Week 2 – setting up your computer and working with crystallographic structures

\*Steps:

Install VESTA, mofchecker,

Exercises (can be inspired by Juarez);

Selected MOFs and COFs (test first) – choose experimental ones, small, that need to be cleaned – how to find them in the database;

Give them an example of a MOF that needs to be cleaned and show the issues (explain the issues and show why we can’t use directly the experimental structures – maybe use my cof as an example, the one with missing hydrogens);

Visualize the MOFs and COFs;

What are the issues that you can find? Are there missing hydrogens? Weird bonds?;

After they check, run mofchecker;

Ask them to try to solve the issues;

Then run mofchecker again;

Ask them to write a simple summary of what they learned – can we just use experimental cifs (elaborate)? What are the issues you came across when cleaning the structures? When using mofchecker, did the issues go away?

\*maybe prepare two weeks – one for simple VESTA/Mercury tutorials, one for cleaning MOFs and COFs; then deliver according to what they already know.