Homework 1 - Update
Due Thursday September 15, 2016
100 points

Purchase a ruler, protractor, compass set, which you will need to draw accurate schematics for assignments and for exams.

Reading assignments: Chapters 1 and 2 Burns and Glazer. Chapter 4 De Graef and McHenry, or any other book that covers the topics covered in this chapter.

1. [8=2×2+4points] Denote the following symmetry operations in the International (Hermann-Mauguin) notation and note the symmetry operation to which they are equivalent (if any):
   a. A four-fold rotation about the **a**-axis applied thrice
   b. A six-fold rotoinversion about the **c**-axis applied thrice
   c. A mirror operation containing both the **b**- and **c**-axes in hexagonal coordinates. Hint: Draw the unit cell, with the **a**-axis pointing down and to the left, and the **b**-axis pointing the right. Then draw the mirror and carefully determine the crystal direction that is perpendicular to the mirror plane. In the International notation, mirrors are always defined by the normal to the mirror plane.

2. [8=4×2 points] Denote the following symmetry operations in the Schoenflies notation and note the symmetry operation to which they are equivalent (if any):
   a. A six-fold rotation about the **c**-axis applied twice
   b. A four-fold rotation-reflection with rotation about and reflection perpendicular to the **c**-axis applied twice
   c. A mirror plane perpendicular to the **c**-axis
   d. A two-fold rotation about the **a**-axis

3. [24=2×12 points] Please use the matrix approach in answering these questions. The matrices for the symmetry operators are given in Appendix 1.
   a. Determine the coordinates of a general point rotated by 240° in a system with a 6-fold rotation axis along the **c**-axis and then reflected in a plane perpendicular to the **a**-axis.
   b. Determine the coordinates of a general point reflected in a mirror perpendicular to the $\left[\bar{1}10\right]$ direction in a reference-frame with mutually perpendicular basis vectors, and then rotated by 180° about [110] axis.

4. [16=5+3+5+3 points] Use the stereographic projection to show the pattern of points. Draw a circle to denote the perimeter of the projection. See Appendix 5 for examples. Denote the height above and below with + and -, respectively. Denote handedness with a comma. Use your ruler, protractor, compass set to make accurate schematics.

a. What pattern of points is created by the application of two intersecting mirrors one normal to the **c**-axis and the other normal to the [110] direction in a rectilinear frame?
b. Is(Are) a new symmetry operator(s) created in (a)? If so, what is(are) this(these) symmetry operator(s) and what is the symmetry element?
c. What pattern of points is created by the application of a two-fold axis perpendicular to a mirror? Take the two-fold axis along the **c**-axis.
d. Is(Are) a new symmetry operator(s) created in (c)? If so, what is(are) this(these) symmetry operator(s) and what is the symmetry element?

5. [44=3+4+2×2+11×3 points] Consider the two conformations of the molecule ethane, C_2H_6 (one conformation has lower energy than another, but this is not a point with which we need be concerned in this question). If the C-C bond is placed along the **c**-axis perpendicular to the page, in one conformation, termed eclipsed, the H atoms are directly above each other. In the second conformation termed staggered, the H atoms on one C atom are rotated 60 degrees relative to the H atoms on the other C atom.
   a. Draw the schematic projection of these two molecular conformations onto the plane of the page. Use your ruler, protractor, compass set to make accurate drawings.
   b. Label your axes on each of your schematics.
   c. List all the symmetry operations for the eclipsed conformation in the table below using both the International (Hermann-Mauguin) and the Schoenflies notations. Describe the Schoenflies symmetry operations in words.

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Operator #	Symbol (ITA)	Symbol (Shoenflies)	Symmetry Operator Description Schoenflies only
1	1	E	Identity
2			
3			
4			
5			
6			
7			
8			
9			
10			
11			
12			

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