

Materials 218/Chem277: Assignment 4

Ram Seshadri (seshadri@mrl.ucsb.edu) Due date: February 12, 2013

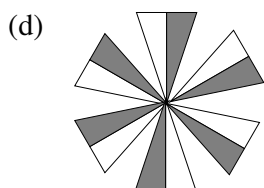
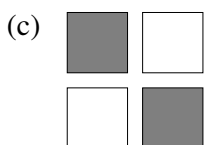
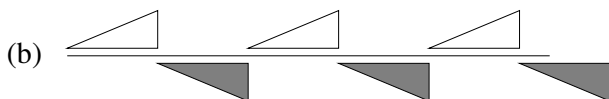
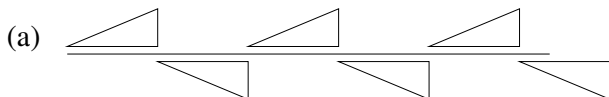
This is a sample midterm exam.

1. The structure of a half-Heusler compound formed from Ti, Co, and Sb is described:
Space group $F4\bar{3}m$ (No. 216) $a = 5.888 \text{ \AA}$.

Atom	Wyckoff Position	x	y	z
Ti	4a	0	0	0
Co	4c	1/4	1/4	1/4
Sb	4b	1/2	1/2	1/2

Note: You should NOT require space group tables.

- What is the formula of the compound ?
 - How many atoms of each kind are there in the unit cell ?
 - Sketch the various sections in the structure.
 - Describe the structure in terms of interpenetrating lattices.
 - How is the structure related to rock salt ?
 - How is the structure related to zinc blende ?
 - What is the coordination of Co in terms of Sb ?
 - What is the coordination of Ti in terms of Sb ?
 - Can you interchange the positions of Ti and Sb without changing the structure ?
 - What would the formula of the compound be for the same atom positions, perhaps different Wyckoff numbers, but in the space group $Fm\bar{3}m$ (the space group of NaCl and CaF_2) ?
2. Sketch the cubic perovskite BaZrO_3 (Ba^{2+} , Zr^{4+} , O^{2-}) with Ba in the corners and Zr in the center of the cube. How many Ba and how many Zr are each O bonded to ? Verify that the rules of electrostatic bond valence are obeyed by considering all bonds coming to oxygen from the cations (remember its Ba^{2+} , Zr^{4+} , and O^{2-}).
3. The questions (a), (b), (c), and (d) correspond to the figures below:



- (a) Identify the line group.
- (b) Identify the line group, including color.
- (c) Identify *all* the mirrors and *all* the rotations (normal symmetry and color symmetry).
- (d) Identify *all* the mirrors and *all* the rotations (normal symmetry and color symmetry).
- (e) Why can't a square lattice be centered (show a sketch) ?
- (f) Can a square lattice with the symmetry $4mm$ support a dipole moment ? [A dipole moment means the centers of positive and negative charges in the unit cell do not coincide].
- (g) What kind of operation (in 2D) is signified by $(0, 0)+$ and $(\frac{1}{2}, \frac{1}{2})+$?
- (h) What kind of operation (in 3D) is signified by $(0, 0, 0)+$; $(0, \frac{1}{2}, \frac{1}{2})+$; $(\frac{1}{2}, 0, \frac{1}{2})+$ and $(\frac{1}{2}, \frac{1}{2}, 0)+$?
- (i) True or false: In 2D systems, 3 and 6-fold symmetries are compatible with glide planes ?
- (j) What new classes of symmetry operations are encountered on going from 1D and 2D, to 3D ? Sketch at least two.