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

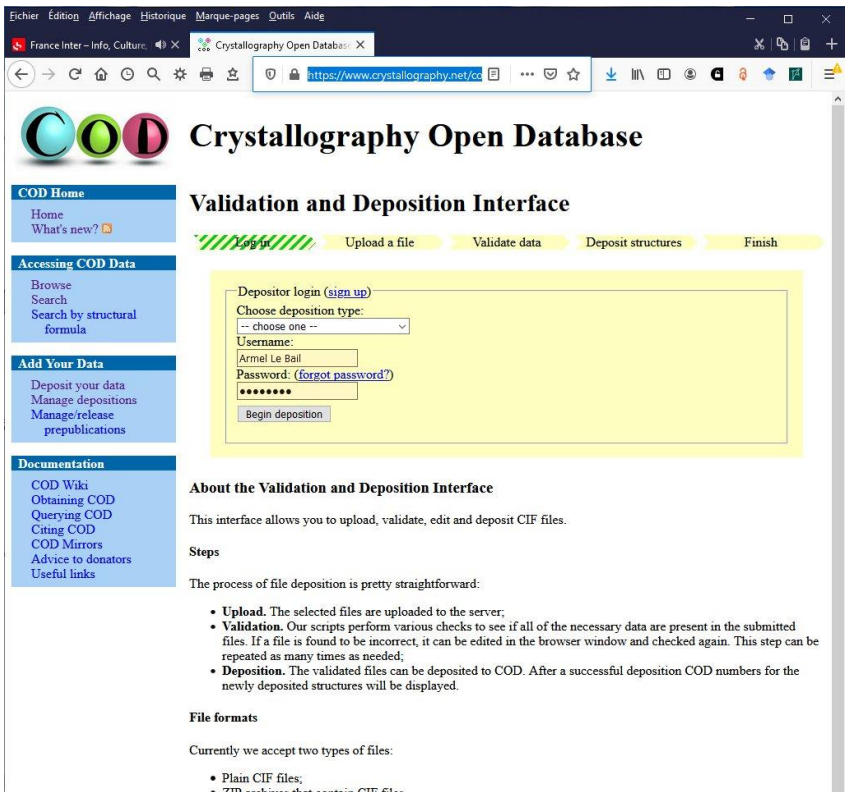
Such CIFs produced by refinement software are generally already almost complete and contain all but the reference to the published text. The COD upload system can add the reference automatically in your CIF provided you have a DOI.

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

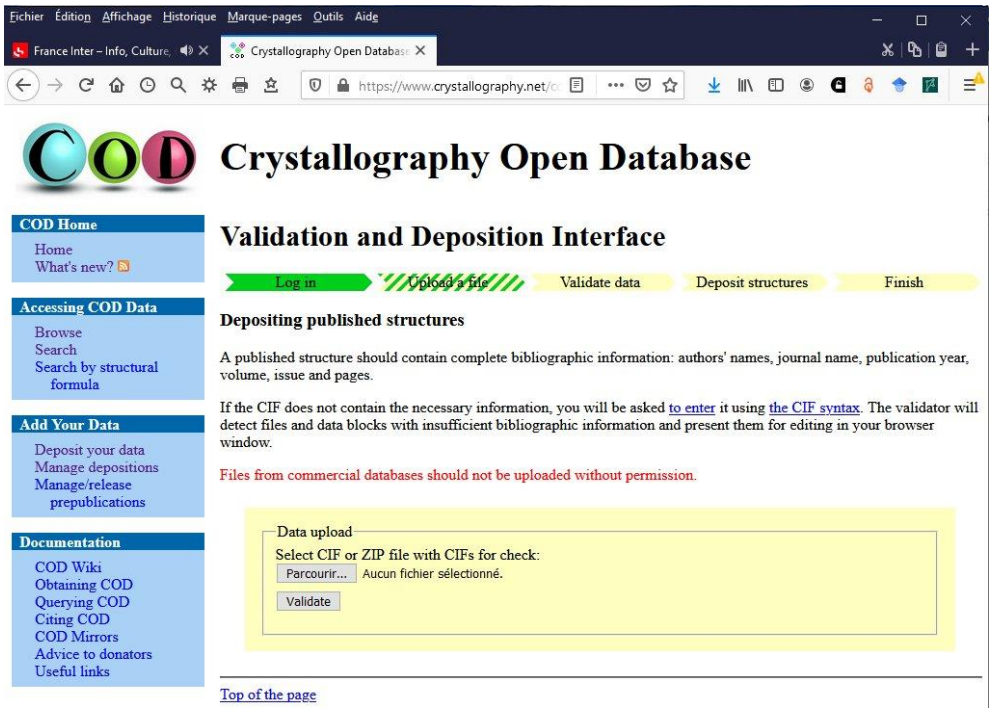
Enter your username and password or sign up in order to obtain them :



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

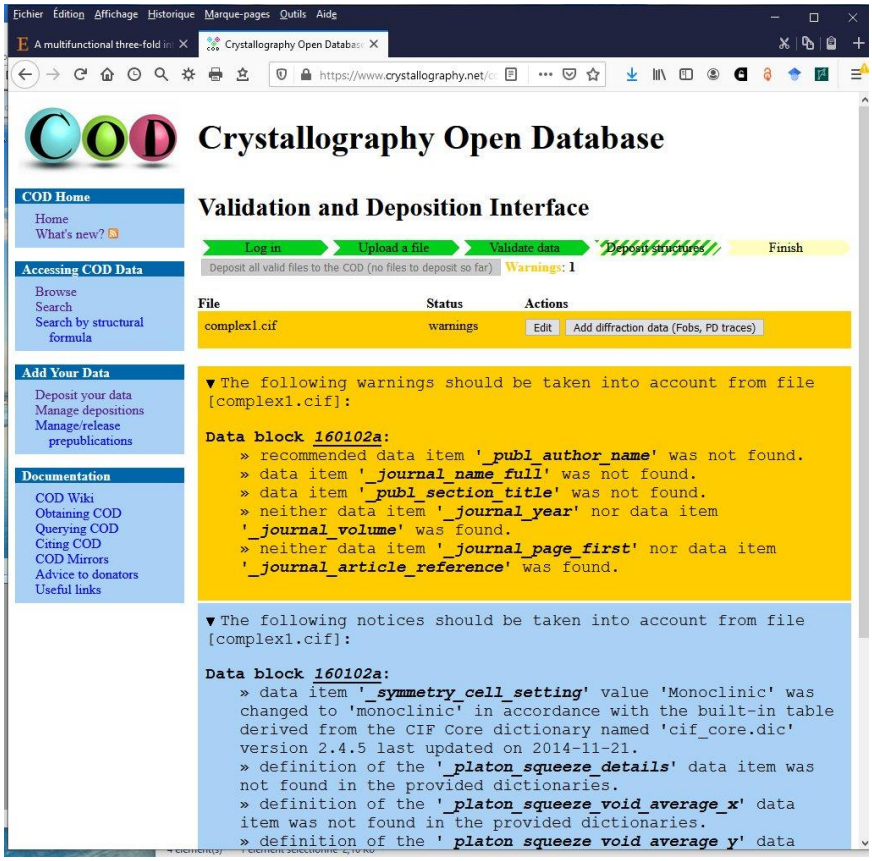
In this case it is « Already published data ».

