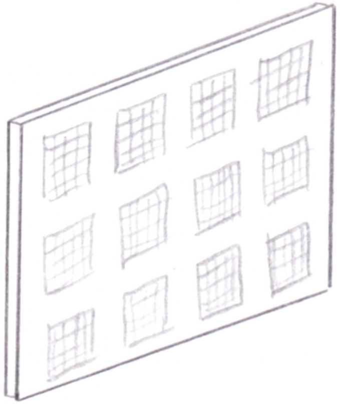
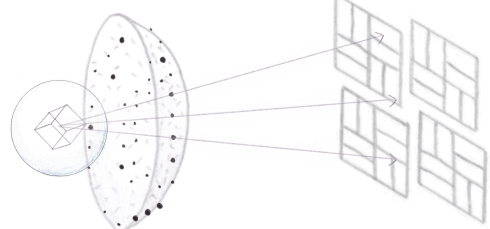
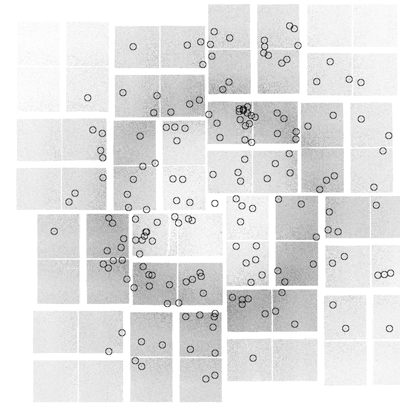
LINEAR ALGEBRA

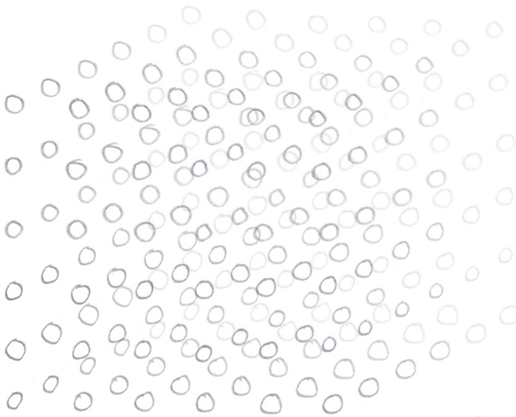
for crystallography.

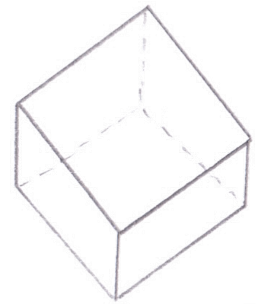
Helen Ginn.

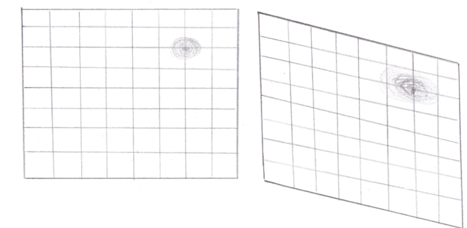


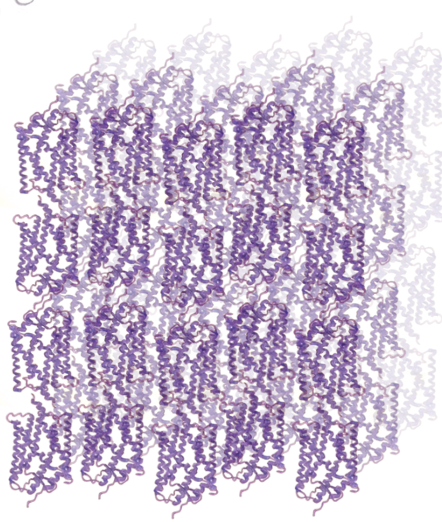


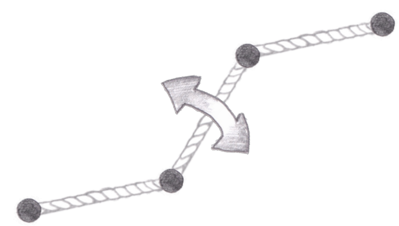










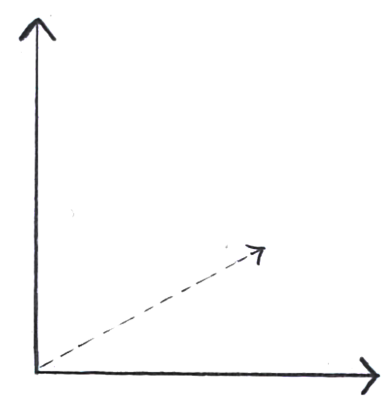


Matrices describe coordinate systems.

