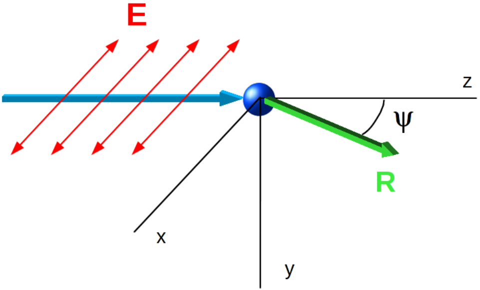
Review: Thomson Scattering

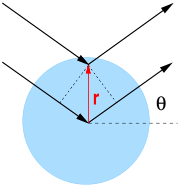


$$\frac{E_{rad}(R,t)}{E_{in}} = -\frac{e^2}{4\pi\epsilon_0 mc^2}\frac{e^{ikR}}{R}cos\psi = -r_o\frac{e^{ikR}}{R}cos\psi$$

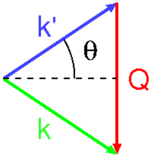
$$r_0 = \frac{e^2}{4\pi\epsilon_0 mc^2} = 2.82 \times 10^{-5}\text{Å}$$

Review: Atomic Scattering

phase shift arises from scattering off different portions of extended electron distribution



$$\Delta\phi(\mathbf{r}) = (\mathbf{k} - \mathbf{k}') \cdot \mathbf{r} = \mathbf{Q} \cdot \mathbf{r}$$

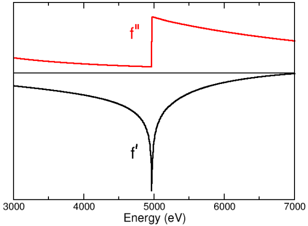


$$|\mathbf{Q}| = 2\,|\mathbf{k}|\, sin\theta = \frac{4\pi}{\lambda} sin\theta$$

Review: Atomic Form Factor

the volume element at $\mathbf{r}$ contributes $-r_o \rho(\mathbf{r}) d^3 r$ with phase factor $e^{i\mathbf{Q}\cdot\mathbf{r}}$
for an entire atom, integrate to get the atomic form factor $f^o(\mathbf{Q})$:

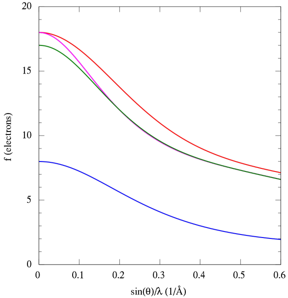
$$-r_o f^o(\mathbf{Q}) = -r_o \int \rho(\mathbf{r}) e^{i\mathbf{Q}\cdot\mathbf{r}} d^3 r$$



the total atomic scattering factor is

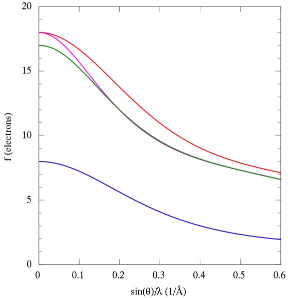
$$f(\mathbf{Q}, \hbar\omega) = f^o(\mathbf{Q}) + f'(\hbar\omega) + if''(\hbar\omega)$$

Atomic Form Factor



The atomic form factor has an angular dependence

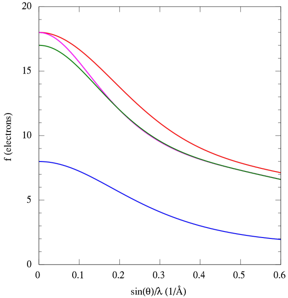
Atomic Form Factor



The atomic form factor has an angular dependence

$$\mathbf{Q} = \frac{4\pi}{\lambda}\sin\theta$$

Atomic Form Factor



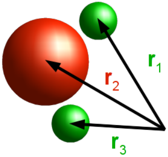
The atomic form factor has an angular dependence

$$\mathbf{Q} = \frac{4\pi}{\lambda} \sin\theta$$

Lighter atoms (blue is oxygen) have wider form factor

Scattering From Molecules

extending to a molecule ...



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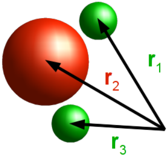

$$F^{molecule}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

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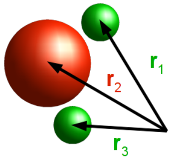

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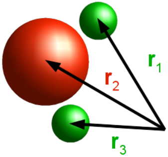

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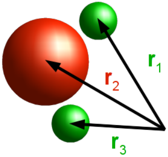

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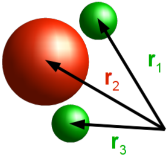

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Scattering from a Crystal

The scattering from a molecule can be extended to a crystal lattice ...