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

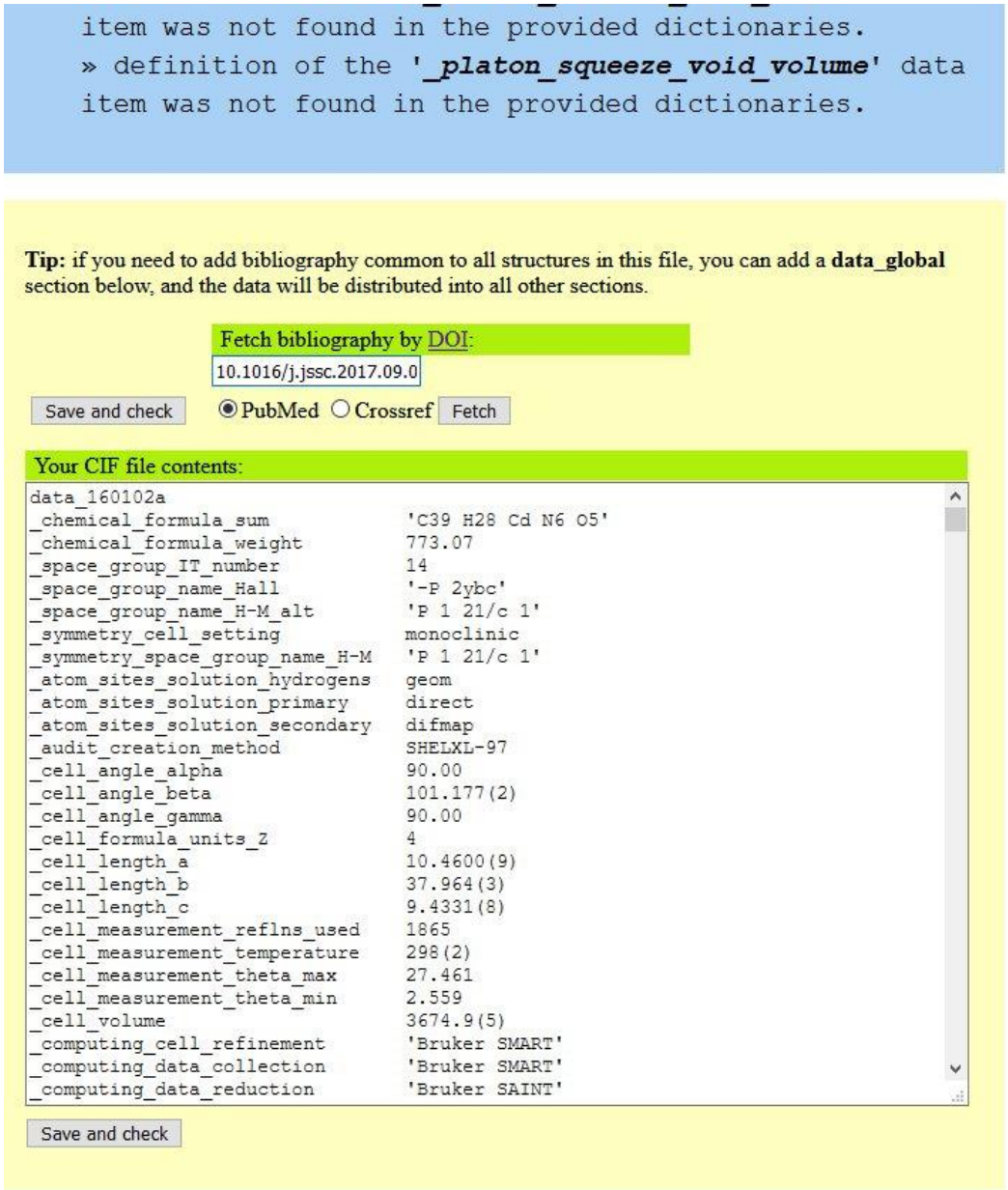


Then select the CIF or ZIP file with CIFs for check and click on « **validate** ».

A first screen of the validation beginning is displayed :



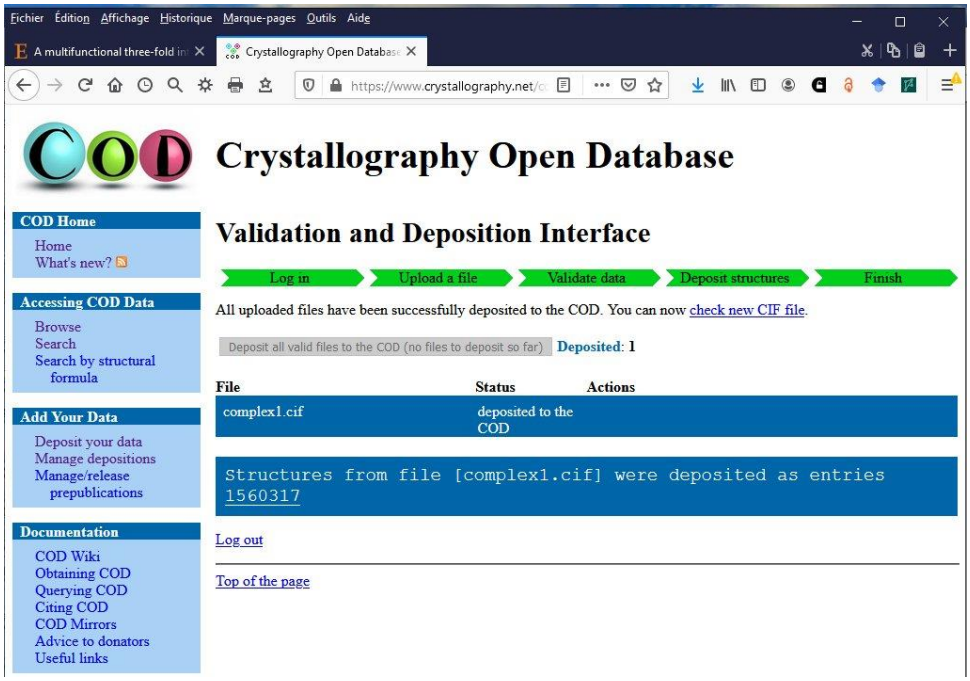
In yellow background, it is said that the CIF tags corresponding to the reference are lacking (author names, journal details, paper title). Then click on « **Edit** » just above the warnings. You see your CIF content appearing and just above you will be offered to « **Fetch bibliography by DOI** ». Enter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



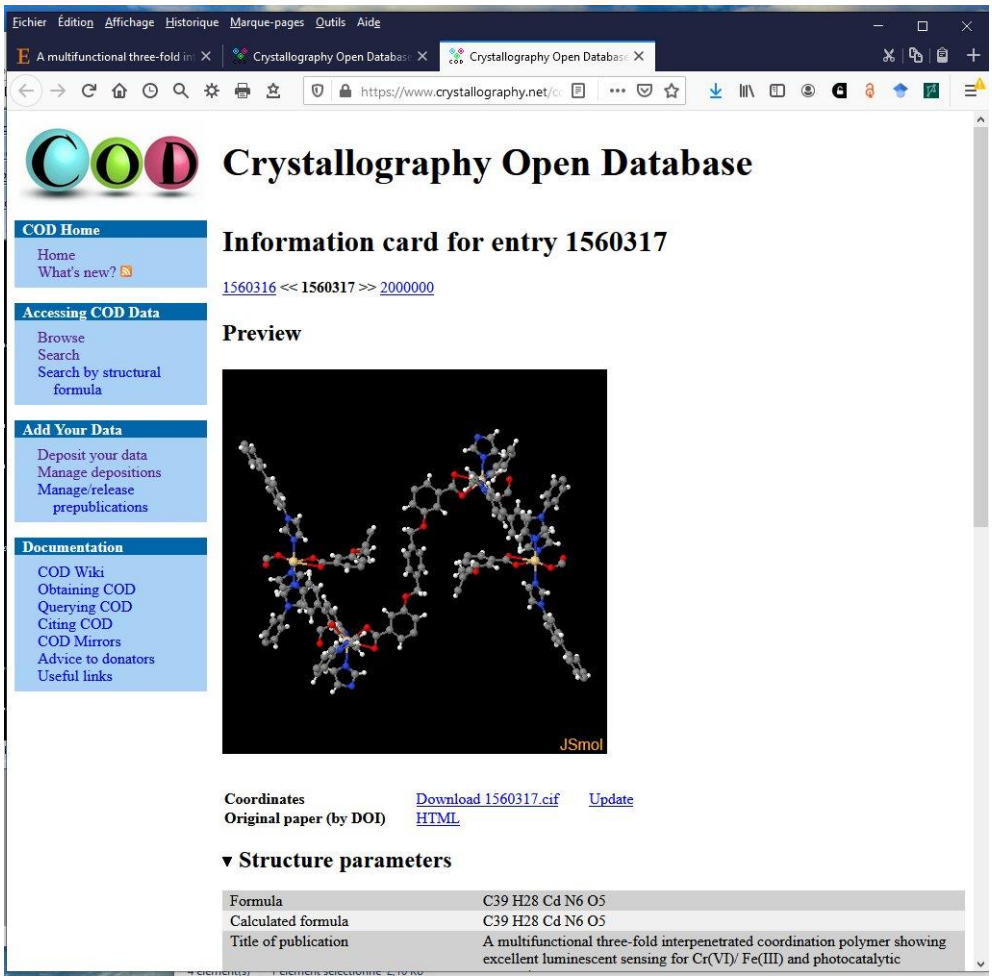
Then you see (in principle…) « **Bibliography was appended successfully** » on a green background and you will see below in the edited CIF the complete bibliography appearing :


