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- Friedel's Law
- Bijvoet (Bay-voot) Pairs
- MAD Phasing
- Quantum Origin of Resonant Scattering

Homework Assignment #7:
Chapter 7: 2, 3, 9, 10, 11
due Thursday, April 23, 2015

PHYS 570 day at 10-ID

1. April 24, 2015, 09:00 – 16:00

PHYS 570 day at 10-ID

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2. Activities
   - Absolute flux measurement
   - Reflectivity measurement
   - EXAFS measurement
   - Rocking curve measurement (possibly)

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5. Let me know when you plan to come!

Single oscillator review

$$f(\vec{Q},\omega) = f^0(\vec{Q}) + \chi(\omega)$$

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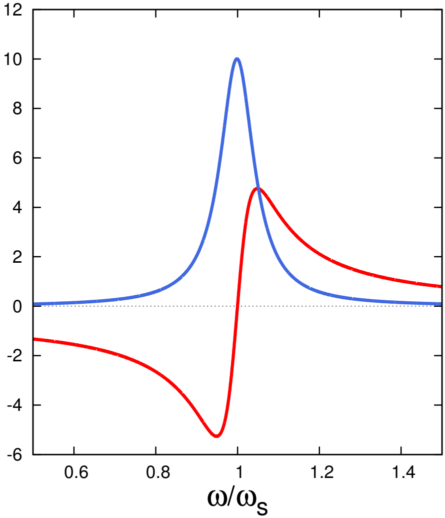
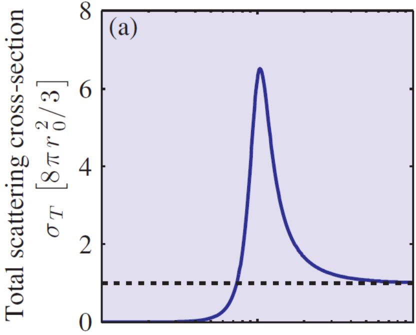
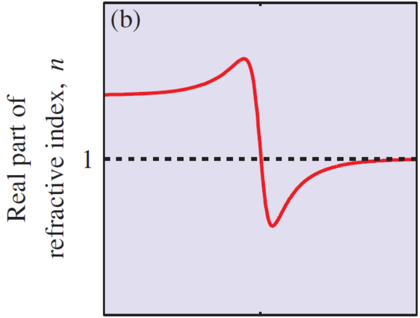


Total cross-section



Refractive index



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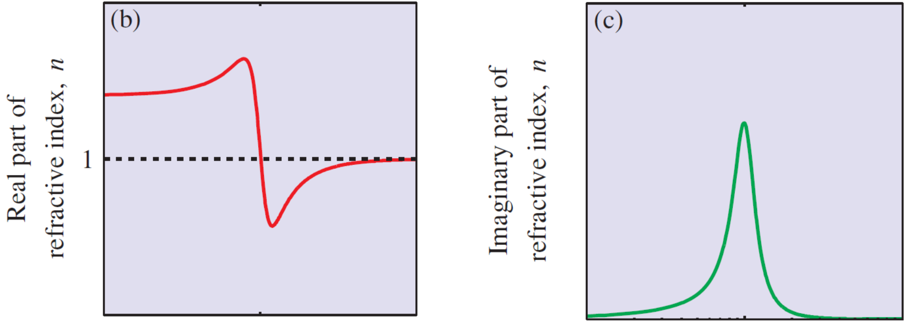
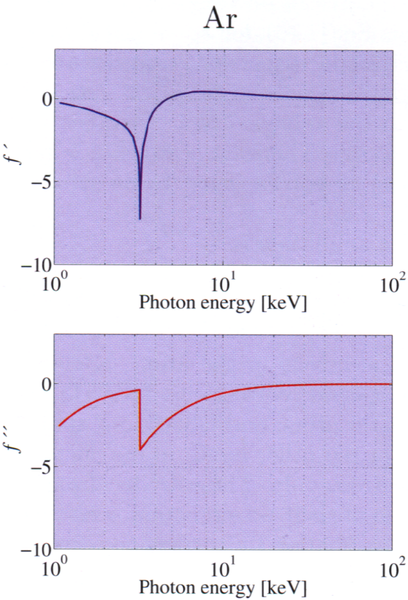
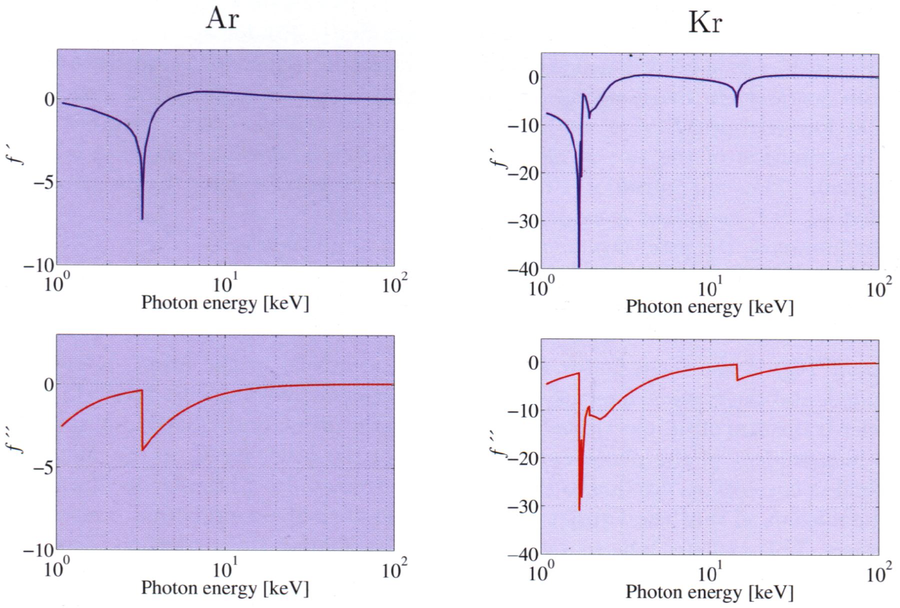


