

# TUTORIAL for UPLOADING CIFs IN COD

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## 1- CIFs from a final refinement result (single crystal – SHELX, etc - or powder - Rietveld method) - **In a few clicks**

Such CIFs produced by refinement software are generally already almost complete and contain all but the reference to the published text. The COD upload system can add the reference automatically in your CIF provided you have a DOI.

**Anyway, remember that the first thing to do is to verify if the entry is not already inside of the COD...**

**So, you have a CIF and a DOI and want to deposit your CIF in COD ?**

Go to the « deposit your data » interface :

[https://www.crystallography.net/cod/initiate\\_deposition.php](https://www.crystallography.net/cod/initiate_deposition.php)

Enter your username and password or sign up in order to obtain them :

The screenshot shows a web browser window displaying the Crystallography Open Database (COD) website. The page title is "Crystallography Open Database" and the main heading is "Validation and Deposition Interface". The interface includes a navigation menu on the left with sections like "COD Home", "Accessing COD Data", "Add Your Data", and "Documentation". The main content area features a progress bar with steps: "Upload a file", "Validate data", "Deposit structures", and "Finish". Below the progress bar is a "Depositor login (sign up)" form with fields for "Choose deposition type", "Username", and "Password", along with a "Begin deposition" button. Below the form is a section titled "About the Validation and Deposition Interface" which explains the process and lists steps: "Upload", "Validation", and "Deposition". It also mentions "File formats" and "Currently we accept two types of files: Plain CIF files; and ZM (zipped CIF files)".

Select the « Deposition type », either « Already published data » or « Prepublication data » or « Personal communication to COD »

In this case it is « Already published data ».

Then click on « **Begin deposition** » :

The screenshot shows the COD website's 'Validation and Deposition Interface'. The page has a navigation bar with 'Log in', 'Upload a file', 'Validate data', 'Deposit structures', and 'Finish'. The 'Validate data' step is currently active. Below the navigation bar, there is a section titled 'Depositing published structures' with instructions on what information a published structure should contain and how to handle missing information. A 'Data upload' box contains a file selection area with a 'Parcourir...' button and a 'Validate' button. The page also includes a sidebar with navigation links and a 'Top of the page' link at the bottom.

Then select the CIF or ZIP file with CIFs for check and click on « **validate** ».

A first screen of the validation beginning is displayed :

The screenshot shows the validation results for a file named 'complex1.cif'. The page displays a table with columns for 'File', 'Status', and 'Actions'. The file 'complex1.cif' has a status of 'warnings'. Below the table, there are two sections of warnings and notices. The first section, titled 'Data block 160102a:', lists several missing data items: '\_publ\_author\_name', '\_journal\_name\_full', '\_publ\_section\_title', '\_journal\_year', and '\_journal\_volume'. The second section, titled 'Data block 160102a:', lists several notices: the '\_symmetry\_cell\_setting' value was changed from 'Monoclinic' to 'monoclinic', and the definitions for '\_platon\_squeeze\_details', '\_platon\_squeeze\_void\_average\_x', and '\_platon\_squeeze\_void\_average\_y' were not found in the provided dictionaries.

In yellow background, it is said that the CIF tags corresponding to the reference are lacking (author names, journal details, paper title). Then click on « **Edit** » just above the warnings. You see your CIF content appearing and just above you will be offered to « **Fetch bibliography by DOI** ». Enter there your DOI, then select just below either « **Pubmed** » or « **Crossref** » (in this JSSC case, select Crossref) and click on « **Fetch** » :

```
item was not found in the provided dictionaries.
» definition of the '_platon_squeeze_void_volume' data
item was not found in the provided dictionaries.
```

**Tip:** if you need to add bibliography common to all structures in this file, you can add a **data\_global** section below, and the data will be distributed into all other sections.

Fetch bibliography by DOI:

10.1016/j.jssc.2017.09.0

Save and check

PubMed  Crossref

Fetch

Your CIF file contents:

```
data_160102a
_chemical_formula_sum      'C39 H28 Cd N6 O5'
_chemical_formula_weight   773.07
_space_group_IT_number     14
_space_group_name_Hall     '-P 2ybc'
_space_group_name_H-M_alt  'P 1 21/c 1'
_symmetry_cell_setting     monoclinic
_symmetry_space_group_name_H-M 'P 1 21/c 1'
_atom_sites_solution_hydrogens geom
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_audit_creation_method     SHELXL-97
_cell_angle_alpha          90.00
_cell_angle_beta           101.177(2)
_cell_angle_gamma          90.00
_cell_formula_units_Z      4
_cell_length_a              10.4600(9)
_cell_length_b              37.964(3)
_cell_length_c              9.4331(8)
_cell_measurement_reflns_used 1865
_cell_measurement_temperature 298(2)
_cell_measurement_theta_max 27.461
_cell_measurement_theta_min 2.559
_cell_volume                3674.9(5)
_computing_cell_refinement  'Bruker SMART'
_computing_data_collection  'Bruker SMART'
_computing_data_reduction   'Bruker SAINT'
```

Save and check

Then you see (in principle...) « **Bibliography was appended successfully** » on a green background and you will see below in the edited CIF the complete bibliography appearing :

Eichier Edition Affichage Historique Marque-pages Outils Aide

A multifunctional three-fold in X Crystallography Open Database X

https://www.crystallography.net/c



# Crystallography Open Database

**Validation and Deposition Interface**

Log in Upload a file **Validate data** Deposit structures Finish

**Edit CIF file: complex1.cif**

Bibliography was appended successfully.

The following warnings should be taken into account from [complex1.cif]:

**Data block 160102a:**

- » recommended data item '\_publ\_author\_name' was not found.
- » data item '\_journal\_name\_full' was not found.
- » data item '\_publ\_section\_title' was not found.
- » neither data item '\_journal\_year' nor data item '\_journal\_volume' was found.
- » neither data item '\_journal\_page\_first' nor data item '\_journal\_article\_reference' was found.

The following notices should be taken into account from [complex1.cif]:

**Data block 160102a:**

- » data item '\_symmetry\_cell\_setting' value 'Monoclinic' was changed to 'monoclinic' in accordance
- item was not found in the provided dictionaries.
- » definition of the '\_platon\_squeeze\_void\_volume' data item was not found in the provided dictionaries.

**Tip:** if you need to add bibliography common to all structures in this file, you can add a **data\_global** section below, and the data will be distributed into all other sections.

Fetch bibliography by DOI:

Save and check  PubMed  Crossref Fetch

**Your CIF file contents:**

```

data_global
loop
  _publ_author_name
  'Zhu, Zheng'
  'Wang, Mei'
  'Xu, Cun-gang'
  'Zong, Zi-ao'
  'Zhang, Dong-mei'
  'Bi, Shuang-yu'
  'Fan, Yu-hua'
  _publ_section_title
  'A multifunctional three-fold interpenetrated coordination polymer showing
  excellent luminescent sensing for Cr(VI)/ Fe(III) and photocatalytic properties'
  _journal_name_full
  'Journal of Solid State Chemistry'
  _journal_page_first
  176
  _journal_page_last
  183
  _journal_paper_doi
  10.1016/j.jssc.2017.09.005
  _journal_volume
  256
  _journal_year
  2017
data_160102a
  _chemical_formula_sum
  'C39 H28 Cd N6 O5'
  _chemical_formula_weight
  773.07
  _space_group_IT_number
  14
  _space_group_name_Hall
  '-P 2ybc'
  _space_group_name_H-M_alt
  'P 1 21/c 1'
  _symmetry_cell_setting
  monoclinic
  _symmetry_space_group_name_H-M
  'P 1 21/c 1'

```

Save and check

Then click on « **Save and check** », the file will be validated, then click on « **Deposit** » and the process should end in a deposited file with an entry number attributed :

The screenshot shows the COD website's 'Validation and Deposition Interface'. At the top, there is a progress bar with five steps: 'Log in', 'Upload a file', 'Validate data', 'Deposit structures', and 'Finish'. Below this, a message states: 'All uploaded files have been successfully deposited to the COD. You can now [check new CIF file](#).' A table shows the deposition status for a file named 'complex1.cif', which has been 'deposited to the COD'. Below the table, a message reads: 'Structures from file [complex1.cif] were deposited as entries 1560317'. The left sidebar contains navigation links for 'COD Home', 'Accessing COD Data', 'Add Your Data', and 'Documentation'.

You may click on that entry number (1560317 here) and make ultimate checks if you wish :

The screenshot shows the 'Information card for entry 1560317' on the COD website. The page title is 'Information card for entry 1560317'. Below the title, there is a navigation path: '1560316 << 1560317 >> 2000000'. A 'Preview' section features a 3D ball-and-stick model of a complex coordination polymer structure, labeled 'JSmol'. Below the model, there are links for 'Coordinates', 'Download 1560317.cif', and 'Update'. A section titled 'Structure parameters' contains a table with the following data:

Formula	C39 H28 Cd N6 O5
Calculated formula	C39 H28 Cd N6 O5
Title of publication	A multifunctional three-fold interpenetrated coordination polymer showing excellent luminescent sensing for Cr(VI)/ Fe(III) and photocatalytic

With some experience, this method takes 1 minute or 2...

