WEEK 2: Visualizing experimental structures

**PART 1: Installing**

0. Download and unzip the folder “ch359-w2”

1. Miniconda (we will check if the system already has it before): download the file in

* + <https://docs.conda.io/projects/conda/en/latest/user-guide/install/linux.html> for linux;
  + <https://docs.conda.io/projects/conda/en/latest/user-guide/install/macos.html> for macos;
  + <https://docs.conda.io/projects/conda/en/latest/user-guide/install/windows.html> for windows;

Then proceed with the following on the terminal (for linux and macos):

bash Miniconda3-latest-Linux-x86\_64.sh

Or for windows:

double click the .exec file

After installing, access the folder “ch359-w2” on the terminal and do:

conda env create -f environment.yml -n myproject

conda activate myproject

2. mofchecker: make sure you are in the conda environment and do

pip install mofchecker

mofchecker --help (to see if it works)

3. manage\_crystal (inside the environment):

pip install manage\_crystal

manage\_crystal --help

4. Avogadro: go to the download page on the website, and proceed with installation

* <https://avogadro.cc>

**PART 2: Visualizing structures on Avogadro**

*be patient, Avogadro unfortunately crashes sometimes*

1. Go to <https://www.ccdc.cam.ac.uk/structures/>

2. Search for a structure that you would like to visualize now – you choose!

3. On the tab “Results”, select the identifier of the structure (if not already selected) and choose Download – Download current entry; fill in with your information and download .cif

4. Open Avogadro

5. Can you tell what is the structure made of?

6. What are the cell parameters (angles, vectors, total number of atoms in the unit cell, number of nonequivalent atoms)?

7. What is the symmetry of the cell?

8. What is the volume of the unit cell?

*hint: you can find information in View – Properties*

9. Select Crystallography – Wrap Atoms to Cell

10. To fill the unit cell, go to Crystallography – Space group – Fill Unit Cell

*9 and 10 are important for cases where the unit cell is not well defined*

11. In View – Crystal View Options – Repeat, change the values of A, B and/or C; set back to A=B=C=1 after

12. Build a supercell in Build – Super Cell Builder

13. What is the difference between repeating the cell and building a supercell?

14. Can you find a way to translate atom positions inside the unit cell?

15. What else can you think of doing with your structure?

*hint: you can find interesting tools in the Crystallography and Extensions section (keep in mind that it’s possible that some of them might crash); example: you might want to try changing the volume of the unit cell – what happens if you do it?*

Explorer mode: If you feel adventurous and up for a (laborious) challenge after class, you can try selecting a paper that has the crystallographic information of the structure and see if you can create a cif file yourself!

**PART 3: What is weird about UiO-66?**

1. Open structure UiO\_66\_orig.cif with Avogadro

2. Can you spot something odd about it?

mofchecker: Checking if your guess was correct

3. On the terminal (it’s best if you are inside the folder “ch359-week2”), type:

jupyter notebook

4. A browser window will open, select the folder “mofchecker” and open the notebook “run-check.ipynb”

5. Replace the name of the structure accordingly and run the lines

*tips: “esc+b” will create a new block of code; “esc+dd” will delete the block of code you’re at; enter will add a new line in the same block of code; shift+enter will run the block of code.*

6. What did you find?

Removing unwanted atoms:

3. Go to Select – Select by element to see which element it is according to color

4.  Select this tool

5. Pressing ctrl (or command on macos) select all atoms you wish to delete and remove it with backspace

6. Take note on the cell parameters (A,B,C and the angles)

7. File – Save as – .xyz (e.g.: test.xyz)

8. Open the .xyz file with any text editor and on the second line add:

CELL: <A> <B> <C> <alpha> <beta> <gamma>

*\*replace <A> with the value of A and so on*

9. Save new file (e.g.: test\_cell.xyz)

Converting to .cif:

10. On the terminal, type:

manage\_crystal test.xyz -o cif

11. Run mofchecker again on the jupyter notebook

12. Were your changes enough to clean the structure?

13. *To think over*: what do we mean by a “clean structure” and why do we need to make sure the structure is properly cleaned?

**PART 4: Do it yourself**

Now practice with structures 1-6 (one of you can select the even structures and the other, the odd ones), repeating PART 3.