Chemistry 208—Spring 2008 **Problem Set 6**
Professor K. N. Raymond **Due 3/17/2008**

1) For the conversion of raw data into structure factors and their standard deviations:

What are the units of F_o^2? (i.e. the observed, unscaled structure factor intensity)

What are the units of $F_{(hkl)}^2$? (i.e. the calculated structure factor, unscaled)

What are the units of the unscaled F_c^2?

How do we scale our observations into what we need?

What are the units of the standard deviation of F_o^2?

What are the units of the variance of F_o^2?

Why do we add variances and not standard deviations?

Why is there a difference in the dependence of the ratio (r) of time (or pixels) for raw count collection (P) versus background (B) when calculating I versus σ(I)?
[e.g. if I = P –rB what is the dependence of σ(I) on r?]

What is the relative size of I versus σ(I) typical of X-ray structures?

2) Note that for the general expression for the structure factor of a reflection,

$$F_{hkl} = \sum_{j=1}^{N} f_j e^{2\pi i(hx_j + ky_j + lz_j)}$$

We can equally well write $F_{h\,k\,l} = A + i\,B$.
For the space groups:
a) Cc
b) $P2_12_12_1$
c) Pnma
Write the simplified forms of A and B by suitably combining those terms involving atom positions related by symmetry.

i) Does this simplified form of the structure factor predict any systematic absences?

ii) Which reflections are of equal intensity? [Note that the problem applies equally well when we consider the integral equation for $F_{h\,k\,l}$ in terms of the continuous electron-density function ρ(x, y, z).]

iii) Is your answer to ii) consistent with the Laue symmetry of the space group?