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$

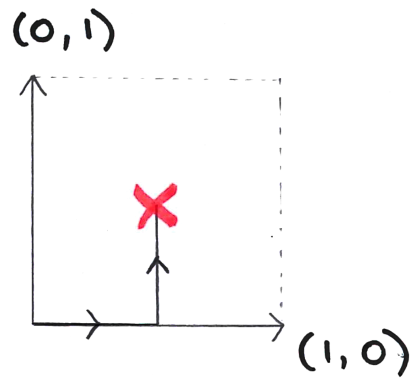
basis vectors

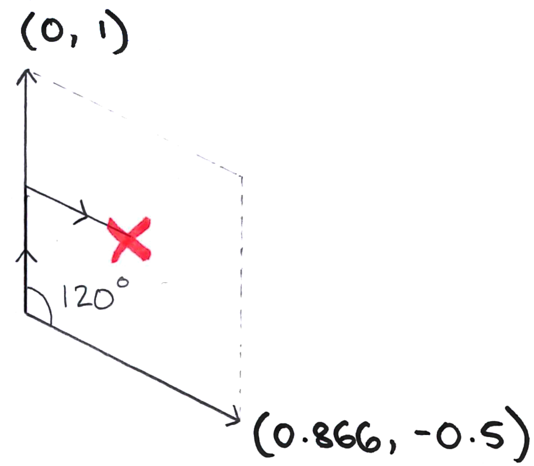
$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



Positions can be described by combinations of basis vectors.

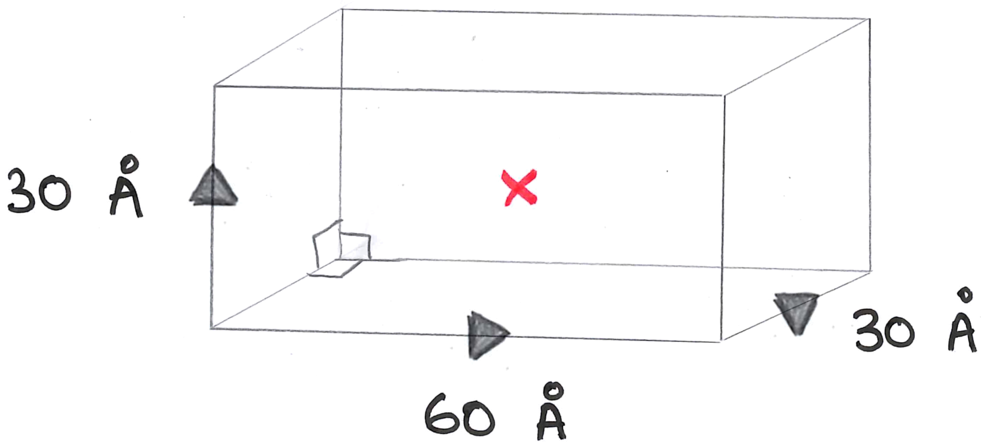
$$\begin{pmatrix} x_0 & y_0 \\ x_1 & y_1 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 0.866 & 0 \\ -0.5 & 1 \end{pmatrix}$$



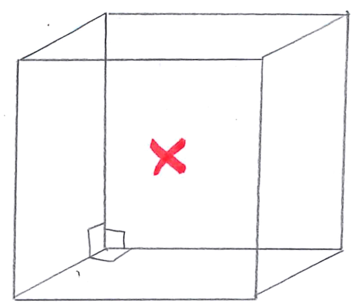


$$\begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} \begin{pmatrix} 0.866 & 0 \\ -0.5 & 1 \end{pmatrix} = \begin{pmatrix} 0.433 \\ 0.25 \end{pmatrix}$$

Orthogonal unit cell described by a matrix.



$$\begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix}$$



$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix} \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix} = \begin{pmatrix} 30 \\ 15 \\ 15 \end{pmatrix}$$