Fichier Édition Affichage Historique Marque-pages Outils Aide
A multifunctional three-fold in
Crystallography Open Databas
https://www.crystallography.net/
Crystallography Open Database
COD Home
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
COD Mirrors
Advice to donators
Useful links
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
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 :



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



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
#----------------------------------------
```

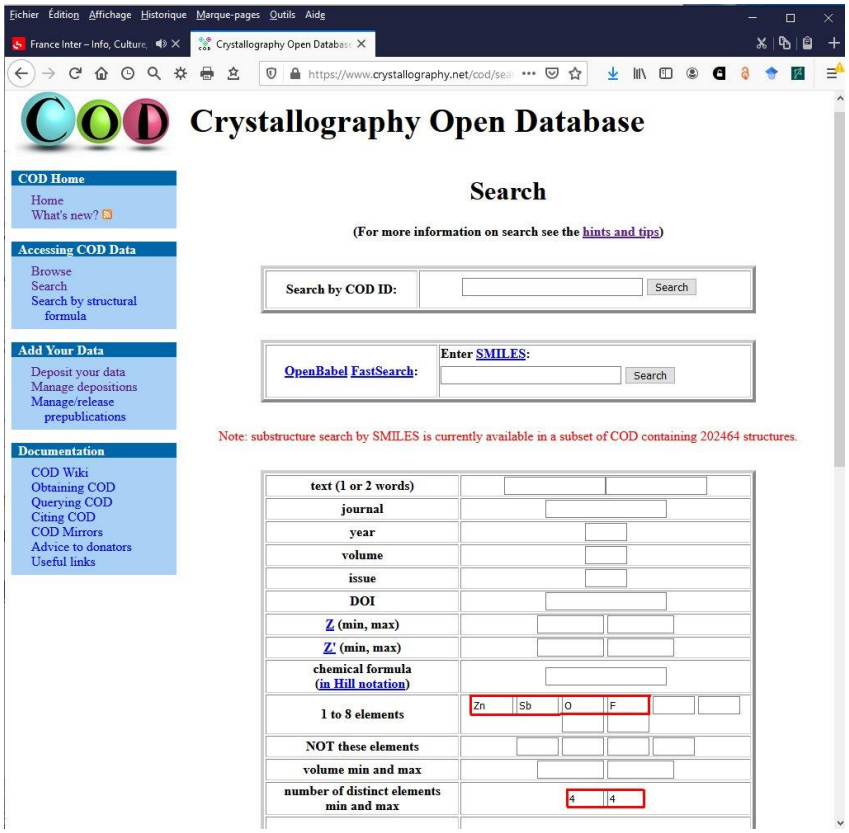
Anyway, the first thing to do is to verify if the entry is not already inside of the COD…

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 :



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
#--

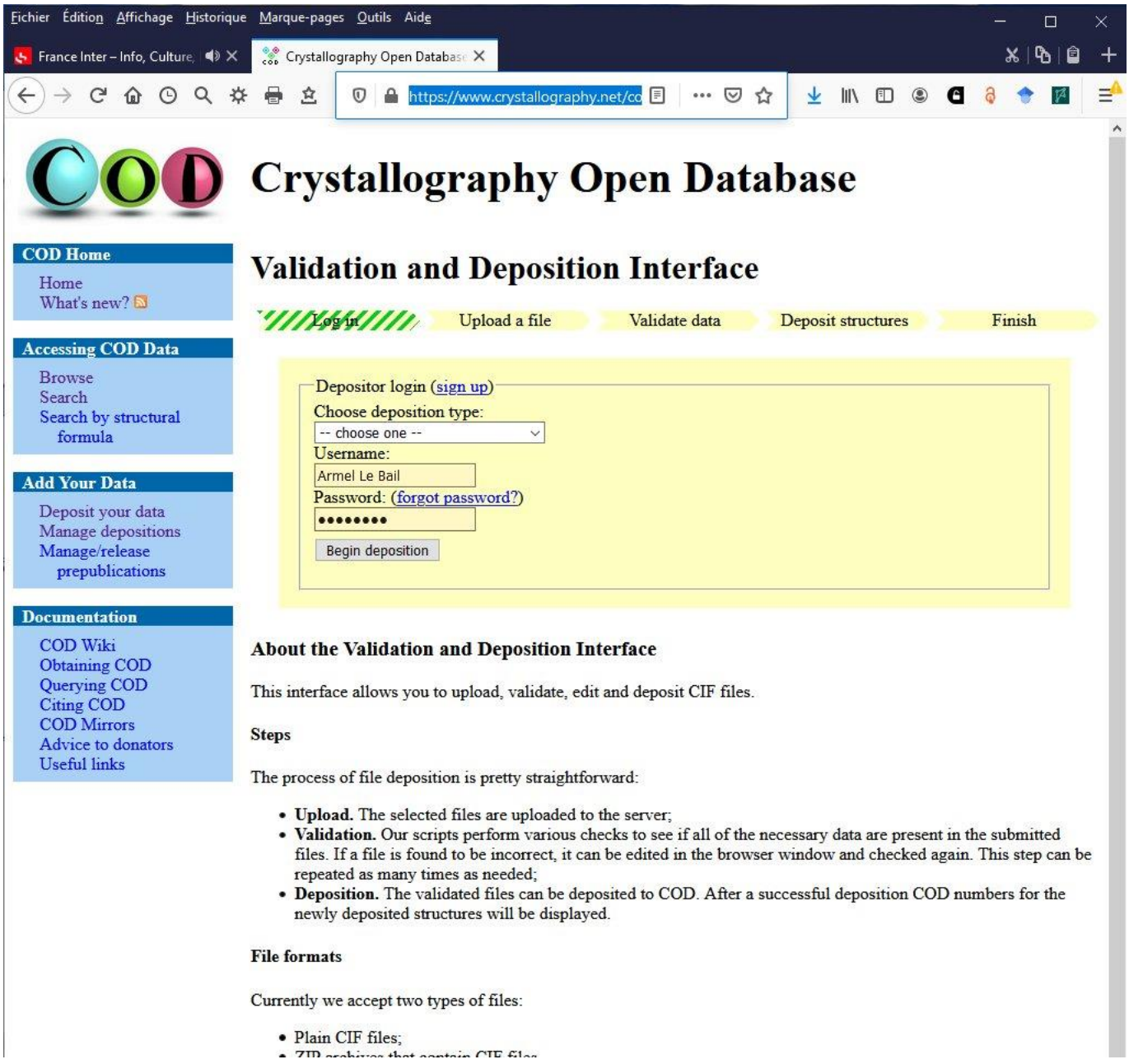