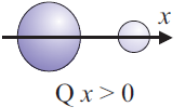
Calculated Cross Sections



Calculated Cross Sections

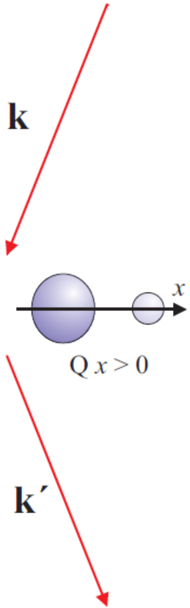


Scattering from Two Unlike Atoms



Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Scattering from Two Unlike Atoms



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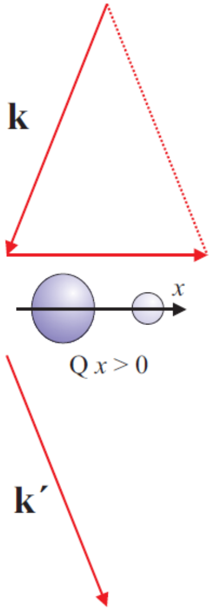
Consider two cases, with the scattering vector Q

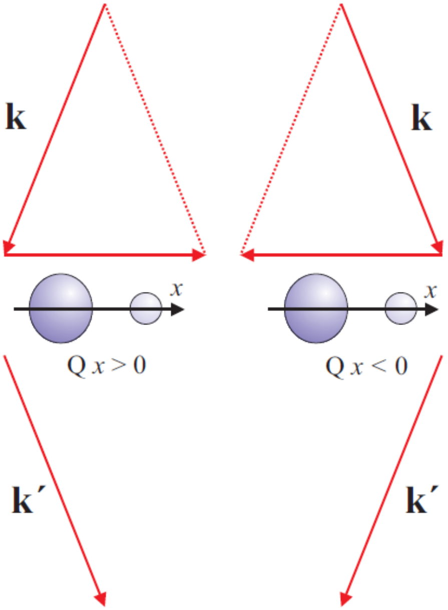
Scattering from Two Unlike Atoms



Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Consider two cases, with the scattering vector Q in the same direction as the orientation vector

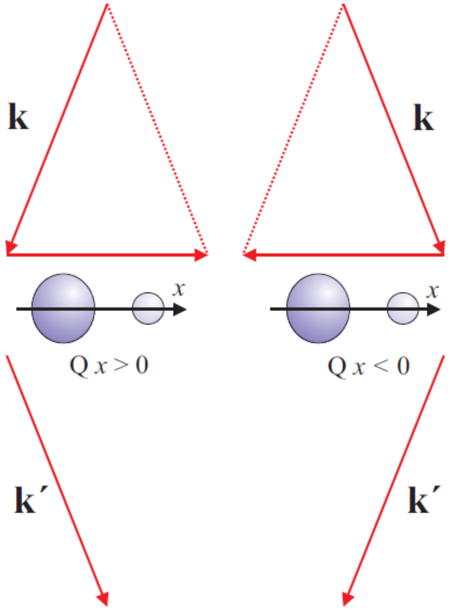
Scattering from Two Unlike Atoms



Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Consider two cases, with the scattering vector Q in the same direction as the orientation vector and opposite to the orientation vector.

