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due Monday, November 28, 2016

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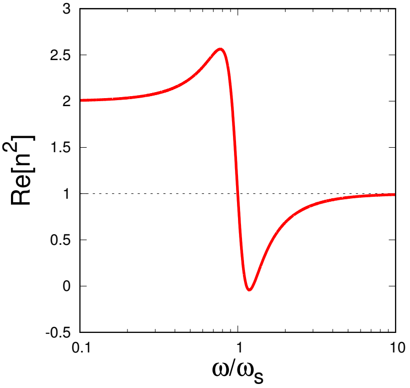

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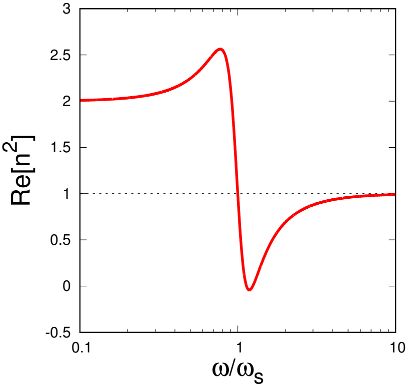

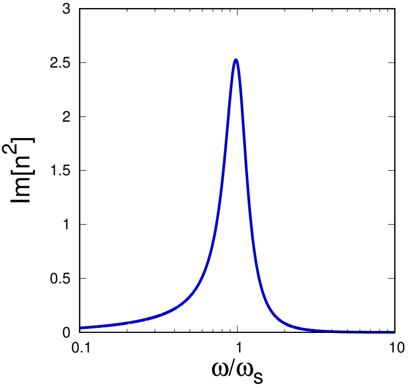

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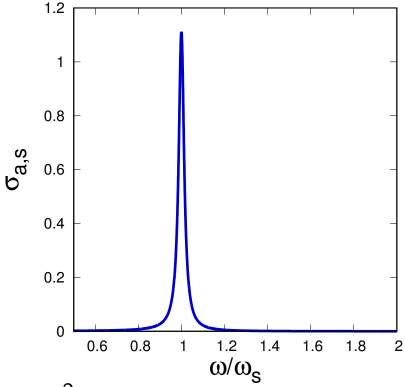

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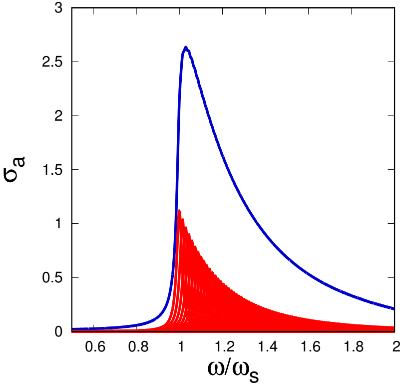

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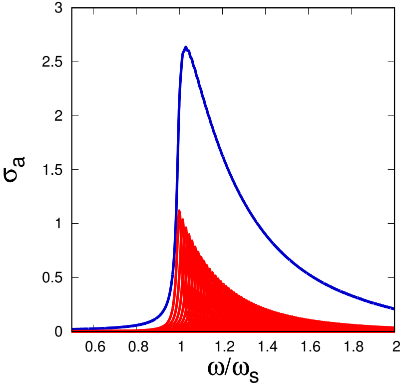

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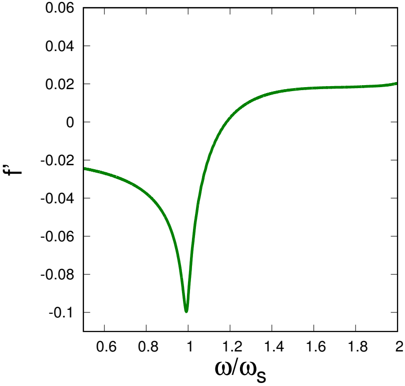

