

MIRION
Connect **21**
Annual Users' Conference





Primer: Spectroscopy Fundamentals

Greg Landry

Product Line Manager – In Vivo

Application Support Manager

Agenda

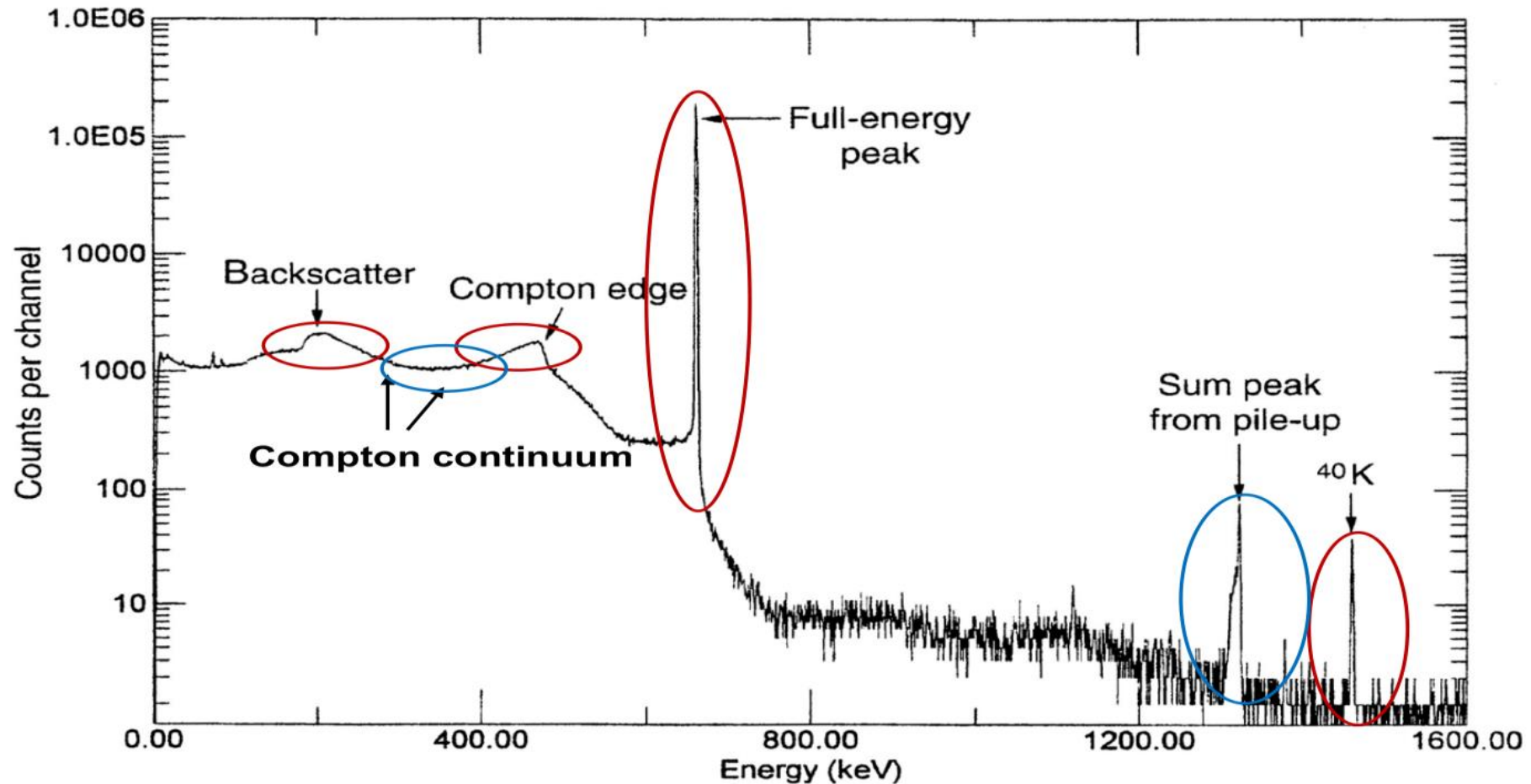
We will discuss fundamental aspects of **Gamma Ray** Spectrometry. This will not include decay physics or electronics

- Common Features in the Gamma Ray Spectrum
- Effects of Summing
- Calibrations

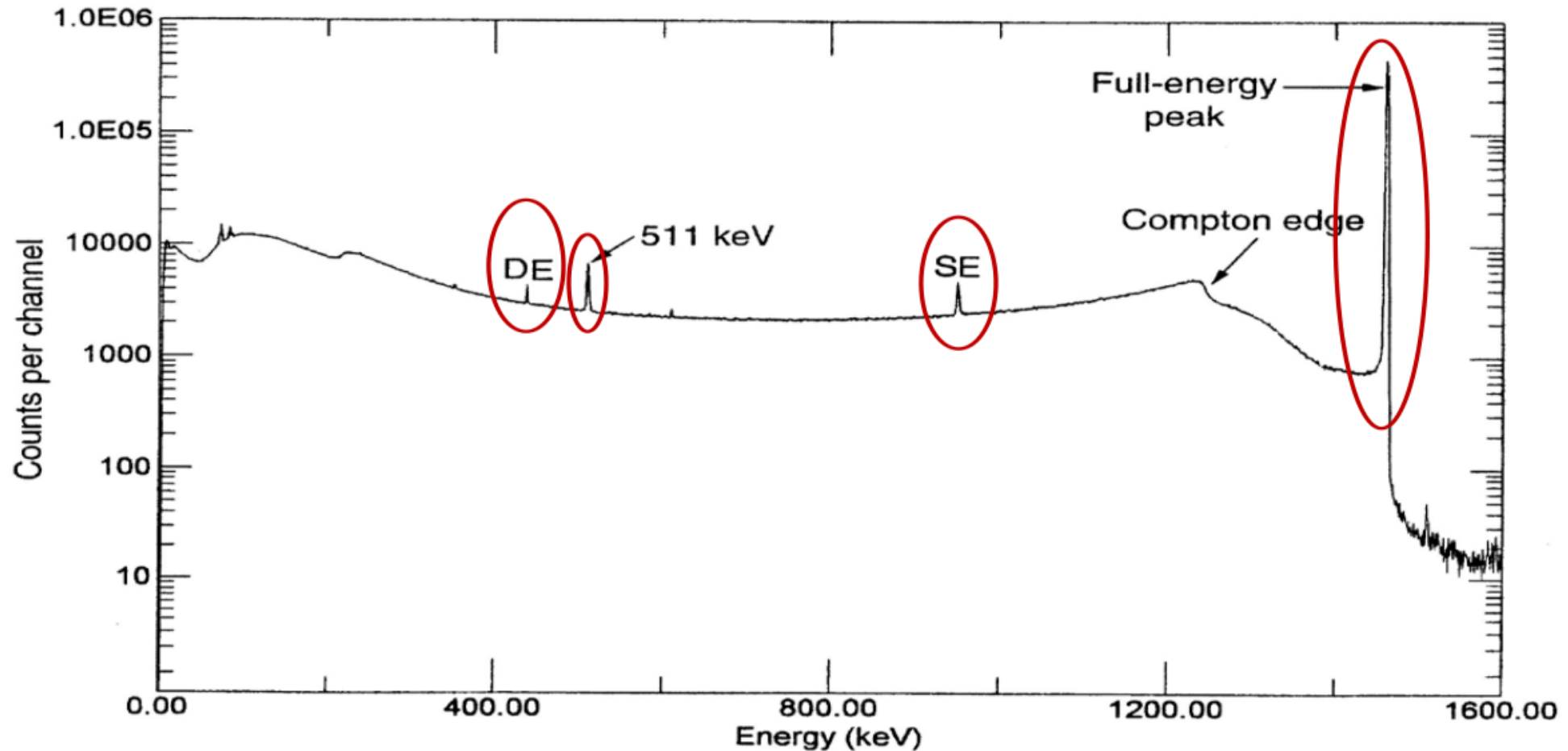
Mirion provides several courses that go through these topics (and more!) over the course of several days. Highly recommended!

