22.54 Neutron Interactions and Applications (Spring 2003)
Lecture 2 (2/11/03)

Neutron Reaction Systematics -- Energy Variations of Cross Sections, Nuclear Data

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References --

Enrico Fermi, *Nuclear Physics*, Lecture Notes compiled by J. Orear, A. H. Rosenfeld, and R. A. Schluter (Univ. Chicago Press, 1949), revised edition, chap. VIII.
Marmier and Sheldon, *Physics of Nuclei and Particles* (Academic Press, New York, 1969), vol. I, pp. 64-95.
S. Pearlstein, "Evaluated Nuclear Data Files", in *Advances in Nuclear Science and Technology* (Academic Press, New York, 1975), vol. 8.

In this lecture we will survey the energy variations of nuclear reaction cross sections, making use of simple results from perturbation theory in quantum mechanics, Fermi's Golden Rules. This is to provide some appreciation of the variety of cross sections that have found useful applications in nuclear science and technology. We will also give a brief description of nuclear data compilation and evaluation, the importance of which cannot be overemphasized since no serious nuclear calculations can be performed without this basic information.

We consider the reaction a + A → b + B, where a is the incoming particle (neutron), A the target nucleus, b the outgoing particle, and B the product nucleus. First we are not concerned with rersonance reaction which is usually treated as a two-step process, involving the formation and subsequent decay of the compound nucleus. This will be taken up later in this lecture. We define the Q-value for the reaction as

$$Q \equiv [(m_a + M_A) - (m_b + M_B)]c^2 \tag{2.1}$$

where m, M are atomic masses, and c is the speed of light. For $Q > 0$, the reaction is exothermic, with energy being given off. For $Q < 0$, the reaction is endothermic, with energy being absorbed. From conservation of total energy, Q also can be written in terms of the kinetic energy of the particles and nuclei,

$$Q = T_b + T_B - (T_a + T_A) \tag{2.2}$$

Notice that despite the appearance of (2.2) which may make one think that Q is dependent on the coordinate system used to measure the kinetic energies (laboratory vs. center-of-mass), Q is independent of the reference frame as shown by (2.1). In most cases, exception is in neutron thermalization discussions, we can ignore the motion of the target nucleus and set $T_A = 0$, a considerable simplification. In the following we will switch notation and use E instead of T for the kinetic energy. For the neturon the kinetic energy is then E (or E_n).

In quantum mechanics the calculation of cross section $\sigma(a,b)$ is usually calculated by applying time-dependent perturbation theory to the reaction A(a,b)B, obtaining the general expressions known as Fermi's Golden Rules. There are two Golden Rules; for our discussion we are concerned with Golden Rule no. 2, which deals with so-called first-order transitions and gives the expression for the transition rate (number of transitions per unit time between initial state a and final state b of the particle) w_{ab},

$$w_{ab} = \frac{2\pi}{\hbar}|H_{ab}|^2 \frac{dn}{dE} \tag{2.3}$$

where H_{ab} is the matrix element of the perturbation H causing the transition from a to b, and dn/dE is the *density of states*, the number of states per unit final energy of the particle. For a particle in vacuum (free particle) with momentum $\underline{p}$, we can readily calculate the density of states. Let the vacuum have a finite volume Ω (we take the system volume to be finite for purpose of simple normalization of the wave function), the number of states with momentum in dp about $\underline{p}$ is

$$dn = 4\pi p^2 dp\Omega/(2\pi\hbar)^3 \tag{2.4}$$

If the outgoing particle b and the product nucleus B have spins I_b and I_B, respectively, then we need to include in Eq.(2.4) a statistical factor, $(2I_b+1)(2I_B+1)$ for the number of spin orientations one can have in the final state. For an outgoing particle with momentum $\underline{p}_b$,

$$dE = v_b dp_b \tag{2.5}$$

Strictly speaking, v_b and p_b should be the velocity and momentum of the final state (b+B) in the center of mass coordinate system (frame of reference), rather than of the outgoing particle b. The difference is small when the product nucleus is heavy compared to the mass of the particle. We can rewrite (2.1) by combining all (2.4), (2.5) and the statistical factor,

$$w_{ab} = \frac{1}{\pi\hbar^4}\frac{p_b^2}{v_b}\Omega\left|H_{ab}\right|^2 (2I_b+1)(2I_B+1) \tag{2.6}$$

