

Depositing and publishing data through the CSD and the ICSD

IUCr25 - CSD and ICSD Workshop – Session 1



CCDC and FIZ Karlsruhe

12th August 2021



Agenda

- Introduction to the CSD and ICSD
- *Show One*: Overview of Deposition
- *Show One*: Demo of Deposition
- *Try One*: Deposition Hands-on
- *Explore More*: After Deposition and data access
- *Explore More*: Quiz
- Summary

Learning outcomes for the session

- Be familiar with the CSD and the ICSD
- Know how to deposit small molecule structural data using our joint
- Know how to check the novelty and integrity of your data
- Know how to access, edit and revise your structures.

What we do at the CCDC

Charitable Objective:

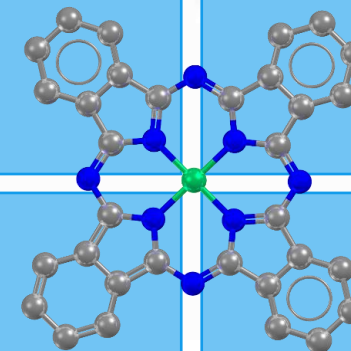
Advancement of chemistry and crystallography for the public benefit through providing high quality information services and software

International
repository of 3D
curated structures

Collaborative
research and
knowledge-based
services

Scientific software

Education and
Outreach



CCDC

What we do at 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.

What is a crystallographic database?

- They usually include:
 - Bibliographic data
 - Crystallographic, chemical and experimental information
 - Atomic coordinates
- What makes a crystallographic data special?
 - Standard agreed file format
 - Every published structure is added to the appropriate database
 - There are established [curated databases](#) rather than just collections of data with some level of [quality control](#) through processing & validation
 - They enable you to learn from the wealth of data they contain



Structural databases



PDB
>175,000
polypeptides,
nucleotides
& saccharides



CSD
>1.1 million
organic and
metal-organic

ICSD
>240,000
(no C-H and C-C
bonds)
Elements,
minerals,
metals

ICDD
Powder
diffraction
files



FIZ Karlsruhe
Leibniz Institute for Information Infrastructure



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The vision

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

Kennard, O. "From Private Data to Public Knowledge." *The Impact of Electronic Publishing on the Academic Community*. Ed. I Butterworth. Portland Press Ltd, 1997. 159-166.



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

The vision

BERNAL'S VISION: FROM DATA TO INSIGHT

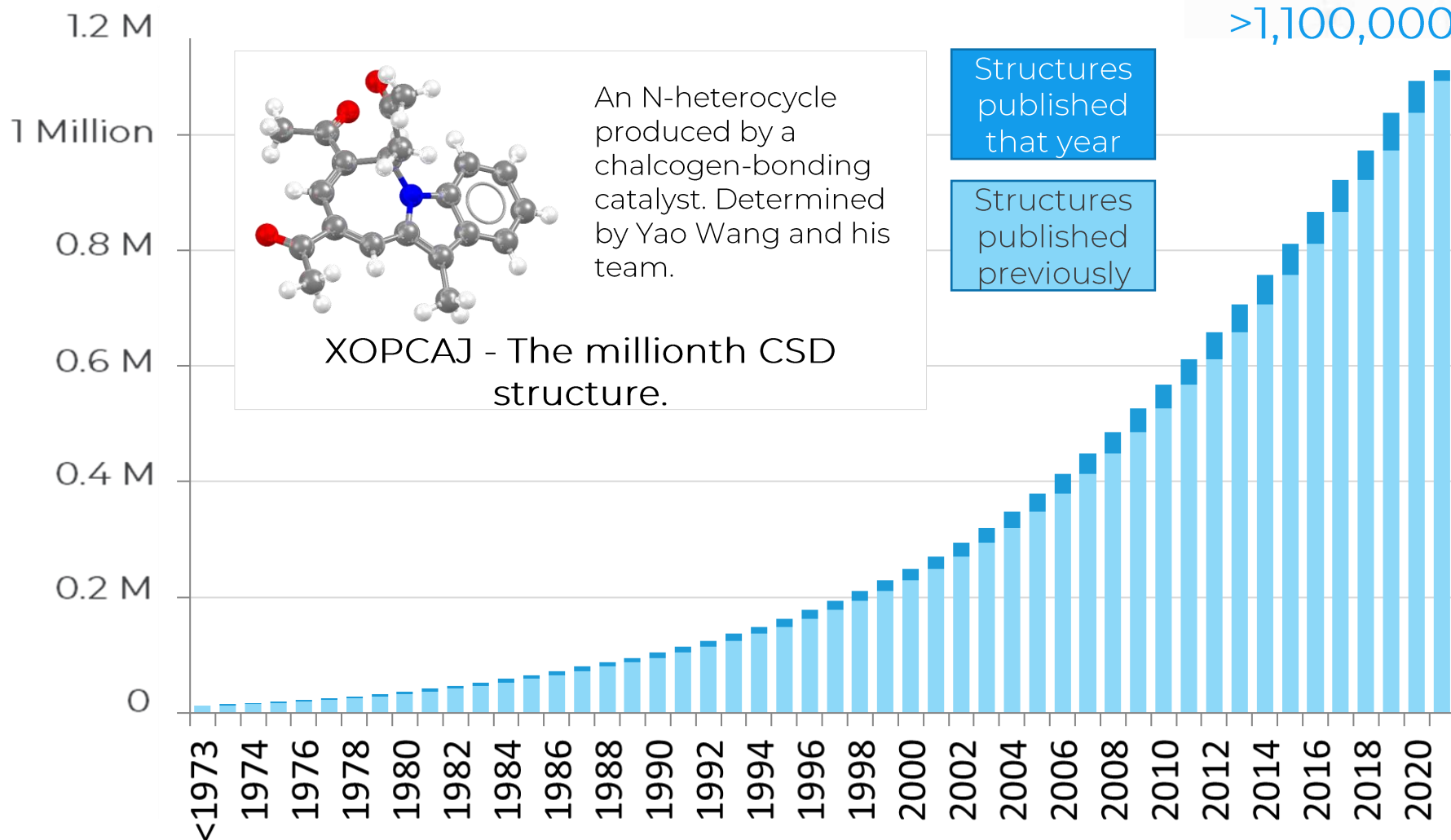
by Dr Olga Kennard OBE FRS

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)

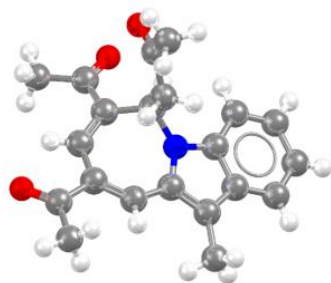


- Every published structure
 - Inc. ASAP & early view
 - CSD Communications
 - Patents
 - University repositories
 - Thesis
- Every entry enriched and annotated by experts
- Discoverability of data and knowledge
- Sustainable for over 55 years
- A trusted CoreTrustSeal repository

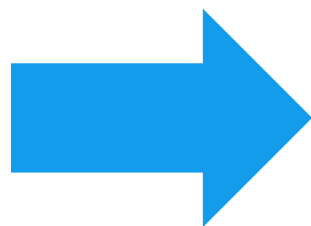


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CSD Refcodes



CSD Refcode -
XOPCAJ



What is XOPCAJ?

- A CSD Refcode
- A database reference code
- Containing 6-8 characters
- Used to identify entries in the CSD

Refcode families

- The same substances are assigned the *same* 6 letter code plus an additional 2 numbers
 - Polymorphs
 - New determinations or re-refinements of the same substance
 - Determinations at different temperatures/pressures
- Stereoisomers or different solvates, co-crystals, etc are assigned *different* refcode families

Some of my favourite refcodes are: KITTEN, BATMAN, DISNEY, GAUTAM, GLYCIN

Inside the Cambridge Structural Database

The CSD is a database of all the published organic and metal-organic experimental crystal structures

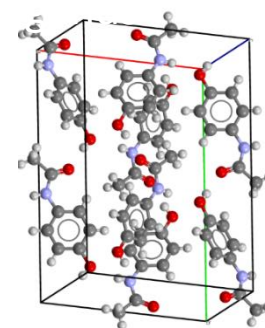
Organic
43%

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

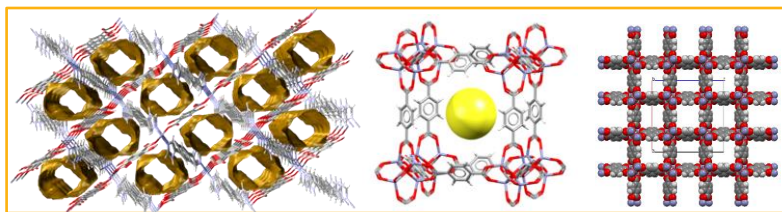
- 11,525 polymorph families
- 171,683 melting points
- 909,992 crystal colours
- 778,663 crystal shapes
- 24,916 bioactivity details
- 11,387 natural source data
- > 250,000 oxidation states

