Angular distributions of scattering kernels and 1st-order intensities with the SAP code

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Visualization of scattering angular distributions with the SAP code

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Angular distributions of scattering intensities with the SAP code

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Summary

- Introduction
- Physical background and mathematical description
- Examples of use of SAP:
  - Angular distributions of scattering differential cross-sections
  - Angular distribution of first order photon scattering flux in transmission and reflection

Introduction: why scattering?

- Rayleigh and Compton scattering (together with photoelectric effect) are the prevailing interactions for x-rays in the energy range (1-1000 keV)
- In x-ray fluorescence experiments, scattering represents background
- Scattering carries information on the target density (scattering investigation techniques)

Introduction: what is SAP?

SAP (Scattering Angular distribution Plot) is a graphical tool to compute and plot the angular distributions of the following quantities (involving Rayleigh and Compton scattering):

- electronic angular differential cross-section
- atomic angular differential cross-section
- form factor (FF) and scattering function (SF)
- reflected and transmitted first-order intensities
- Rayleigh to Compton ratio (R/C) for transmission and reflection

Angular differential cross-sections: single element

- *Rayleigh scattering*

$$\frac{d\sigma_R}{d\vartheta} = \frac{r_e^2 N}{2A}\left(1+\cos^2\vartheta\right) F^2(X,Z) \qquad \left[cm^2/g\right]$$

Form Factor

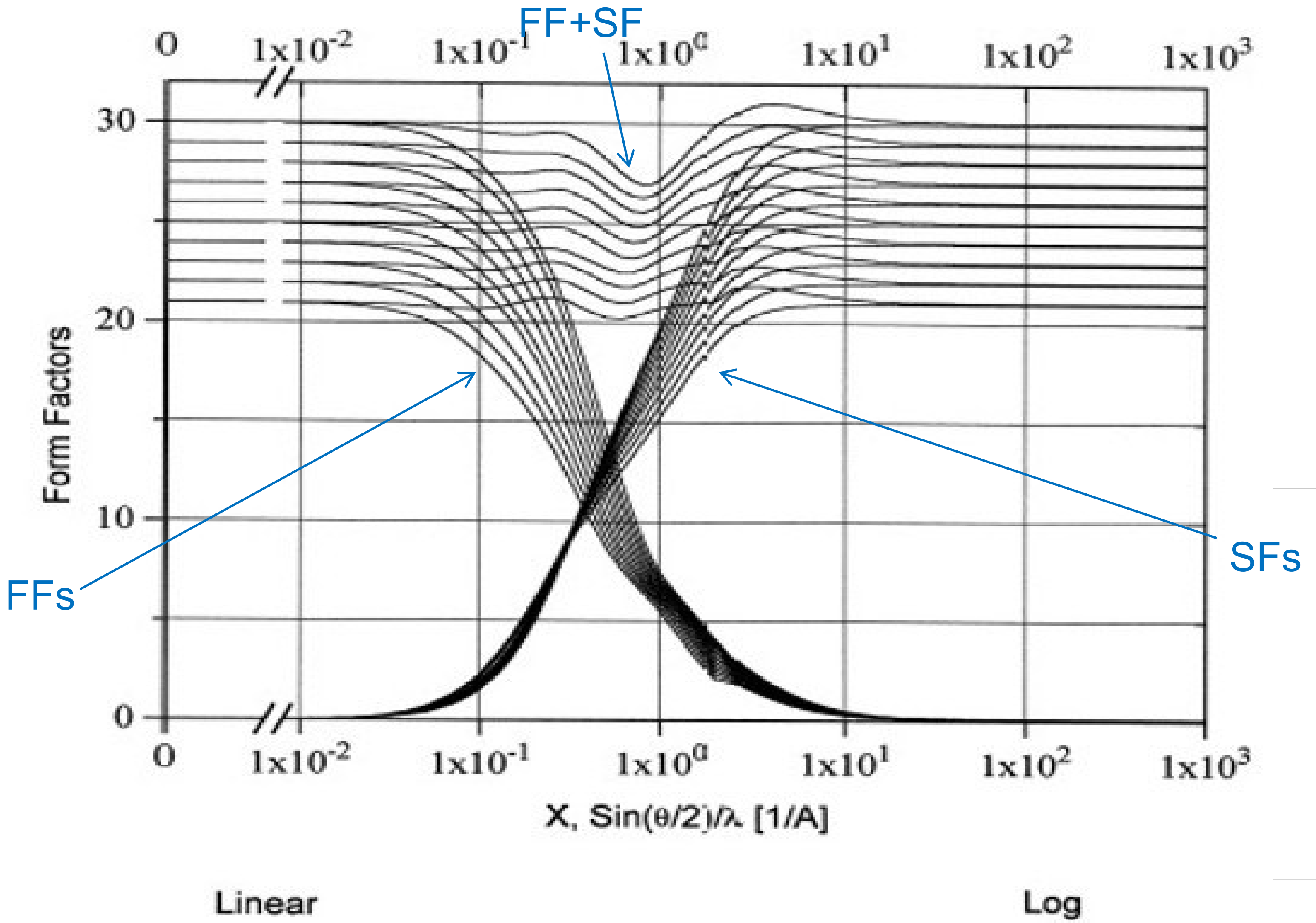
- *Compton scattering*

$$\frac{d\sigma_C}{d\vartheta} = \frac{r_e^2 N}{2A}\left(\frac{E_P}{E}\right)^2\left(\frac{E_P}{E}+\frac{E}{E_P}-\sin^2\vartheta\right) S(X,Z) \qquad \left[cm^2/g\right]$$

Scattering Function

Form Factors and Scattering Functions

As a function of the transferred momentum for selected atomic numbers: from 21 (Sc) to 30 (Zn)



Angular differential cross-sections: compound or mixture

Rayleigh

- Electronic $$\left(\frac{d\sigma_R}{d\vartheta}\right)_{el,comp} = \sum_{i=1}^{n} w_i \left(\frac{d\sigma_R}{d\vartheta}\right)_{el,i}$$
- Atomic $$\left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at,comp} = \sum_{i=1}^{n} w_i \left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at,i}$$

