

University of Windsor
Chemistry and Biochemistry
Chemistry 59-553, Fall Term 2014

Project

Due: November 28, 2014

For the project component of this course, you are required to solve, refine a crystal structure and to write a brief report in the style of a crystal structure communication such as those found in *Acta Crystallographica Section C or E* (<http://journals.iucr.org/e/journalhomepage.html> - there is an application called publCIF that you can use to generate the style correctly). Be sure to include all the details of the solution and refinement as part of your discussion. As a further part of the “Discussion” section, you are expected to compare the metrical parameters determined in your structure to appropriate comparable values reported in the CSD. You must include pictures of the molecular structure (and a packing diagram of some sort). Be sure to include a copy of the tables you generate from the CIF file, the CIF file and a copy of the checkCIF validation report that you generate for the CIF file. Make sure that you reference the software that you have used for the solution, refinement and presentation of your structure. In addition, please supply me with an electronic copy of the final RES file and CIF file from your project.

If required, I will provide each of you with a data set (and the associated information) required for this project.