THEORETICAL INVESTIGATION OF THE EFFICIENCY OF NAI(Tl) CRYSTALS EXPOSED TO 1MeV GAMMA RAYS BY THE MONTE CARLO METHOD.

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c Zahra Ghorayshi

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ABSTRACT

THEORETICAL INVESTIGATION OF THE EFFICIENCY OF NaI(Tl) CRYSTALS EXPOSED TO 1MeV GAMMA RAYS BY THE MONTE CARLO METHOD.

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The objective of this thesis is to develop a computer program using the Monte Carlo method to calculate the efficiency of the right circular cylindrical NaI(Tl) detectors of different sizes, for monoenergetic gamma-rays incident along the axis of the cylinder.

Here the number of photons depositing all of their energy in a 3"X3" crystal is compared to the number incident on the crystal. The photon deposits energy by a series of collisions with the electrons in the crystal. The case histories of many photons travelling inside the crystal are followed using the Monte Carlo method

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CHAPTER 1

INTRODUCTION

PRINCIPLE OF OPERATION OF A CRYSTAL SCINTILLATION SYSTEM.

A photon interacting in a scintillation crystal produces electrons by photoelectric and Compton effect. These charged particles in turn produce excitation and ionization of atoms along their tracks. De-excitation of the atoms occur by the emission of photons. These photons are transmitted through a shaped pipe (fig. 1.1.)[1] to the photocathode of a photomultiplier. There photons release electrons which are accelerated and focused onto the first dynode. For each primary electron hitting a dynode, two to five secondary electrons are released. Up to 14 multiplying stages are used, and overall amplification of up to 10^9 can be achieved. Thus one incident photn can produce a measurable voltage pulse at the output of the multiplier. The pulse height is proportional to the total energy deposited in the scintillator by the entering gamma-ray.

A few remarks are in order concerning the mechanism of observation of gamma-rays in NaI(Tl) crystals. For a gamma-ray of less than 1MeV, only the photoeffect and Compton effect have to be considered. The photoeffect results in an electron with an energy $E_e = E_\gamma - E_b$, where E_b is the binding energy of the electron before it was ejected by the photon. The Compton effect produces electrons by collision. Here the

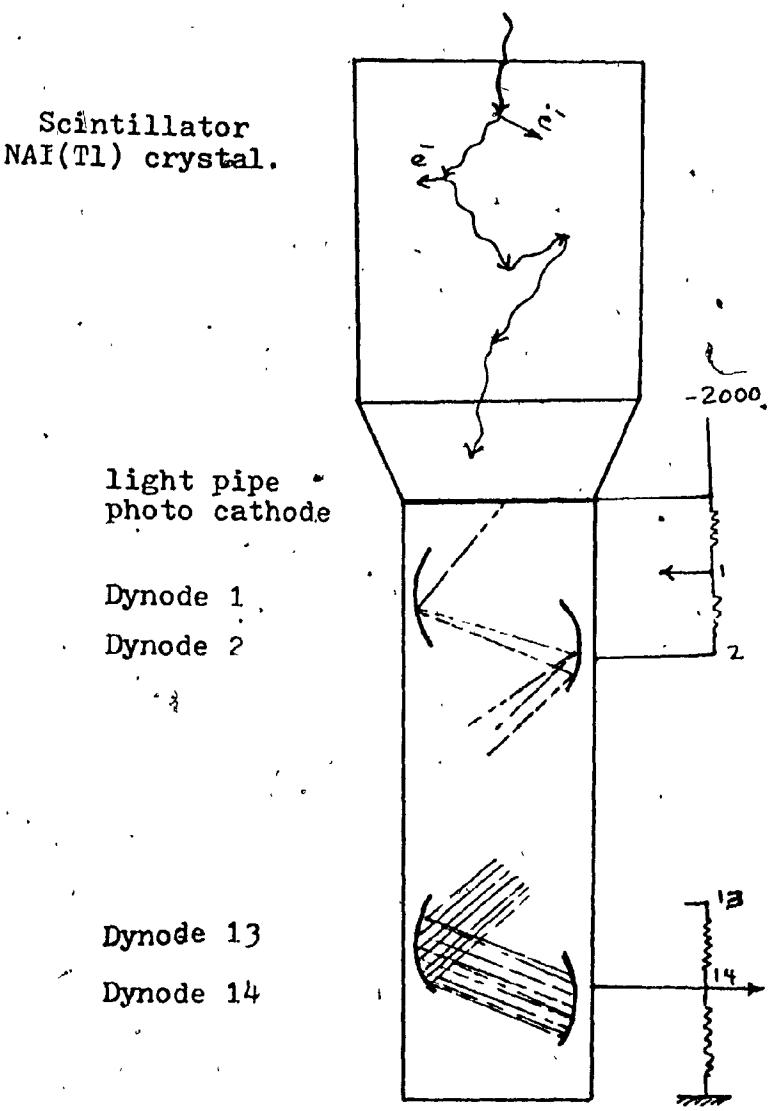


Fig. 1.1. Scintillation counter. A particle passing through the scintillator produces light which is transmitted through a light pipe onto a photomultiplier.

Klein-Nishina formula[2] gives the relationship between the recoil photon energy and the electron kinetic energy. The electrons will as a rule be completely absorbed in the crystal. The energy deposited in the crystal gives rise to a number of light quanta that are seen by the photomultiplier. In turn, these photons result in a pulse proportional to the total electron energy deposited E_e and with a certain ΔE due to a variation in gain in the photomultiplier. If the incident photon loses all of its energy in the crystal it gives rise to a peak. This photon or full-energy peak is shown in fig. 1.2.[1] In many Compton interactions the energy of the recoil photon is sufficient for it to escape from the crystal. The energy deposited in the crystal in this case is much less than the full photon energy and is equal to the energy of the recoil electron. The energy of the electrons produced by the Compton effect depends on the angle at which they are scattered. The Compton effect therefore gives rise to the lower portion of the spectrum as shown in fig. 1.2.

The width of the full-energy peak, measured at half-height, depends on the number of light quanta produced by the incident gamma-ray. Typically $\Delta E/E_\gamma$ is of the order of 6-8% at 1MeV for a 2 inch crystal.

The aim of this work is the theoretical evaluation of NaI(Tl) detector efficiency (The ratio of the number of gamma rays under the full-energy peak to the total number of

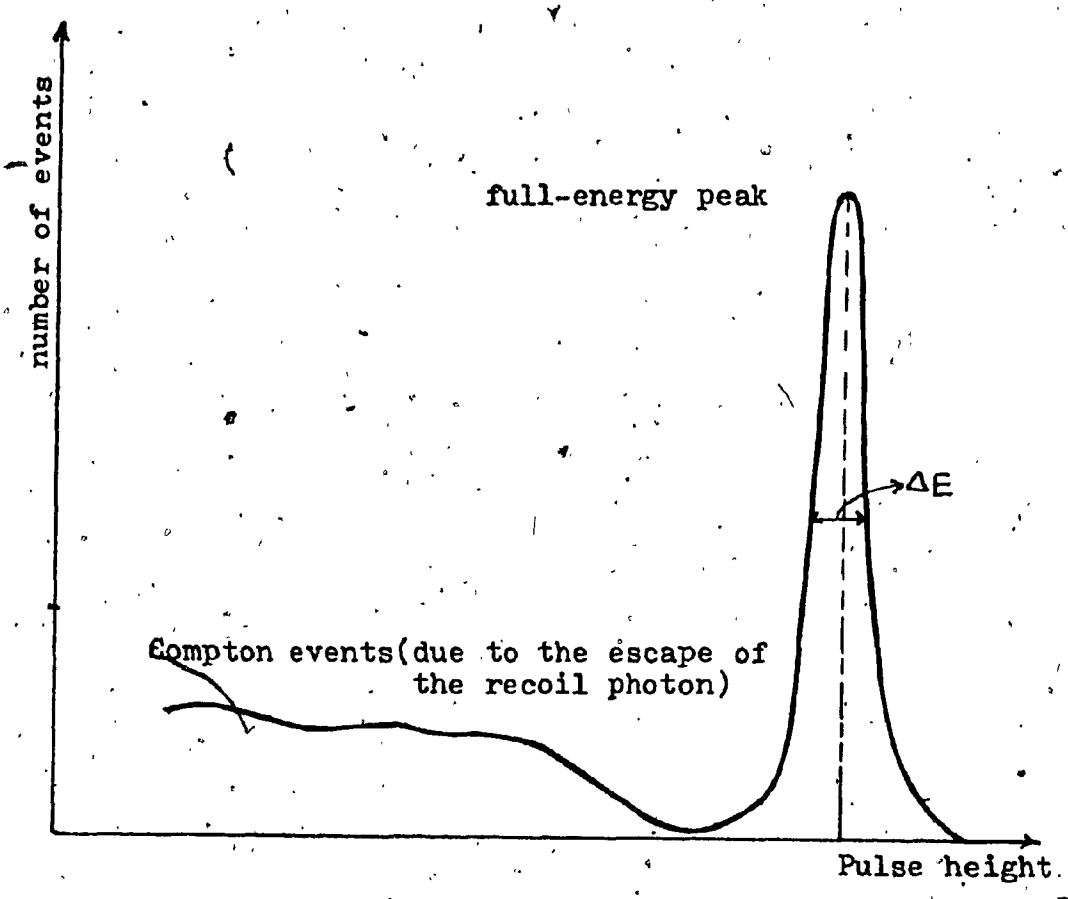


Fig. 1.2. Scintillation spectrum, NaI(Tl) crystal.

incident gamma-rays) as a function of energy for a scintillation detector by Monte Carlo method.

Because of multiple interactions by Compton effect it is impossible to calculate the radiation transport by analytical methods. The problem which must be solved for this purpose is the calculation of the transport of gamma radiation through the detector material taking the creation of secondary radiations and photon scattering into account. Such calculations have been reported by Miller and Snow[3], Zerby and Moran[4], and Seltzer and Berger[5] for point isotropic sources located on the axis of right circular cylindrical detectors. Marshall[6] has written a program for calculating the response of scintillators in complex detector geometries but few details are given.

This paper describes a Monte Carlo calculation which determines the photopeak detector efficiency of a right circular cylindrical NaI(Tl) detector for monoenegetic gamma rays incident along the axis of the cylinder. The analysis considers only Compton and photoelectric interactions, pair production was not taken into account because the calculation was done for gamma-rays with energies below the pair production threshold. In all calculations, the creation of bremsstrahlung and Rayleigh scattering was neglected. Rayleigh scattering is negligible because of the small energy loss associated with this event, bremsstrahlung losses are small for most electron energies considered here.

CHAPTER 2

2. INTERACTION OF RADIATION WITH MATTER

2.1. ABSORPTION OF GAMMA-RAYS

The basic property of the absorption of gamma-rays is the exponential decrease in the intensity of radiation as a homogeneous beam of gamma-rays passes through a thin slab of matter. When a beam of gamma-ray photons is incident on a thin absorber, each photon that is removed from the beam is removed individually in a single event. The event may be an actual absorption process (fig. 2.1.)[7], in which case the photon disappears, or the photon may be scattered out of the beam. The "one-shot" nature of the removal process is responsible for the exponential absorption. The number of photons removed in passing through a thickness Δx of absorber is proportional to Δx and to the number of photons reaching Δx.

When N_0 gamma-rays are incident on a slab of thickness Δx, the number of interactions of gamma-rays as they pass through the slab is proportional to the thickness and to the number of incident photons;

$$dN = -N\mu\, dx \qquad (2\text{-}1)$$

where the proportionality constant μ is called the attenuation coefficient. Integration of the above equation gives;

$$N/N_0 = e^{-\mu x}$$

This equation gives the number of photons N remaining after a beam of initial number N_0 has travelled a thickness x of a given material(fig. 2.1.)

The characteristic exponential absorption curve given by equation (2-2) is shown in fig. 2.1. Thus we see that a beam of gamma-rays will never be completely stopped by a finite thickness of matter, but its intensity will be reduced.

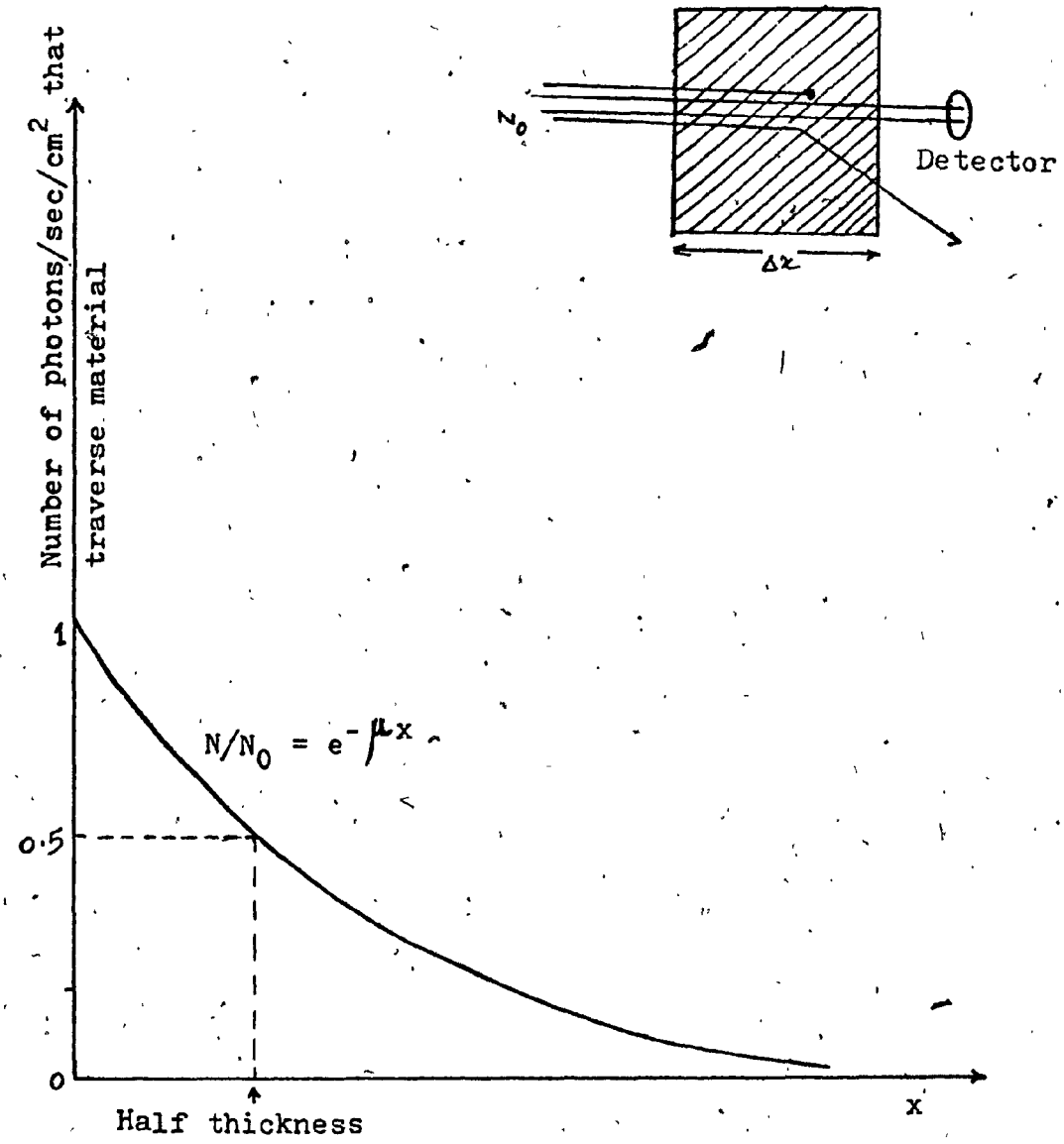


Fig. 2.1. Absorption of a narrow beam of X or gamma radiation passing through matter.

