1)

b)

$$S_{hkl} := \sum_{j=1}^{N} f_j \, e^{i2\pi(hu_j + kv_j + lw_j)}$$

Si: $S_{hkl} = \sum_{j=1}^{8} f_{Si} \, e^{i2\pi(hu_j + kv_j + lw_j)}$

$$= f_{Si}\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)} + e^{\frac{i\pi}{2}(h+k+l)} + e^{\frac{i\pi}{2}(3h+3k+l)} + e^{\frac{i\pi}{2}(3h+k+3l)} + e^{\frac{i\pi}{2}(h+3k+3l)}\right)$$

$$= f_{Si}\left(1 + (-1)^{(h+k)} + (-1)^{(h+l)} + (-1)^{(k+l)} + i^{(h+k+l)} + i^{(3h+3k+l)} + i^{(3h+k+3l)} + i^{(h+3k+3l)}\right)$$

$$= f_{Si}\left(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l} + i^{h+k+l} + (i^2)^{h+k} \, i^l + (i^2)^{h+l} \, i^k + (i^2)^{k+l} \, i^h\right)$$

$$= f_{Si}\left(1 + i^{h+k+l}\right)\underbrace{\left(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right)}_{\neq 0 \text{ falls alle gerade oder alle ungerade}}$$

h,k,l gerade: $1 + i^{h+k+l}$ real

$\Rightarrow \neq 0$ falls $h+k+l = 4n$, $n \in \mathbb{N}$

h,k,l ungerade: $1 + i^{h+k+l}$ komplex ↯

=> Auswahlregeln: h,k,l gerade
$h+k+l = 4n$, $n \in \mathbb{N}$

c)

$$S_{hkl} := \sum_{j=1}^{N} f_j \, e^{i2\pi(hu_j + kv_j + lw_j)}$$

Gaks: $S_{hkl} = \sum_{j=1}^{8} f_j \, e^{i2\pi(hu_j + kv_j + lw_j)}$

$$= f_{Ga}\left(1 + e^{i\pi(h+k)} + e^{i\pi(h+l)} + e^{i\pi(k+l)}\right) + f_{As}\left(e^{\frac{i\pi}{2}(h+k+l)} + e^{\frac{i\pi}{2}(3h+3k+l)} + e^{\frac{i\pi}{2}(3h+k+3l)} + e^{\frac{i\pi}{2}(h+3k+3l)}\right)$$

$$= f_{Ga}\left(1 + (-1)^{(h+k)} + (-1)^{(h+l)} + (-1)^{(k+l)}\right) + f_{As}\left(i^{(h+k+l)} + i^{(3h+3k+l)} + i^{(3h+k+3l)} + i^{(h+3k+3l)}\right)$$

$$= \left(f_{Ga} + f_{As} \, i^{h+k+l}\right)\underbrace{\left(1 + (-1)^{h+k} + (-1)^{h+l} + (-1)^{k+l}\right)}_{\neq 0 \text{ falls alle gerade oder alle ungerade}}$$

h,k,l gerade: $f_{Ga} + f_{As} \, i^{h+k+l}$ real

h,k,l ungerade: $f_{Ga} + f_{As} \, i^{h+k+l}$ komplex

=> Auswahlregeln: h,k,l gerade

2)

a)

$\vec{a}_1 = (a,0,0)^T \qquad \vec{a}_2 = (0,a,0)^T \qquad \vec{a}_3 = (\frac{a}{2}, \frac{a}{2}, \frac{a}{2})^T$

$$\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) = (a,0,0)^T \cdot (\tfrac{a^2}{2}, 0, -\tfrac{a^2}{2}) = \frac{a^3}{2}$$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}(1,0,-1)^T$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{2\pi}{a}(0,1,-1)^T$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} = \frac{4\pi}{a}(0,0,1)^T$$