**CEM 913 SPRING 2002**

**Course in X-ray crystallography**

**Homework 4, 100 points**

**Due by March 14**

1 LiF is cubic with a = 4·026 Å. A crystal of LiF is mounted on a simple single crystal diffractometer with the [001] axis parallel to the axis of rotation and perpendicular to the plane defined by the incident X-ray beam and the axis of the detector. Initially the (100) face of the crystal is perpendicular to the incident beam. Through what angle must the crystal be rotated from this position to enable to the 420 reflection to be observed with CuKα radiation (λ = 1.5418 Å)? At what angle will the detector then be inclined to the forward direction of the incident X-ray beam? (30 points)

2 A material wih the empirical formula $KAg_3As_2S_5$ crystallizes in the orthorhombic space group *Pnma* with a=19.21 Å, b=16.867 Å, c=6.349 Å and a unit cell volume of 2057.2 $Å^3$. Its density was measured to be 4.34 $g/cm^3$.

(a) Calculate Z (i.e. how many times does this empirical formula fit into the unit cell).

(b) Calculate how many reflections exist inside the Ewald sphere using (I) CuKα radiation for which λ = 1.5418 Å, and (ii) MoKα radiation for which λ = 0.7071 Å.

(c) Up to what 2θ angle must one go for data collection for each type of radiation in order to measure *hkl* reflections with d spacing of 0.7 Å?

(d) List all the equivalent space groups which arise when the a-, b- and c-crystallographic axes in the cell of $KAg_3As_2S_5$ above are chosen in different ways, the axial system being right handed.

(40 points)

3 Using moving-film methods, the reciprocal lattice of a triclinic crystal was found to have the following unit-cell constants: $a^* = 0.176\ Å^{-1}$, $b^* = 0.213\ Å^{-1}$, $c^* = 0.268\ Å^{-1}$, $a^* = 89.5°$, $\beta^* = 49.0°$, and $\gamma^* = 90.0°$. What are the corresponding unit-cell constants of the crystal lattice? (30 points)