Common Features in the Gamma Ray Spectrum

Common Features in Gamma Ray Spectrum

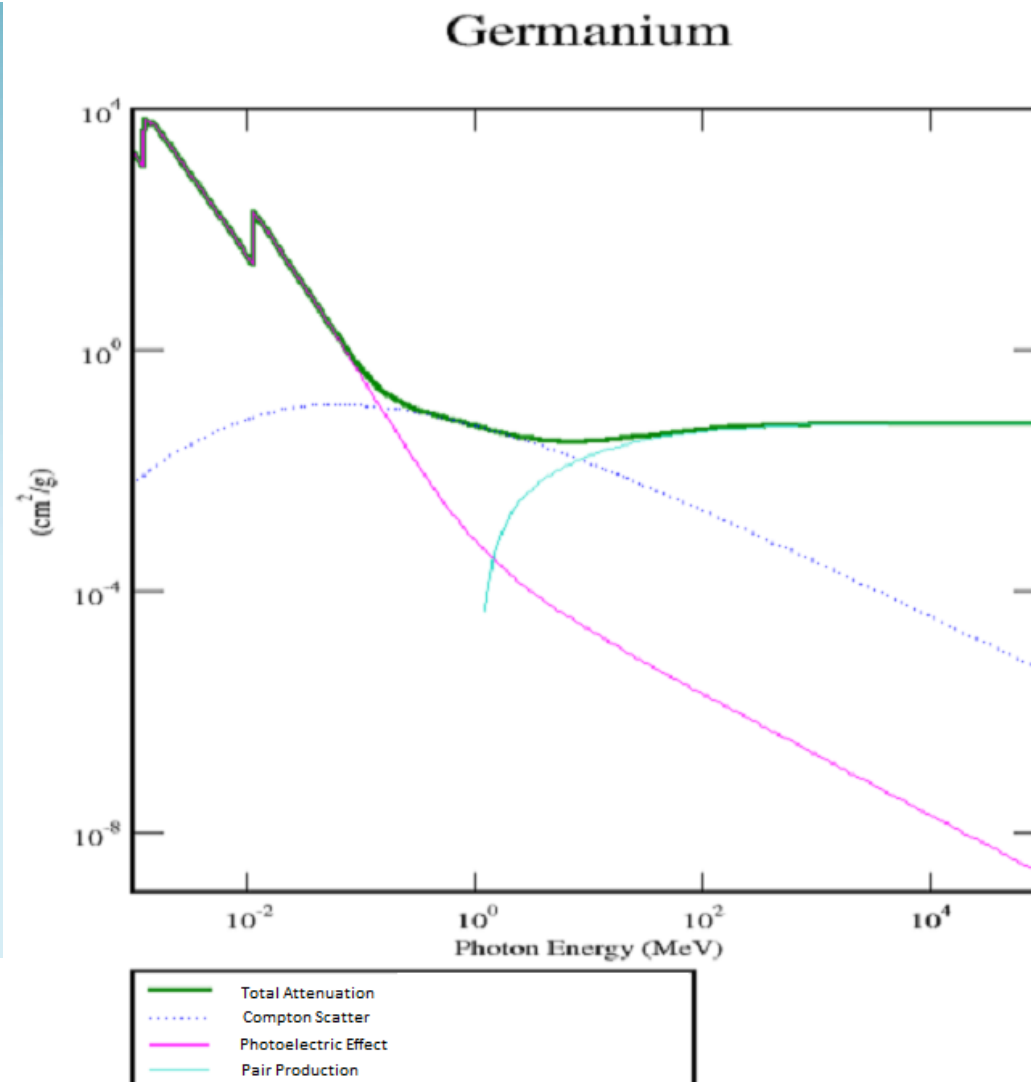


Spectral Features Including Escape and Annihilation Peaks

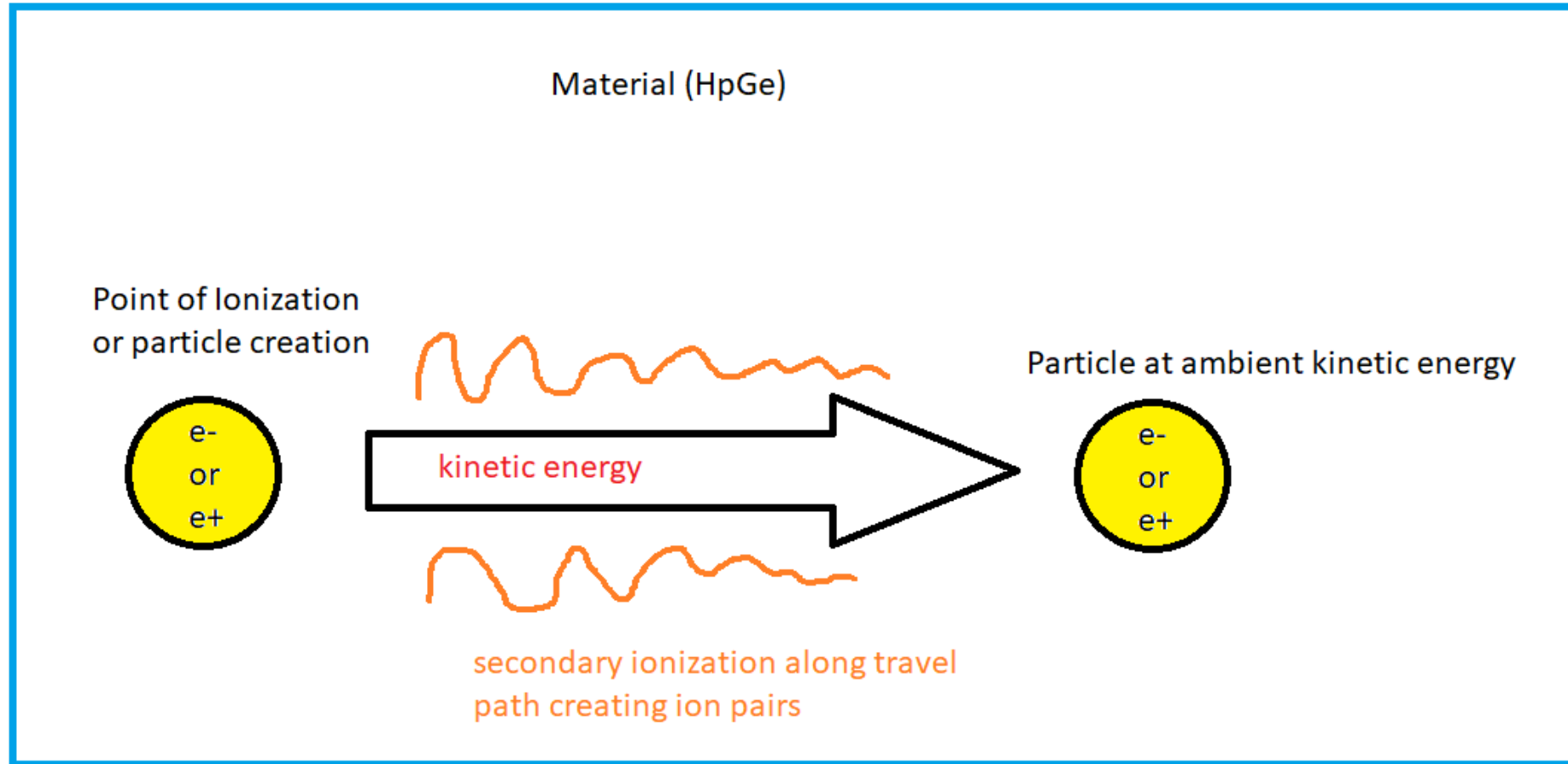


Gamma Ray Interactions with Matter

Photoelectric effect
Compton scattering
Pair production

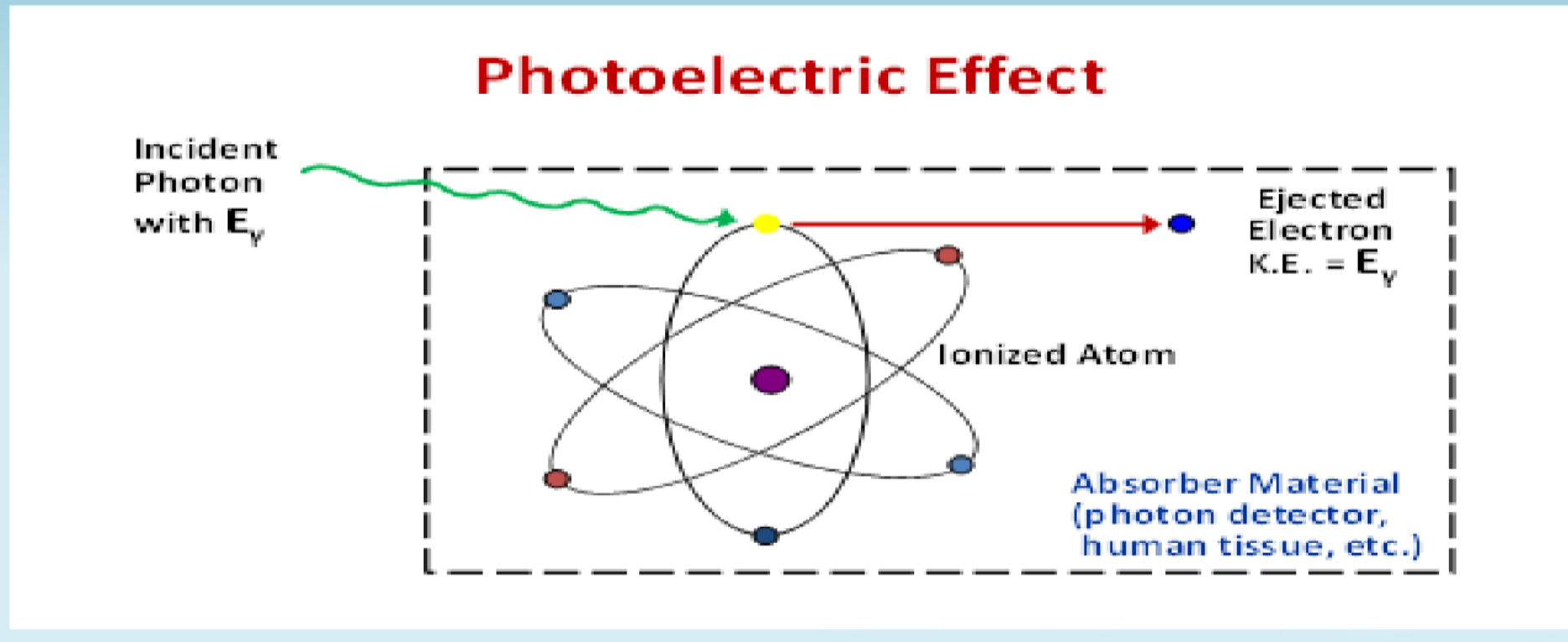


Signal Pulse from Interaction

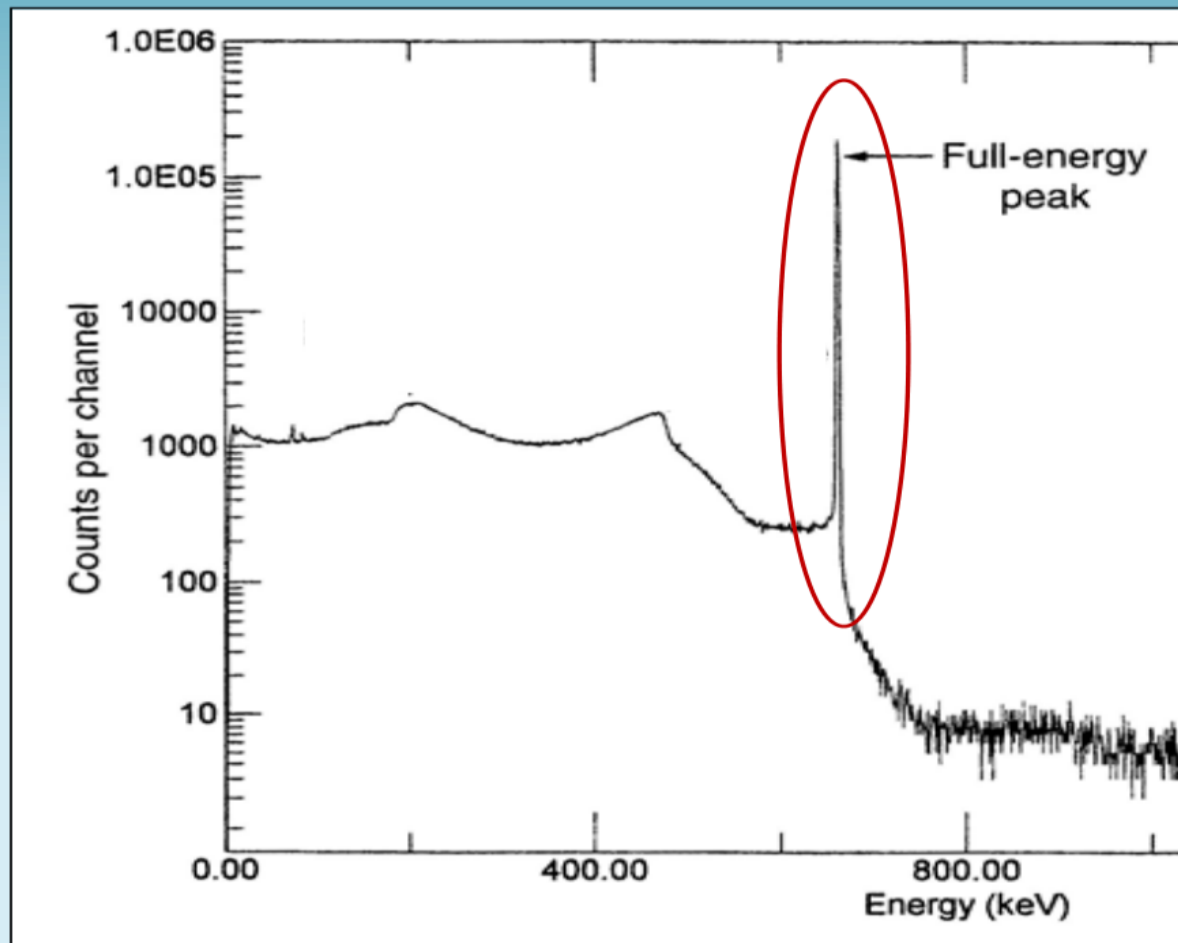


Photoelectric Effect

- **Principal interaction mechanism of relatively low energy incident photons, less than about 200 keV**



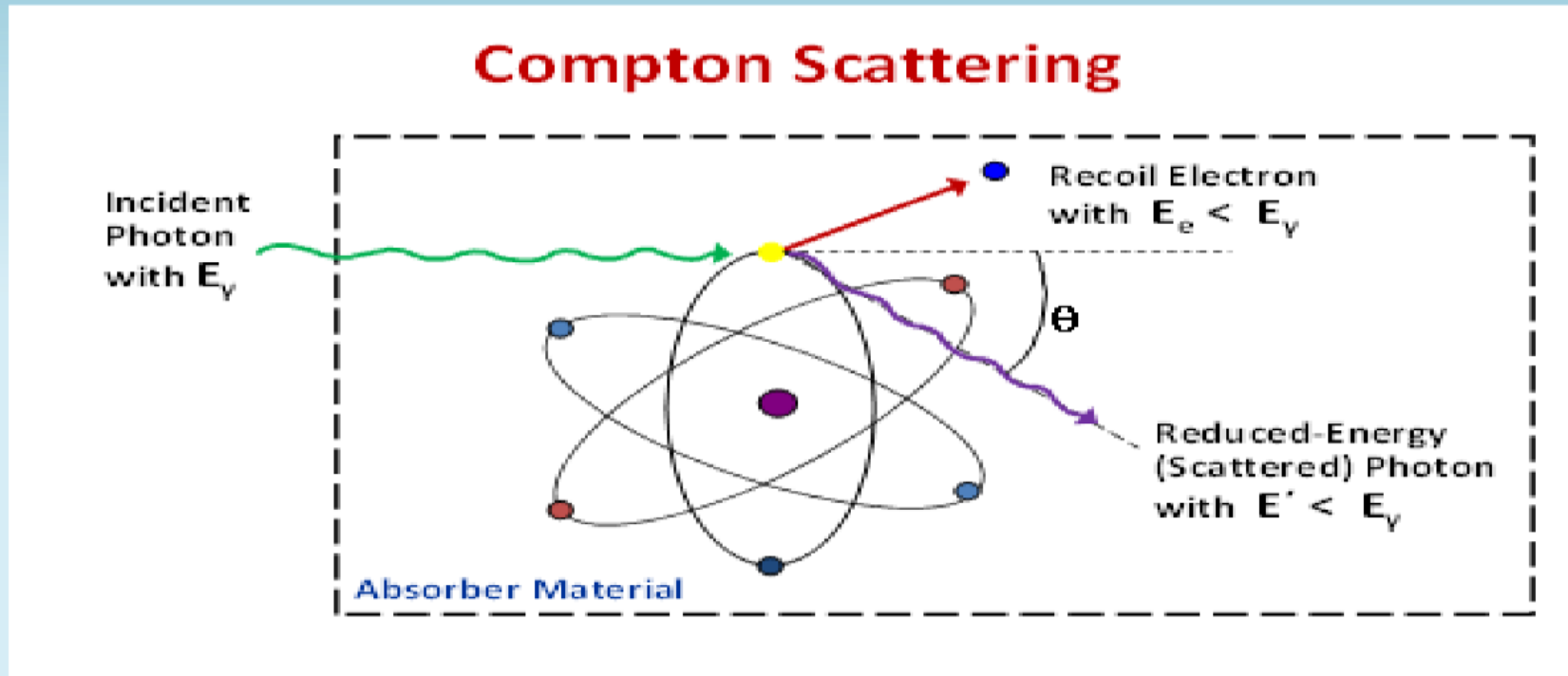
Full Energy Peak



- ▶ **Primary spectral feature representing decay events with deposition of the full gamma ray energy in the detector**
- ▶ **Net peak area values are used to calculate activity for identified nuclides**

