**1. Consider the compound CaF2, which has the Ca atoms face centered and the F atoms form a simple cube within the Ca fcc cube. It has atoms described by the following positions (see picture of the conventional cell):**

**Ca: four atoms, one at 0,0,0; one at ½, ½, 0; one at ½, 0, ½; one at 0, ½, ½**

**F: eight atoms at: 1/4, 1/4, 1/4 ; 3/4, 1/4, 1/4 ; 1/4, 3/4, 1/4; 3/4, 3/4, 1/4;**

**1/4, 1/4, 3/4; 3/4, 1/4, 3/4; 1/4, 3/4, 3/4; 3/4, 3/4, 3/4**

**i. e. each F atom has four Ca atoms tetrahedrally associated with it. CaF2 has a cube edge of 5.462 Å**

**Figure 1: conventional cell, large (white gray) spheres are the F, smaller (yellow) spheres are Ca.**

**a.) (2 pts) what is the physical mass density, units of g/cm3, of CaF2, if the molar mass of Ca is 40.078 g and of F 18.998 g?**

**in one unit cell, vol=a3=162.95 Å3**

**in this cell are 4 Ca atoms (=1/8 \* 8 for the cube corners and 6x1/2 for the 6 faces) plus 8 F atoms. The masses are 4 \*(40.078 g/mole)/6.022x1023 atoms/mole and 8\*18.998 gmole/6.022 1023 atoms/mole = (26.62+25.24)x10-23 g/162.95 10-24 cm3=3.18 g/cm3**

**b.) (2 pts) Using fCa and fF for the atomic form factors of Ca and F respectively, write down the structure factor, SG, using the 12 atom positions given above for the basis,**

**SG = Σj fj exp(-i2π[ hxj + kyj + lzj ]) where the sum is over j=1 to 12 for the basis atoms and the positions of the basis atoms are**

**rj =** x**ja1 +** y**ja2 +** z**ja3 and the ai are the conventional cell vectors.**

**SG=fCa(1 + exp(-iπ(h+k)) + exp(-iπ(h+l)) + exp(-iπ(k+l))) + fF(exp(-πi(h + k + l)/2) + exp(-πi(3h + k + l)/2) + exp(-πi(h + 3k + l)/2) + exp(-πi(3h + 3k + l)/2) + exp(-πi(h + k + 3l)/2) + exp(-πi(3h + k + 3l)/2) + exp(-πi(h + 3k + 3l)/2) + exp(-πi(3h + 3k + 3l)/2))**

**c.) 4 pts What is the structure factor for the following (hkl) values:**

**(hkl) = (100), (001), (110), (103), (112), (200), (210) ? (please convert to numbers, rather than leaving it as, for example, an answer that contains exp(iπ) (which is -1) or exp(-i2π/3) which is -0.5 -i√3/2. So, if the answer should be 0, and you have the sum of a bunch of exponentials that would add to zero if you did the conversions, you don't get credit.)**

**plug these hkl into answer to b. and look for a pattern**

**100 gives fCa(1-1-1+1) + fF(-i+i-i+i-i+i-i+i) = 0**

**001 gives fCa(1+1-1-1) + fF(-i-i-i-i+i+i+i+i) = 0**

**110 gives fCa(1+1-1-1) + fF(-1+1+1-1-1+1+1-1)=0**

**103 gives fCa(1-1+1-1) + fSi(1-1+1-1-1+1-1+1)=0**

**112 gives fCa(1+1-1-1) + fF(+1-1-1+1+1-1-1+1)=0**

**200 give fCa(1+1+1+1) + fF(-1-1-1-1-1-1-1-1)=4fCa -8fF, so this is finite when S\*S is calculated, and of course fCa ≠ fF**

**210 gives fCa(1-1+1-1) + fF(i+i-i-i+i+i-i-i) = 0**

**d.) 2 pts For full credit, can you see a pattern? For which general rule of (hkl) is SG finite or zero?**

**Clearly, 400, 600 etc. are finite.**