But if that way « **In a few clicks** » fails... then try the following « **By hands** » way :

## 2- CIFs from a final refinement result (single crystal – SHELX, etc - or powder - Rietveld method) – **By hands**

Such CIFs produced by refinement software are generally already almost complete and contain all but the reference to the published text. Then, before uploading such CIFs into the COD, one needs to complete the CIF with the following list of CIF tags :

```
#-----  
loop_  
_publ_author_name  
,  
_publ_section_title  
;  
;  
_journal_name_full  
_journal_page_first  
_journal_page_last  
_journal_volume  
_journal_year  
_journal_paper_doi  
#-----
```

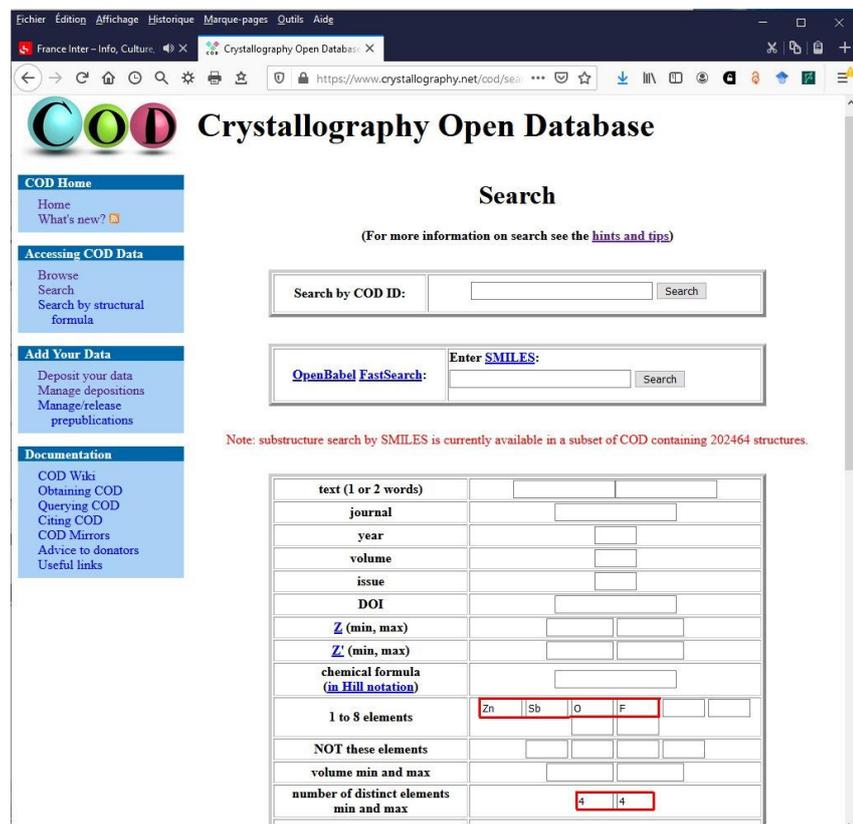
Anyway, the first thing to do is to verify if the entry is not already inside of the COD...

The example used here corresponds to a 2017 paper in JSSC, volume 256, pp 158-161.

So, log in the COD and verify by a search either on the journal reference or/and on the authors, the chemical formula if that compounds ( $Zn_3Sb_4O_6F_6$ ) has not yet an entry :

<https://www.crystallography.net/cod/search.html>

Here the choice for the search is the chemical content, Zn, Sb, O, F and exactly four different elements :



The screenshot shows the Crystallography Open Database search page. The search form is titled "Search" and includes a note: "(For more information on search see the [hints and tips](#))". The search options are as follows:

text (1 or 2 words)	<input type="text"/>
journal	<input type="text"/>
year	<input type="text"/>
volume	<input type="text"/>
issue	<input type="text"/>
DOI	<input type="text"/>
Z (min, max)	<input type="text"/> <input type="text"/>
Z' (min, max)	<input type="text"/> <input type="text"/>
chemical formula (in Hill notation)	<input type="text"/>
1 to 8 elements	<input type="text"/> Zn <input type="text"/> Sb <input type="text"/> O <input type="text"/> F <input type="text"/>
NOT these elements	<input type="text"/>
volume min and max	<input type="text"/> <input type="text"/>
number of distinct elements min and max	<input type="text"/> 4 <input type="text"/> 4

In case of an organic or organometallic compound, the best choice for a search would not be necessarily the chemical content, but in this case it works and the result is negative : no such entry in the COD.

Then you can get the CIF from the supplementary material of the paper (unless you are the author so you have it already) and complete the lacking tags.

Once many useless tags in the original CIF removed (these tags being ended by ' ?') the file first lines are the following :

```
#-----  
data_1  
  
_chemical_formula_sum      'F6 O6 Sb4 Zn3'  
_chemical_formula_weight   893.1  
  
_symmetry_cell_setting     cubic  
_symmetry_space_group_name_H-M 'I -4 3 m'  
_symmetry_space_group_name_Hall 'I -4 2 3'  
_symmetry_Int_Tables_number 217  
  
Etc  
#-----
```

And after adding the reference tags (in red the text added to the tags by copy-paste from the published paper) :

Care that the lines should not be longer than 80 characters...

```
#-----  
data_1  
  
loop_  
_publ_author_name  
'Sk Imran Alia'  
'Weiguo Zhangb'  
'P. Shiv Halasyamanib'  
'Mats Johnsson'  
  
_publ_section_title  
;  
Zn3Sb4O6F6: Hydrothermal synthesis, crystal structure and nonlinear  
optical properties  
;  
  
_journal_name_full      'Journal of Solid State Chemistry'  
_journal_page_first     158  
_journal_page_last      161  
_journal_volume         256  
_journal_year           2017  
  
_journal_paper_doi      10.1016/j.jssc.2017.08.033  
  
_chemical_formula_sum      'F6 O6 Sb4 Zn3'  
_chemical_formula_weight   893.1  
  
_symmetry_cell_setting     cubic  
_symmetry_space_group_name_H-M 'I -4 3 m'
```

\_symmetry\_space\_group\_name\_Hall 'I -4 2 3'  
\_symmetry\_Int\_Tables\_number 217

Etc

#-----

The text editor used here is simply « Bloc-Notes » from Microsoft.

At this stage, before the deposition in COD, it is not useless to test/check the CIF with a software able to do that (PLATON, ENCIFER, etc).

If no error or warning is detected then proceed to the CIF upload in COD (otherwise, correct the errors...).

Go to the « deposit your data » interface :

[https://www.crystallography.net/cod/initiate\\_deposition.php](https://www.crystallography.net/cod/initiate_deposition.php)

Enter your username and password or sign up in order to obtain them :

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France Inter – Info, Culture, X Crystallography Open Database X

https://www.crystallography.net/cod/initiate\_deposition.php

# Crystallography Open Database

## Validation and Deposition Interface

Log in Upload a file Validate data Deposit structures Finish

Depositor login ([sign up](#))

Choose deposition type:  
-- choose one --

Username:  
Armel Le Bail

Password: ([forgot password?](#))  
.....

Begin deposition

### About the Validation and Deposition Interface

This interface allows you to upload, validate, edit and deposit CIF files.

#### Steps

The process of file deposition is pretty straightforward:

- **Upload.** The selected files are uploaded to the server;
- **Validation.** Our scripts perform various checks to see if all of the necessary data are present in the submitted files. If a file is found to be incorrect, it can be edited in the browser window and checked again. This step can be repeated as many times as needed;
- **Deposition.** The validated files can be deposited to COD. After a successful deposition COD numbers for the newly deposited structures will be displayed.

#### File formats

Currently we accept two types of files:

- Plain CIF files;
- ZIP archives that contain CIF files.

Select the « Deposition type », either « Already published data » or « Prepublication data » or « Personal communication to COD »

In this case it is « Already published data ».

Then click on « Begin deposition » :

The screenshot shows the COD website's 'Validation and Deposition Interface'. The page has a navigation bar with 'Log in', 'Upload a file', 'Validate data', 'Deposit structures', and 'Finish'. The 'Validate data' step is currently active. Below the navigation bar, there is a section titled 'Depositing published structures' with instructions on what information a published structure should contain and how to handle missing information. A warning states: 'Files from commercial databases should not be uploaded without permission.' Below this is a 'Data upload' form with a file selection button ('Parcourir...') and a 'Validate' button. The left sidebar contains links for 'COD Home', 'Accessing COD Data', 'Add Your Data', and 'Documentation'.