To go from the rate of transition to the cross section, we simply write

$$w_{ab} = n_a v_{rel}\sigma(a,b) \tag{2.7}$$

which essentially introduces and therefore defines the cross section. Compare this argument with Eq.(1.3) in Lec 1. In (2.7), n_a is the density of incoming particle and v_{rel} is the relative velocity in the initial state (a+A). Again, if the target nucleus is massive compared to the incoming particle, then to a good approximation v_{rel} is given by v_a, the velocity of the incoming particle in CMCS. Combining (2.6) and (2.7) we obtain

$$\sigma(a,b) = \frac{1}{\pi\hbar^4}\left|\Omega H_{ab}\right|^2 \frac{p_b^2}{v_a v_b}(2I_b+1)(2I_B+1) \tag{2.8}$$

This formula is useful for deducing the qualitative variation of the cross section with energy for a number of typical reactions, without knowing much about the really complicated part of the calculation, the matrix element of the perturbation H between initial and final states.

We now assume that there are two parts to the transition matrix element, one involving nuclear interactions among the nucleons and the other pertains to electrostatic (Coulomb) interactions between the incoming or outgoing particle, if it were a charged particle, and the nucleus (either the target or the product as the case may be). We further assume that the nuclear interactions, however complicated, may be taken to be a constant for the purpose of estimating the energy variation of $\sigma(a,b)$. What is left in H_{ab} is the Coulomb interaction. The effect of this can be estimated by using the model of a charged particle tunneling through a Coulomb barrier. (Recall from 22.101 that such a model was introduced to calculate the decay constant for $\alpha -$decay.) For a positively charged particle, charge z with velocity v, to penetrate a nucleus, charge Z, the transmission factor is exp(-G/2), where [Fermi's Notes, p. 143]

$$G/2 \approx \frac{\pi Zze^2}{\hbar v} \tag{2.9}$$

where G is called the Gamow factor. Accordingly, if the incoming and outgoing particles are both charged, we will write

$$\left|H_{ab}\right|^2 \approx \overline{U}^2 \exp(-G_a - G_b) \tag{2.10}$$

where $\overline{U}$ is the nuclear interaction part, which we will take to be energy independent.

Now we are ready to examine the variation with energy of incoming particle of various neutron reactions at low energies, say eV range. Eq.(2.8) shows that there are two parts which can vary with energy, the kinematical factor, $p_b^2 / v_a v_b$, and the transmission factors, if present. We can distinguish four types of neutron interactions of interest.

1. **Elastic scattering (n,n)**

With incoming and outgoing particles being uncharged, the transmission factor is unity. Also, with $v_a = v_b$, the kinematical factor $p_b^2 / v_a v_b$ is a constant. Eq.(3.8) then predicts the cross section to be a constant, as shown in Fig. 3-1(a). Notice that elastic scattering is, strictly speaking, not a proper reaction.

2. **Charged-Particle Emission (exothermic)**

Since Q is typically a few MeV, while the incoming neutron energy is of order eV, $p_b^2 / v_a v_b \approx 1/v_a$. $\left|H_{ab}\right|^2 \approx \overline{U}^2 \exp(-G_b) \approx$ constant. So $\sigma \approx 1/v_n$; this is the '1/v' behavior often seen in reactions like (n,α), (n,γ), etc.

3. **Inelastic scattering (n,n')**

Since the product nucleus is left in an excited state, this is an endothermic reaction that requires a threshold value for the neutron energy, E* = -Q ~ 1 MeV. Velocity of the outgoing neutron is $v_{n'}$, with $v_{n'}^2$ = (excess energy above threshold)/(m_n/2) ~ (E_n - E*). Thus,

$$\sigma(n,n') \propto v_{n'} \sim (E_n - E^*)^{1/2}$$

An example here is $O^{16}(n,\alpha)C^{13}$, with Q = -2.215 MeV.

4. **Charged-Particle Emission (endothermic)**

This reaction is like the endothermic reaction of inelastic neutron scattering, except there is now a Coulomb factor,

$$\sigma(n,b) \sim e^{-G_b}(E_n - E^*)^{1/2}$$

with $G_b \sim 1/v_b$.