Compton

- Electronic $$\left(\frac{d\sigma_C}{d\vartheta}\right)_{el,comp} = \sum_{i=1}^{n} w_i \left(\frac{d\sigma_C}{d\vartheta}\right)_{el,i}$$
- Atomic $$\left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at,comp} = \sum_{i=1}^{n} w_i \left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at,i}$$

Computation of FFs and SFs

- *Single element*
  - **From table**: logarithmic interpolation of the EPDL97 database (Cullen et al. 1997)
  - **Computed** (Fernandez 2000): combination of analytical calculations (Veigele et al. 1966), and semi-analytical formulas (Cromer et al. 1969,1974) (Smith et al. 1975)
- *Mixture or compound*

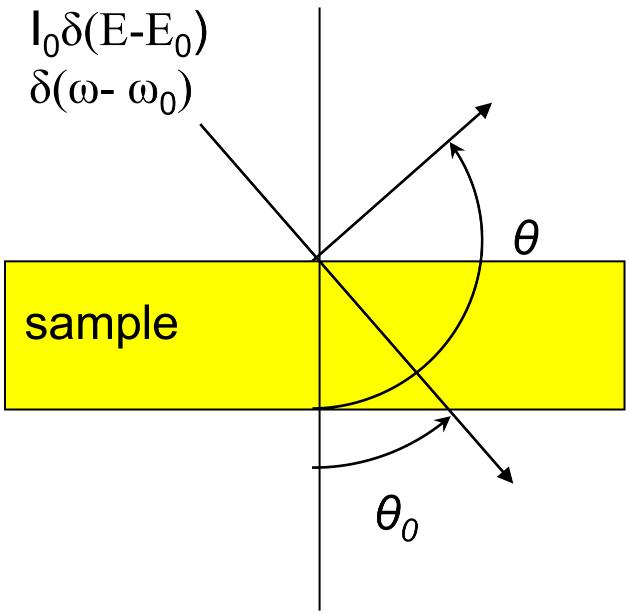
$$\left\langle F^2(X,Z_i)\right\rangle_{comp} = \frac{\left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at,comp}}{\left(\frac{d\sigma_R}{d\vartheta}\right)_{el,comp}} = \sum_{i=1}^{n}\alpha_i^{at}F^2(X,Z_i)$$

$$\left\langle S(X,Z_i)\right\rangle_{comp} = \frac{\left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at,comp}}{\left(\frac{d\sigma_C}{d\vartheta}\right)_{el,comp}} = \sum_{i=1}^{n}\alpha_i^{at}S(X,Z_i)$$

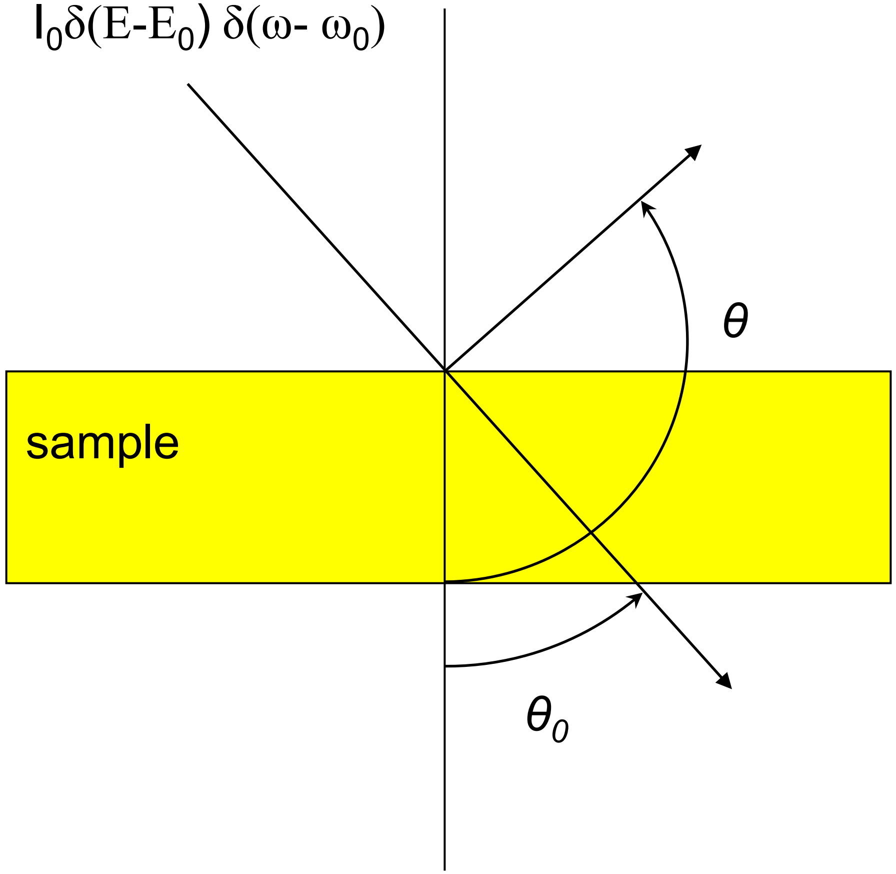
$$\alpha_i^{at} = \frac{\frac{w_i}{A_i}}{\sum_{i=1}^{n}\frac{w_i}{A_i}}$$

Physical and geometrical model

- Specimen:
  - Homogeneous
  - 1D geometry
- Source:
  - Monochromatic excitation
  - Collimated beam
  - Energy range 1-1000 keV
- First order Rayleigh and Compton scattering (no multiple scattering)
- No polarization effects considered



Physical and geometrical model



d = sample thickness

$$\eta_0 = \cos\theta_0 \qquad \alpha_0 = \frac{\mu(E_0)}{|\eta_0|}$$

$$\eta = \cos\theta \qquad \alpha = \frac{\mu(E')}{|\eta|}$$

Outgoing energy

- *Rayleigh scattering*

$$E' = E_0$$

- *Compton scattering*

$$E' = \frac{E_0}{1 + \frac{E_0}{mc^2}(1 - \cos\vartheta)}$$

First order scattering flux

- ***Reflection***
  - *Semi-Infinite Target*

$$I_S = \frac{I_0}{|\eta||\eta_0|}\frac{1}{\alpha+\alpha_0}\left(\frac{d\sigma_{S,at}}{d\vartheta}\right)_{comp}$$