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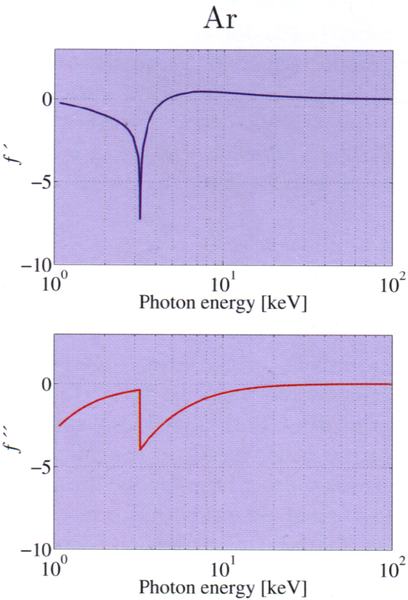
Calculated cross-sections



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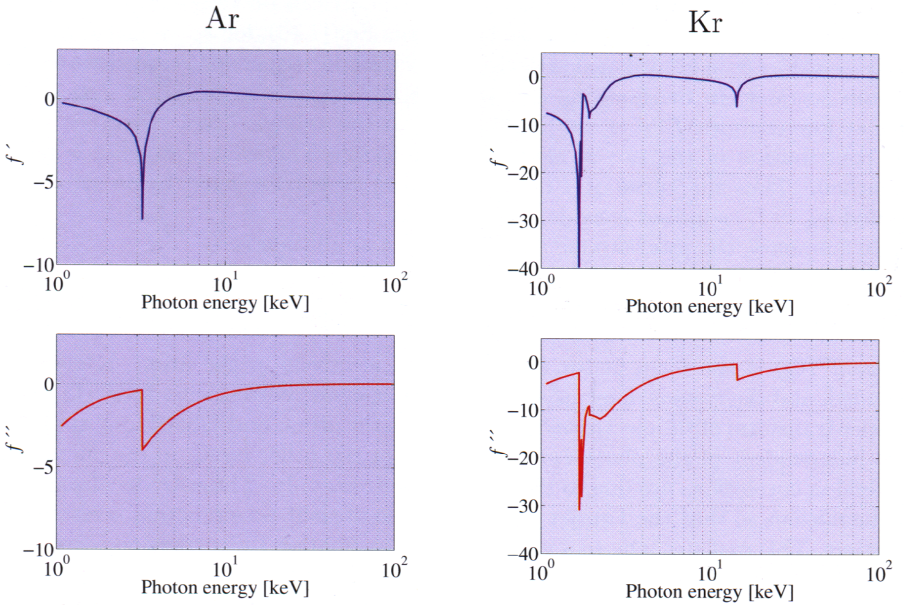
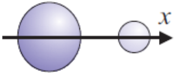


Scattering from two unlike atoms



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

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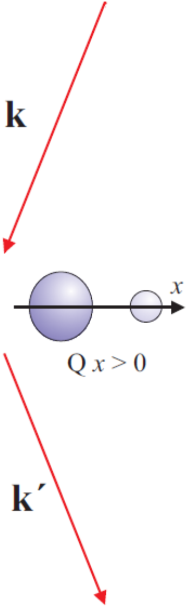
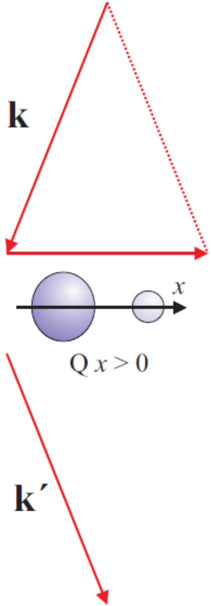


Two unlike atoms with scattering factors f_1 and f_2 are oriented by a vector pointing from the larger to the smaller.

