Chemistry 832 - Spring 2000

Final Exam, Take Home

Name:_____ Student Number:_____

This is a open book exam. Clearly show all of your work. If you have any questions, please ask me for clarification. *On questions where you have choices, **clearly** indicate the choice(s) you want me to grade.*

This is a take home/open book exam.

However, you may ***not*** discuss it with anyone but myself until after noon on Friday June 9th when it is due in!!!!!

/ 100 Points Total

1. (20 points) Answer *two out of three* of the following questions.

(a) During routine x-ray data collection an a crystal you only observed useful data out to 45 degrees. Suggest several approaches that would allow you to collect data out to higher angles.

(b) If a crystal was being damaged by the x-radiation, how would this affect the data as it was being collected and how could you minimize this radiation damage?

(c) What is meant by the term Mosaic spread and how does it affect the diffraction data?

3. (15 points in total) Answer *three out of four* of the following questions.

(a) If you had a crystal of a tungsten alloy, would it be better to use a copper or a molybdenum x-ray tube? Give your reasoning.

(b) What do the six anisotropic displacement parameters (i.e. U_{11} U_{22} U_{33} U_{12} U_{13} U_{23}) tell you about the atom?

(c) What is meant by the term thermal diffuse scattering and how does it affect the diffraction data?

(d) What is meant by the term Convergence and, when you are refining your structure by XL, how can you tell that Convergence has occurred?