2.2. CROSS-SECTION AND ATTENUATION COEFFICIENT

One of the most important measurments that must be made in a nuclear or atomic reaction is the probability that the reaction will occur under given experimental conditions. The reaction probability is usually expressed in terms of an effective area. This area is called the cross-section (σ) which has the dimensions of an area, and is expressed in units of barns ($1b = 10^{-24}$ cm^2).

The concept of an atomic cross-section can be most easily visualized as the "target area" presented by an atom to an incident particle. Each atom is pictured as having an effective area towards the incident particles and can be very different from the geometrical area of the atom. The cross section for an atomic reaction of one type, or for a particular scattering process, is defined by :

$$\sigma = \frac{\text{Number of events of a given type/sec/atom}}{\text{Number of incident photons/sec/cm}^2}$$

For an incident collimated beam of N' photons/sec/cm^2 striking a target of thickness dx containing n target atoms /cm^3, the fraction of incident photons (fig. 2.2.) removed from the beam is :

$$dN'/N' = \sigma n dx \qquad (2\text{-}3)$$

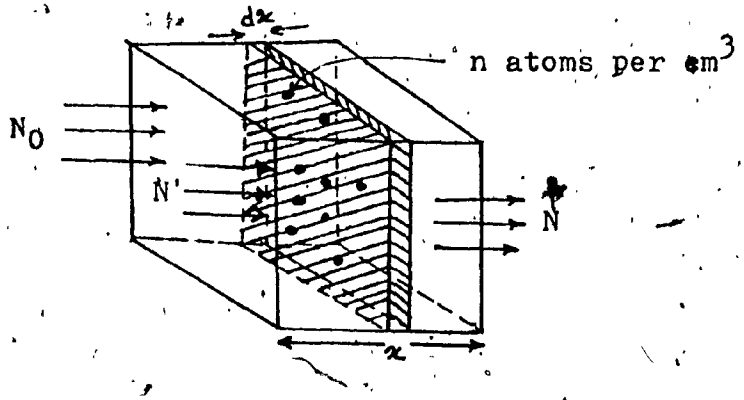


Fig. 2.2. Cross-section for atomic reaction as geometrical areas.

For a slab of material of thickness x the attenuation of a photon beam containing N_0 photons/cm^2/sec is obtained by integration of equation (2-3), from x =0 to x =x,

$$N = N_0 e^{-\sigma n x} = N_0 e^{-\mu x}$$

where N is the number of incident photons/cm^2/sec which pass through the slab without interaction.

The total cross-section can be written as a sum of several partial cross-sections which represent the contribution of the various distinct and independent processes. The total atomic cross-section may be written :

$$\mu = \mu_{com} + \mu_{photo}$$

$$\mu = \sigma + \tau$$

The attenuation coefficient may be defined as the probability

per unit path length that a photon will interact with matter. This quantity depends on the photon energy $h\nu$, the density and the atomic number Z of the material.

The attenuation coefficient has dimension of $(\text{length})^{-1}$. the attenuation coefficient is usually denoted by μ, where the units are cm^{-1}, by μ/ρ for cm /gm, by $e\mu$ for cm^2/electron, and by $a\mu$ for cm^2/atom.

Also, it is given by;

$$a\mu = Z e\mu$$

$$\mu/\rho = n\sigma/\rho = N(Z/A)e\mu = (N/A)a\mu$$

$$\mu = \rho N (Z/A) e\mu = (\rho N/A) a\mu$$

where Z is the atomic number, A is the atomic weight, N is Avogadro's number, and ρ is the density in gm/cm^3.

Fig. 2.3.[7] illustrates the mass attenuation coefficient for sodium iodide.

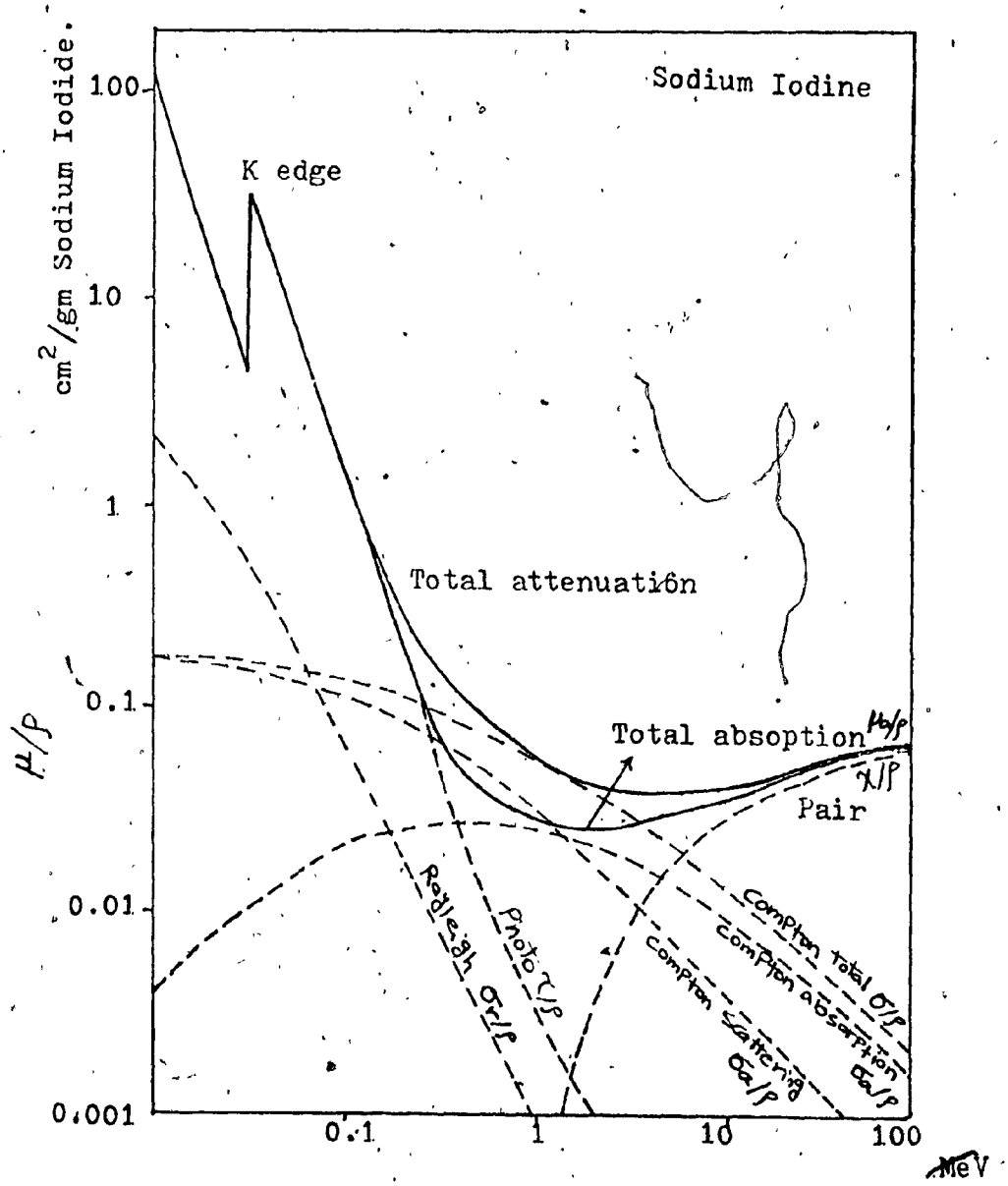


Fig. 2.3. Mass attenuation coefficients for sodium iodide. The "Compton total" attenuation coefficient $(\sigma/\rho) = (\sigma_a/\rho) + (\sigma_s/\rho)$ is shown explicitly, because of its usefulness in computing the behavior of NaI(Tl) scintillators. Linear attenuation coefficients for NaI may be obtained by using $\rho = 3.67$ gm/cm^3 NaI.

2.3. CLASSIFICATION OF INTERACTIONS

Interactions of photons with matter, by which individual photons are removed or deflected from a primary beam of X- or-gamma-radiation, may be classified according to:

1)The kind of target,e.g., electrons, atoms, or nuclei, with which the photon interacts, and,

2) The type of event,e.g., scattering, absorption,pair production,etc., which takes place.

There are many possible types of interaction between electromagnetic radiation and atoms, electrons and nuclei. Among all these the three which usually predominate below 10 MeV, are the photoelectric, Compton, and pair production interactions. The relative importance of these three varies with the energy of the incident photon and with the atomic number Z of the struck atoms. The curves in fig.2.4.[7] are the boundaries between three regions of $h\nu$ and Z within each of which one of the three principal modes of interaction is dominant.

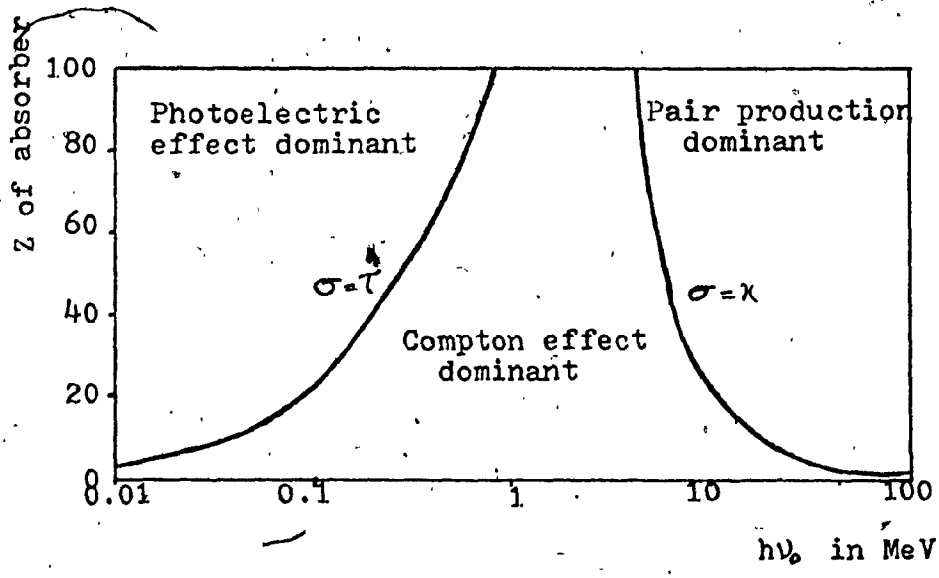


Fig. 2.4. Locus of equal atomic cross-sections for Compton and photoelectric interaction ($\sigma = \tau$) and for Compton and pair-production interaction ($\sigma = \kappa$). The incident photon energy is $h\nu_0$, and Z is the atomic number of the atom in the absorber. Compton collisions have larger cross-section than any other mode of interaction in the entire domain of medium energy photons marked "Compton effect dominant".

2.3.1. ATOMIC PHOTOEFFECT(PHOTOELECTRIC ABSORPTION), FLUORESCENT RADIATION, THE AUGER EFFECT.

In the atomic photoeffect, a photon disappears and an electron is ejected from an atom(fig. 2.5.)

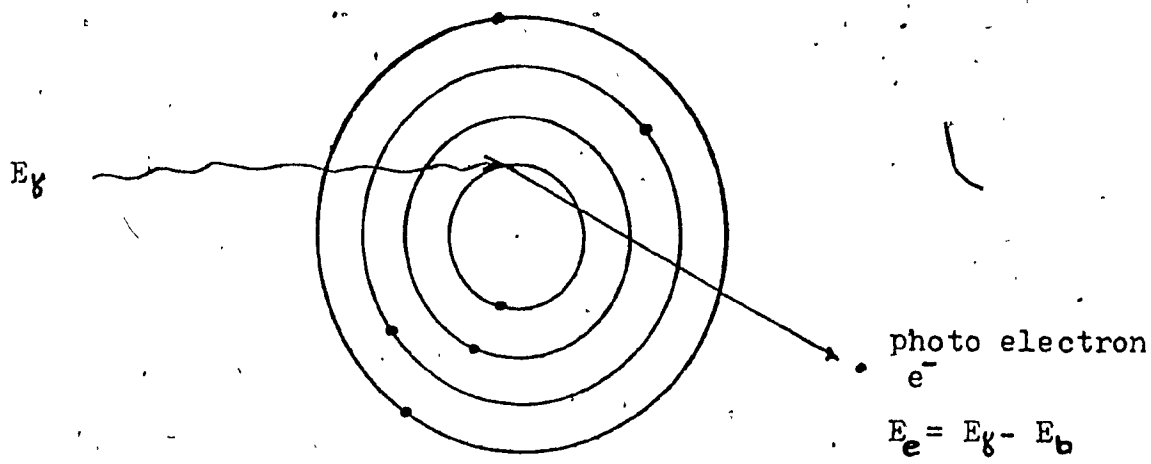


Fig. 2.5. The photoelectric effect sometimes called external conversion.

The electron carries away all the energy of the absorbed photon, minus the energy binding the electron to the atom. If the photon energy drops below the binding energy of a given shell, an electron from that shell cannot be ejected. Photoelectric absorption cannot take place with a free electron because a third body is needed to share, and hence conserve, the momentum. The remaining ion provides this third body.

The process is most efficient when the energy of the photon is just sufficient to eject the tightly bound electron. The K shell electrons, which are most tightly bound, are the most important for this effect in the energy region considered in this report. If the incident gamma photon has an energy less than that required to remove a K-electron from the atom, there may be photoelectric absorption with a less tightly electron in another shell.

We shall now consider two phenomena that are commonly associated with the photoelectric absorption of X-rays, although both are actually quite independent of the photo-electric process. The first of these is the phenomenon of fluorescent radiation accompanying the excitation of the atoms by the photoelectric process. This radiation is of course just the characteristic radiation of the absorber. For a given wavelength of incident radiation, those series of the characteristic spectrum will appear whose initial levels can be excited by this radiation (fig. 2.6a.). This process is called X-ray fluorescence because the radiated quanta are characteristic of the absorbing material rather than of the incident radiation, just as in ordinary optical fluorescence.

The other phenomenon associated with photoelectric absorption is called the Auger-effect. In this effect, an atom which is in an excited state reduces its excitation by simultaneouly dropping an electron from an upper shell into the vacant electronic state and ejecting another electron from a yet higher shell from the atom (fig. 2.6b.).

It should be emphasized that the second electron is not ejected by photoelectric absorption, but it happens directly in the process of readjustment of the atom. This form of readjustment of an excited atom is called an Auger transition and the electron ejected is called an Auger electron. Auger transitions occur with quite high probability ; an atom may emit two or more Auger electrons in a sequence of Auger transitions from an excited state.

