

# Lattice classification

## 1 Face Centered cubic. Primitive

$$a_1 = (1/2, 1/2, 0), \quad a_2 = (1/2, 0, 1/2), \quad a_3 = (0, 1/2, 1/2)$$

Internal angles all 60 degrees ( $\cos \theta = 1/2$ ). 45 degrees with respect to two cardinal axis ( $\cos \theta = \sqrt{2}/2$ ), Orthogonal with respect to last. All lengths equal ( $\sqrt{2}/2$ )

## 2 Body centered cubic. Primitive

$$a_1 = (1, 0, 0), \quad a_2 = (0, 1, 0), \quad a_3 = (1/2, 1/2, 1/2)$$

Internal angles:  $a_1$  and  $a_2$  are orthogonal.  $a_1$  or  $a_2$  with  $a_3$  has  $\cos \theta = \sqrt{3}/3$  (roughly 54.74 degrees). Two vectors have length 1, last has length  $\sqrt{3}/2$ .

## 3 Tetragonal Body centered

Increase z-coordinate on  $a_3$ . Say  $a_3 = (a/2, a/2, b/2)$ . Then  $\cos \theta = a/\sqrt{2a^2 + b^2}$ , and  $|a_3| = \frac{\sqrt{2a^2 + b^2}}{2}$ , or  $\cos \theta = |a_1|/2|a_3|$ :

$$a_1 = (a, 0, 0), \quad a_2 = (0, a, 0), \quad a_3 = (a/2, a/2, b/2) \quad (3.1)$$

$$|a_1| = a = |a_2|, \quad |a_3| = \frac{\sqrt{2a^2 + b^2}}{2}, \quad (3.2)$$

$$\cos \theta_{12} = 0, \quad \cos \theta_{23} = \cos \theta_{31} = \frac{|a_1|}{2|a_3|} = \frac{|a_2|}{2|a_3|} \quad (3.3)$$

## 4 Tetragonal Face centered

$$a_1 = (a/2, a/2, 0), \quad a_2 = (a/2, 0, b/2), \quad a_3 = (0, a/2, b/2), \quad (4.1)$$

$$|a_1| = \frac{\sqrt{2}}{2}a, \quad |a_2| = \frac{\sqrt{a^2 + b^2}}{2} = |a_3|, \quad (4.2)$$

$$\cos \theta_{12} = \frac{|a_1|}{2|a_2|} = \cos \theta_{31} = \frac{|a_1|}{2|a_3|}, \quad \cos \theta_{23} = \frac{b^2}{a^2 + b^2} = \frac{2a_2^2 - a_1^2}{2a_2^2} = \frac{2a_3^2 - a_1^2}{2a_3^2} \quad (4.3)$$

## 5 Tetragonal base centered

$$a_1 = (a/2, a/2, 0), \quad a_2 = (0, a, 0), \quad a_3 = (0, 0, b) \quad (5.1)$$

$$|a_1| = \frac{\sqrt{2}}{2}a, \quad |a_2| = a, \quad |a_3| = b \quad (5.2)$$

$$\cos \theta_{12} = \frac{\sqrt{2}}{2}, \quad \cos \theta_{31} = \cos \theta_{23} = 0 \quad (5.3)$$

## 6 Orthorhombic

Let's assume the conventional unit cell has  $a_1 = (a, 0, 0)$ ,  $a_2 = (0, b, 0)$ ,  $a_3 = (0, 0, c)$

### 6.1 Body centered

$a_3 = (a/2, b/2, c/2)$ . Lengths:  $|a_1| = a$ ,  $|a_2| = b$ ,  $|a_3| = \frac{\sqrt{a^2+b^2+c^2}}{2}$ . Angles:

$$\cos \theta_{12} = 0, \quad \cos \theta_{31} = \frac{a}{\sqrt{a^2+b^2+c^2}} = \frac{|a_1|}{2|a_3|}, \quad \cos \theta_{23} = \frac{b}{\sqrt{a^2+b^2+c^2}} = \frac{|a_2|}{2|a_3|} \quad (6.1)$$

And the spacing is  $c^2 = 4a_3^2 - a_1^2 - a_2^2$

These two last are also angles with respect to x-axis and y-axis respectively. Angle with z is  $\cos \theta_{3z} = \frac{c}{\sqrt{a^2+b^2+c^2}} = 2(4a_3^2 - a_1^2 - a_2^2)/|a_3|$