Consider two cases, with the scattering vector Q

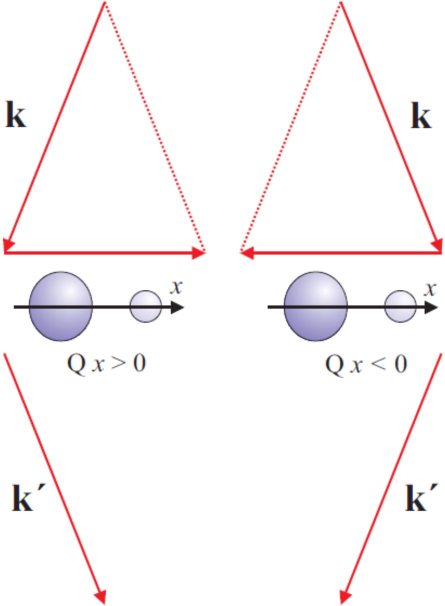
Scattering from two unlike atoms



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

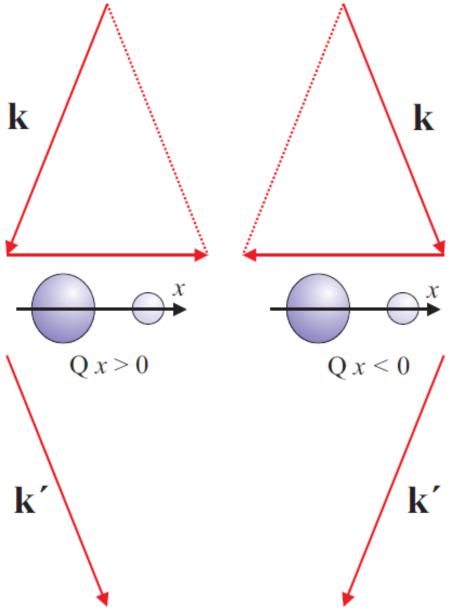
Scattering from two unlike atoms



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



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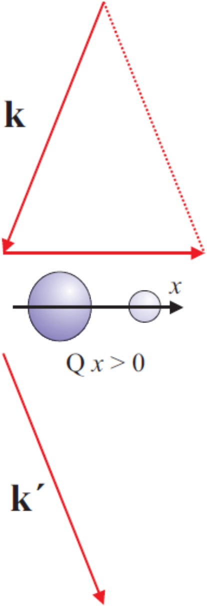
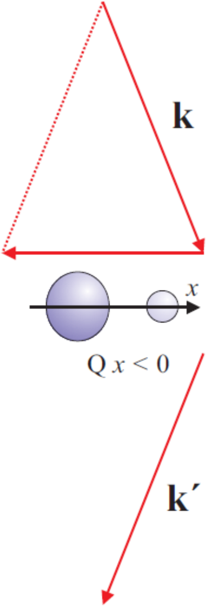
Now compute the scattered intensity in each case, assuming scattering factors are purely real.

Friedel's Law





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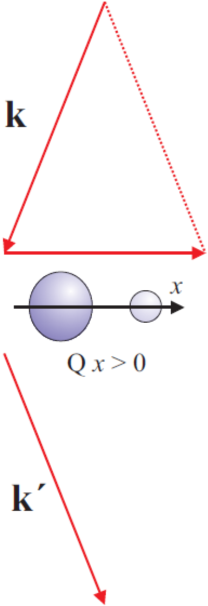
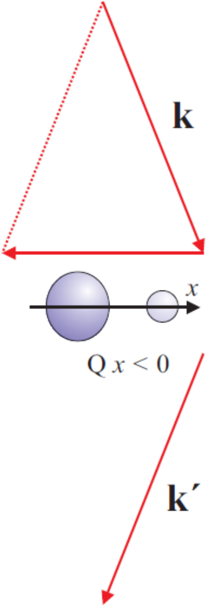


$$A(+Q) = f_1 + f_2 e^{+iQx}$$

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



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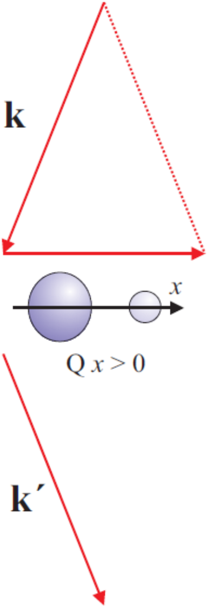

$$A(+Q) = f_1 + f_2 e^{+iQx}$$

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

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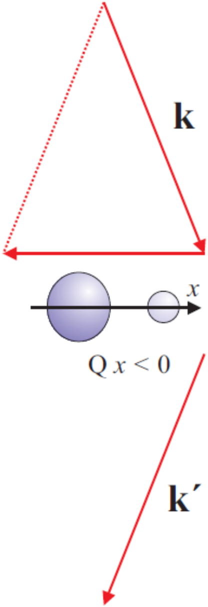

