The cuprite, a copper oxide, has the structure shown in the figure, where oxygen and copper atoms are indicated by the small dark and larger gray circles, respectively.

1. Which is the chemical formula of the compound?

2. Which is the crystalline lattice formed by the oxygen atoms? and the one formed by the copper atoms? Which is the Bravais lattice of the compound?

3. Is the cubic cell shown in the figure the primitive one? How many atoms are in the primitive cell? Write the primitive vectors and the basis.
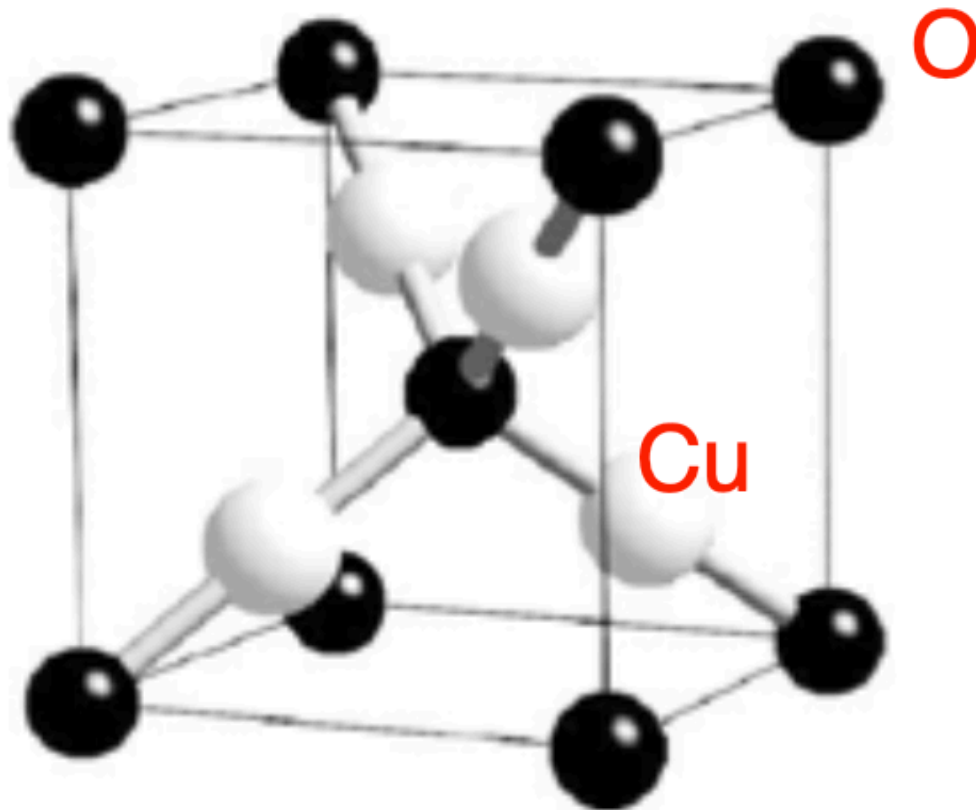
4. What are the coordinates of the largest interstitial hole in this structure? (Hint: where should we put an extra atom if we were looking for the most room?) How many of these sites are there per unit cell?
