Chemistry 208—Spring 2008 **Problem Set 2**
Professor K. N. Raymond **Due 02/09/09**

1) You have obtained a beautiful, crystalline sample which is insoluble in most organic solvents. Unfortunately, you have become reckless in your notebook-keeping and do not know for certain the molecular formula of the compound you have isolated. Cursing your oversight, you set out to set right your mistake.

a) You are able to suspend your crystals in a mixture of 65 mL benzene (density = 0.88 g/mL) and 35 mL CH_2Cl_2 (1.33 g/mL). Describe the calculation or experimental procedure that might be used to calculate the density of your crystal.

b) X-ray diffraction on your crystal provides you with lattice constants a, b, and c for your orthorhombic crystal. How can you use this information to calculate the formula weight for your compound? Solve for the formula weight in terms of the lattice constants, experimental density ($\rho_{crystal}$) and any other variables you would need (which you should define explicitly).

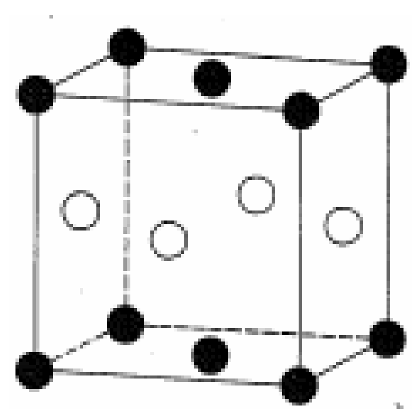
2) Addition of two waves with different phases and amplitudes can be accomplished in two different ways. Consider the two waves, **A** (offset $\phi = 45^o$, amplitude $|F| = 12$) and **B** (offset $\phi = 100^o$, amplitude $|F| = 8$). These waves can be represented as $F(\theta)=\cos(\theta+\phi)$.

a) The simplest solution to this problem involves the addition of two vectors with magnitude $|F|$ and angle ϕ (from the x-axis). Use a vector diagram to generate **A+B** and find ϕ and $|F|$ for the sum.
b) Trigonometric analysis is a more complicated but still satisfying way to solve for the waves sum **A+B**. Differentiation of the function $F(\theta)$ with respect to θ (for the sum of **A** and **B**) will allow you to solve for the phase shift where the amplitude is a maximum (i.e., the wave crest). Use this technique to find the amplitude and phase shift for the wave sum.
c) If the offset of wave **B** is instead 225^o, this same problem becomes completely trivial. Why is this, and what is this phenomenon called?

3) For each of the space groups below identify the unit cell type (triclinic, monoclinic, orthorhombic, tetragonal, trigonal/hexagonal, or cubic), the point symmetry of the crystal and the Laue symmetry of the lattice.

Space group	Unit cell	Point Symmetry	Laue Symmetry
$P2_12_12_1$			
$P2_1/m$			
$P\bar{1}$			
P4nc			
P1			
Pccm			
Amm2			
P31c			
$Fm\bar{3}$			

4) While copper is miscible with gold (most gold is alloyed with Cu or Ni), a separate phase CuAu crystallizes with tetragonal symmetry, reduced from the cubic symmetry of the parent elements. The structure shown is a C centered tetragonal cell. If you look in the International Tables you will find no C centered tetragonal cells, only P and I. Can you propose an alternative cell choice to explain this conundrum? What is the space group? Suggest the atom coordinates for the two elements, including the Wyckoff notation.



5) The volume of the unit cell (in Å^3) is given by the vector equation V = **a**•(**b**x**c**). [For an explanation of the math see: http://en.wikipedia.org/wiki/Cross_product] Use the vector definitions of **a***, etc. to prove that a similar equation (replace V by V*, **a** by **a***, etc.) gives the volume of the reciprocal cell in Å^{-3}.

a) Show that V* = 1/V.

b) In the cell of problem 4 what does **b**x**c** represent**?**