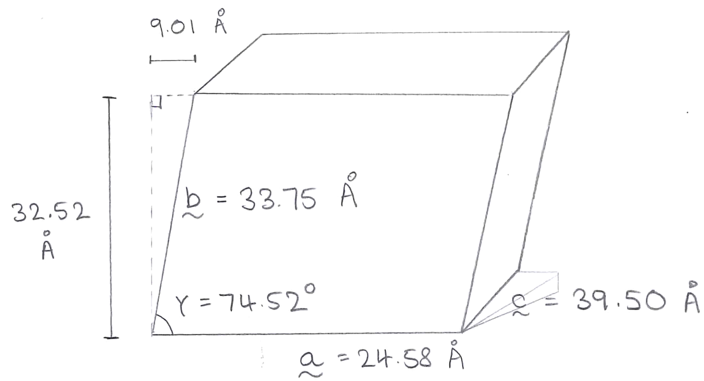
Triclinic unit cell described by a matrix.

5i40 (P1)

$a, b, c = ?$

$\alpha, \beta, \gamma = ?$

$$
\begin{array}{ccc}
\left(\begin{matrix} 24.58 & 9.01 & 11.34 \\ 0 & 32.52 & 10.56 \\ 0 & 0 & 36.34 \end{matrix}\right) \\
\uparrow \quad\quad \uparrow \quad\quad \uparrow \\
\underset{\sim}{a} \quad\quad \underset{\sim}{b} \quad\quad \underset{\sim}{c}
\end{array}
$$



$$|\underset{\sim}{a}| = \text{sqrt}(24.58^2 + 0^2 + 0^2) = 24.58 \text{ Å}$$

$$|\underset{\sim}{b}| = \text{sqrt}(9.01^2 + 32.52^2 + 0^2) = 33.75 \text{ Å}$$

$$\cos(\alpha) = \frac{\underset{\sim}{b} \cdot \underset{\sim}{c}}{|\underset{\sim}{b}||\underset{\sim}{c}|} = \frac{(9.01 \times 11.34 + 32.52 \times 10.56 + 0 \times 36.34)}{33.75 \times 39.50}$$

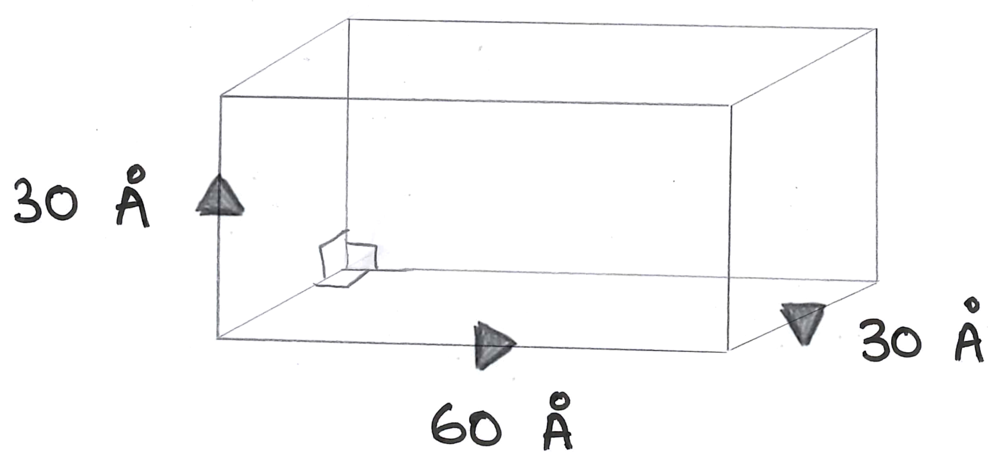
$$\alpha = \cos^{-1}(0.3342) = 70.47°$$

Coordinate system from unit cell dimensions.