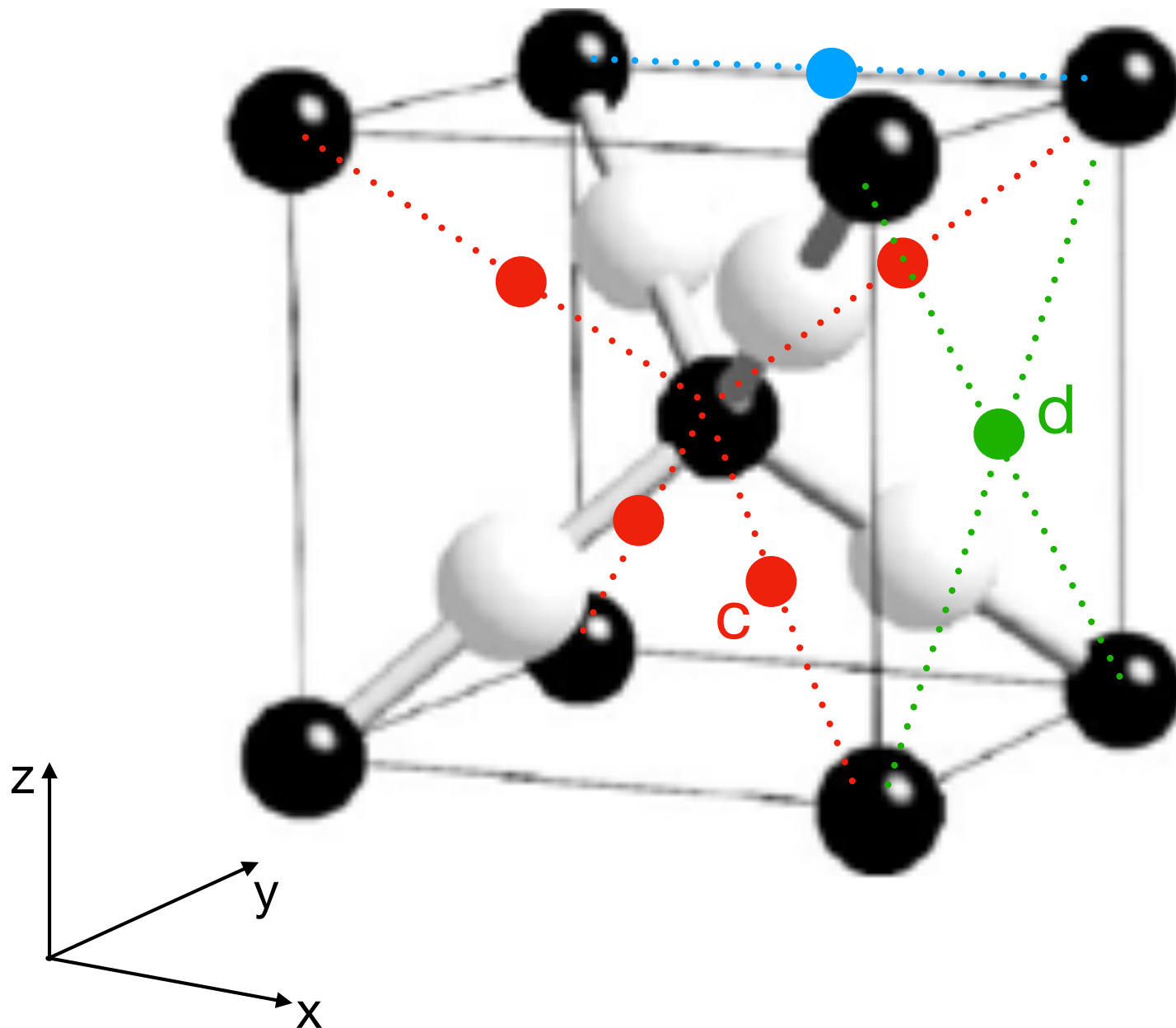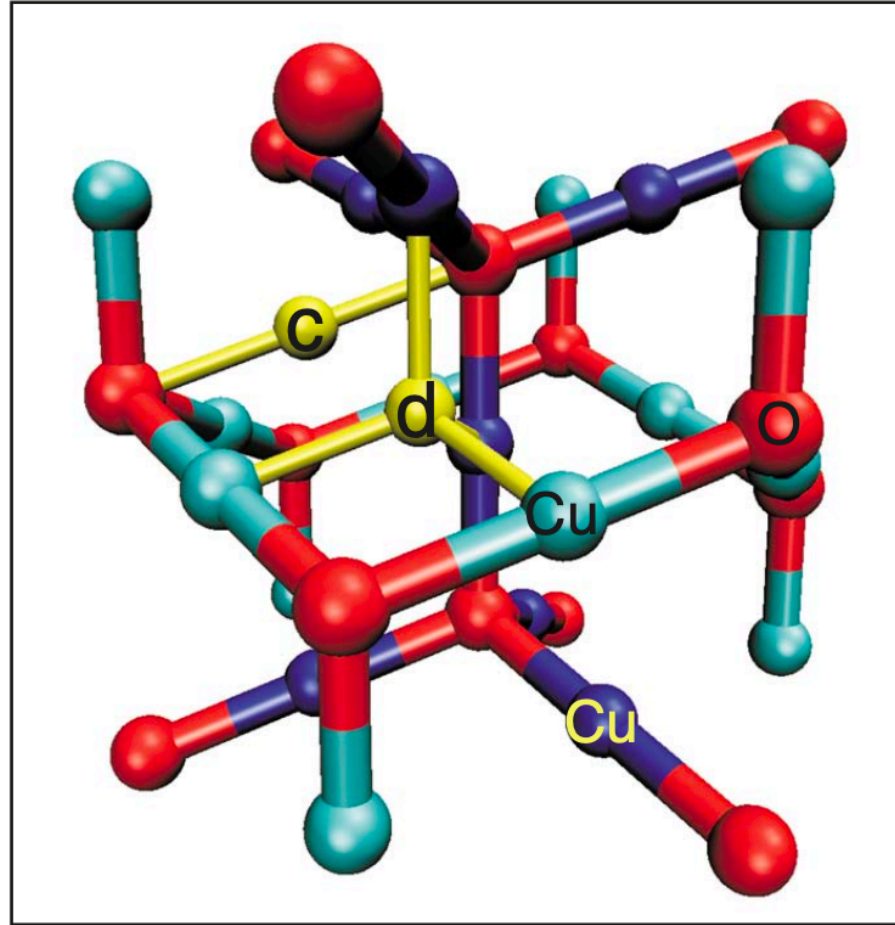
FIG. 1. (Color online) The cuprite structure of Cu_2O and possible interstitial positions. Cu and O atoms are given as blue and red spheres, respectively. The cuprite structure consists of two interpenetrating cristobalite lattices that are