Then select the CIF or ZIP file with CIFs for check and click on « validate ».

A first screen of the validation beginning is displayed :

The screenshot shows the COD website's validation progress screen. The navigation bar now shows 'Validating: 1' and 'Validation in progress'. Below the navigation bar, there is a table with columns 'File', 'Status', and 'Actions'. The table contains one entry: 'JSSC-2017-256-158.cif' with status 'validating' and an action 'Add diffraction data (Fobs, PD traces)'. Below the table, a message states: 'File [JSSC-2017-256-158.cif] is being validated now'. The left sidebar remains the same as in the previous screenshot.

Then if all is OK, the COD system says that your file is valid (if not, you may have to modify some parts of the CIF...):

The screenshot shows the COD website's 'Validation and Deposition Interface'. A progress bar at the top indicates the steps: Log in, Upload a file, Validate data, Deposit structures (highlighted in green), and Finish. Below the progress bar, a table shows the file 'JSSC-2017-256-158.cif' with a status of 'valid'. The 'Actions' column for this file includes 'Edit', 'Add diffraction data (Fobs, PD traces)', and 'Deposit to the COD'. A green banner below the table states 'File [JSSC-2017-256-158.cif] is correct'. A notice follows, stating that certain data items in the file have been automatically corrected to lowercase: '\_diffrn\_radiation\_probe' to 'x-ray' and '\_expt1\_absorpt\_correction\_type' to 'multi-scan'. The interface also includes a sidebar with navigation options like 'COD Home', 'Accessing COD Data', 'Add Your Data', and 'Documentation'.

In that case, the COD system has automatically changed some useless capital letters in normal ones.

If you have diffraction data (Fobs, Powder pattern) you may add them there.

Then you have to click on « Deposit all valid files to the COD » :

The system says the File is being deposited now :

This screenshot shows the same COD interface but in a 'deposition in progress' state. The progress bar now shows 'Deposit structures' as the active step. The table below shows the file 'JSSC-2017-256-158.cif' with a status of 'depositing'. A large grey banner at the bottom of the main content area displays the message: 'File [JSSC-2017-256-158.cif] is being deposited now. Time elapsed: 00:11, time left: 00:04 (estimated)'. Below this message is a green progress bar that is approximately 73% full. The sidebar and navigation elements remain the same as in the previous screenshot.

And the COD system provides already the new COD entry number : here 1560299 :

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https://www.crystallography.net/cod



# Crystallography Open Database

**Validation and Deposition Interface**

Home What's new?

Accessing COD Data

- Browse
- Search
- Search by structural formula

Add Your Data

- Deposit your data
- Manage depositions
- Manage/release prepublications

Documentation

- COD Wiki
- Obtaining COD
- Querying COD
- Citing COD

Log in Upload a file Validate data Deposit structures Finish

All uploaded files have been successfully deposited to the COD. You can now [check new CIF file](#).

Deposit all valid files to the COD (no files to deposit so far) **Deposited: 1**

File	Status	Actions
JSSC-2017-256-158.cif	deposited to the COD	

Structures from file [JSSC-2017-256-158.cif] were deposited as entries  
1560299

[Log out](#)

[Top of the page](#)

The job is done, the CIF has been deposited. You may click on the entry number for a preview, an ultimate check and for eventually update some things if necessary (in case an error is obvious in the paper title or authors names, etc...) :

Fichier Édition Affichage Historique Marque-pages Outils Aide

France Inter – Info, Culture. Crystallography Open Database X

https://www.crystallography.net/cod

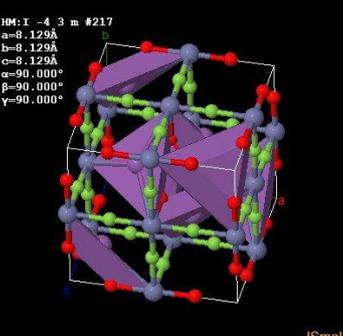


# Crystallography Open Database

**Information card for entry 1560299**

1560298 << 1560299 >> 2000000

Preview



HMgT - 4 3 m #217  
 a=8.129Å  
 b=8.129Å  
 c=8.129Å  
 α=90.000°  
 β=90.000°  
 γ=90.000°

Coordinates [Download 1560299.cif](#) [Update](#)  
 Original paper (by DOI) [HTML](#)

▼ Structure parameters

Formula	F6 O6 Sb4 Zn3
Calculated formula	F6 O6 Sb4 Zn3
Title of publication	Zn3Sb4O6F6: Hydrothermal synthesis, crystal structure and nonlinear optical properties

Done, congratulations !!!

With experience, this kind of deposit takes 5 minutes only.

### 3- CIF to be built completely from an old published crystal structure (for instance from Acta Chemica Scandinavica)

Such a complete built needs for a complete (minimal) CIF template :

```
#####
```

```
data_1
```

```
loop_
```

```
_publ_author_name
```

```
,
```

```
_publ_section_title
```

```
;
```

```
;
```

```
_journal_name_full      'Acta Chemica Scandinavica'
```

```
_journal_page_first
```

```
_journal_page_last
```

```
_journal_volume        43
```

```
_journal_year          1989
```

```
_journal_paper_doi
```

```
_chemical_name_common
```

```
;
```

```
;
```

```
_chemical_formula_sum    "
```

```
_chemical_formula_weight
```

```
_symmetry_cell_setting
```

```
_symmetry_space_group_name_H-M  "
```

```
_cell_length_a
```

```
_cell_length_b
```

```
_cell_length_c
```

```
_cell_angle_alpha
```

```
_cell_angle_beta
```

```
_cell_angle_gamma
```

```
_cell_formula_units_Z
```

```
_cell_volume
```

```
_diffraction_ambient_temperature
```

```
_diffraction_radiation_probe      x-ray
```

```
_diffraction_radiation_type       MoK\alpha
```

```
_diffraction_radiation_wavelength 0.71069
```

```
_exptl_crystal_density_diffraction
```

```
_exptl_crystal_F_000
```

```
_exptl_absorption_coefficient_mu
```

\_refine\_ls\_number\_parameters  
\_refine\_ls\_number\_reflns  
\_refine\_ls\_R\_factor\_gt  
\_refine\_ls\_wR\_factor\_gt

\_refine\_ls\_R\_factor\_all  
\_refine\_ls\_wR\_factor\_ref  
\_refine\_ls\_goodness\_of\_fit\_ref

\_pd\_proc\_ls\_prof\_R\_factor  
\_pd\_proc\_ls\_prof\_wR\_factor  
\_pd\_proc\_ls\_prof\_wR\_expected  
\_refine\_ls\_R\_I\_factor  
\_refine\_ls\_R\_Fsqd\_factor

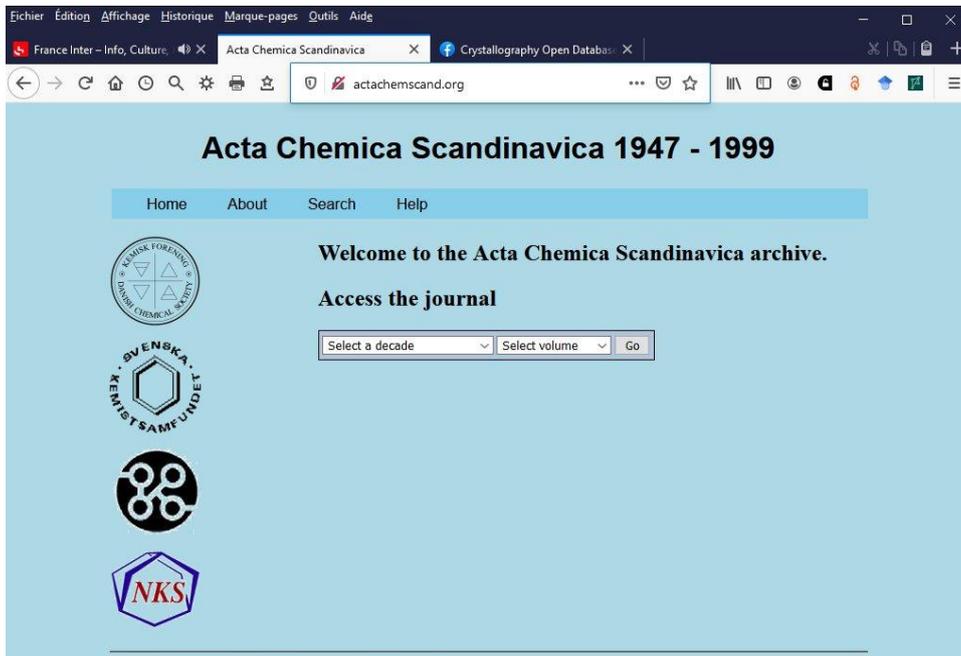
loop\_  
\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_U\_iso\_or\_equiv

loop\_  
\_atom\_site\_aniso\_label  
\_atom\_site\_aniso\_U\_11  
\_atom\_site\_aniso\_U\_22  
\_atom\_site\_aniso\_U\_33  
\_atom\_site\_aniso\_U\_23  
\_atom\_site\_aniso\_U\_13  
\_atom\_site\_aniso\_U\_12