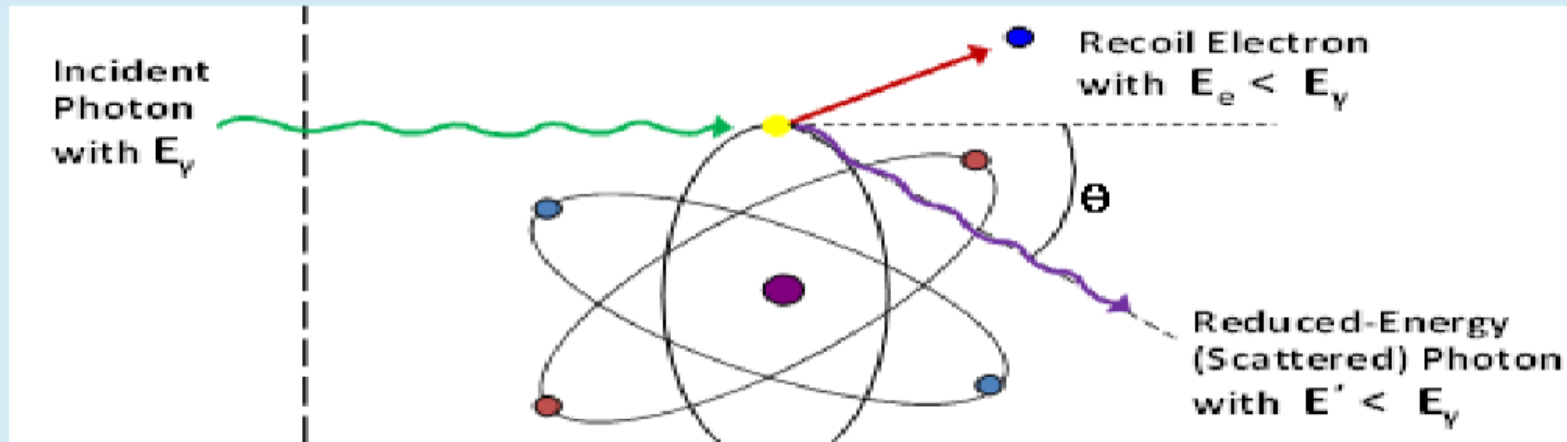
Compton Scattering

Primary interaction mechanism for photons of medium energy, roughly between 200 and 2000 keV

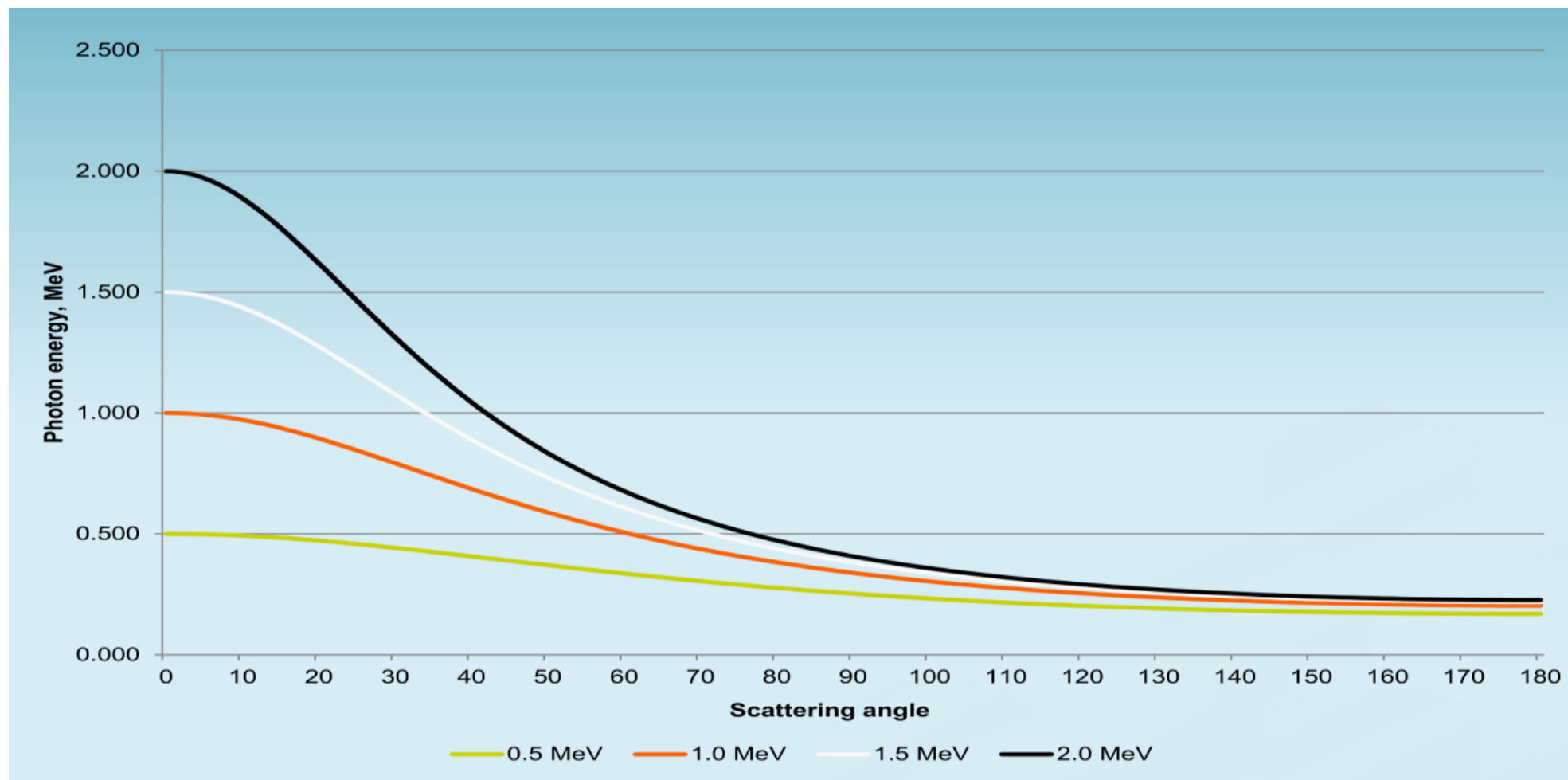


Compton Scattering – Energy of Scattered Photon

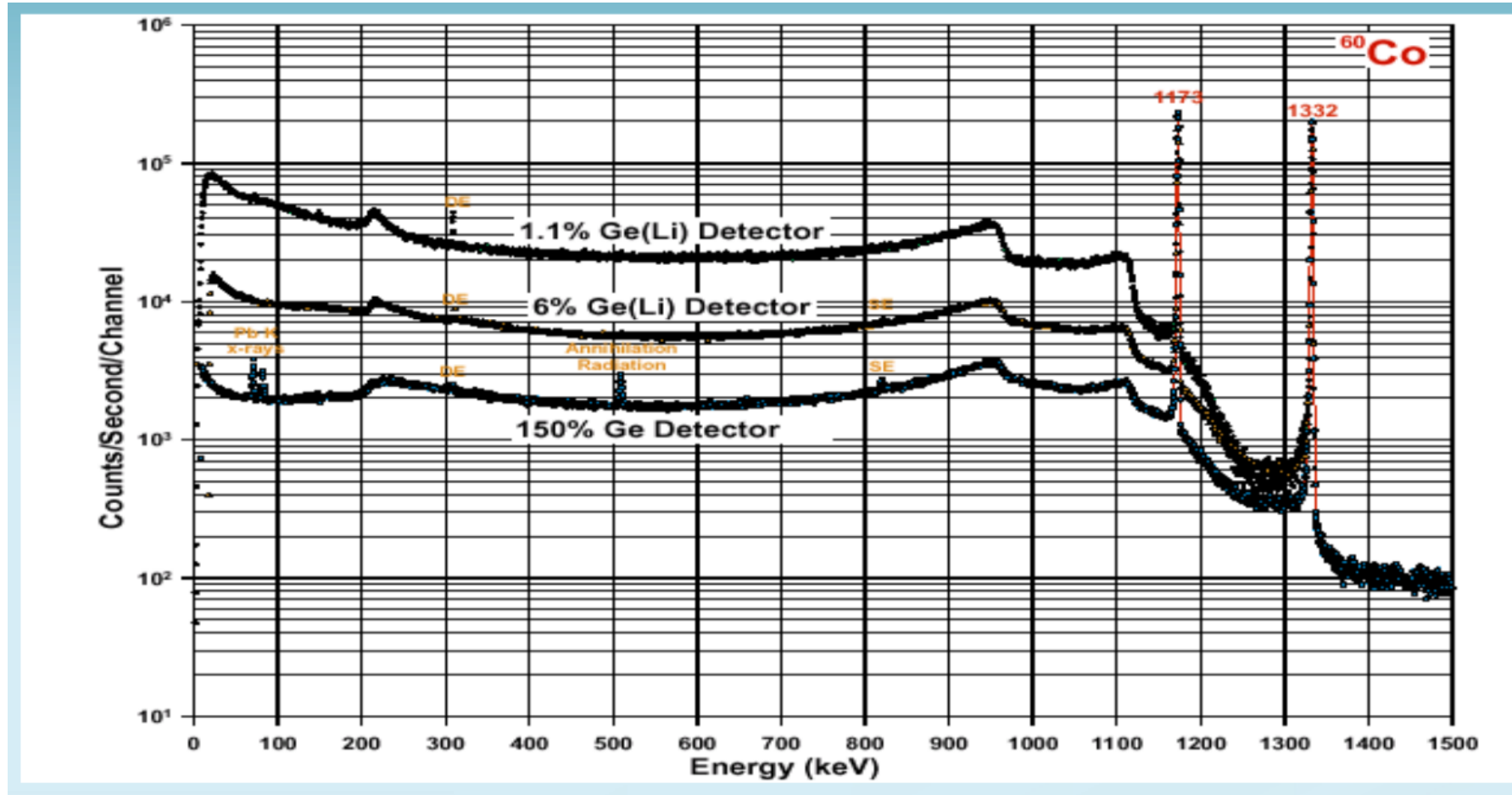
$$E_{scat} = \frac{E_{\gamma}}{1 + \left(\frac{E_{\gamma}}{m_0 c^2} \right) [1 - \cos(\theta)]}$$