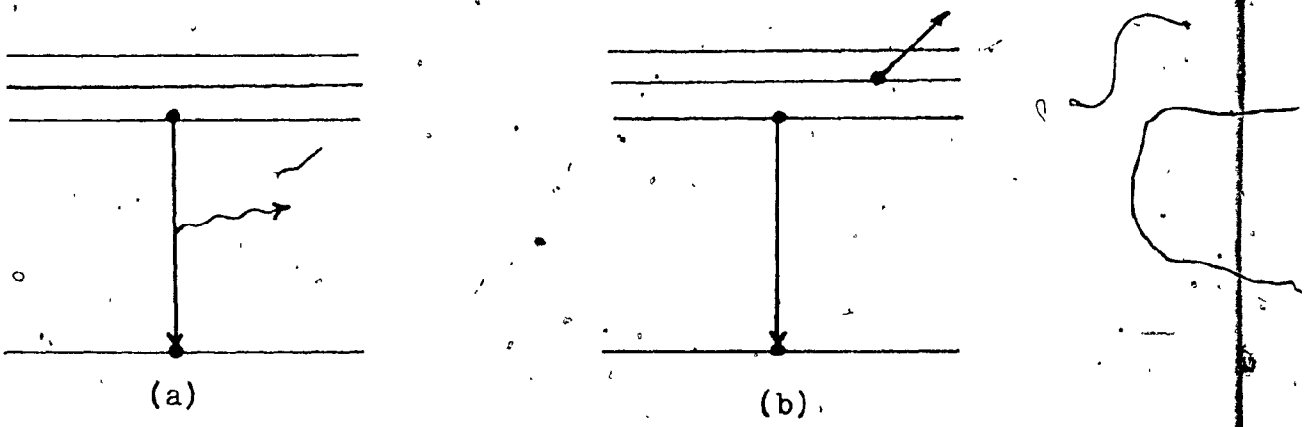


Fig. 2.6. An atom ionized by the photoelectric effect has an inner shell vacancy and hence an energy equal to the binding energy of the shell containing the vacancy. This energy is released by two competing processes. (a) fluorescence radiation, (b) Auger electron.

Photoelectric absorption occurs mostly with gamma rays of low energy and with elements of high atomic number, because their inner electrons are more tightly bound. The photoelectric cross-section of an atom varies very roughly with $1/A^2$ and Z^5 . It is because of this fact that lead

(Z = 82) or uranium (Z = 92) are often chosen as shields against electromagnetic radiation.

2.3.2. COMPTON SCATTERING

In Compton scattering, a photon collides with an electron, loses some of its energy and is deflected from its original direction of travel. The basic theory of this effect, assuming the electron to be initially free and at rest, is that of Klein and Nishina. This theory has been well confirmed experimentally.

Over most of the region in which Compton scattering is a major part of the total cross section, the Klein-Nishina[2] theory is directly applicable.

The relationship between deflection and energy loss for Compton scattering, assuming the electron to be initially free and stationary, is determined from conservation of momentum and energy between the photon and the recoiling electron. This relation can be expressed as:

$$A/A_0 = \frac{1}{1 + A_0 (1 - \cos\theta)}$$

Where A_0 and A are the energies of the photon before and after the scattering in mc^2 units, m_0c^2 is the electron rest energy and θ is the photon deflected angle, (fig. 2.7). If a photon of energy 1MeV is scattered in the backward direction, the maximum electron energy in a Compton interaction is about .025 MeV less than the incident photon energy.

The electron can only be scattered in a forward direction. Since energy is conserved, energy of the scattered photon plus the kinetic energy of the Compton electron is equal to the energy of the incident photon.

The cross section for a Compton interaction increases linearly with the atomic number of the scattering material, and decreases slowly with increasing gamma energy. The effect is relatively more significant than photoelectric absorption at intermediate gamma energies, and in light elements (see fig.2.4.).

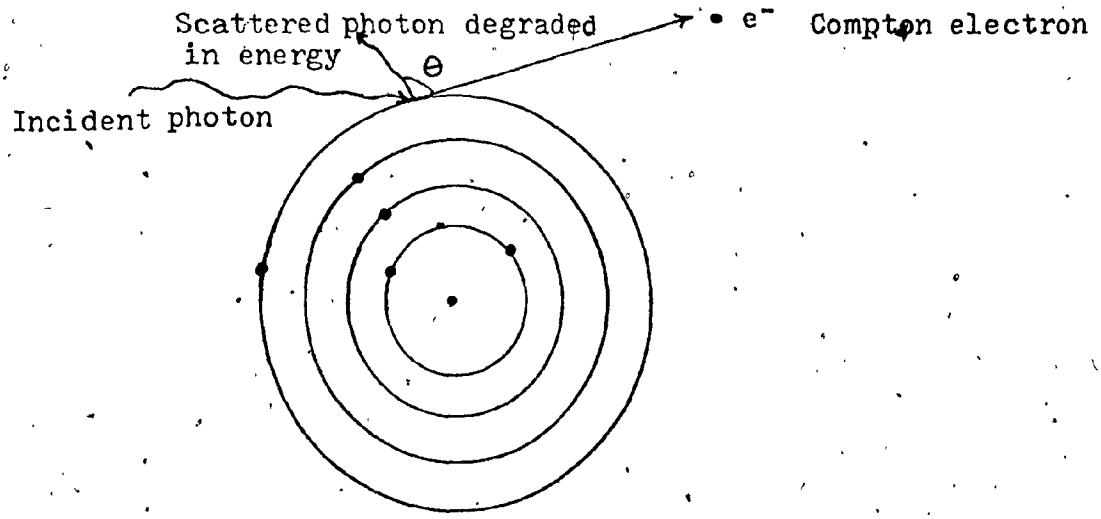


Fig. 2.7. The photon after being scattered has a lower energy corresponding to a longer wavelength.

2.3.3. COHERENT SCATTERING

For sufficiently small angle scattering, or low energy photons, the Klein-Nishina[2] differential cross-section reduces to the classical Thomson cross-section. Then there is no appreciable change in photon energy, or wavelength, on scattering, and the energy transfered to the electron is insufficient for it to escape from its orbit. The atom as a whole absorbs the momentum recoil. Under these conditions the wavelength of the radiation scattered by each of the electrons in the atom is the same. There is a fixed phase relationship between the scattered and the incident radiation. This process is called coherent scattering because it depends upon the co-operative action of all the electrons in one atom.

Compton collisions involve only incoherent scattering, in which each electron acts entirely independently, and there is no fixed phase nor wavelength relationship between the radiations scattered by different electrons in the same atom. Compton(modified) scattering decreases as Z increases.

CHAPTER 3

USE OF THE MONTE CARLO METHOD

3.1. PRINCIPLE OF MONTE CARLO METHOD

The Monte Carlo method consists of following and categorizing a large number of photon histories from emission at the source to absorption within the detector. Random number and probability theory, combined with known transport distributions are used to locate the photon collision site, as well as trajectory, energy and direction throughout each history. Then it is necessary to have a source of random numbers which scan the interval zero to one. Each history is begun and terminated by two steps.

1) We consider the photon flux to be incident along the central axis of the cylinder and each incident gamma-ray is forced to interact within the bounds of the detector, i.e., photons are not allowed to escape from the detector before making at least one collision (see section 3.2. for further explanation).

2) Each history is terminated when the energy of the photon falls below a specified minimum (e.g., 0.01 MeV), or the photon escapes from the crystal.

After entrace of the photon, the following has to be studied:

a) How far does the photon travel before it interacts with the detector ?

b) What new energy and direction does the photon have after undergoing an interaction ?

Part (a) and (b) are repeated until either the photon weight or energy drops below the appropriate threshold value, or the photon is not within the bounds of the detector.

3.2. CALCULATION OF INTERACTION PATH LENGTH

If N_0 photons are sent into a detector and N photons pass through without interacting in the crystal, the relation between N and N_0 can be written as:

$$\frac{N}{N_0} = e^{-\mu x}$$

Where μ is the attenuation coefficient and x is the path length. N/N_0 is the probability that a photon will not interact in the crystal, hence $1-N/N_0$ is the probability of an interaction in travelling a distance x, we can call this distance x the path length Δl.

Then $1-e^{-\mu \Delta l}$ = probability of interation(P).

We can use this in a Monte Carlo method by saying that if we draw a random number $R < P$ the photon interacts, if $R > P$ no interaction occurs. We have:

$$1-e^{-\mu \Delta l} = P$$

Then $1-P = e^{-\mu \Delta l}$

By taking the natural logs of both sides, we get;

$$\ln(1-P) = -\mu \Delta l,$$

$$\text{or } \Delta l = \frac{\ln(1-P)}{\mu}$$

By choosing values of (1-P) at random, equivalent values of Δl can be derived

3.2.1 METHOD OF FORCING PHOTON TO INTERACT IN THE CRYSTAL

In order to collect reasonable statistics it is necessary to follow many case histories. Since each of these uses time on the computer, it is important to minimize processing where possible. A useful first step is to eliminate photons which do not interact in the crystal.

From the previous section the probability of a photon interacting in the crystal is $1-e^{-\mu x}$ where x is the thickness of the crystal. Expressing the thickness of the crystal in g/cm^2 and using the mass attenuation coefficient (μ/ρ), for a $2\frac{1}{2}$" crystal and 1 MeV photons the probability of an interaction is:

$$1-e^{18.355 \times 5.80 \times 10^{-2}} = 0.65514$$

where the crystal thickness is 18.355 gm/cm^2 and 5.80×10^{-2} is the mass attenuation coefficient for 1 MeV photons in NaI.

This is equivalent to saying that if random numbers between 0 and 0.65514 are drawn, the path length Δl will always be less than the thickness of the crystal and so at least have one interaction of interest.

By this method we have eliminated the 35% of the incident photons which do not interact.

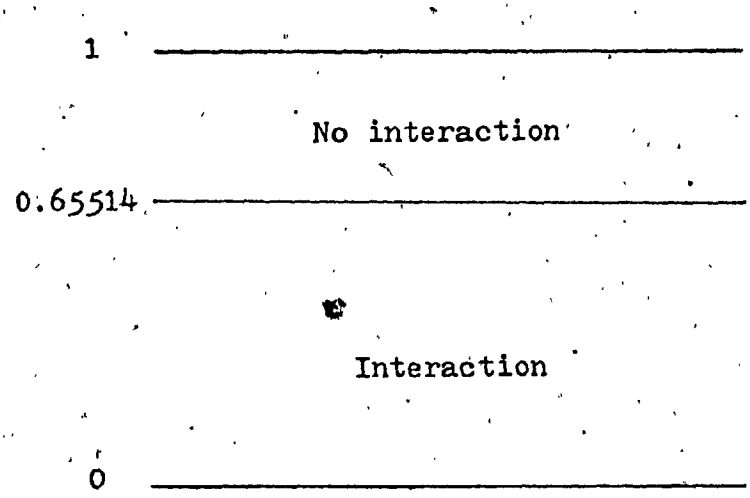


Fig. 3.1. Probability of having or not having an interaction.

3.2.2. THE FIRST INTERACTION

Having selected the depth of the first interaction Δl, the type of interaction must be chosen. For 1 MeV the cross section for the photoelectric and Compton interaction in sodium iodide are 366×10^{-3} cm^2/g and 543×10^{-2} cm^2/g respectively. Normalising their sum to one, the respective fractions of the total cross section are 0.063 and 0.937 . Hence if a random number between 0 and 1 is chosen, one of the interactions can be selected.

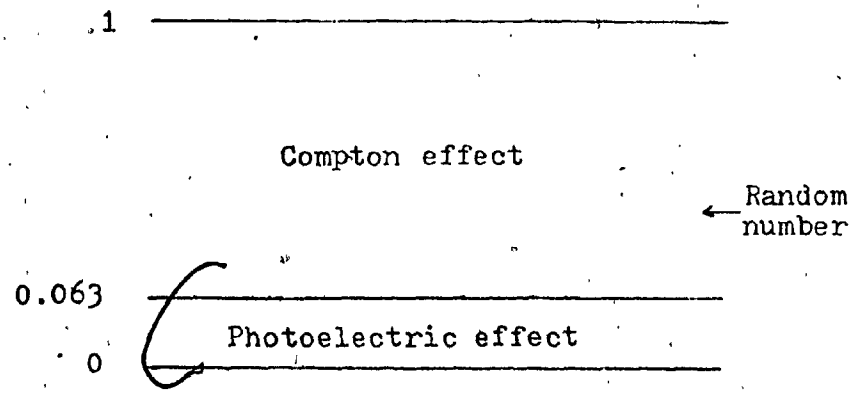


Fig. 3.2. Illustrating the selection of a Compton interaction

3.2.3. INTERACTION BY A PHOTOELECTRIC ABSORPTION

In this case some computer time is saved by subdividing the 0.063 range into subdivisions representing various interactions. Firstly the range can be divided between interactions in sodium and iodine (see fig. 3.3). Next, interactions in the various shells in iodine are considered. Interactions in the various shells of the sodium atom were not considered. Using cross section data from J.H.Hubbell[8] and J.H.Scofield.[9]

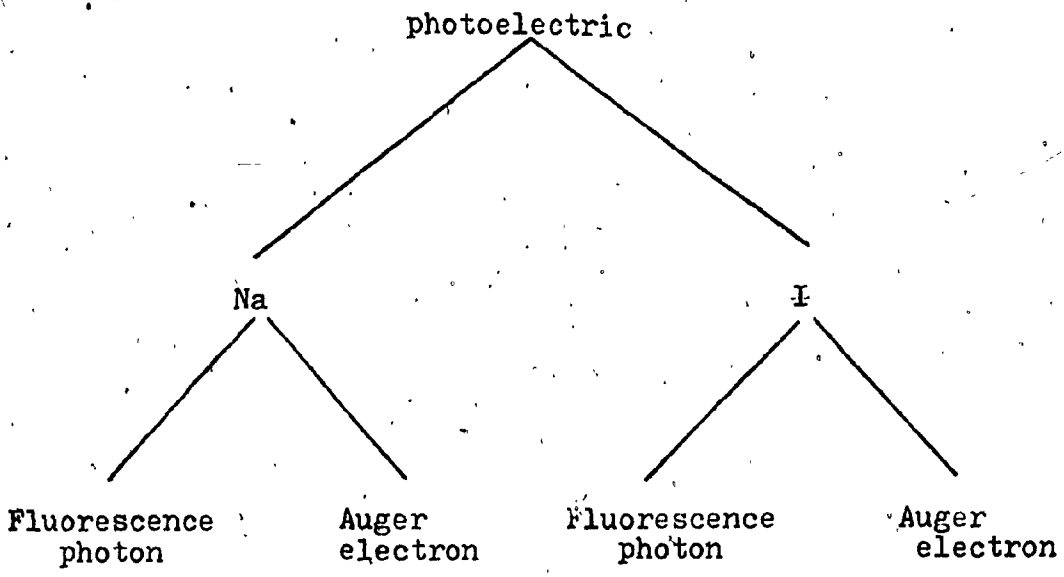


Fig. 3.3 Division of the photoelectric interaction.

$\sigma_{Na} = 5.58 \times 10^{-5}$ b/atom $= 5.58 \times 10^{-5}$ 0.0262 cm^2/gm

$= 1.462 \times 10^{-5}$ cm^2/gm

$\sigma_I = 9.11 \times 10^{-1}$ b/atom $= 9.11 \times 10^{-1}$ 0.004746 cm^2/gm

$= 4.324 \times 10^{-3}$ cm^2/gm

To find the cross-section of Na and I out of the total photoelectric cross-section, we use their atomic weights.

