MSAE E4100 Crystallography
Fall 2016
Barmak

Homework 2 – Update 2
Due Thursday September 22, 2016
100 points

Reading assignments: Chapters 1-3 Burns and Glazer. Chapters 4 and 5 De Graef and McHenry, or any other book that covers the topics covered in this chapter.

1. [52 points] Consider the two conformations of the molecule rhenium chloride, Re_2Cl_8. If the Re-Re bond is placed along the **c**-axis perpendicular to the page, in one conformation, termed eclipsed, the Cl atoms are directly above each other. In the second conformation termed staggered, the Cl atoms on one Re atom are rotated 45 degrees relative to the Cl atoms on the other Re atom.
    a. Draw the schematic projection of these two molecular conformations onto the plane of the page. Use your ruler, protractor, compass (RPC) set to make accurate drawings.
    b. Label your axes on each of your schematics. For the staggered configuration pay particular attention to the symmetry of the molecule. Location of the axes requires some careful thought or you will not be able to do part (c) correctly.
    c. List all the symmetry operations for the staggered conformation in the table below, using both the International (Hermann-Mauguin) and the Schoenflies notations. Include the symmetry axis [uvw]. Describe the ITA symmetry operations in words.

Operator #	Symbol (ITA)	Symbol (Schoenflies)	Symmetry Operator Description – Schoenflies only
1			
2			
3			
4			
5			
6			
7			
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9			
10			
11			
12			
13			
14			
15			
16			

d. Using the symmetry operators above, create the symmetry-related points to a general point on a stereographic projection. Be certain to show the pictorial symbol for the symmetry operators.
e. What do you observe about the number of symmetry operators and the number of symmetry related points on your stereogram?

2. [10 points] β-Sn is the high-temperature polymorph of tin, stable at temperatures above 286.4 K. It assumes the *tI* Bravais lattice with lattice constants a = 0.58315 nm and c =

0.31814 nm. Because of its tetragonal structure, as opposed to diamond cubic structure of other group IV elements, β-Sn is a semi-metal (near metal) rather than a semiconductor. Use the metric tensor for the following calculations.

a. What is the angle between the [111] and [$\bar{1}$23] directions?
b. What is the length of the vector connecting a corner atom to the body center atom?

3. [20 points] Assuming the presence of a $\bar{4}^3(S_4)$ symmetry operation, prove using the martices in Appendix 1, that a = b and that $\alpha = \beta = \gamma = 90°$. In other words, the presence of the given symmetry operator requires the equality of two axial lengths and the mutual orthogonality of the three basis vectors.

4. [8 points] The coordinates of a point in the hexagonal unit cell are (1/3/,2/3,2/3). What are the coordinates of this point in the obverse rhombohedral unit cell?

5. [10 points] Show that $\frac{3}{m}$ and $\bar{6}$ are equivalent. Use stereographic projections to demonstrate. Make accurate schematics using your RPC set.