Homework set #6 *X-ray crystallography. Due in my mailbox any time before the end of next week!*

(1) What is the packing criterion that will likely lead to each of the following physical properties for a given crystal:

a) Triboluminescence:
b) "Organic metals":
c) Organic magnets:
d) Ion-pair charge transfer absorption bands in coordination compounds:
e) Au(I)-based photoluminescence:

(2) Identify the type of intermolecular interactions in crystals of compounds that exhibit each of the above physical properties.

a) Triboluminescence:
b) "Organic metals":
c) Organic magnets:
d) Ion-pair charge transfer absorption bands in coordination compounds:
e) Au(I)-based photoluminescence:

(3) Give an example from the literature for an article that contains a crystal structure which demonstrates the relevant packing criterion in Question 1. Make sure you read the paper and see the crystal structure (don't completely rely on citations given in class or elsewhere). Just provide the citation for the journal article below.

a) Triboluminescence:
b) "Organic metals":
c) Organic magnets:
d) Ion-pair charge transfer absorption bands in coordination compounds:
e) Au(I)-based photoluminescence:

(4) We did in class an example that illustrates 2_1, 3_1, and 3_2 screw axes.

a) What are the 8 remaining possible screw axes?

b) Demonstrate the application of these eight screw axes on a separate piece of paper in the same manner we followed for the three examples we did in class.

(5) Draw on a separate piece of paper an enlarged version of a two-dimensional crystal with a ***p4*** symmetry. Assume that the motif is an open circle. In order to answer this question, it is easiest that you distinguish the different circles in the crystal structure with numbers even though they are identical (for example, make a 5x5 matrix of open circles and label each circle with numbers 1-25). Choose a unit cell in the middle of the crystal (label the a and b vectors by arrows) and then answer the following questions:

a) Justify the ***p4*** symbol given to the space symmetry:

b) Reproduce the drawing of graphical symbols for the symmetry elements given in your notes for the ***p4*** unit cell (on page 6 of the first set of X-ray notes handed out to you and posted on the course web site; keep in mind that the symbols in the middle don't pass through lattice points). This should give a total of 17 symmetry elements (5 C_4 rotations, 4 C_2 rotations, 8 reflections). Give a legend or a label to each of these 17 symmetry elements (for example, label them with letters).

c) What happens to the unit cell you chose when you apply each of the 17 symmetry operations (for example say that numbers (7,8,12,13) become (12,13,7,8) when the vertical reflection denoted as ?? is applied).

d) Apply a glide operation to the same ***p4*** primitive square lattice and draw the resulting crystal structure when you fill the new lattice with the same open circle motif used above. Keep the old numbers you used for the circles in the original crystal structure but don't label the new circles at the new lattice points generated by the glide operation. It is essential that you are accurate in your drawing regarding the distances and angles separating the different circles (you might want to use graph paper but you don't have to if you are accurate enough).

e) Justify whether the centering you did in part d leads to a new crystal symmetry or whether the resulting symmetry will remain as ***p4***.