Atomic weight of Na = 23

Atomic weight of I = 127

$$\sigma_{Na} = \frac{1.462 \times 10^{-5} \times 23}{127 + 23} = 2.242 \times 10^{-6} \quad cm^2/gm$$

$$\sigma_I = \frac{4.324 \times 10^{-3} \times 127}{127 + 23} = 3.661 \times 10^{-3} \quad cm^2/gm$$

$$= \sigma_I + \sigma_{Na} = 3.661 \times 10^{-3} + 2.242 \times 10^{-6} = 3.661242 \quad 10^{-3} cm^2/gm$$

The percentage of random number of Na = 6.12×10^{-3}

The percentage of random number of I = 0.999388

These percentages are out of the total random number of the photoelectric part which occupies 0.063 of total random number. Then portion of random numbers for Na and I is :

R of I = $0.999388 \times 0.63172 = 0.0631333$

R of Na = $6.12 \times 10^{-4} \times 0.063172 = 0.0000387$

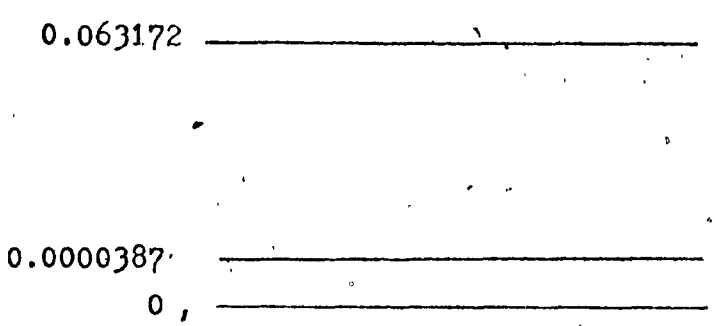


Fig. 3.4. Illustrating the selection of a I or Na atom interaction in a photoelectric absorption.

When there is a photoelectric absorption, a photon or an Auger electron could be produced, then it should be established which one of these two is produced, and from which shell it is coming. Since almost all of the photo-electric absorptions are with iodine(I) atom, the calculations are performed just for I.

To determine the shell that the collision occurs, the relative probabilities of interaction in each shell are used,

	K shell	L1 shell	L2 shell	L3 shell
(b/atom)	0.75201	0.081289	0.0057057	0.0061475

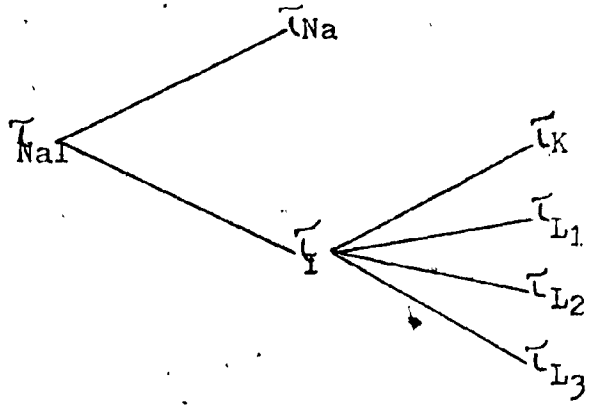


Fig. 3.5. Division of photoelectric cross-section for NaI.

$\tau_K + \tau_{L_1} + \tau_{L_2} + \tau_{L_3} = 0.8451504$ b/atom

The fraction of cross-section for each shell is :

$F_k = 0.75201/0.8451504 = 0.8897943$

$F_{L_1} = 0.081289/0.8451504 = 0.0961829$

$F_{L_2} = 0.0057057/0.8451504 = 0.0067511$

$F_{L_2} = 0.0061457/0.8451504 = 0.0072717$

The range of random numbers for interactions in each shell is normalized so that their sum equals the total photoelectric probability, and it is given below;

$R_I = 0.063172 - 0.0000387 = 0.0631333$

$R_k = 0.0631333 \times 0.8897943 = 0.0561757$

$R_{L_1} = 0.0631333 \times 0.0961829 = 0.0060723$

$R_{L_2} = 0.0631333 \times 0.0067511 = 0.0004262$

$R_{L_3} = 0.0631333 \times 0.0072717 = 0.0004591$

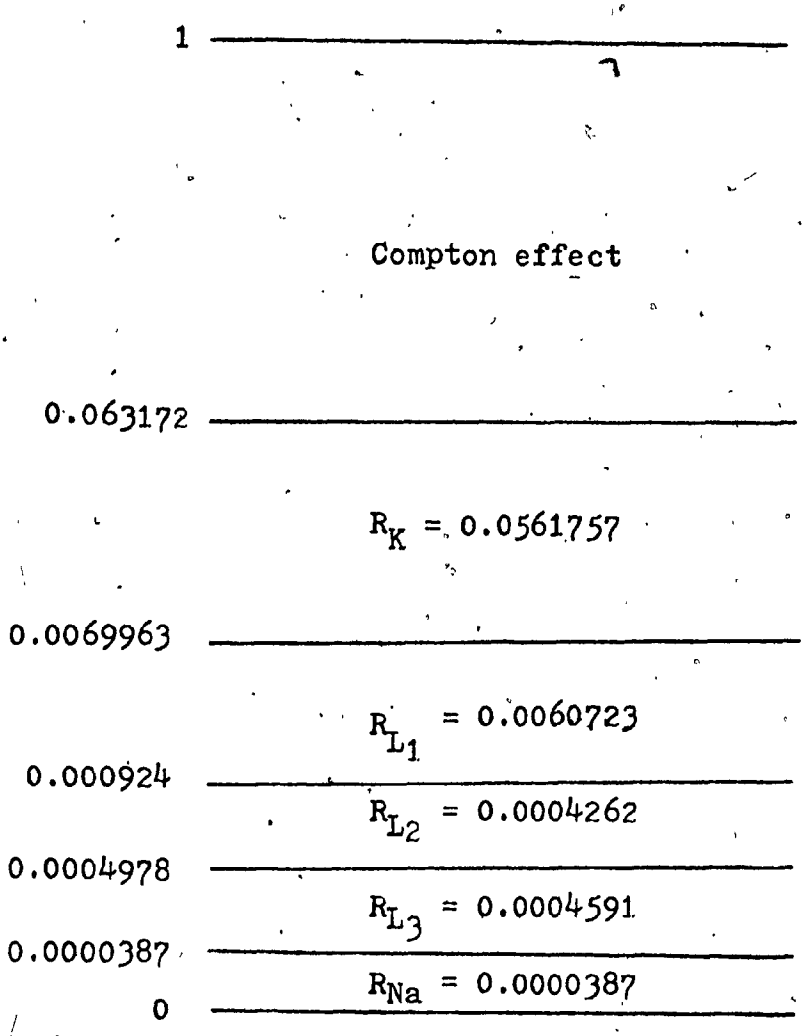


Fig. 3.6. When random number falls into one of these different regions, then that is the reaction which occurs.

We now know, if a photoelectric interaction occurs, in which atom and in which shell the collision occurs.

The ejected photoelectron leaves a vacancy in the atom which is filled by an electron transition from an upper shell. Here two possible mechanisms compete, radiative and Auger transitions.

If a fluorescence photon is emitted then it will have to be followed further in the crystal, whereas if an Auger electron is produced, it is assumed that all of its energy is deposited in the crystal.

The relative numbers of fluorescence photons for K and L shell vacancies are given by the fluorescence yields $\omega_{K,L}$ which are defined as the fraction of vacancies filled by radiative transitions. Value of $\omega_{K,L}$ are available from W.Bambynek[10] et al. and are given in Table 3.1.

The energies of fluorescence photons and their relative intensities for iodine atoms are given in Table 3.2. These were taken from Storm and Israel.[11] It can be seen that the photons fall into two groups with similar energies, K-L and K-M. Only these two groups were considered in the program. Fig. 3.7 summarizes the relative probabilities of various emissions following K-shell transition by photoelectric effect.

Shell	K	L_1	L_2	L_3
Probability of having a photon(ω).	0.882	0.058	0.091	0.097
Probability of having an Auger electron.	0.118	0.942	0.909	0.903

Table. 3.1. Fraction of vacancies filled by radiative transition.

E transferred from K to L or M shell.	K-L_2	K-L_3	K-M_2	K-M_3
Energy in KeV.	28.318	28.613	32.239	32.294
Relative intensities of kX-rays.	54.1	100	9.39	0.0914

Table. 3.2. The energies of fluorescence photons and their relative intensities for iodine atoms.

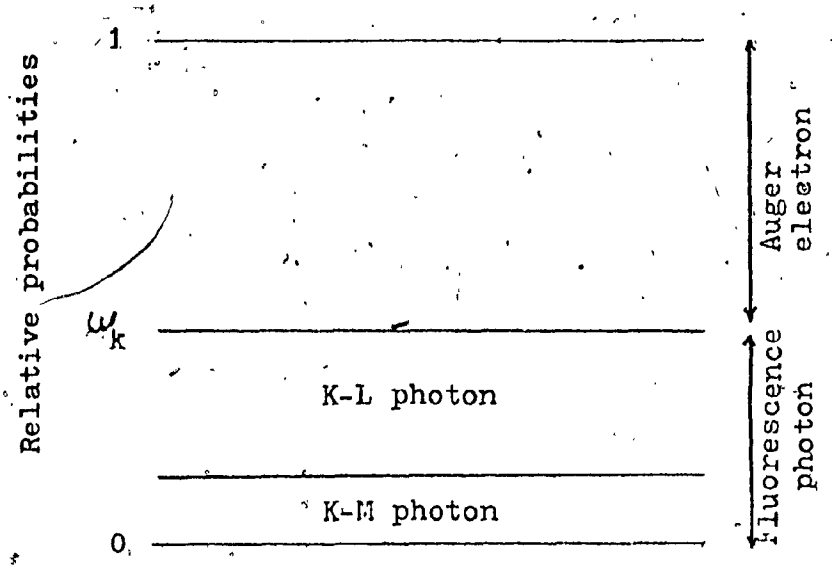


Fig. 3.7. The relative probabilities of the emitted particle following the photoelectric interaction in the K-shell of iodine.
By choosing a random number from 0 to 1, one of these possibilities is selected.

3.2.4. THE COMPTON EFFECT

If an interaction takes place by the Compton effect then it is necessary to select the energy of the recoil photon (A) by drawing a random number. Once A is known then the recoil electron energy (deposited in the crystal) is just $A_0 - A$, where A_0 is the energy of the photon before the collision. From a knowledge of A_0 and A the angle through which the photon is scattered is also deduced by the equation;

$$A = A_0/(1 + A_0(1-\cos\theta))$$

To select the recoil photon energy, integrals of the differential cross section in A divided by the total cross section were compared to random numbers. This is illustrated in fig. 3.8. The cross section $\frac{d\sigma}{dA}$ was integrated from the minimum A value $A_0/1+2A_0$ up to a selected value of A. If this expression as a fraction of the total cross section was less than the random number the range of the integral was extended to A + dA and the comparison repeated. Finally this can be written as;

$$R \leqslant \frac{\int_{A_{min}}^{A} (d\sigma/dA)\,dA}{\int_{A_{min}}^{A_0} (d\sigma/dA)\,dA} = \frac{\int_{A_{min}}^{A} (d\sigma/dA)\,dA}{\sigma_T}$$

Energy of A and A_0 is in mc^2 units.

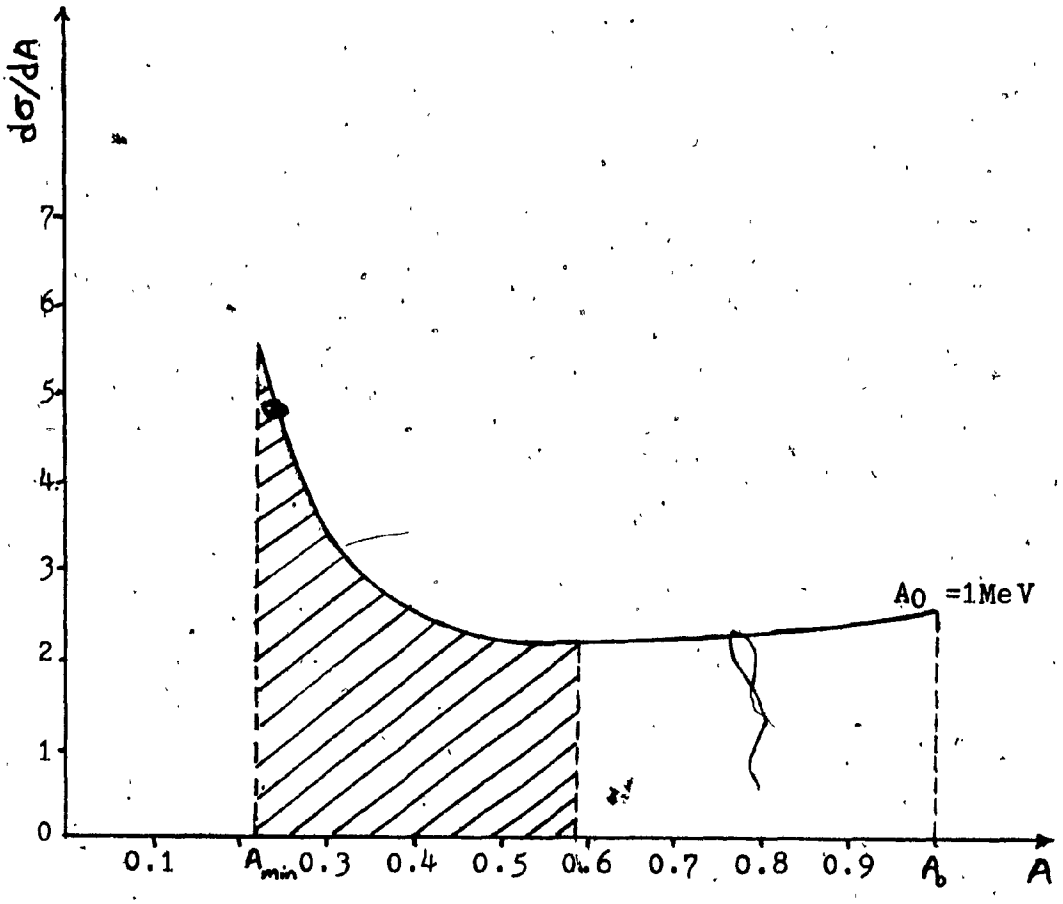


Fig. 3.8. Method of finding the energy of the recoil photon A by drawing a random number. A is the recoil photon energy, if $\int_{A_{min}}^{A}(d\sigma/dA)dA / \int_{A_{min}}^{A_0}(d\sigma/dA)dA$ exceeds the random number drawn. The ratio in this case is the shaded area under the curve to the total area under the curve

σ_T is given by Nelms[2] as :

$$\sigma_T = (\pi r_o^2/A_o^2)\left[A\left(\frac{2}{A_o}+\frac{1}{A_o^2}\right)-\left(2+\frac{2}{A_o}-A_o\right)\left(\ln A-\ln\frac{A_o}{1+2A_o}\right)\right.$$
$$\left.-\frac{1}{A_o}-\frac{A^2}{2A_o}-\frac{1}{1+2A_o}\left(2+\frac{1}{A_o}+\frac{A_o}{2(1+2A_o)}\right)+\frac{1+2A_o}{A_o}\right]$$

and;

$$\frac{d\sigma}{dA}=\frac{\pi r_o^2}{A_o^2}\left(\frac{2}{A_o}-\frac{2}{A}+\frac{1}{A_o^2}+\frac{1}{A^2}-\frac{2}{A_oA}-\frac{A_o}{A}+\frac{A}{A_o}\right)$$

Where r_o is the classical radius of the electron. Hence;

$$R(N)=\frac{\pi r_o^2}{\sigma_T A_o^2}\left[A(n)\left(\frac{2}{A_o}+\frac{1}{A_o^2}\right)-\left(2+\frac{2}{A_o}-A_o\right)\left(\ln A(n)-\right.\right.$$
$$\left.\ln\frac{A_o}{1+2A_o}\right)-\left(\frac{1}{A(n)}+\frac{A^2(n)}{2A_o}\right)-\frac{1}{1+2A_o}$$
$$\left.\left(2+\frac{1}{A_o}+\frac{A_o}{2(1+2A_o)}\right)+\left(1+\frac{2A_o}{A_o}\right)\right]$$

Initially 100 intervals from A_{min} to A_0 were used but it was found that these ranges are not fine enough for our purposes. To improve the accuracy of the selection in the above method, a second comparison was made. The first series of integrations allow the determination of the photon energy in the range A to $A + dA$. This range of width dA

was then subdivided into another 100 intervals and the process described above repeated. This is equivalent to using 100×100 intervals but saves a great deal of computing time.