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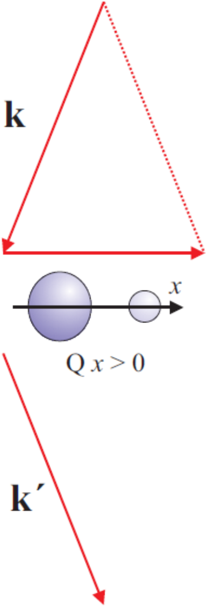

$$A(+Q) = f_1 + f_2 e^{+iQx}$$

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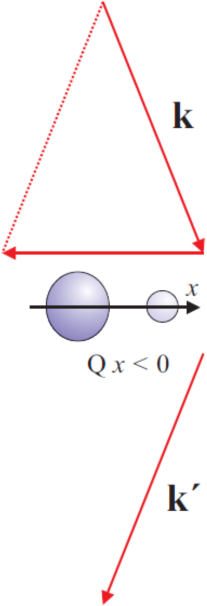
$$= f_1^2 + f_2^2 + 2 f_1 f_2 \cos(Qx)$$



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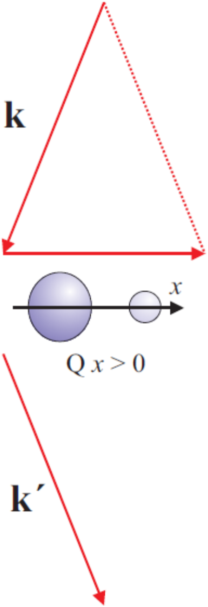
Friedel's Law



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

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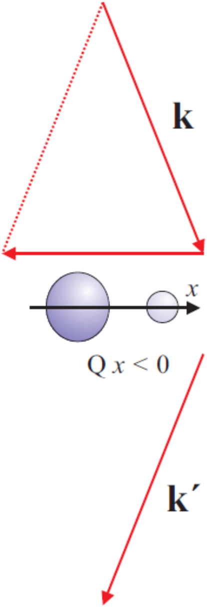

Breakdown of Friedel's Law

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$$F = r_1 e^{-i(\phi_1 + Qx_1)} + r_1 e^{-i(\phi_1 - Qx_1)} + r_2 e^{-i(\phi_2 + Qx_2)} + r_2 e^{-i(\phi_2 - Qx_2)}$$

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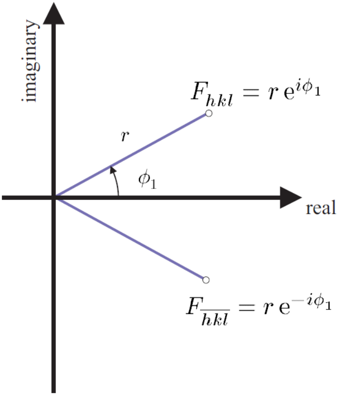
$$

Argand diagram

This can all be described graphically using an Argand diagram:



