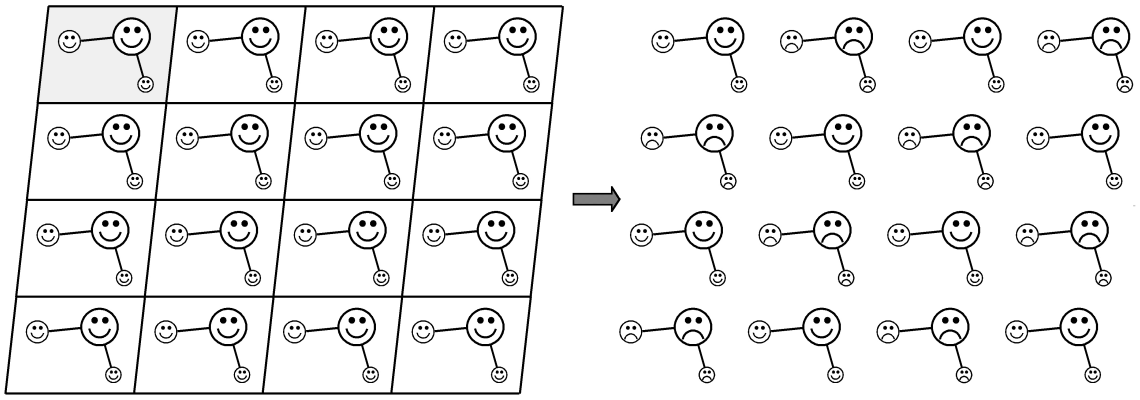
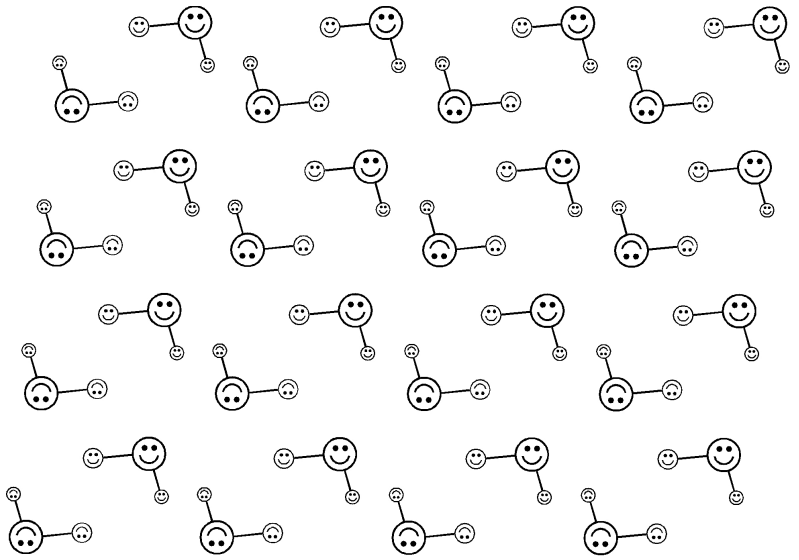
Assignment 1
Due Tuesday, February 6, 2018

(1) Consider a two-dimensional lattice shown below left. One half of the molecules in this lattice have been modified in a regular way so that their atoms now have sad faces, as shown at right. This could be a schematic illustrating the formation of a magnetically ordered structure, where happy and sad faces represent opposite directions of magnetic moments. Suggest the most probable unit cell in this new lattice assuming that the correct unit cell in the original lattice is shown by a shaded parallelogram.



(2) Consider the two-dimensional lattice shown below. Draw the smallest possible unit cell for this 'structure' that uses an angle as close to (but greater than) 90˚. Using the proper symbols, draw all the symmetry operations in (and on the borders of) the cell and assign the correct plane group to the 'structure'. Recall that when possible, the origin of a cell is usually chosen to reside on an inversion center, if any exist.



(3) Consider the following relationships between lattice parameters: $a \neq b \neq c$, $\alpha \neq \beta \neq 90°$ or 120° and $\gamma = 90°$ potentially define a "diclinic" crystal system (two angles ≠ 90°). Is this an eighth crystal system? Explain your answer.

(4) Give an explanation, in your own words, for each of the following (some mathematics may help, but not much is necessary):

(a) The angle (2θ) dependence of atomic X-ray scattering does not affect the condition for constructive interference in diffraction experiments (i.e., it doesn't change the fact that the beam must be diffracted by a reciprocal lattice vector).

(b) X-ray diffraction using radiation from a tube with a molybdenum target can yield more information than diffraction using radiation from a tube with a copper target.

(c) Although the process of diffraction involves a much shorter time scale than IR absorption, it is much easier to study short time scale processes (< 1 μs) with IR spectroscopy than with X-ray diffraction.

(5) There are two ways to identify systematic absences for C-centered orthorhombic lattice. *Clearly show that these two approaches give the same results*.