CHAPTER 4

THE PASSAGE OF A PHOTON IN THE CRYSTAL

4.1. INTRODUCTION

The path of the photon, its position of interaction and the energy lost at each interaction must be followed as the photon travels through the crystal. In addition each point of interaction must be tested to see if the photon is still inside the crystal.

At each collision it is necessary to know the direction the photon is travelling before the interaction (direction cosines $\cos\alpha$, $\cos\beta$, $\cos\gamma$), the distance travelled from the previous interaction Δl_i, and the position of the previous interaction X_i, Y_i, Z_i. From these it is possible to test if the interaction takes place in the crystal. If it does, then the type of interaction is determined as discussed in the previous chapter, and the energy lost by the interaction is calculated..

If the interaction at X_{i+1}, Y_{i+1}, Z_{i+1} is by the photoelectric effect it is assumed that any fluorescence photon emitted is isotropic so that the polar angle is selected randomly from values between 0° and 180° and the azimuthal angle from values between 0° and 360°.

For the Compton effect the polar angle θ is given by the energy of the recoil photon and the azimuthal angle is assumed to be uniformly distributed between 0° and 360°.

The relationships between the scattering angle and

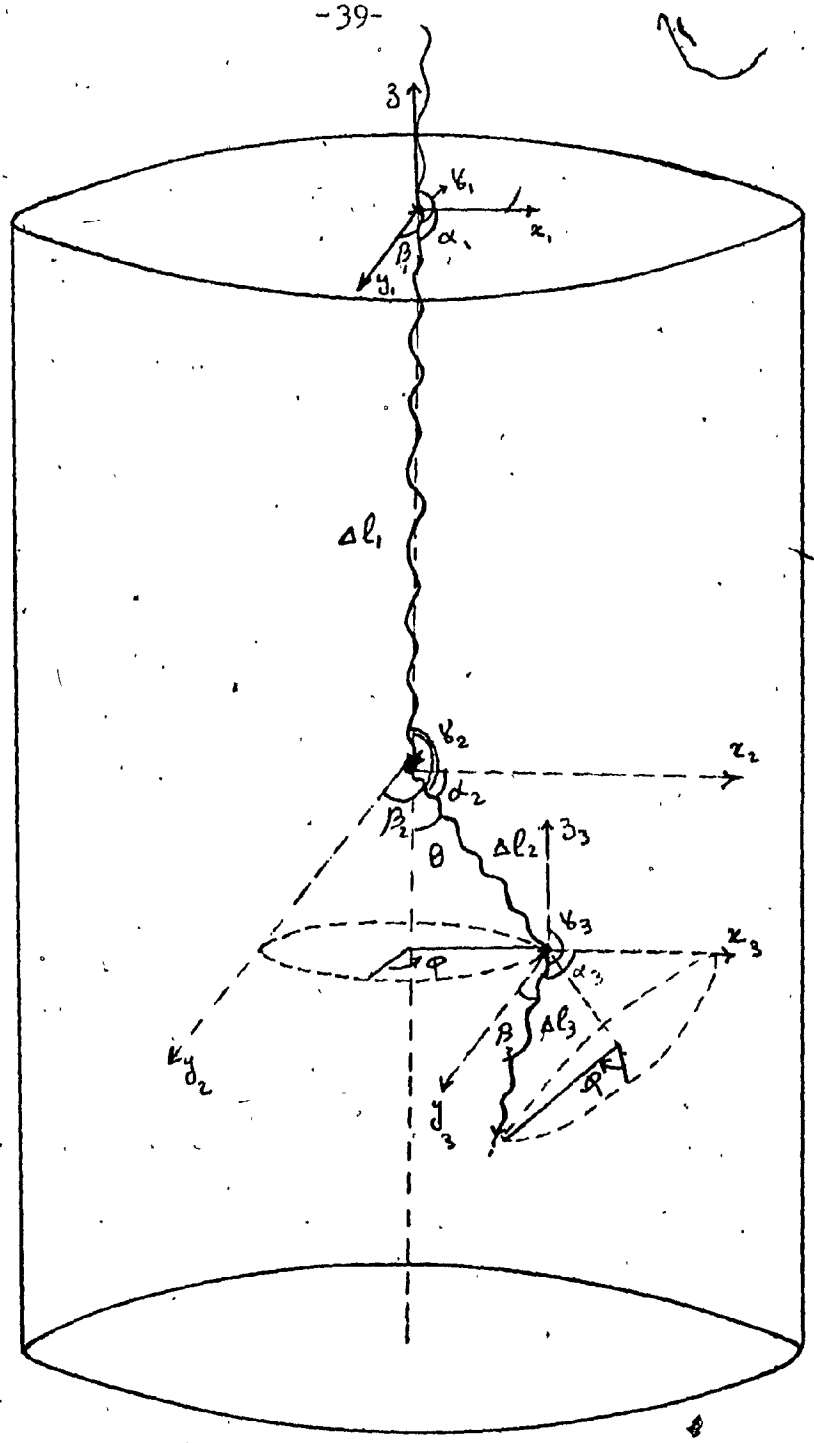


Fig. 4.1. The geometry used; α, β, γ are the direction cosines, Δl_i is the path length of the photon passing through the crystal, θ is the polar angle, and Φ is the azimuthal angle.

the distance travelled are shown in fig. 4.1.

4.2. THE FIRST INTERACTION

Each photon enters the crystal along the Z axis and forces to interact in the crystal by an appropriate choice of random numbers. The co-ordinates of the first interactions are:

$X_0 = 0$

$Y_0 = 0$

$Z_0 = \Delta l_1$

and the initial direction is:

$\cos\alpha_1 = 0$

$\cos\beta_1 = 0$

$\cos\gamma_1 = 1$

From the interaction the new direction of travel is determined by selection of the polar angle θ and the azimuthal angle ϕ. The new set of direction cosines($\cos\alpha_2$, $\cos\beta_2$, $\cos\gamma_2$) is given by the standard transformation.[12]

$$\cos\alpha_2 = \cos\theta\cos\alpha_1 + (\sin^2\theta/\sin^2\gamma_1)^{\frac{1}{2}}(\cos\alpha_1\cos\gamma_1\cos\phi - \cos\beta_1\sin\phi)$$

$$\cos\beta_2 = \cos\theta\cos\beta_1 + (\sin^2\theta/\sin^2\gamma_1)^{\frac{1}{2}}(\cos\beta_1\cos\gamma_1\cos\phi + \cos\alpha_1\sin\phi)$$

$$\cos\gamma_2 = \cos\theta\cos\gamma_1 - (\sin^2\theta/\sin^2\gamma_1)^{\frac{1}{2}}(\sin^2\gamma_1)\cos\phi$$

Except when $(1-\cos^2\gamma_1)$ approaches zero, in which case :

$\cos\alpha_2 = \sin\theta\cos\varphi$

$\cos\beta_2 = \sin\theta\sin\varphi$

$\cos\gamma_2 = (\cos\gamma_1/|\cos\gamma_1|)\cos\theta$

4.3. THE SECOND AND SUBSEQUENT INTERACTION

The first interaction will produce a photon with a new energy so that in order to determine its path length before it interacts a new set of mass attenuation coefficients is needed. These are interpolated from data already read in by the program(see Table. 5.1, 2.). The path length to the next interaction is defined from:

$$\Delta l_2 = \frac{\lambda \rho R}{\mu}$$

The co-ordinate of the interaction are given by:

$X_2 = \Delta l_2 \cdot \cos\alpha_2 + X_1$

$Y_2 = \Delta l_2 \cdot \cos\beta_2 + Y_1$

$Z_2 = \Delta l_2 \cdot \cos\gamma_2 + Z_1$

To test if this location is in the crystal, we define:

$S_2^2 = X_2^2 + Y_2^2$

If S_2 is greater than the radius of the crystal then the interaction has taken place outside of the crystal, i.e. the photon has escaped. The energy deposited in the crystal by the first interaction is recorded and the next photon entering the crystal is considered. In addition if Z_2 is greater than the thickness of the crystal the photon has escaped.

If the site of interaction is in the crystal then the type of interaction (Compton or photoelectric) is chosen, new angles and photon energy found etc,and the process repeated.

Photons were followed until they escaped from the crystal or their energy dropped below 10 Kev, in which case it was assumed they were absorbed in the crystal.

The total energy deposited by each photon was recorded and the resulting spectrum is shown in the next chapter.

CHAPTER 5

RESULTS AND DISCUSSION

5.1. RESULT

Using the method described previously a FORTRAN program was written to track the passage of individual photons through a sodium iodide crystal. All cross sections of the Compton and photoelectric interactions were taken from tabulation by J.H. Hubbell[8] which is shown in Tables 5.1, 5.2. A Flow Chart of the Program is shown in Appendix 1.

The program was run for 1MeV photons incident along the axis of a 3"×3" sodium iodide crystal and the output gave the energy deposited in the crystal as a fraction of the incident photon energy in 100 intervals. The results are shown in fig. 5.1. for 10,000 interacting photons. It can be seen that the figure divides into two parts. The large peak is due to photons stopping in the crystal and depositing all of their energy. The lower section of the curve is caused by the escape of photons from crystal. Here the photons deposit only a fraction of their energy.

The number of photons in the main peak expressed as a fraction of the total numbers incident gives the counting efficiency. In this case for 10,000 photons interacting in the crystal there are 1843 counts in this peak. In order to calculate the efficiency it is necessary to know the number of incident photons that produce 10,000 interactions.

The number of photons passing through the crystal will

be given by the familiar equation;

$$N = N_0 e^{-\mu x}$$

where N_0 is the number incident, μ is the attenuation coefficient for 1MeV photons in NaI($\mu = 5.8 \times 10^{-2}$) and x is the thickness of the crystal (x = 3"), the number interacting (10,000) is given by $N_0 - N$, or:

$$10,000 = N_0 - N$$
$$= N_0 - N_0 e^{-\mu x}$$
$$= N_0(1 - e^{-\mu x})$$

Hence N_0, the numbers incident in order to give 10,000 interactions is equal to 15,264.

Using this value for the number incident and the 1,843 counts under the peak gives 0.0059 as the absolute efficiency of the crystal This absolute efficiency compares well with the absolute efficiency, 0.0055, calculated by R.L.Heath[13].

Fig. 5.2. shows the comparison of theoretical and experimental results.

5.2. DISCUSSION

In any Monte Carlo program compromises between the running time and approximation have to be made. Here it has been assumed that all electrons produced are stoped in the crystal and that photons below 10 keV are stopped in the crystal. The bremsstrahlung production was not taken into account and followed.

These approximation even if they seem to be reasonable can cause discrepancies compared with experimental data.

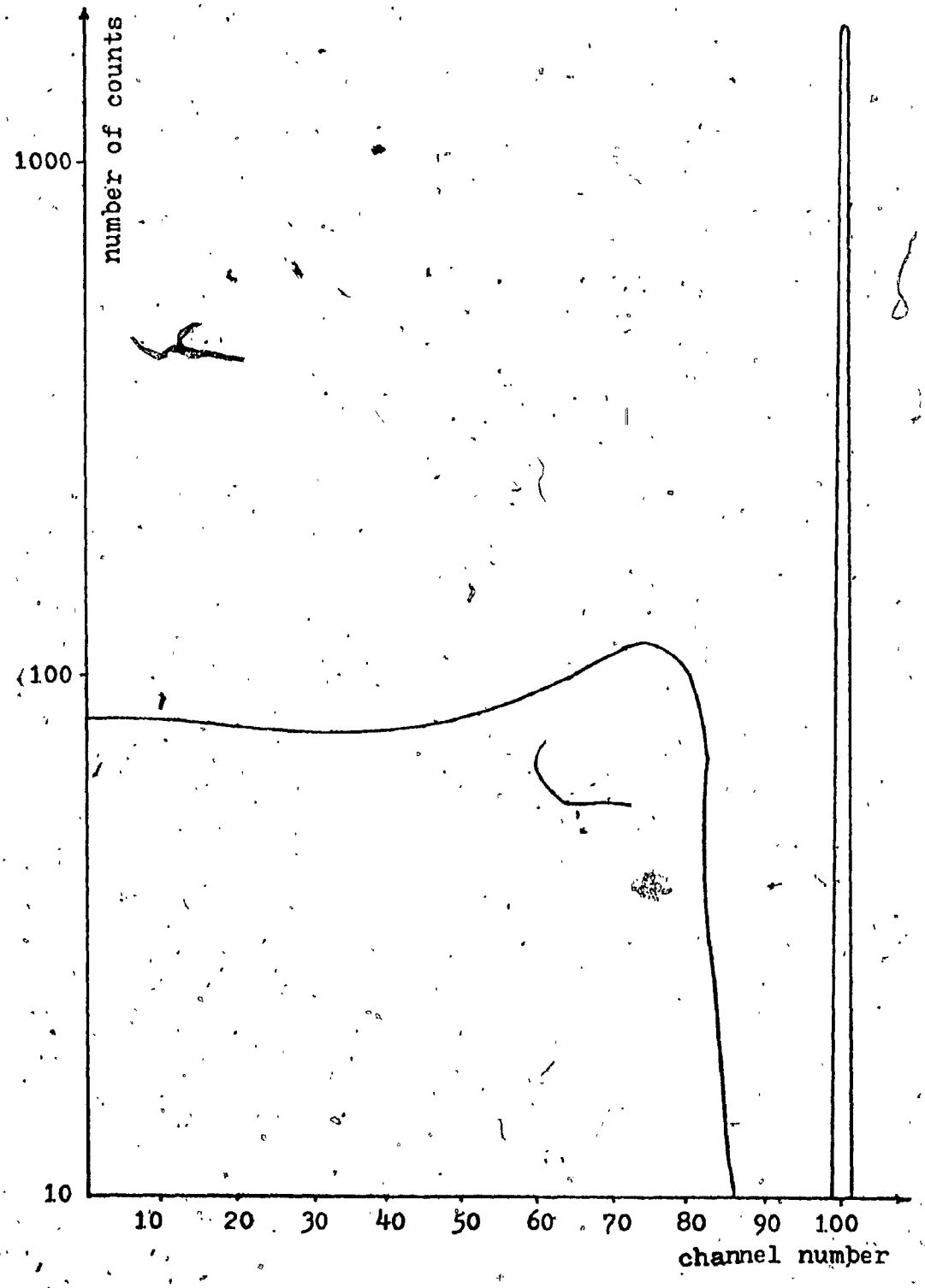


Fig. 5.1. Absolute number of counts per channel.

