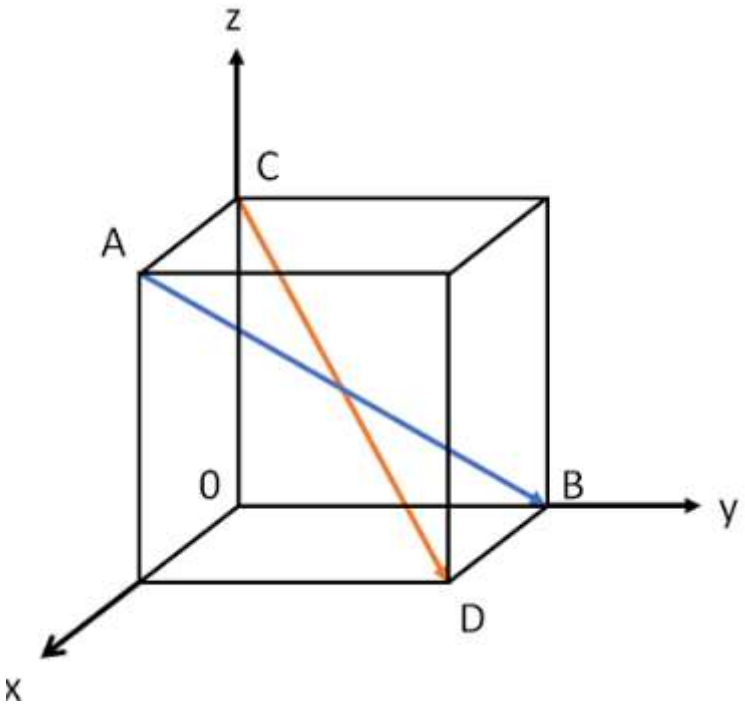
Problem 2.1

Problem 2.1 The tetrahedral bond angle of diamond is given by the angle between the body diagonals of a cube.

2.1.1 Use vector analysis to find the angle. (3 points)



We can find this angle using $\cos\theta = \frac{\vec{a}\cdot\vec{b}}{|\vec{a}||\vec{b}|}$

$$\vec{a} = (1,1,1)/\sqrt{3}$$
$$\vec{b} = (1,1,-1)/\sqrt{3}$$
$$\cos\theta = (1+1-1)/\sqrt{3}$$
$$\theta = \cos^{-1}\frac{1}{\sqrt{3}} = 1.23\text{rad} \rightarrow 70.5^\circ$$

Or $180 - 70.5 = 109.5^\circ$ for the larger angle

Problem 2.2

Problem 2.2 Consider a cubic crystal.

2.2.1 Calculate the angles between the following planes: (8 points)

- (100) and (110)
- (100) and (111)
- (100) and (010)
- (111) and (113)

Miller indicies represent a vector which is normal to the associated plane, so we can simply treat them as vectors

1. $$\begin{pmatrix}1\\0\\0\end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix}1\\1\\0\end{pmatrix} = \frac{1}{\sqrt{2}}$$
$$\theta = \cos^{-1} \frac{1}{\sqrt{2}} = \pi/4$$

2. $$\begin{pmatrix}1\\0\\0\end{pmatrix} \cdot \frac{1}{\sqrt{3}} \begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{3}}$$
$$\theta = \cos^{-1} \frac{1}{\sqrt{3}} = 0.95$$

3. Clearly a right angle $\pi/2$

4. $$\frac{1}{\sqrt{3}} \begin{pmatrix}1\\1\\1\end{pmatrix} \cdot \frac{1}{\sqrt{11}} \begin{pmatrix}1\\1\\3\end{pmatrix} = \frac{5}{\sqrt{33}}$$
$$\theta = \cos^{-1} \frac{5}{\sqrt{33}} = 0.51$$

Problem 2.3

Problem 2.3 For the four crystal structures on the following page, identify:

2.3.1 type of lattice (crystal system and centering type) (3 points)

2.3.3 position of all atoms in basis (3 points)

2.3.3 number of each type of atom per unit cell (3 points)

I'll answer 2.3 by the crystal rather than go back and forth. Sorry for breaking order!