The text editor used here is simply « Bloc-Notes » from Microsoft.

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

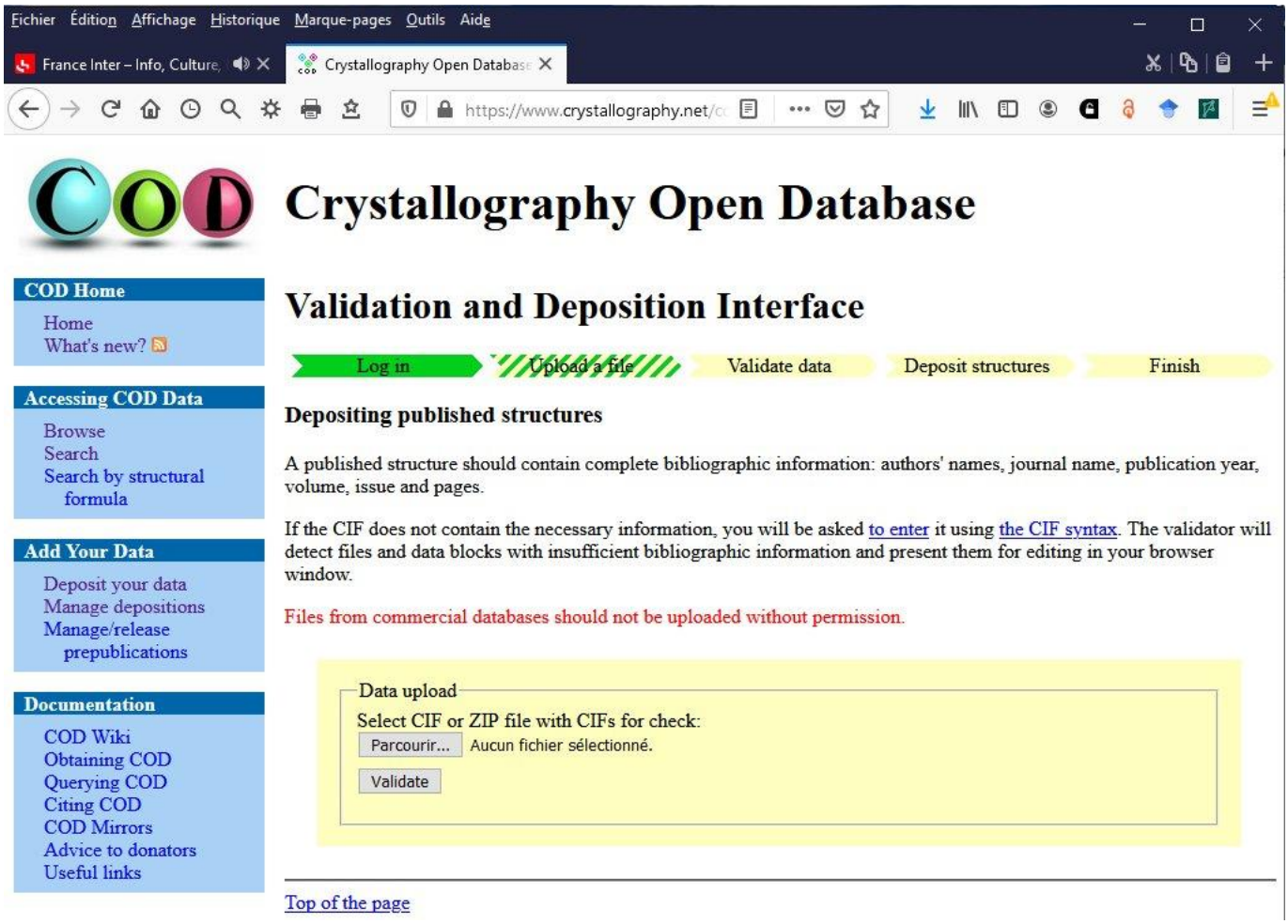
Enter your username and password or sign up in order to obtain them :



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

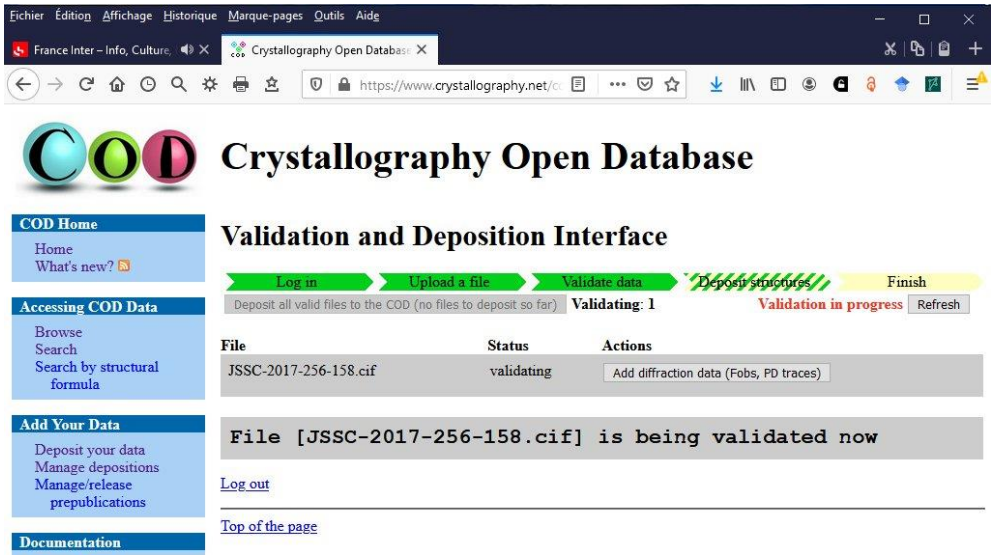
In this case it is « Already published data ».

Then click on « Begin deposition » :

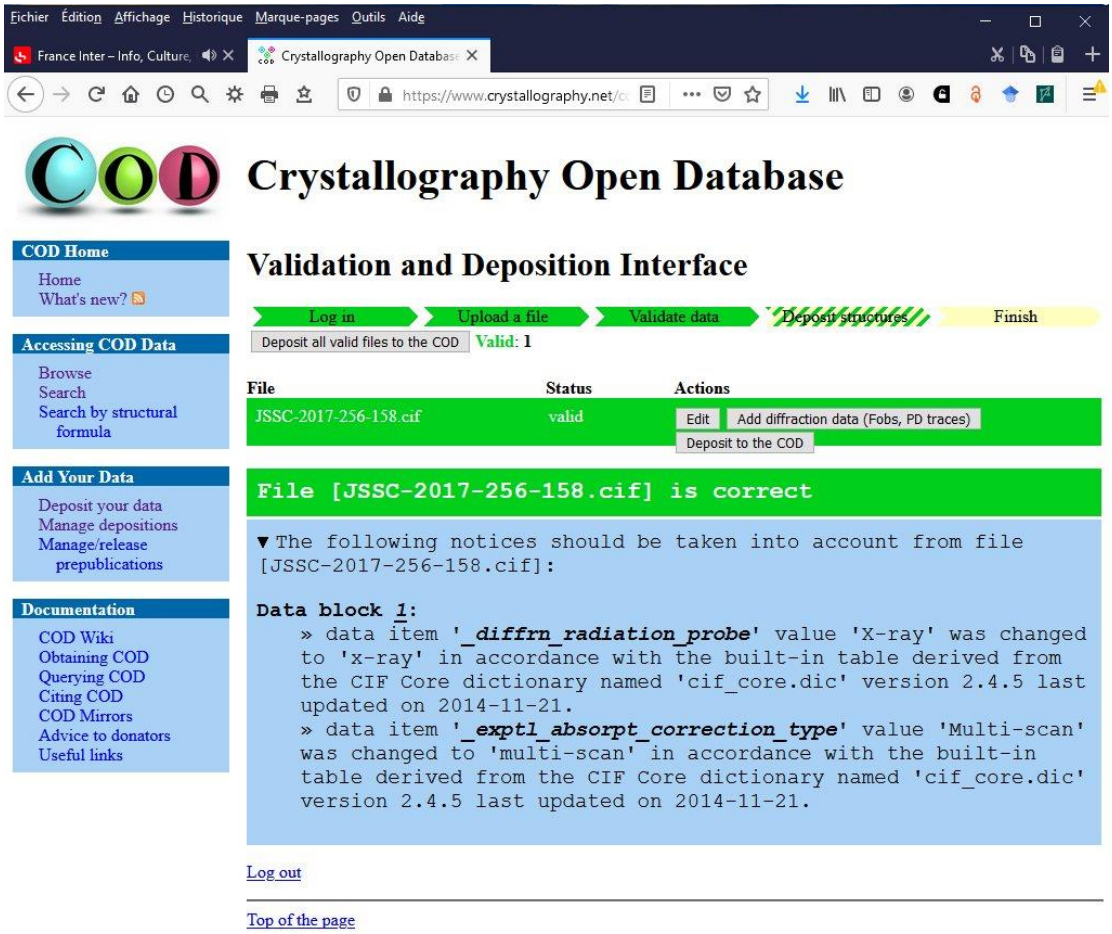


Then select the CIF or ZIP file with CIFs for check and click on « validate ».

A first screen of the validation beginning is displayed :



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…) :

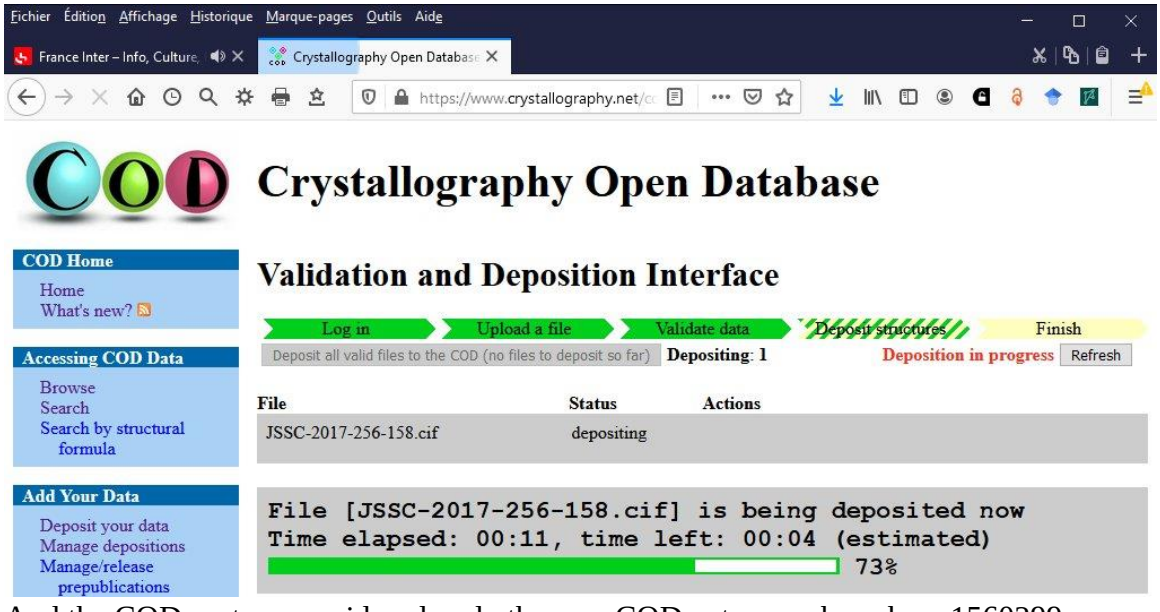


In that case, the COD system has automatically changed some useless capital letters in normal ones.

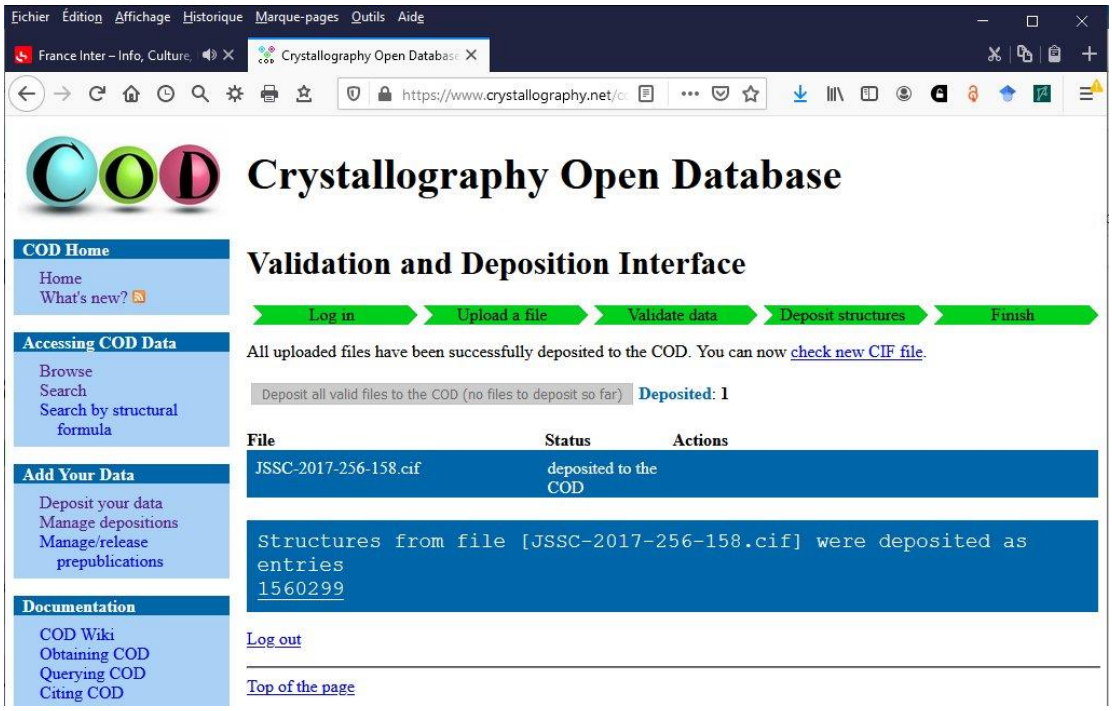