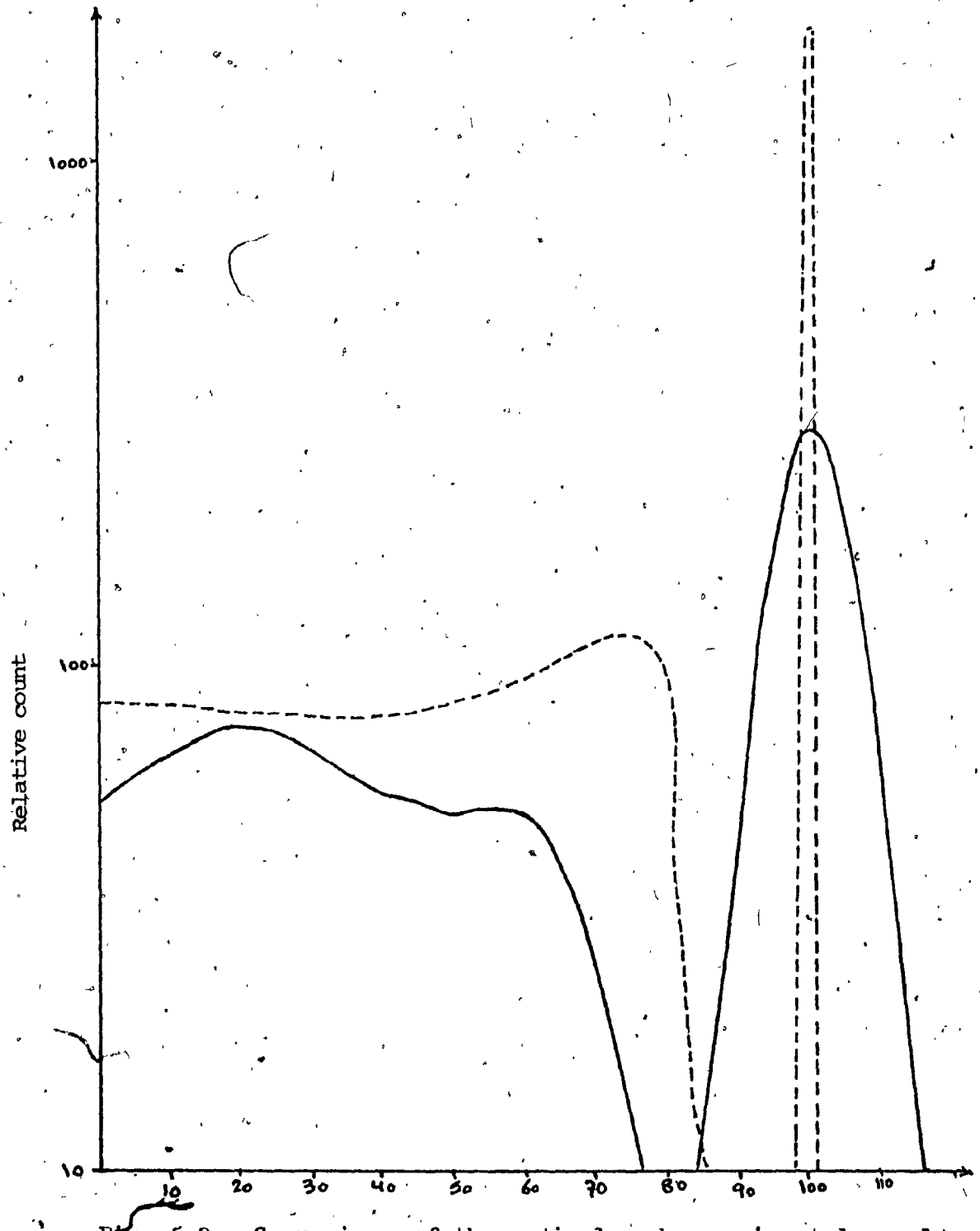


Fig. 5.2. Comparison of theoretical and experimental results.

PHOTON ENERGY	COMP(T)	PHOTO(T)	TOTAL	I(PHOT)	NA(PHOT)
1.00E-02	1.65E+01	1.36E+02	1.36E+02	1.58E+02	1.50E+01
2.00E-02	1.59E-01	2.11E+01	2.12E+01	2.46E+01	1.70E+00
3.00E-02	1.54E-01	6.70E+00	6.86E+00	7.83E+00	4.66E-01
3.32E-02	1.52E-01	5.03E+00	5.19E+00	5.88E+00	3.00E-01
3.32E-02	1.52E+01	3.03E+01	3.04E+01	3.57E+01	2.00E-01
4.00E-02	1.49E-01	1.88E+01	1.89E+01	2.21E+01	1.88E-01
5.00E-02	1.44E-01	1.03E+01	1.05E+01	1.22E+01	9.25E-02
6.00E-02	1.40E-01	6.28E+00	6.42E+00	7.40E+00	5.21E-02
8.00E-02	1.33E-01	2.87E+00	3.00E+00	3.39E+00	2.07E-02
1.00E-01	1.27E-01	1.52E+00	1.64E+00	1.79E+00	1.01E-02
1.50E-01	1.14E-01	4.76E-01	5.90E-01	5.60E-01	2.78E-03
2.00E-01	1.05E-01	2.09E-01	3.14E-01	2.47E-01	1.12E-03
3.00E-01	9.09E-02	6.68E-02	1.58E-01	7.88E-02	3.25E-04
4.00E-01	8.15E-02	3.10E-02	1.12E-01	7.88E-02	1.39E-04
5.00E-01	7.44E-02	1.77E-02	9.21E-02	2.09E-02	7.49E-05
6.00E-01	6.88E-02	1.14E-02	8.02E-02	1.34E-02	4.66E-05
8.00E-01	6.05E-02	5.88E-03	6.63E-02	6.93E-03	2.36E-05
1.00E+00	5.43E-02	3.66E-03	5.80E-02	4.32E-03	1.46E-05

Table. 5.1 Tabulation of cross-sections for energies less than 1MeV for Compton, photoelectric, total ($\sigma_{comp} + \tau_{Photo}$), for iodine and sodium(when there is photoelectric effect). All the cross sections are in units of cm^2/gm.

PHOTON ENERGY (MeV)	K-SHELL	L-SHELL	M-SHELL
1.0000E-02	0.0000E+00	2.8968E+04	5.5148E+03
1.5000E-02	0.0000E+00	8.4945E+03	1.0165E+03
2.0000E-02	0.0000E+00	4.0637E+03	8.1735E+02
3.0000E-02	0.0000E+00	1.3046E+03	2.6161E+02
3.3134E-02	0.0000E+00	9.8497E+02	1.9745E+02
3.3399E-02	6.0611E+03	9.6297E+02	1.9308E+02
4.0000E-02	3.8135E+03	5.7688E+02	1.1557E+02
5.0000E-02	2.1201E+03	3.0486E+02	6.1044E+01
6.0000E-02	1.2942E+03	1.8055E+02	3.6142E+01
8.0000E-02	5.8464E+02	7.7647E+01	1.5743E+01
1.0000E-01	3.1211E+02	4.1170E+01	8.2420E+00
1.5000E-01	9.8370E+01	1.2687E+01	2.5414E+00
2.0000E-01	4.3309E+01	5.5355E+00	1.1094E+00
3.0000E-01	1.3911E+01	1.7643E+00	3.5384E-01
4.0000E-01	6.4163E+00	8.1019E-01	1.6247E-01
5.0000E-01	3.6209E+00	4.5546E-01	9.1338E-02
6.0000E-01	2.3201E+00	2.9077E-01	5.8304E-02
8.0000E-01	1.2031E+00	1.4980E-01	3.0024E-02
1.0000E+00	7.5201E-01	9.3141E-02	1.8656E-02

Table. 5.2 Tabulation of photoelectric cross-section for energies less than 1Mev for K, L, and M shell of iodine. All the cross-sections are in units of cm^2/gm.

REFERENCES

1) H.Frauenfeler and E.M.Henly, Sub Atomic Physics. P.Hall, Inc.Englewood Cliffs, New Jersy, 1974.

2) A.T.Nelms, NBS Circular 542(1953).

3) W.F.Miller and W.J.Snow, ANL-6318. Argonne National Laboratory(1961).

4) C.D.Zerby and H.S.Moran, Nucl. Instr and Meth 14,115(1962).

5) J.M.Seltzer and M.J.Berger, ANS trans 14.124(1971).

6) J.D.Marshal. ANS trans 13,873(1970).

7) R.D.Evans, Compton Effect. In Handbook of Physics.XXXIV. S.Flugge, Berlin.Gottingen.Heidelberg,1958.

8) J.H.Hubbel, Stand. Ref. Data. Ser. NSRDS. 29(1969).

9) J.H.Scofield, UCRL. 51326(1973).

10) W.Bambynek, B.Crasemann, R.W.Fink, H.U.Freund, H.Mark, R.E.Price, and P.Venugopala Rao, Rev. Mod. Phys., 44,716-813(1972).

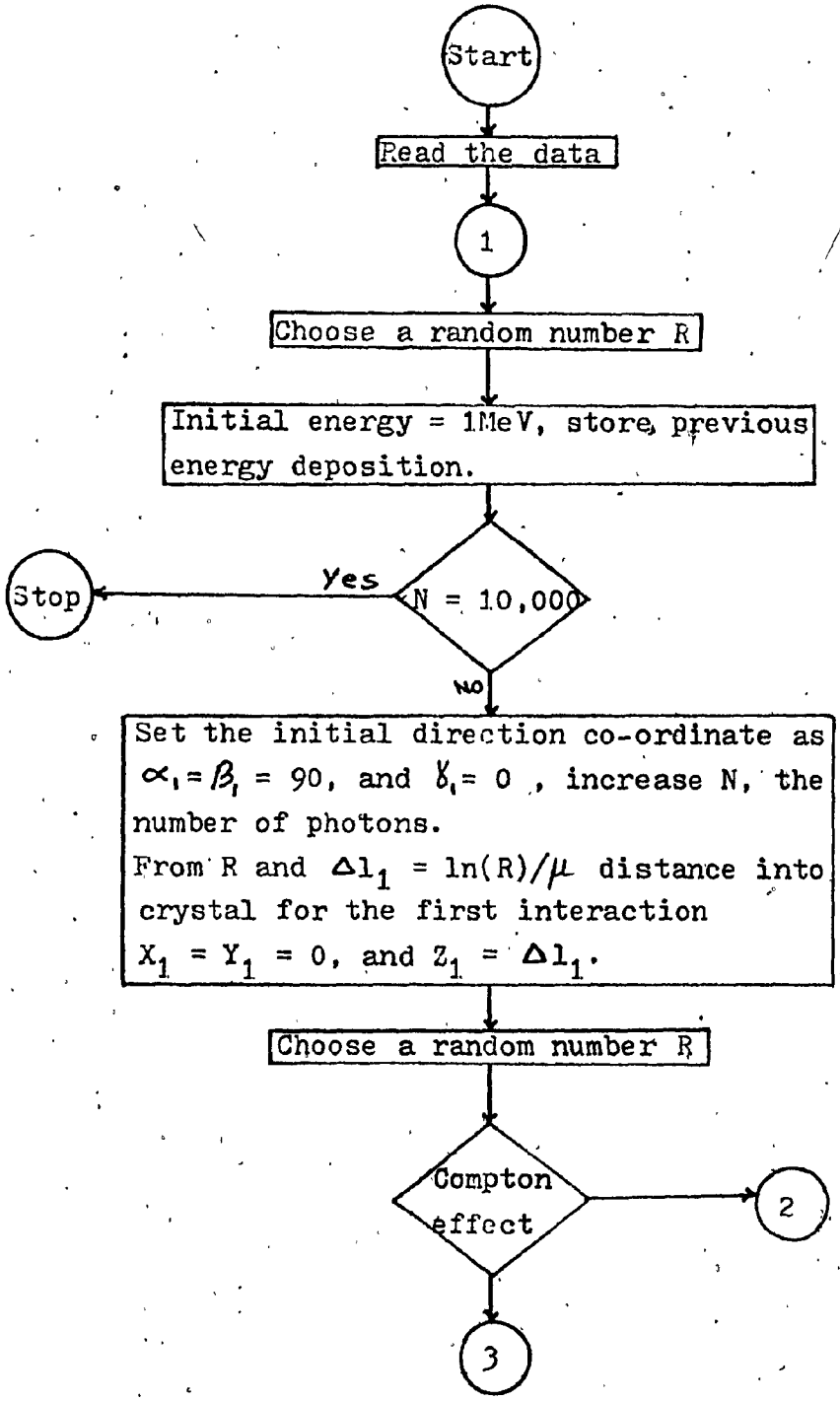
11) E.Storm and H.I.Israel, Nucl Data Tables A7, 565-681 (1972).

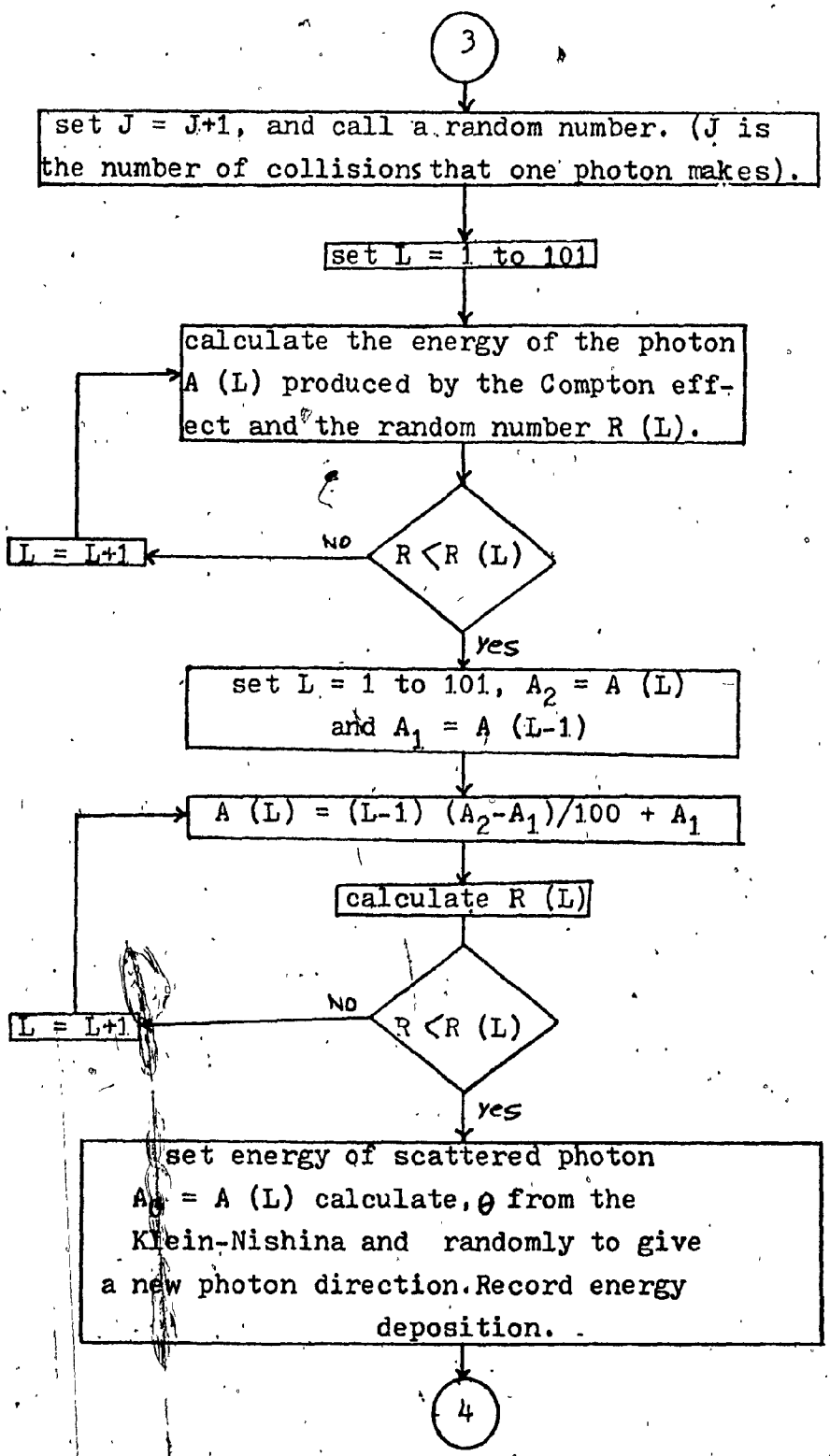
12) B.Grosswendt and E.Waible, Nucl. Instr and Meth, 131,143-156(1975).