Not Polymeric
89%

Polymeric: 11%

Metal-Organic

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

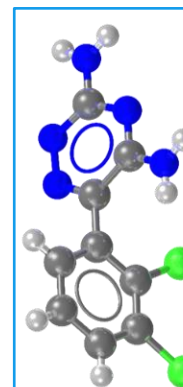


Single
Component
56%

Multi
Component
44%

Links and subsets

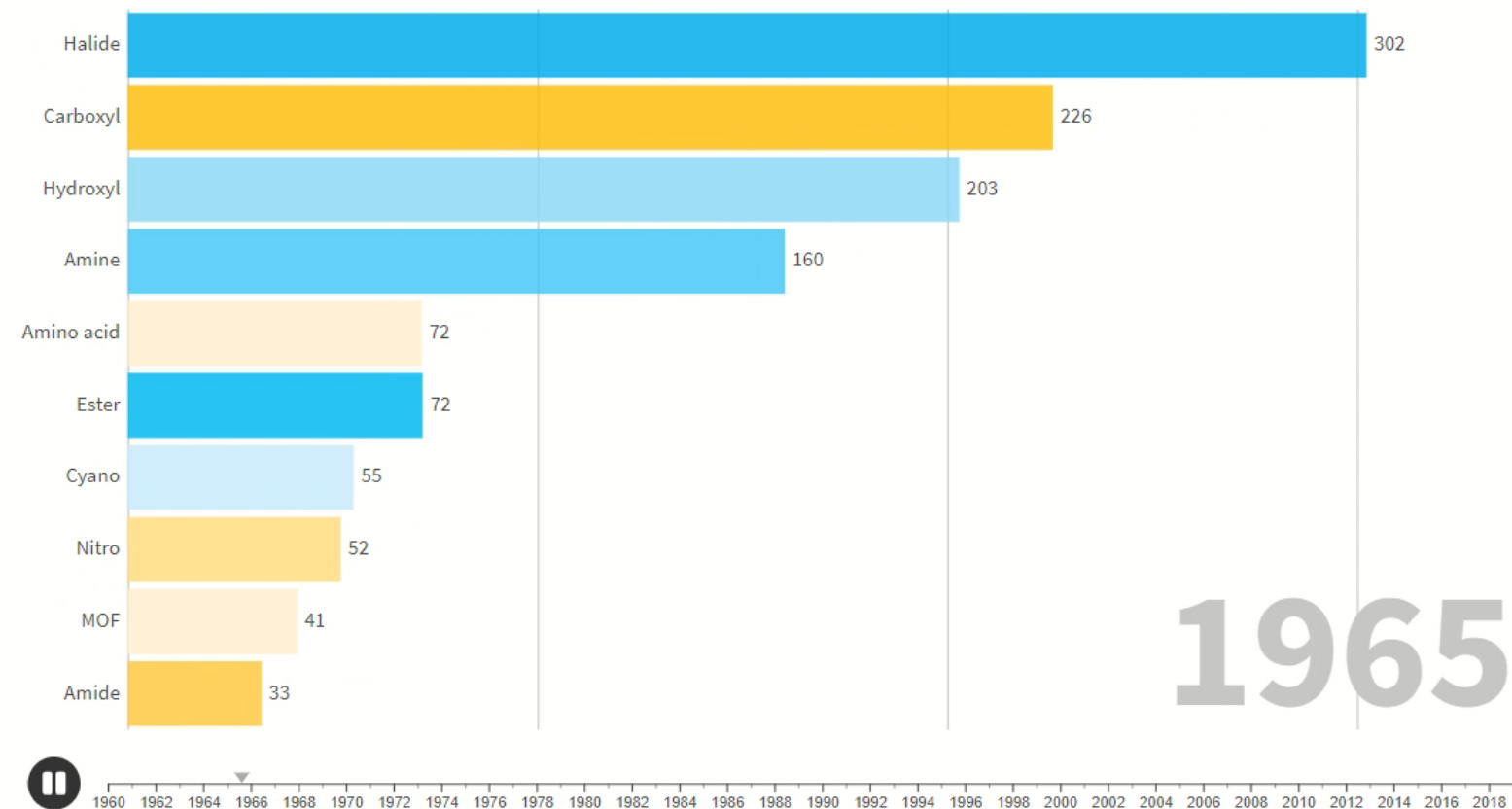
- DrugBank
- Druglike
- MOFs
- PDB ligands
- PubChem
- ChemSpider
- Pesticide PDB



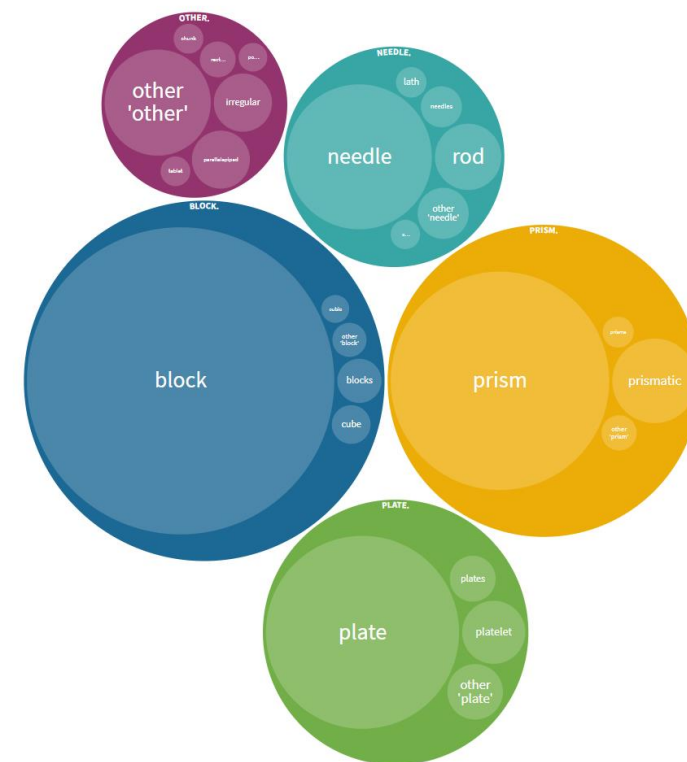
Exploring the CSD

Chemistry in the CSD

Number of structures containing certain chemical groups



Crystal shapes in the CSD



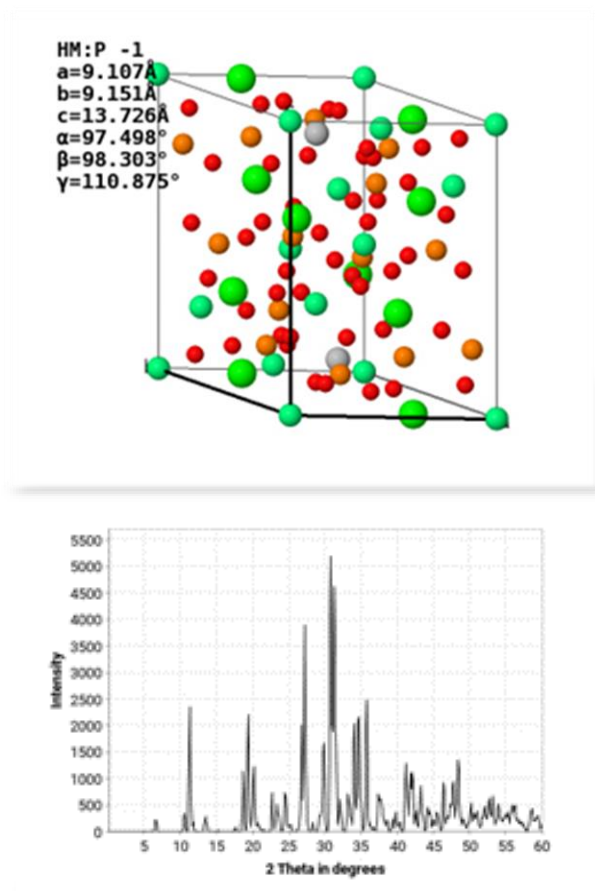
ICSD has a history of 40 years

- 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)



Picture: Wendelin Detemple, FIZ Karlsruhe

Scope of ICSD



ICSD = world's largest database for fully determined inorganic crystal structures

ICSD contains the following types of crystal structures:

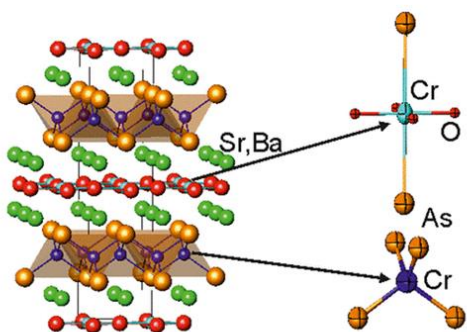
- Experimentally determined inorganic structures (dating back to 1913)
- Experimentally determined organometallic structures (since 2018)
- Theoretically calculated inorganic structures (since 2016)

Inorganic structures also include metals and intermetallic compounds, which were increasingly recorded from 2003 onwards.

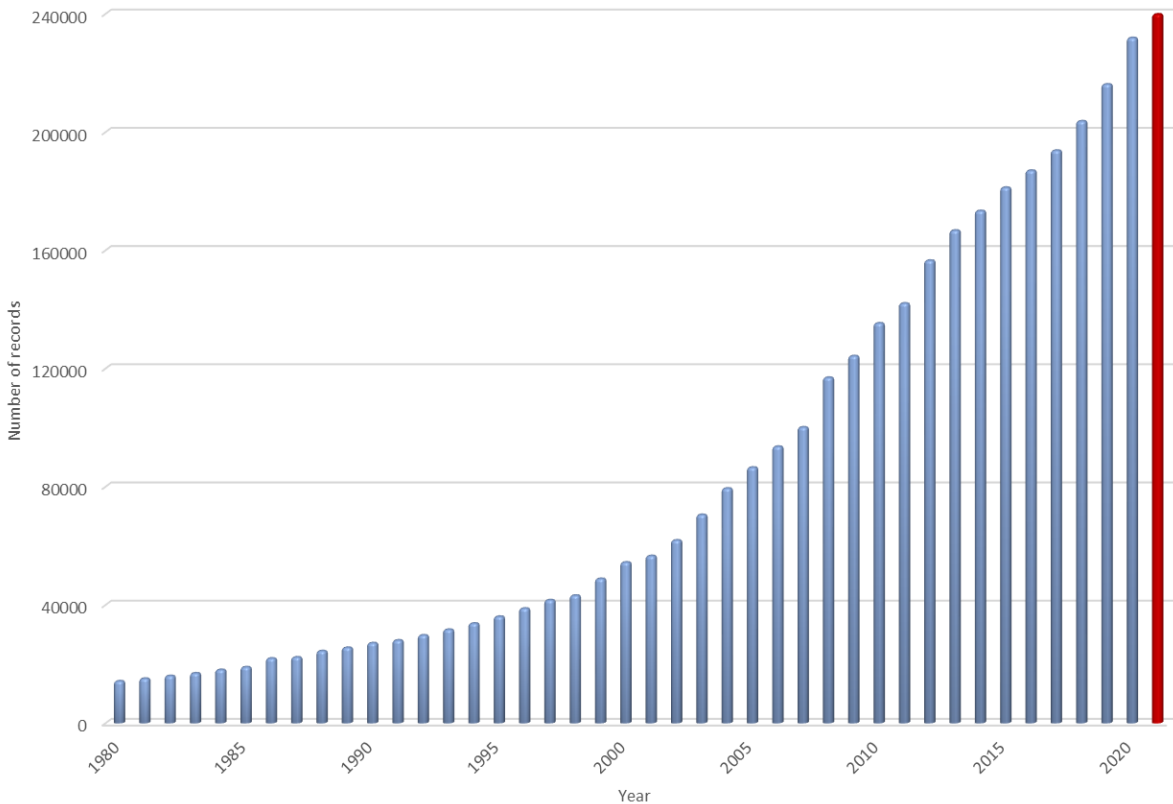
ICSD growth - 1980 – 2021

FIZ Karlsruhe has added the 250,000th crystal structure to the ICSD database

The structure is a complex transition metal compound containing an oxide and an anion of a more electronegative element (arsenides).