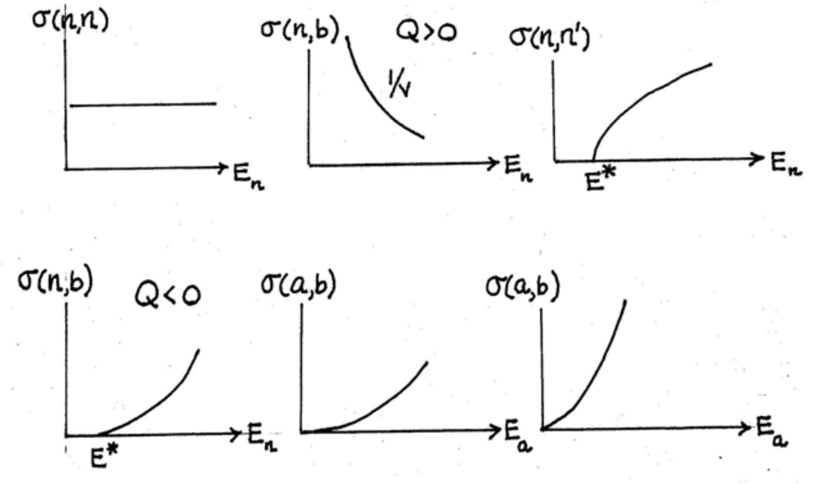

Fig. 2-1. Schematic energy variations of cross sections, the first four correspond to neutron elastic scattering, neutron-induced reaction (exothermic), neutron inelastic scattering, and neutron-induced reaction (endothermic). The last two reactions are charged particle and uncharged particle, and charged particles in and out, both reactions being exothermic.

In addition, we can consider exothermic reactions with incoming charged particles. If the outgoing particle is uncharged, then with Ea << Q, $p_b^2 / v_a v_b$ ~1/va, pb ~ constant, we have

$$\sigma(a,b) \sim \frac{1}{v_a} e^{-G_a}$$

An example would be the inverse reaction to that already mentioned, $C^{13}(\alpha,n)O^{16}$, Q = 2.215 MeV. If the outgoing particle is also charged, as in (α,p), $p_b^2 / v_a v_b$ ~1/va, and

$$\sigma(a,b) \sim \frac{1}{v_a} e^{-(G_a+G_b)}$$

Both cases are also shown in Fig. 2-1.

Resonance Reactions

The energy variations we have discussed are qualitative and smooth behavior; they are not intended to apply to resonances which are sharp features of the energy dependence of the cross sections. To describe resonances one can apply Golden Rule no. 1 which curiously deals with second-order transitions. Instead of going from initial to final state directly in a transition, as in the case of Golden Rule no. 2, we consider a two-step process where the incoming particle interacts with the target nucleus to form a *compound nucleus* which exists for a finite period and then *decays* to the final state consisting of an outgoing particle and the product nucleus,

$$a + A \rightarrow C \rightarrow b + B \tag{2.11}$$

Without going into details, we will simply give the results for two neutron resonances which are quite commonly encountered, elastic scattering (n,n) and radiative capture (n,γ). The cross sections for these two reactions have the form of so-called Breit-Wigner resonances.

For elastic scattering,

$$\sigma(n,n) = \pi \lambda\!\!\!^{-}{}^2 f_o \frac{\Gamma_n^2}{(E-E_\gamma)^2 + \Gamma^2/4} + 4\pi \lambda\!\!\!^{-} \Gamma_n a f_o \frac{E-E_\gamma}{(E-E_\gamma)^2+\Gamma^2/4} + \sigma_p \tag{2.12}$$

where $\lambda\!\!\!^{-} = 2\pi / k$, k being the neutron wave number, $E = \hbar^2 k^2 / 2m$, a is the scattering length which appears in the definition of the potential scattering cross section $\sigma_p = 4\pi a^2$ (we will come back to discuss what we mean by potential scattering in more detail), and $f_o = (2J+1)/2(2I+1)$ is the statistical factor for spin orientations, I being the spin of the target and J is the total spin, $I \pm 1/2$. The other quantities in (2.12) are the resonance energy E_γ, and the neutron and total resonance width, Γ_n and $\Gamma = \Gamma_n + \Gamma_\gamma + \ldots$, with Γ_γ being the radiation width; these are typically known as resonance parameters, they are part of the nuclear data and are tabulated for a given target nucleus. Eq.(2.12) shows there are three contributions to elastic scattering, the first term is the resonance contribution, called resonance elastic scattering, the second term is an interference term between resonance scattering and potential scattering, the latter being the ordinary scattering in the absence of any resonance. The third term is the potential scattering which is typically taken to be a constant, depending only on the scattering length, a basic property of the nucleus (more discussion will be given in the lectures on cross section calculation and neutron-proton scattering).