CsCl:

- Lattice: Cubic.
- Basis atom Positions:
  Cl: $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
  1/8Cs: One in each corner $\{(x_1, x_2, x_3)\}$ for $x_1, x_2, x_3 \in \{0, 1\}$
- Number: 1x Cs, 1x Cl

NaCl:

- Lattice: FCC
- Basis Positions:
  1/8Cl $\{(x_1, x_2, x_3)\}$ for $x_1, x_2, x_3 \in \{0, 1\}$
  1/2Cl $\left\{\left(\frac{1}{2}, \frac{1}{2}, x\right), \left(\frac{1}{2}, x, \frac{1}{2}\right), \left(x, \frac{1}{2}, \frac{1}{2}\right)\right\}$ for $x \in \{0, 1\}$
  1/4Na $\left\{\left(\frac{1}{2}, x_1, x_2\right), \left(x_1, \frac{1}{2}, x_2\right), \left(x_1, x_2, \frac{1}{2}\right)\right\}$ for $x_1, x_2 \in \{0, 1\}$
  Na $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
- Number: 4x Na, 4x Cl

CaF_2:

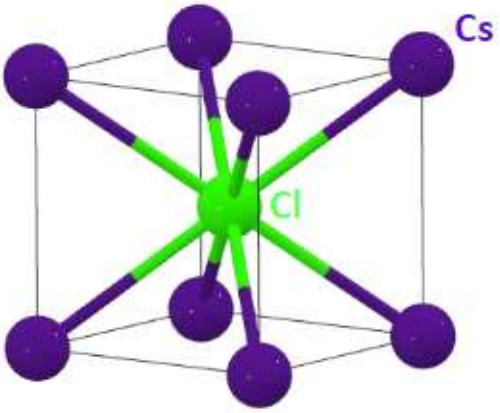
- Lattice: FCC
- Basis Positions:
  1/8Ca $\{(x_1, x_2, x_3)\}$ for $x_1, x_2, x_3 \in \{0, 1\}$
  1/2Ca $\left\{\left(\frac{1}{2}, \frac{1}{2}, x\right), \left(\frac{1}{2}, x, \frac{1}{2}\right), \left(x, \frac{1}{2}, \frac{1}{2}\right)\right\}$ for $x \in \{0, 1\}$
  F $\left\{\left(\frac{2 \pm 1}{4}, \frac{2 \pm 1}{4}, \frac{2 \pm 1}{4}\right)\right\}$
- Number: 4x Ca, 8x F

$BaTiO_3$:

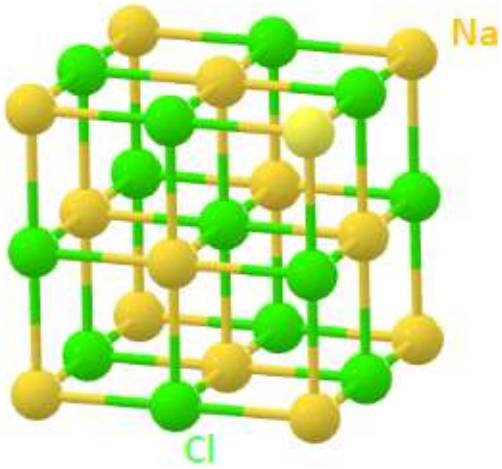
- Lattice: Cubic
- Basis Positions:
  1/8Ba $\{(x_1, x_2, x_3)\}$ for $x_1, x_2, x_3 \in \{0, 1\}$
  1/2O $\left\{\left(\frac{1}{2}, \frac{1}{2}, x\right), \left(\frac{1}{2}, x, \frac{1}{2}\right), \left(x, \frac{1}{2}, \frac{1}{2}\right)\right\}$ for $x \in \{0, 1\}$
  Ti: $\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)$
- Number: 1x Ba, 1x Ti, 3x O

Yay we're done!

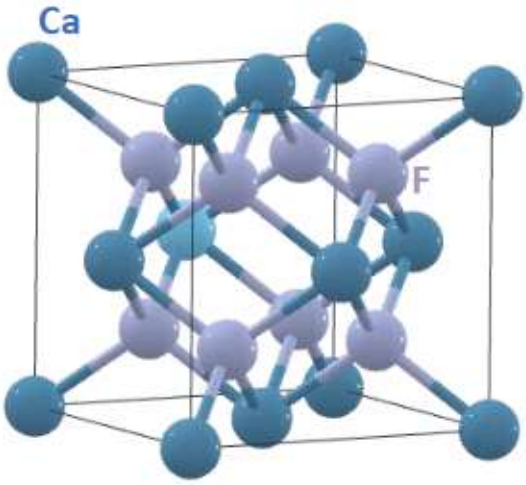
Cesium Chloride (CsCl)



Sodium Chloride (NaCl)



Calcium Fluoride (CaF_2)



Barium Titanate ($BaTiO_3$)