distinguished by using two different shades for Cu atoms in each of the lattices. Interstitial atoms are labeled "c" and "d" (yellow spheres) according to their Wyckoff positions (symmetries D_{3d} and D_{2d}, respectively).
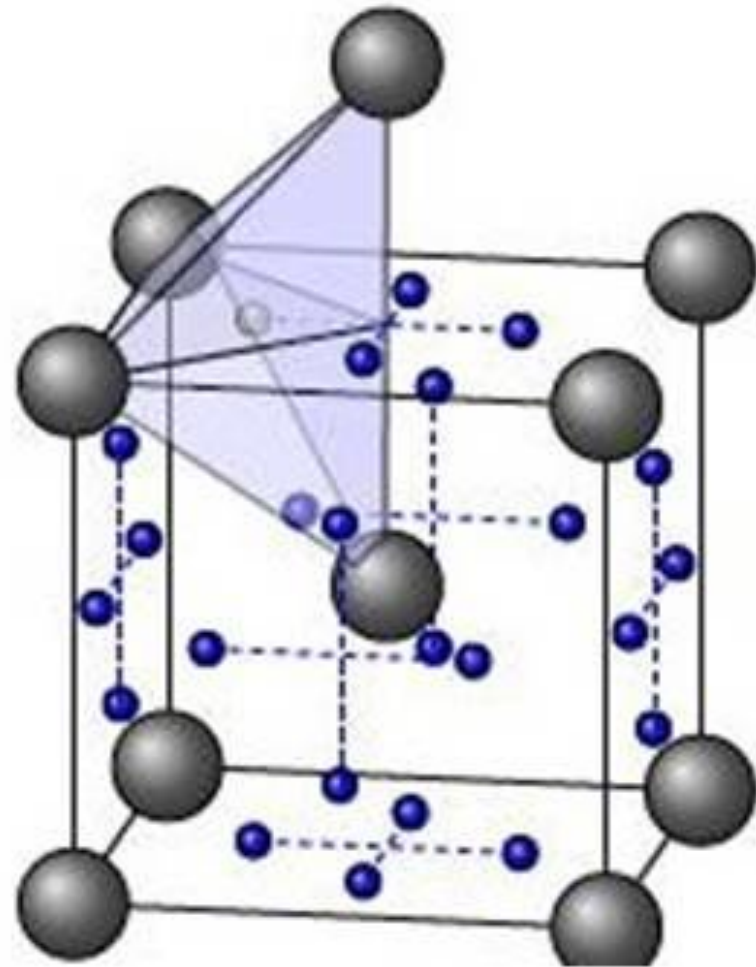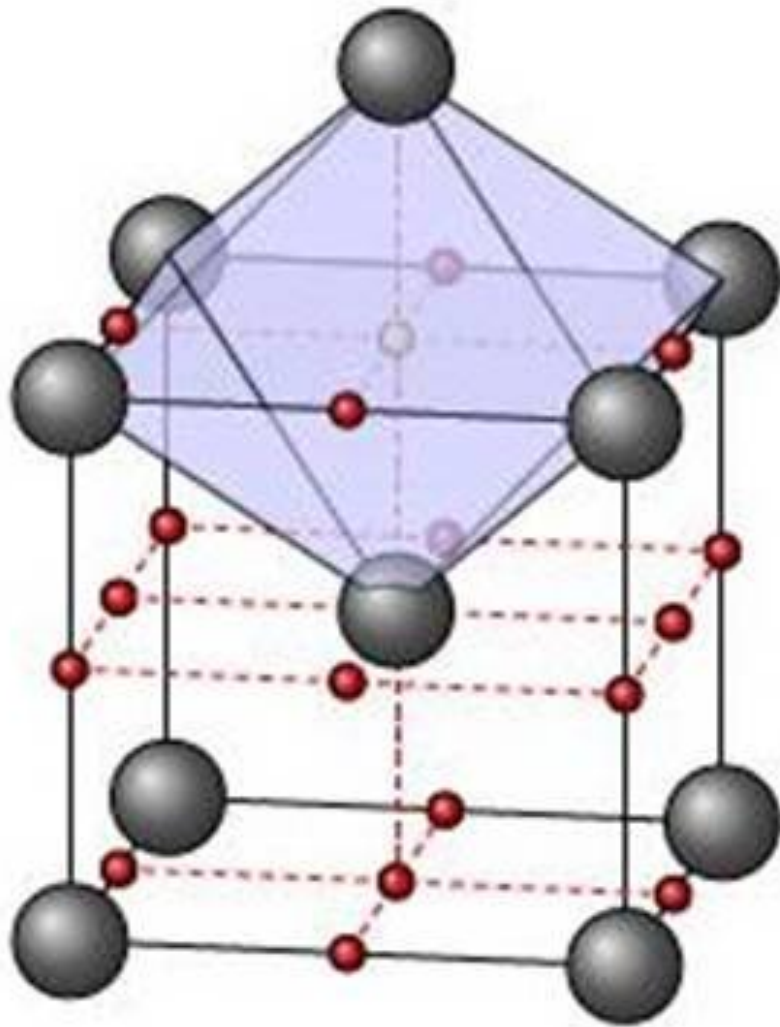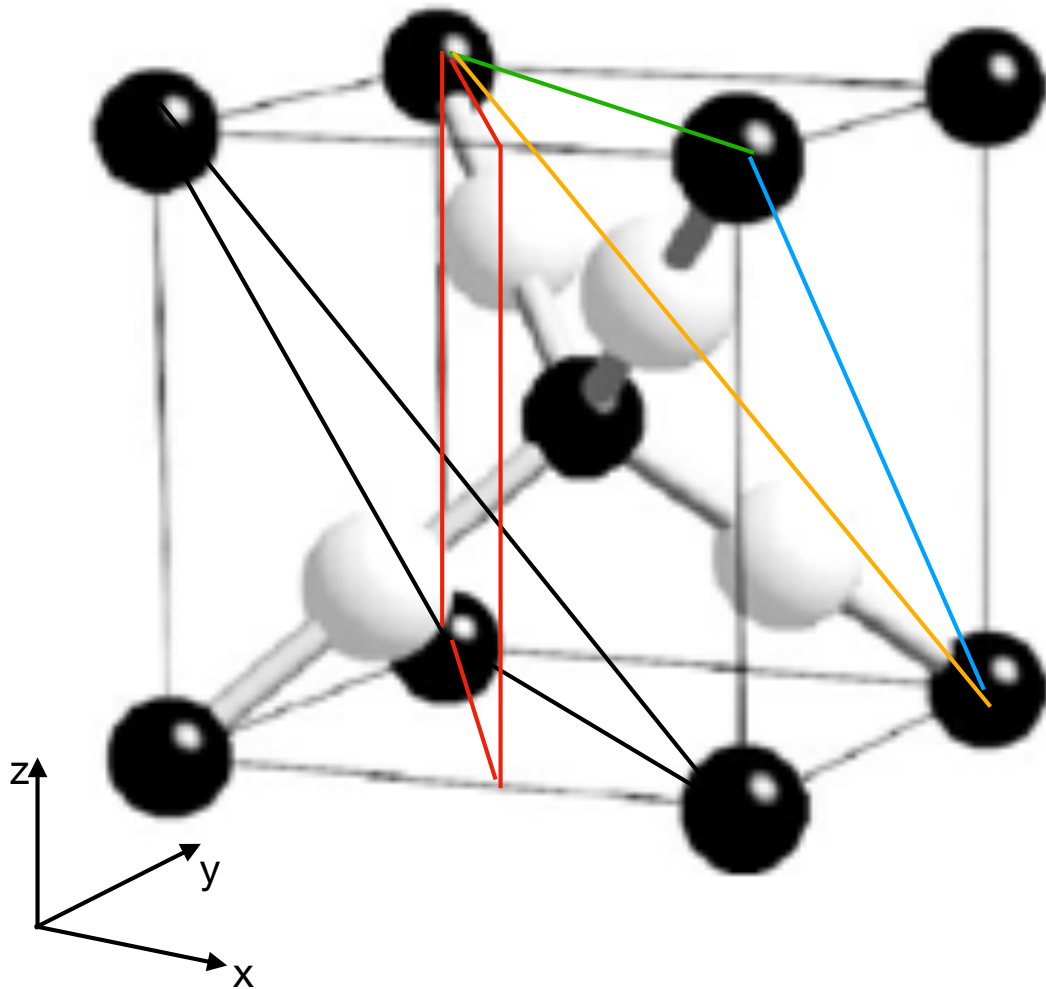
bcc lattice sites

