xiu; Xu	Dalton Transactions (2018
3529	C 1 2/c 1	C6 H2 O4 Pb S		Phosphorescence emissio	He, Jin-Yu; Deng, Zheng-R	Dalton Transactions (2018
3604	P 1 21/n 1	C24 H26 N4 O4 Pb S2		Heterocyclic lead(II) thioure	Ketchemen, Kevin I.Y.; Mlo	Inorganica Chimica Acta (2
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 Anorganisch
4562	P 1 21/c 1	Pb4 I4 (C2 H4 O2)2		Two new oxyiodoplumbate	Xiao, Hong; Zhou, Jian; Hu	Dalton Transactions (2018
6334	P -1	C65 H143 Cl15 N8 Pb4		Blue emitting single crystal	Zhou, Chenkun; Lin, Haora	Journal of the American Ch
7068	C 1 2/c 1	C6 H12 I6 N6 Ni1 Pb2		Solvothermal synthesis, cr	Zhang, Limei; Tang, Chuny	European Journal of Inorga

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

Research paper

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

Jun-Xia Xiao [a], De-Yun Ma [b]

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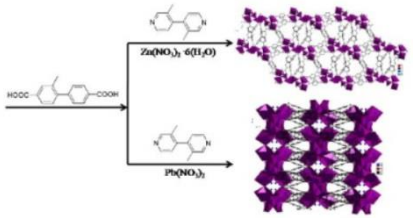
Inorganica Chimica Acta

Volume 483, 1 November 2018, Pages 6-11

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

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.



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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 in 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, [a] Alireza Salimi *[a] and Jered C. Garrison[b]

Article information

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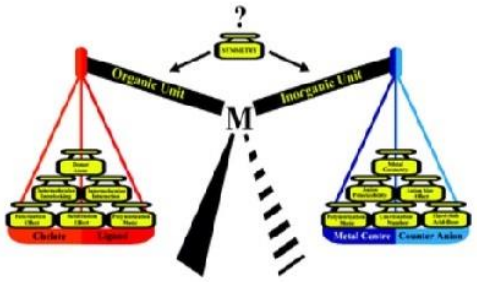

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Thank you for your attention and stay healthy!

Your comments and suggestions are welcome as well as theoretical CIF files which you can send to: crysdata@fiz-karlsruhe.de

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Zertifikat seit 2016
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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

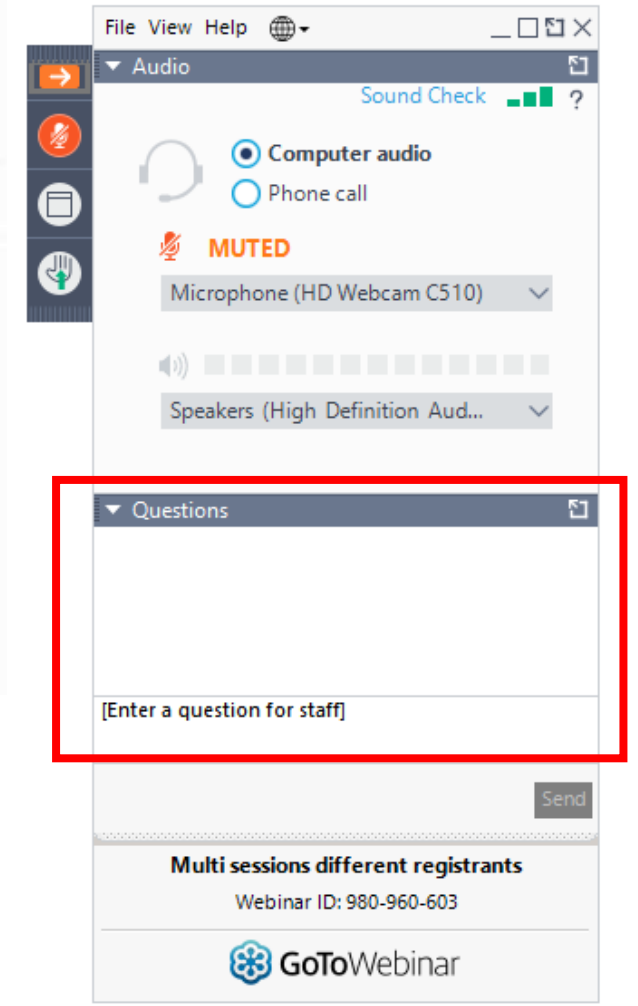
What next?

- 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 7th October 2020

CCDC

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



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Thank you

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