no resonant terms

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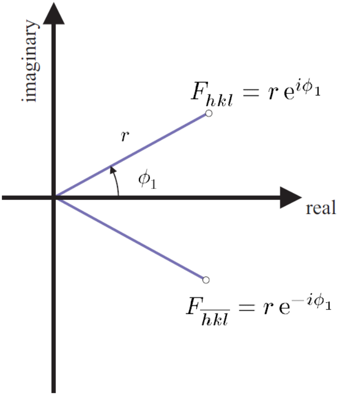
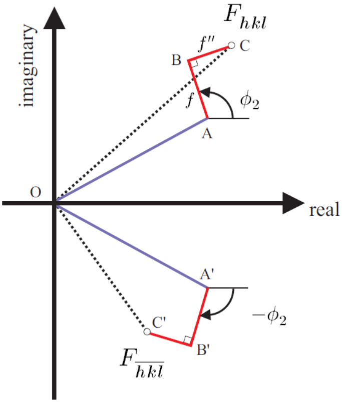
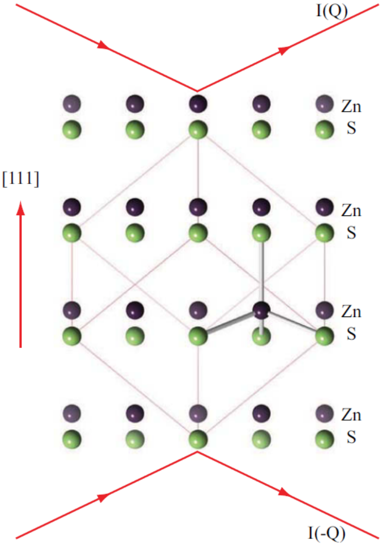


no resonant terms



including resonant terms

ZnS example



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

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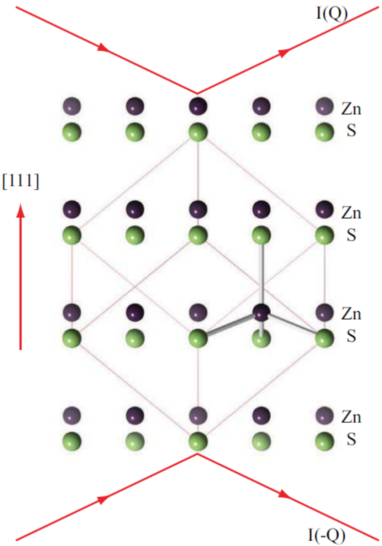

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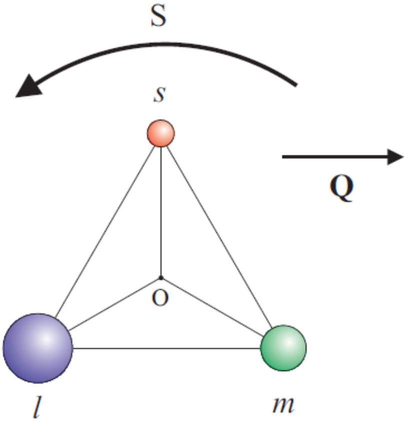
Scattering from opposite faces of a single crystal of ZnS gives a different scattering factor and one can deduce the terminating surface atom.