The 250,000 ICSD structure: the antiferromagnetic properties of two transition metal compounds as a function of temperature. (DOI: 10.1021/acs.inorgchem.0c02415)



Welcome to ICSD Web. Logged in: Rehme, Silke

FIZ Karlsruhe | Contact
Change Password | Logout

Back to Query
Back to List

CCDC
Export Cif
Print
Feedback to Editor

Entry 1 of 1

Collection Code 53815

Summary

Struct. formula	Na Cl	Structure type	NaCl
Cell parameter	5.63 5.63 5.63 90. 90. 90.	Space group	F m -3 m (225)
Cell volume	178.45 [Å³]	Z	4
Temperature	room temperature	Pressure	atmospheric
Data quality	Standard quality	Title	Structure of some crystals
Author	Bragg, W.H.; Bragg, W.L.	DOI	10.1098/rspa.1913.0040
Reference	Proceedings of the Royal Society of London, Series A: Mathematical and Physical and Engineering Sciences (1913) 88, (1) Article ID * (p. 428-428)		

Details

Expand all
Collapse all

Visualization

Published Crystal Structure

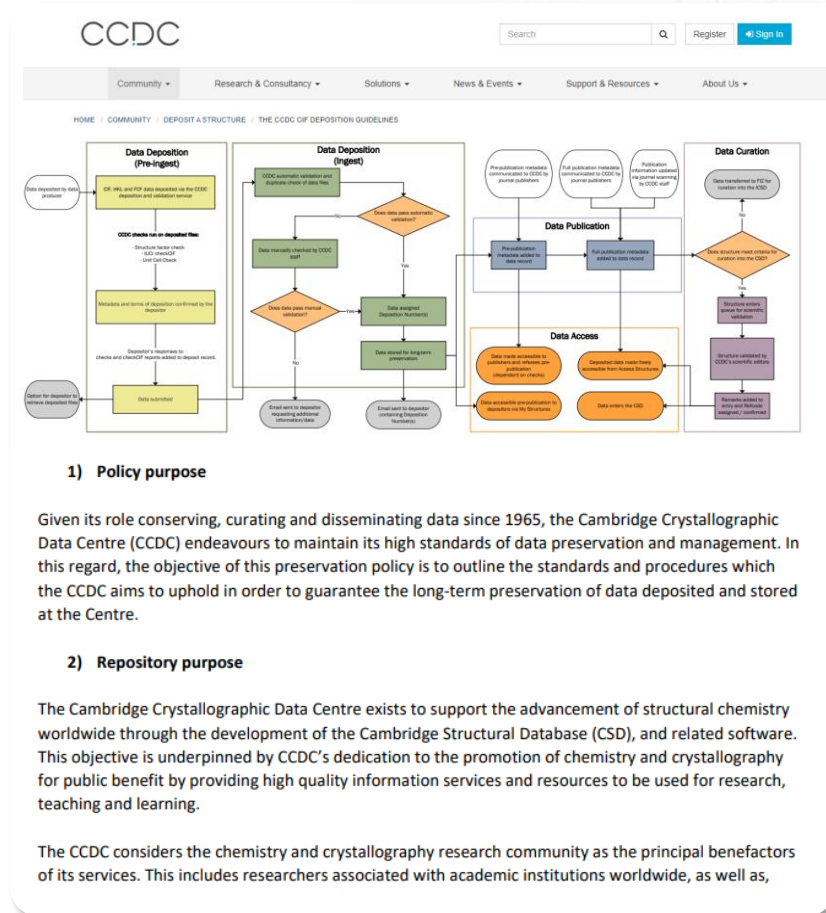
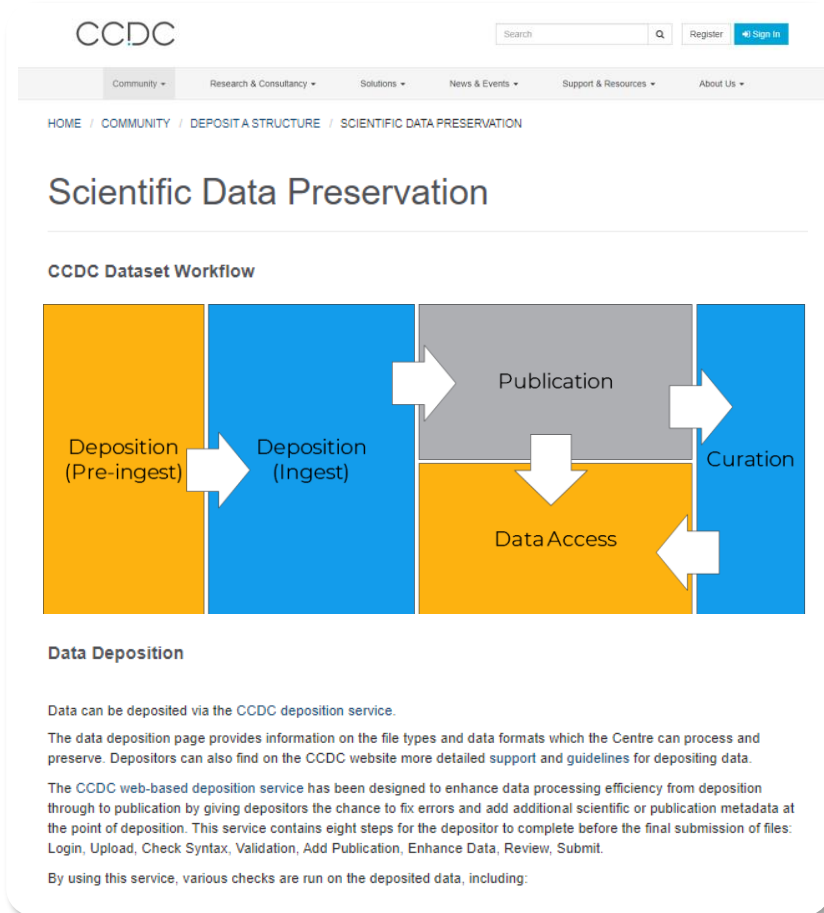
HM: F m -3 m
a=5.630 Å
b=5.630 Å
c=5.630 Å
α=90.000°
β=90.000°
γ=90.000°

Powder Pattern

Agenda

- Introduction to the CSD and ICSD
- *Show One: Overview of Deposition*
- *Show One: Demo of Deposition*
- Try One: Deposition Hands-on
- Explore More: After Deposition and data access
- Explore More: Quiz
- Summary

A data preservation policy



CCDC

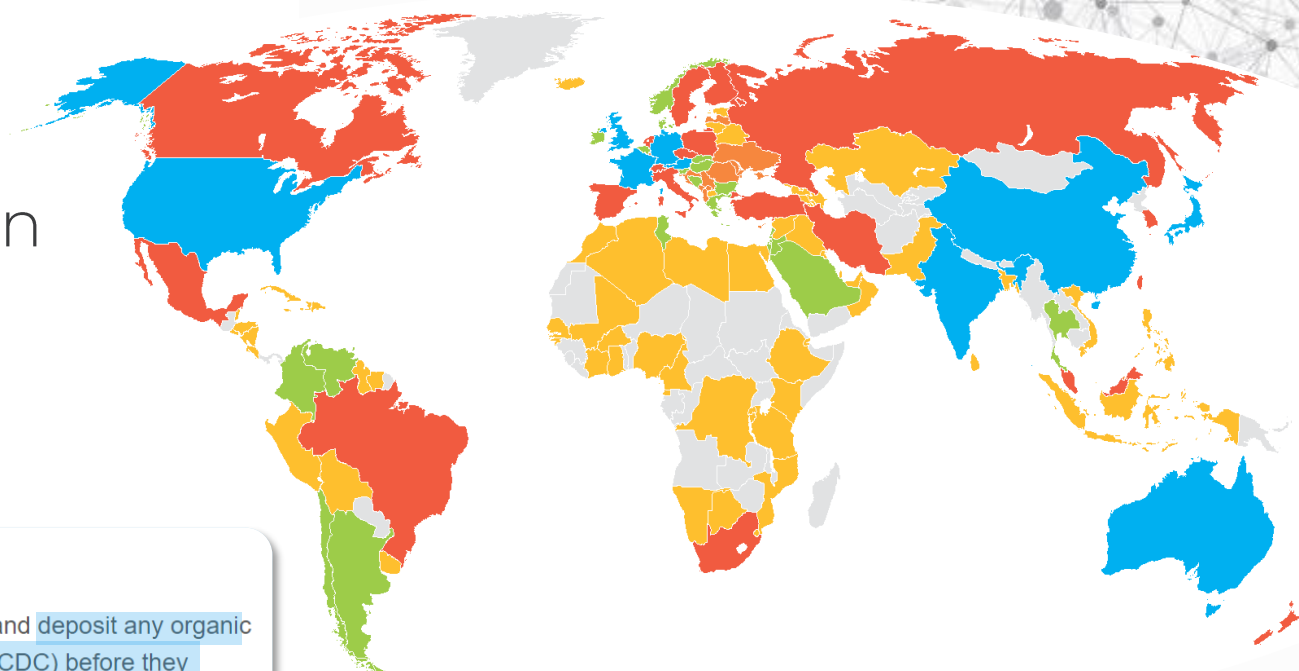
Deposition

- Data deposited pre-publication
 - Enables links to data sets at the point of publication
 - Tailored deposition service

Small molecule single crystal data

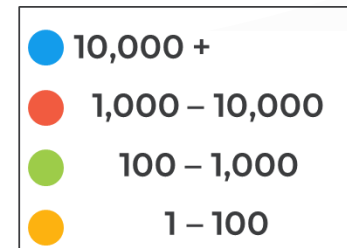
Authors should present their crystal data in a CIF (Crystallographic Information File) format and deposit any organic or organometallic structural information with the [Cambridge Crystallographic Data Centre \(CCDC\)](#) before they submit their manuscript to us. Data will be held in the CCDC's confidential archive until publication of the article, when data for organic and organometallic compounds will be entered into the Cambridge Structural Database. Authors are encouraged to deposit inorganic crystal structures with the [ICSD](#), hosted by FIZ Karlsruhe.