To see the cross section variation with neutron energy in elastic scattering, we note that $\lambda\!\!\!^{-}$ ~ v or $\sqrt{E}$, $\Gamma_n \sim \sqrt{E}$, Γ_γ ~ constant. Imagine there is a resonance at energy E_γ, for neutron energy much less or much greater than E_γ the first and second terms do not contribute, so the cross section is a constant. In the vicinity of E_γ the cross section has a variation shown in Fig. 2-2. Notice that the interference effect is *destructive* at energies just below the resonance, and *constructive* at energies above. This is a characteristic feature of resonance reaction which sometimes are observed in actual cross section measurements.

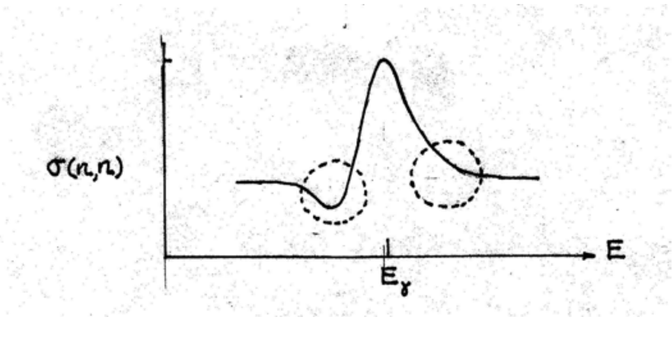

Fig. 2-2. Schematic energy variation of neutron elastic scattering showing interference effects between resonant and potential scattering.

For radiative capture the cross section has the pure Breit-Wigner form,

$$\sigma(n,\gamma) = \pi ƛ^2 f_o \frac{\Gamma_n \Gamma_\gamma}{(E - E_\gamma)^2 + \Gamma^2/4} \tag{2.13}$$

One can see that well below the resonance the cross section behaves like 1/v, and the full width at half maximum of the resonace peak is Γ, as shown in Fig. 2-3.

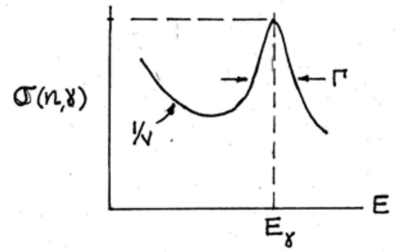

Fig. 2-3. Schematic energy variation of a neutron capture resonance, showing a characteristic 1/v behavior below the resonance and a full width at half maximum of Γ.

To conclude our brief survey of neutron cross sections we show the actual cross sections for a few nuclei which are of definite interest to nuclear engineering students. The first example is U^{235}, an isotope of uranium which is fissile (capable of undergoing fission when bombarded by thermal neutrons).

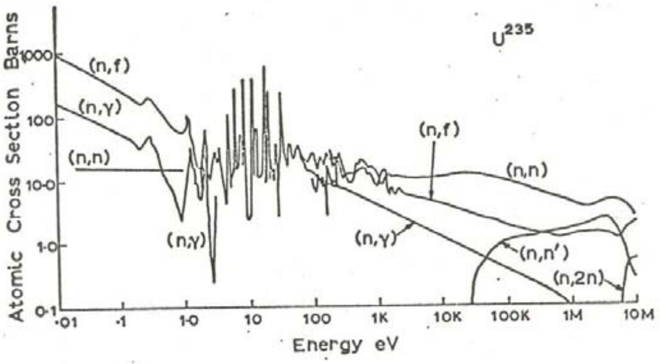

Fig. 2-4. Various cross sections of the uranium isotope 235, fission (n,f), radiative capture (n,γ), elastic scattering (n,n), inelastic scattering (n,n'), and a stripping reaction (n,2n).

In Fig. 2-4 one can pick out some of the characteristic features discussed above, energy-independent behavior for potential scattering, 1/v variation for capture and fission below the resonances, and threshold behavior for inelastic scattering. The student should also pay attention to the magnitudes of the cross sections and the wide energy range covered. In the thermal region, around 0.025 eV, the energy dependence is rather simple, all monotonic variations. Starting at about 1 eV and extending up to about 1 KeV, there are many sharp resonances. Above 10 KeV the cross sections return to smooth behavior. In the context of using uranium as the fuel for a nuclear reactor, we can see the reason for building thermal reactors - to take advantage of the large fission cross sections. Since neutrons from fission are emitted in the MeV range, one also has the problem of slowing down the neutrons past the resonance region where there is a high probability of capture down to the thermal range in order to continue the chain reaction.