  - *Finite Target*

$$I_S = \frac{I_0}{|\eta||\eta_0|}\frac{1-\exp\left[-(\alpha+\alpha_0)d\right]}{\alpha+\alpha_0}\left(\frac{d\sigma_{S,at}}{d\vartheta}\right)_{comp}$$

- ***Transmission***
  - *Finite Target*

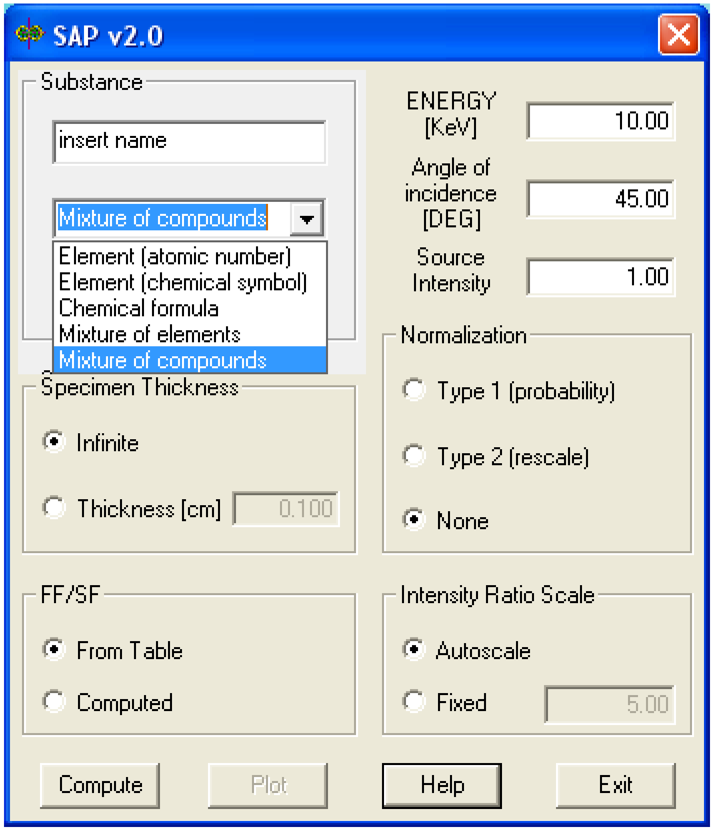
$$I_S = \frac{I_0}{|\eta_0||\eta|}\frac{\exp\left[-(\alpha_0-\alpha)d\right]-1}{\alpha-\alpha_0}\exp\left(-\alpha\, d\right)\left(\frac{d\sigma_{S,at}}{d\vartheta}\right)_{comp}$$

with $\alpha_0 = \frac{\mu(E_0)}{|\eta_0|}$ $\alpha = \frac{\mu(E')}{|\eta|}$

SAP (Scattering Angular distribution Plot)

Every computation consists of four stages

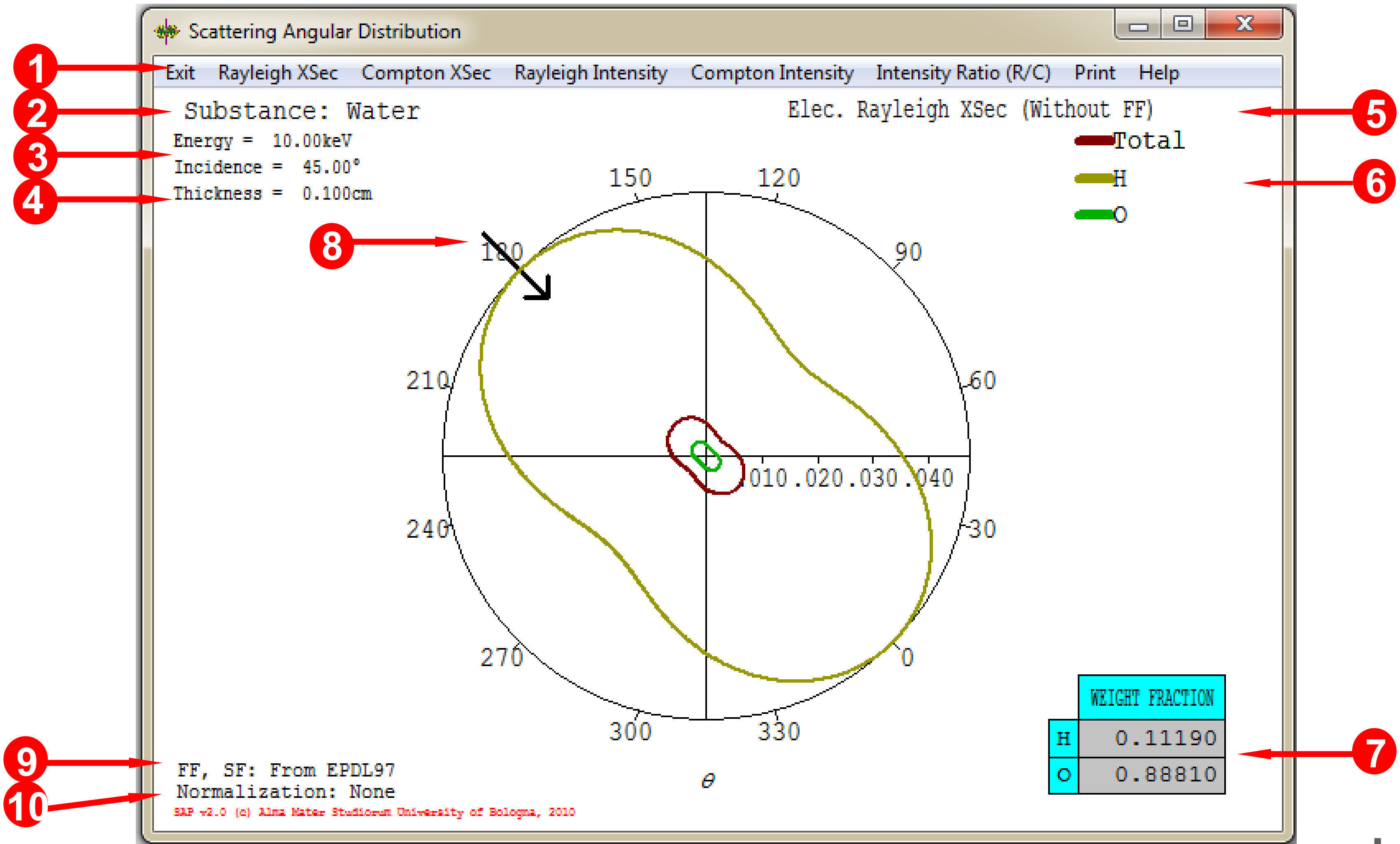
- definition of the required parameters
- computation with automatic saving of the results in the report file sap_out.txt
- graphical visualization of the results
- saving of the plot as encapsulated postscript (eps) file