During submission of a manuscript to the Royal Society of Chemistry using our online submission system, authors will be asked to provide CCDC reference numbers; CIFs should not be submitted with the manuscript (these should have already been deposited with the CCDC/ICSD, see above). Any revised CIFs obtained subsequently should be deposited directly with the CCDC before the revised manuscript is submitted to us. CCDC or ICSD numbers should be included in the manuscript prior to submission.



Countries contributing data

Analysis based on sampling of email addresses



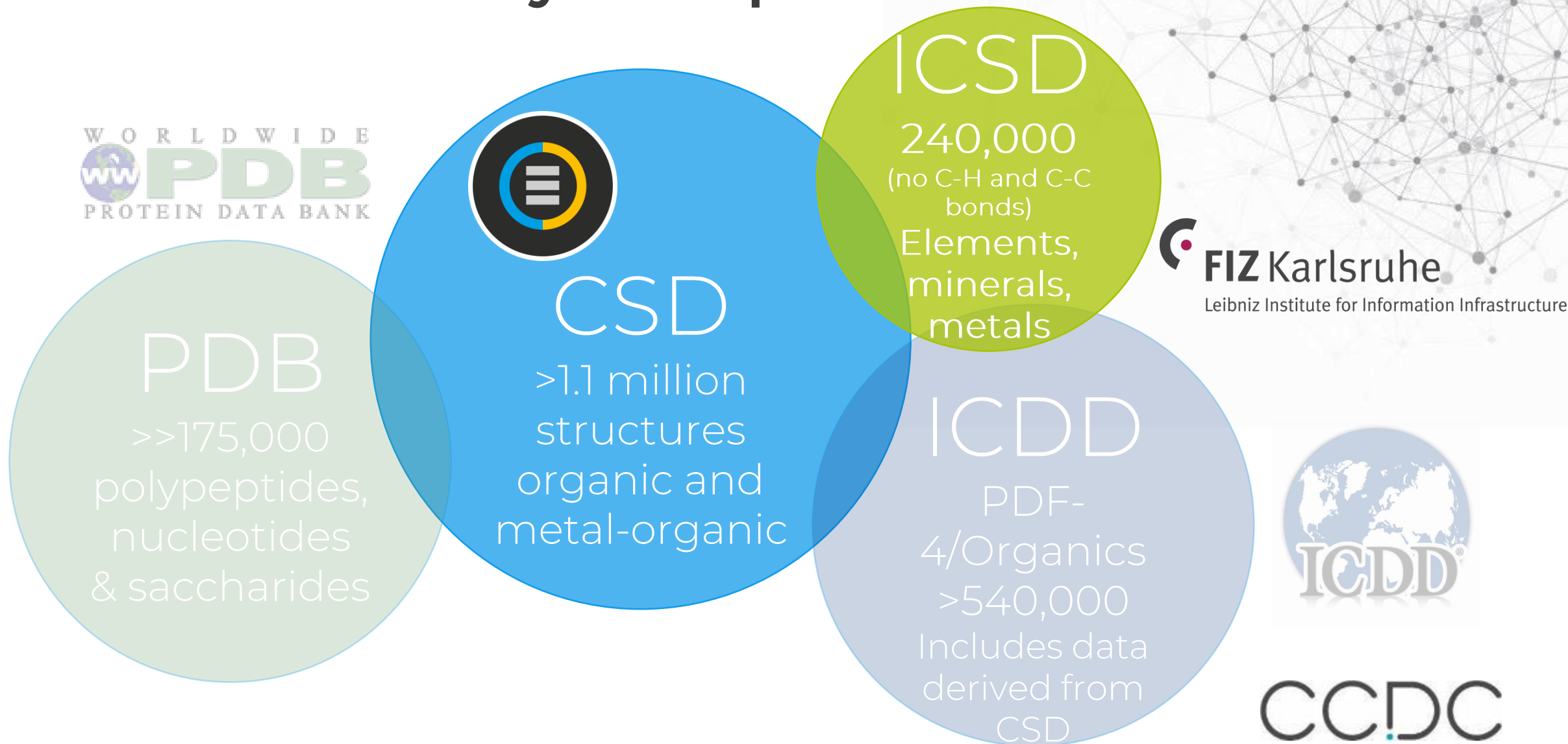
>30% of depositions from China

www.ccdc.cam.ac.uk/deposit

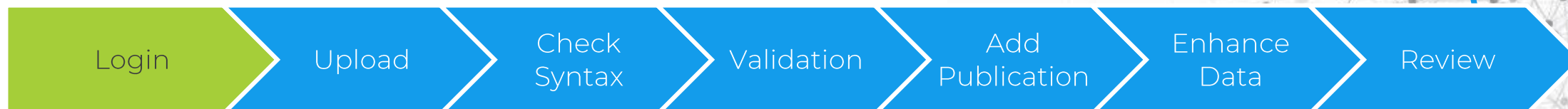
When should you deposit data?

- **Pre-publication** – when you have finished a structure is when you know most about the dataset
- Enables you to **check and correct data** prior to inclusion in a manuscript
- Deposited data is stored **privately** at the CCDC prior to publication
- Most publishers require data to be deposited **before manuscript submission**
 - Enables publishers and referees secure access to the data during the peer review process
 - Enables links to the data to be added at the point of publication

What data can you deposit with us?



Deposition



CIF deposition and validation service

[Click here to continue to the deposition process without signing in.](#)

If you have not registered for a CCDC account before you can register using the button below. To find out more about CCDC accounts and what you are able to do once you have logged in, please see our [support page](#).

Sign in with your CCDC account

Username or Email

ward@ccdc.cam.ac.uk

Password

.....

☐ Remember me?

Sign In

Register

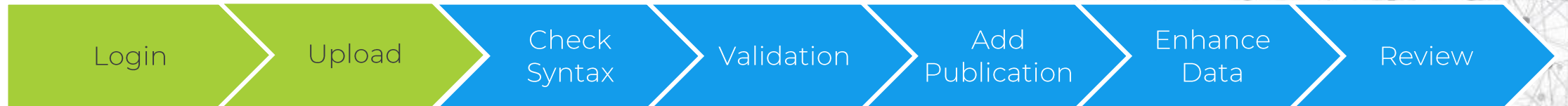
[Forgotten Username or Password](#)

If you don't want an account on our website you can click [here](#)

Why register?

- Simplifies deposition
- Gives you access to see, edit and share your data
- Enables you to link your CSD licence to use WebCSD

Deposition



CIF deposition and validation service

First name(s)

Last name(s)

Your email address

Additional email addresses

Institution (e.g. University/Company)

Deposition number(s) for revision

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

4.42 KB

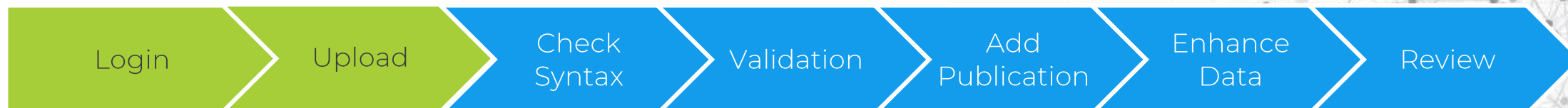
Details ☐ Remember my details

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

Along with your **personal details** you are asked to add:

- Your **ORCID ID**
 - A persistent **digital identifier** that distinguishes you from every other **researcher**
 - Enable you to add your data into your ORCID ID
 - Displayed on our Access Structures service alongside your data
- Your **files**
 - In **CIF format** – the standard file format for crystallographic data
- **Two options**
 - **Remember your details**
 - **Run checkCIF** – a service to check the integrity of your data

Deposition



CIF deposition and validation service

No Structure Factor data have been uploaded.

Structure Factor data are an essential part of the deposition. You should click 'Go Back' to add Structure Factor data to your deposition. If you are unable to embed Structure Factor data into your CIF automatically, you can upload this data as separate files alongside your CIF.

If in exceptional circumstances you are unable to include Structure Factor data with your deposition you may continue by clicking 'Proceed to Next Step', however you must use the comment box below to explain why this data is not available. The text you enter will be automatically embedded into your deposited CIFs.

Reason why your deposition does not include Structure Factor data (this comment will automatically be added into your deposited CIFs): *

← Go Back

Proceed to Next Step →

Structure Factor data check

- The experimental data which were used to determine the 3D structure
- Structure factor data enables
 - Rigorous validation of the structure-determination results
 - Their preservation and continued accessibility
- Data should either be appended to the CIF or in .FCF or .HKL format
- If data is missing you need to add a comment explaining why

Structure factors

Structure factors: what

The CCDC and FIZ Karlsruhe strongly encourage the inclusion of structure factor data in the IUCr's Crystal Structure Database (ICSD), in line with recommendations from the IUCr's Commission on Crystallographic Nomenclature (CCN).

What are structure factors?

Structure factors are created from experimental crystallographic data. For detailed information, see the IUCr's Commission on Crystallographic Nomenclature (CCN).

Currently, there are two types of information that CCDC and IUCr encourage to be included in the CIF file: structure factor intensities (.hkl). They can also be appended to the CIF file as structure factor amplitudes (.mtz).

