

# CSD Communications



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.

## CSD Communications

Today I would like to present to you: *CSD Communications*!

今天我给大家介绍一下 CSD 通讯!

*CSD Communications* are a fast alternative to publish your data. If you deposit your data as a *CSD Communication*, it will be immediately accessible today with no need for an associated scientific paper!

CSD 通讯是一条快速发表数据的通道! 如果您选择以 CSD 通讯发表所存储的数据, 它们将立即对公众开放而无需相关联的科学论文!

<https://www.ccdc.cam.ac.uk/Community/csd-communications/>

## Guidelines - 存储准则页面

HOME / COMMUNITY / DEPOSIT A STRUCTURE / THE CCDC CIF DEPOSITION GUIDELINES

### The CCDC CIF Deposition Guidelines

When preparing your CIF for deposition please include as much information as possible and check it carefully. This is especially true for *CSD Communications* where there is no paper to describe the chemistry and experimental details leading to your structure. If you choose to publish your data as a *CSD Communication* please remember to provide all the authors/crystallographers/chemists who contributed to the crystallographic experiment as authors of the data. The co-authors of a *CSD Communication* should be all those persons who have made significant scientific contributions to the work reported, including the ideas and their execution, and who share responsibility and accountability for the results. Suggested contributors that could be included as authors include:

- Crystallographer
- Data Collection/Data solution/Refinement Scientist
- Synthetic Chemist
- Recrystallisation Scientist
- Principal Investigator/Supervisor

By publishing data as a *CSD Communication* you are also certifying that you are the owner of the data and your contribution is your original work; that all authors concur with and are aware of the submission; and that all workers involved in the study are listed as authors and given proper credit.

If we are unable to validate your structure from the information you have provided we may contact you. If we cannot resolve the issue, unfortunately, we may not be able to add your structure to the [CSD](#).

 [Guidelines in Chinese](#)

#### In This Section

[The CCDC CIF Deposition Guidelines.pdf](#)

#### Related Topics

[Deposit a Structure](#)

[Structure Deposition Information](#)

[Correcting CIFs](#)

[CSD Communications](#)

<https://www.ccdc.cam.ac.uk/Community/depositastructure/cif-deposition-guidelines/>

If you are new to depositing data, we have some handy, easy to follow guidelines and these are especially important for data deposited as *CSD Communications* as there is no scientific paper to accompany it. Ensuring researchers get the credit they deserve is important so if you are publishing *CSD Communications* make sure the list of authors includes everyone that contributed to the dataset including the Crystallographer, Data Collection/Data solution/Refinement Scientist, Synthetic Chemist, Supervisor and so on. Once your *CSD Communication* is deposited with us, we will include it

in the Cambridge Structural Database (or CSD for short) and it will be scientifically checked and it will undergo a standard procedures such as validation and curation.

如果您是我们的新用户， 请参看这些简单， 方便的存储准则。由于没有相关的科学论文， 遵循这些准则对 CSD 通讯尤为重要。为确保所有与该数据相关的研究人员都得到相应的信酬， 请在作者名单中包括所有与该数据相关的人员姓名， 包括晶体学家， 合成化学家， 导师等。完成 CSD 通讯的存储操作以后， 该数据将经过 CCDC 专家们的验证， 整理等常规程序最终收录于剑桥结构数据库 (CSD)中。