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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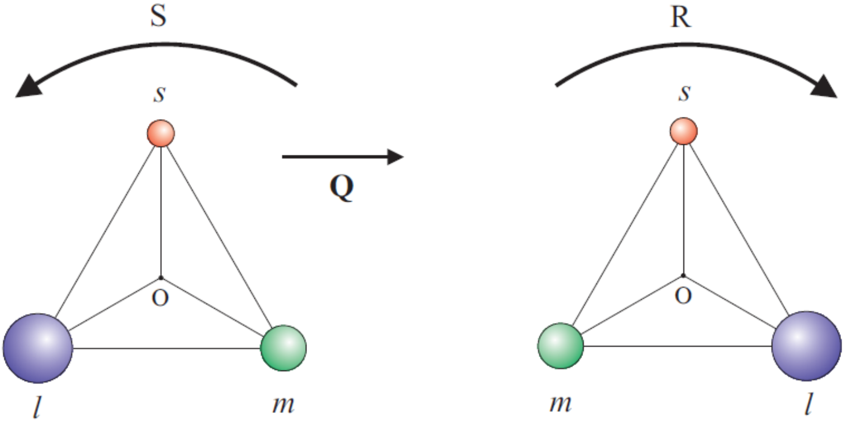
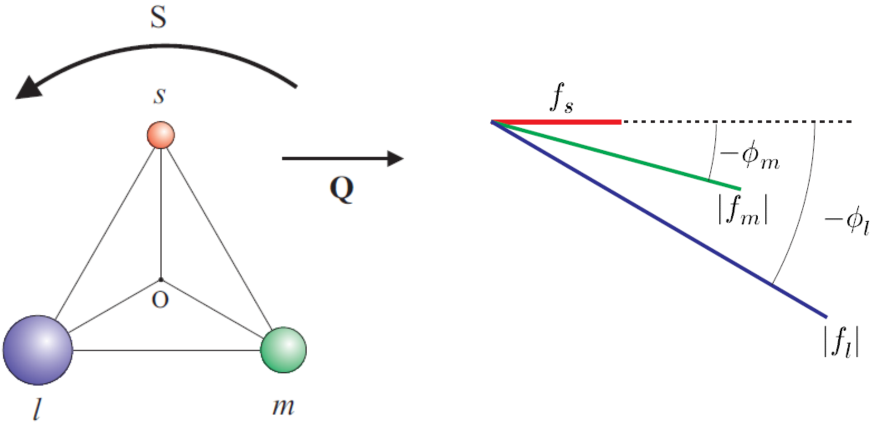
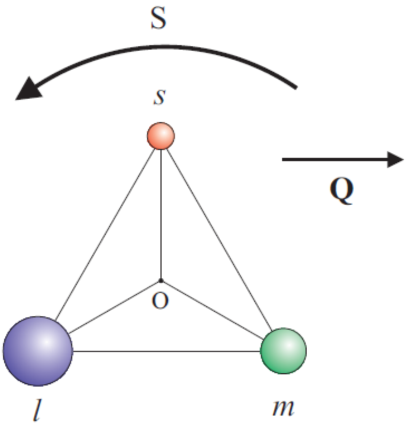


Atomic scattering factors

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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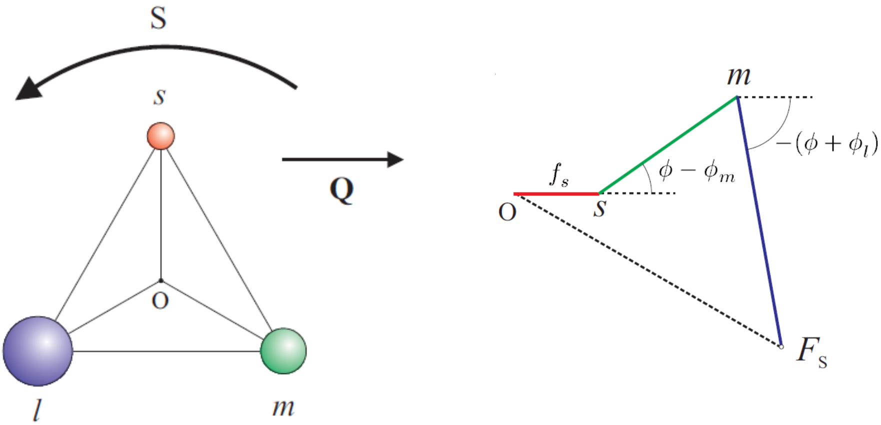

$$F_S = |f_s| + |f_m|e^{-i\phi_m}e^{i\phi} + |f_l|e^{-i\phi_l}e^{-i\phi}$$

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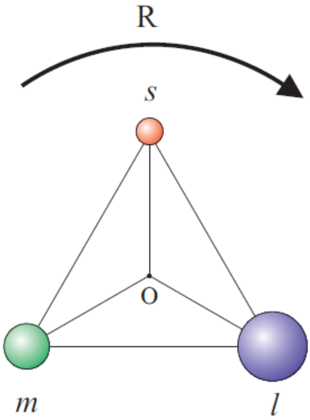