\_cod\_depositor\_comments

;  
;  
#####

The entry Web page for the Acta Chem. Scand. Papers :

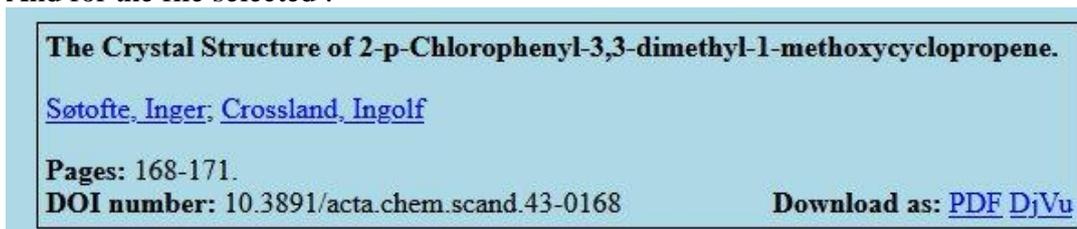


The paper selected for deposit is Acta Chem. Scand. (1989) 43, 168-171.  
The absence of this crystal structure in COD was first verified.

Page for 1989 :



And for the file selected :



Well... The CIF building starts here by copy-paste into the template renamed  
Acta-Chem-Scand-1989-43-168.cif :

In red the added text in the template CIF tags, in blue some explanation

#####

loop\_  
\_publ\_author\_name

'Sotofte, Inger'  
'Crossland, Ingolf'

Sorry for the character ø in Søtøfte.... No time for a perfect job here

\_publ\_section\_title

The Crystal Structure of 2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene

\_journal\_name\_full 'Acta Chemica Scandinavica'  
\_journal\_page\_first 168  
\_journal\_page\_last 171  
\_journal\_volume 43  
\_journal\_year 1989

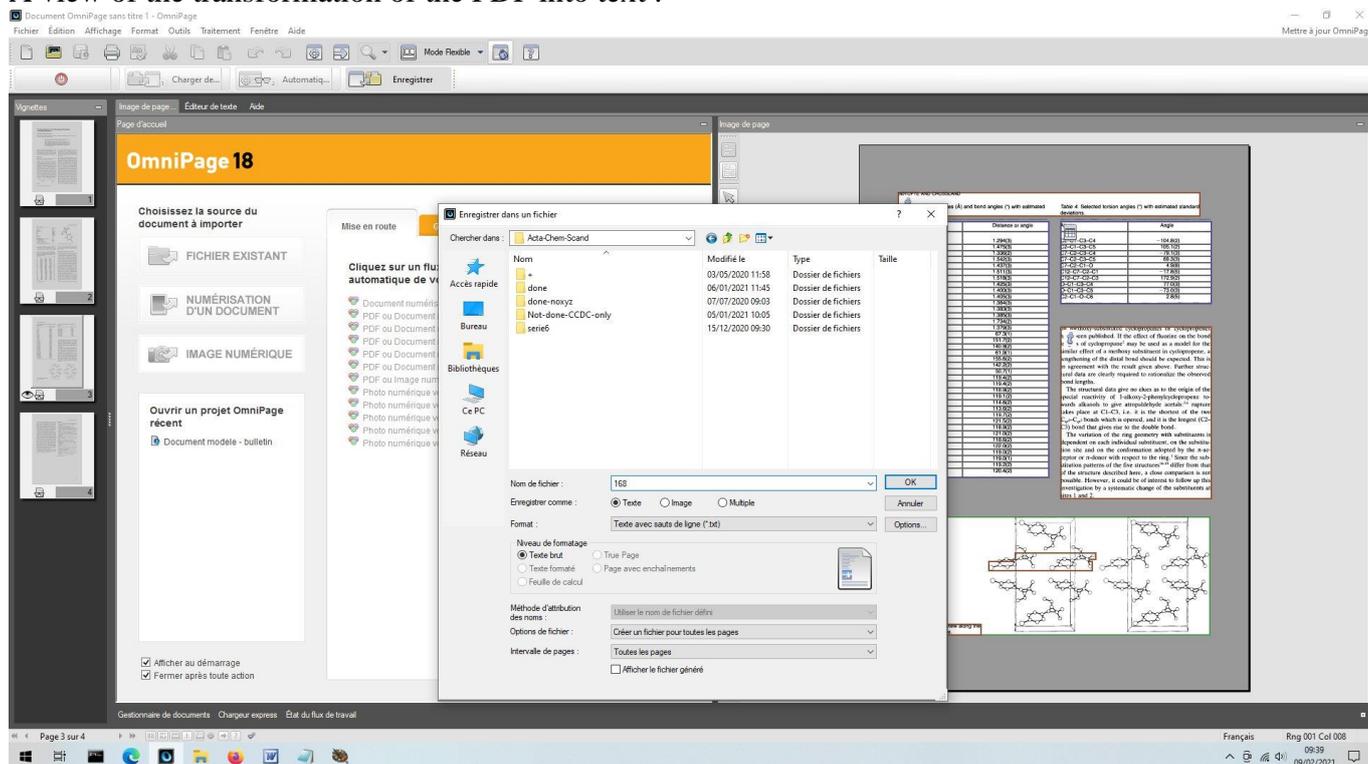
\_journal\_paper\_doi 10.3891/acta.chem.scand.43-0168

\_chemical\_name\_common

2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene

#####

Then we have to look inside of the paper itself. It is a PDF file built from images so we have to OCRized it (more modern recent PDFs may admit simple copy-paste). The software used here is OMNIPAGE 18. A view of the transformation of the PDF into text :



Continuing to enter values into the CIF, it may be sometimes as fast as a copy-paste to type the individual values found in the original paper like in the following Table :

Table 1. Crystal data.

Formula	C <sub>12</sub> H <sub>13</sub> ClO
<i>M<sub>r</sub></i>	208.7
μ(MoKα)/cm <sup>-1</sup>	3.08
Crystal system	Monoclinic
<i>V</i> /Å <sup>3</sup>	1105.9
<i>a</i> /Å	9.939(5)
<i>b</i> /Å	19.099(4)
<i>c</i> /Å	5.828(4)
β/°	91.60(5)
Space group	<i>I</i> <i>c</i> (No. 9)
<i>D<sub>s</sub></i> /g cm <sup>-3</sup>	1.25
<i>Z</i>	4
Total number of refl.	1844
Number of independent refl. with <i>I</i> ≥ 2σ( <i>I</i> )	1520
Number of variables	177
<i>R</i> = Σ(  <i>F<sub>o</sub></i>   -   <i>F<sub>c</sub></i>  ) / Σ  <i>F<sub>o</sub></i>	0.027
<i>R<sub>w</sub></i> = [Σ <i>w</i> (  <i>F<sub>o</sub></i>   -   <i>F<sub>c</sub></i>  ) <sup>2</sup> / Σ <i>w</i>   <i>F<sub>o</sub></i>   <sup>2</sup> ] <sup>1/2</sup>	0.032
<i>S</i> = [Σ <i>w</i> (  <i>F<sub>o</sub></i>   -   <i>F<sub>c</sub></i>  ) <sup>2</sup> / (N <sub>obs</sub> - N <sub>var</sub> )] <sup>1/2</sup>	1.15
Equiv. positions (0,0,0; ½,½,½): <i>x</i> , <i>y</i> , <i>z</i> ; <i>x</i> , <i>y</i> , ½ + <i>z</i>	

CYCLOPROPENE STRUCTURE

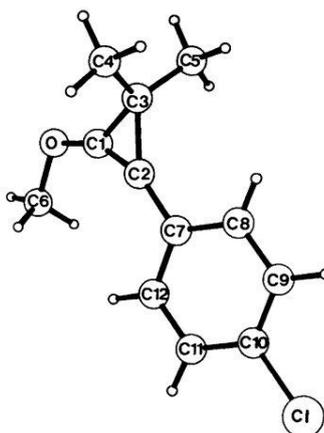


Fig. 1. The structure viewed along the *b*-axis.