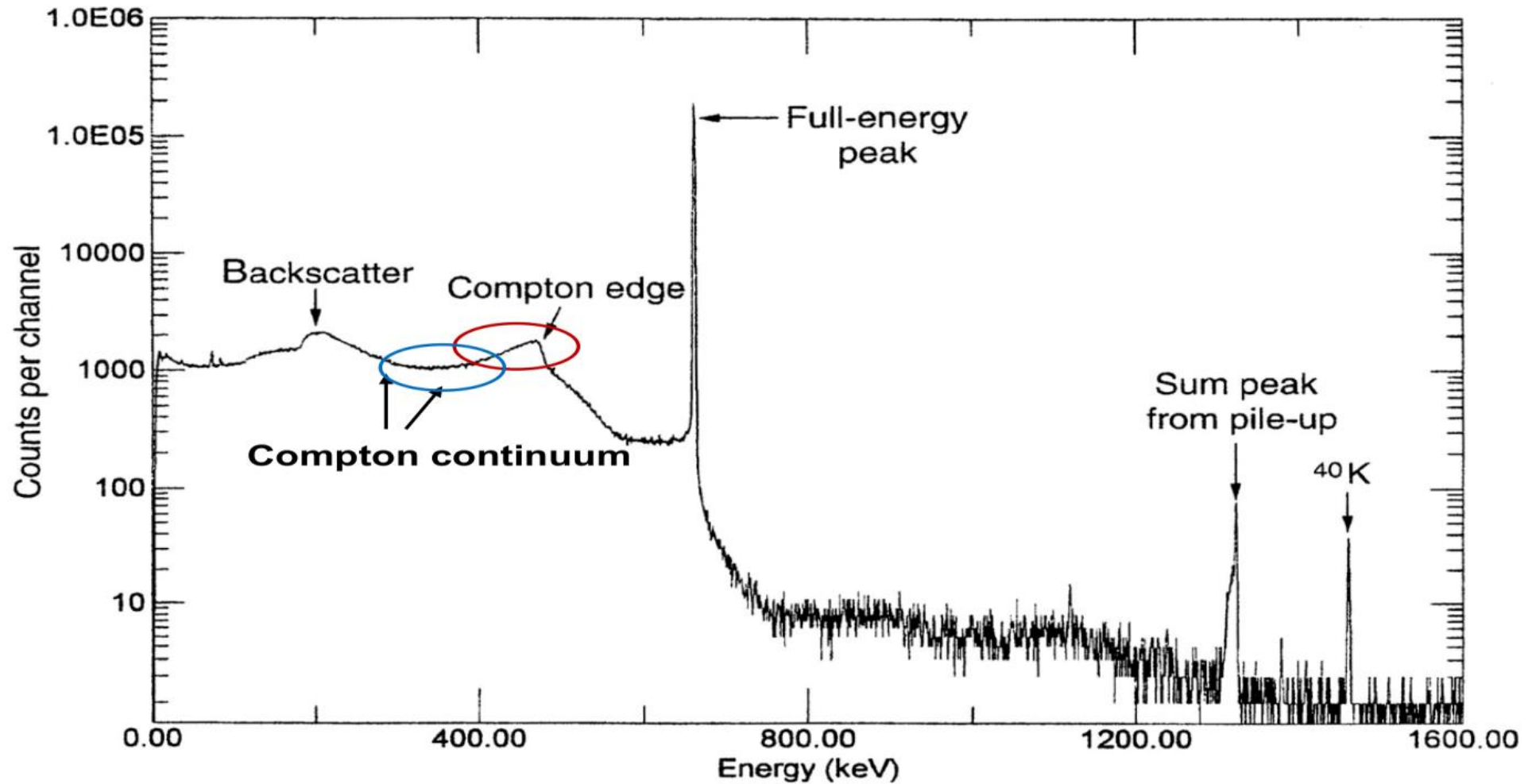
Compton Scattering – Energy of Scattered Photon



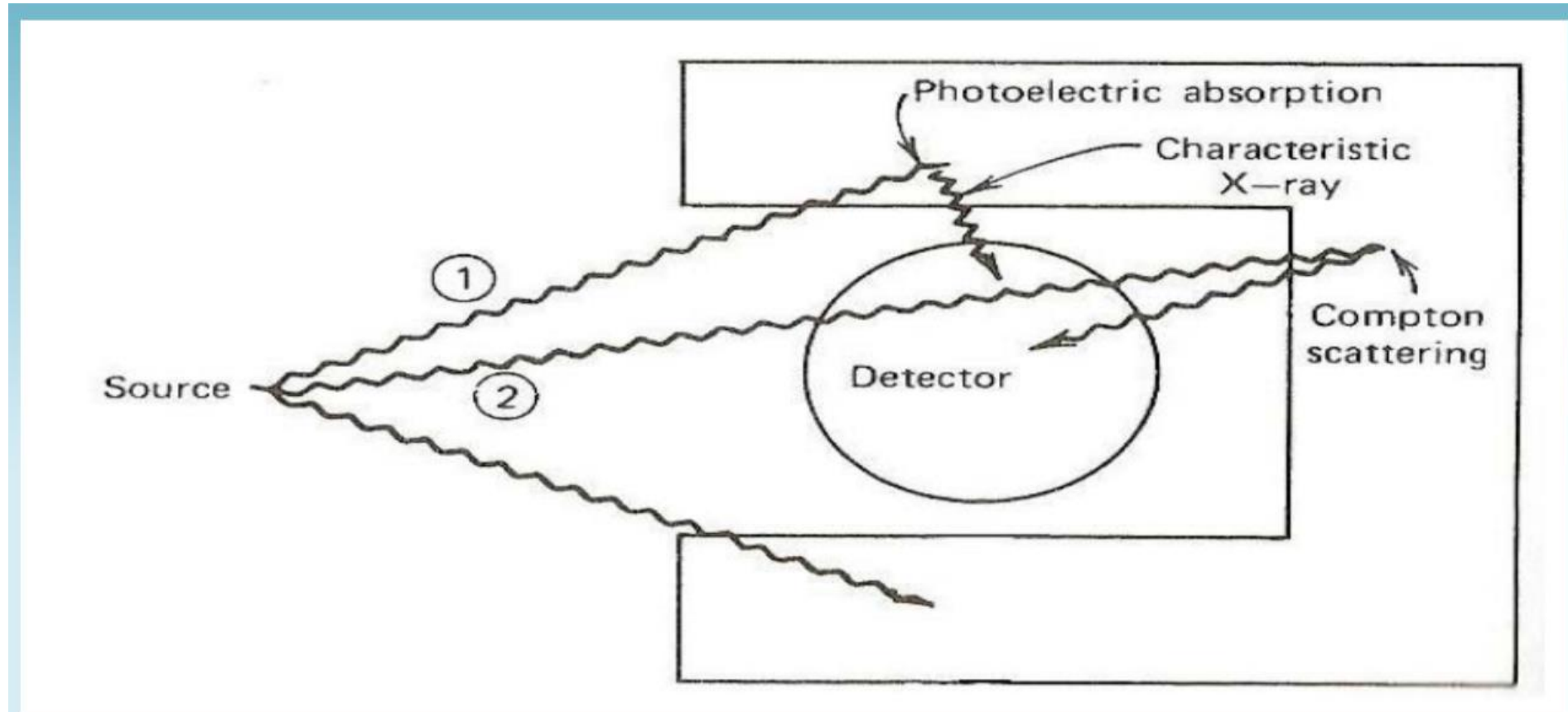
Effect of Detector Size on Compton Scattering



