Question A2, 1998:

Explain carefully the meaning of the terms *rotation axis of symmetry*, *mirror plane* and *center of symmetry*. Draw a plan on (001) of cubic $BaTiO_3$ (perovskite structure) showing a 2x2 block of unit cells with a common vertical edge. Add to one unit cell of the plan the traces of the mirror planes containing [001]. Identify the rotation axes parallel to [001] that pass through $\frac{1}{2}\frac{1}{2}0$ and $\frac{1}{2}00$. Write down the coordinates of the centres of symmetry.

The properties *pyroelectricity*, *piezoelectricity* and *ferroelectricity* all involve the production of a dipole moment. Explain carefully the difference between these properties and discuss how a knowledge of the symmetry elements shown by a crystalline compound will indicate whether or not that compound may display one of these properties.

Above 120 ^{o}C, $BaTiO_3$ is cubic with $a = 3.906\mathring{A}$. At 120 ^{o}C, it undergoes a displacive transition to a tetragonal phase with $a = 3.994\mathring{A}$ and $c = 4.033\mathring{A}$. In what direction is the Ti^{4+} ion displaced in the tetragonal form. Indicate how the symmetry elements of the tetragonal cell are related to those of the cubic cell.

Assuming that the ions are fully ionised, estimate the net polarisation per unit volume of the tetragonal phase, given that the displacements of the ions, relative to the O^{2-} ions with the same z coordinate as the Ti^{4+} ion in the cubic phase, are as follows:
Ti^{4+}: $+11 \times 10^{-12}$ m; Ba^{2+}: $+6 \times 10^{-12}$ m; O^{2-}: -3×10^{-12} m;