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# Visualization of scattering angular distributions with the SAP code

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ABSTRACT

SAP (Scattering Angular distribution Plot) is a graphical tool developed at the University of Bologna to compute and plot Rayleigh and Compton differential cross-sections (atomic and electronic), form-factors (FFs) and incoherent scattering functions (SFs) for single elements, compounds and mixture of compounds, for monochromatic excitation in the range of 1–1000 keV. The computation of FFs and SFs may be performed in two ways: (a) by interpolating Hubbell's data from EPDL97 library and (b) by using semi-empirical formulas as described in the text. Two kinds of normalization permit to compare the plots of different magnitudes, by imposing a similar scale. The characteristics of the code SAP are illustrated with one example.

## 1. Introduction

The atomic differential cross-section of Rayleigh and Compton scattering has been well described by Hubbell et al. [1] in terms of the so called form-factors (FFs) and incoherent scattering functions (SFs), which add the collective effect of many electrons to the electronic cross-section. As a consequence, the angular dependence of the electronic cross-section may be heavily modified by the FFs and SFs distributions. The graphical representation of the scattering angular distributions is important to get an immediate picture of the preferred directions of X-ray photons after scattering. The polar angle represents the only relevant magnitude to describe the angular distributions because they are uniformly distributed in terms of the azimuthal angle.

This paper introduces the code SAP (Scattering Angular distribution Plot) developed at the University of Bologna. SAP is a graphical tool to compute and plot Rayleigh and Compton differential cross-sections (atomic and electronic), expressed in [cm$^2$/g], and FFs and SFs, for single and multi-element specimens. All calculations are performed for monochromatic excitation in the range of 1–1000 keV. FFs and SFs may be computed in two ways: (a) by interpolating Hubbell's data from EPDL97 library [2] and (b) by using semi-empirical formulas as described by Fernandez [3].

Since the computed quantities may have very different plot scales, two kinds of normalization can be used to simplify the representation and to compare plots of different magnitudes.

## 2. The code SAP

For each element in a substance and for a specific energy, the code SAP computes and visualizes a polar plot (as a function of the scattering angle $\vartheta$) of the following quantities:

- The electronic angular differential cross-section for Rayleigh and Compton scattering
- The atomic angular differential cross-section for Rayleigh and Compton scattering
- The angular distribution of the FF for Rayleigh scattering
- The angular distribution of the SF for Compton scattering

Every computation consists of four stages which are interactively activated by the user:

- Definition of the required parameters (substance name and composition, monochromatic excitation energy, eventual normalization of the results, data source used to compute FFs and SFs);
- Computation of the mentioned angular distributions with automatic saving of the results in the report file sap_out.txt which contains:
  - ○ A header with date and time, composition of the substance in terms of atomic elements, excitation energy, type of normalization and used data base;
  - ○ A data section for the total quantities of the substance
  - ○ A data section for each element present in the substance
  - ○ Each row in the data section contains the following columns: Polar angle, electronic Rayleigh x-sec, electronic Compton x-sec, atomic Rayleigh x-sec, atomic Compton x-sec, FF, SF

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  - All quantities in a data section are computed for a fix grid of 500 uniformly distributed polar angles between 0 and $\pi$.
- Graphical visualization of the results:
  - Polar plots of the interest magnitudes can be selected from a list menu in the plot window;
  - Each plot shows a closed curve corresponding to a section of the 3D angular distribution (which may be obtained by rotating this curve around the symmetry axis);
  - In case of mixtures or compounds, the same graph shows together the total distribution and the contributions of the single elements;
  - Normalization is always performed with respect to the total distribution;
- Saving of the plot as encapsulated postscript (eps) file.

## 3. Electronic angular differential cross-sections

For a pure element, the electronic angular differential cross-sections for Rayleigh scattering is given by

$$\left(\frac{d\sigma_R}{d\vartheta}\right)_{el}=\frac{r_e^2N}{2A}(1+\cos^2\vartheta) \tag{1}$$

For Compton scattering, it is:

$$\left(\frac{d\sigma_C}{d\vartheta}\right)_{el}=\frac{r_e^2N}{2A}\left(\frac{E_P}{E}\right)^2\left\{\frac{E}{E_P}+\frac{E_P}{E}-\sin^2\vartheta\right\} \tag{2}$$

where $E$ is the excitation energy and $E_p$ is the well known expression for the energy of the Compton peak-center

$$E_P=\frac{E}{1+\frac{E}{mc^2}(1-\cos\vartheta)} \tag{3}$$

In all the equations, $r_e$ is the classical electron radius, $A$ the atomic weight of the element, $N$ the Avogadro's number, $m$ the electron mass, $c$ the speed of light in vacuum and $\vartheta$ the scattering angle.