● 18 octahedral sites => 6 in the cubic conventional cell

● 24 tetrahedral sites => 12 in the cubic conventional cell

5. Sketch in the cubic unit cell the planes (111) and (210).

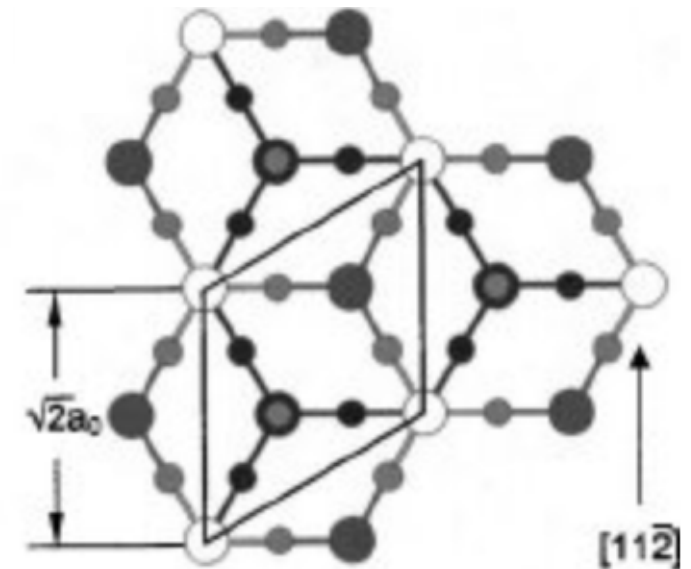6. How many different [110]-type directions lie in the (111) plane? Write out the indices for each such direction.

