

Midterm Exam

1. Imagine that you are working on a new compound for which there is considerable controversy in the literature as to which space group it belongs. Although this material only has one space group, different authors report it to belong to space groups $Ama2$, $P4_2/ncm$, $P6_3cm$, $P2_1$, $P2_1/m$, $Pnn2$, Cc , $Ibca$, $R\bar{3}c$, $Fd\bar{3}$, $P31c$, or $I4_1/acd$. You obtain a perfect single crystal of this material and cut three thin parallel plates from faces on the crystal that are mutually perpendicular. You label the plates **A**, **B**, and **C**. As the space group is not known, the Miller indices of the faces of the three plates that you cut are not known, but you proceed to make some measurements on them nonetheless. You change the temperature of the three single crystal plates by a temperature ΔT and measure the polarization that develops on the faces of the three plates. The table below shows the polarization in $\mu C/cm^2$ that you measure on the three plates as a function of ΔT .

Plate	$\Delta T=0$	$\Delta T=100\text{ }^\circ C$	$\Delta T=200\text{ }^\circ C$	$\Delta T=300\text{ }^\circ C$
A	0	0.5	1.4	3.5
B	0	2.1	3.0	3.5
C	0	0	0	0

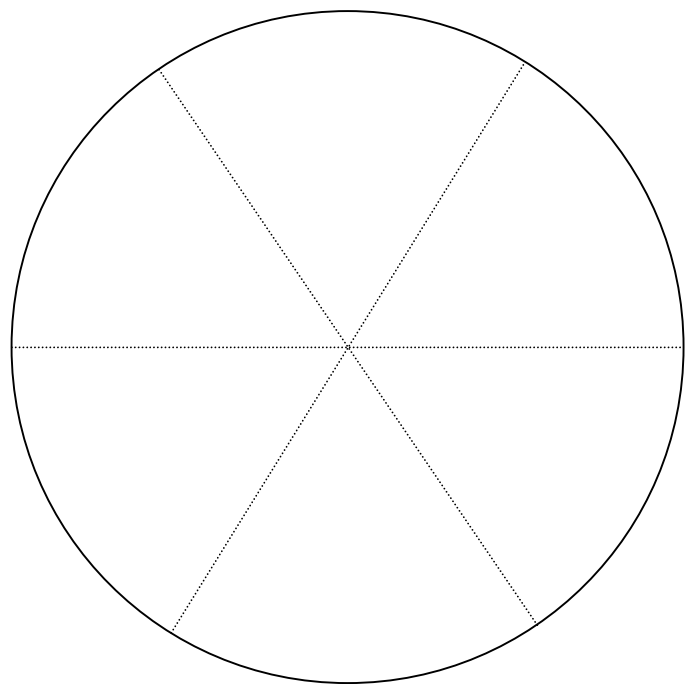
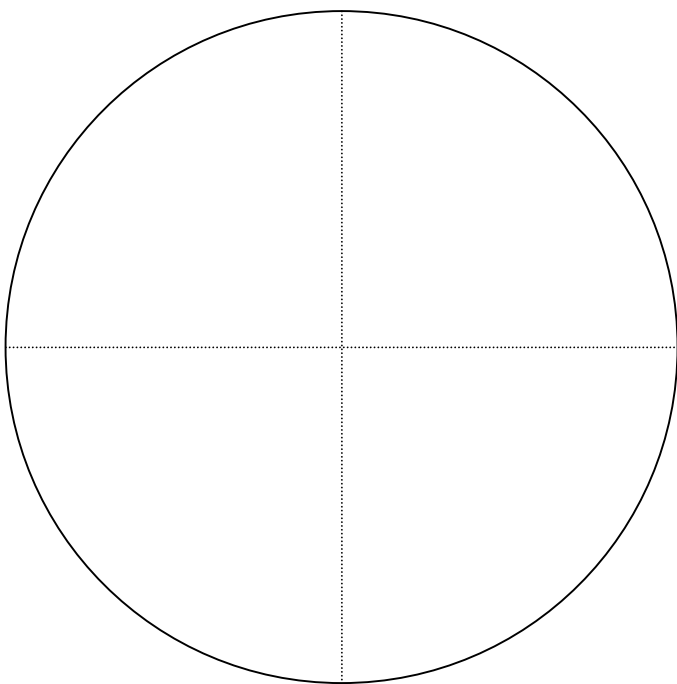
- a. Give an equation that defines the relevant tensor involved in these measurements. Define all terms in your equation. For each term, indicate its rank, whether it is a polar or axial tensor, and whether it is a tensor property or tensor variable. (5 Points)
- b. Do these measurements allow you to reduce the possible space groups that the material can belong to? Explain. (12 Points)

- c. Do these measurements allow you to conclude anything about the directions of the crystal physics axes? About the directions of the crystallographic axes? Explain. (8 Points)

