

## MATRL 218/CHEM277: Assignment 2

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1. Explain  $a$ ,  $n$  and  $d$  glides in 3D crystals using sketches.
2. Cubic cells always have a  $\bar{3}$  or 3 in the space group label. What is the  $\bar{3}$  symmetry element in a cube?
3. What is the difference between the  $6_1$  and  $6_5$  symmetry operations? Distinguish with a sketch. It is helpful to use a low-symmetry motif such as the letter 'R' for your illustration.
4. In addition to normal symmetry operations, Shubnikov has described elements of color symmetry. For example, the mirror  $m'$  would take a black object and reflect it to a white one as shown below. Sketch 2D objects, if you can, with the following symmetries: (i)  $4mm$  (ii)  $4'm'm'$  (iii)  $2m'm'$  (iv)  $3'$ . Hint: The last case is "frustrated". What does this say about spins (as in magnetism) at the corners of a triangle?



5. Illustrate the relationship between  $fcc$  and  $ccp$  by sketching layers with hexagonal cells.
6. Calculate the efficiency of packing in the diamond structure. Remember that there are 8 atoms in the cell, and that the atom at  $(0,0,0)$  touches the atom at  $(1/4,1/4,1/4)$ .
7. Under extreme cryogenic conditions, a light isotope of helium,  $^3\text{He}$ , forms crystals with fascinating physical properties. Using the International Crystal Tables, sketch (by hand, with tiles) a particular polymorph of  $^3\text{He}$ : space group  $P6_3/mmc$  (194), with  $a = 3.46 \text{ \AA}$ , and  $c = 5.60 \text{ \AA}$ . The helium atom sits at  $(0, 0, 0)$  in the unit cell. Is the resulting structure  $hcp$  (hexagonal close packed)? Verify your answer with VESTA.
8. Use VESTA to draw all the structures whose data have been presented to you (from  $\alpha\text{-Po}$  to ...)