

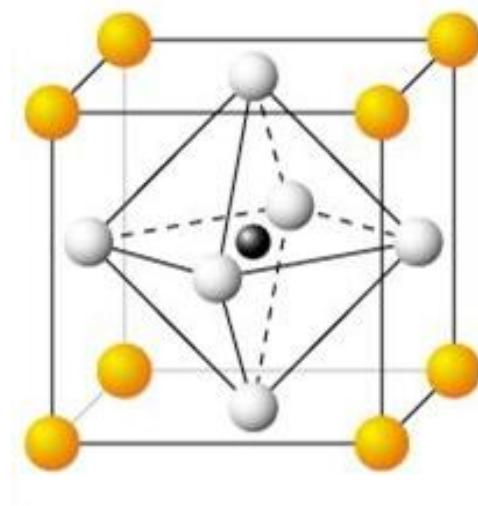
## Question 1

- (i) A crystal lattice has a square top and an elongated body. The angles between all sides are  $90^\circ$ . What is the shape of the unit cell?
- (ii) Which flavours (primitive, body centered, face centered, base centered) are seen in monoclinic cells?
- (iii) Which is the only unit cell type to show all four flavours?
- (iv) A unit cell has all sides of equal length and all angles equal but not  $90^\circ$ . What is the shape of this unit cell?
- (v) A crystal structure consists of planes of spheres stacked tightly together with stacking order ABABAB... What type of crystal structure is this?
- (vi) Which of the Bravais lattices is most commonly observed in nature?

## Question 2

The diagram below shows the unit cell for the crystal structure of  $\text{BaTiO}_3$ . This structure is called a perovskite. Barium (in orange) sits at the corners, titanium (black) sits in the very centre, and oxygen in the centre of each face. The lattice parameter is 0.3996nm

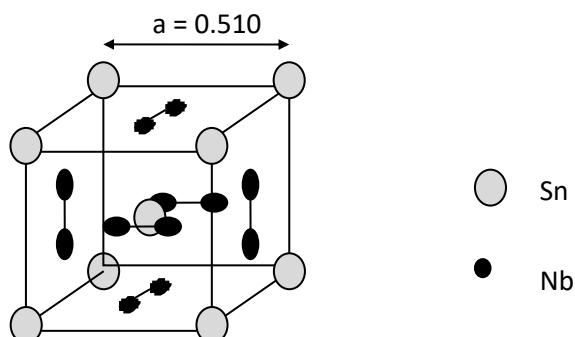
- (i) what is the shape of the unit cell?
- (ii) is it primitive, base-, body-, or face-centered?
- (iii) what is the bravais lattice type for this structure?
- (iv) how many atoms each of Ba, Ti, and O are there per unit cell?
- (v) What is the distance between the barium ions and the surrounding oxygen ions?
- (vi) Can you see any symmetries in this crystal structure?



### Question 3

The diagram below shows the unit cell for the crystal structure of  $\text{Nb}_3\text{Sn}$  (incidentally, still the most widely used superconducting material). Sn atoms are at the corners of the unit cell and there is also an Sn atom in the very center of the unit cell. Pairs of Nb atoms are in the center of each face of the unit cell.

- (i) what is the shape of the unit cell?
- (ii) is it primitive, base-, body-, or face-centered?
- (iii) what is the bravais lattice type for this structure?
- (iv) how many atoms of Sn and how many of Nb are there per unit cell?
- (v) show the (100) plane of the unit cell and draw a picture of the arrangement of atoms on this plane.
- (vi) if the atomic weight of Nb is 92.91g/mol and the atomic weight of Sn is 118.69g/mol, calculate the theoretical density of this material. [10,024kg/m<sup>3</sup>]



$$[\text{mass of proton} = 1.6606 \times 10^{-27} \text{kg}]$$

### Question 4

The diagram below shows the crystal structure of cristobalite, a common phase of silica.

- (i) what are the positions of the atoms labelled one and two?
- (ii) calculate the distance in nanometres between them. [0.171nm]
- (iii) in what direction is the line from atom 1 to atom 2?
- (iv) if the crystal is cleaved so that the (110) plane is on the surface, draw a diagram to show what this surface will look like.
- (v) what is the shape of the unit cell?
- (vi) is it simple, body centered, base centered, or face centered?
- (vii) how many atoms of silicon and of oxygen are there per unit cell?
- (viii) what is the packing fraction of this structure given  $\text{RSi}_4^+ = 0.039 \text{ nm}$  and  $\text{RO}_4^- = 0.132 \text{ nm}$ . [31.7%]
- (ix) given the atomic weights,  $M_{\text{Si}} = 28.09 \text{ g/mol}$  and  $M_{\text{O}} = 16.00 \text{ g/mol}$ , calculate the density of this crystal. [1630kg/m<sup>3</sup>]

790 nm )