[1,-1,0] [-1,1,0]

[0,1,-1] [0,-1,1]

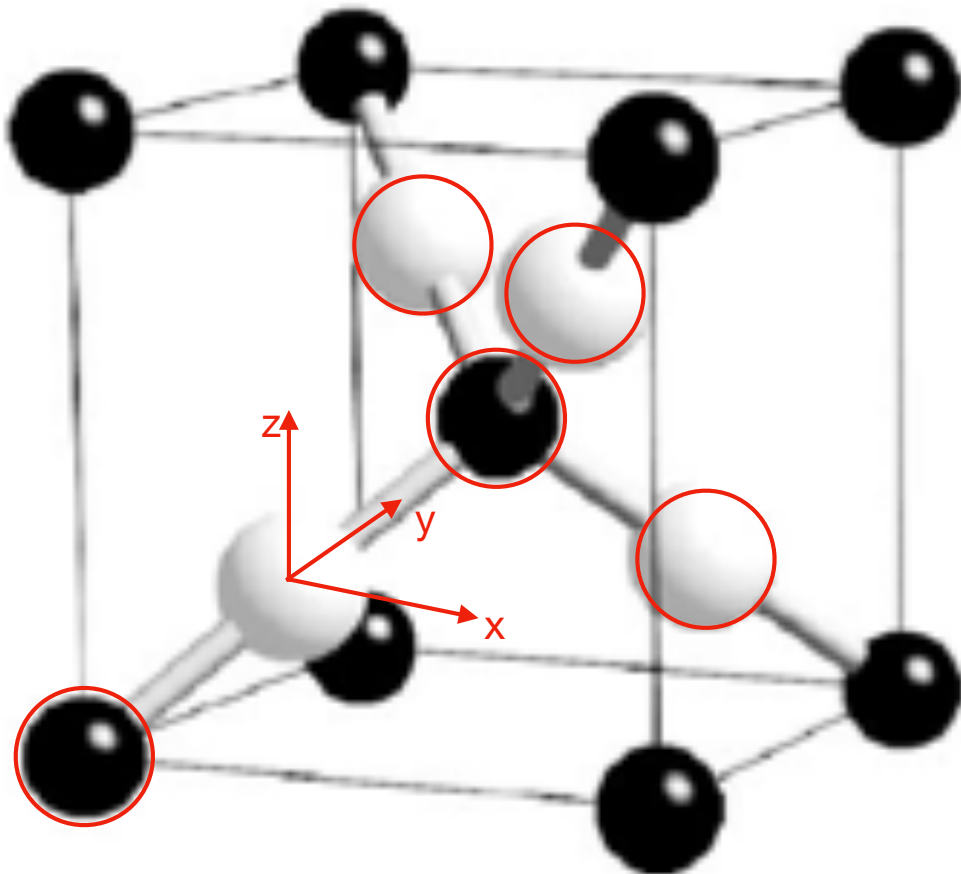[1,0,-1] [-1,0,1]

top view of the (111) plane

$\sqrt{2}a_0$

$[11\bar{2}]$

7. Is it possible to choose the origin such that the structure factor is real? In case of positive answer, make this choice. In any case, write the structure factor.

(hint: if the *inversion center* is placed in the *origin…*)

[1,-1,0] [-1,1,0]

[0,1,-1] [0,-1,1]

[1,0,-1] [-1,0,1]

top view of the (111) plane