Supplemental Problems for Chapter 3

1) Consider a structure with space group $P4_2cm$ (no. 101), and c = 4a.
(i) Name the point group from which this space group is derived, and sketch a diagram illustrating the general equivalent positions.
(ii) Explain the orientation and action of the operators 4_2, c, and m in this space group.
(iii) Find a general equation for the interplanar spacings in this lattice (d-spacings).
(iv) Draw a sketch comparing the direct lattice to the reciprocal lattice for this structure, projected along [010]. (include at least four unit cells in the plane and label all points and vectors)
(v) In this structure, what direction is perpendicular to the (011) plane?

2) List the coordinates of all of the special positions in point group 4/m.

3) Use eqn. 3.2 to determine the 3x3 rotation matrix for a triad along the <111> axis of a cubic system.
(ii) Starting from the general coordinate x,y,z, what other coordinates are generated by this operator?
(iii) How many other triads are there in a cubic point group? What are their rotation matrixes?

4) The compound $LaMnO_3$ crystallizes in the structure described in the table below.
(i) What is the Bravais lattice of this structure?
(ii) Are the general positions of this group occupied?
(iii) Sketch a projection of this structure along the [001] axis.
(iv) Define the meanings of "n" and the "a" in the space group symbol. Explain exactly where these operators are in the unit cell and define their action.
(vi) This group also contains a screw diad (2_1) that is not specified in the name. Where is this located in the unit cell?

Table 1: The structure of $LaMnO_3$

Formula unit	$LaMnO_3$	
Space group:	Pnma (no. 62)	
Cell dimensions:	a = 5.453 Å b = 7.672 Å c = 5.447 Å	
Cell contents:	4 formula units per cell	
Atomic positions:	La in (4a)	0,0,0; 1/2,0,1/2; 0,1/2,0; 1/2,1/2,1/2
	Mn in (4c)	x, 1/4, z; $\bar{x}$ +1/2, 3/4, z +1/2;
		$\bar{x}$, 3/4, $\bar{z}$; x +1/2, 1/4, $\bar{z}$ +1/2
		x = 0.5436 and z = 0.0064
	O1 in (4c)	x = -0.0108 and z = -0.0734
	O2 in (8d)	x, y, z; $\bar{x}$ +1/2, $\bar{y}$, z +1/2;
		$\bar{x}$, y+1/2, $\bar{z}$; x+1/2, $\bar{y}$+1/2, $\bar{z}$ +1/2;
		$\bar{x}$, $\bar{y}$, $\bar{z}$; x +1/2, y, $\bar{z}$ +1/2;
		x, $\bar{y}$+1/2, z; $\bar{x}$ +1/2, y+1/2, z+1/2;
		x = 0.3015; y = 0.0385, z = 0.2258