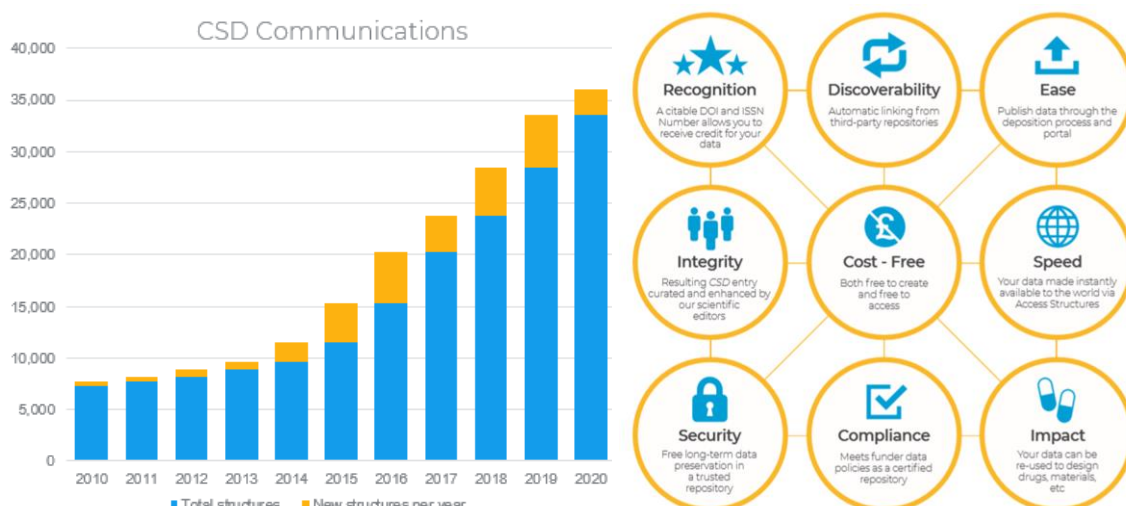
With over 30% of deposits now coming from China we have also made these guidelines available in Chinese.

目前超过 30%的数据来自中国， 因此我们特意准备了存贮准则的中文版本。

<https://www.ccdc.cam.ac.uk/Community/depositastructure/cif-deposition-guidelines/the-ccdc-cif-deposition-guidelines.pdf>

## Benefits - 优点

<https://www.ccdc.cam.ac.uk/Community/csd-communications/CSDCommunicationsInformation/>



*CSD Communications* are completely free to deposit, publish and access and have been available to our users since 1976. We currently have over 30,000 datasets deposited and published in this way and last year we were the number one place to publish structures. *CSD Communications* provide instant recognition for authors and enhanced discoverability for each dataset and as an author you get a citable reference and data DOI. You can also trust your data will be valued by the community and others can learn it, so you never know your *CSD Communication* may go on to help identify a new drug or catalyst that could help millions around the world.

自 1976 年以来， CSD 通讯就以免费存储， 出版， 访问的形式面向广大用户。迄今已收录超过 30, 000 套数据， 去年还登上了发表结构数据总量的第一名。 CSD 通讯的作者可以得到即时的认可， 数据的可见度得以大幅度提高， 每套数据还为作者带来可以作为引证的数据 DOI。毫无疑问， 您的数据将为全世界广大同行们的研究带来不可估量的价值， 它们也许能在新药研发， 新型催化剂的研制中起到关键作用。

How to deposit as CSD Communication? - 那么我们怎样存贮 CSD 通讯数据呢?

## How to deposit CSD Communications data

1. During the deposition process using "Publish in a Database"
2. After deposition through our MyStructures service

The deposition of the *CSD Communication* data can be a part of the normal deposition process. You can check the integrity and uniqueness of data through tools such as CheckCIF or our Reduced Cell Check that are available as a part of the online deposition.

CSD 通讯数据的存储可以通过我们通常使用的数据存储过程来完成。其中包含的线上服务 CheckCIF 和晶胞检测可以用来验证数据的完整性和唯一性。

For full deposition process please see our resources on how to deposit data:

关于如何存储数据的完整过程请观看我们‘如何存储数据’的教程。

- <https://www.ccdc.cam.ac.uk/Community/depositastructure/>
- <https://www.youtube.com/watch?v=bxDbLdNaJ7M>
- <https://www.ccdc.cam.ac.uk/Community/educationalresources/workshop-materials/csd-community-workshops/CSDC-Deposition.pdf>



## CIF deposition and validation service

This web service enables you to submit CIF files and associated structure factor files to the joint CCDC and FIZ Karlsruhe deposition service.