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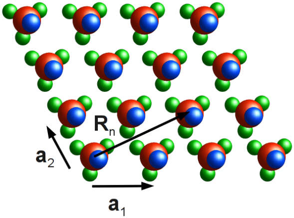

... which is simply a periodic array of molecules

$$F^{crystal}(\mathbf{Q}) = F^{molecule} F^{lattice}$$

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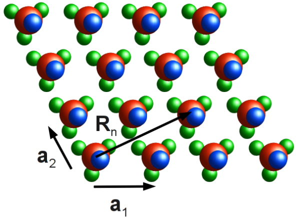

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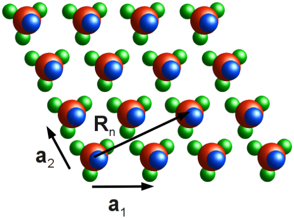
Scattering from a Crystal

The scattering from a molecule can be extended to a crystal lattice ...



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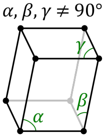
$$F^{crystal}(\mathbf{Q}) = \sum_j f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j} \sum_n e^{i\mathbf{Q}\cdot\mathbf{R}_n}$$

$\sum e^{i\mathbf{Q}\cdot\mathbf{R}_n}$ is always small
unless $\mathbf{Q} \cdot \mathbf{R}_n = 2\pi m$
where $\mathbf{R}_n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ is a real space lattice vector

Crystal Lattices

There are 7 possible real space lattices: triclinic,



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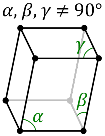

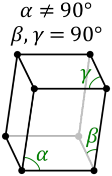

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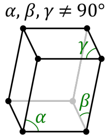

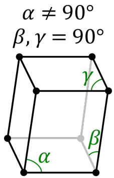

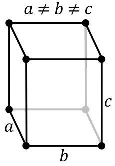

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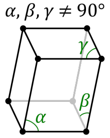

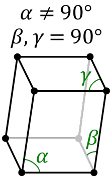

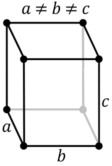

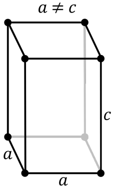

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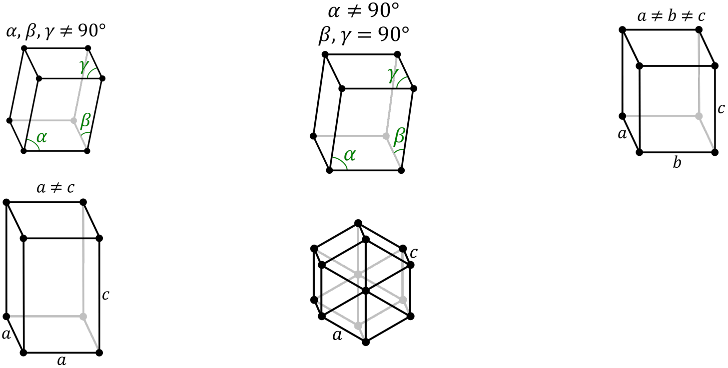

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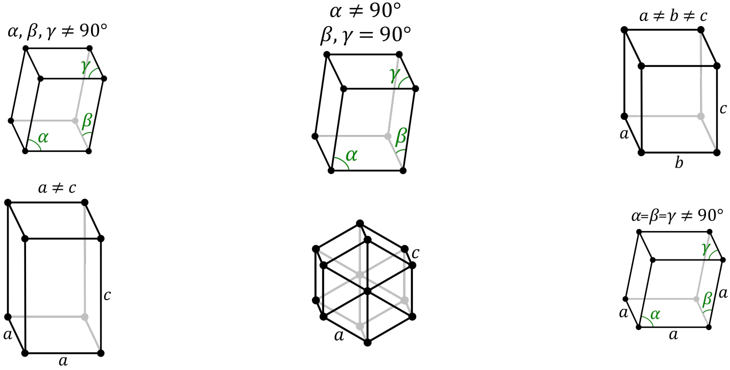