(a) Find the reciprocal lattice, treating the centered lattice as if it were primitive, i.e.,

$$\mathbf{a} = (a/2)\hat{\mathbf{x}} - (b/2)\hat{\mathbf{y}}$$
$$\mathbf{b} = (a/2)\hat{\mathbf{x}} + (b/2)\hat{\mathbf{y}}$$
$$\mathbf{c} = c\hat{\mathbf{z}}$$

(b) Use a the conventional cell and the structure factor expression, with two atoms per cell:

$\mathbf{a} = a\hat{\mathbf{x}}$

$\mathbf{b} = b\hat{\mathbf{y}}$ atoms at positions: $(0,0,0)$, $(\frac{1}{2},\frac{1}{2},0)$

$\mathbf{c} = c\hat{\mathbf{z}}$

The following table explaining space group symbols will be useful for problems below:

Order of Symbols in the International Symbol

System	1	2	3
Triclinic	Only one symbol used		
Monoclinic	1st setting: c axis unique 2nd setting: b axis unique - generally used		
Orthorhombic	2 or $\bar{2}$ along **a**	2 or $\bar{2}$ along **b**	2 or $\bar{2}$ along **c**
Tetragonal	4 or $\bar{4}$ along **c**	2 or $\bar{2}$ along **a** & **b**	2 or $\bar{2}$ along [110] & [1$\bar{1}$ 0]
Trigonal	3 or $\bar{3}$ along **c**	2 or $\bar{2}$ along **a, b** and [110]	2 or $\bar{2}$ ⊥ to **a, b** and [110]
Hexagonal	6 or $\bar{6}$ along **c**	2 or $\bar{2}$ along **a, b** and [110]	2 or $\bar{2}$ ⊥ to **a, b** and [110]
Cubic	4, $\bar{4}$, 2 or $\bar{2}$ along **a, b,** and **c**	3 or $\bar{3}$ along ⟨111⟩	2 or $\bar{2}$ along ⟨110⟩

(6) Consider the space group *Pnma*.

(a) Derive the condition for systematic absences for each of the glide planes shown in the symbol.

(b) What is the symmetry of the reciprocal lattice in the Hermann-Mauguin notation? (This is called the Laue class; the symmetry conforms to a point group with respect to the origin in reciprocal space.)

(7) Consider the space groups *Amm*2, *Bmm*2, *Cmm*2, *Am*2*m*, *Bm*2*m*, *Cm*2*m*, *A*2*mm*, *B*2*mm*, and *C*2*mm*. How many truly distinct space groups are there in this list? To be "truly distinct", the space group can not be related to another space group by merely relabeling the axes. Identify and list together sets of all the equivalent space groups – those that are really the same as others by such a relabeling.

(8) $2\bar{2}2$, $\bar{3}/m2$, $43\bar{2}$ and are unusual descriptions of the symmetry of three crystallographic point groups. What are the conventional symbols? What do these point groups have in common?

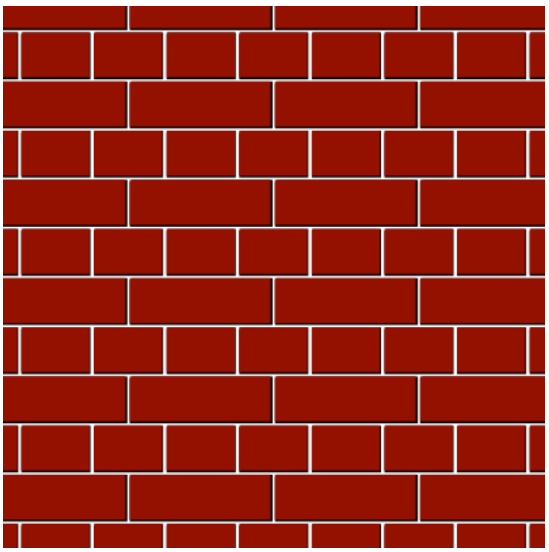
(9) In the patterns on the following page (*a-f*) you will find some of the seventeen 2D plane groups represented. In each case, identify the applicable plane group, and draw a diagram showing the location of at least one of each unique symmetry element for that group.

(10) (a)-(i) Download (or view in a browser) the .mp4 files the 12 crystal structures in the "handouts" part of the class web page. For each case, print out a view of the structure (you will need to do a screen shot) that you can use to identify each of the symmetry elements that appears in the space group. See http://img.chem.ucl.ac.uk/sgp/mainmenu.htm for a list of space groups; this link has nice diagrams as well!

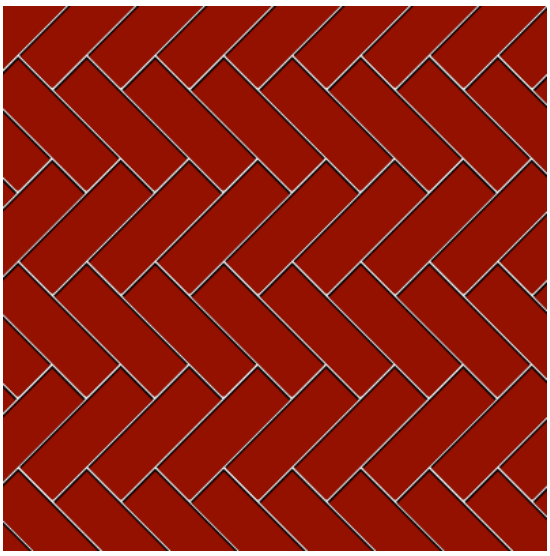
(11)The crystal structure of a material is described in space group symmetry $P\bar{6}2m$ with the following atomic coordinates. The lattice parameters are $a = b = 7.7517$, $c = 3.6262$ Å.

