# Structure and Properties of Functional Materials

## Homework Set 3

*Due Wednesday, 30 January, 2013 by 4 p.m.*

**Problem 1: Terms and definitions** (8 marks)

Explain the following terms or concepts, giving an example of their significance in condensed matter physics:
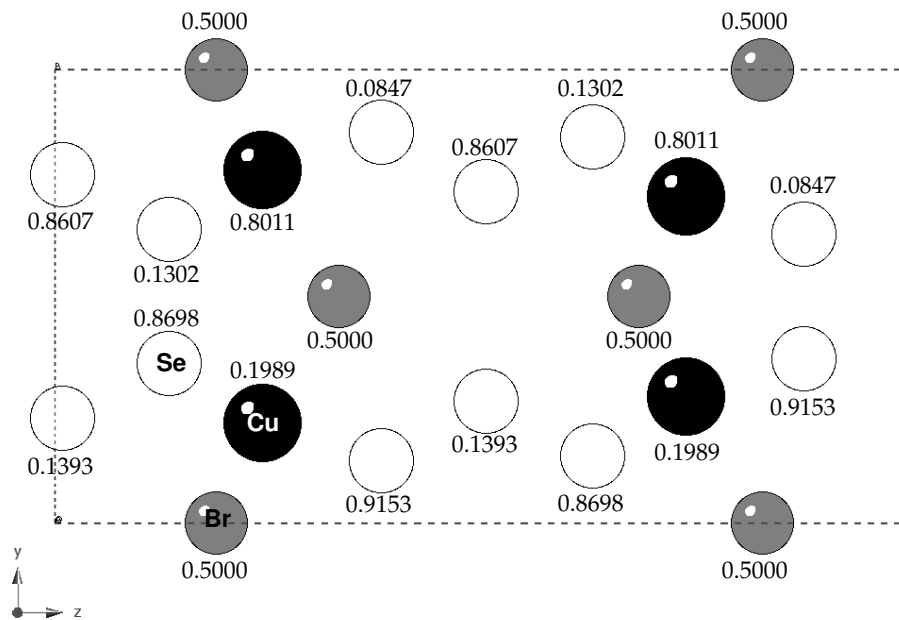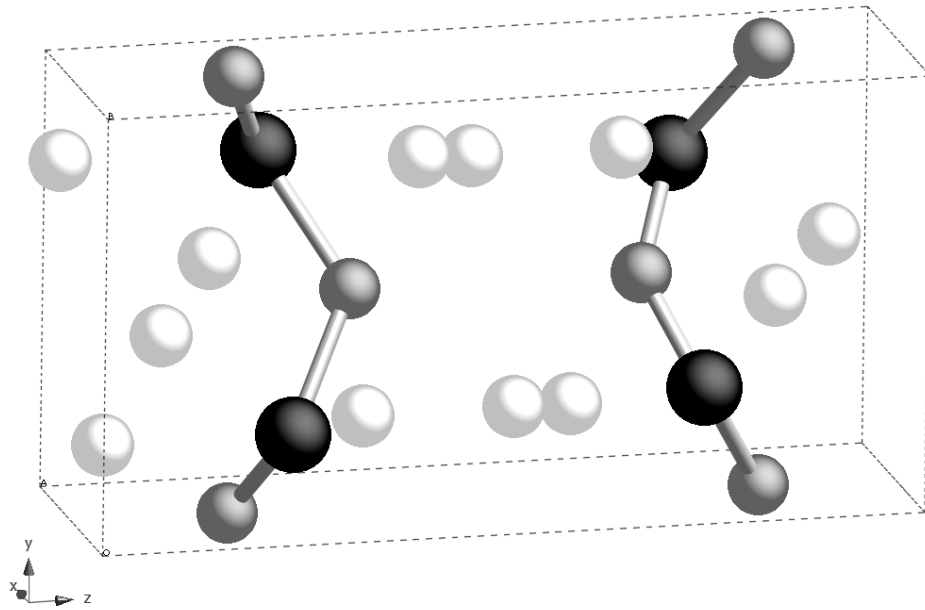
(a) Laue class (4)

(b) Systematic absence (4)

**Problem 2: Symmetry in real space** (13 marks)

The structure of $CuBrSe_3$ has been reported from X-ray powder diffraction data (Sakuma *et al.*, *J. Phys. Soc. Jpn.* **60** (1991), 1608–1611) and is shown below, first in projection onto the *yz* plane with *x* coordinates indicated, then in 3D perspective. Cu atoms are shown in black, Br in grey, and Se in white.

(a) Find the three symmetry elements (other than the identity) of this structure, and give their symbol and location (*e.g.*, "*m* at $(x, \frac{1}{2}, y)$"). (Hint: one way of approaching this is to choose any one of the four Cu atoms; the three symmetry operations will transform it into the three others.) (9)

(b) Hence identify this compound's space group. (2)

(c) What point group will the diffraction pattern of this compound have? (2)

**Problem 3: Symmetry in reciprocal space** (9 marks)
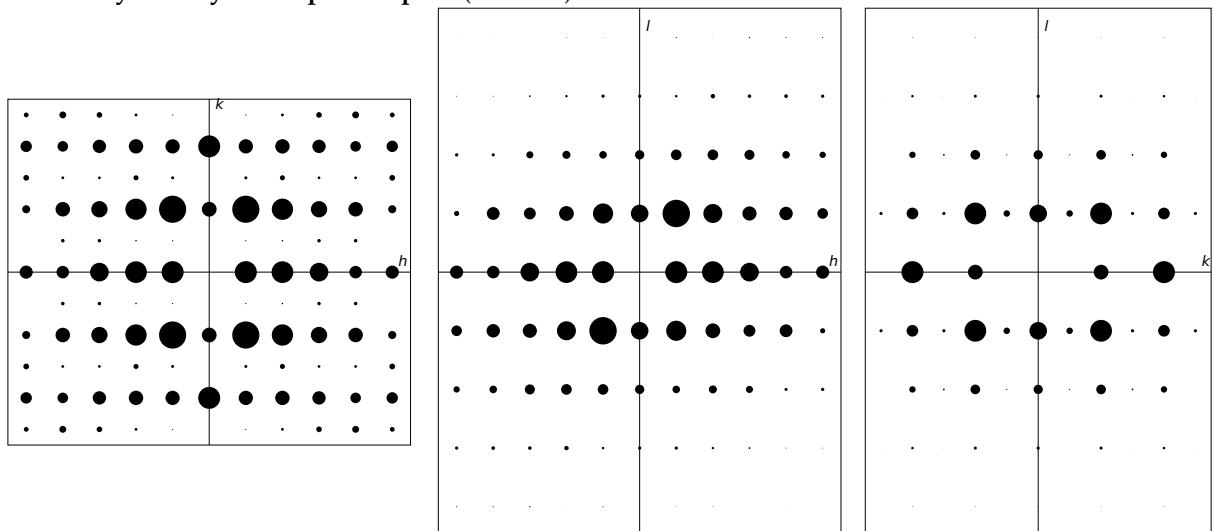


Shown above are the $(hk0)$, $(h0l)$ and $(0kl)$ planes of the diffraction pattern of silver cyanate, AgNCO.

(a) What is the Laue class of this crystal (*i.e.*, the point group of its diffraction pattern)? (Warning: look carefully to see whether symmetry elements you identify are really present!) (2)

(b) Given that the crystal is known to be centrosymmetric, determine its point group. (2)

(c) Write down the reflection conditions needed to account for all systematic absences in the diffraction pattern, and hence determine the space group. (5)