Here these values are reported by hand in the CIF :

#####

\_chemical\_formula\_sum 'C12 H13 Cl O'  
\_chemical\_formula\_weight 208.7

\_symmetry\_cell\_setting monoclinic  
\_symmetry\_space\_group\_name\_H-M 'I c'

\_cell\_length\_a 9.939(5)  
\_cell\_length\_b 19.099(4)  
\_cell\_length\_c 5.828(4)  
\_cell\_angle\_alpha 90.  
\_cell\_angle\_beta 91.60(5)  
\_cell\_angle\_gamma 90.  
\_cell\_formula\_units\_Z 4  
\_cell\_volume 1105.9

\_diffn\_ambient\_temperature 120  
\_diffn\_radiation\_probe x-ray  
\_diffn\_radiation\_type MoK\α  
\_diffn\_radiation\_wavelength 0.71069

care to give in K

sometimes you find 0.71073

\_exptl\_crystal\_density\_diffn 1.25  
\_exptl\_crystal\_F\_000 ?  
\_exptl\_absorpt\_coefficient\_mu 0.308

care it should be μ/mm<sup>-1</sup>, not cm<sup>-1</sup>

\_refine\_ls\_number\_parameters 177  
\_refine\_ls\_number\_reflns 1520  
\_refine\_ls\_R\_factor\_gt 0.027  
\_refine\_ls\_wR\_factor\_gt 0.032

\_refine\_ls\_R\_factor\_all ?  
\_refine\_ls\_wR\_factor\_ref ?  
\_refine\_ls\_goodness\_of\_fit\_ref 1.15

#####

Then comes the problem of the coordinates which are a mixture of values  $\times 10^4$  or  $\times 10^3$ , needing some hand-work from the OCRized table... The original Table :

Table 2. Atomic coordinates  $\times 10^4$ . The estimated standard deviations  $\times 10^4$  are given in parentheses. The values of the hydrogen atoms are multiplied by  $10^3$ . The isotropic temperature factors for the non-hydrogen atoms are estimated from the anisotropic values (Ref. 22).

Atom	x	y	z	$B_{eq}^a$
C1	6513(2)	8166(1)	-4865(3)	2.0
C2	5857(2)	8540(1)	-3422(3)	1.8
C3	7403(2)	8610(1)	-3412(3)	2.0
C4	8020(3)	9260(1)	-4423(5)	3.0
C5	8232(2)	8278(1)	-1473(4)	2.7
C6	5275(3)	7428(1)	-7252(4)	2.8
C7	4690(2)	8769(1)	-2229(3)	1.7
C8	4850(2)	9142(1)	-172(3)	1.8
C9	3746(2)	9348(1)	1056(3)	2.0
C10	2474(2)	9181(1)	201(3)	2.0
C11	2278(2)	8823(1)	-1848(4)	2.1
C12	3382(2)	8616(1)	-3059(3)	2.0
O	6564(2)	7685(1)	-6526(3)	2.5
Cl	1082	9435(1)	1725	2.7
H1	823(3)	960(2)	-323(6)	3.9
H2	739(4)	950(2)	-550(6)	4.8
H3	893(3)	915(2)	-510(5)	3.4
H4	912(4)	813(2)	-204(6)	4.2
H5	841(3)	863(2)	-35(5)	3.4
H6	777(3)	786(2)	-83(6)	4.0
H7	474(3)	780(2)	-790(5)	3.4
H8	540(4)	707(2)	-835(7)	6.0
H9	479(3)	722(2)	-598(6)	4.2
H10	572(3)	922(1)	44(4)	2.1
H11	387(3)	963(1)	251(5)	2.7
H12	140(3)	872(1)	-253(4)	2.4
H13	325(3)	836(1)	-448(5)	2.3

$$^a B_{eq} = \frac{4}{3} \sum_i \sum_j b_i \cdot b_j \cdot a_i \cdot a_j$$

And the OCR-ized Table :

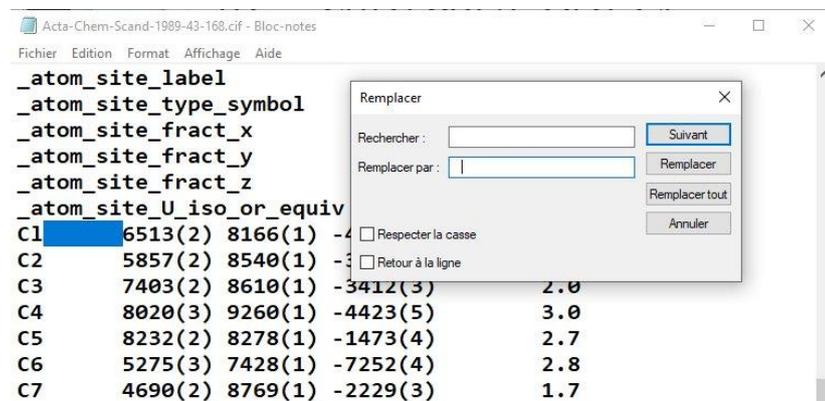
C1	6513(2)	8166(1)	-4865(3)	2.0
C2	5857(2)	8540(1)	-3422(3)	1.8
C3	7403(2)	8610(1)	-3412(3)	2.0
C4	8020(3)	9260(1)	-4423(5)	3.0
C5	8232(2)	8278(1)	-1473(4)	2.7
C6	5275(3)	7428(1)	-7252(4)	2.8
C7	4690(2)	8769(1)	-2229(3)	1.7
C8	4850(2)	9142(1)	-172(3)	1.8
C9	3746(2)	9348(1)	1056(3)	2.0
C10	2474(2)	9181(1)	201(3)	2.0
C11	2278(2)	8823(1)	-1848(4)	2.1
C12	3382(2)	8616(1)	-3059(3)	2.0
O	6564(2)	7685(1)	-6526(3)	2.5
Cl	1082	9435(1)	1725	2.7
H1	823(3)	960(2)	-323(6)	3.9
H2	739(4)	950(2)	-550(6)	4.8
H3	893(3)	915(2)	-510(5)	3.4
H4	912(4)	813(2)	-204(6)	4.2
H5	841(3)	863(2)	-35(5)	3.4
H6	777(3)	786(2)	-83(6)	4.0
H7	474(3)	780(2)	-790(5)	3.4
H8	540(4)	707(2)	-835(7)	6.0
H9	479(3)	722(2)	-598(6)	4.2
H10	572(3)	922(1)	44(4)	2.1
H11	387(3)	963(1)	251(5)	2.7
H12	140(3)	872(1)	-253(4)	2.4
H13	325(3)	836(1)	-448(5)	2.3

So, a copy-paste of the OCR-ized text into the CIF template gives :

```
loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
C1 6513(2) 8166(1) -4865(3) 2.0
C2 5857(2) 8540(1) -3422(3) 1.8
C3 7403(2) 8610(1) -3412(3) 2.0
```

C4	8020(3)	9260(1)	-4423(5)	3.0
C5	8232(2)	8278(1)	-1473(4)	2.7
C6	5275(3)	7428(1)	-7252(4)	2.8
C7	4690(2)	8769(1)	-2229(3)	1.7
C8	4850(2)	9142(1)	-172(3)	1.8
C9	3746(2)	9348(1)	1056(3)	2.0
C10	2474(2)	9181(1)	201(3)	2.0
C11	2278(2)	8823(1)	-1848(4)	2.1
C12	3382(2)	8616(1)	-3059(3)	2.0
0	6564(2)	7685(1)	-6526(3)	2.5
Cl	1082	9435(1)	1725	2.7
H1	823(3)	960(2)	-323(6)	3.9
H2	739(4)	950(2)	-550(6)	4.8
H3	893(3)	915(2)	-510(5)	3.4
H4	912(4)	813(2)	-204(6)	4.2
H5	841(3)	863(2)	-35(5)	3.4
H6	777(3)	786(2)	-83(6)	4.0
H7	474(3)	780(2)	-790(5)	3.4
H8	540(4)	707(2)	-835(7)	6.0
H9	479(3)	722(2)	-598(6)	4.2
H10	572(3)	922(1)	44(4)	2.1
H11	387(3)	963(1)	251(5)	2.7
H12	140(3)	872(1)	-253(4)	2.4
H13	325(3)	836(1)	-448(5)	2.3

Needing hand-work. First replacing the tabulations by spaces :



With that result :

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
Cl 6513(2) 8166(1) -4865(3) 2.0
C2 5857(2) 8540(1) -3422(3) 1.8
C3 7403(2) 8610(1) -3412(3) 2.0
C4 8020(3) 9260(1) -4423(5) 3.0
C5 8232(2) 8278(1) -1473(4) 2.7
C6 5275(3) 7428(1) -7252(4) 2.8

```

C7 4690(2) 8769(1) -2229(3) 1.7  
 C8 4850(2) 9142(1) -172(3) 1.8  
 C9 3746(2) 9348(1) 1056(3) 2.0  
 C10 2474(2) 9181(1) 201(3) 2.0  
 C11 2278(2) 8823(1) -1848(4) 2.1  
 C12 3382(2) 8616(1) -3059(3) 2.0  
 O 6564(2) 7685(1) -6526(3) 2.5  
 Cl 1082 9435(1) 1725 2.7  
 H1 823(3) 960(2) -323(6) 3.9  
 H2 739(4) 950(2) -550(6) 4.8  
 H3 893(3) 915(2) -510(5) 3.4  
 H4 912(4) 813(2) -204(6) 4.2  
 H5 841(3) 863(2) -35(5) 3.4  
 H6 777(3) 786(2) -83(6) 4.0  
 H7 474(3) 780(2) -790(5) 3.4  
 H8 540(4) 707(2) -835(7) 6.0  
 H9 479(3) 722(2) -598(6) 4.2  
 H10 572(3) 922(1) 44(4) 2.1  
 H11 387(3) 963(1) 251(5) 2.7  
 H12 140(3) 872(1) -253(4) 2.4  
 H13 325(3) 836(1) -448(5) 2.3

Also it may be necessary to change some possible special characters such as – by - .

Adding dots, reajusting, adding the atom site symbol, correcting errors produced at the OCR-ization stage, take care about thermal parameters, U or B, etc...

Final result in that case (not two identical cases...) ; Really a lot of job here... :

#####