Scattering from Two Unlike Atoms

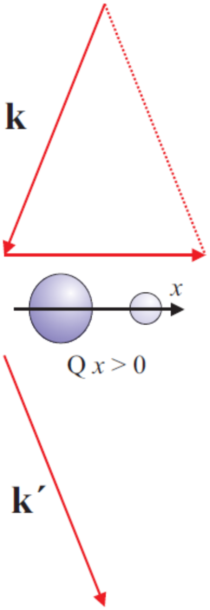


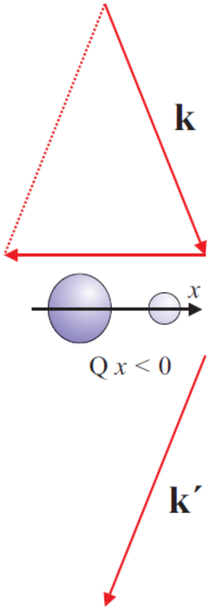
Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Consider two cases, with the scattering vector Q in the same direction as the orientation vector and opposite to the orientation vector.

Now compute the scattered intensity in each case, assuming scattering factors are purely real.

Friedel's Law





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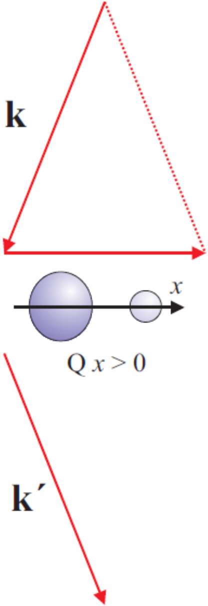
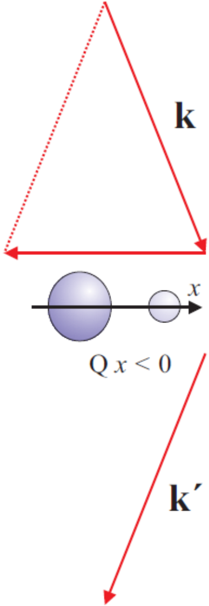


$$A(+Q) = f_1 + f_2 e^{+iQx}$$

$$A(-Q) = f_1 + f_2 e^{-iQx}$$



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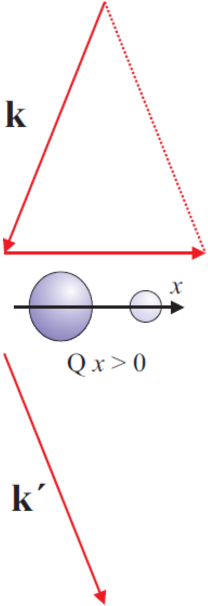

$$A(+Q) = f_1 + f_2 e^{+iQx}$$

$$I(+Q) = (f_1 + f_2 e^{+iQx})(f_1 + f_2 e^{-iQx})$$

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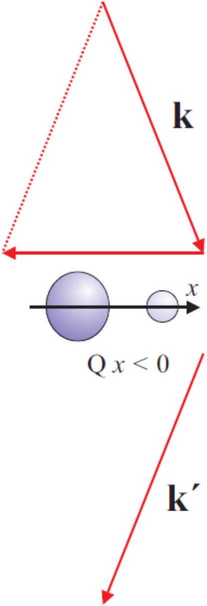

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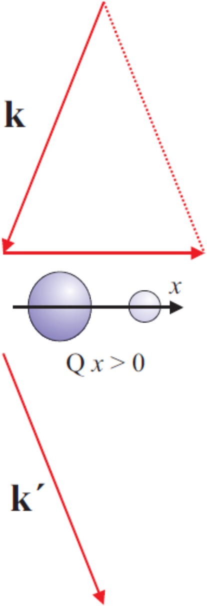

$$A(+Q) = f_1 + f_2 e^{+iQx}$$

$$\begin{aligned} I(+Q) &= (f_1 + f_2 e^{+iQx})(f_1 + f_2 e^{-iQx}) \\ &= f_1^2 + f_2^2 + 2 f_1 f_2 \cos(Qx) \end{aligned}$$