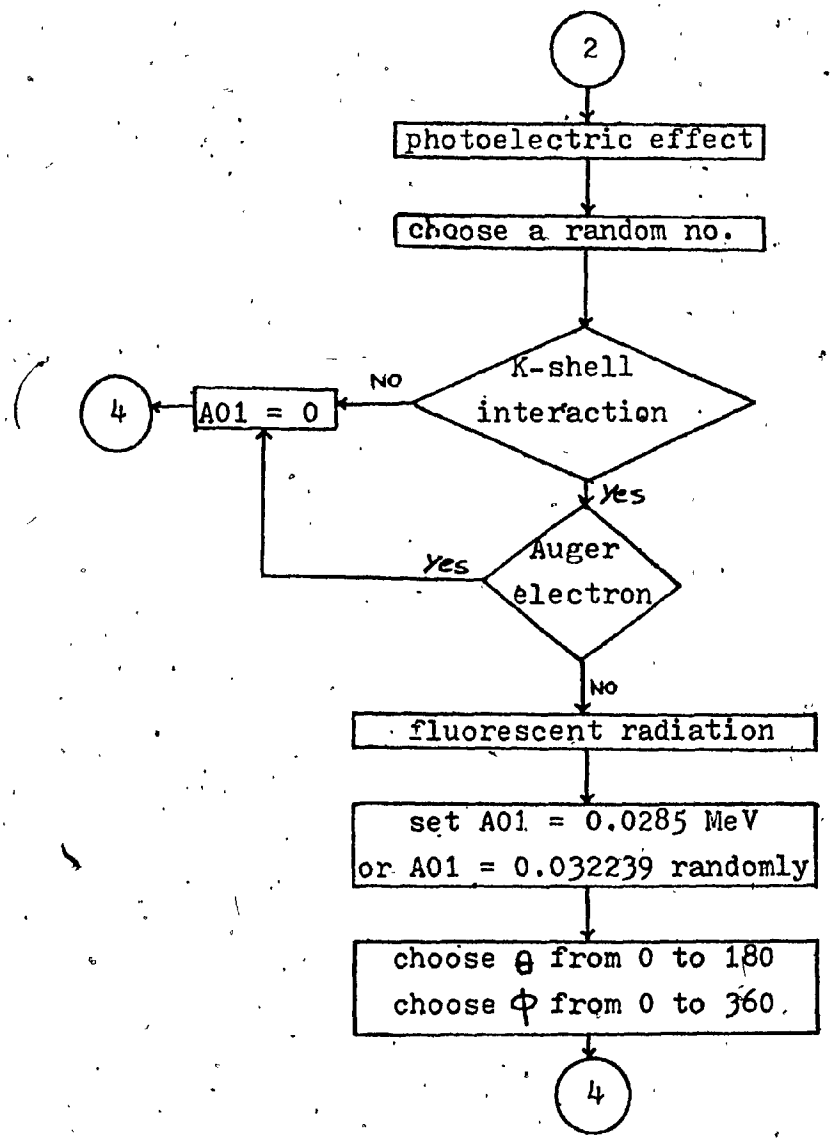
13) R.L.Heath, Scintillation Spectrometry, U.S.Atomic Energy Commission, 1,1964.

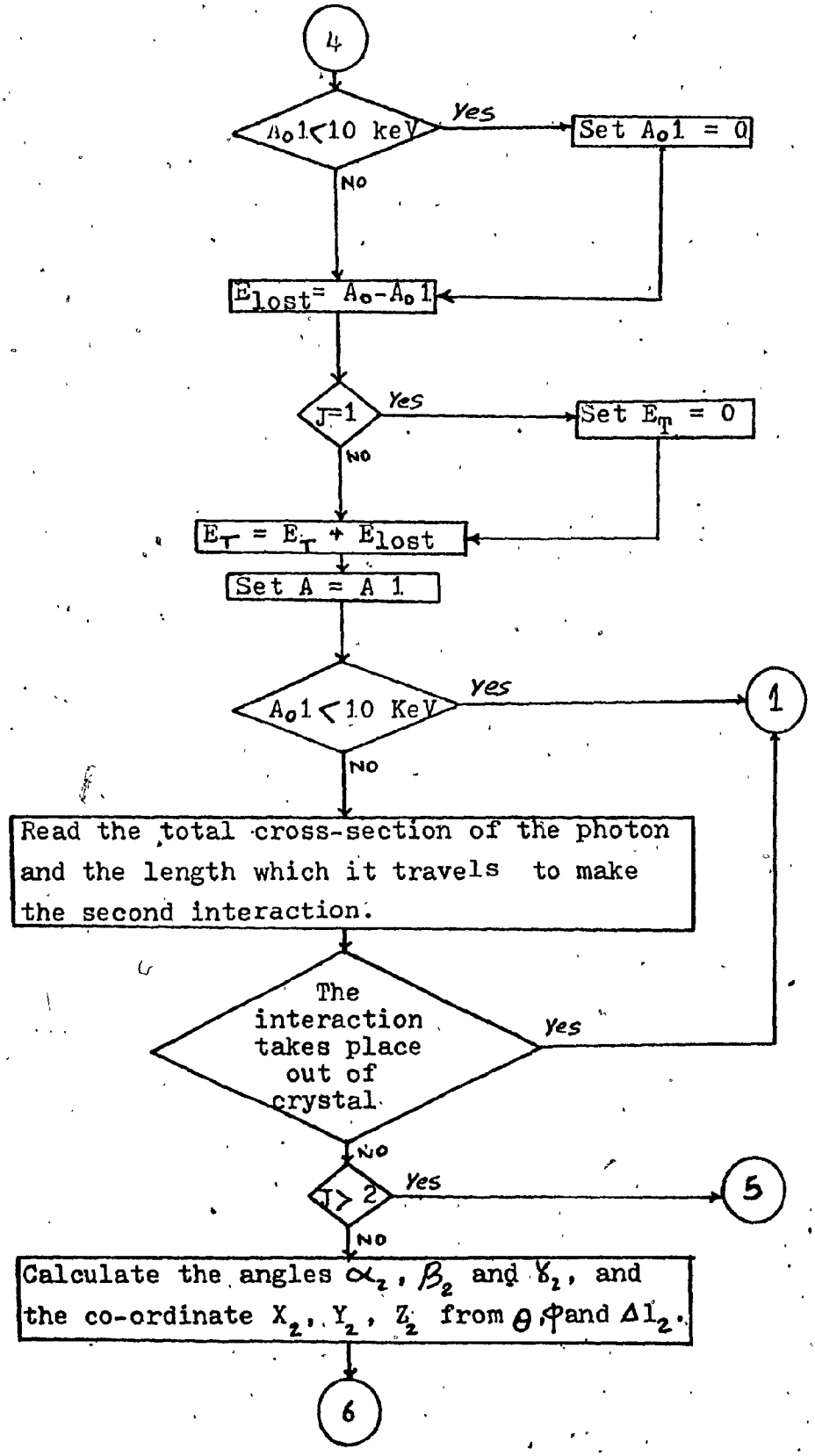
APPENDIX "1"

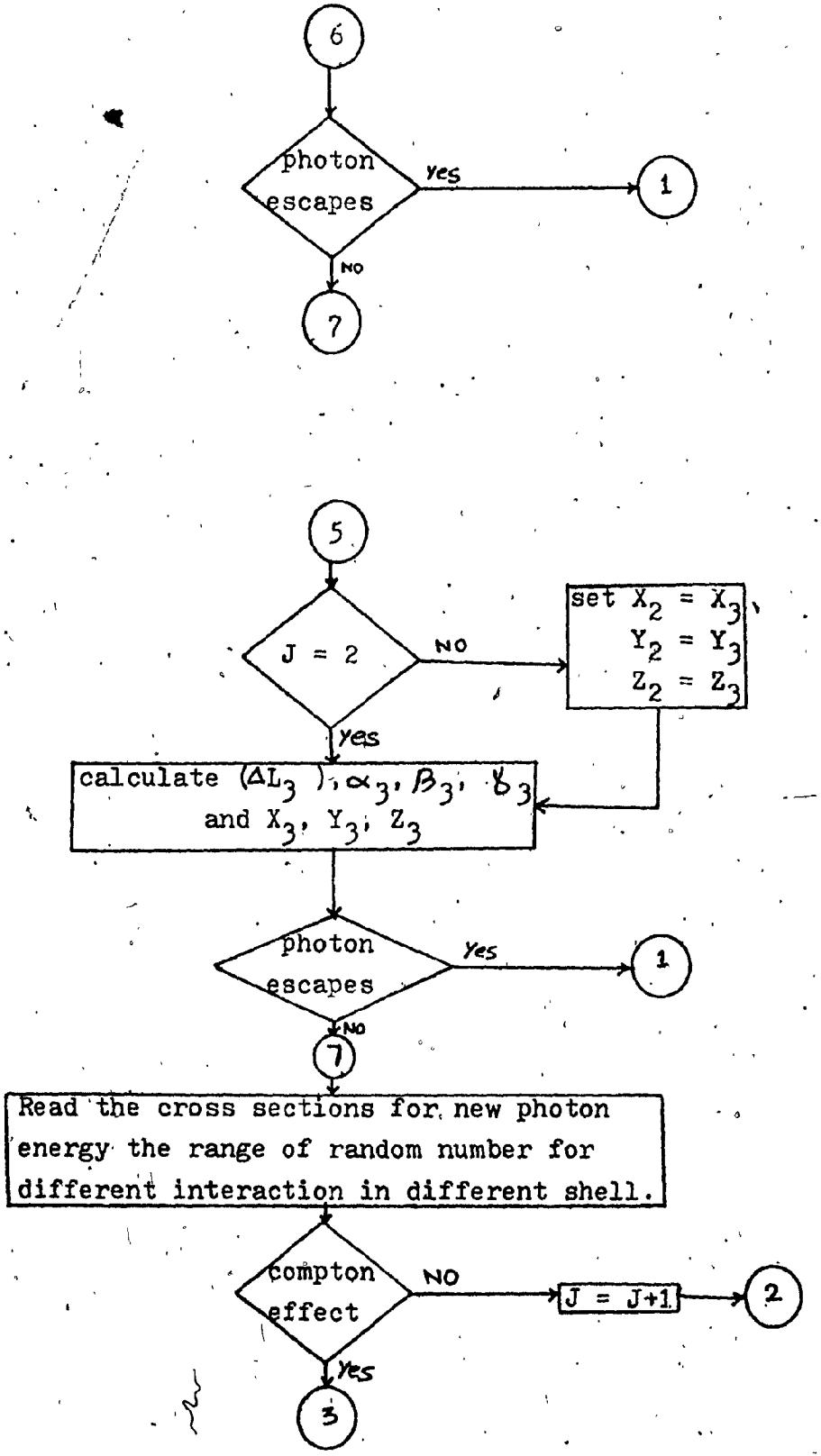
THE FLOW CHART OF THE PROGRAM.


Start
Read the data
1
Choose a random number R
Initial energy = 1MeV, store previous energy deposition.
N = 10,000
Yes
Stop
No
Set the initial direction co-ordinate as $\alpha_1 = \beta_1 = 90$, and $\gamma_1 = 0$, increase N, the number of photons.
From R and $\Delta l_1 = \ln(R)/\mu$ distance into crystal for the first interaction
$X_1 = Y_1 = 0$, and $Z_1 = \Delta l_1$.
Choose a random number R
Compton effect
2
3


3
set J = J+1, and call a random number. (J is the number of collisions that one photon makes).
set L = 1 to 101
calculate the energy of the photon A (L) produced by the Compton effect and the random number R (L).
R <R (L)
NO
L = L+1
yes
set L = 1 to 101, A_2 = A (L) and A_1 = A (L-1)
A (L) = (L-1) (A_2-A_1)/100 + A_1
calculate R (L)
R <R (L)
NO
L = L+1
yes
set energy of scattered photon A_6 = A (L) calculate, θ from the Klein-Nishina and randomly to give a new photon direction. Record energy deposition.
4


2
photoelectric effect
choose a random no.
K-shell interaction
NO
A01 = 0
4
Yes
Auger electron
yes
NO
fluorescent radiation
set A01 = 0.0285 MeV
or A01 = 0.032239 randomly
choose θ from 0 to 180
choose Φ from 0 to 360
4


4
A_o1<10 keV
Yes
Set A_o1 = 0
NO
E_{lost}= A_o-A_o1
J=1
Yes
Set E_T = 0
NO
E_T = E_T + E_{lost}
Set A = A 1
A_o1 < 10 KeV
Yes
1
NO
Read the total cross-section of the photon and the length which it travels to make the second interaction.
The interaction takes place out of crystal
Yes
NO
J> 2
Yes
5
NO
Calculate the angles α_2, β_2 and γ_2, and the co-ordinate X_2, Y_2, Z_2 from θ, ϕ and Δl_2.
6


6
photon escapes
yes
1
NO
7
5
J = 2
NO
set $X_2 = X_3$, $Y_2 = Y_3$, $Z_2 = Z_3$
yes
calculate (ΔL_3), α_3, β_3, γ_3 and X_3, Y_3, Z_3
photon escapes
Yes
1
NO
7
Read the cross sections for new photon energy the range of random number for different interaction in different shell.
compton effect
NO
J = J+1
2
Yes
3

APPENDIX "2"

LIST OF THE PROGRAM FOR CALCULATING THE EFFICIENCY OF Na(Tl) CRYSTALS EXPOSED TO 1MeV GAMMA RAYS BY MONTE CARLO METHOD.