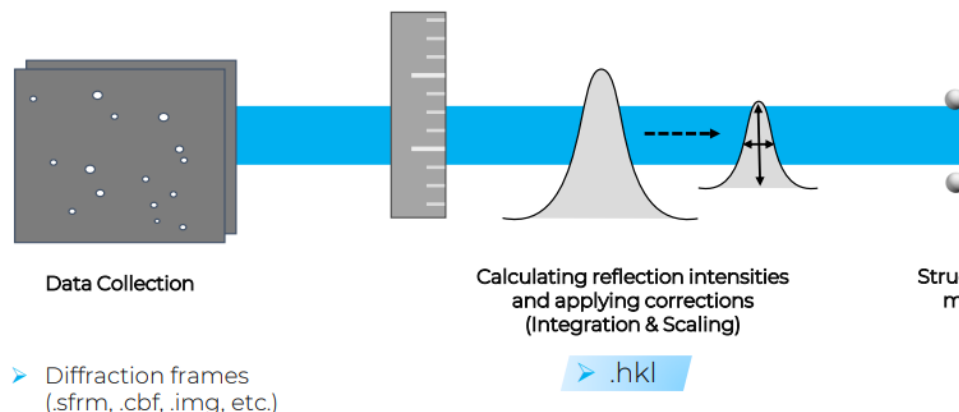
- The **.hkl** file contains the intensity and standard uncertainty values: h , k and l - to identify the reflection. This information is used to calculate the structure factors.
- The **.fcf** file contains the structure factors, which can be recreated using the .hkl and .res file. This last one contains constraints that have been applied). The .fcf file is used for refinement.

These files provide more information about the crystal structure, as part of the publications standard.

Why is it important to share structure factor data?

- It's good data practice - by sharing the data used to create the structure, then it is already stored, especially if you move the data to another repository.
- CheckCIF (the IUCr's CIF checking service) can do checks on the .res in the CIF allows such checks to be performed.
- Several journals require the deposition of structure factor data.

A number of different files are created at each stage of a crystallographic experiment – here we have listed some of the main ones. Files may have different names/some may be combined in different crystallographic software.



If the diffraction frames have been deposited in another repository, the DOI can be associated with your dataset during deposition under "Raw Data DOI"

Files for CCDC deposition:

- **Mandatory**
- **Recommended**

If no structure factor data has been uploaded, you should:

- Go back and upload a new dataset which includes structure factors
- Most refinement software now embeds this into a CIF
- If it is historic data and no structure factor data is available, you need to add a comment before proceeding.

Deposition

Login

Upload

Check
Syntax

Validation

Add
PublicationEnhance
Data

Review

CIF deposition

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 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/d'
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 10.7085(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

Checking the syntax

- Uses enCIFer syntax checking
- Syntax colour coded
 - Field names
 - Loops
 - Data
- Errors highlighted
- Syntax errors need fixing before proceeding
- Once fixed save and recheck errors

```
1 data_5_93GPa
2
3 _audit_creation_method          CRYSTALS_ver_12.80
4 _chemical_name_systematic       '2-hydroxybenzaldehyde oxime'
5 _chemical_name_common           salicylaldoxime
6 _chemical_formula_moiety        'C7 H7 N1 O2'
7 _chemical_formula_sum           'C7 H7 N1 O2'
8 _chemical_formula_weight        137.14
9 _chemical_melting_point         59-61
10 _symmetry_cell_setting          Monoclinic
11 _symmetry_space_group_name_H-M  'P 1 21/n 1 '
12 _symmetry_space_group_name_Hall '-P 2yn'
13 loop_
14 _symmetry_equiv_pos_as_xyz
15
16 x,y,z
17 -x,-y,-z
18 -x+1/2,y+1/2,-z+1/2
19 x+1/2,-y+1/2,z+1/2
20 ;
21 _cell_length_a                  7.677(3)
22 _cell_length_b                  5.7731(8)
23
24 _cell_length_c                  12.159(3)
25
26 _cell_angle_alpha               90
27
28 _cell_angle_beta                110.62(2)
29
30 _cell_angle_beta                110.62(2)
```

You can easily see if the CIF format is broken by looking at the colour coding

```
loop_
  symmetry_equiv_pos_as_xyz
;
x,y,z
-x,-y,-z
-x+1/2,y+1/2,-z+1/2
x+1/2,-y+1/2,z+1/2
;
```

```
_cell_length_a          7.677(3)
_cell_length_b          5.7731(8)
_cell_length_c          12.159(3)
_cell_angle_alpha       90
_cell_angle_beta        110.62(2)
```

[← Go Back](#)[Save & Recheck File](#)[Proceed to Next Step →](#)

Please click on the error message to navigate to the location of the error in the CIF

Error	302	Text block finished at end of file without final ';
Error	-1	The CIF contains no data blocks recognised as crystal structure data

You can easily navigate to errors

Deposition



CIF deposition

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 below have syntax errors. Please click on the file name to view the error details. For more information, see the [FAQ](#).

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
structure01.cif		
data_1	View Report Enter Response	View Hits
structure02.cif		
data_sa2906c	View Report Enter Response	View Hits
data_sa2906a	View Report Enter Response	View Hits
data_sa2906b	View Report Enter Response	View Hits
data_sa2906g	View Report No Response Required	View Hits

[Go Back](#)
[Save & Recheck File](#)
[Proceed to Next Step](#)

Error 44 No terminating (") quote

CheckCIF

- Checks consistency and integrity of the data
- Generates alerts that should either be corrected or explained
- Report and explanations can be embedded in a CIF

Deposition



CIF deposition

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 have syntax errors. Please click on the file name to view the error details. 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
structure01.cif	data_1 View Report Enter Response View Hits	
structure02.cif	data_sa2906c data_sa2906a data_sa2906b data_sa2906g	

Level A

Most likely a serious problem, resolve or explain

Level B

A potentially serious problem, consider carefully

Level C

Check. Ensure it is not caused by an omission or oversight

Level G

General information/check it is not something unexpected

CheckCIF

- Checks consistency and integrity of the data
- Generates alerts that should either be corrected or explained
- Report and explanations can be embedded in a CIF

What to do if you have a checkCIF alert?

Alerts provide potential errors, unusual findings and suggestions for improvement

- All alerts should be checked
- Then decide if you need to improve your model/dataset or add a comment providing more information about the reason for the alert

Alert level A

<u>PLAT183</u>	<u>ALERT_1</u>	<u>A</u>	Missing _cell_measur
<u>PLAT184</u>	<u>ALERT_1</u>	<u>A</u>	Missing _cell_measur
<u>PLAT185</u>	<u>ALERT_1</u>	<u>A</u>	Missing _cell_measur

● Alert level B
PLAT029 ALERT 3 B diff

● **Alert level C**
ABSMU01 ALERT 1 C The

Alerts are hyperlinked to more information about the alert and what action should be taken

There are a number of
online resources available
to learn more about
checkCIF.....



CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

checkCIF validation software to learn more about checkCIF.....

checkCIF validation software

how to respond to checkCIF alerts

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Supporting information: this article has supporting information at journals.iucr.org/e



IUCr Journals

CRYSTALLOGRAPHY JOURNALS ONLINE

checkCIF/PLATON report

Authors of a paper that is expected to not only interpret, but also format the experiment. Additionally, an IUCr review of a submitted manuscript from the deposited CIF file, unusual findings, but a review of the submitted CIF file, information on the structure have been acted on already. The associated paper and readers and users of the interpretation of the calculations with the associated CIF file (findable, accessible, interoperable, *Struct. Dyn.* **6**, 05430). In pointing to and avoid pitfalls. The IUCr web-based on data upload *checkCIF* version is a determination process. There is also a short e web server or with the provides additional basic additional details for a them.

checkCIF Frequently-Asked Questions (FAQ)

- What is checkCIF?

checkCIF on the Web

- How do I use checkCIF?
- What options are available?
- Can I use checkCIF to submit a paper?

Data Validation checks

- What is Data Validation?
- What does Alert Level A signify?
- What does Alert Level B signify?
- What does Alert Level C signify?
- What is a Validation Response Form?

What is checkCIF?

checkCIF is the IUCr service for checking submissions in CIF format to its own and other journals. Prospective authors may submit their CIF manuscripts by email or via a web interface, and receive a check report by return email or as a web page.

checkCIF on the web

How do I use checkCIF?

Web interface

checkCIF is at

- checkCIF for full publication checks
- checkCIF for basic structural checks.

Enter the full path name of a CIF on your local computer system in the text entry box, or use the **Browse...** button to locate the desired file. Send the file for processing by clicking on the **Send CIF for checking** button. Processing and return of the results may take several minutes, depending on file sizes, available network bandwidth and load on the server computer.

- Acta E, Volume 76| Part 1| January 2020| Pages 1-11
<https://doi.org/10.1107/S2056989019016244>
- <https://journals.iucr.org/services/cif/checking/checkfaq.html>

Deposition



CIF deposition

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 below have syntax errors. Please click on the file name to view the error details. 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
structure01.cif		
data_l	View Report Enter Response	View Hits
structure02.cif		
data_sa2906c	View Report Enter Response	View Hits
data_sa2906a	View Report Enter Response	View Hits
data_sa2906b	View Report Enter Response	View Hits
data_sa2906g	View Report No Response Required	View Hits

← Go Back
Save & Recheck File
Proceed to Next Step →

Error 44 No terminating (") quote

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

Style: Ball and Stick
 Labels: No Labels
 Packing: None
 Measure: None

Chemical diagram

View group symbols key

What if my compound is already in a database?

- You can still deposit your data – it's still useful for research!
- Once deposited you can either:
 - Publish your new structure in an associated scientific article
 - Publish directly through the CSD or ICSD without an associated scientific article, known as a **CSD Communication** or **ICSD Communication**

Did you know **glycine** is the **most commonly deposited substance** in the CSD? The structure of glycine has been determined so many times there are two different refcode families!