Definition of the parameters: Main dialog

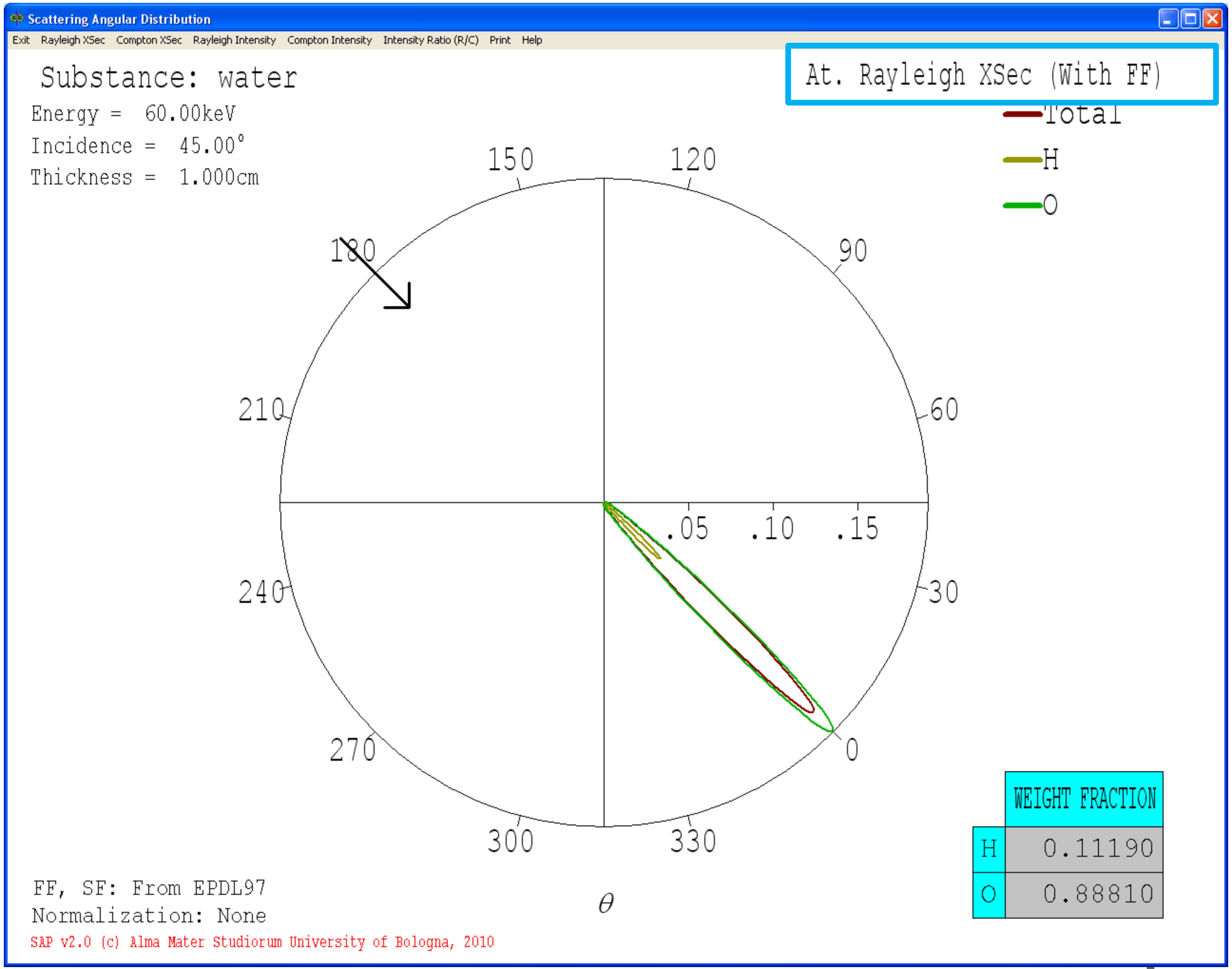
- substance properties
- source properties
- specimen thickness
- table or semi-analytical FF/SF computation
- kernel normalization (if any)
- scale for the R/C reprensentation