Spectral Features for Compton Scatter

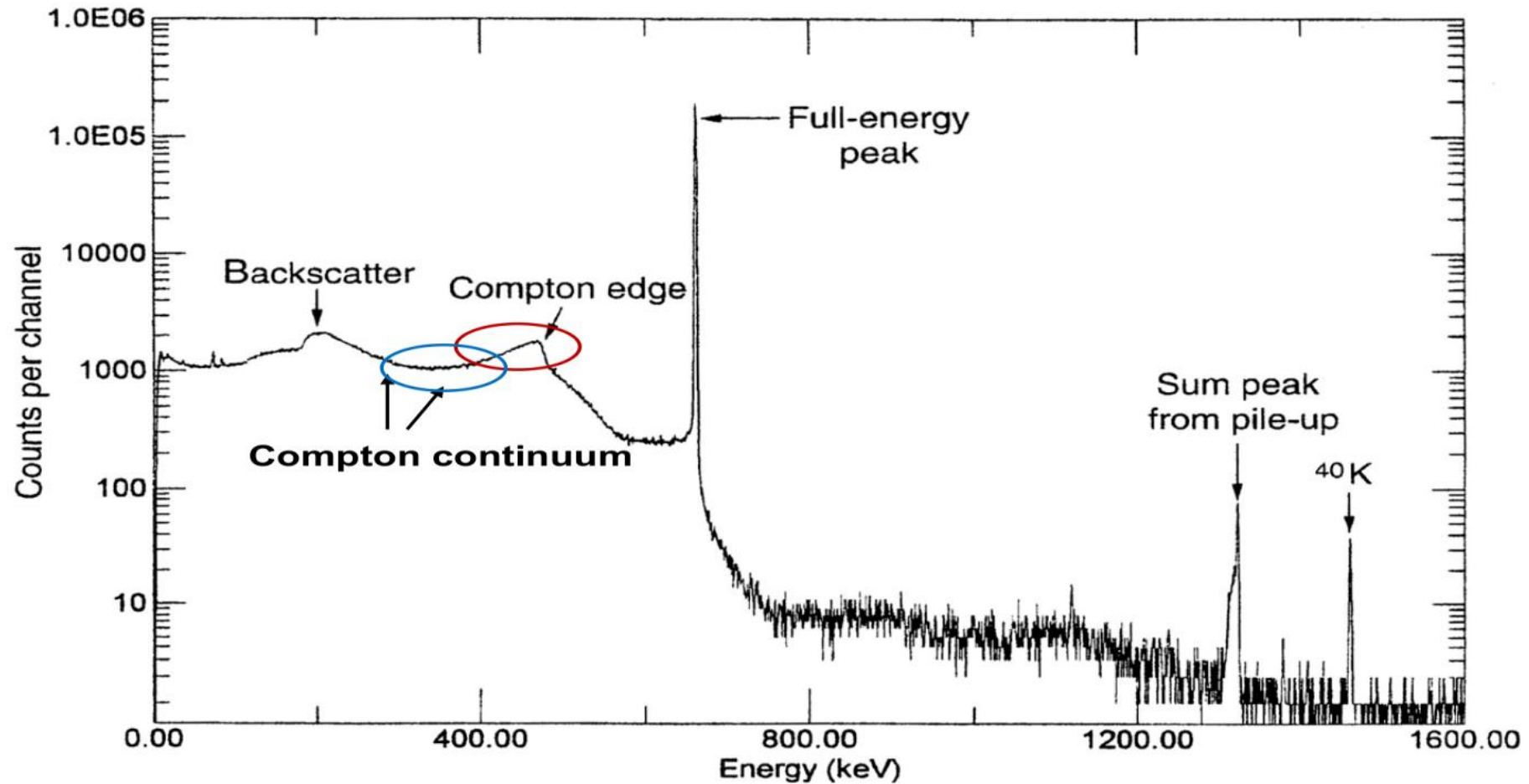


Compton Scatter – Backscatter Effects

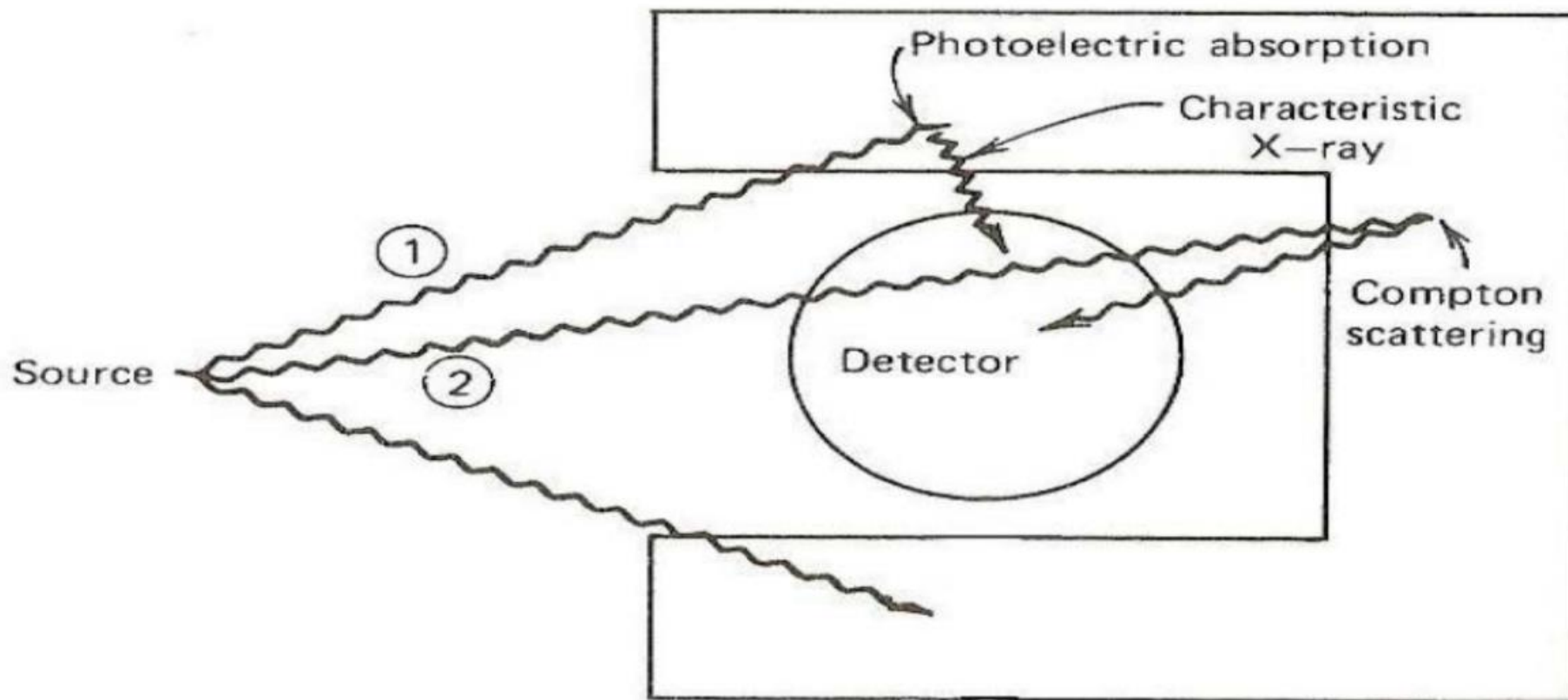


Source: "Radiation Detection and Measurement", Glenn Knoll; used with permission

Spectral Features from Compton Scatter

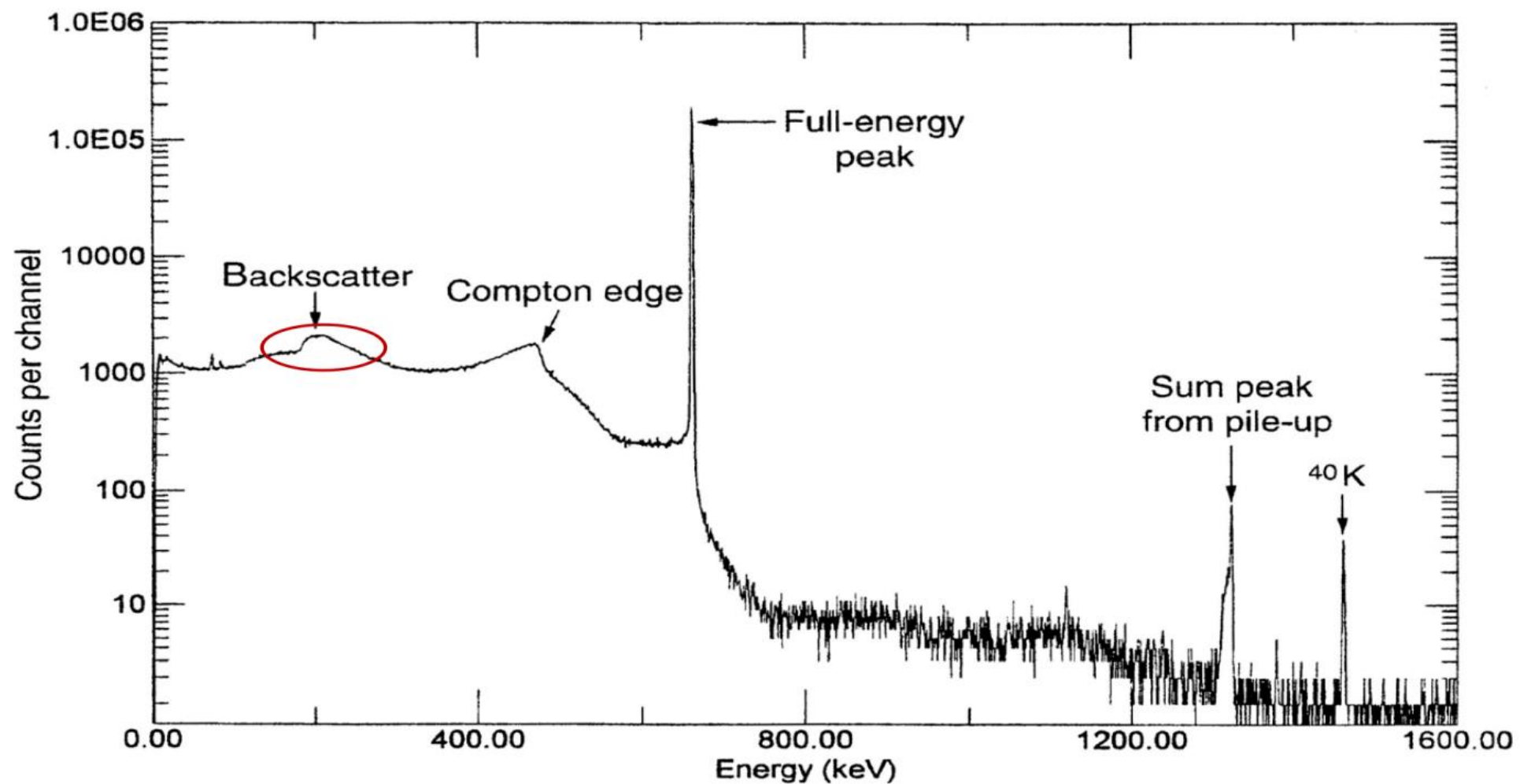


Compton Scattering – Backscatter Effect



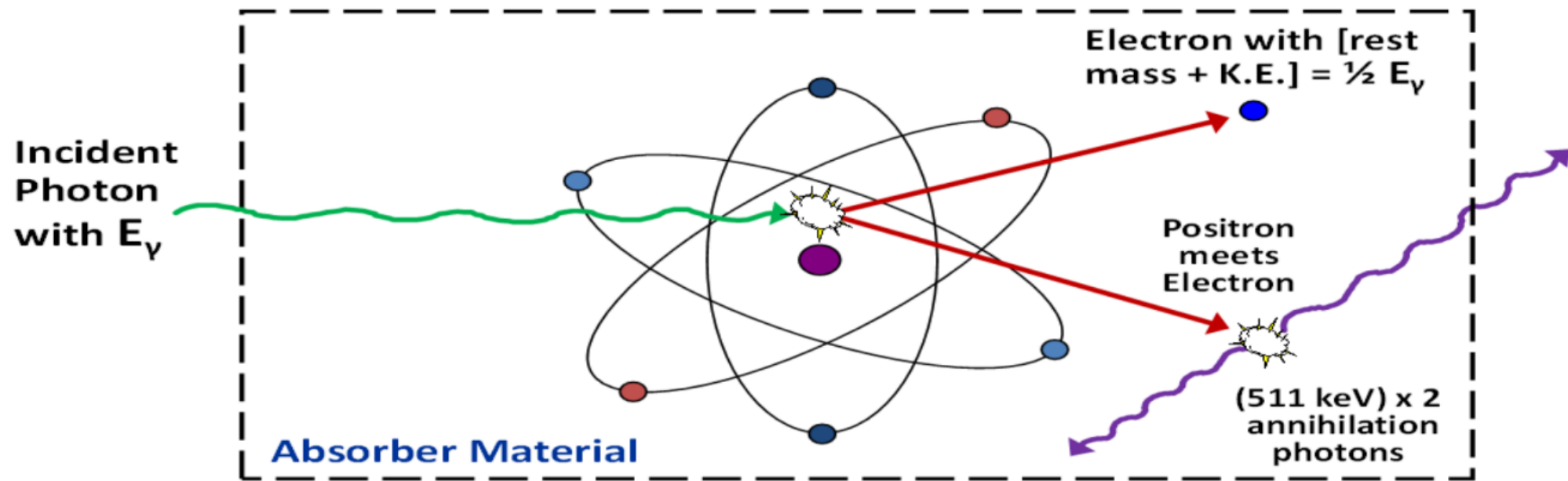
Source: "Radiation Detection and Measurement", Glenn Knoll; used with permission