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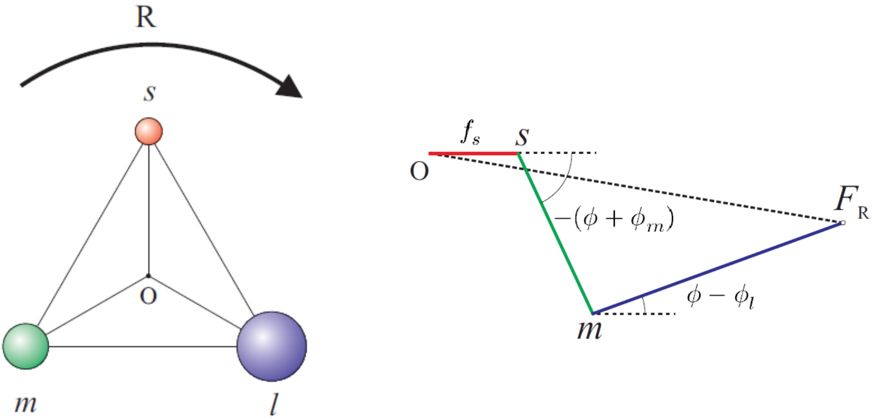
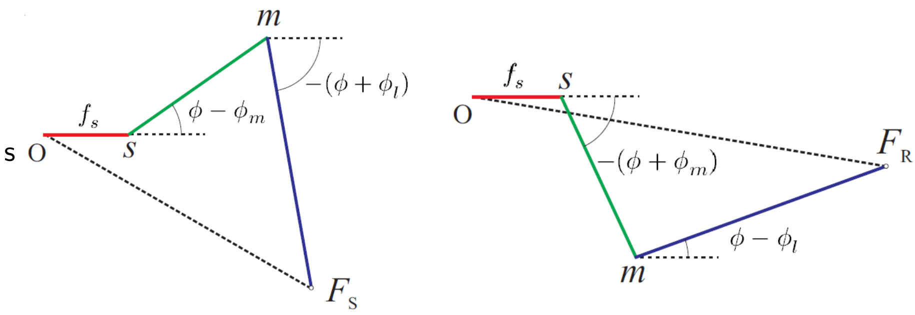


$$F_R = |f_s| + |f_m|e^{-i\phi_m}e^{-i\phi} + |f_l|e^{-i\phi_l}e^{i\phi}$$

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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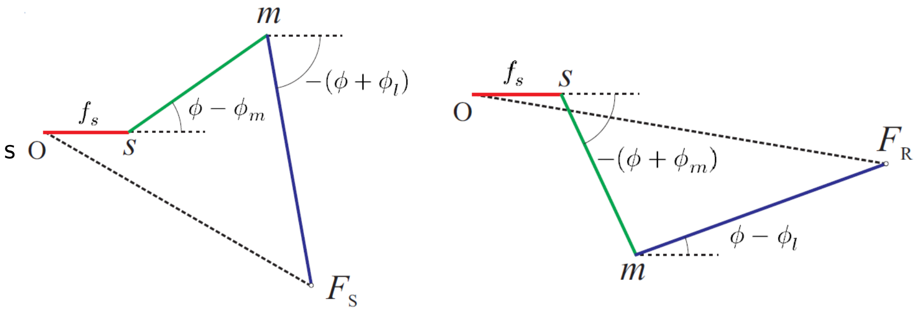
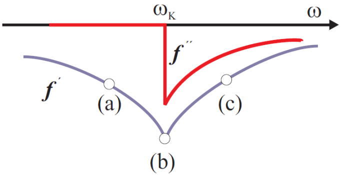
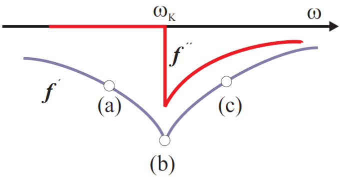


$$\left| |f_s| + |f_m| e^{-i\phi_m} e^{i\phi} + |f_l| e^{-i\phi_l} e^{-i\phi} \right|^2 \neq \left| |f_s| + |f_m| e^{-i\phi_m} e^{-i\phi} + |f_l| e^{-i\phi_l} e^{i\phi} \right|^2$$