- Files should be in **CIF, HKL, RES, FCF, Word** format and may be included in a ZIP file
- At least one CIF file must be included in the submission
- All files submitted on one form should correspond to **one publication only**
- There is a limit of **50 MB** per file and a limit of **100 MB** for the total size of files uploaded. [Click here](#) if your data exceeds these limits
- If possible structure factor data for all structures should be included in the deposition
- You may also revise unpublished structures using this service
- For more information please see our [Structure Deposition Information](#) page

### During the Deposition process – 在存储过程中

As you are depositing your data – the option of submitting your deposition as *CSD Communication* is right there at the step 5 Add publication – all you need to do is add the authors and click the ‘Publish in a Database’ button.

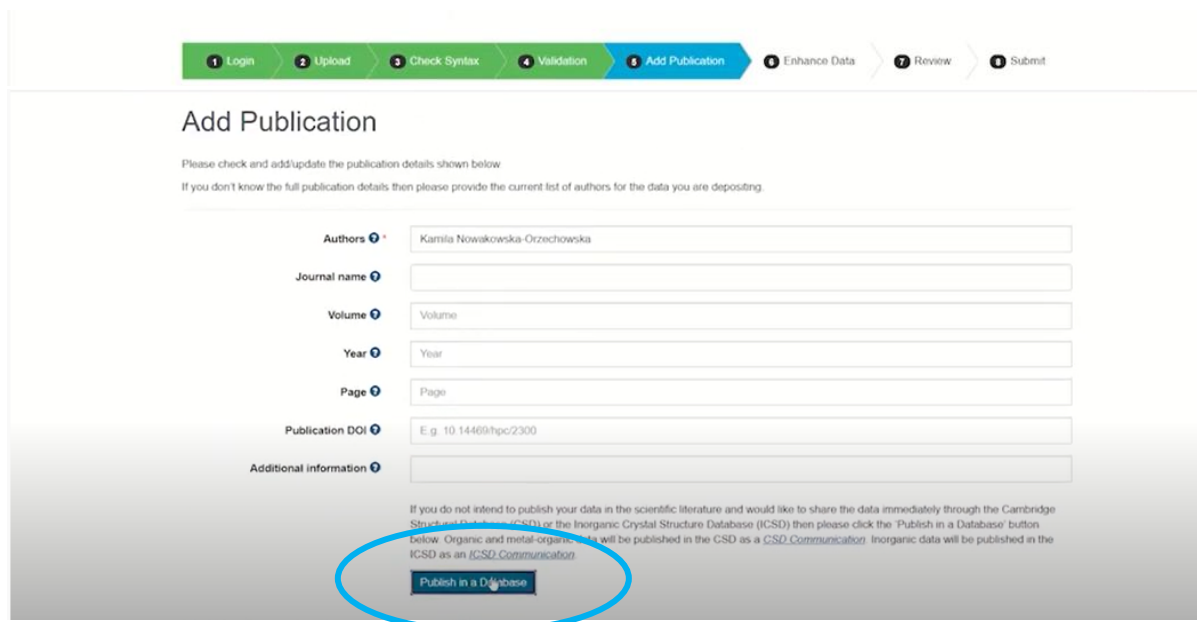
在您存储数据的过程中-提交数据作为 CSD 通讯的选项存在于第 5 步“添加出版物”-您需要做的就是添加作者名称并点击“在数据库中发表”按钮。

One click and you can Publish in a Database!

点击此键，您就可以在数据库中发表该结构!

**Note:** If you intend to publish your data in an associated scientific article, then you do NOT need to select this option. If your data is published, our workflows with publishers will mean your data is automatically updated with publication details and made available through the CSD when your manuscript is published.

**注意：**如果您计划在科学论文中发表该数据，则无需选择这一选项。如果您的数据是伴随文章所投的稿，那么一旦文章得以正式发表，我们和相关出版商合作的工作流程将会自动更新数据的出版物详情。



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

### 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

Journal name

Volume

Year

Page

Publication DOI

Additional information

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

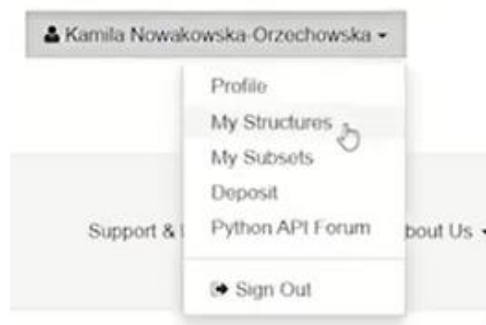
[Publish in a Database](#)

## How to update already deposited unpublished data - 如何更新已经存入但还未发表的数据

If you are registered on our website, you can access your deposited structures by logging in and then go to My Structures on the dropdown menu.