### 6.2 Face centered

$a_1 = (a/2, b/2, 0)$ ,  $a_2 = (a/2, 0, c/2)$ ,  $a_3 = (0, b/2, c/2)$ .

$$|a_1| = \frac{\sqrt{a^2+b^2}}{2}, \quad |a_2| = \frac{\sqrt{a^2+c^2}}{2}, \quad |a_3| = \frac{\sqrt{b^2+c^2}}{2} \quad (6.2)$$

$$\cos \theta_{12} = \frac{a^2}{\sqrt{a^2+c^2} \cdot \sqrt{a^2+b^2}}, \quad \cos \theta_{31} = \frac{b^2}{\sqrt{b^2+c^2} \cdot \sqrt{a^2+b^2}}, \quad \cos \theta_{23} = \frac{c^2}{\sqrt{a^2+c^2} \cdot \sqrt{b^2+c^2}} \quad (6.3)$$

And the spacings are

$$a^2 = 2(a_1^2 + a_2^2 - a_3^2), \quad b^2 = 2(a_1^2 - a_2^2 + a_3^2), \quad c^2 = 2(-a_1^2 + a_2^2 + a_3^2) \quad (6.4)$$

As such the angles can be written

$$\cos \theta_{12} = \frac{a_1^2 + a_2^2 - a_3^2}{2 \cdot |a_1| \cdot |a_2|}, \quad \cos \theta_{31} = \frac{a_1^2 - a_2^2 + a_3^2}{2 \cdot |a_1| \cdot |a_3|}, \quad \cos \theta_{23} = \frac{-a_1^2 + a_2^2 + a_3^2}{2 \cdot |a_2| \cdot |a_3|} \quad (6.5)$$

### 6.3 Base centered

$a_1 = (a, 0, 0)$ ,  $a_2 = (a/2, b/2, 0)$ ,  $a_3 = (0, 0, c)$ .

Spacings and angles

$$|a_2|^2 = \frac{a^2+b^2}{4}, \quad b^2 = 4a_2^2 - a_1^2. \quad \cos \theta_{12} = \frac{a}{\sqrt{a^2+b^2}} = \frac{|a_1|}{2|a_2|}, \quad \cos \theta_{31} = \cos \theta_{23} = 0 \quad (6.6)$$

## 7 Simple monoclinic

[https://en.wikipedia.org/wiki/Monoclinic\\_crystal\\_system#/media/File:Monoclinic.svg](https://en.wikipedia.org/wiki/Monoclinic_crystal_system#/media/File:Monoclinic.svg)

$$|a_1| = a, \quad |a_2| = b, \quad |a_3| = c, \quad \cos \theta_{12} = \cos \theta_{23} = 0, \quad \cos \theta_{31} \neq 0 \quad (7.1)$$

$a_1$  and  $a_2$  are along x and y.  $a_3 = c \cdot (\cos \theta_{31}, 0, \sin \theta_{31})$

## 8 Base centered monoclinic

$a_1 = (a, 0, 0)$ ,  $a_2 = (a/2, b/2, 0)$ ,  $a_3 = c \cdot (\cos \theta_{31}, 0, \sin \theta_{31})$ .

$$|a_1| = a, \quad |a_2| = \frac{\sqrt{a^2+b^2}}{2}, \quad |a_3| = c \quad \cos \theta_{12} = \frac{|a_1|}{2|a_2|}, \quad \cos \theta_{23} = \frac{a \cos \theta_{31}}{\sqrt{a^2+b^2}} = \frac{a_1 \cdot a_3}{2 \cdot |a_2| \cdot |a_3|} \quad (8.1)$$

## 9 Hexagonal

$a_1 = (1, 0, 0)$ ,  $a_2 = (1/2, \sqrt{3}/2, 0)$ ,  $a_3 = (0, 0, a)$ .  $a_1$  and  $a_2$  are orthogonal to  $a_3$ , and 60 degrees between them.  $|a_1| = |a_2| \neq |a_3|$   $\cos \theta_{12} = 1/2$ ,  $\cos \theta_{31} = \cos \theta_{23} = 0$

## 10 Triclinic

$|a_1| \neq |a_2| \neq |a_3|$ . And  $\theta_{12} \neq \theta_{31} \neq \theta_{23}$

## 11 Rhombohedral

$|a_1| = |a_2| = |a_3|$  and  $\theta_{12} = \theta_{31} = \theta_{23}$  but they're not right angles Examples:

$$a_1 = (a, b, b), \quad a_2 = (b, a, b), \quad a_3 = (b, b, a) \quad (11.1)$$