Graphical visualization of the results



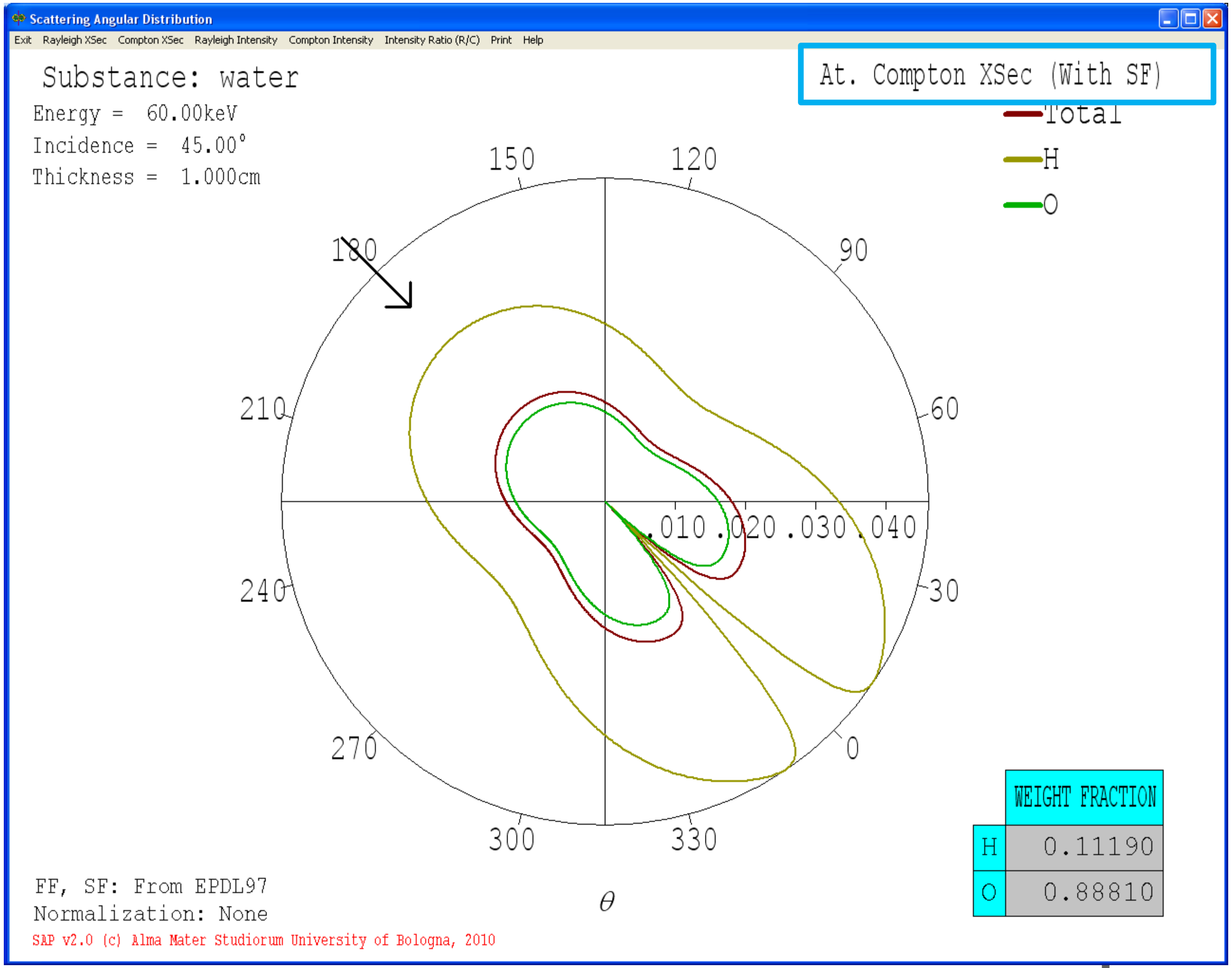
Example: Rayleigh kernel
Water 60 keV

Substance: Water
Composition: H_2O
Energy: 60 keV
Normalization: None
FF/SF: From EPDL97



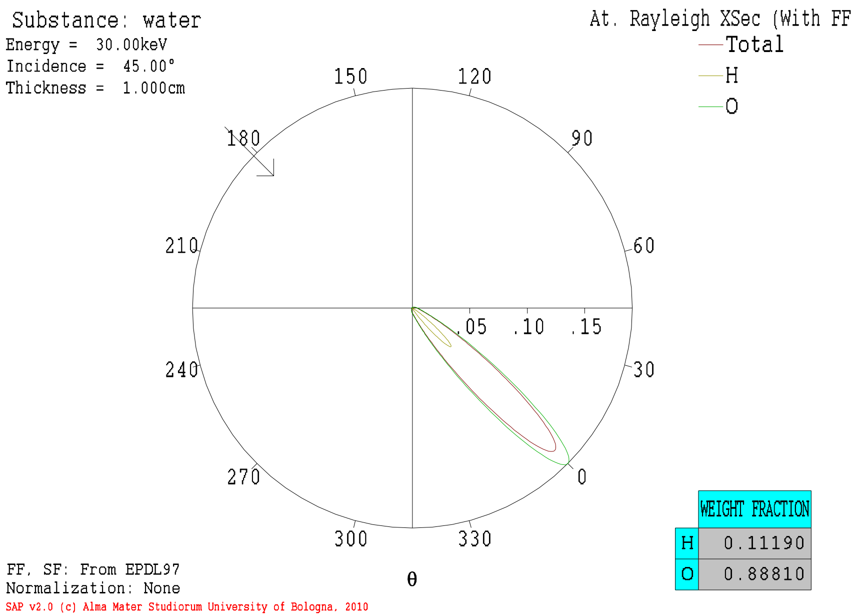
Example: Compton kernel
Water 60 keV

Substance: Water
Composition: H_2O
Energy: 60 keV
Normalization: None
FF/SF: From EPDL97