If you have diffraction data (Fobs, Powder pattern) you may add them there.

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

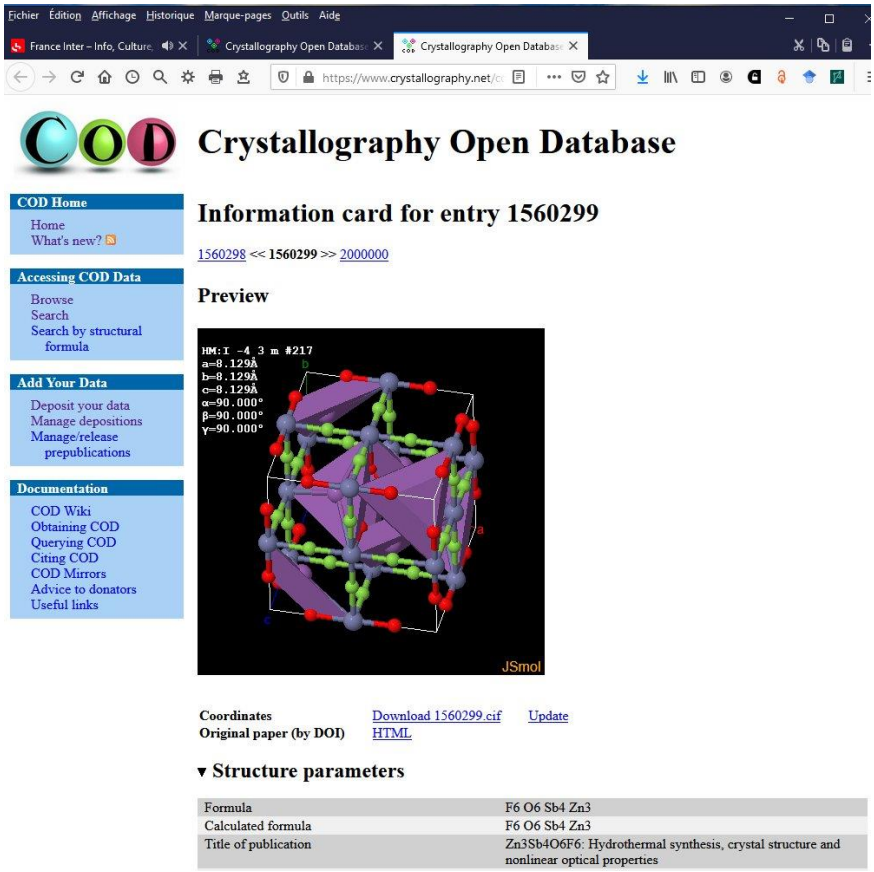
The system says the File is being deposited now :



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



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…) :



Done, congratulations !!!

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

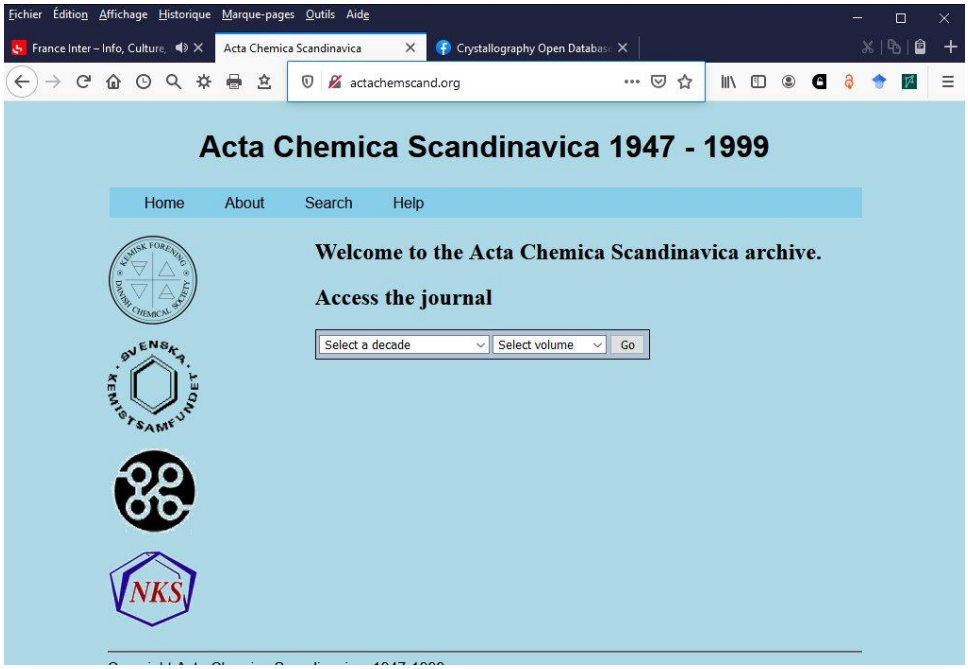
3- CIF to be built completely from an old published crystal structure (for instance from Acta Chemica Scandinavica)

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

_diffrn_ambient_temperature
_diffrn_radiation_probe         x-ray
_diffrn_radiation_type          MoK\a
_diffrn_radiation_wavelength     0.71069

_exptl_crystal_density_diffrn
_exptl_crystal_F_000
_exptl_absorpt_coefficient_mu
```

