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SCHOOL OF PHYSICS AND ASTRONOMY

Structure and Properties of Functional Materials

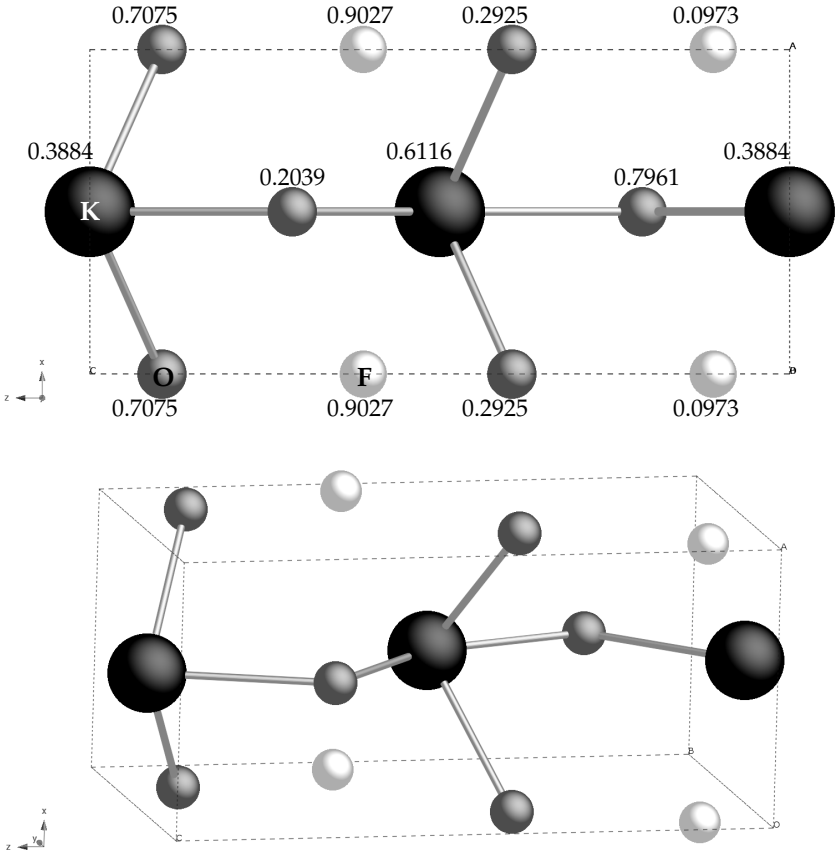
Exercise Set 3

Friday, 25 January, 2013

1. (a) Draw sphere diagrams for the point groups $2/m$ and $mm2$. Hence show that each group has four members.

   (b) For the four elements of each group, write down the symbol (using International notation, as we've learnt in class) for the symmetry element and the position to which it would map a general point (x, y, z).

2. Anhydrous potassium fluoride has the sodium chloride structure, but this compound also forms crystals containing water molecules hydrogen-bonded into the ionic structure. The structure of potassium fluoride dihydrate is shown below, first in projection onto the xz plane with y coordinates indicated, then in 3D perspective. K atoms are shown in black, O in grey, and F in white; H atoms, for clarity, are not shown (they lie along the O−K bonds).



Find the three symmetry elements (other than the identity) of this structure, and hence identify its space group. What point group will the diffraction pattern of this compound have?

3. (a) Prove that, if a structure contains a *c*-glide plane perpendicular to the x axis, the $(0kl)$ diffraction peaks will have nonzero intensity only if l is even.

   (b) Prove that, for a face-centred cubic structure, the structure factor $F(hkl)$ is zero unless h, k, and l are either all odd or all even.

   (c) Diffraction of Mo $K\alpha$ radiation ($\lambda = 0.709\,26$ Å) from a crystalline sample of nickel gave diffraction peaks at $2\theta = 20.0760°$, $23.2220°$, $33.0738°$, $38.9945°$, and $40.8037°$. Bearing in mind your result from the previous part, show that nickel metal has a face-centred cubic structure, determine the (hkl) index of each peak, and calculate the lattice parameter a of nickel.