```

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_B_iso_or_equiv
C1 C .6513(2) .8166(1) -.4865(3) 2.0
C2 C .5857(2) .8540(1) -.3422(3) 1.8
C3 C .7403(2) .8610(1) -.3412(3) 2.0
C4 C .8020(3) .9260(1) -.4423(5) 3.0
C5 C .8232(2) .8278(1) -.1473(4) 2.7
C6 C .5275(3) .7428(1) -.7252(4) 2.8
C7 C .4690(2) .8769(1) -.2229(3) 1.7
C8 C .4850(2) .9142(1) -.0172(3) 1.8
C9 C .3746(2) .9348(1) .1056(3) 2.0
C10 C .2474(2) .9181(1) .0201(3) 2.0
C11 C .2278(2) .8823(1) -.1848(4) 2.1
C12 C .3382(2) .8616(1) -.3059(3) 2.0
O O .6564(2) .7685(1) -.6526(3) 2.5
Cl Cl .1082 .9435(1) .1725 2.7
H1 H .823(3) .960(2) -.323(6) 3.9
H2 H .739(4) .950(2) -.550(6) 4.8
H3 H .893(3) .915(2) -.510(5) 3.4
H4 H .912(4) .813(2) -.204(6) 4.2

```

```

H5 H .841(3) .863(2) -.035(5) 3.4
H6 H .777(3) .786(2) -.083(6) 4.0
H7 H .474(3) .780(2) -.790(5) 3.4
H8 H .540(4) .707(2) -.835(7) 6.0
H9 H .479(3) .722(2) -.598(6) 4.2
H10 H .572(3) .922(1) .044(4) 2.1
H11 H .387(3) .963(1) .251(5) 2.7
H12 H .140(3) .872(1) -.253(4) 2.4
H13 H .325(3) .836(1) -.448(5) 2.3
#####

```

By chance the hydrogen atomic coordinates are given in that paper (not always the case).  
 No available anisotropic thermal parameters so the job is almost finished.  
 To do now is checking, then re-checking and checking again...

### First check of the CIF using ENCIFER :

The screenshot shows the ENCIFER software window titled "Acta-Chem-Scand-1989-43-168.cif - enCIFer". The main window displays a ball-and-stick model of a molecule with a red oxygen atom, a green chlorine atom, and several grey carbon atoms with white hydrogen atoms. Below the model, there is a status bar that says "Now showing structure for block 'data\_1'".

At the bottom of the window, there is a panel with two tabs: "Editor" and "Visualiser". The "Visualiser" tab is active, showing a list of warnings:

- Errors - none
- Warnings - none
- Remarks - none

Below the warnings, there is a list of messages for hydrogen atoms:

- Atom H8: will be treated isotropically: stored type was: missing
- Atom H9: will be treated isotropically: stored type was: missing
- Atom H10: will be treated isotropically: stored type was: missing
- Atom H11: will be treated isotropically: stored type was: missing
- Atom H12: will be treated isotropically: stored type was: missing
- Atom H13: will be treated isotropically: stored type was: missing

By chance, no warning, no error, no remark... and the molecule looks normal.

If you are unlucky, the most frequent problems are :

- a remark concerning the molecule weight in error in the paper and proposed different by ENCIFER
- a molecule displayed strange because of errors in atomic coordinates in the paper, then you may locate the error and try to guess what the error was... You should insert a « comment from the COD depositor » into the CIF.
- various possible « errors » about which you will have to take initiatives...

This is not the end because the CIF does not contain interatomic distances and lack some other details requested at the COD deposit time (equivalent positions corresponding to the space group, etc).

The way to complete the CIF is to use the famous PLATON checking software used in any CHECKCIF stage requested by editors when you try to publish a crystal structure paper. Read your CIF by PLATON, make a new CIF by PLATON, and use that new CIF to complete your starting one...

Below is your actual CIF to be read by PLATON :

```
#####  
data_1  
  
loop_  
_publ_author_name  
'Sotofte, Inger'  
'Crossland, Ingolf'  
  
_publ_section_title  
;  
The Crystal Structure of 2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene  
;  
  
_journal_name_full      'Acta Chemica Scandinavica'  
_journal_page_first     168  
_journal_page_last      171  
_journal_volume         43  
_journal_year           1989  
  
_journal_paper_doi     10.3891/acta.chem.scand.43-0168  
  
_chemical_name_common  
;  
2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene  
;  
  
_chemical_formula_sum   'C12 H13 Cl O'  
_chemical_formula_weight 208.7  
  
_symmetry_cell_setting  monoclinic  
_symmetry_space_group_name_H-M 'I c'  
  
_cell_length_a          9.939(5)  
_cell_length_b          19.099(4)  
_cell_length_c          5.828(4)  
_cell_angle_alpha       90.  
_cell_angle_beta        91.60(5)  
_cell_angle_gamma       90.  
_cell_formula_units_Z   4  
_cell_volume            1105.9  
  
_diffrn_ambient_temperature 120  
_diffrn_radiation_probe     x-ray  
_diffrn_radiation_type      MoK\alpha  
_diffrn_radiation_wavelength 0.71069  
  
_exptl_crystal_density_diffrn 1.25  
_exptl_crystal_F_000         ?  
_exptl_absorpt_coefficient_mu 0.308  
  