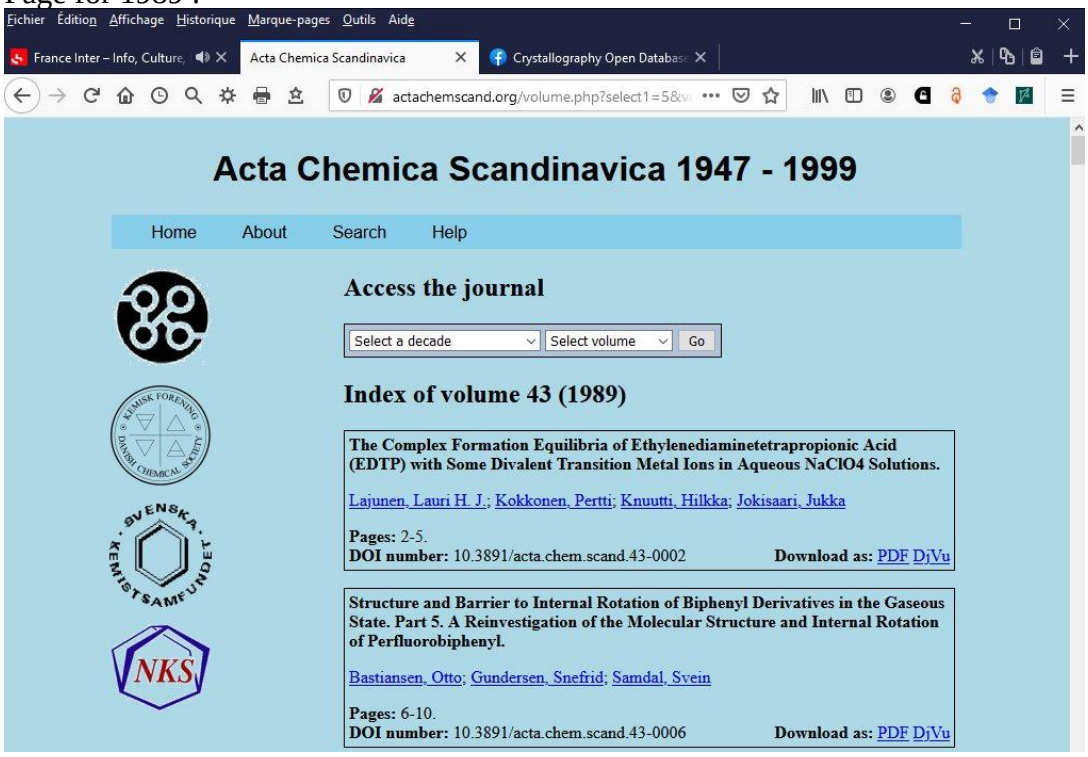
```
_refine_ls_number_parameters
_refine_ls_number_reflns
_refine_ls_R_factor_gt
_refine_ls_wR_factor_gt

_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 :

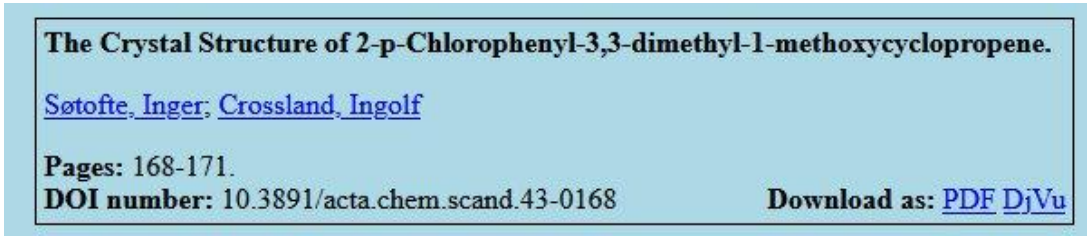


The paper selected for deposit is Acta Chem. Scand. (1989) 43, 168-171.
The absence of this crystal structure in COD was first verified.

Page for 1989 :



And for the file selected :

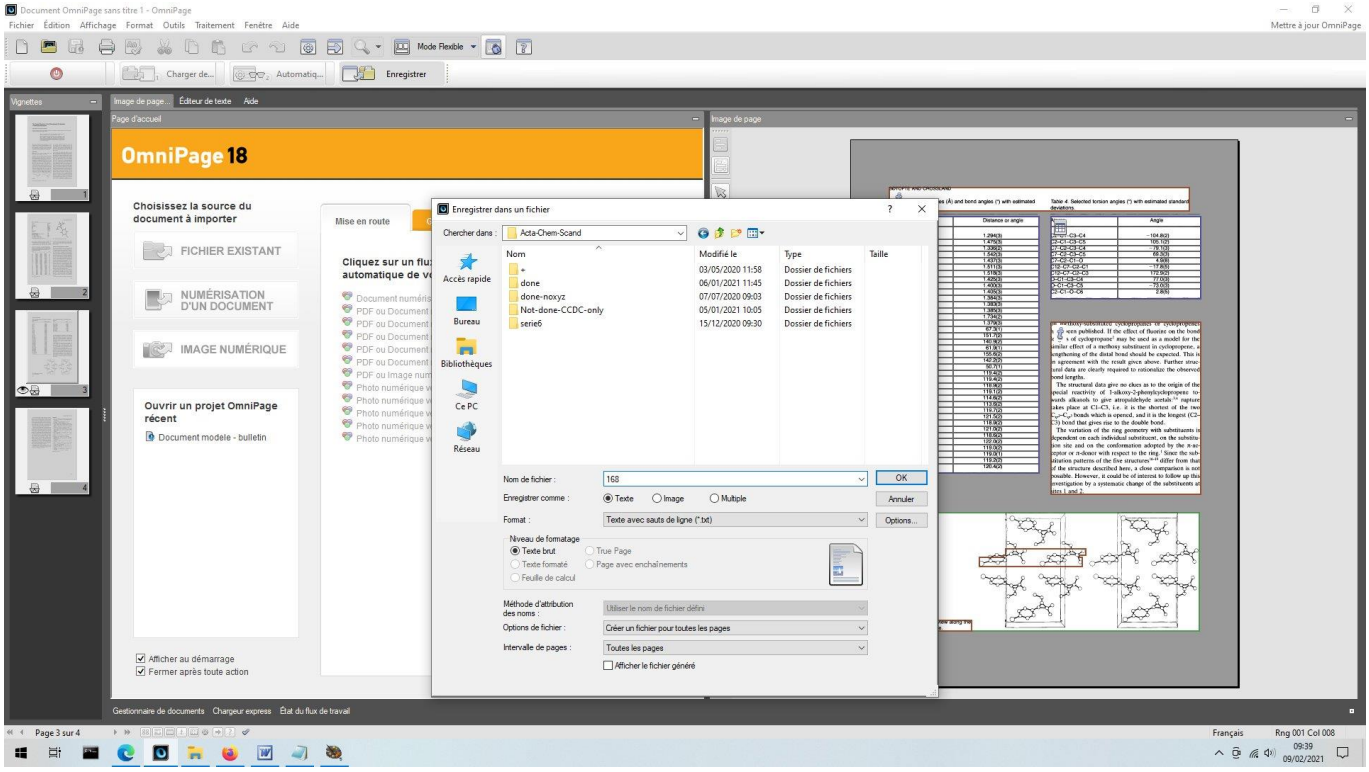


Well… The CIF building starts here by copy-paste into the template renamed
Acta-Chem-Scand-1989-43-168.cif :

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