Unit cell = $a, b, c, \alpha, \beta, \gamma$

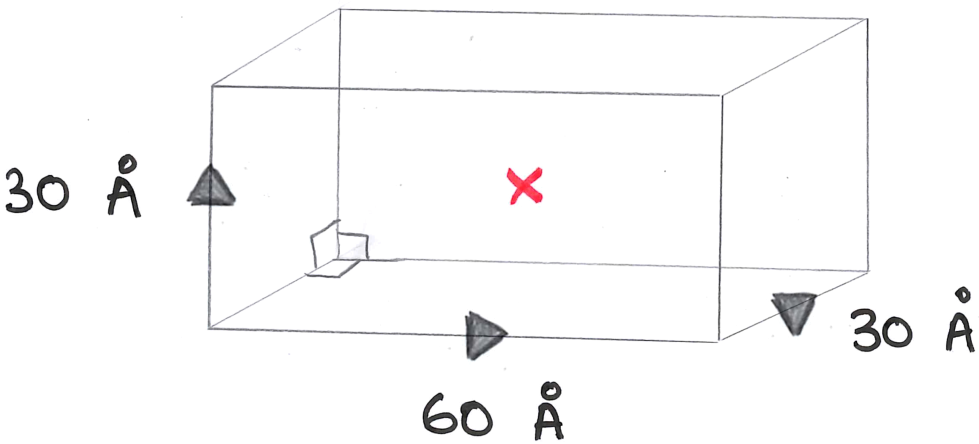
$$\text{Matrix} = \begin{pmatrix} a & b \cdot \cos\gamma & c \cdot \cos\beta \\ 0 & b \cdot \sin\gamma & \dfrac{c \cdot (\cos\alpha - \cos\beta \cdot \cos\gamma)}{\sin\gamma} \\ 0 & 0 & \dfrac{\text{volume}}{a \cdot b \cdot \sin\gamma} \end{pmatrix}$$

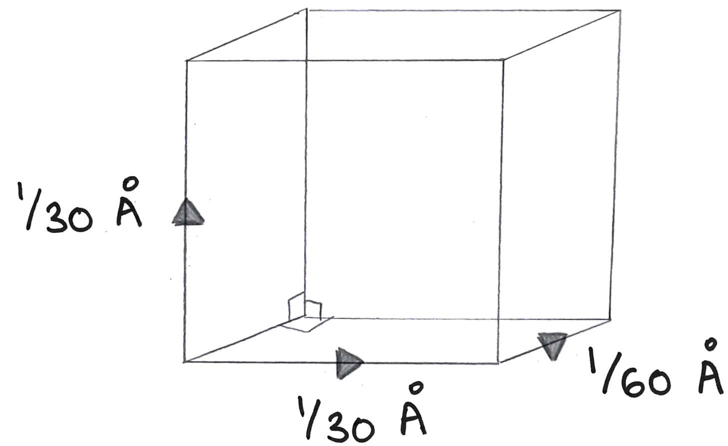
$$\text{volume} = a \cdot b \cdot c \cdot \text{sqrt}(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)$$