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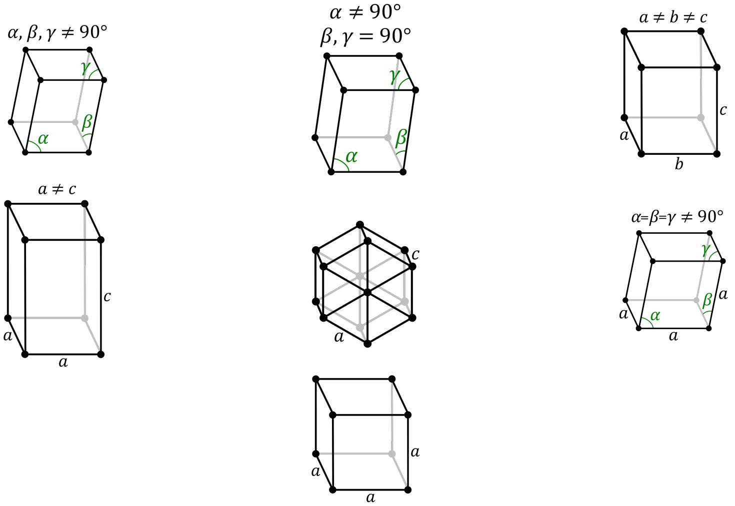
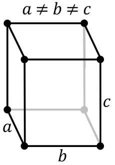


Lattice Volume

Consider the orthorhombic lattice for simplicity (the others give exactly the same result).



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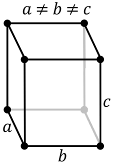

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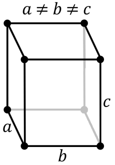

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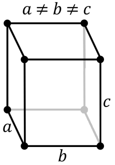

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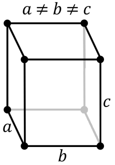

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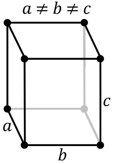

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A simple way of calculating the volume of the unit cell!

Reciprocal Lattice

Define the reciprocal lattice vectors in terms of the real space unit vectors

$$
\begin{aligned}
\mathbf{a}_1^* &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \\
\mathbf{a}_2^* &= 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)} \\
\mathbf{a}_3^* &= 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}
\end{aligned}
$$

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\mathbf{a}_3^* &= 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)}
\end{aligned}$$

In analogy to $\mathbf{R}_n$, we can construct an arbitrary reciprocal space lattice vector $\mathbf{G}_{hkl}$

$$\mathbf{G}_{hkl} = h\mathbf{a}_1^* + k\mathbf{a}_2^* + l\mathbf{a}_3^*$$

Laue Condition

Because of the construction of the reciprocal lattice

$$\mathbf{G}_{hkl} \cdot \mathbf{R}_n = 2\pi(hn_1 + kn_2 + ln_3) = 2\pi m$$

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and therefore, the crystal scattering factor is non-zero **only** when

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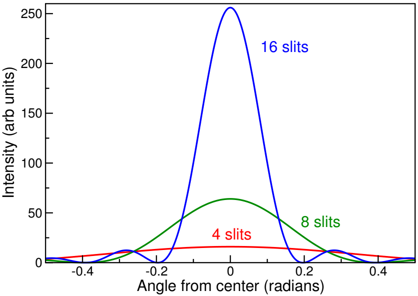
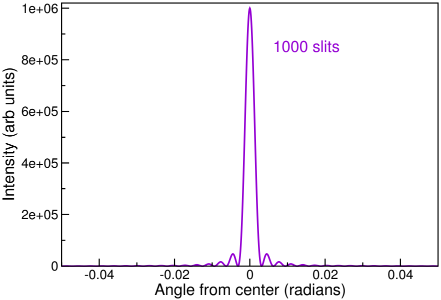
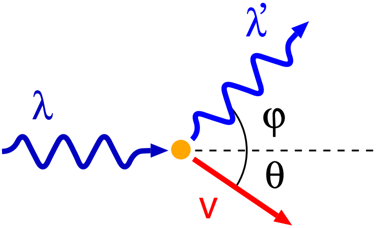




Compton Scattering

A photon-electron collision



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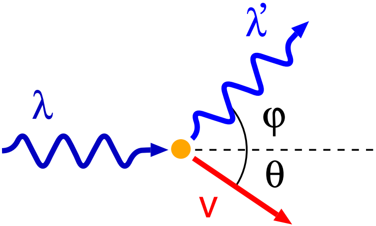

$$\mathbf{p} = \hbar \mathbf{k} = 2\pi\hbar/\lambda$$

$$\mathbf{p}' = \hbar \mathbf{k}' = 2\pi\hbar/\lambda'$$

$$|\mathbf{k}| \neq |\mathbf{k}'|$$

Treat electron relativistically and conserve energy and momentum

$$mc^2 + \frac{hc}{\lambda} = \frac{hc}{\lambda'} + \gamma mc^2 \qquad \text{(energy)}$$

$$\frac{h}{\lambda} = \frac{h}{\lambda'} \cos\phi + \gamma mv \cos\theta \qquad \text{(x-axis)}$$

$$0 = \frac{h}{\lambda'} \sin\phi + \gamma mv \sin\theta \qquad \text{(y-axis)}$$