Atom	*x*	*y*	*z*
Fe	0	0	0
Te	1/3	2/3	0.5
Zr1	0.5961	0	0
Zr2	0.2428	0	0.5

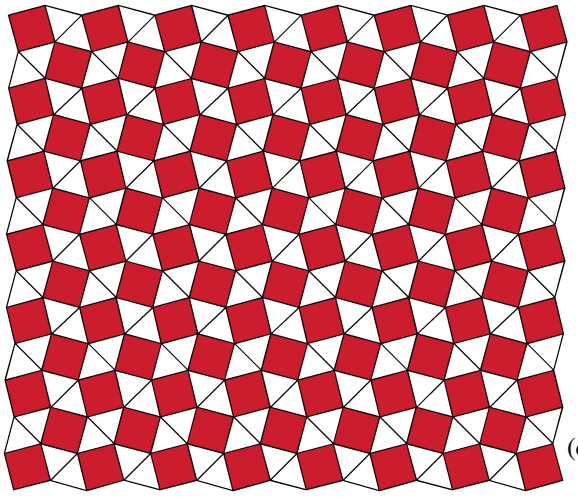
Using the International Tables for Crystallography, describe every atom in terms of the multiplicities and Wyckoff letters of their site positions and establish the content of the unit cell, the simplest chemical formula and the number of formula units (Z) per unit cell. By explicit calculation, determine the nearest Fe–Zr, Fe–Fe, and Zr–Te distances in this compound. Find *all* unique angles, ∠Zr-Fe-Zr, ∠Zr-Te-Zr.



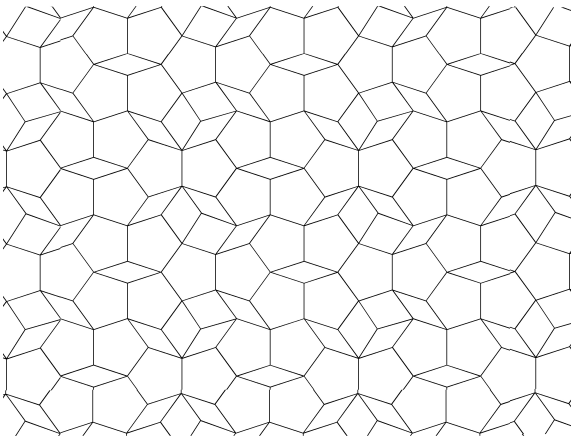
(a)



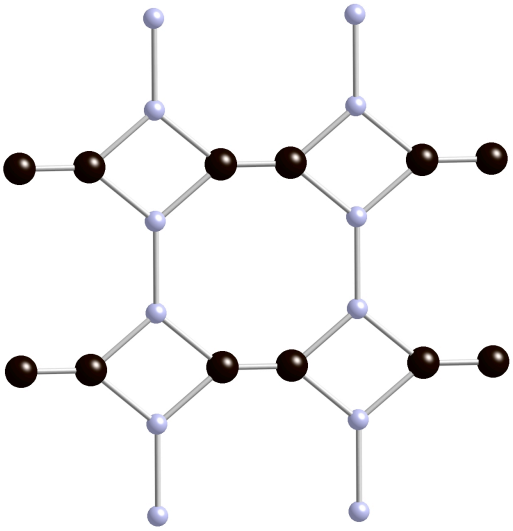
(b)



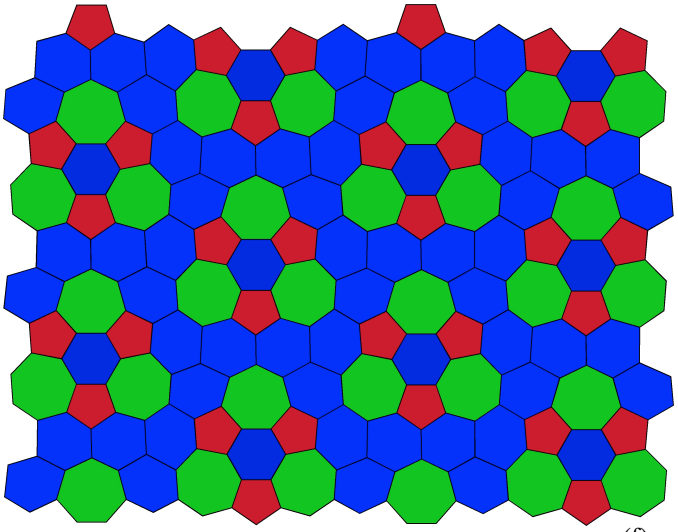
(c)



(d)



(e)



(f)