Thus, the optimum design of a nuclear system, whether it is a nuclear reactor, a particle accelerator, or anything else, often comes down to a matter of materials properties, or in this case the cross sections.

When one compares the cross sections of U^{235} with those of another isotope U^{238}, shown in Fig. 2-5, several features can be noted. The absence of thermal fission reaction in U238 results in rather low cross section values in the thermal energy region. In the resonance region, the characteristic interference behavior in elastic scattering is even more pronounced than that sketched in Fig. 2-2. In the Mev region, fast fission is seen to be a threshold process. U^{238} is a fertile nucleus in the sense that when it captures a neutron, it becomes U239 which undergoes two β -decays to reach Pu^{239} which is fissile.

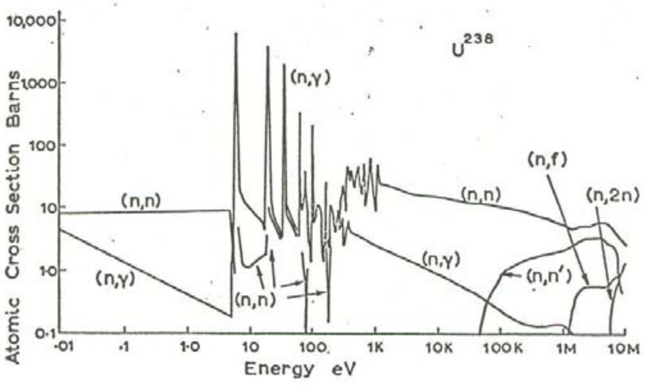

Fig. 2-5. Cross sections of uranium isotope 238.

At the opposite extreme of a light nucleus we can consider the cross section of the proton, the nucleus of hydrogen atom, shown in Fig. 2-6. The most notable feature here is the essentially constant value of the cross section at 20 barns over an extended energy from about 1 eV to well beyond 10 KeV. Given that the thermal absorption cross section is 0.3 barns, the entire 20 barns can be attributed to potential scattering. An interesting question is since the proton is the smallest possible nucleus, why should its scattering cross section be so large, about a factor of 2 or more compared to all the other nuclei. This clearly suggests that in the case of neutron scattering by hydrogen, the cross section is not determined only by the size of the nucleus. As we will see later, the answer lies in the contribution to the cross section from the coupling of the neutron and proton spins (each has spin 1/2). This explanation is fully consistent with our knowledge of nuclear interactions as being spin-dependent

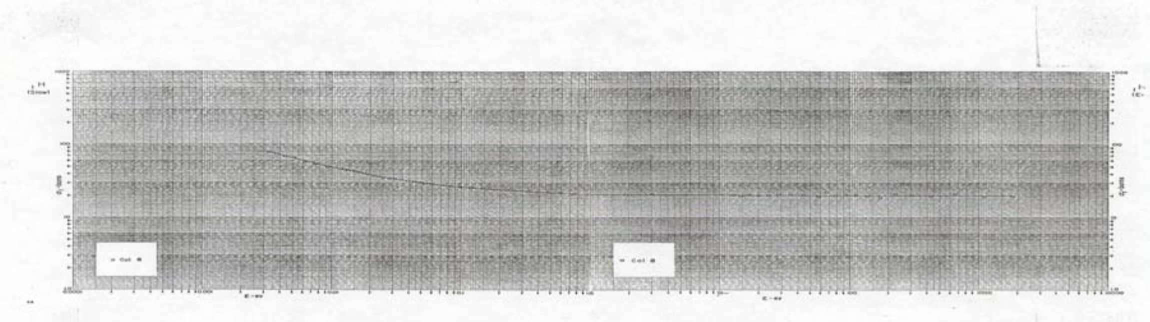

Fig. 2-6. Neutron scattering cross section of hydrogen in the low-energy region.

In contrast to the hydrogen cross section, the cross section of carbon, shown in Fig. 2-7, shows features which arise from the physical state of target atoms. In this case the target is a crystalline sample. One sees a sharp edge in the cross section variation which arises from Bragg scattering, a constructive interference effect. Below the edge, the cross section behaves like 1/v and is temperature-sensitive, higher magnitude at higher temperature. Beyond about 0.1 eV the cross section reaches a constant at about 5 barns, the same potential scattering behavior as mentioned above. We will come back to discuss these features in more detail later.