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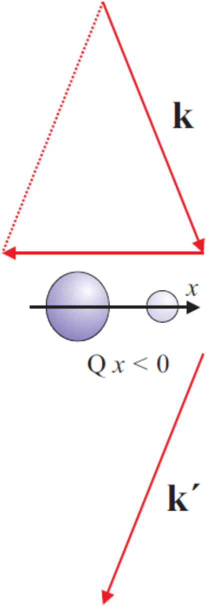

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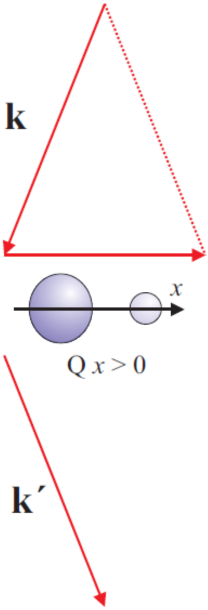

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$I(+Q) = I(-Q)$ Friedel's Law

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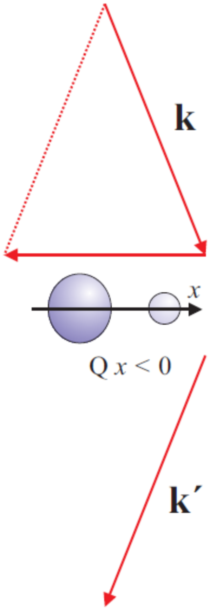

Breakdown of Friedel's Law

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If the scattering factor has resonant terms which are not negligible, we have to include them in the computation

$$f_j = f_j^0 + f_j' + if_j'' = r_j e^{i\phi_j} \qquad j = 1, 2 \qquad r_j = |f_j|$$

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&= r_1^2 + r_2^2 + r_1 r_2 e^{i\phi_1} e^{-i\phi_2} e^{-iQx} + r_1 r_2 e^{-i\phi_1} e^{i\phi_2} e^{iQx} \\
&= |f_1|^2 + |f_2|^2 + r_1 r_2 \big(e^{-(Qx+\phi_1-\phi_2)} + e^{+(Qx+\phi_1-\phi_2)}\big)
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$$\begin{aligned} I(Q) &= (r_1 e^{i\phi_1} + r_2 e^{i\phi_2} e^{iQx})(r_1 e^{-i\phi_1} + r_2 e^{-i\phi_2} e^{-iQx}) \\ &= r_1^2 + r_2^2 + r_1 r_2 e^{i\phi_1} e^{-i\phi_2} e^{-iQx} + r_1 r_2 e^{-i\phi_1} e^{i\phi_2} e^{iQx} \\ &= |f_1|^2 + |f_2|^2 + r_1 r_2 (e^{-(Qx+\phi_1-\phi_2)} + e^{+(Qx+\phi_1-\phi_2)}) \end{aligned}$$

$$I(Q) = |f_1|^2 + |f_2|^2 + 2 r_1 r_2 \cos(Qx + \phi_1 - \phi_2)$$

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&= |f_1|^2 + |f_2|^2 + r_1 r_2 (e^{-(Qx+\phi_1-\phi_2)} + e^{+(Qx+\phi_1-\phi_2)}) \\
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Thus, Friedel's Law breaks down unless there is a center of symmetry:

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Thus, Friedel's Law breaks down unless there is a center of symmetry:

