27. FILE 27. ATOMIC FORM FACTORS OR SCATTERING FUNCTIONS

27.1. General Description

The ENDF system for neutron and photon production data allows two alternatives for storing angular distribution data. One is by probability per unit cos θ vs. cos θ, and the other is by Legendre coefficients. Actually, neither of these is a "natural" method for photons. The natural method would be atomic form factors or incoherent scattering functions. These are discussed briefly below.

a. ***Incoherent Scattering***. The cross section for incoherent scattering is given by

$$\frac{d\sigma_i(E,E',\mu)}{d\mu} = S(q;Z)\frac{d\sigma_i(E,E',\mu)}{d\mu}, \qquad (27.1)$$

where $d\sigma_c/d\mu$ = the Klein-Nishina cross section[1] which can be written in a closed form.
$S(q;Z)$ = the incoherent scattering function. At high momentum transfer (q), S approaches Z. In the other limit, S(0,Z) = 0.
q = the momentum of the recoil electron (in inverse angstroms[2]).

$$q = \alpha\left[1+\left(\frac{\alpha'}{\alpha}\right)^2 - 2\mu\left(\frac{\alpha'}{\alpha}\right)\right]^{1/2} \qquad (27.2)$$

where $\alpha = E_\gamma/m_0c^2$,
E_γ' = scattered photon energy,
$\mu = \cos\theta$.

The angular distribution can then easily be calculated, given a table of S(q;Z) are tabulated as a function of q in File 27. The user presumably will have subroutines available for calculating q for energies and angles of interest and for calculating Klein-Nishina cross sections. The user will then generate the cross sections for the appropriate cases by calculating q's, looking up the appropriate values of S, and substituting them in the above formula.

b. ***Coherent Scattering.*** The coherent scattering cross section is given by

$$\frac{d\sigma_{coh}(E,E',\mu)}{d\mu} = \pi r_0^2\left(1+\mu^2\right)\left[\left(F(q;Z)+F'(E)\right)^2 + F''(E)^2\right], \qquad (27.3)$$

where $q = \alpha[2(1-\mu)]^{1/2}$, the recoil momentum of the atom (in inverse angstroms),
$r_0 = e^2/m_0c^2$, the classical radius of the electron.
$F'(E)$ = the real anomalous scattering factor.
$F''(E)$ = the imaginary anomalous scattering factor.

The quantity F(q;Z) is a form factor. This quantity is also easily tabulated. At high momentum transfer (q), F approaches zero. In the other limit F(0;Z)=Z. The anomalous scattering factors are assumed to be isotropic. In addition, they smoothly approach zero at 1.0 MeV and can be assumed to be zero at higher energies.

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[1] O. Klein and Y. Nishina, Z. Phys. 52, 853 (1929).
[2] In ENDF, q is given in inverse angstroms, as customarily reported in the literature. The above equation shows q in m_0c units. See Appendix H for unit conversions.

An alternative way of presenting the photon scattering data, then, would be to tabulate incoherent scattering functions and form factors. Users could then provide processing codes to generate the cross sections from this information. The calculation is quite straightforward and allows the user to generate all his scattering data from a relatively small table of numbers. The incoherent and coherent scattering data should always be presented as scattering functions and form factors, respectively, whether or not data are included in File 6.

27.2. Formats

The structure of a section is very similar to that of File 3 (and 23) and is

```
[MAT, 27, MT/  ZA,  AWR,  0,  0,  0,  0] HEAD
[MAT, 27, MT/ 0.0,    Z,  0,  0, NR, NP/ q_int / H(q;Z)] TAB1
[MAT, 27,  0/ 0.0,  0.0,  0,  0,  0,  0] SEND
```

The general symbol H(q;Z) is used for either F(q;Z) or S(q;Z) for coherent and incoherent scattering, respectively, or for the anomalous factors

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[MAT, 27, MT/  ZA,  AWR,  0,  0,  0,  0] HEAD
[MAT, 27, MT/ 0.0,    Z,  0,  0, NR, NP/ E_int / F(E)] TAB1
[MAT, 27,  0/ 0.0,  0.0,  0,  0,  0,  0] SEND
```

27.3. Procedures

1. Values of H(q;Z) should be entered in each case for the entire energy range for which integrated coherent and incoherent cross sections are given in File 23. This is true even though the respective values may be 0.0 or Z over most of the (higher) energy range.
2. The value of Z is entered in floating-point format.