Spectral Features Related to Backscatter

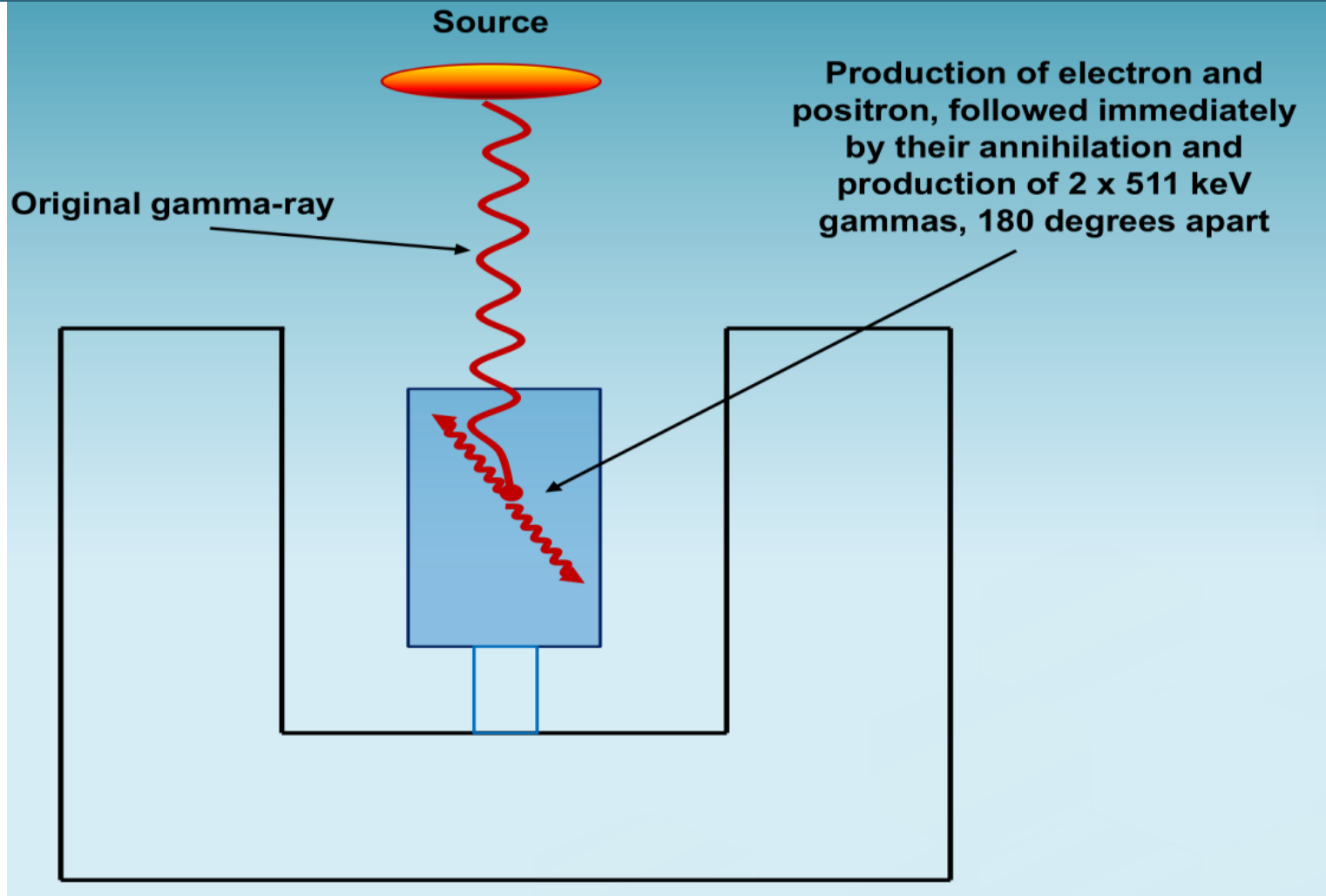


Pair Production

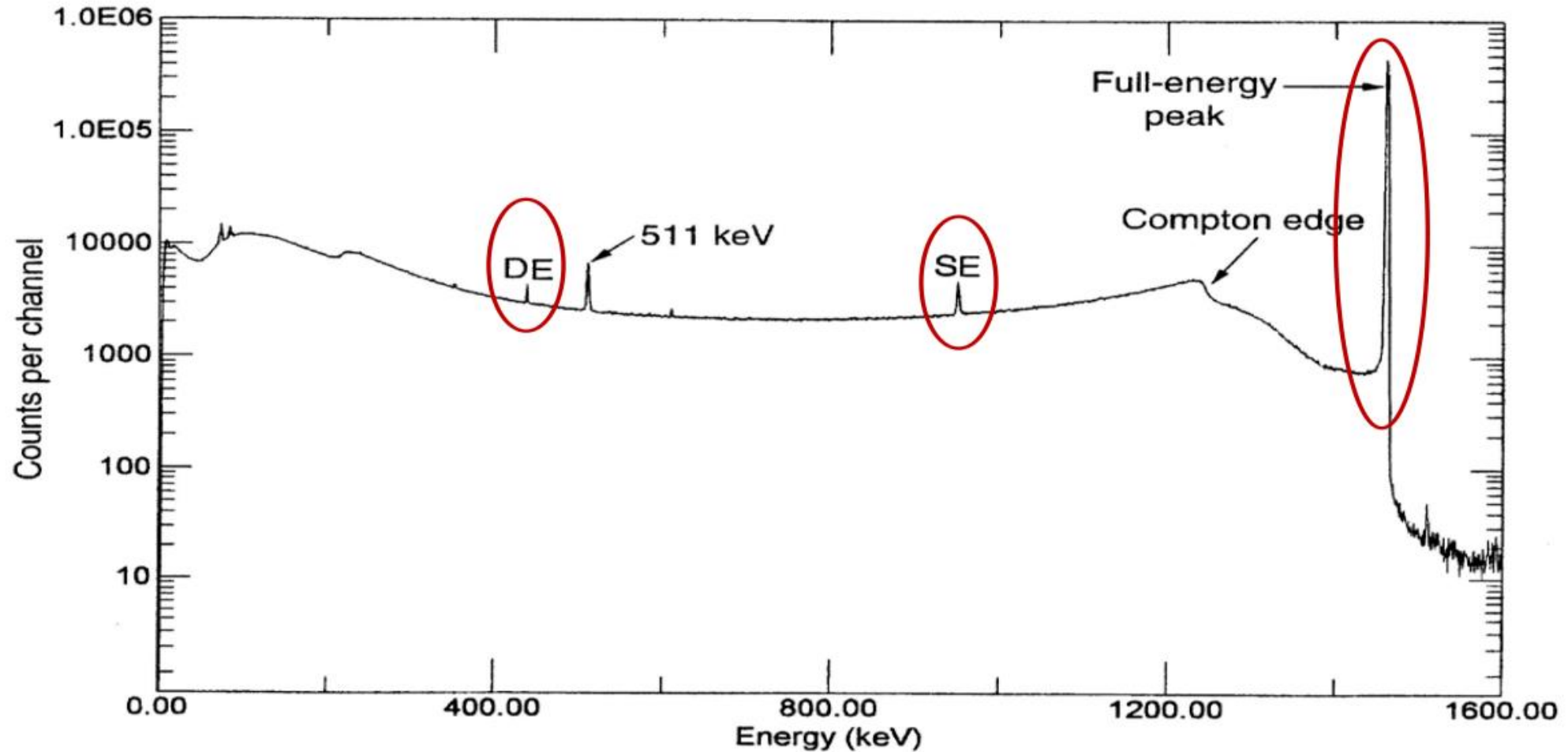
Primary interaction mechanism for photons of high energy, usually > 2000 keV, with a threshold of 1022 keV



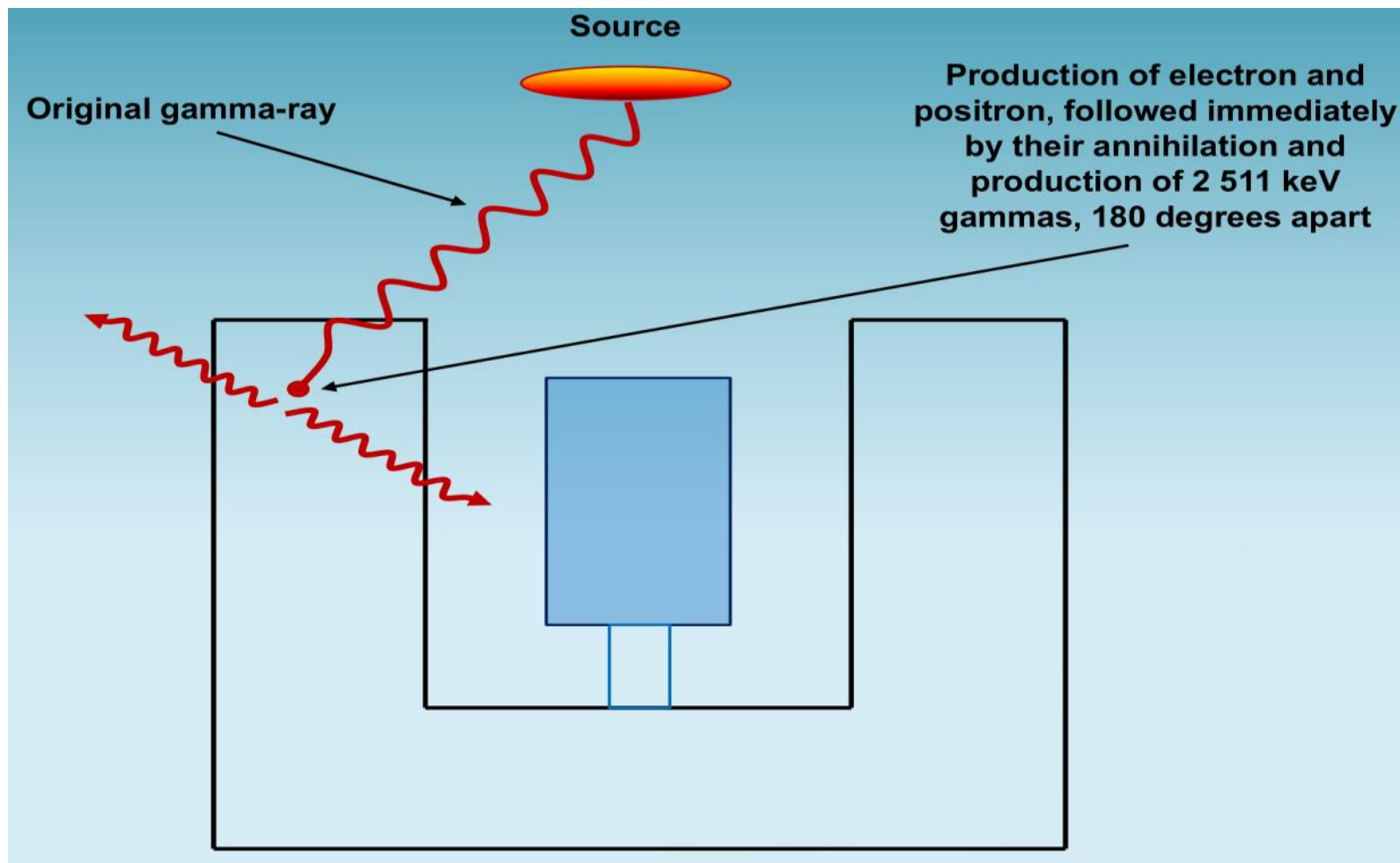
Pair Production



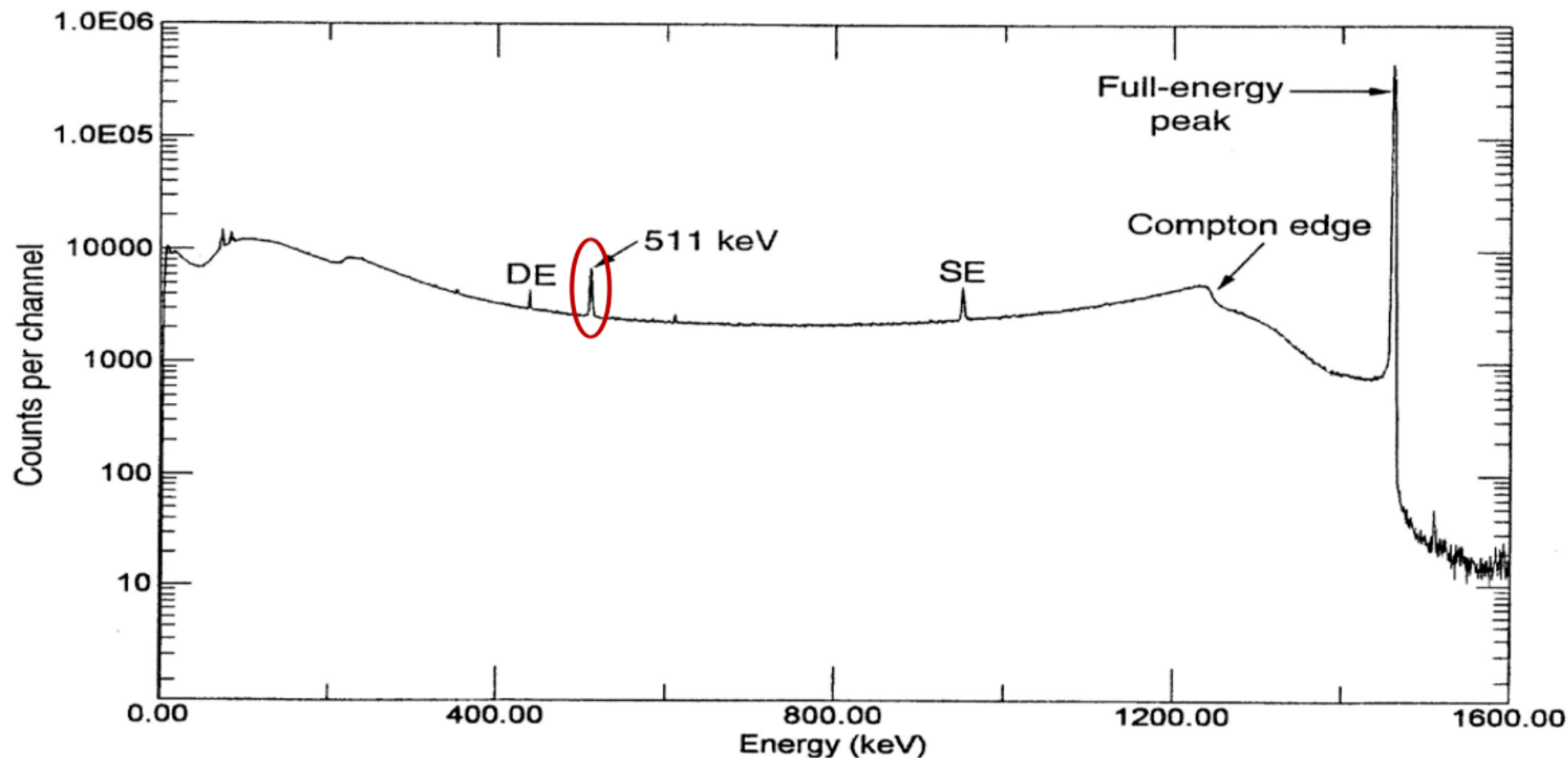
Spectral Features – Pair Production



Pair Production – Environmental 511 keV Peak



Pair Production – Environmental 511 keV Peak



Effects of Summing

Random Summing

If two or more gamma-ray photons from *two or more separate decay events* are absorbed by the detector during a pulse sampling cycle, the sum of the energies of the two (or more) is recorded in the spectrum.

Since the two gamma rays are *not related in any way*, this is called *random coincidence summing*. Random coincidence sum peaks can be formed at double the energy of the primary peaks (single nuclide) or the sum of primary peaks (multiple nuclides).

Random Summing

Any full-energy photon that is summed with another pulse is not recorded in the single full energy photon peak and represents a loss of counts or efficiency in that full energy peak.

This loss is count-rate dependent and therefore geometry dependent. Moving the sample farther from the detector reduces the count rate and therefore reduces the effect of random summing.

True Coincidence (Cascade Summing)

If two or more gamma-ray photons from *the same decay event* are absorbed by the detector during a pulse sampling cycle, the sum of the energies of the two (or more) is recorded in the spectrum. Since the two gamma rays are *from the same decay event*, this is called *true coincidence or cascade summing*.