Simple Search Structure Search Unit Cell Search Formula Search

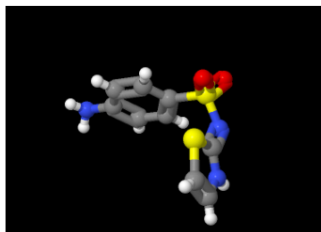
Your query was: Identifier(s): SUTHAZ and the search returned more than 30 records. [Back to Search List](#) [Modify Search](#) [New Search](#)

Results

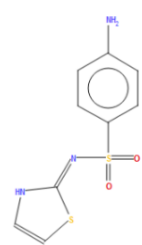
Database Identifier	Deposition Number
☒ SUTHAZ	1264861
☒ SUTHAZ01	1264862
☒ SUTHAZ02	1264863
☒ SUTHAZ03	1264864
☒ SUTHAZ04	1264865
☒ SUTHAZ05	137993
☒ SUTHAZ06	1264866
☒ SUTHAZ07	637211
☒ SUTHAZ08	637215
☒ SUTHAZ09	637212
☒ SUTHAZ10	637216
☒ SUTHAZ11	637213
☒ SUTHAZ12	637217
☒ SUTHAZ13	637214
☒ SUTHAZ14	637218
☒ SUTHAZ16	687586
☒ SUTHAZ17	687587

SUTHAZ : N'-2-Thiazolyl-sulfanilamide
Space Group: P 2₁/c (14), Cell: a 8.235(4)Å b 8.550(4)Å c 15.558(8)Å, α 90° β 93.67(1)° γ 90°

3D viewer



Chemical diagram



View group symbols key

Additional details

Deposition Number	1264861
Synonyms	Sulfathiazole, DrugBank: DB06147
Deposited on	31/12/1971

For example there are over 46 sulfathiazole structures in the CSD
Refcode family SUTHAZ

Deposition



Publish in a Database
Clicking here, you are publishing your data as *CSD Communications* or *ICSD Communications*. Click it **only** if you don't intend to publish your data in a journal article.

Add Publication

Please check and add/update the publication details shown below.

If you don't know the full publication details then please provide the current list of authors for the data you

Authors ? *

William Porter, John Morris

Journal name ?

Volume ?

Year ?

Page ?

Publication DOI ?

Additional information ?

E.g. 10.14469/hpc/2300

If you do not intend to publish your data in the scientific literature and/or through the Cambridge Structural Database (CSD) or the Inorganic Crystallographic Database (ICSD) please click the 'Publish in a Database' button below. Organic and Inorganic data will be published in the CSD as a *CSD Communication*. Inorganic data will be published in the ICSD as an *ICSD Communication*.

Publish in a Database

Authors' names format

- Same order as on publication.
- Each name should be separated by a comma and space.
- No any additional characters, titles, or salutation.
- You can use initials or expand the first name; if you are using initials, then you do not need spaces between them.

Examples of correct authors' names in the CSD e.g.: *C.A.Tovee*, *C.A.Kilner*, *J.A.Thomas*, *M.A.Halcrow* or *Clare A. Tovee*, *Colin A. Kilner*, *Jim A. Thomas*, *Malcolm A. Halcrow*.

Deposition

www.ccdc.cam.ac.uk/community/csd-communications/

Login

Upload

Check
Syntax

Validation

Add
Publication

Enhance
Data

Review

Add Publication

Please check and add/update the publication details shown below.

If you don't know the full publication details then please provide the current list of authors for the data you are depositing.

Authors ? *

William Porter, John Morris

Journal name ?

Volume ?

Volume

Year ?

Year

Page ?

Page

Publication DOI ?

E.g. 10.14469/hpc/2300

Additional information ?

If you do not intend to publish your data in the scientific literature and would like to deposit your data through the Cambridge Structural Database (CSD) or the Inorganic Crystal Structure Database (ICSD), please click the 'Publish in a Database' button below. Organic and metal-organic frameworks will be published in the CSD as a *CSD Communication*. Inorganic data will be published in the ICSD.

Publish in a Database

CSD Communications

ISSN 2631-9888



CSD Communications is a collection of small molecule crystallographic data which has been shared by depositors through the Cambridge Structural Database (CSD) without an associated scientific article.

This may include new data collections of novel structures or new determinations or re-refinements of previously published compounds. *CSD Communications* have an ISSN number and each entry contains the author list and crystallographer details as supplied by the depositor. This allows authors and data producers to get credit for their data, as their structure receives a full CCDC citation including DOI and publication year. The objective of *CSD Communications* is to help scientists contribute to the quantity of crystallographic data available to the public. So far *CSD Communications* have provided the scientific community with access to more than 28,000 crystallographic structures which may never have otherwise been made public.

More information about the benefits of *CSD Communications* is available [here](#) and we also have a series of blog posts about *CSD Communications* and data sharing in general if you want to learn more about this initiative.

Archive

The *CSD Communications* archive contains all of the data published directly through the Cambridge Structural Database (CSD) by the Cambridge Crystallographic Data Centre (CCDC) as *CSD Communications* (previously known as *Private Communications*). Select a year to view all *CSD Communications* published in that year.

2021

2020

2019

2018

2017

2016

2015



In This Section

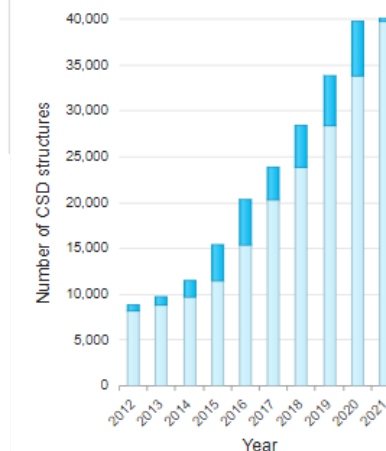
CSD Communications Information

CSD Communications

This Year: 290

To Date: 40,077

CSD Communications growth



Deposition

Login

Upload

Check
Syntax

Validation

Publication

Enhance
Data

Review

CIF deposition

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

The files highlighted in red have errors. Please click on any red file name before proceeding to the next stage. For more information, see the help page.

Pick file to edit

structure01.cif

structure02.cif

Validation

View reports

Structure

structure01.cif

data_1

structure02.cif

data_sa2906c

data_sa2906a

data_sa2906b

data_sa2906d

data_sa2906e

57 _cell_volume 2230.91
58 _cell_formula_units_Z 1
59

Go Back Save & Recheck

Error 44 No terminating (') quote

Add Publication

Please check and add publication information. If you don't know the journal name, please enter the journal abbreviation.

Journal

Publication

Additional information

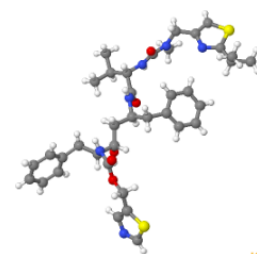
Enhance Data

Pick a structure to edit

YIGPIO03.cif

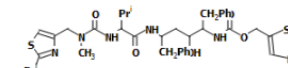
data_YIGPIO03

3D viewer



JSmol

Chemical diagram



data_YIGPIO03

```

16 data_YIGPIO03
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

```

Associated DOIs

Raw data DOI

Data fields

Compound name

Synonyms/other names

Crystal colour

During this stage:

- Check
- Enhance

Each data set by updating info in the data fields

CCDC

Raw data DOIs

Associated DOIs

Raw data DOI ?

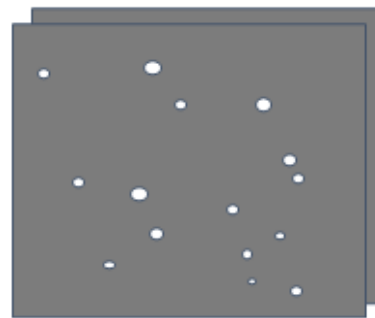
Data fields

Compound name ?

Bis(acetonitrile- λ N)-{(2R_p,2''R_p)-1,1''-[1,2-ethanediylbis(nit

Synonyms/other names ?

Crystal colour ?



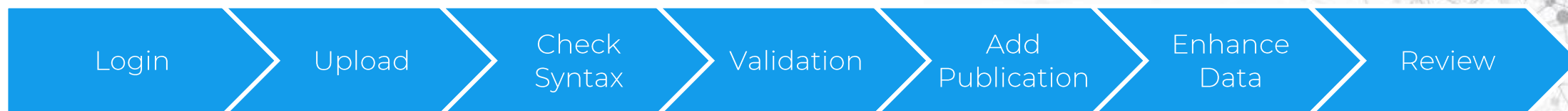
Raw data DOIs are for data created during data collection

- Diffraction frames e.g. .sfrm, .cbf, .img, etc

- We do not accept **diffraction frame data** during deposition
- But you can choose to upload your diffraction frames in another repository or institution repository
 - If you do publish your diffraction frames you should add the DOI to “Raw data DOI”
- Raw data DOI should **not** include the DOI of associated articles

Joint ICSD/CSD deposition service

Deposit your crystal structures ready for publication using our joint deposition service – we'll handle entry into the CSD or ICSD



Our deposition service aims to make it easy for you to:

- Follow community recommendations
- Provide reliable data and metadata
- Deposit all organic, inorganic and metal-organic data
- Publish directly through a database

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/FIZ Karlsruhe

www.ccdc.cam.ac.uk/deposit

CCDC

Try One

It's your turn!

- Try [examples 1 and 2](#) from the handout.
- Your tutors are on hand to help you!
- The handout and example CIFs are available on the web page
- To ask questions during this time [type a message in the chat box](#).



2020.0 CSD Release



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Agenda

- Introduction to the CSD and ICSD
- *Show One*: Overview of Deposition
- *Show One*: Demo of Deposition
- *Try One*: Deposition Hands-on
- *Explore More*: After Deposition and data access
- *Explore More*: Quiz
- Summary



Dataset identifiers

Deposition Numbers should be included in manuscripts

Deposition Numbers - Message (HTML)

File Message Insert Options Format Text Review Help Tell me what you want to do

From: deposit_reply@ccdc.cam.ac.uk

To: Depositor

Cc:

Subject: Deposition Numbers

Dear Depositor,

Thank you for depositing your crystal structure(s) at the Cambridge Crystallographic Data Centre. The data have been assigned to the following deposition numbers.