$$
F = r_1 e^{-i(\phi_1 + Qx_1)} + r_1 e^{-i(\phi_1 - Qx_1)} + r_2 e^{-i(\phi_2 + Qx_2)} + r_2 e^{-i(\phi_2 - Qx_2)}
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&= r_1^2 + r_2^2 + r_1 r_2 e^{i\phi_1} e^{-i\phi_2} e^{-iQx} + r_1 r_2 e^{-i\phi_1} e^{i\phi_2} e^{iQx} \\
&= |f_1|^2 + |f_2|^2 + r_1 r_2 (e^{-(Qx+\phi_1-\phi_2)} + e^{+(Qx+\phi_1-\phi_2)}) \\
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&= [2r_1 \cos(Qx_1)] e^{-i\phi_1} + [2r_2 \cos(Qx_2)] e^{-i\phi_2}
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&= |f_1|^2 + |f_2|^2 + r_1 r_2 (e^{-(Qx+\phi_1-\phi_2)} + e^{+(Qx+\phi_1-\phi_2)}) \\
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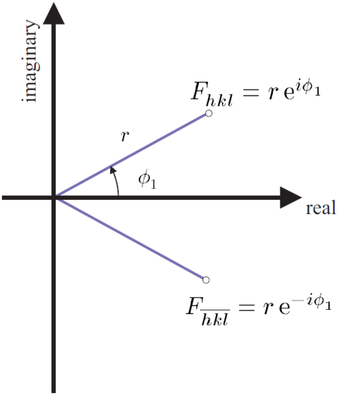
&= [2r_1 \cos(Qx_1)]e^{-i\phi_1} + [2r_2 \cos(Qx_2)]e^{-i\phi_2} \\
I(Q) &= 4|f_1|^2 + 4|f_2|^2 + 8|f_1||f_2| \cos(Qx_1)\cos(Qx_2)\cos(\phi_2 - \phi_1)
\end{aligned}
$$

Argand Diagram

This can all be described graphically using an Argand diagram:



no resonant terms

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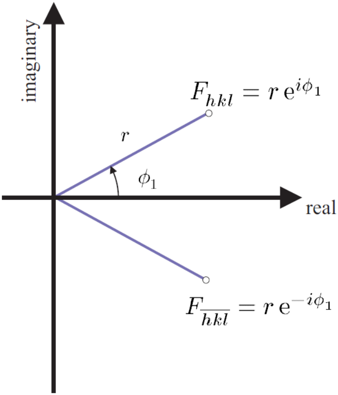
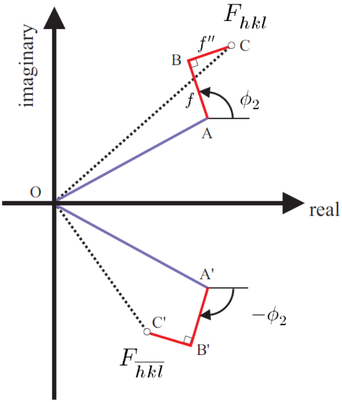
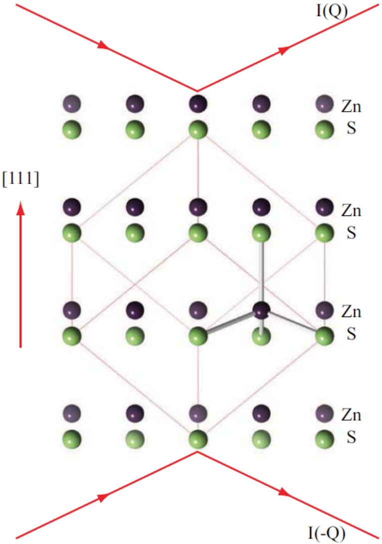


no resonant terms



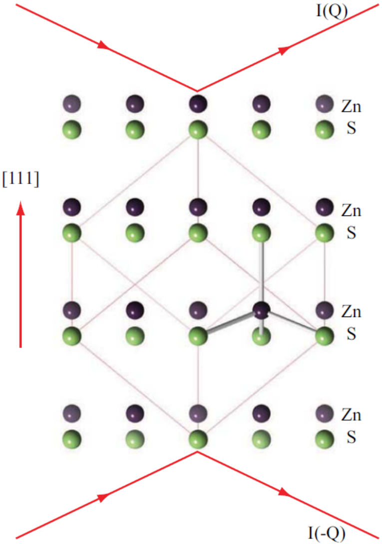
including resonant terms

ZnS Example



The ZnS structure is not centrosymmetric and when viewed along the $\langle 111 \rangle$ direction, it shows alternating stacked planes of Zn and S atoms.

ZnS Example

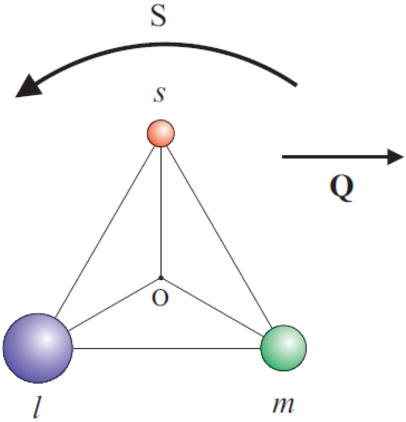


The ZnS structure is not centrosymmetric and when viewed along the $\langle 111 \rangle$ direction, it shows alternating stacked planes of Zn and S atoms.