$$\begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix}$$

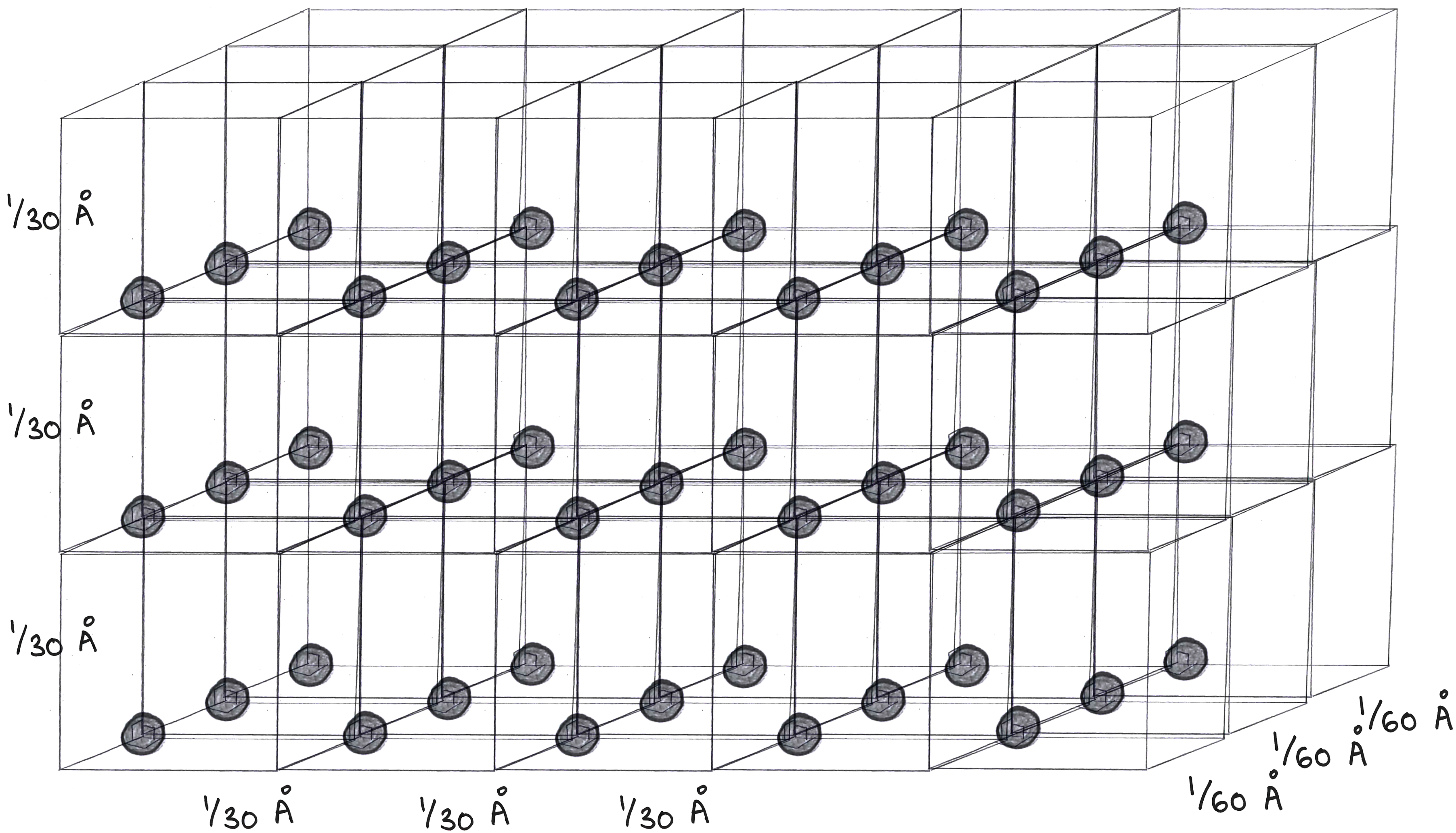
Real space to reciprocal unit cell coordinates.

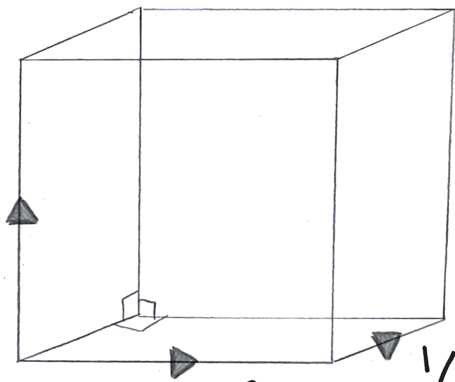




$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} 30 \\ 15 \\ 15 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}$$