```
##########################################################
loop_
_publ_author_name
'Sotofte, Inger'                    Sorry for the character ø in Søtofte…. No time for a perfect job here
'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
;
##########################################################
```

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	$C_{12}H_{13}ClO$
M_r	208.7
μ(Mo$K\alpha$)/cm^{-1}	3.08
Crystal system	Monoclinic
V/Å^3	1105.9
a/Å	9.939(5)
b/Å	19.099(4)
c/Å	5.828(4)
β/°	91.60(5)
Space group	$I\,c$ (No. 9)
D_c/g cm^{-3}	1.25
Z	4
Total number of refl.	1844
Number of independent refl. with $I \geq 2\sigma(I)$	1520
Number of variables	177
$R = \Sigma(\|F_o\|-\|F_c\|)/\Sigma\|F_o\|$	0.027
$R_w = [\Sigma w(\|F_o\|-\|F_c\|)^2/\Sigma w\|F_o\|^2]^{\frac{1}{2}}$	0.032
$S = [\Sigma w(\|F_o\|-\|F_c\|)^2/(N_{obs}-N_{var})]^{\frac{1}{2}}$	1.15

Equiv. positions (0,0,0; $\frac{1}{2},\frac{1}{2},\frac{1}{2}$): x,y,z; $x,\bar{y}$, $\frac{1}{2}+z$

CYCLOPROPENE STRUCTURE

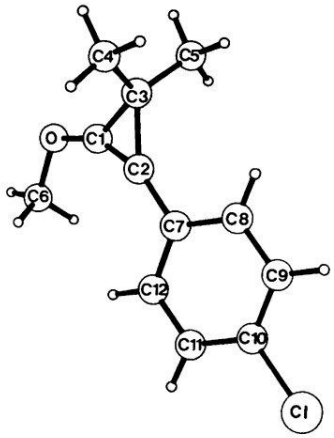


Fig. 1. The structure viewed along the *b*-axis.

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

_diffrn_ambient_temperature     120                    care to give in K
_diffrn_radiation_probe         x-ray
_diffrn_radiation_type          MoK\a
_diffrn_radiation_wavelength    0.71069                sometimes you find 0.71073

_exptl_crystal_density_diffrn   1.25
_exptl_crystal_F_000            ?
_exptl_absorpt_coefficient_mu   0.308                  care it should be µ/mm-1, not cm-1

_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 $x10^4$ or $x10^3$, needing some hand-work from the OCRized table… The original Table :

Table 2. Atomic coordinates × 10^4. The estimated standard deviations × 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] $B_{eq} = \frac{4}{3}\sum_i \sum_j b_{ij}\,(\mathbf{a}_i \cdot \mathbf{a}_j)$.

And the OCR-ized Table :

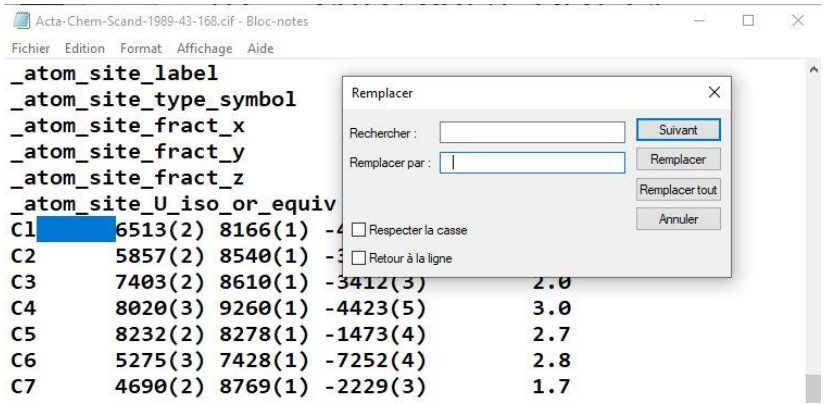
```
Cl      6513(2) 8166(1) -4865(3)        2.0
C2      5857(2) 8540(1) -3422(3)        1.8
C3      7403(2) 8610(1) -3412(3)        2.0
C4      8020(3) 9260(1) -4423(5)        3.0
C5      8232(2) 8278(1) -1473(4)        2.7
C6      5275(3) 7428(1) -7252(4)        2.8
C7      4690(2) 8769(1) -2229(3)        1.7
C8      4850(2) 9142(1) -172(3) 1.8
C9      3746(2) 9348(1) 1056(3) 2.0
Cl 0    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
```

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
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
Cl 0 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
Cl 0 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
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…

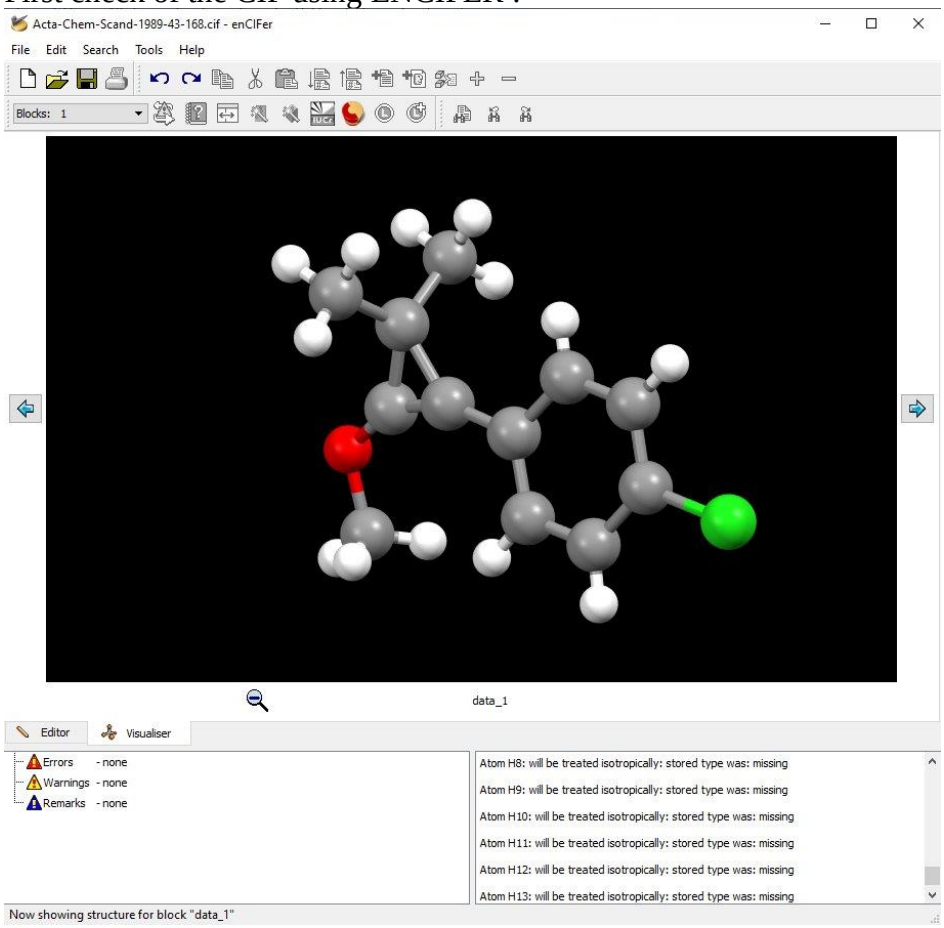
Final result in that case (not two identical cases…) ; Really a lot of job here… :

