

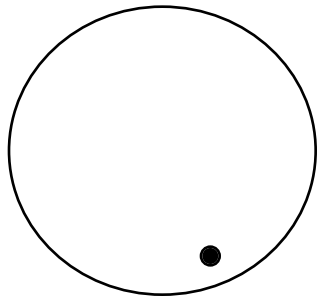
**Question #1 (25 points)**

**1.a)** Consider the molecule of benzene ( $C_6H_6$ ) a planar cyclic molecule, where the carbon atoms form a perfect hexagon (each carbon is hybridized  $sp^2$  and each hydrogen is therefore in the same plane as all the carbon atoms).

Determine **all** the symmetry elements that this molecule possesses. (please, show using a sketch where the symmetry elements are). **(6 points)**

**1.b)** A tetragonal crystal is defined by the point group  $4/m\bar{m}2$ . Assuming that the 4-fold axis is normal to the surface of the paper, locate the points that are obtained when the symmetry operations of that point group are applied to the point shown on the drawing. Indicate how you transform one point into another. (Use empty circles for points below the planes and filled circles for points above the plane, if necessary).

**(7 points)**

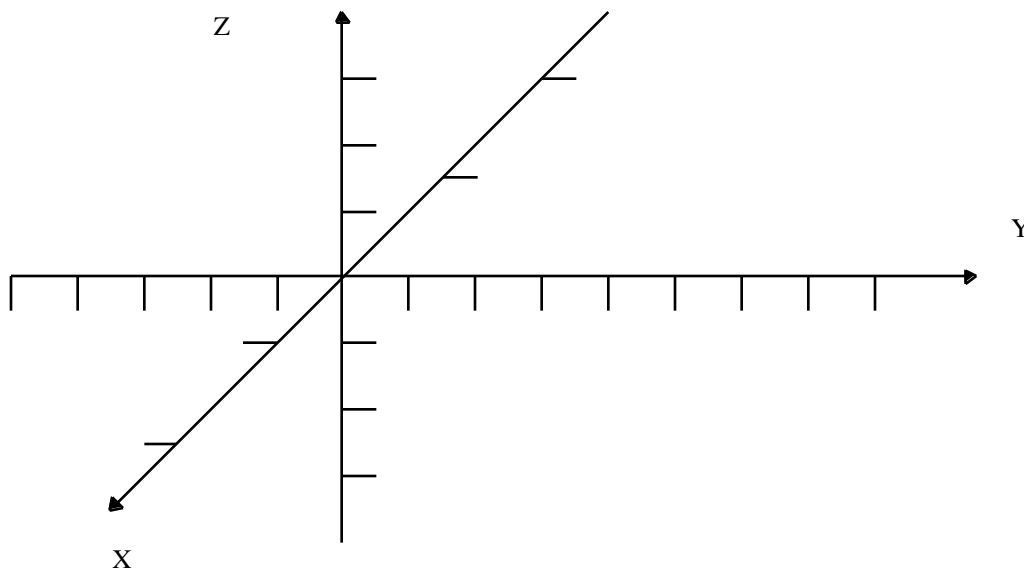


**1.c)** Indicate, for the point group discussed above, all the other symmetry operations (these which were not directly mentioned in  $4/m\bar{m}2$  but which are implicit). **(6 points)**

**1.d)** If you are told a crystal has the structure  $I4_1/acd$ . What can you say about this crystal and its symmetry elements (just explain what these symbols mean). **(6 points)**

**Question #2 (25 points, 5 points each)**

**2.a)** On the following set of axes, draw the  $(1\bar{3}2)$  plane. Draw the  $[1\bar{3}2]$  direction. The tick marks in each direction represent the unit cell dimension in that direction.



**2.b)** Assuming that the basis vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  of a crystal lattice are defined in a cartesian coordinate system by  $\mathbf{a} = (1, 0.5, 0)$ ,  $\mathbf{b} = (0.5, -1, 0)$ ,  $\mathbf{c} = (0.5, 0.5, 2)$ . Calculate the volume of the unit cell.

**2.c)** Determine the reciprocal lattice vectors  $\mathbf{a}^*$ ,  $\mathbf{b}^*$ ,  $\mathbf{c}^*$  associated with the direct lattice vectors  $\mathbf{a}$ ,  $\mathbf{b}$ ,  $\mathbf{c}$  (defined in 2.b)

**2.d)** What is the distance between planes having Miller indices (222) ? (defined in terms of lattice vectors given in 2.b)

**2.e)** What is the angle between the direction of the normal to the (222) plane and the direction given by [222] ?

**Question #3 (25 points)**

**3.a)** Tobacco seed globulin forms face centered cubic crystals with a unit cell dimension of 12.3 nm and a density of  $1.287 \text{ g.cm}^{-3}$ . Determine the molar mass of Tobacco seed globulin. **(5 points)**

**3.b)** The coordinates in units of  $\mathbf{a}$ , of the A atoms with scattering factors  $f_A$  in a cubic lattice are (0,0,0), (1,0,0), (0,1,0), (0,0,1) (0,1,1) (1,0,1) (1,1,0) and (1,1,1). There is also a B atom with scattering factor  $f_B$  at (1/2, 1/2, 1/2). Calculate the structure factor  $F_{hkl}$  for a general plane of Miller indices (hkl). **(5 points)**

**3.c)** Determine the form of the polycrystalline or powder diffraction pattern (i.e. which planes actually diffract) when:

**A)**  $f_A = f$  and  $f_B = 0$  (**5 points**)

**B)**  $f_B = 0.5 f_A$  (**5 points**)

**C)**  $f_A = f_B = f$  (**5 points**)

**Question #4. (25 points, 5 points each)**

In a given crystal, the following Burgers vectors of two distinct dislocations have been identified as :

$$\frac{a}{2} [111] \text{ and } \frac{a}{2} [\bar{1} \bar{1} 1]$$

- a) Which Bravais lattice would you expect this crystal to belong to and why ?
- b) Assuming that these two dislocations have the same slip plane, what is the slip plane ?
- c) If these two dislocations combine with one another, what is the resulting Burgers vector ?
- d) Is the energy of the resulting dislocation lower or higher than the total energy of the two separate dislocations ?

- e)      A) What are the main differences between screw and edge dislocations ?
- B) Is the following statement correct and Why ? In a single component “pure” crystal there are always more interstitials than vacancies and both can be annealed away at high temperature.