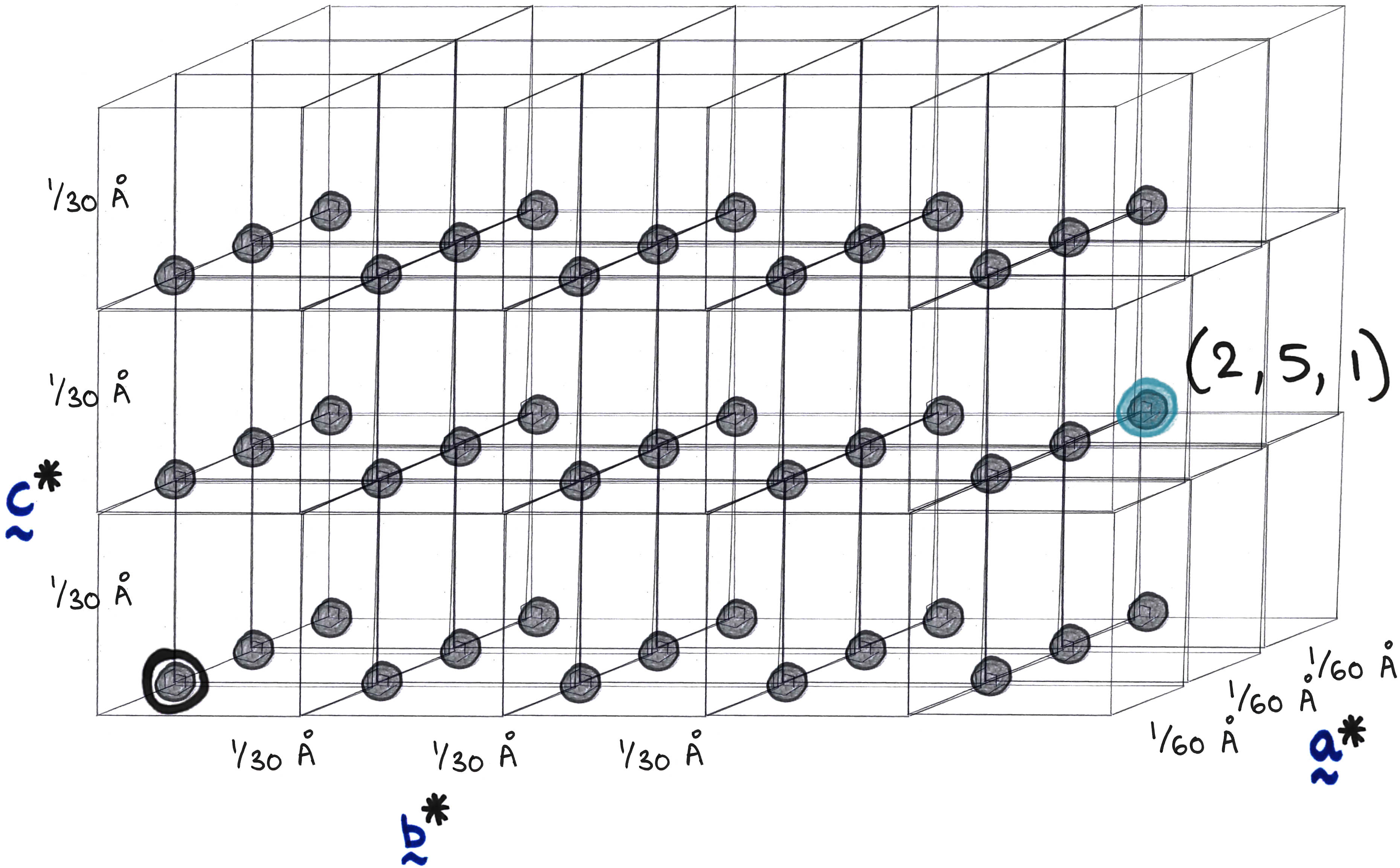
Position of a Miller index in reciprocal space.