```
##########################################
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 :



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).

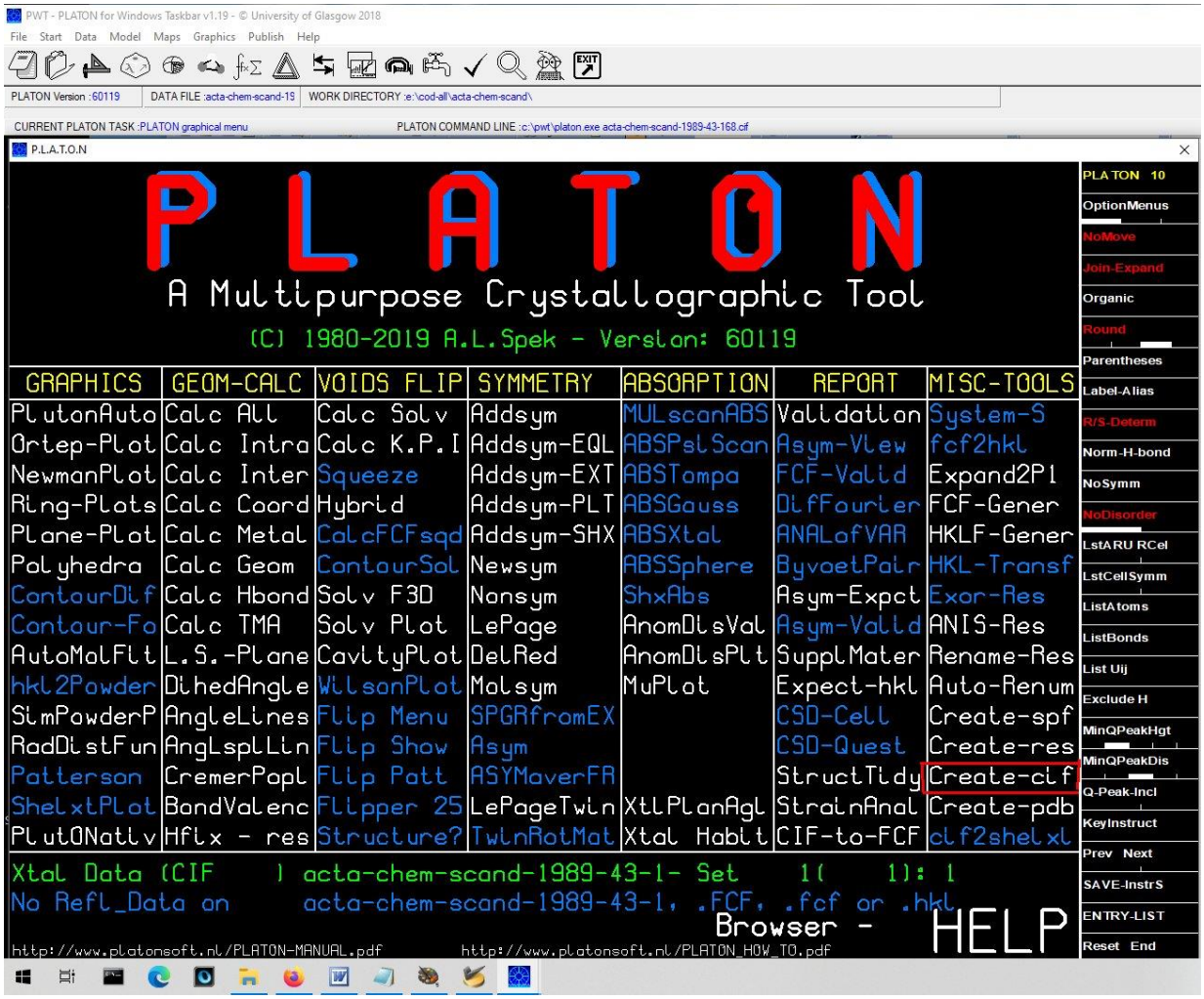
The way to complete the CIF is to use the famous PLATON checking software used in any CHECKCIF stage requested by editors when you try to publish a crystal structure paper. Read your CIF by PLATON, make a new CIF by PLATON, and use that new CIF to complete your starting one…

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\a
_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_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_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_
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_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\a
_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
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_geom_bond_site_symmetry_1
_geom_bond_site_symmetry_2
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 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
Cl	C10	C9	119.03(15)	.	.	yes
Cl	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

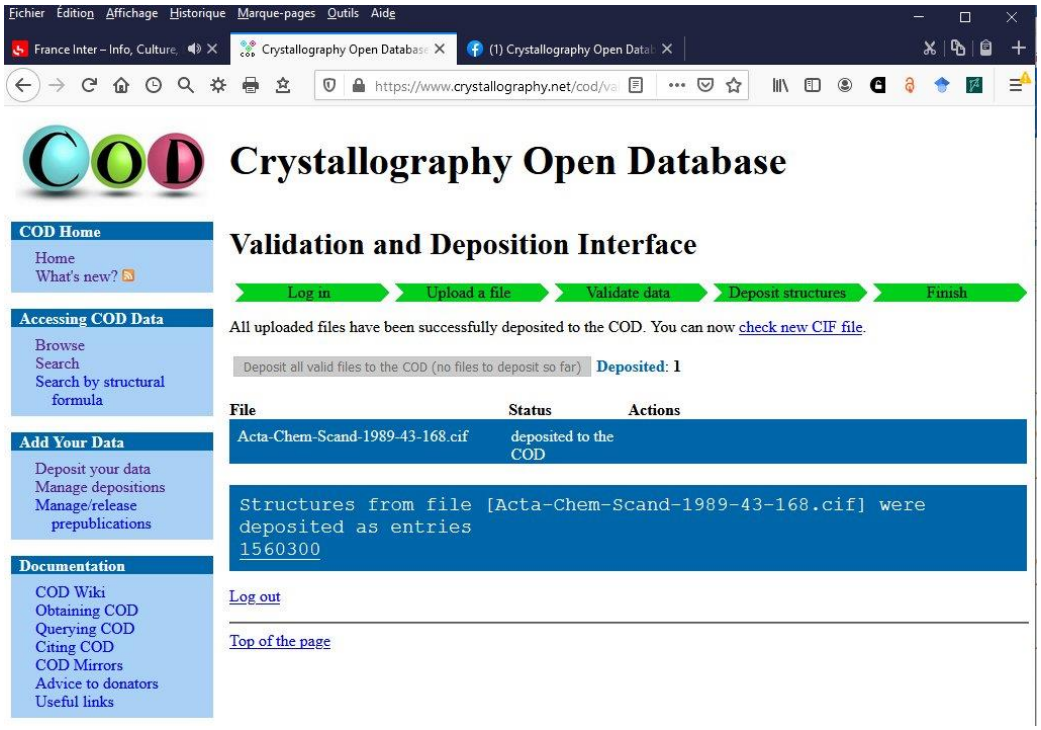
C3	C5	H4	110(2)	.	.	.	no
C3	C5	H5	108(2)	.	.	.	no
C3	C5	H6	111.6(19)	.	.	.	no
H4	C5	H5	106(3)	.	.	.	no
H4	C5	H6	109(3)	.	.	.	no
H5	C5	H6	113(3)	.	.	.	no
O	C6	H7	110(2)	.	.	.	no
O	C6	H8	108(2)	.	.	.	no
O	C6	H9	111.9(19)	.	.	.	no
H7	C6	H8	111(3)	.	.	.	no
H7	C6	H9	109(3)	.	.	.	no
H8	C6	H9	107(3)	.	.	.	no
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	Cl	179.91(17)	.	.	.	no
C8	C9	C10	C11	-0.8(3)	.	.	.	no
Cl	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 usefull before the final deposition into the COD. If no new error, then go :



Done… Self-congratulations…
With experience, that whole stuff will take between 15 and 30 minutes for building one CIF…

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 !