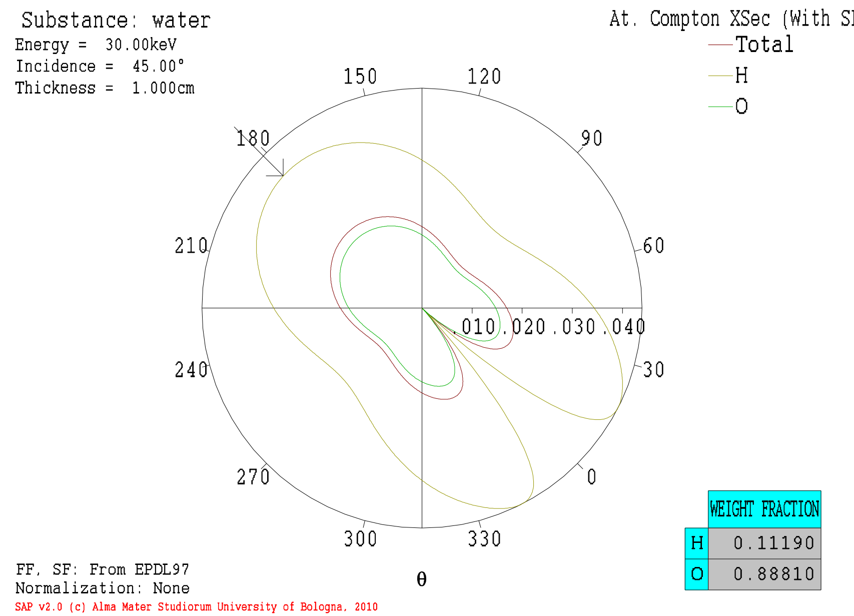


Influence of energy on kernels

Rayleigh kernel



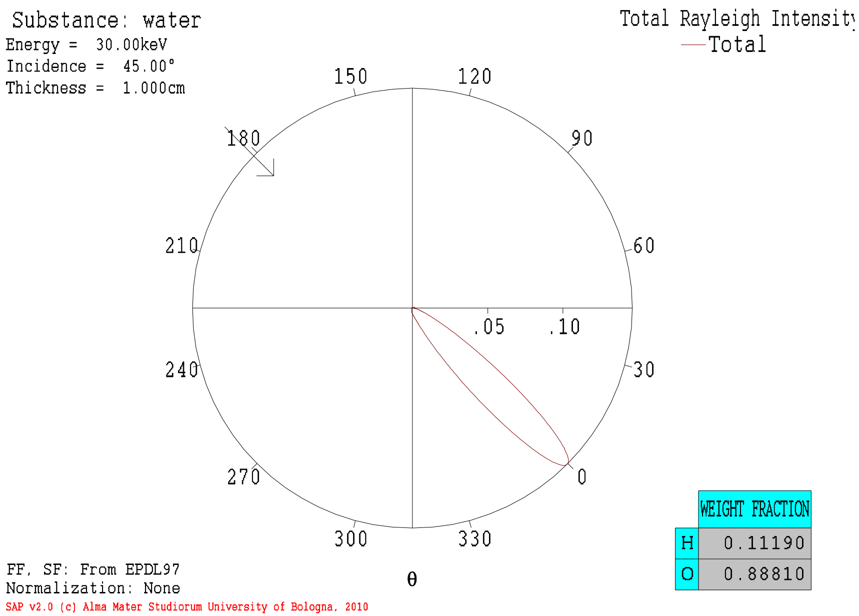
Compton kernel



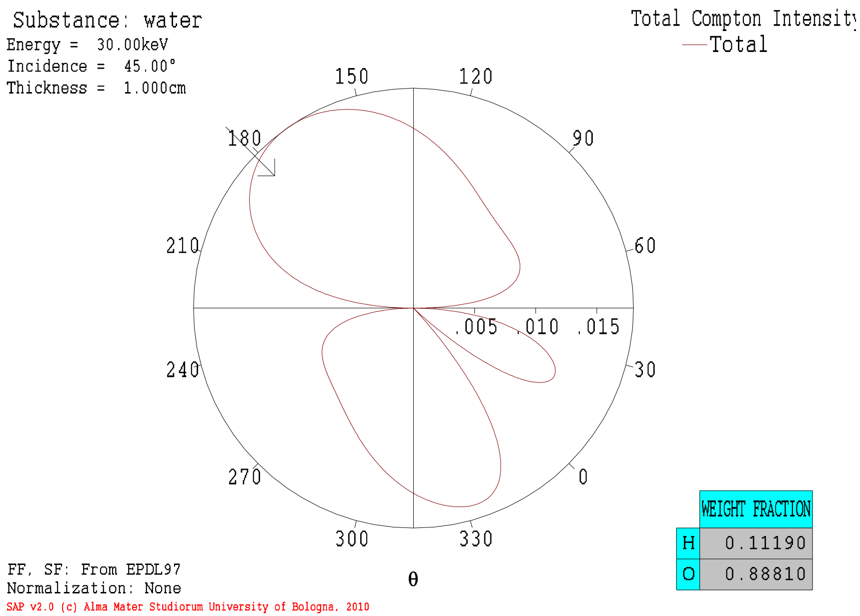
Substance: Water
Composition: H_2O
Energy: 10 keV - 20 keV - 30 keV
Normalization: None
FF/SF: From EPDL97

