3.60 Symmetry, Structure and Tensor Properties of Materials

Problem Set 9

The following problems are intended to give a few examples of how space group properties may be used to obtain information about the structure and behavior of crystals.

(1) Sodium chloride, NaCl, has a density of 2.16 gr/cm^3. X-ray diffraction reveals that crystals are cubic, with space group Fm3m and a lattice constant equal to 5.640 Å.

  (a) How many atoms are contained within a unit cell?

  (b) Which equipoints must be occupied in the space group?

  (c) Sketch the arrangement of Na and Cl ions in a unit cell.

(If you get this much correct, you may award yourself the 1915 Nobel Prize for Physics.)

(2) A molecular crystal has space group P4/mnc. An organic chemist decides, on chemical grounds, that three possible configurations seem likely for the structure of the molecules which are packed to build this crystal.

Computation of the unit cell contents from the density of the crystal and its lattice constants (as in the preceding problem) reveals that four molecules are contained within the cell.

Using the properties of the space group and the type of position which must be occupied by the molecule, decide which of the three structures sketched below might be correct. Can you say anything about the orientation of the molecule within the cell? [Hint: The arrangement of atoms in the space around a special position must conform to the point group of that special position.]
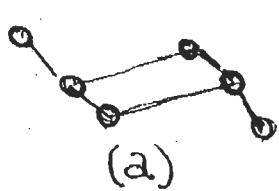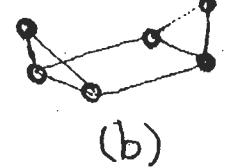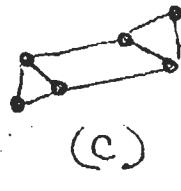
(a)   (b)   (c)
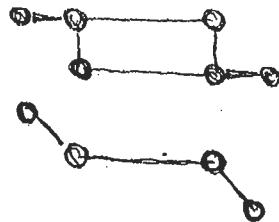
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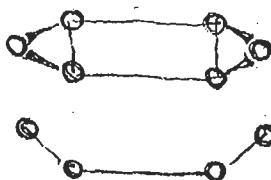
SIDE VIEWS

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