_refine_ls_number_parameters 177  
_refine_ls_number_reflns     1520
```

\_refine\_ls\_R\_factor\_gt 0.027  
\_refine\_ls\_wR\_factor\_gt 0.032

\_refine\_ls\_R\_factor\_all ?  
\_refine\_ls\_wR\_factor\_ref ?  
\_refine\_ls\_goodness\_of\_fit\_ref 1.15

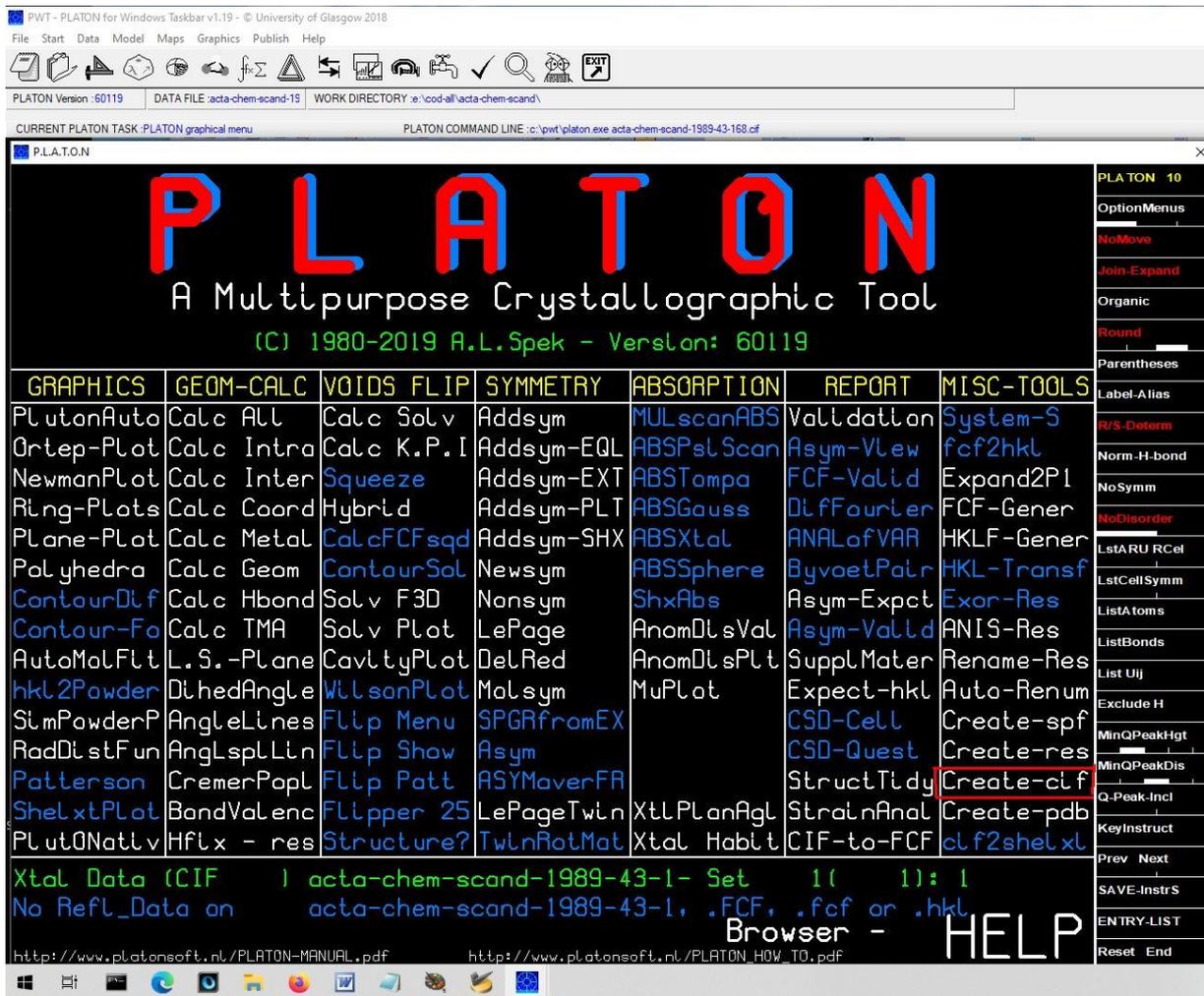
loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_B\_iso\_or\_equiv

C1	C	.6513(2)	.8166(1)	-.4865(3)	2.0
C2	C	.5857(2)	.8540(1)	-.3422(3)	1.8
C3	C	.7403(2)	.8610(1)	-.3412(3)	2.0
C4	C	.8020(3)	.9260(1)	-.4423(5)	3.0
C5	C	.8232(2)	.8278(1)	-.1473(4)	2.7
C6	C	.5275(3)	.7428(1)	-.7252(4)	2.8
C7	C	.4690(2)	.8769(1)	-.2229(3)	1.7
C8	C	.4850(2)	.9142(1)	-.0172(3)	1.8
C9	C	.3746(2)	.9348(1)	.1056(3)	2.0
C10	C	.2474(2)	.9181(1)	.0201(3)	2.0
C11	C	.2278(2)	.8823(1)	-.1848(4)	2.1
C12	C	.3382(2)	.8616(1)	-.3059(3)	2.0
O	O	.6564(2)	.7685(1)	-.6526(3)	2.5
Cl	Cl	.1082	.9435(1)	.1725	2.7
H1	H	.823(3)	.960(2)	-.323(6)	3.9
H2	H	.739(4)	.950(2)	-.550(6)	4.8
H3	H	.893(3)	.915(2)	-.510(5)	3.4
H4	H	.912(4)	.813(2)	-.204(6)	4.2
H5	H	.841(3)	.863(2)	-.035(5)	3.4
H6	H	.777(3)	.786(2)	-.083(6)	4.0
H7	H	.474(3)	.780(2)	-.790(5)	3.4
H8	H	.540(4)	.707(2)	-.835(7)	6.0
H9	H	.479(3)	.722(2)	-.598(6)	4.2
H10	H	.572(3)	.922(1)	.044(4)	2.1
H11	H	.387(3)	.963(1)	.251(5)	2.7
H12	H	.140(3)	.872(1)	-.253(4)	2.4
H13	H	.325(3)	.836(1)	-.448(5)	2.3

#####

So start PLATON, select your CIF, make appear the command system and click on « Create-CIF » :



Here is your new CIF after having added the complement of information built by PLATON. In red the additions or replacement to be performed :

```
#####
data_1

loop_
  _publ_author_name
  'Sotofte, Inger'
  'Crossland, Ingolf'

  _publ_section_title
  ;
  The Crystal Structure of 2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene
  ;

  _journal_name_full      'Acta Chemica Scandinavica'
  _journal_page_first    168
  _journal_page_last     171
  _journal_volume        43
  _journal_year          1989