Scattering from opposite faces of a single crystal of ZnS gives a different scattering factor and one can deduce the terminating surface atom.

Bijvoet Pairs - Chiral Molecules

Consider a tetrahedral molecule of carbon with four different species at each corner, oriented so the lightest is projected to the origin.



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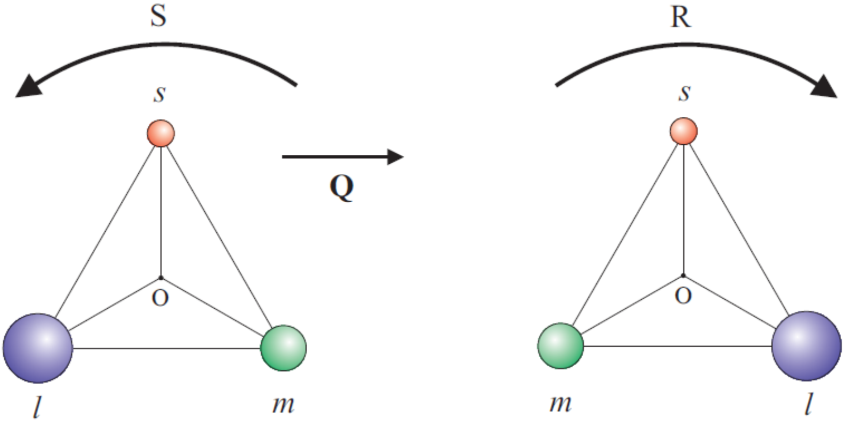
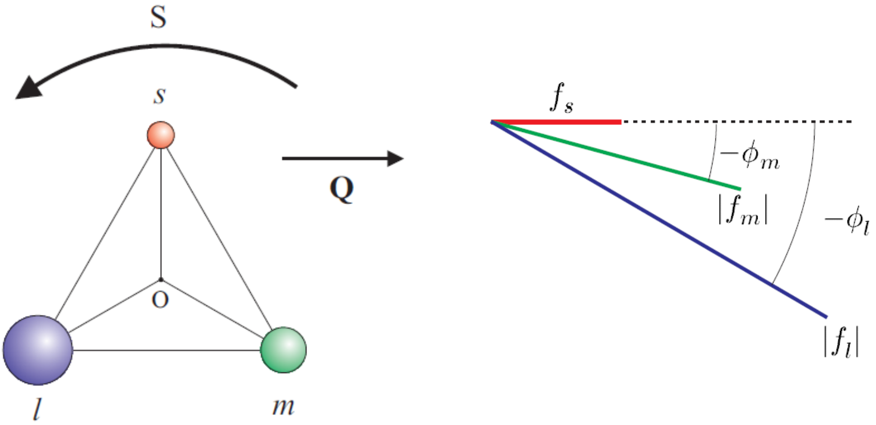
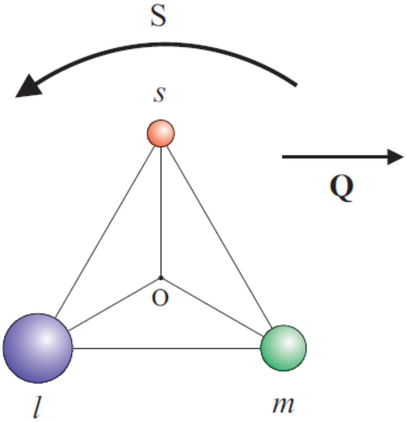


Each of the three atoms not at the origin has a scattering factor for $\vec{Q}$ as shown



Left Handed Scattering Factor



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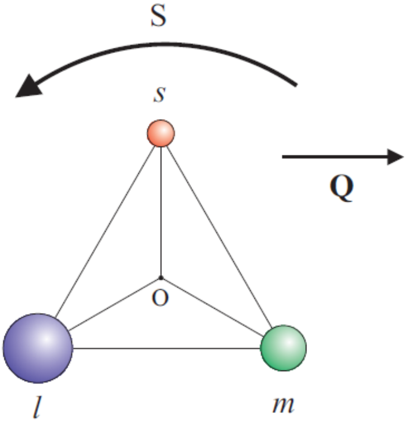
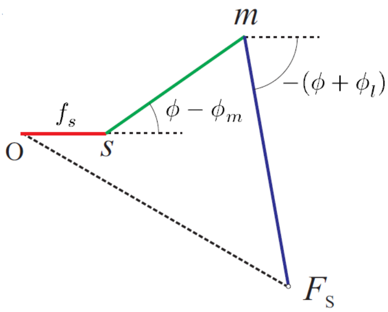
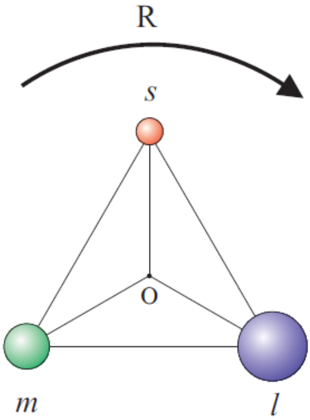