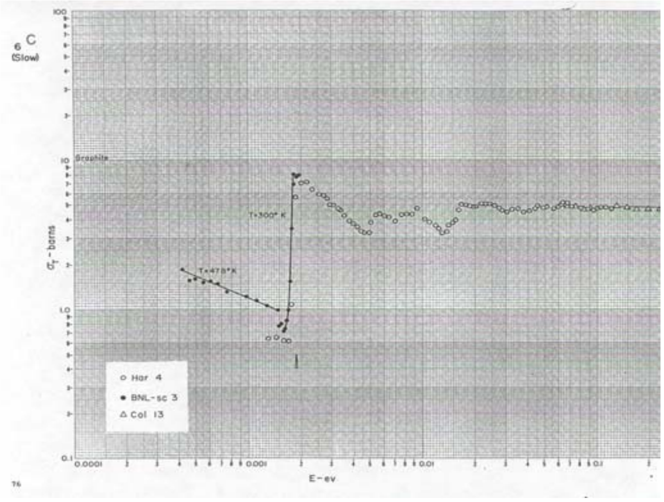

Fig. 2-7. Neutron scattering cross section of a polycrystal of natural carbon in the low-energy region.

Nuclear Data Compilation and Evaluation

As the last part of this lecture we take up the important topic of how information on nuclear data is gathered, analyzed, and made available to users on a world-wide basis. Given the importance of having accurate knowledge of cross sections and other data in nuclear calculations, it is not surprising that there is a whole industry on nuclear data technology that has been long established and continues to be active in maintaining and improving the database. The student should beware that our discussion is based on source material dated around the mid 70's; it is quite possible that significant changes have since taken place. While detailed information may have changed over the years, the role of nuclear data in nuclear system analysis and design remains as vital as ever.

Compilation and evaluation of nuclear data are carried out at many national laboratories and research centers all over the world. In the U.S. the focal point of this activity has been the National Neutron Cross Section Center at the Brookhaven National Laboratory. Perhaps the most important contribution of this Center is a library of evaluated nuclear data, known as the Evaluated Nuclear Data File (**ENDF**), which was developed for the storage and retrieval of nuclear data needed for neutronic and photonic calculations. There are two libraries. ENDF/A is a collection of useful evaluated data sets. **ENDF/B** contains the reference data sets recommended by the Cross Section Evaluation Working Group. At any given time there is only evaluated data set for a particular material. Most users are concerned only with the B version.

Evaluation of nuclear data means the assignment of the most credible value after consideration of all the pertinent information. The evaluation is supported by documentation giving a description of how the value was determined and an estimate of its uncertainty. As of 1975 the information contained in ENDF consists of: Resonance parameters, cross section tables, angular distributions, energy distributions, double differential data in angle and energy, scattering law data, and fission parameters.

Four primary centers with responsibilities for collecting and disseminating nuclear data information have been established to serve the world-wide community. The Neutron Cross Section Center, Brookhaven National Laboratory, serves U.S. and Canada. The Neutron Data Compilation Center, Saclay, France, serves Western Europe and Japan. The Nuclear Data Center, Obninsk, USSR, serves the Soviet Union. The Nuclear Data Section, IAEA, serves essentially the rest of the world.

For a brief look at the contents of ENDF/B library, we note that ENDF/B-II contains 3 basic types of data stored on 13 magnetic tapes.

1. Scattering law data for 12 moderator materials. For example, $S(\alpha, \beta)$ for a series of temperatures, 10 temperatures between 296^{o}K and 2000^{o}K in the case of graphite.

2. Neutron cross sections for 78 fissile, fertile, structural, and other materials, each being an element or an isotope -- total and any significant partial cross sections, reactions producing outgoing neutrons, angular and energy distributions, radioactive decay chain data, fission product yield, $\nu(E)$.

3. Photon interaction cross sections for 87 elements from Z = 1 to 94 -- photon cross sections, angular and energy distributions of secondary photons.

Over the years a number of active compilation groups have issued library files: KEDAK from Karlsruhe, Germany, JAERI (Japan), UKNDL from England, and various libraries from U.S. national laboratories such as Oak Ridge, Los Alamos, and Lawrence Livermore.