CCDC XXXXXXXX-XXXXXX

Summary of Data CCDC XXXXXXXX

Formula: C_x H_y O_z

Unit Cell Parameters: a XXXX b XXXX c XXXX Space Group

Summary of Data CCDC XXXXXXXX

16 M. A. Meador, H. Hart, *J. Org. Chem.* 1989, **54**, 2336–2341.

CrossRef | CAS | Web of Science® Times Cited: 16 | 'ejournals@cambridge - find full text'

17 CCDC 1543805 (16) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

McKervey, A. R. Maguire, S. M. Tuladhar and M. Fiona Twohig, *J. Chem. Soc.* 1047–1054 DOI: [10.1039/P19900001047](https://doi.org/10.1039/P19900001047); (b) H. Duddeck, *J. Chem. Soc.*, 1055–1063 DOI: [10.1039/P19900001055](https://doi.org/10.1039/P19900001055); (c) P. Panne and J. M. Fox, *J. Am. Chem. Soc.* 1989, **111**, 1047–1054. For ESI and crystallographic data in CIF or other electronic format see DOI: [10.1039/b82615536](https://doi.org/10.1039/b82615536)

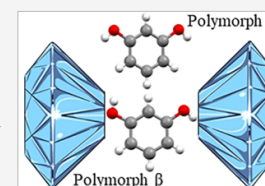
Footnote

† Electronic supplementary information (ESI) available: Experimental procedures and spectroscopic data. For ESI and crystallographic data in CIF or other electronic format see DOI: [10.1039/b82615536](https://doi.org/10.1039/b82615536)

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Abstract

Polymorph α of resorcinol, at ambient pressure stable to 365 K when it transforms to polymorph β , is exceptionally resistant to high pressure. The crystals of polymorph α can be compressed to over 4 GPa without transforming to the β phase. We have performed high-pressure recrystallization of resorcinol aqueous and methanol solutions, and they yielded polymorph α below 0.5 GPa and polymorph β 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 α above 0.5 GPa, consistent with the calorimetric and NMR results. The high-temperature, high-pressure polymorph β 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... π bonds. The large temperature and pressure hysteresis of the polymorphs α and β are connected with the different topologies of their O-H...O networks.



Synopsis

The pressure- and temperature-dependent transition between resorcinol polymorphs α and β 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.^[1,2] Until today, the resorcinol crystals belong to the best known examples of polymorphs.^[3]

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

Revising data

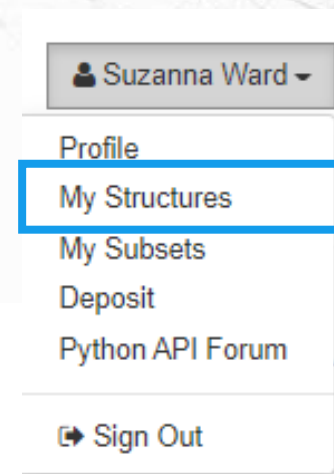
- You can revise your data prior to publication
- During deposition:
 - If logged in:
 1. Click for revision
 2. Add deposition number to revise / select deposition number you wish to revise
 - If not logged in:
 1. Add deposition number to Deposition Number(s) for revision box
- Revised dataset will be assigned the same deposition number
- Old revisions will no longer be visible

This screenshot shows the interface for a user who is logged in. At the top, there are two tabs: '1 Login' (highlighted in green) and '2 Upload' (highlighted in blue). Below the tabs, the text 'Select mode of deposition ?' is followed by two buttons: 'New Deposit' (grey) and 'Click for Revision' (blue). Below these buttons is a blue button labeled 'Add Deposition Number to Revise'. Underneath, the 'Deposition Number:' is followed by a dropdown menu showing '1584792'. At the bottom, there is a link that says 'Check details for the selected structure'.

This screenshot shows the interface for a user who is not logged in. At the top, there are two tabs: '1 Login' (highlighted in green) and '2 Upload' (highlighted in blue). Below the tabs, the text 'Deposition number(s) for revision ?' is followed by a large, empty text input box.

What happens to your data after deposition?

- It is [stored privately until published](#) in an associated scientific article or you decide to publish directly through the CSD or ICSD
- If you have registered on our website you can access your data at any time using our [My Structures](#) service
 - Enables you to view and retrieve datasets
 - Enables you to edit and update datasets
 - Enables you to share your datasets with co-workers
 - Enables you to create your own institutional database
 - Enables you to publish your data directly through the CSD/ICSD
- If you have not published your data [after one year](#), we will [email](#) you to ask if you would like to publish it



My Structures – view, edit, retrieve, share

My Structures

Search by Deposition Number



Clear Filters

Save Settings

Reset Settings

Suzanna Ward

Profile

My Structures

My Subsets

Deposit

Python API Forum

Sign Out

After depositing structures they may take a few minutes to appear in the table. If you are still unable to see your structures after you have received your Deposition Numbers please contact deposit@ccdc.cam.ac.uk

To change the displayed columns or filter results you should click on the down arrow of the relevant column heading. To order the results by a particular column click on the column heading you wish to order your results by.

You can select which structures are displayed by using the dropdown box below. Different subsets can be created using the 'Add to Subset' button and you can view or export these subsets.

All structures

Default Data View

My Downloads

Associate More Structures

Add to Subset

Share Structures

☐		Deposition ...	Datablock	Deposited On	Deposited By	Refcode	Formula	Embargoed...	Status
☐	Details		data_tBu10kbar	28/04/2021			C11 H15 N1 O2	28/02/2022 ?	Unpublished
☐	Details		data_5_93GPa	28/04/2021			C7 H7 N1 O2	28/02/2022 ?	Unpublished
☐	Details	1584792	data_tBu10kbar	09/11/2017			C11 H15 N1 O2	29/11/2019 ?	Unpublished
☐	Details	825801	data_2007may0...	06/06/2011	ward@ccdc.cam...	YIFTUD01	C9 H10 O3		Published in the CSD
☐	Details	825800	data_2007may0...	06/06/2011	ward@ccdc.cam...	EPAHOT	C8 H5 N1 O3		Published in the CSD

My Structure Details

44

Datablock: tBu10kbar

Space Group: I2/a, Cell: a 14.811Å b 6.456Å c 19.759Å, α 90° β 94.060(8)° γ 90°

Formula: C11 H15 N1 O2, Temperature: 298 K

▼ User Details

Reliability Score 3

2D Diagram True

2D/3D Match Full

2D/3D Last Edited

User Compound Name 2-t-butyl-6-[(hydroxyimino)methyl]phenol

User Identifier [Click to add some data](#)

▼ Additional Details

Deposition

Refcode

Compound

Deposited On 28/04/2021

Additional Depositors

Status Unpublished

Embargoed Date 28/04/2022

Unpublished

[Publish in a Database](#)

Status

Embargoed Date ?

28/04/2022

[Extend](#)

[Publish in a Database](#)

[Extend](#)

CCDC

Curating the data into the CSD and ICSD

After publication your data is enhanced and curated

- Every entry undergoes both automated and manual processes
- Enhanced and curated by experts at CCDC and FLZ Karlsruhe
- Ensuring accessibility, discoverability and re-usability of the data

```
data_b:

_andit_creation_method SHELXL-97
_chemical_name_systematic ?
_chemical_name_common ?
_chemical_melting_point ?
_chemical_formula_moiety ?
_chemical_formula_sum 'C23 H23 N4 O10'
_chemical_formula_weight 515.45

loop
  _atom_type_symbol
  _atom_type_description
  _atom_type_scat_dispersion_real
  _atom_type_scat_dispersion_imag
  _atom_type_scat_source
C C 0.0033 0.0016 'International Tables Vol C
H H 0.0000 0.0000 'International Tables Vol C
N N 0.0061 0.0033 'International Tables Vol C
O O 0.0106 0.0060 'International Tables Vol C

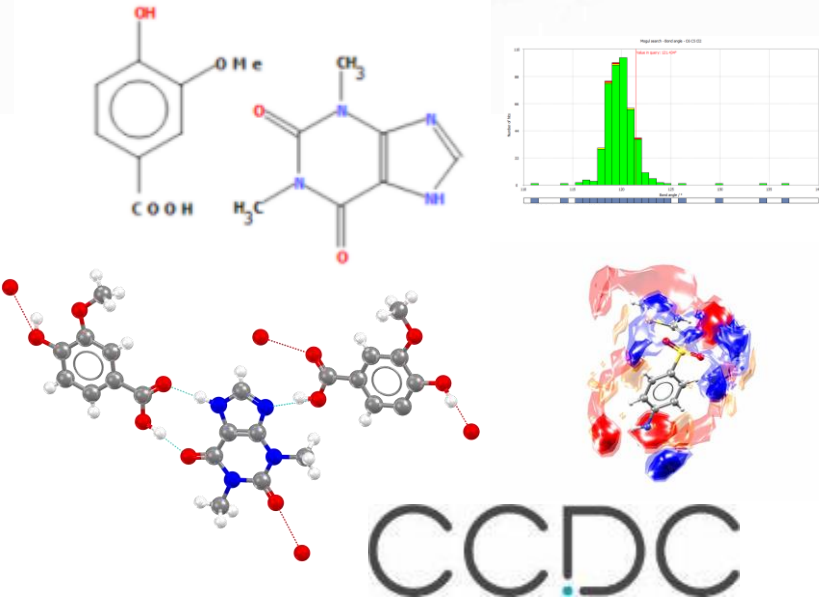
_symmetry_cell_setting Monoclinic
_symmetry_space_group_name_H-M P21/c

loop
  _symmetry_equiv_pos_as_xyz
  'x, y, z'
  'x, y+1/2, -z+1/2'
  'x, -y, -z'
  'x, -y+1/2, z-1/2'

_cell_length_a 11.2741(6)
_cell_length_b 15.7712(10)
_cell_length_c 13.3746(8)
_cell_angle_alpha 90.00
_cell_angle_beta 90.572(2)
_cell_angle_gamma 90.00
_cell_volume 2375.0(2)
_cell_formula_units_Z 4
_cell_measurement_Temperature 173(2)
_cell_measurement_reflns_used 29773
_cell_measurement_theta_min 1.81
_cell_measurement_theta_max 28.33
```



