Problem sets 4

1. Fluorite (CaF_2) is face-centered cubic a=5.45Å , with 4 CaF_2 per unit cell at Ca 000; F 1/4 1/4 1/4, 3/4 3/4 3/4, and other positions given by the face-centering translations. (Warren 3.7)
   (a) Derive simplified expressions for the structure factor F.
   (b) From the tables evaluates F^2 for the reflections 111 and 222.

2. Cu_3Au is cubic with 1 unit of Cu_3Au per unit cell. In the ordered form the positions are Au at (000)and Cu at (1/2,/1/2,0), (1/2, 0, ½), (0, ½ , ½). In the disordered form the same positions are occupied at random; consider this to be statistically equivalent to 1/4 Au and 3/4 Cu at each position. (Warren 3.10)
   (a) Derive simplified expressions for F for the ordered form.
   (b) Derive simplified expressions for F for the disordered from
   (c) For what reflections will F be the same in the two forms, and for what reflections will they differ?

3. Graphite is hexagonal with 4 atoms per cell in the positions 000; 1/3 2/3 0; 0 0 1/2; 2/3 1/3 1/2.
   (a) Show that the structure factor is given by,

$$l = even, \quad F = 4f \cos^2 \pi(h+2k)/3$$
$$l = odd, \quad F = 2if \sin 2\pi(h+2k)/3$$

   (b) For what combinations of hkl will the structure factor vanish? (Warren 3.8)