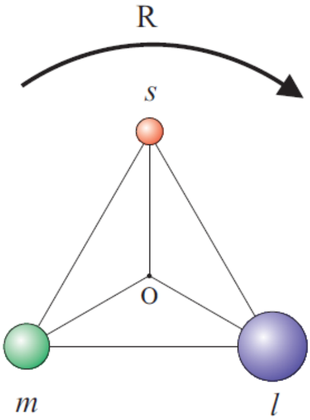


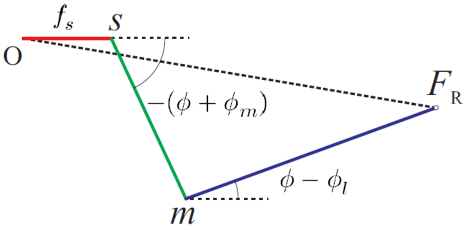
$$F_S = |f_s| + |f_m|e^{-i\phi_m}e^{i\phi} + |f_l|e^{-i\phi_l}e^{-i\phi}$$

Right Handed Scattering Factor



Right Handed Scattering Factor

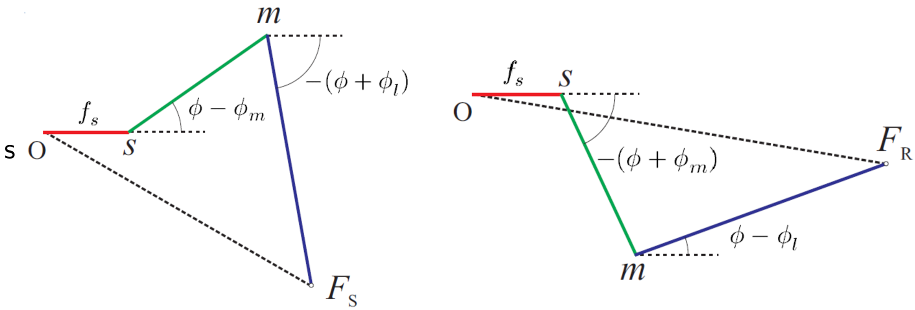




$$F_R = |f_s| + |f_m|e^{-i\phi_m}e^{-i\phi} + |f_l|e^{-i\phi_l}e^{i\phi}$$

Scattering Factor Comparison

It is thus possible to tell the difference in handedness of chiral molecule simply by x-ray scattering



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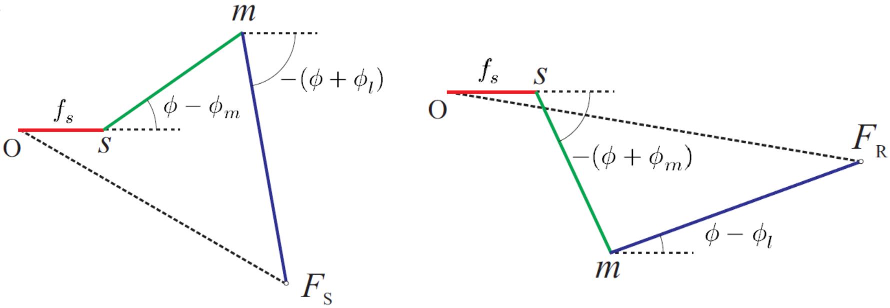
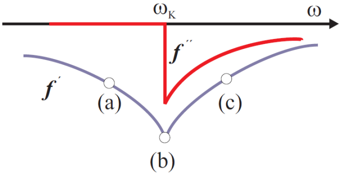
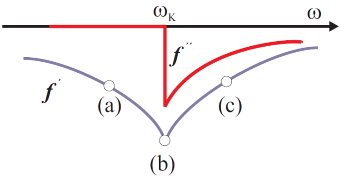
s 