  _journal_paper_doi     10.3891/acta.chem.scand.43-0168

  _chemical_name_common
  ;
```

2-p-Chlorophenyl-3,3-dimethyl-1-methoxycyclopropene

;

\_chemical\_formula\_sum 'C12 H13 Cl O'  
\_chemical\_formula\_weight 208.67

loop\_

\_atom\_type\_symbol  
\_atom\_type\_description  
\_atom\_type\_scatter\_dispersion\_real  
\_atom\_type\_scatter\_dispersion\_imag  
\_atom\_type\_scatter\_source  
C C 0.0033 0.0016  
' International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
H H 0.0000 0.0000  
' International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
Cl Cl 0.1484 0.1585  
' International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
O O 0.0106 0.0060  
' International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting monoclinic  
\_symmetry\_space\_group\_name\_Hall 'I -2yc'  
\_symmetry\_space\_group\_name\_H-M 'I c'  
\_symmetry\_Int\_tables\_number 9

loop\_

\_space\_group\_symop\_id  
\_space\_group\_symop\_operation\_xyz  
1 x,y,z  
2 x,-y,1/2+z  
3 1/2+x,1/2+y,1/2+z  
4 1/2+x,1/2-y,z

\_cell\_length\_a 9.939(5)  
\_cell\_length\_b 19.099(4)  
\_cell\_length\_c 5.828(4)  
\_cell\_angle\_alpha 90.  
\_cell\_angle\_beta 91.60(5)  
\_cell\_angle\_gamma 90.  
\_cell\_formula\_units\_Z 4  
\_cell\_volume 1105.9(10)

\_diffrn\_ambient\_temperature 120  
\_diffrn\_radiation\_probe x-ray  
\_diffrn\_radiation\_type MoK $\alpha$   
\_diffrn\_radiation\_wavelength 0.71069

\_exptl\_crystal\_density\_diffrn 1.253  
\_exptl\_crystal\_F\_000 440  
\_exptl\_absorpt\_coefficient\_mu 0.308

\_refine\_ls\_number\_parameters 177  
\_refine\_ls\_number\_reflns 1520  
\_refine\_ls\_R\_factor\_gt 0.027  
\_refine\_ls\_wR\_factor\_gt 0.032

\_refine\_ls\_R\_factor\_all ?

\_refine\_ls\_wR\_factor\_ref ?  
\_refine\_ls\_goodness\_of\_fit\_ref 1.15

loop\_

\_atom\_site\_label  
\_atom\_site\_type\_symbol  
\_atom\_site\_thermal\_displace\_type  
\_atom\_site\_fract\_x  
\_atom\_site\_fract\_y  
\_atom\_site\_fract\_z  
\_atom\_site\_occupancy  
\_atom\_site\_U\_iso\_or\_equiv  
\_atom\_site\_calc\_flag  
\_atom\_site\_refinement\_flags  
\_atom\_site\_disorder\_assembly  
\_atom\_site\_disorder\_group  
Cl Cl Uiso 0.10820 0.94350(10) 0.17250 1.000 0.0342 . . . .  
O O Uiso 0.6564(2) 0.76850(10) -0.6526(3) 1.000 0.0317 . . . .  
C1 C Uiso 0.6513(2) 0.81660(10) -0.4865(3) 1.000 0.0253 . . . .  
C2 C Uiso 0.5857(2) 0.85400(10) -0.3422(3) 1.000 0.0228 . . . .  
C3 C Uiso 0.7403(2) 0.86100(10) -0.3412(3) 1.000 0.0253 . . . .  
C4 C Uiso 0.8020(3) 0.92600(10) -0.4423(5) 1.000 0.0380 . . . .  
C5 C Uiso 0.8232(2) 0.82780(10) -0.1473(4) 1.000 0.0342 . . . .  
C6 C Uiso 0.5275(3) 0.74280(10) -0.7252(4) 1.000 0.0355 . . . .  
C7 C Uiso 0.4690(2) 0.87690(10) -0.2229(3) 1.000 0.0215 . . . .  
C8 C Uiso 0.4850(2) 0.91420(10) -0.0172(3) 1.000 0.0228 . . . .  
C9 C Uiso 0.3746(2) 0.93480(10) 0.1056(3) 1.000 0.0253 . . . .  
C10 C Uiso 0.2474(2) 0.91810(10) 0.0201(3) 1.000 0.0253 . . . .  
C11 C Uiso 0.2278(2) 0.88230(10) -0.1848(4) 1.000 0.0266 . . . .  
C12 C Uiso 0.3382(2) 0.86160(10) -0.3059(3) 1.000 0.0253 . . . .  
H1 H Uiso 0.823(3) 0.960(2) -0.323(6) 1.000 0.0494 . . . .  
H2 H Uiso 0.739(4) 0.950(2) -0.550(6) 1.000 0.0608 . . . .  
H3 H Uiso 0.893(3) 0.915(2) -0.510(5) 1.000 0.0431 . . . .  
H4 H Uiso 0.912(4) 0.813(2) -0.204(6) 1.000 0.0532 . . . .  
H5 H Uiso 0.841(3) 0.863(2) -0.035(5) 1.000 0.0431 . . . .  
H6 H Uiso 0.777(3) 0.786(2) -0.083(6) 1.000 0.0507 . . . .  
H7 H Uiso 0.474(3) 0.780(2) -0.790(5) 1.000 0.0431 . . . .  
H8 H Uiso 0.540(4) 0.707(2) -0.835(7) 1.000 0.0760 . . . .  
H9 H Uiso 0.479(3) 0.722(2) -0.598(6) 1.000 0.0532 . . . .  
H10 H Uiso 0.572(3) 0.9220(10) 0.044(4) 1.000 0.0266 . . . .  
H11 H Uiso 0.387(3) 0.9630(10) 0.251(5) 1.000 0.0342 . . . .  
H12 H Uiso 0.140(3) 0.8720(10) -0.253(4) 1.000 0.0304 . . . .  
H13 H Uiso 0.325(3) 0.8360(10) -0.448(5) 1.000 0.0291 . . . .

loop\_

\_geom\_bond\_atom\_site\_label\_1  
\_geom\_bond\_atom\_site\_label\_2  
\_geom\_bond\_distance  
\_geom\_bond\_site\_symmetry\_1  
\_geom\_bond\_site\_symmetry\_2  
\_geom\_bond\_publ\_flag  
Cl C10 1.734(2) . . . . yes  
O C1 1.337(3) . . . . yes  
O C6 1.425(4) . . . . yes  
C1 C2 1.294(3) . . . . no  
C1 C3 1.475(3) . . . . no  
C2 C3 1.542(3) . . . . no  
C2 C7 1.437(3) . . . . no  
C3 C4 1.512(3) . . . . no

C3	C5	1.519(3)	.	.	no
C7	C8	1.400(3)	.	.	no
C7	C12	1.405(3)	.	.	no
C8	C9	1.384(3)	.	.	no
C9	C10	1.383(3)	.	.	no
C10	C11	1.385(3)	.	.	no
C11	C12	1.379(3)	.	.	no
C4	H1	0.97(4)	.	.	no
C4	H2	0.99(4)	.	.	no
C4	H3	1.02(3)	.	.	no
C5	H4	0.99(4)	.	.	no
C5	H5	0.95(3)	.	.	no
C5	H6	1.00(4)	.	.	no
C6	H7	0.96(3)	.	.	no
C6	H8	0.95(4)	.	.	no
C6	H9	0.98(3)	.	.	no
C8	H10	0.94(3)	.	.	no
C9	H11	1.01(3)	.	.	no
C11	H12	0.97(3)	.	.	no
C12	H13	0.97(3)	.	.	no

loop\_

_geom_angle_atom_site_label_1					
_geom_angle_atom_site_label_2					
_geom_angle_atom_site_label_3					
_geom_angle					
_geom_angle_site_symmetry_1					
_geom_angle_site_symmetry_2					
_geom_angle_site_symmetry_3					
_geom_angle_publ_flag					
C1	O	C6	113.57(19)	.	yes
O	C1	C2	151.7(2)	.	yes
O	C1	C3	140.9(2)	.	yes
C2	C1	C3	67.32(15)	.	no
C1	C2	C3	61.97(15)	.	no
C1	C2	C7	155.6(2)	.	no
C3	C2	C7	142.12(17)	.	no
C1	C3	C2	50.71(13)	.	no
C1	C3	C4	119.45(18)	.	no
C1	C3	C5	119.42(17)	.	no
C2	C3	C4	119.00(19)	.	no
C2	C3	C5	119.11(16)	.	no
C4	C3	C5	114.55(19)	.	no
C2	C7	C8	119.69(18)	.	no
C2	C7	C12	121.44(17)	.	no
C8	C7	C12	118.85(18)	.	no
C7	C8	C9	120.99(19)	.	no
C8	C9	C10	118.56(17)	.	no
C1	C10	C9	119.03(15)	.	yes
C1	C10	C11	118.99(16)	.	yes
C9	C10	C11	121.98(19)	.	no
C10	C11	C12	119.21(19)	.	no
C7	C12	C11	120.39(18)	.	no
C3	C4	H1	111(2)	.	no
C3	C4	H2	112(2)	.	no
C3	C4	H3	111(2)	.	no
H1	C4	H2	105(3)	.	no
H1	C4	H3	104(3)	.	no
H2	C4	H3	114(3)	.	no

C3	C5	H4	110(2)	.	.	.	no
C3	C5	H5	108(2)	.	.	.	no
C3	C5	H6	111.6(19)	.	.	.	no
H4	C5	H5	106(3)	.	.	.	no
H4	C5	H6	109(3)	.	.	.	no
H5	C5	H6	113(3)	.	.	.	no
O	C6	H7	110(2)	.	.	.	no
O	C6	H8	108(2)	.	.	.	no
O	C6	H9	111.9(19)	.	.	.	no
H7	C6	H8	111(3)	.	.	.	no
H7	C6	H9	109(3)	.	.	.	no
H8	C6	H9	107(3)	.	.	.	no
C7	C8	H10	119.2(14)	.	.	.	no
C9	C8	H10	119.6(15)	.	.	.	no
C8	C9	H11	120.4(17)	.	.	.	no
C10	C9	H11	121.0(17)	.	.	.	no
C10	C11	H12	123.9(15)	.	.	.	no
C12	C11	H12	116.9(15)	.	.	.	no
C7	C12	H13	120.1(18)	.	.	.	no
C11	C12	H13	119.5(18)	.	.	.	no

loop\_

_geom_torsion_atom_site_label_1							
_geom_torsion_atom_site_label_2							
_geom_torsion_atom_site_label_3							
_geom_torsion_atom_site_label_4							
_geom_torsion							
_geom_torsion_site_symmetry_1							
_geom_torsion_site_symmetry_2							
_geom_torsion_site_symmetry_3							
_geom_torsion_site_symmetry_4							
_geom_torsion_publ_flag							
C6	O	C1	C2	2.8(5)	.	.	no
C6	O	C1	C3	179.1(2)	.	.	no
O	C1	C2	C3	177.5(4)	.	.	no
O	C1	C2	C7	4.7(8)	.	.	no
C3	C1	C2	C7	-172.8(5)	.	.	no
O	C1	C3	C2	-178.1(3)	.	.	no
O	C1	C3	C4	77.0(3)	.	.	no
O	C1	C3	C5	-73.0(3)	.	.	no
C2	C1	C3	C4	-104.9(2)	.	.	no
C2	C1	C3	C5	105.1(2)	.	.	no
C1	C2	C3	C4	105.8(2)	.	.	no
C1	C2	C3	C5	-105.7(2)	.	.	no
C7	C2	C3	C1	175.2(3)	.	.	no
C7	C2	C3	C4	-79.0(3)	.	.	no
C7	C2	C3	C5	69.4(3)	.	.	no
C1	C2	C7	C8	161.3(4)	.	.	no
C1	C2	C7	C12	-17.6(5)	.	.	no
C3	C2	C7	C8	-8.3(4)	.	.	no
C3	C2	C7	C12	172.8(2)	.	.	no
C2	C7	C8	C9	-177.72(18)	.	.	no
C12	C7	C8	C9	1.1(3)	.	.	no
C2	C7	C12	C11	178.03(19)	.	.	no
C8	C7	C12	C11	-0.8(3)	.	.	no
C7	C8	C9	C10	-0.4(3)	.	.	no
C8	C9	C10	C1	179.91(17)	.	.	no
C8	C9	C10	C11	-0.8(3)	.	.	no
C1	C10	C11	C12	-179.59(17)	.	.	no

```

C9  C10  C11  C12    1.1(3)  .  .  .  .  no
C10 C11  C12  C7    -0.3(3) .  .  .  .  no

```

#####

At this stage, an ultimate check by ENCIFER is useful before the final deposition into the COD. If no new error, then go :

**Crystallography Open Database**

**Validation and Deposition Interface**

Log in → Upload a file → Validate data → Deposit structures → Finish

All uploaded files have been successfully deposited to the COD. You can now [check new CIF file](#).

Deposit all valid files to the COD (no files to deposit so far) **Deposited: 1**

File	Status	Actions
Acta-Chem-Scand-1989-43-168.cif	deposited to the COD	

Structures from file [Acta-Chem-Scand-1989-43-168.cif] were deposited as entries  
1560300

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[Top of the page](#)

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**4- If you are too lazy, then send me your CIF file together with the DOI...**

**Preferably compressed into a .zip file**

**By email to : alb@cristal.org**

Insert the DOI into the email

Thanks !