Author(s)	A. Jacobs, F.M.A. Noa
Reference	CrystEngComm (2015), 17, 98
Publication DOI	10.1039/C4CE01795A
Deposition	CCDC 1022107
Formula	2(C ₈ H ₈ O ₄), C ₇ H ₈ N ₄ O ₂
Compound	bis(4-Hydroxy-3-methoxybenzoic acid) 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
Synonym	bis(Vanillic acid) theophylline
Spacegroup	Name: P21/c Number: 14
Cell	a: 11.274(4) b: 15.771(1) c: 13.375(4) alpha: 90.00 beta: 90.57(1) gamma: 90.00 Volume: 2377.967
Reduced Cell	a: 11.274 b: 13.375 c: 15.771 alpha: 90.00 beta: 90.00 gamma: 90.57 Volume: 2377.967
Molecular Volume	594.492
Chemical Units	2
Z, Z'	Z: 4.0 Z': 1.0
R-Factor (%)	4.7
Disorder	C7A, O4A and C5A, O5A disordered over two sites with occupancies 0.812/0.188.
Temperature (K)	173
Density	CCDC: 1.443 Author: 1.44
Intensity Meas	diffractometer
Average Sigma (C-C)	0.001-0.005Å
Colour	colorless
Habit	rectangle
Recryst. Solvent	water



Access Structures

www.ccdc.cam.ac.uk/structures

- Access Structures allows you to search **CSD** and **ICSD**
- Every individual dataset is free to view and download



Simple Search Structure Search Unit Cell Search Formula Search

Simple text and numeric searching

Welcome to WebCSD. This service now includes the ability to search for inorganic structures through the CCDC's and FIZ Karlsruhe's joint Access Service using the Simple Search tab. 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

Identifier(s)

Compound name

DOI

Authors

Journal

Publication details
 Year Volume Page

Database to search
☒ Entire published collection ☐ CSD ☐ ICSD ☐ Teaching subset

POWVEF : catena-[(μ-phenylphosphonato)-zinc(II)]
 Space Group: P 2₁/c (14), Cell: a 14.8549(8)Å b 5.1581(3)Å c 10.5471(6)Å, α 90° β 105.816(2)° γ 90°

3D viewer

Chemical diagram

View group symbols key

Additional details

Deposition Number	1951130
Data Citation	L. Falvello, P. Lotti, C. Massera, S.C. Tarantino, M. Zema, H. Puschmann, M.Y. Agbahoungbata, J. Andreo, S.A. Sahadevan, A. Bismuto, G. Bonfant, S.A.S. Bonou, C. Carraro, M.D. Zotti, A. di Biase, R. Fantini, I. Ferraboschi, J.M.F. Custodio, M. Frigerio, G. Gallo, S. Gjyli, M. Goudjil, F. Igao, E. Kahveci, M. Kalienko, S. Lorenzon, L. Macera, J.J.M. Fajardo, E. Nushi, S. Ouatta, E. Parisi, L. Pasqualetto, E. Pesko, G. Pierri, R. Pinalli, R. Poppe, A. Santoro, E. Smirnova, S. Sorbara, L. Tensi, G. Tusha CCDC 1951130: Experimental Crystal Structure Determination, 2019, DOI: 10.5517/ccdc.csd.cc23h9pm
Deposited on	03/09/2019

Simple Search Structure Search Unit Cell Search Formula Search

Your query was: DOI: 10.1039/C4CE01795A and the search returned 7 records.

Modify Search

New Search

Results

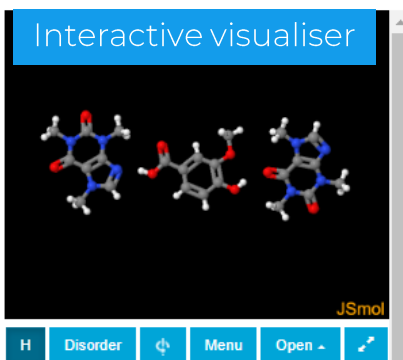
☒	Database Identifier	Deposition Number
☒	ZOYBEW	1022106
☒	ZOYBIA	1022107
☒	ZOYBOG	1022108
☒	ZOYCAT	1022109
☒	ZOYCEX	1022110
☒	ZOYCIB	1022111
☒	ZOYCOH	1022112

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identifiersData citation and
DOIQuery
highlighted and
DOI links to
publicationZOYBEW : 4-hydroxy-3-methoxybenzoic acid bis(1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione)
Space Group: $P \bar{1} (2)$, Cell: a 10.110(2)Å b 10.525(2)Å c 12.221(2)Å, α 77.69(3)° β 81.26(3)° γ 82.69(3)°

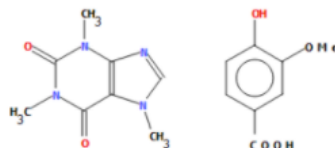
3D viewer

Interactive visualiser

H Disorder Menu Open ▾
Style: Ball and Stick Labels: No Labels Packing: None

Chemical diagram

Curated diagram



View group symbols key

Identifier and key details. Banner colour coded
depending on databaseAdditional chemical, crystal and experimental
details

Additional details

Deposition Number	1022106
Data Citation	Ayesha Jacobs, Francoise M. Amombo Noa CCDC 1022106: Experimental Crystal Structure Determination, 2014, DOI: 10.5517/cc139155
Synonyms	vanillic acid bis(caffeine)
Deposited on	30/08/2014

Associated publications

Ayesha Jacobs, Francoise M. Amombo Noa, *CrystEngComm*, 2015, 17, 98, DOI: [10.1039/C4CE01795A](https://doi.org/10.1039/C4CE01795A)

Chemical details

Formula $2(C_8H_{10}N_4O_2) \cdot C_8H_8O_4$

Crystal details

Space group	$P \bar{1} (2)$
Unit cell	a 10.110(2)Å b 10.525(2)Å c 12.221(2)Å α 77.69(3)° β 81.26(3)° γ 82.69(3)°
Cell volume	1249.69
Reduced cell	a 10.110Å b 10.525Å c 12.221Å α 77.690° β 81.260° γ 82.690°
Z, Z'	2, 1
Habit	rectangle
Recrystallisation solvent	Re-crystallisation from solvent: ethyl methylketone
Colour	colorless

Experimental details

R-factor (%)	5.42
Temperature (K)	173

Wiley Online Library

16 M. A. Meador, H. Hart, *J. Org. Chem.* 1989, **54**, 2336–2341.
CrossRef | CAS | Web of Science® Times Cited: 16 | 'ejournals@cambridge - find full text'

17 CCDC 1543805 (16) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

18 Nitrile oxide **18** could be stored at –18 °C for at least one month.

Outline

Abstract

Graphical abstract

1. Introduction

2. Results and dis

3. Conclusions

4. Experimental

Acknowledgements

Supplementary data

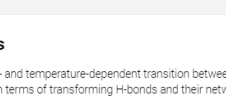
Research Data

References and notes



ACS Publications
Most Trusted. Most Cited. Most Read.

Polymorph α



Polymorph β

with the calorimetric and NMR results. The high-temperature, high-pressure polymorph β 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... π bonds. The large temperature and pressure hysteresis of the polymorphs α and β are related to the different topologies of their O—H...O networks.

Synopsis

The pressure- and temperature-dependent transition between resorcinol polymorphs α and β 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 (1,2). Until today, the resorcinol crystals belong to the best known examples of polymorphs (3).

ARTICLE SECTIONS

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CCDC: 1913241
CCDC: 1913242

Keywords: celecoxib; active pharmaceutical ingredient; API; solvate; crystal structure; isostructurality; disorder; *PIXEL*; anti-inflammatory.

CCDC references: 2011633; 2011634; 2011635; 2011636; 2011637; 2011638

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 Cambridge Crystallographic Data Center
Crystallographic data
Data associated with the article:
[CCDC 689113: Experimental Crystal Structure Determination](#)

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☒	ZOYBEW	1022106
☒	ZOYBIA	1022107
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#####

data_b:
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_citation_doi
_citation_year
10.1039/C4CE01795A 2015
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2014-08-30 deposited with the CCDC.    2021-01-22 downloaded from the CCDC.
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'-x, -y, -z'
'x, -y-1/2, z-1/2'

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_cell_angle_gamma           90.00
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_cell_measurement_temperature 173 (2)
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_cell_measurement_theta_min 1.81
_cell_measurement_theta_max 28.33
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What have we learnt?

- What data you can find in the CSD and the ICSD
- Familiarity in depositing a crystal structure ready for publication
 - Following the 8 step deposition process in the demo and hands on example
- The basics of how to check the novelty and integrity of your data
 - Duplicate check
 - checkCIF
 - Syntax checking
- How to revise and access deposited datasets

Want to explore more?

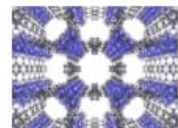
Training and Educational Resources

The wealth of information contained within the Cambridge Structural Database (CSD) extends far beyond a collection of crystal structures. Knowledge derived from these materials informs much of chemistry, biochemistry, and biology. Chemical and structural concepts are often difficult to grasp without real world, interactive examples for students to explore.

The CCDC and our colleagues continually produce educational materials for use in classroom and computer lab settings, or as independent study modules. Many of these materials make use of the Teaching Subset - a freely available set of over 750 structures that can be investigated with the free version of our Mercury visualisation and analysis program. Of course, our database of over one million entries are available for free through our Access Structures portal.

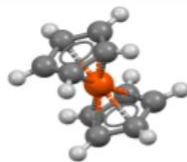
If you are an educator looking for supplementary teaching materials, find out more about the Teaching Database [here](#). If you have developed your own modules using the CSD and would like to share them with the broader community, please contact us at education@ccdc.cam.ac.uk.

To keep up to date with the latest news from education and outreach at the CCDC, sign up for the Education and Outreach Newsletter [here](#).



CSD-Community

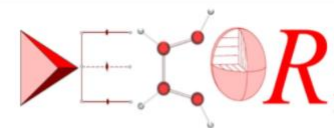
Freely accessible tools from the CCDC.



Information on the Teaching Subset



Access a series of teaching modules for use in the classroom



DECOR: Educational Resources for Teaching Crystallography

Self-guided workshops



Download a series of self-guided workshop materials for CCDC tools and features



Watch software training and support videos

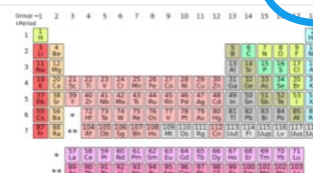


CSD University modules

On-demand modules with completion certificate



Access fun science activities for kids through the CCDC Home learning page



Explore the Periodic Table through Crystal Structures

YouTube and LabTube channels

CCDC