Influence of energy on intensity

Rayleigh Total Intensity



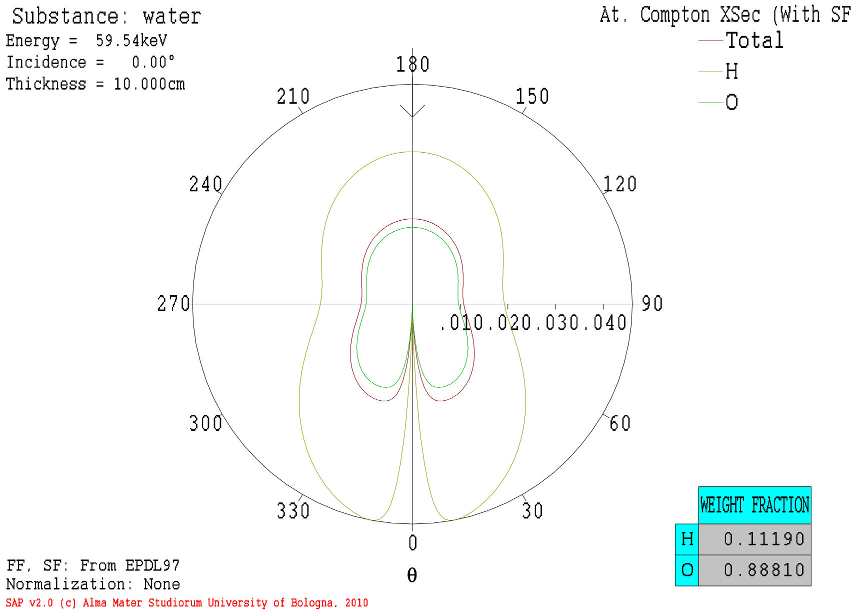
Compton Total Intensity



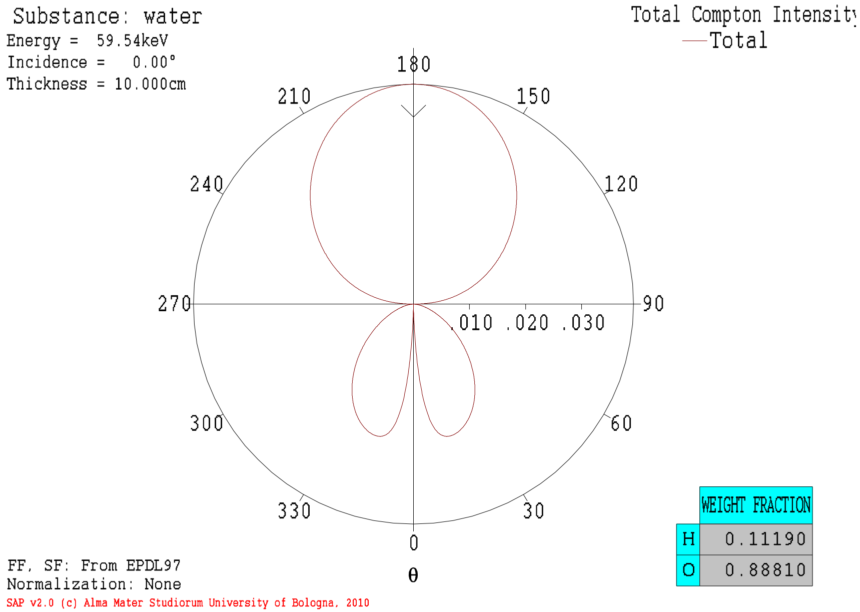
Substance: Water
Composition: H2O
Energy: 10 keV – 20 keV – 30 keV
Thickness: 1 cm
FF/SF: From EPDL97

Influence of sample thickness on Compton intensity

Reference Compton kernel



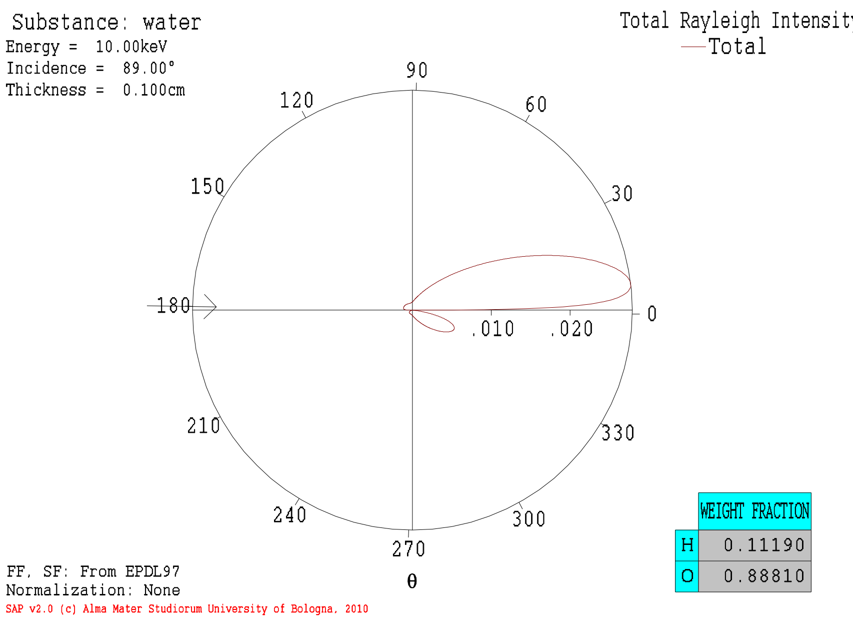
Compton Total Intensity



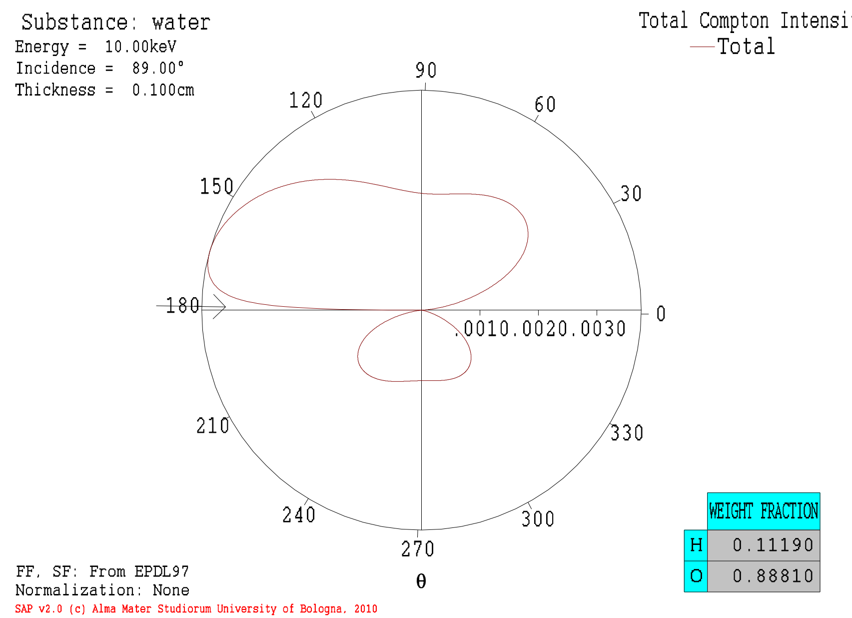
Substance: Water
Composition: Compound (chemical formula) → H2O
Energy: 59.54 keV
Thickness: 0.05 cm – 0.5 cm – 1 cm – 10 cm
FF/SF: From EPDL97