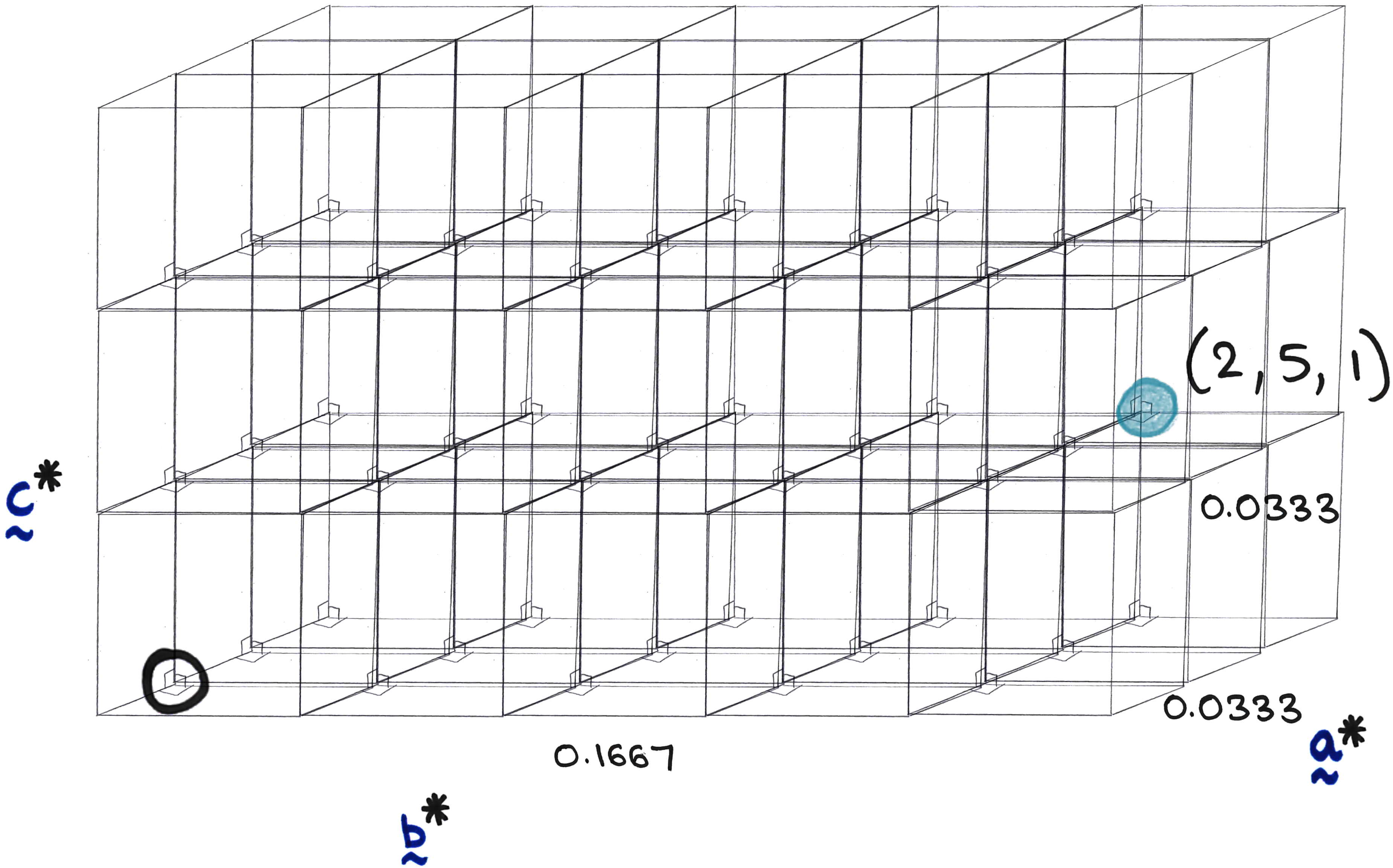


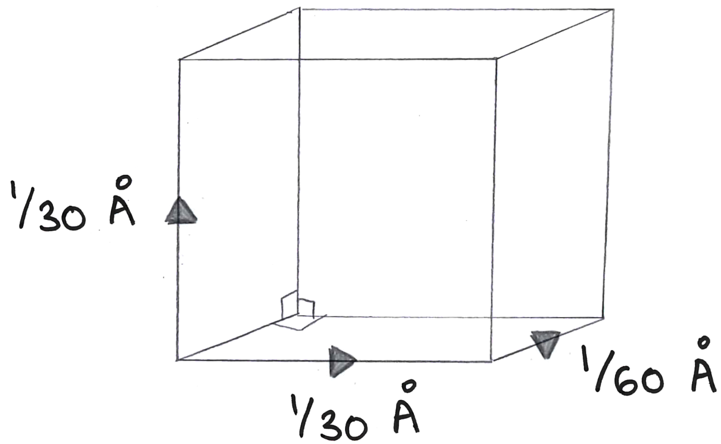
d of (2, 5, 1)?

$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} 2 \\ 5 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.0333 \\ 0.1667 \\ 0.0333 \end{pmatrix}$$



1/30 Å
1/30 Å
1/30 Å
c*
(2, 5, 1)
1/30 Å
1/30 Å
1/30 Å
b*
1/60 Å
1/60 Å
1/60 Å
a*


(2, 5, 1)
c*
0.0333
0.0333
a*
0.1667
b*



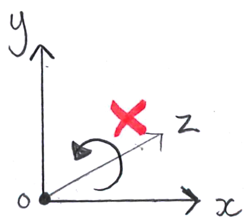
d of (2, 5, 1)?