Compton Scattering Derivation

Squaring the momentum equations

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \cos^2\theta$$

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using $\sin^2\theta + \cos^2\theta = 1$

$$\left(\frac{h}{\lambda} - \frac{h}{\lambda'} \cos\phi\right)^2 = \gamma^2 m^2 v^2 \left[1 - \frac{\left(\frac{h}{\lambda'} \sin\phi\right)^2}{\gamma^2 m^2 v^2}\right]$$

Compton Scattering Derivation

Squaring the momentum equations

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$$\left(\tfrac{h}{\lambda} - \tfrac{h}{\lambda'}\cos\phi\right)^2 = \gamma^2 m^2 v^2 \left[1 - \frac{\left(\frac{h}{\lambda'}\sin\phi\right)^2}{\gamma^2 m^2 v^2}\right]$$

$$\tfrac{h^2}{\lambda^2} - \tfrac{2h^2}{\lambda\lambda'}\cos\phi + \tfrac{h^2}{\lambda'^2}\cos^2\phi = \gamma^2 m^2 v^2 - \tfrac{h^2}{\lambda'^2}\sin^2\phi$$

$$\tfrac{h^2}{\lambda^2} - \tfrac{2h^2}{\lambda\lambda'}\cos\phi + \tfrac{h^2}{\lambda'^2} = \tfrac{m^2 v^2}{1-\beta^2} = \tfrac{m^2 c^2 \beta^2}{1-\beta^2}$$

Compton Scattering Derivation

Now take the energy equation and square it

$$\left(mc^2 + \frac{hc}{\lambda} - \frac{hc}{\lambda'}\right)^2 = \gamma^2 m^2 c^4 = \frac{m^2 c^4}{1-\beta^2}$$

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$$\beta^2 = \frac{\left(mc^2+\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)^2 - m^2c^4}{\left(mc^2+\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)^2} = \frac{2mc^2\left(\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)+\left(\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)^2}{\left(mc^2+\frac{hc}{\lambda}-\frac{hc}{\lambda'}\right)^2}$$

Compton Scattering Derivation

Combining and reducing, we obtain

$$\frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}\cos\phi = 2m\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'}\right) + \frac{h^2}{\lambda^2} + \frac{h^2}{\lambda'^2} - \frac{2h^2}{\lambda\lambda'}$$

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$$\Delta\lambda = \frac{h}{mc}(1-\cos\phi)$$

Compton Scattering Results

$$\lambda_c = \hbar/mc = 3.86 \times 10^{-3}\text{Å for an electron}$$

Comparing to the Thomson scattering length: $r_o/\lambda_C = 1/137$

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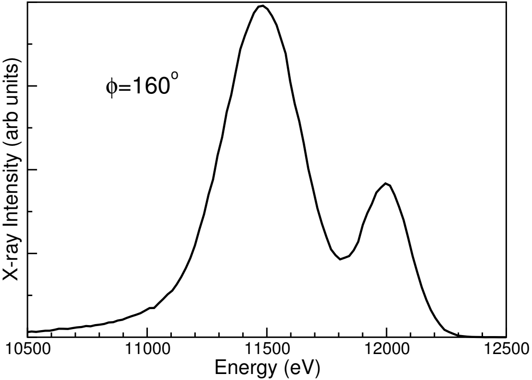
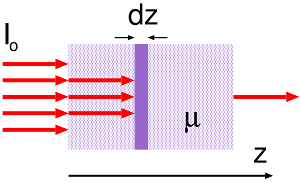


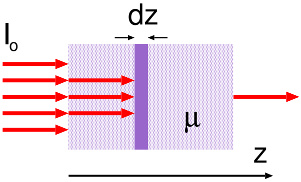
X-Ray Absorption



Absorption coefficient μ, thickness dz x-ray intensity is attenuated as

$$dI = -I(z)\mu dz$$

X-Ray Absorption



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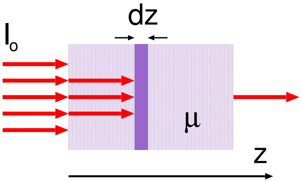

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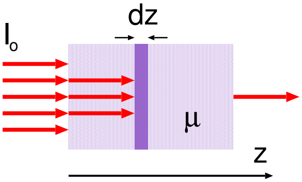

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$$\mu = \rho_a\sigma_a = \left(\frac{\rho_m N_A}{A}\right)\sigma_a$$

with mass density ρ_m , Avogadro's number N_A, atomic number A