如果已在我们的网站上注册，您可以登录后在下拉菜单中的“我的结构”中访问已保存的结构。

Once your data is deposited with us and remains unpublished – you can make it available as *CSD Communication* via MyStructures.



如果已存入的结构还保持在‘未发表’的状态-您可以通过‘我的结构’来将该数据以 CSD 通讯的形式发表

(1) First load all your structures in MyStructures view and (2) then select the dataset you wish to make a *CSD Communication*. (3) Open the record by clicking on details and (4) scroll down to the publication. If your data has never been published before you will see this button “Publish in a Database”.

(1)首先在‘我的结构’中加载所有结构，(2)然后选中要发表为 CSD 通信的数据。(3)通过单击‘详细信息’打开数据详情，(4)并向下滚动到出版物。如果此数据还未发表过，您将看到“在数据库中发布”按钮。

(5) Once you press this button & (6) add all the authors according to our guidelines, the year will be added, and the data will be made available immediately!

(5) 点击此按钮, (6) 并按照存储准则中的规定添加作者姓名, 信息存盘后, 出版年份将会自动更新, 数据将立即对公众开放。

### My Structures

Search by Deposition Number

After depositing structures they may take a few minutes to appear in the table. If you are still unable to see your structures, contact [deposit@ccdc.cam.ac.uk](mailto: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 subsets.

**1** → All structures

<input type="checkbox"/>	Deposition ...	Datablock	Deposited On	Deposited By	Refcode	Formula
<input type="checkbox"/>	<input type="button" value="Details"/>	data_03scw020	22/09/2020	kamita@ccdc.ca...		C7 H4 F1 O2
<input type="checkbox"/>	<input type="button" value="Details"/>	data_a	22/08/2018			C10 H13 Cs0.3 Se3.2

**2** → **3** →

### My Structure Details

**3** →

Datablock: 03scw020  
**Space Group:** Pbcn, **Cell:** a 12.06Å b 11.603Å c 15.434Å,  $\alpha$  90.00°  $\beta$  90.00°  $\gamma$  90.00°  
**Formula:** C7 H4 F1 O2 1-, C5 H7 N2 1+, Temperature: 120 K

**User Details**

Reliability Score	2
2D Diagram	True
2D/3D Match	Full
2D/3D Last Edited	
User Compound Name	
User Identifier	

**Additional Details**

Deposition Number	
Refcode	
Compound Name	2-Aminopyridinium 2-fluorobenzoate salt
Deposited On	22/09/2020
Additional Depositors	
Status	Unpublished <input type="button" value="Publish in a Database"/>
Embargoed Date	22/09/2021 <input type="button" value="Extend"/>

**Associated Publications**

**4** → **5** →

**6** →

**Publish in a Database**

By choosing to Publish in a Database your structure will be made publicly available via our Access Structures service. Organic and Metal-Organic structures will be published in the CSD as a *CSD Communication*. Inorganic structures will be published in the ICSD as an *ICSD Communication*. Please check the author details are correct before pressing 'Save' or press 'Cancel' if you do not wish to publish your structure directly through a database.

**Authors**

Please bear in mind that the year of the publication is always set to a current year by default.

请记住，默认情况下，发表年份始终设置为当前年份。

Each year we also send thousands of emails to the depositors of the unpublished data to remind them of this possibility so if you have unpublished data we will contact you!

我们每年都会发送上千份邮件给拥有未发表数据的作者们，提醒她们可以将数据作为 CSD 通讯加以发表，所以如果您在 CCDC 拥有未发表的数据我们将会联系您。