

- 1.) Your group is examining a crystal yields the following precession photographs:
- | | | | | |
|-------|-------|----|--------------|--|
| photo | $h0l$ | 2 | (C_2) | symmetry, no systematic absences |
| | $h1l$ | 2 | (C_2) | symmetry, no systematic absences |
| | $hk0$ | mm | (C_{2v}) | symmetry, $0k0, k=2n$ |
| | $hk1$ | m | (C_s) | symmetry (\perp to b), no systematic absences |
- a) What symmetry elements are suggested by these photographs? Explain clearly.
b) Suggest the space group for your crystal. Is there any ambiguity?
c) By coincidence, another group has used the same crystal samples and taken photographs with identical indexes and systematic absences. Strangely, this other group has obtained different cell constants! Your a and b values are identical ($a = 8.23, b = 7.86$) but your other values are different ($c = 13.16 \text{ \AA}, \beta = 116.6^\circ$, while they obtain $c = 15.82 \text{ \AA}, \beta = 132.2^\circ$). How is this possible? (Hint: Garnish your explanation with a drawing of the ac-faces of the two settings and their relationship.)
d) Write a transformation matrix which transforms your unit cell to that of the rival group.
e) What is the determinant of the matrix you wrote in d)? What is the significance of this value?
- 2.) Rh_2B crystallizes in space group Pnma with $a = 5.42, b = 2.98, c = 7.44 \text{ \AA}, Z = 4$. Consider the space group diagram for Pnma. Show that if no two Rh atoms may approach within 2.5 \AA of each other, they cannot lie on general positions. Where might the Rh atoms be placed? Illustrate your answer with a sketch showing possible positions for these atoms in projection on (010).
- 3.) Powder diffraction experiments are remarkably similar to x-ray diffraction experiments, using instead a sample which is polycrystalline (enough so that it contains truly random orientation of the constituent microcrystals. While much information is lost due to this random orientation, this remains a powerful technique.
- a) Provide a diagram of the Ewald Sphere construction. What is the purpose of this mathematical construction in a single-crystal x-ray diffraction experiment?
b) In a random polycrystalline sample, the reciprocal lattice (like the real lattice) is oriented randomly. As a result, the single spots that would be present for a single crystal are instead 'smeared out' by these rotations. Instead of spots, what shapes will be produced by the reciprocal lattice of a polycrystalline sample?
c) As a result of your answer in b), what will the intersections of the reciprocal lattice and the Ewald Sphere look like?
d) What information do you think would be available from a powder diffraction pattern, and what information is lost (from a single crystal diffraction experiment)? Explain your reasoning.

(continued on reverse)

4.) A crystal is tetragonal, space group $P4bm$, with $a = 4.00$, $c = 12.00 \text{ \AA}$. Draw diagrams of the $0kl$, $1kl$, $h0l$, and $h1l$ precession photographs. Use the same scale for all four diagrams. Omit reflections or mark those which are forbidden by the space group rules.