Influence of incidence angle on intensity

Rayleigh Total Intensity

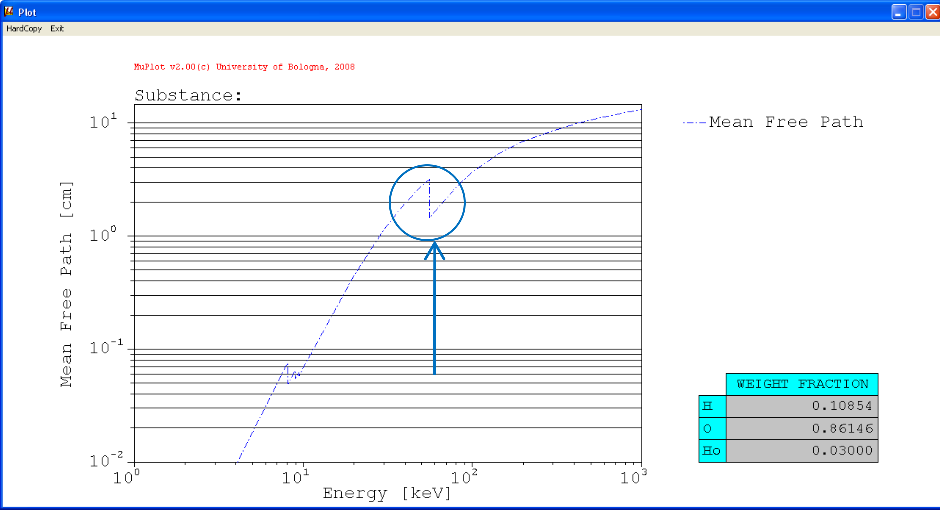


Compton Total Intensity



Substance: Water
Composition: H2O
Energy: 10 keV **Thickness:** 0.1 cm
Incidence angle: 0° - 30° - 45° - 60° - 89°
FF/SF: From EPDL97

mpton intensity of
mpound



Composition: H_2O (97%)
Ho (3%)

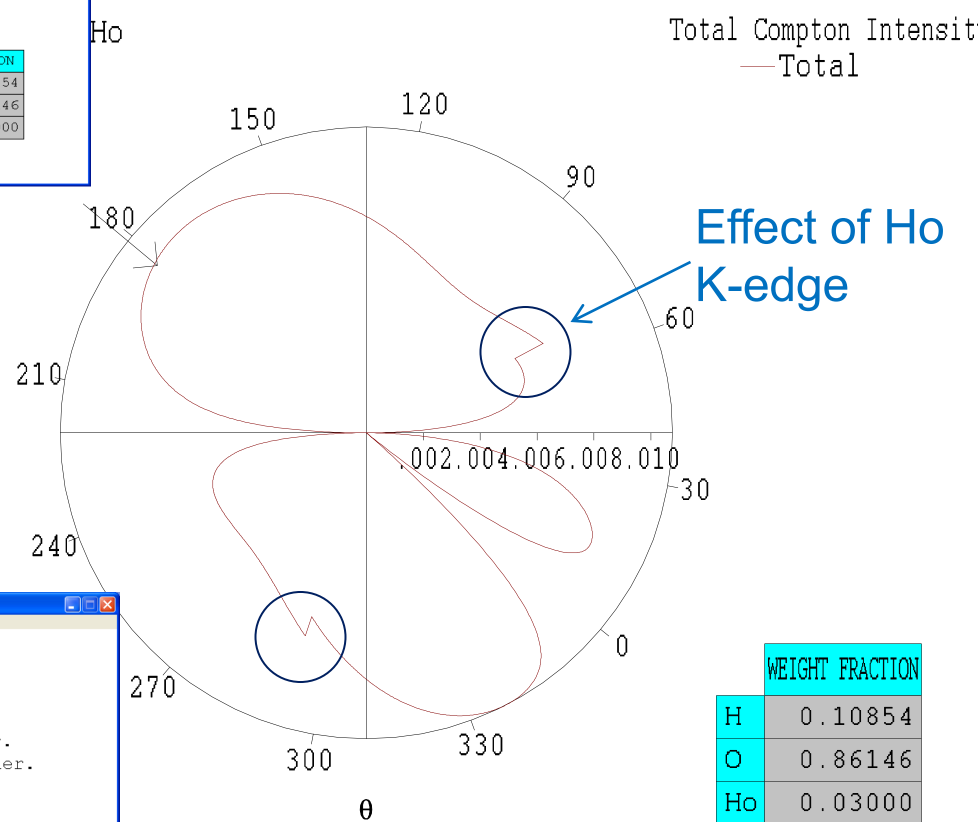
Energy: 59.54 keV

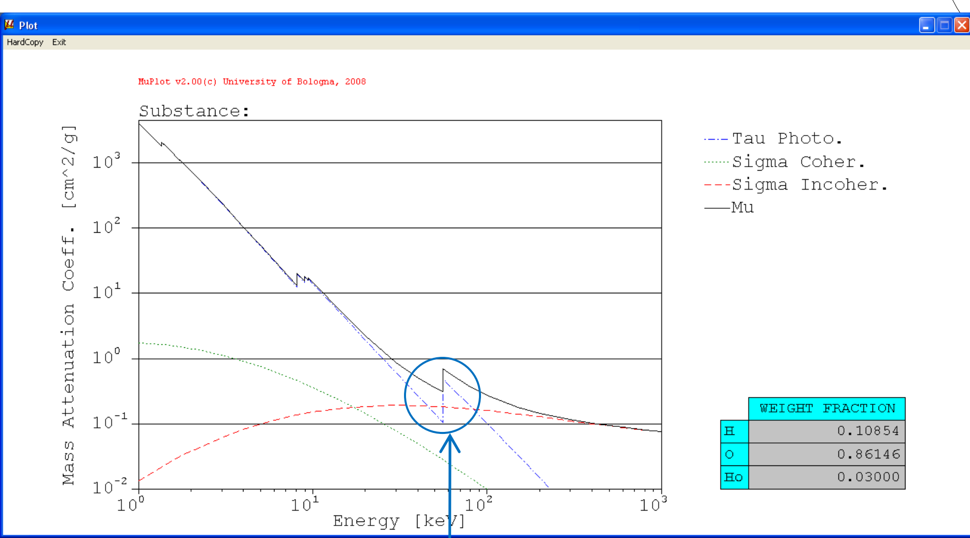
Thickness: 0.5 cm

Incidence angle: 50°

FF/SF: From EPDL97

Ho K-edge 55.62 keV





Conclusions

- The code SAP computes and plots:
  - angular distribution of first order Rayleigh and Compton intensities for reflection and transmission
  - angular distributions of FFs and SFs
  - angular distributions of electronic and atomic scattering kernels
- Useful tool to determine the optimal position of the detector in a scattering experiment
- Applications on industry, medicine and non-destructive testing (NDT) with scattering techniques

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