Cascade sum peaks can be formed at the sum of any of the two (or more) coincident gamma-ray energies. All counts in a sum peak are necessarily taken from a full energy peak, and thus the counts (and apparent activity) of the full energy peak are reduced.

True Coincidence (Cascade Summing)

The probability of true coincidence summing is almost entirely geometry dependent and can be calibrated for and normalized.

This loss is *not* count-rate dependent, but since it is geometry dependent, whereby the two or more cascade gammas must reach the detector at the same time, moving the sample farther from the detector reduces the effect of coincidence summing.

Effects of Summing

Two Primary Consequences of Summing

Summing In and Summing Out

Summing In – the sum of the energies of all of the summed gamma-rays are collected **IN** a single observation. Repeated observations create a sum peak.

Summing Out – each of gamma-rays that contribute to a sum peak are observations left **OUT** of the peak that would otherwise represent that gamma-ray.

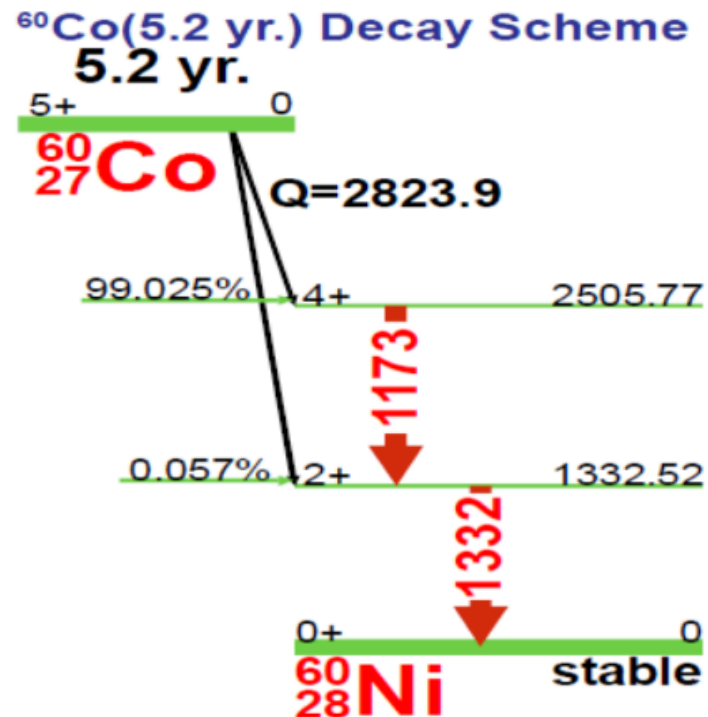
Consequences of Summing

The primary consequence of Summing In is the presence of a peak that we do not readily recognize.

The primary consequence of Summing Out is the reduction of data in peaks that we do recognize – and therefore we underestimate the activity represented by that peak.

True Coincidence Summing Example

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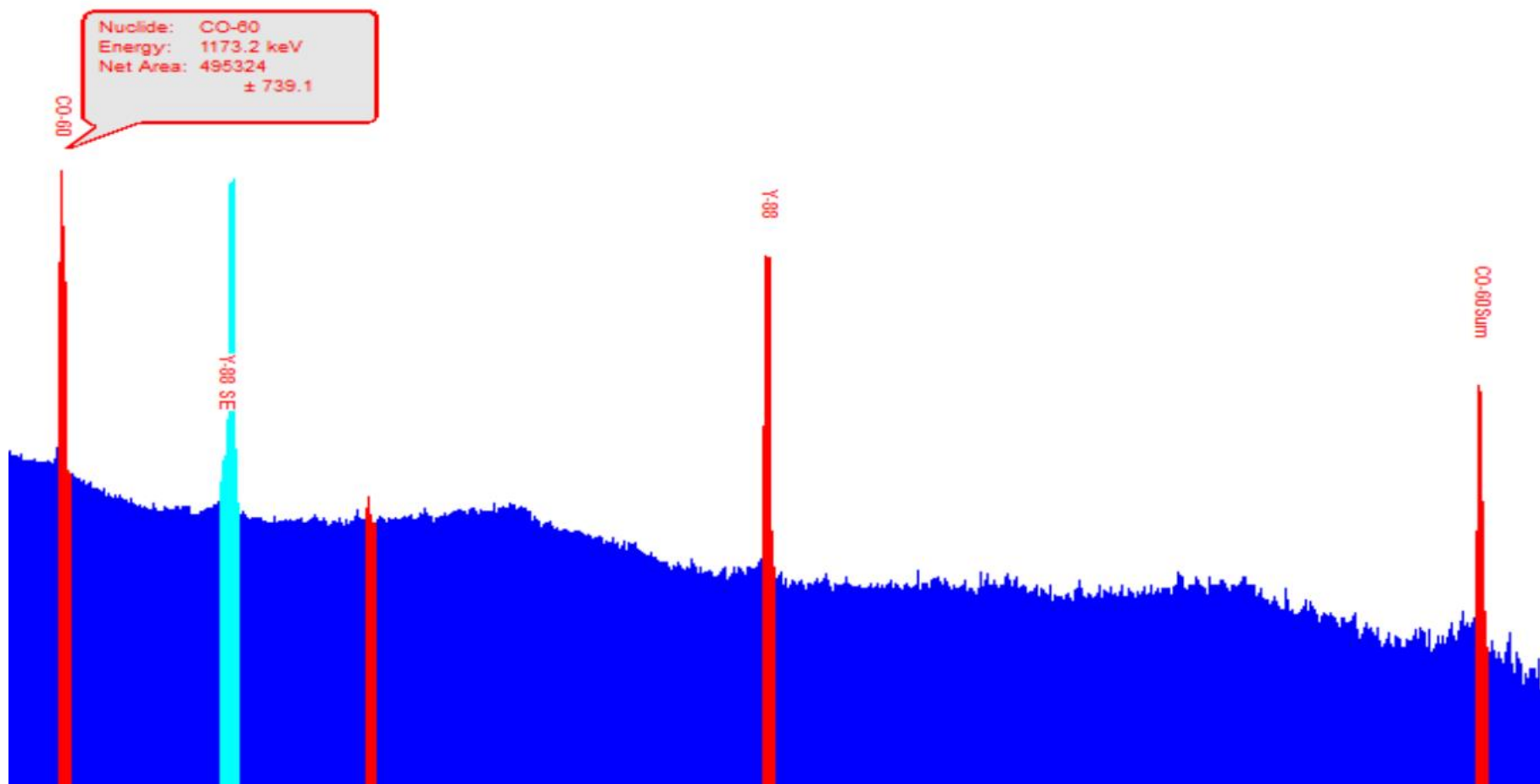
GAMMA-RAY ENERGIES AND INTENSITIES

Nuclide: ^{60}Co Half Life: 5.2714(5) yr.
Detector: 55 cm³ coaxial Ge (Li) Method of Production: $^{59}\text{Co}(n,\gamma)$

E_γ (keV)	σE_γ	I_γ (rel)	I_γ (%)	σI_γ	S
346.93	0.07		0.0076	0.0005	4
826.28	0.09		0.0076	0.0008	4
1173.237	0.004	100	99.9736	0.0007	1
1332.501	0.005	100	99.9856	0.0004	1
2158.77	0.09		0.0011	0.0002	4
2505.					4

E_γ , σE_γ , I_γ , σI_γ - 1998 ENSDF Data

True Coincidence Summing Example



True Coincidence Summing Example

The data 'missing' from the 1173 and 1332 keV peak areas is represented in the 2505 keV peak area. This allows us to empirically determine the 'correct' values for the 1173 and 1332 keV peak areas. This can be a relatively simple process or a very difficult process, depending on the contributions to the sum peak.

True Coincidence Summing Example

The peak area at 2505 keV shows 19955 net counts. Each of these counts is from one each 1173 gamma-ray and one each 1332 keV gamma-ray. Thus, nominally 19955 counts are from ‘missing’ from each of the two individual gamma peaks (1173 and 1332 keV). Simply add these counts back into the peak areas to apply the appropriate correction.

Note – this is actually an oversimplification, as there are other summing events that contribute to the summing out but are not obvious; for example, full energy plus Compton summing.

Gamma and X-ray radiation:

	Energy (keV)	Intensity (%)	Dose (MeV/Bq-s)
XR l	4.29	15.7 % 8	6.7E-4 3
XR kα2	30.625	33.9 % 10	0.0104 3
XR kα1	30.973	62.2 % 18	0.0193 6
XR kβ3	34.92	5.88 % 17	0.00205 6
XR kβ1	34.987	11.4 % 3	0.00397 11
XR kβ2	35.818	3.51 % 10	0.00126 4
	53.1622 6	2.14 % 3	0.001138 17
	79.6142 12	2.65 % 5	0.00211 4
	80.9979 11	32.9 % 3	0.0267 3
	160.6120 16	0.638 % 5	0.001025 9
	223.2368 13	0.453 % 3	0.001011 8
	276.3989 12	7.16 % 5	0.01979 13
	302.8508 5	18.34 % 13	0.0555 4
	356.0129 7	62.05 %	0.2209
	383.8485 12	8.94 % 6	0.03432 24

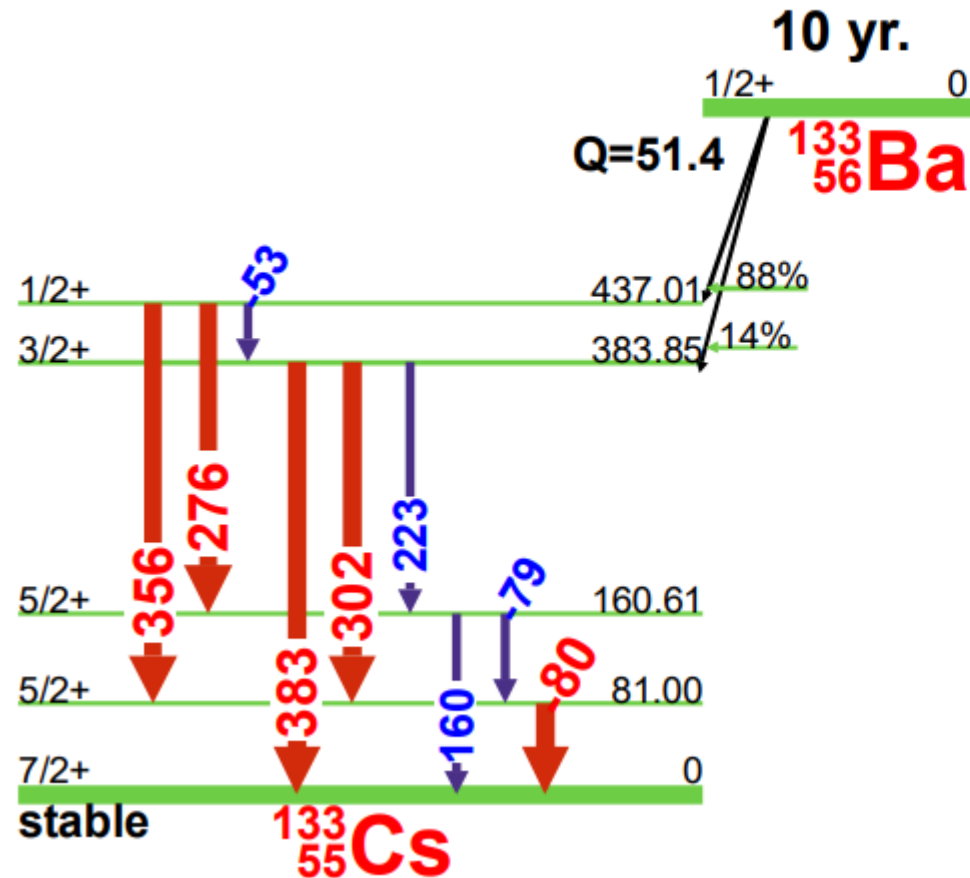
Parent Nucleus	Parent E(level)	Parent Jπ	Parent T _{1/2}	Decay Mode	GS-GS Q-value (keV)	Daughter Nucleus
¹³³ ₅₆ Ba	0.0	1/2+	10.551 y 11	ε: 100 %	517.5 10	¹³³ ₅₅ Cs

BA-133

Gamma Coincidence Data:

For each gamma, the list of gammas in coincidence is given.
If experimentally known, an estimate of the average time interval (in seconds) between both gammas is given.

