Lattice classification

1 Face Centered cubic. Primitive

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

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

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

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 $a_3 = (a/2, a/2, b)$. Then $\cos\theta = a^2/\sqrt{2a^2+b^2}$, and $|a_3| = \frac{\sqrt{2a^2+b^2}}{2}$, or $\cos\theta = |a_1|/2|a_3|$

4 Tetragonal Face centered

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

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

$$\cos\theta_{12} = \frac{|a_1|}{2|a_2|} = \cos\theta_{13} = \frac{|a_1|}{2|a_3|}, \quad \cos\theta_{23} = \frac{b^2}{a^2+b^2} = \frac{2a_2^2 - a_1^2}{2a_2^2} = \frac{2a_3^2 - a_1^2}{2a_3^2} \tag{4.3}$$

5 Orthorhombic

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

5.1 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:

$$\cos\theta_{12} = 0,\ \cos\theta_{13} = \frac{a}{\sqrt{a^2+b^2+c^2}} = \frac{|a_1|}{2|a_3|},\ \cos\theta_{23} = \frac{b}{\sqrt{a^2+b^2+c^2}} = \frac{|a_2|}{2|a_3|} \tag{5.1}$$

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 $\cos\theta_{3z} = \frac{c}{\sqrt{a^2+b^2+c^2}} = 2(4a_3^2 - a_1^2 - a_2^2)/|a_3|$

5.2 Face centered

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

$$|a_1| = \frac{\sqrt{a^2+b^2}}{2}, \ |a_2| = \frac{\sqrt{a^2+c^2}}{2}, \ |a_3| = \frac{\sqrt{b^2+c^2}}{2} \tag{5.2}$$

$$\cos\theta_{12} = \frac{a^2}{\sqrt{a^2+c^2}\cdot\sqrt{a^2+b^2}}, \ \cos\theta_{13} = \frac{b^2}{\sqrt{b^2+c^2}\cdot\sqrt{a^2+b^2}}, \ \cos\theta_{23} = \frac{c^2}{\sqrt{a^2+c^2}\cdot\sqrt{b^2+c^2}} \tag{5.3}$$

And the spacings are

$$a^2 = 2(a_1^2 + a_2^2 - a_3^2), \ b^2 = 2(a_1^2 - a_2^2 + a_3^2), \ c^2 = 2(-a_1^2 + a_2^2 + a_3^2) \tag{5.4}$$

As such the angles can be written

$$\cos\theta_{12} = \frac{a_1^2 + a_2^2 - a_3^2}{2\cdot|a_1|\cdot|a_2|}, \quad \cos\theta_{13} = \frac{a_1^2 - a_2^2 + a_3^2}{2\cdot|a_1|\cdot|a_3|}, \quad \cos\theta_{23} = \frac{-a_1^2 + a_2^2 + a_3^2}{2\cdot|a_2|\cdot|a_3|} \tag{5.5}$$

5.3 Base centered

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

Spacings and angles

$$|a_2|^2 = \frac{a^2+b^2}{4}, \ b^2 = 4a_2^2 - a_1^2. \quad \cos\theta_{12} = \frac{a}{\sqrt{a^2+b^2}} = \frac{|a_1|}{2|a_2|}, \ \cos\theta_{13} = \cos\theta_{23} = 0 \tag{5.6}$$

6 Simple monoclinic

https://en.wikipedia.org/wiki/Monoclinic_crystal_system#/media/File:Monoclinic.svg

$$|a_1| = a, \ |a_2| = b, \ |a_3| = c, \quad \cos\theta_{12} = \cos\theta_{23} = 0, \ \cos\theta_{13} \neq 0 \tag{6.1}$$

a_1 and a_2 are along x and y. $a_3 = c\cdot(\cos\theta_{13}, 0, \sin\theta_{13})$

7 Base centered monoclinic

$a_1 = (a, 0, 0), \ a_2 = (a/2, b/2, 0), \ a_3 = c\cdot(\cos\theta_{13}, 0, \sin\theta_{13})$.

$$|a_1| = a, \ |a_2| = \frac{\sqrt{a^2+b^2}}{2}, \ |a_3| = c \quad \cos\theta_{12} = \frac{|a_1|}{2|a_2|}, \ \cos\theta_{23} = \frac{a\cos\theta_{13}}{\sqrt{a^2+b^2}} = \frac{a_1\cdot a_3}{2\cdot|a_2|\cdot|a_3|} \tag{7.1}$$

8 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. $|a_1| = |a_2| \neq |a_3| \quad \cos\theta_{12} = 1/2, \ \cos\theta_{13} = \cos\theta_{23} = 0$

9 Triclinic

$|a_1| \neq |a_2| \neq |a_3|$. And $\theta_{12} \neq \theta_{13} \neq \theta_{23}$

10 Rhombohedral

$|a_1| = |a_2| = |a_3|$ and $\theta_{12} = \theta_{13} = \theta_{23}$ but they're not right angles