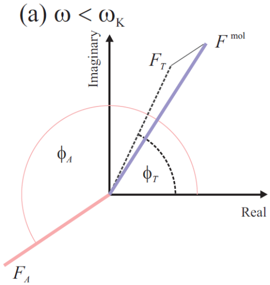
MAD phasing



MAD phasing

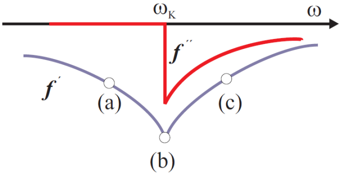


ω_K
ω
f''
f'
(a)
(b)
(c)

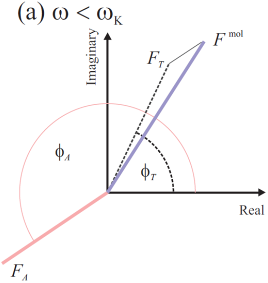


(a) $\omega < \omega_K$
Imaginary
F^{mol}
F_T
ϕ_A
ϕ_T
Real
F_A

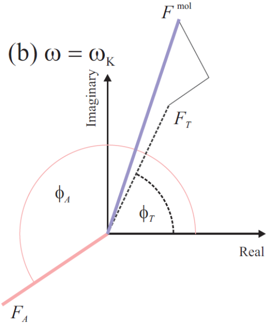
MAD phasing



ωK
ω
f''
f'
(a)
(b)
(c)

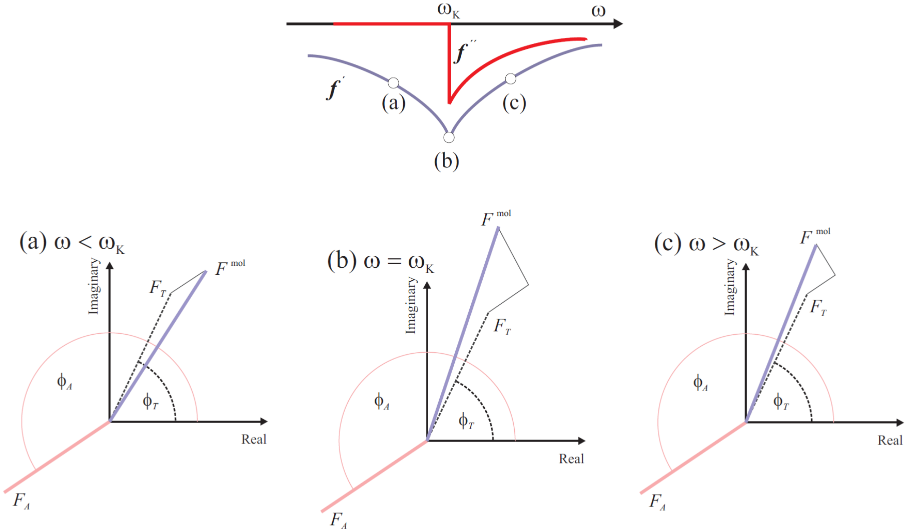


(a) ω < ωK
Imaginary
Real
F mol
F T
ϕA
ϕT
FA



(b) ω = ωK
Imaginary
Real
F mol
F T
ϕA
ϕT
FA

MAD phasing

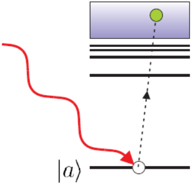


ω_K
ω
f''
f'
(a)
(c)
(b)
(a) ω < ω_K
Imaginary
F_T
F mol
ϕ_A
ϕ_T
Real
F_A
(b) ω = ω_K
Imaginary
F mol
F_T
ϕ_A
ϕ_T
Real
F_A
(c) ω > ω_K
Imaginary
F mol
F_T
ϕ_A
ϕ_T
Real
F_A

Comparison of matrix elements

Absorption

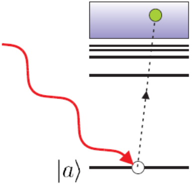
$$\frac{e\vec{A}\cdot\vec{p}}{m}$$



Comparison of matrix elements

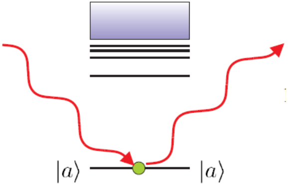
Absorption

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



Thomson scattering

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



Comparison of matrix elements

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