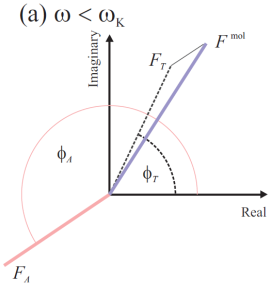
$$\left| |f_s| + |f_m|e^{-i\phi_m}e^{i\phi} + |f_l|e^{-i\phi_l}e^{-i\phi} \right|^2 \neq \left| |f_s| + |f_m|e^{-i\phi_m}e^{-i\phi} + |f_l|e^{-i\phi_l}e^{i\phi} \right|^2$$

MAD Phasing

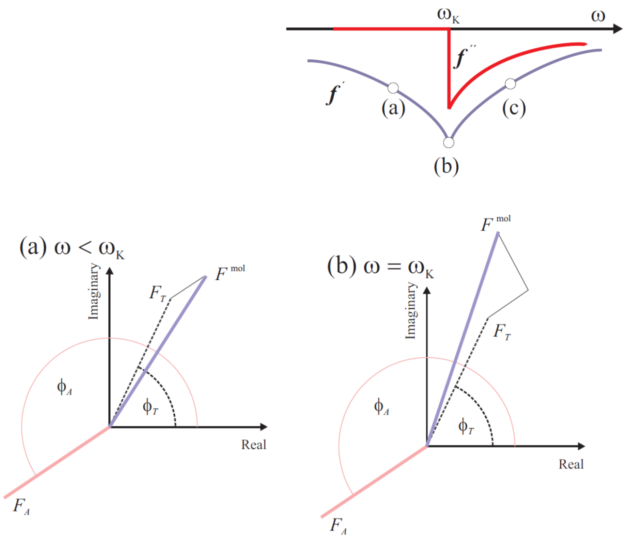


MAD Phasing



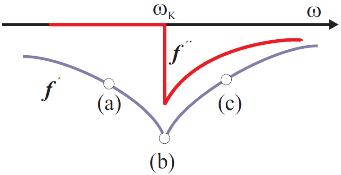


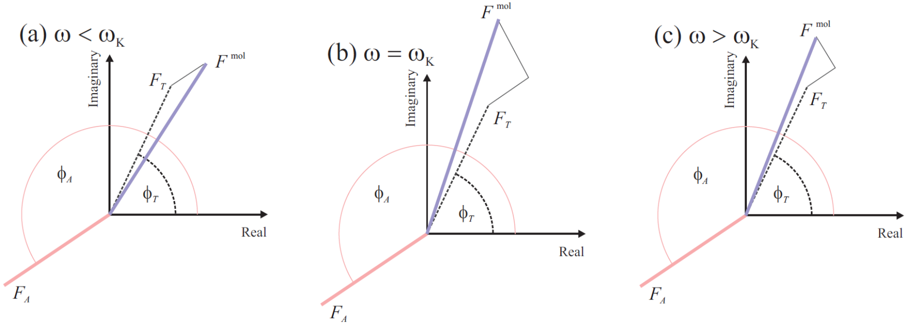
MAD Phasing



ω_K
ω
f''
f'
(a)
(b)
(c)
(a) $\omega < \omega_K$
Imaginary
F^{mol}
F_T
ϕ_A
ϕ_T
Real
F_A
(b) $\omega = \omega_K$
Imaginary
F^{mol}
F_T
ϕ_A
ϕ_T
Real
F_A

MAD Phasing

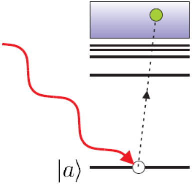




Comparison of Matrix Elements

Absorption

$$\frac{e\vec{A}\cdot\vec{p}}{m}$$



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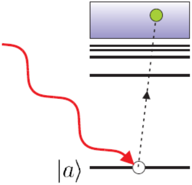
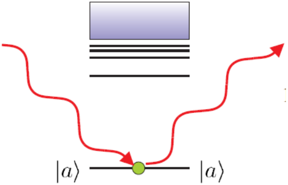


Thomson scattering

$$\frac{e^2A^2}{2m}$$



Comparison of Matrix Elements

Absorption	Thomson scattering	Resonant scattering
$\dfrac{e\vec{A}\cdot\vec{p}}{m}$	$\dfrac{e^2A^2}{2m}$	$\left(\dfrac{e\vec{A}\cdot\vec{p}}{m}\right)^2$