The Klein-Nishina cross-section [4] is usually defined in terms of energy as follows:

$$K_{KN}=\left(\frac{E_P}{E}\right)^2\left\{\frac{E}{E_P}+\frac{E_P}{E}-\sin^2\vartheta\right\} \tag{4}$$

By using the definition of $\alpha$

$$\alpha=\frac{E}{m_ec^2}=\frac{h\nu}{m_ec^2}=\frac{hc}{\lambda}\frac{1}{m_ec^2} \tag{5}$$

it is possible to rewrite Eq. (4) as

$$K_{KN}(\alpha,\vartheta)=\frac{1}{[1+\alpha(1-\cos\vartheta)]^2}\left[1+\cos^2\vartheta\frac{\alpha^2(1-\cos\vartheta)^2}{1+\alpha(1-\cos\vartheta)}\right] \tag{6}$$

In this last expression it is clear that for small values of $\alpha$, i.e. when the incoming energy becomes negligible compared to the electron mass rest energy, the electronic Compton cross-section approaches the Rayleigh one.

For a sample containing $n$ elements, the electronic angular differential cross-sections for Rayleigh and Compton scattering are given, respectively, by

$$\left(\frac{d\sigma_R}{d\vartheta}\right)_{el,comp}=\sum_{i=1}^{n}w_i\left(\frac{d\sigma_R}{d\vartheta}\right)_{el,i} \quad \text{(Rayleigh scattering)} \tag{7}$$

$$\left(\frac{d\sigma_C}{d\vartheta}\right)_{el,comp}=\sum_{i=1}^{n}w_i\left(\frac{d\sigma_C}{d\vartheta}\right)_{el,i} \quad \text{(Compton scattering)} \tag{8}$$

where $w_i$ is the weight fraction of the $i^{\text{th}}$ element.

## 4. Atomic angular differential cross-sections

For a pure element, the atomic angular differential cross-sections for Rayleigh and Compton scattering are given, respectively, by

$$\left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at}=\frac{r_e^2N}{2A}(1+\cos^2\vartheta)F^2(q,Z) \quad \text{(Rayleigh scattering)} \tag{9}$$

$$\left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at}=\frac{r_e^2N}{2A}\left(\frac{E_P}{E}\right)^2\left\{\frac{E}{E_P}+\frac{E_P}{E}-\sin^2\vartheta\right\}S(q,Z) \quad \text{(Compton scattering)} \tag{10}$$

$F(q, Z)$ and $S(q, Z)$ denote, respectively, the FF and the SF representing the collective effect of many electrons in the atom as a function of the atomic number $Z$ and the transferred momentum

$$q=\frac{E[\text{keV}]}{hc}\sin\left(\frac{\vartheta}{2}\right)$$

As a consequence of the coherent overlapping of the single electron contributions, the atomic cross-section for Rayleigh scattering (Eq. (9)) depends on the square FF $F^2(q, Z)$ which gives atomic contributions significantly greater than $Z$ times the contribution from one single electron. Some special limits of the FF are $F(0, Z)=Z$ and $F(\infty, Z)=0$.

In contrast, the electronic contributions to the atomic cross-section for Compton scattering (Eq. (10)) add incoherently, giving the so-called Waller-Hartree SF $S(q, Z)$. Special limits of the SF are $S(0, Z)=0$ and $S(\infty, Z)=Z$.

Hubbell et al. [1] have reviewed exhaustively the computation of both, the FF and the SF.

For a sample containing $n$ elements, the electronic angular differential cross-sections for Rayleigh and Compton scattering are given by

$$\left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at,comp}=\sum_{i=1}^{n}w_i\left(\frac{d\sigma_{R,FF}}{d\vartheta}\right)_{at,i} \quad \text{(Rayleigh scattering)} \tag{11}$$

$$\left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at,comp}=\sum_{i=1}^{n}w_i\left(\frac{d\sigma_{C,SF}}{d\vartheta}\right)_{at,i} \quad \text{(Compton scattering)} \tag{12}$$

## 5. Computation of FFs and SFs

The form factor (FF) for Rayleigh scattering and the scattering function (SF) for Compton scattering can be computed in two ways: using the tables in the EPDL97 library [2] and using the semi-analytical method described by Fernandez [3].

### 5.1. *From table*

SAP reads the tables extracted from the EPDL97 database and, using logarithmic interpolation, computes the values for $F(q, Z)$ and $S(q, Z)$.

The Evaluated Photon Data Library, 1997 version (EPDL97) [2] includes photon interaction data for all elements with atomic number between $Z=1$ and 100 over the energy range 1 eV to 100 GeV. From this library, SAP uses the Hubbell's nonrelativistic values of FFs and SFs for all the elements $Z=1$–92, in the energy subrange 1–1000 keV, tabulated as a function of the momentum transfer.

### 5.2. *From semi-empirical equations*

FFs and SFs are computed using the method described by Fernandez [3]. It consists of a combination of analytical calculations by Veigele et al. [5], and semi-analytical formulas due to Cromer and Waber [6,7] and Smith et al. [8].