APROGRAM FOR CALCULATING THE EFFICIENCY OF NaI(Tl) CRYSTALS EXPOSED TO 1MeV GAMMA-RAYS BY MONTE CARLO METHOD FOR A 3"×3" INCH CRYSTAL.

```
00010       PROGRAM CORRECT(INPUT,OUTPUT,TAPE6=OUTPUT,TAPE5)
00020       DIMENSION NCOMP(101),NPHOTO(101),KPHOT(101),BO(20)
00030+      ,XMU1(20),SIGMAPH(20),SIGMAC(20),SIGMANA(20),
00040+      SIGMAI(20),A(301),R(301),CO(20),SIGMAK(20),
00050+      SIGMAL1(20),SIGMAL2(20),SPECT(101),KPPHOT(101)
00060+      ,KAPHOT(101)
00070       RAD=3/2
00080       RAD=RAD*3.667
00090       DEPTH=3.
00100       DEPTH=(DEPTH)*3.667
00110       XN=0.
00120       NCOMP(N)=0
00130       NPHOTO(N)=0
00140       ET=0.0
00150       READ,TABLE7
00160       CALL GET(5HTAPE5,TABLE7,0,0)
00170       READ(5,99)TOPIC
00180   99  FORMAT(A11)
00190       DO 23 I=1 , 19
00200       READ(5,25)BO(I),SIGMAC(I),SIGMAPH(I),XMU1(I)
00210+      ,SIGMAI(I),SIGMANA(I)
00220   25  FORMAT(6(E8.2,3X))
00230   23  BO(I)=BO(I)/0.511006
00240       READ,TABLE8
00250       CALL GET(5HTAPE5,TABLE8,0,0)
00260       READ(5,99)TOPIC
00270       DO 24 I=1,19
00280       READ(5,26)CO(I),SIGMAK(I),SIGMAL1(I),SIGMAL2(I)
00290   26  FORMAT(E10.4,5X,3(E10.4,2X))
00300   24  CO(I)=CO(I)/0.511006
00310       DO 90 KK=1 , 101
00320   90  SPECT(KK)=0.
00330       NRAND=21175
00340   10  CALL RANDU(NRAND,NRAND,RANDOM)
00350       Y=RANDOM
00360       AO=1./0.511006
00370       KK=(ET/AO)*100+1
00380  103  FORMAT(F10.4,3X,I4)
00390       SPECT(KK)=SPECT(KK)+1
00400       IF(XN.GT.100.)GO TO 40
00410       XMU=5.80/(10.**2)
00420       H=0.79428E-25
00430*      RO**2=H
00440       J=0
```

```
00450       P=(2.71828182B)**(-XMU*DEPTH)
00460       Y=Y*(1-P)+P
00470       XN=XN+1
00480       DELTA1=(-ALOG(Y))/XMU
00490       ALFA1=90.*(3.141592654/180.)
00500       BETA1=90.*(3.141592654/180.)
00510       GAMA1=0.
00520       X1=0.
00530       Y1=0.
00540       Z1=DELTA1
00550       CALL RANDU(NRAND,NRAND,RANDOM)
00560       Y=RANDOM
00570       IF(Y.LE.0.063172)GO TO 60
00580*      ------------------------------------------------------
00590*
00600*                    COMPTON EFFECT
00610*
00620*      ------------------------------------------------------
00630 100   NCOMP(N)=NCOMP(N)+1
00640       SIGCT=2.*3.141592654*(H)*(((1.+A0)/A0**2)*(((2.
00650+            *(1.+A0))/(1.+2.*A0))-((ALOG(1.+2.*A0))
00660+            /A0))+(ALOG(1.+2.*A0))/(2.*A0)-(1.+3.*A0)/
00670+            ((1.+2.*A0)**2))
00680       B=(3.141592654*H)/SIGCT
00690       J=J+1
00700       CALL RANDU(NRAND,NRAND,RANDOM)
00710       Y=RANDOM
00720       DO 41 N=1 , 101
00730       A(N)=((N-1)*(A0-(A0/(1.+(2.*A0)))))/100+A0/(1.+
00740+            (2.*A0))
00750       R(N)=(B/(A0**2))*(A(N)*((2./A0)+(1./(A0**2)))-
00760+           (2.+(2./A0)-A0)*(ALOG(A(N))-ALOG(A0/(1.+
00770+           (2.*A0))))-(1./A(N))+((A(N)**2)/(2.*A0))-
00780+           (1./(1.+(2.*A0)))*(2.+(1./A0)+(A0/(2.*(1.
00790+           +(2.*A0)))))+((1.+(2.*A0))/A0))
00800       IF(Y.LT.R(N))GO TO 42
00810   41  CONTINUE
00820   42  A2=A(N)
00830       A1=A(N-1)
00840       DO 43 N=1, 101
00850       A(N)=(N-1)*(A2-A1)/100+A1
00860       R(N)=(B/(A0**2))*(A(N)*((2./A0)+(1./(A0**2)))-
00870+           (2.+(2./A0)-A0)*(ALOG(A(N))-ALOG(A0/(1.+
00880+           (2.*A0))))-(1./A(N))+((A(N)**2)/(2.*A0))-
00890+           (1./(1.+(2.*A0)))*(2.+(1./A0)+(A0/(2.*(1.
00900+           +(2.*A0)))))+((1.+(2.*A0))/A0))
00910       IF(Y.LT.R(N)) GO TO 45
```

```
00920   43  CONTINUE
00930   45  A01=A(N)
00940       TATA=ACOS(1.+1./A0-1./A01)
00950       CALL RANDU(NRAND,NRAND,RANDOM)
00960       Y=RANDOM
00970       FUY=Y*(2.*3.141592654)
00980       GO TO 20
00990*      ------------------------------------------------------
01000*
01010*                  PHOTOELECTRIC EFFECT
01020*
01030*      ------------------------------------------------------
01040   60  NPHOTO(N)=1
01050       J=1
01060       IF(Y.LE.0.063172.AND.Y.GT.0.0069963)GO TO 66
01070*       THE SCATTERING IS ON THE K SHELL
01080       IF(Y.LE.0.0069963.AND.Y.GT.0.0009240)GO TO 79
01090*      THE SCATTERING IS ON THE L1 SHELL
01100       IF(Y.LE.0.0009240.AND.Y.GT.0.0004978)GO TO 79
01110*      THE SCATTERING IS ON L3 SHELL
01120       IF(Y.LE.0.0004978.AND.Y.GT.0.000038700)GO TO 79
01130*      THE SCATTERING IS ON L2 SHELL
01140       IF(Y.LE.0.000038700)GO TO 79
01150*      THE SCATTERING IS WITH THE SODIUM ATOM
01160   55  CALL RANDU(NRAND,NRAND,RANDOM)
01170       Y=RANDOM
01180       IF(Y.LE.0.0580) GO TO 62
01190       IF(Y.GT.0.0580) GO TO 64
01200*      K-M2 OR K-M3 TRANSITION
01210   62  A01=0.032239/0.511006
01220       GO TO 11
01230   64  A01=0.028514/0.511006
01240*      K-L2 OR K-L3 TRANSITION
01250   11  CALL RANDU(NRAND,NRAND,RANDOM)
01260       Y=RANDOM
01270       TATA=Y*3.141592654
01280       CALL RANDU(NRAND,NRAND,RANDOM)
01290       Y=RANDOM
01300       FUY=Y*(2.*3.141592654)
01310   20  IF(A01.LT.(.01/0.511006))A01=0.
01320       ELOST=A0-A01
01330       IF(J.EQ.1)ET=0.0
01340       ET=ET+ELOST
01350       A0=A01
01360   29  IF(A01.LT.(0.01/0.511006))GO TO 10
01370       DO 27 I=1 , 19
01380       IF(A01.LT.B0(I)) GO TO 28
01390   27  CONTINUE
```

```
01400   28  XMUE=((A01-B0(I-1))/(B0(I)-B0(I-1)))*(XMU1(I)-
01410+                XMU1(I-1))+XMU1(I-1)
01420       IF(J.GE.2)GO TO 6
01430       CALL RANDU(NRAND,NRAND,RANDOM)
01440       Y=RANDOM
01450       DELTA2=(-ALOG(Y))/XMUE
01460       ALFA2=ACOS(SIN(TATA)*COS(FUY))
01470       BATA2=ACOS(SIN(TATA)*SIN(FUY))
01480       GAMA2=ACOS((COS(GAMA1)/ABS(COS(GAMA1)))*COS(TATA))
01490       X2=(DELTA2)*(COS(ALFA2))
01500       Y2=(DELTA2)*(COS(BATA2))
01510       Z2=(DELTA2*COS(GAMA2))+Z1
01520       S=SQRT((X2)**2+(Y2)**2)
01530       IF(S.GT.RAD)GO TO 10
01540       IF(Z2.LT.0.0.OR.Z2.GT.DEPTH)GO TO 10
01550       GO TO 33
01560   92  FORMAT(3(F8.4,3X),1X,F10.4,3X,F10.4,2X,F10.4,
01570+          3X,F10.4)
01580    6  CALL RANDU(NRAND,NRAND,RANDOM)
01590       Y=RANDOM
01600       DELTA3=(-ALOG(Y))/XMUE
01610       IF(J.EQ.2)GO TO 9
01620       ALFA2=ALFA3
01630       BATA2=BATA3
01640       GAMA2=GAMA3
01650    9  IF(ABS(COS(GAMA2)).EQ.1.)GO TO 13
01660       ALFA3=ACOS(COS(TATA)*COS(ALFA2)+(SIN(TATA)
01670+            /SIN(GAMA2))*(COS(ALFA2)*COS(GAMA2)*COS(FUY)
01680+             - COS(BATA2)*SIN(FUY)))
01690       BATA3=ACOS(COS(TATA)*COS(BATA2)+(SIN(TATA)
01700+            /SIN(GAMA2))*(COS(BATA2)*COS(GAMA2)*COS(FUY)
01710+            +COS(ALFA2)*SIN(FUY)))
01720       GAMA3=ACOS(COS(TATA)*COS(GAMA2)-(SIN(TATA)/
01730+             SIN(GAMA2))*(1-(COS(GAMA2))**2)*COS(FUY))
01740       GO TO 14
01750   13  ALFA3=ACOS(SIN(TATA)*COS(FUY))
01760       BATA3=ACOS(SIN(TATA)*SIN(FUY))
01770       GAMA3=ACOS(COS(GAMA2)/ABS(COS(GAMA2))*COS(TATA))
01780   14  IF(J.EQ.2)GO TO 19
01790       X2=X3
01800       Y2=Y3
01810       Z2=Z3
01820   19  X3=(DELTA3)*(COS(ALFA3))+X2
01830       Y3=(DELTA3)*(COS(BATA3))+Y2
01840       Z3=((COS(GAMA3))*(DELTA3))+Z2
01850   21  IF((ABS(X3)).GT.RAD.OR.(ABS(Y3)).GT.RAD.OR.
01860+          Z3.LT.0.0.OR.Z3.GT.DEPTH)GO TO 10
```

```
01870*-------------------------------------------------------------------
01880*     IN THIS PART OF PROGRAM THE COMPUTER GOES
01890*     THROUGH THE TABLES AND BY KNOWING THE VALUE
01900*     OF ENERGY IT CALCULATES THE CROSSPONDING
01910*     VALUES OF CROSS-SECTIONS .
01920*     P=PHOTOELETRIC CROSS SECTION FOR ENERGY A01 .
01930*     C=COMPTON CROSS SECTION FOR ENERGY A01 .
01940*-------------------------------------------------------------------
01950  33  P=((A01-B0(I-1))/(B0(I)-B0(I-1)))*(SIGMAPH(I)-
01960+     SIGMAPH(I-1))+SIGMAPH(I-1)
01970      C=((A01-B0(I-1))/(B0(I)-B0(I-1)))*(SIGMAC(I)-
01980+       SIGMAC(I-1))+SIGMAC(I-1)
01990      SIGNA=((A01-B0(I-1))/(B0(I)-B0(I-1)))*(SIGMANA(I)-
02000+          SIGMANA(I-1))+SIGMANA(I-1)
02010      SIGI=((A01-B0(I-1))/(B0(I)-B0(I-1)))*(SIGMAI(I)-
02020+          SIGMAI(I-1))+SIGMAI(I-1)
02030      DO 35 I=1 , 19
02040      IF(A01.LT.C0(I))GO TO 16
02050  35  CONTINUE
02060  16  SIGK=((A01-C0(I-1))/(C0(I)-C0(I-1)))*(SIGMAK(I)
02070+         -SIGMAK(I-1))+SIGMAK(I-1)
02080      SIGL1=((A01-C0(I-1))/(C0(I)-C0(I-1)))*(SIGMAL1(I)
02090+          -SIGMAL1(I-1))+SIGMAL1(I-1)
02100      SIGL2=((A01-C0(I-1))/(C0(I)-C0(I-1)))*(SIGMAL2(I)
02110+         -SIGMAL2(I-1))+SIGMAL2(I-1)
02120*-------------------------------------------------------------------
02130*     IN THIS PART OF PROGRAM THE PORTION OF RANDOM
02140*     NUMBER FOR THE COMPTON EFFECT , PHOTOELECTRIC
02150*     EFFECT, SODIUM AND IODINE WILL BE CALCULATED .
02160*     T IS THE TOTAL CROSS SECTION .
02170*     FP IS THE FRACTION OF PHOTOELECTRIC EFFECT .
02180*     FC IS THE FRACTION OF COMPTON EFFECT .
02190*     TNA IS THESODIUM CROSS SECTION PER ELECTRON .
02200*     TI IS THE IODINE CROSS SECTION PER ELECTRON .
02210*     FNA IS THE FRACTION OF OF NA .
02220*     FI IS THE FRACTION OF ) .
02230*     YNA AND YI ARE THE PORTION OF RANDOM NUMBER
02240*     FOR NA AND I .
02250*-------------------------------------------------------------------
02260      T=P+C
02270      YP=P/T
02280      YC=C/T
02290      CALL RANDU(NRAND,NRAND,RANDOM)
02300      Y=RANDOM
02310      IF(Y.GT.YP) GO TO 100
02320      NPHOTO(N)=NPHOTO(N)+1
02330      J=J+1
02340      TNA=(SIGNA*23)/150.
```

```
02350        TI=(SIGI*127)/150.
02360        FI=TI/(TNA+TI)
02370        YI=FI*YP
02380        FK=SIGK/(SIGL1+SIGL2+SIGK)
02390        YK=YI*FK
02400        IF(Y.LE.YK)GO TO 79
02410   66   KPHOT(N)=KPHOT(N)+1
02420        CALL RANDU(NRAND,NRAND,RANDOM)
02430        Y=RANDOM
02440        IF(Y.LE.0.118) GO TO 80
02450        KFPHOT(N)=KFPHOT(N)+1
02460        GO TO 55
02470   80   KAPHOT(N)=KAPHOT(N)+1
02480   79   A01=0.0
02490        GO TO 20
02500   40   DO 97 KK=1 , 101
02510   97   WRITE(6,91)KK,SPECT(KK)
02520   91   FORMAT(10X,I4,10X,F6.0)
02530        STOP
02540        END
02550*
02560*           RANDOM NUMBER FUNCTION
02570*
02580        SUBROUTINE RANDU(IX,IY,YFL)
02590        DATA M/2814749767106S5/
02600        N=2147483651*IX
02610        IY=MOD(N,M)
02620        YFL=IY
02630        YFL=YFL*.35527136E-14
02640        RETURN
02650        END
READY.
```