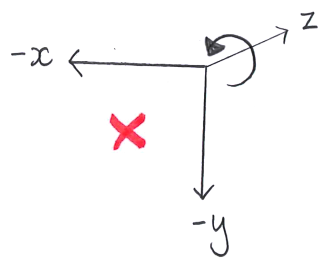
$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} 2 \\ 5 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.0333 \\ 0.1667 \\ 0.0333 \end{pmatrix}$$

$$d^* = \mathrm{sqrt}(0.0333^2 + 0.1667^2 + 0.0333^2)$$
$$= \mathrm{sqrt}(0.03) = 0.173$$

$d = 5.77$ Å resolution

Matrices that rotate vectors around the origin.





$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$\uparrow \quad \uparrow \quad \uparrow$

basis vectors

$\theta \quad \phi \quad \psi$

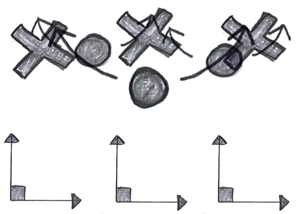
$(x, y, z) + \theta$

axis angle

$$\begin{pmatrix} 0.977 & -0.158 & -0.144 \\ 0.094 & 0.922 & -0.374 \\ 0.192 & 0.352 & 0.916 \end{pmatrix}$$

Is a matrix a rotation matrix?

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$



$$x_0^2 + x_1^2 + x_2^2 = 1$$
$$y_0^2 + y_1^2 + y_2^2 = 1$$
$$z_0^2 + z_1^2 + z_2^2 = 1$$

$$\underset{\sim}{x} \cdot \underset{\sim}{y} = 0$$
$$\underset{\sim}{y} \cdot \underset{\sim}{z} = 0$$
$$\underset{\sim}{x} \cdot \underset{\sim}{z} = 0$$

Inversion of a rotation matrix

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix} \qquad \begin{pmatrix} x_0 & x_1 & x_2 \\ y_0 & y_1 & y_2 \\ z_0 & z_1 & z_2 \end{pmatrix}$$

Rotation matrix from Tait-Bryan angles.

$$R_x(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix}$$

$$R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix}$$

$$R_z(\gamma) = \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R_x(\alpha)\,R_y(\beta)\,R_z(\gamma) = \begin{pmatrix} \cos\beta\cos\gamma & -\sin\gamma\cos\beta & \sin\beta \\ \cos\alpha\sin\gamma + \sin\alpha\sin\beta\cos\gamma & \cos\alpha\cos\gamma - \sin\alpha\sin\beta\sin\gamma & -\sin\alpha\cos\beta \\ \sin\alpha\sin\gamma - \cos\alpha\sin\beta\cos\gamma & \sin\alpha\cos\gamma + \cos\alpha\sin\beta\sin\gamma & \cos\alpha\cos\beta \end{pmatrix}$$

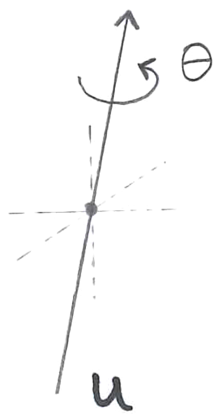
$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$

$$\sin\beta = z_0$$

$$\cos\alpha\cos\beta = z_2$$

$$\cos\beta\cos\gamma = x_0$$

Rotation matrix from angle around axis.



$$\begin{pmatrix} \cos\theta + u_x^2(1-\cos\theta) & u_x u_y(1-\cos\theta) - u_z\sin\theta & u_x u_z(1-\cos\theta) + u_y\sin\theta \\ u_y u_x(1-\cos\theta) + u_z\sin\theta & \cos\theta + u_y^2(1-\cos\theta) & u_y u_z(1-\cos\theta) - u_x\sin\theta \\ u_z u_x(1-\cos\theta) - u_y\sin\theta & u_z u_y(1-\cos\theta) + u_x\sin\theta & \cos\theta + u_z^2(1-\cos\theta) \end{pmatrix}$$

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$

$$x_0 + y_1 + z_2 = \cos\theta + u_x^2(1-\cos\theta) + \cos\theta + u_y^2(1-\cos\theta) + \cos\theta + u_z^2(1-\cos\theta)$$

$$= 3\cos\theta + (1-\cos\theta)\underbrace{(u_x^2 + u_y^2 + u_z^2)}_{\text{unit vector}}$$

$$x_0 + y_1 + z_2 = 2\cos\theta + 1.$$