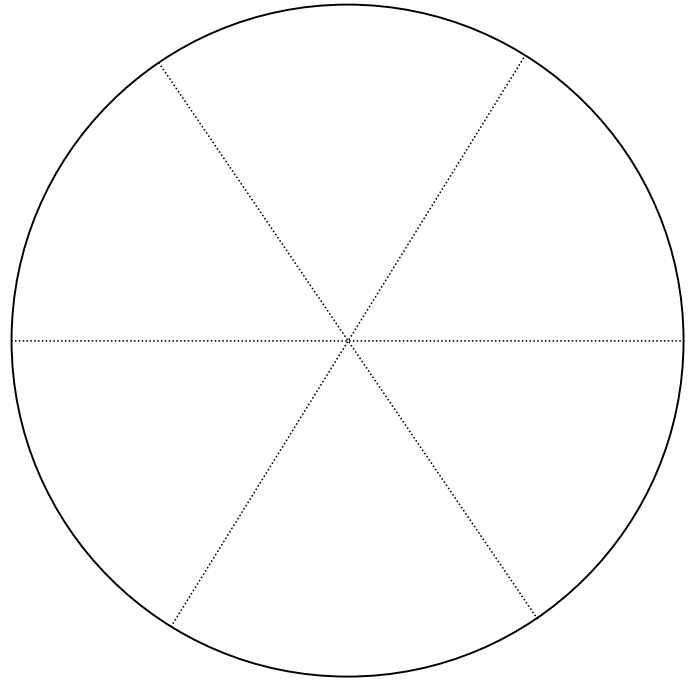
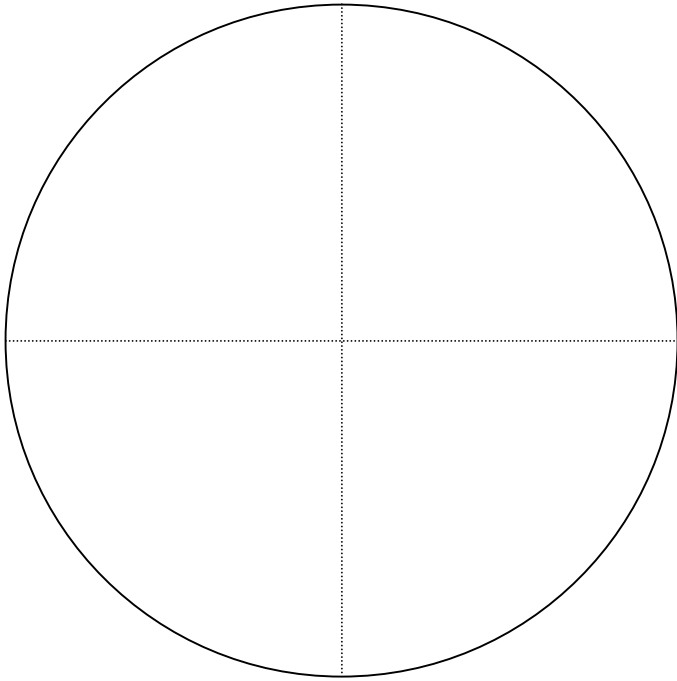
2. A single crystal of tungsten carbide, WC, has space group $P\bar{6}m2$.

- a. To which crystal system does WC belong? (2 Points)

- b. On either of the stereographic projections below (whichever you find easier to draw on) show the symmetry-equivalent poles of a single crystal of WC. (10 Points)



- c. On either of the stereographic projections below (whichever you find easier to draw on) *clearly* indicate the position of the symmetry elements (all of them), the location of the crystallographic axes (a , b , and c), and the location of the crystal physics axes (Z_1 , Z_2 , and Z_3) of a single crystal of WC. Make your drawing with the same relative orientation as your stereographic projection of part (b). (10 Points)



- d. Give the transformation matrix (i.e., the \mathbf{a} matrix) of the point group symmetry element of WC that involves (i.e., is either parallel to or perpendicular to) the Z_1 axis? (5 Points)
- e. Give the transformation matrix (i.e., the \mathbf{a} matrix) of the point group symmetry element of WC that involves (i.e., is either parallel to or perpendicular to) the Z_2 axis? (5 Points)

- f. Give the transformation matrix (i.e., the \mathbf{a} matrix) of the point group symmetry element of WC that involves (i.e., is either parallel to or perpendicular to) the Z_3 axis? (5 Points)
- g. Does WC have a center of inversion? (2 Points)
- h. Is pyroelectricity a null property for WC? Explain. (5 Points)
3. Imagine that you are hired by the Colombian government to determine some of the physical properties of cocaine, $C_{17}H_{21}NO_4$. A single crystal of cocaine has space group $P12_11$, at both room temperature and 77 K.
- a. Use Neumann's principle to determine the pyroelectric tensor of cocaine. (5 Points)
- b. If the crystallographic axes of a single crystal of cocaine are unknown, what is the minimum number of measurements needed to establish the full pyroelectric tensor of cocaine? (3 Points)
- c. Will making the number of measurements specified in part (b) allow you to conclude anything about the directions of the crystallographic axes? Explain. (3 Points)

4. In measuring the pyroelectric coefficient of a single crystal, you measure non-zero (and significant) values of the pyroelectric coefficient along the Z_1 , Z_2 , and Z_3 directions. To which point group(s) must the material belong? (4 Points)
5. This problem involves starting with a totally randomly-oriented powder of the mineral dreyerite, BiVO_4 , and processing it. The crystal structure of BiVO_4 has space group $I4_1/amd$ at all temperatures in which the sample is processed in the parts that follow. At each step of the process described below, indicate the point group symmetry of the polycrystalline BiVO_4 sample.
- What is the point group symmetry of the initial (totally randomly-oriented) BiVO_4 sample? If there is more than one possibility for the limited information given, state the possibilities and explain. (4 Points)
 - The BiVO_4 sample is first exposed to a uniaxial stress (along the Z_3 direction) by being stretched. What is the point group symmetry of the BiVO_4 sample following stretching? If there is more than one possibility for the limited information given, state the possibilities and explain. (4 Points)
 - The BiVO_4 sample is then hot-pressed uniaxially along a direction inclined at an angle of 32° with respect to the stretching axis. What is the point group symmetry of the BiVO_4 sample following this step in the process? If there is more than one possibility for the limited information given, state the possibilities and explain. (4 Points)
 - An electric field is then applied at an angle of 90° with respect to the stretching axis. What is the point group symmetry of the BiVO_4 sample following this step in the process? If there is more than one possibility for the limited information given, state the possibilities and explain. (4 Points)