E(γ)	Coincidence
53.1622	79.6142 (2.16E-10), 80.9979 (6.49E-9), 160.6120 (2.16E-10), 223.2368 (4.39E-11), 302.8508 (4.39E-11), 383.8485 (4.39E-11)
79.6142	53.1622 (2.16E-10), 80.9979 (6.28E-9), 223.2368 (1.72E-10), 276.3989 (1.72E-10)
80.9979	53.1622 (6.49E-9), 79.6142 (6.28E-9), 223.2368 (6.45E-9), 276.3989 (6.45E-9), 302.8508 (6.28E-9), 356.0129 (6.28E-9)
160.6120	53.1622 (2.16E-10), 223.2368 (1.72E-10), 276.3989 (1.72E-10)
223.2368	53.1622 (4.39E-11), 79.6142 (1.72E-10), 80.9979 (6.45E-9), 160.6120 (1.72E-10)
276.3989	79.6142 (1.72E-10), 80.9979 (6.45E-9), 160.6120 (1.72E-10)
302.8508	53.1622 (4.39E-11), 80.9979 (6.28E-9)
356.0129	80.9979 (6.28E-9)
383.8485	53.1622 (4.39E-11)

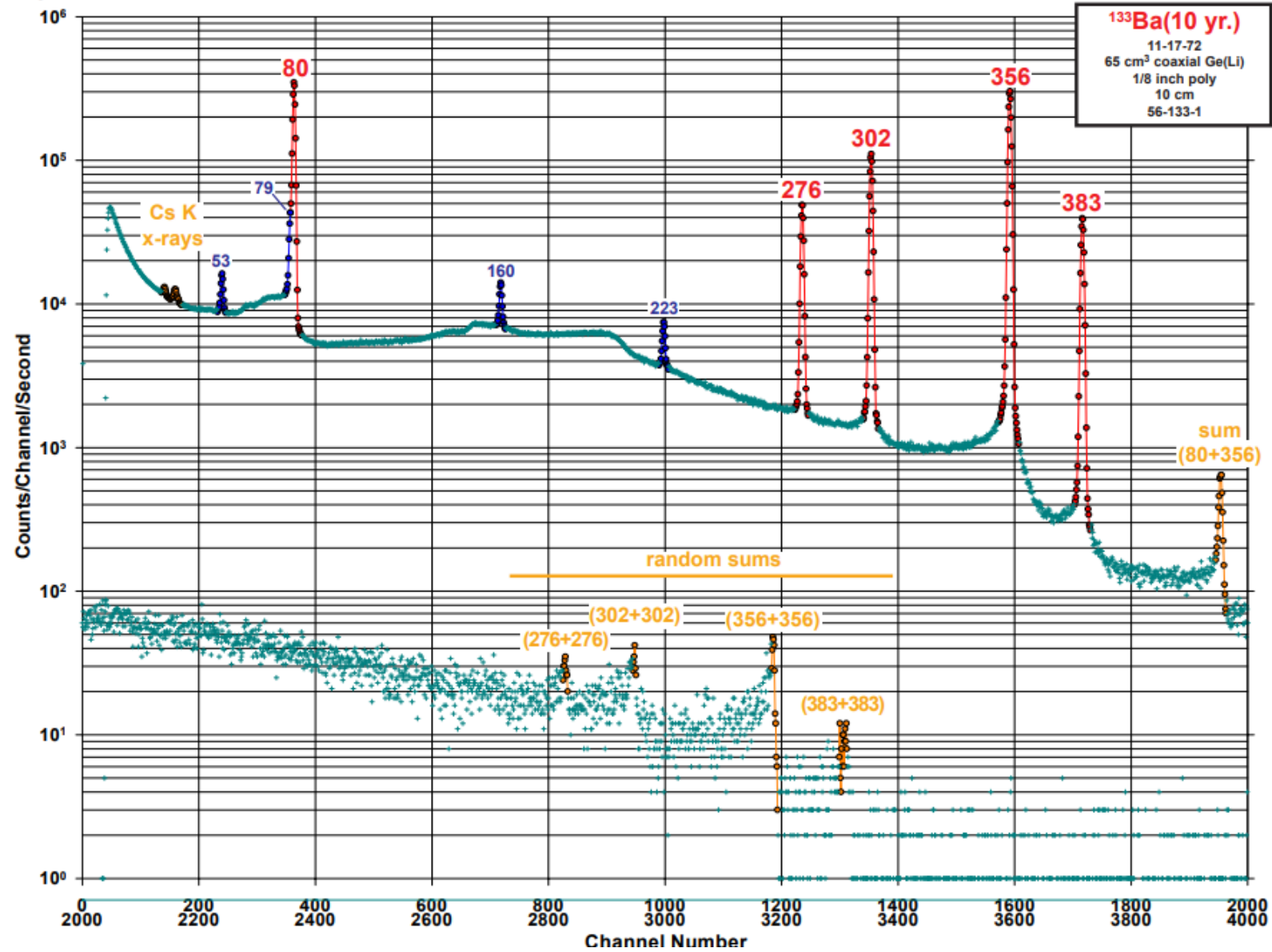
^{133}Ba (10 yr.) Decay Scheme**GAMMA-RAY ENERGIES AND INTENSITIES**Nuclide: ^{133}Ba

Half Life: 10.51(5) yr.

Detector: 65 cm³ coaxial Ge (Li)Method of Production: $^{132}\text{Ba}(n,\gamma)$

E_γ (keV)	σE_γ	I_γ (rel)	I_γ (%)	σI_γ	S
53.162	0.001	3.0	2.199	0.022	3
79.614	0.001	5.6	2.62	0.06	3
80.997	0.001	52.0	34.06	0.27	1
160.611	0.002	1.12	0.645	0.008	3
223.237	0.001	0.85	0.45	0.004	3
276.400	0.001	11.69	7.164	0.022	1
302.851	0.001	29.78	18.33	0.06	1
356.013	0.001	100.	62.05	0.19	1
383.848	0.001	14.43	8.94	0.03	1

 $E_\gamma, \sigma E_\gamma, I_\gamma, \sigma I_\gamma$ - 1998 ENSDF Data



Affects of Geometry

How Does Geometry Affect True Coincidence Summing?

Larger detectors

→ *more Summing*

(for fixed sample size and fixed separation)



← Sample →



← Detector →



▶ *Smaller sample size*

→ *more Summing*

(for same detector size and fixed separation)



← Sample →



← Detector →



▶ *Less separation*

→ *more Summing*

(for same detector and fixed sample size)



← Separation →



Calibrations

Calibrations – 3 Types Required

Energy (versus spectrum channel number)

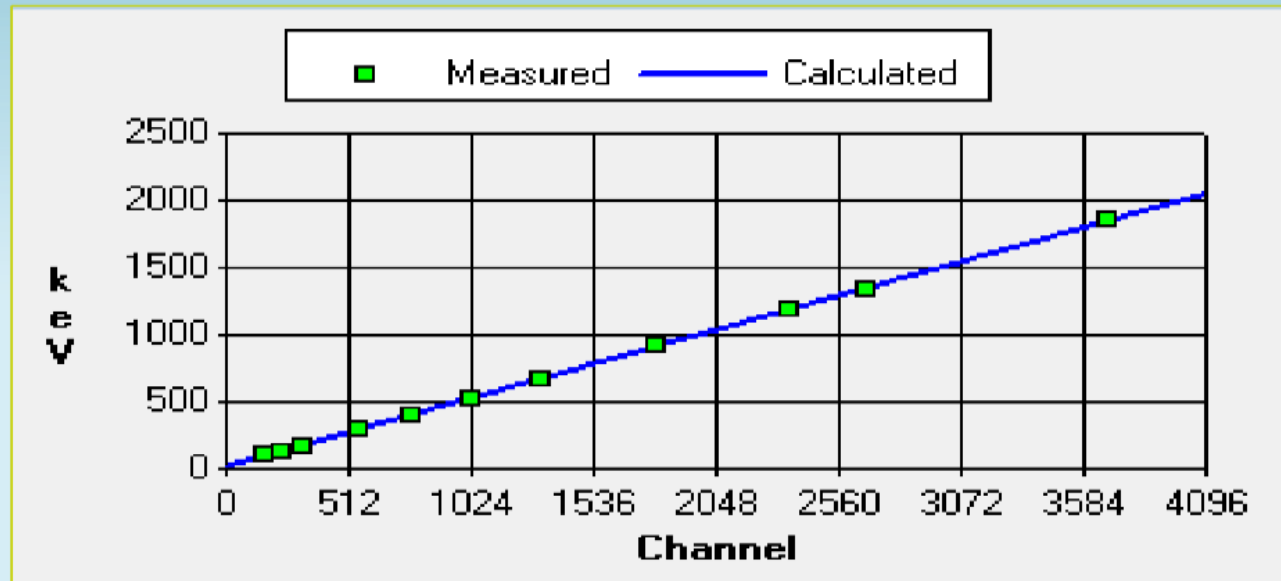
Peak Shape (versus gamma-ray energy)

Efficiency (versus gamma-ray energy)



Energy Calibration - Purpose

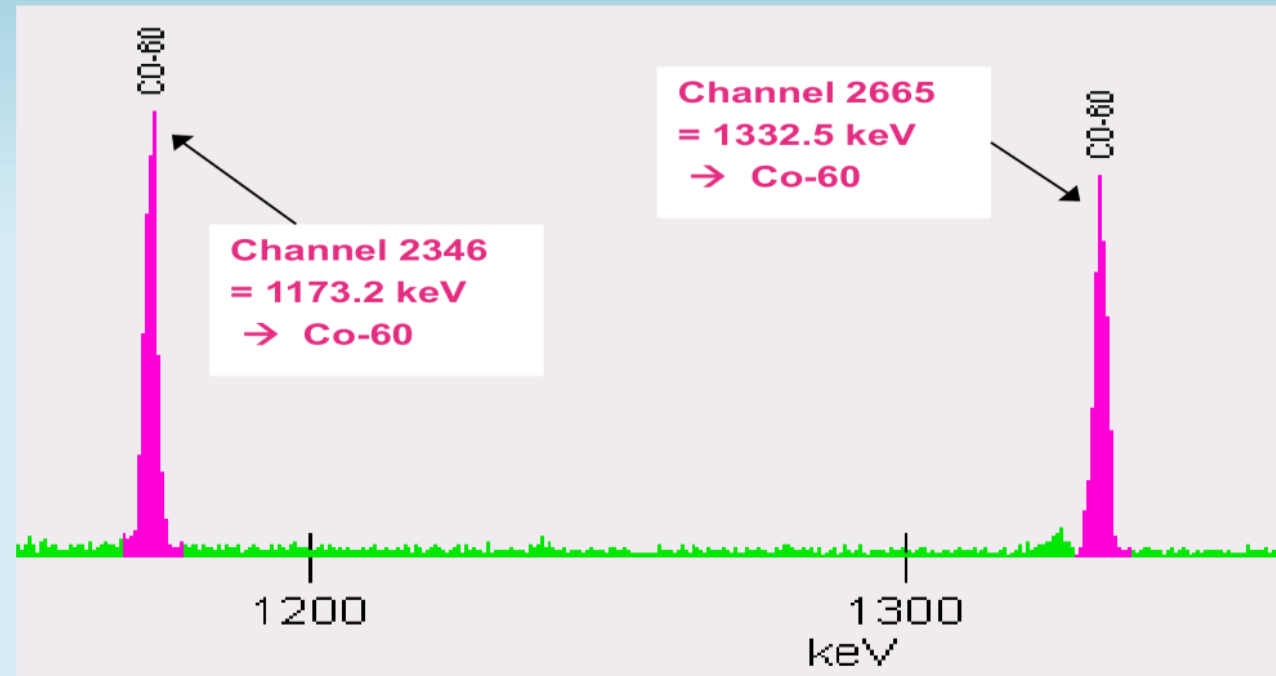
Establish a mathematical relationship between channel number and gamma-ray energy



Use that calibration to assign gamma-ray energies to peaks in a spectrum, based on peak channel location

Energy Calibration Allows Proper Nuclide Identification

Knowing the energy of gamma-ray peaks in the spectrum allows proper identification of the nuclides that emitted those gamma rays



Basic Energy Calibration Equation

The relationship between energy and channel may be expressed in terms of an equation

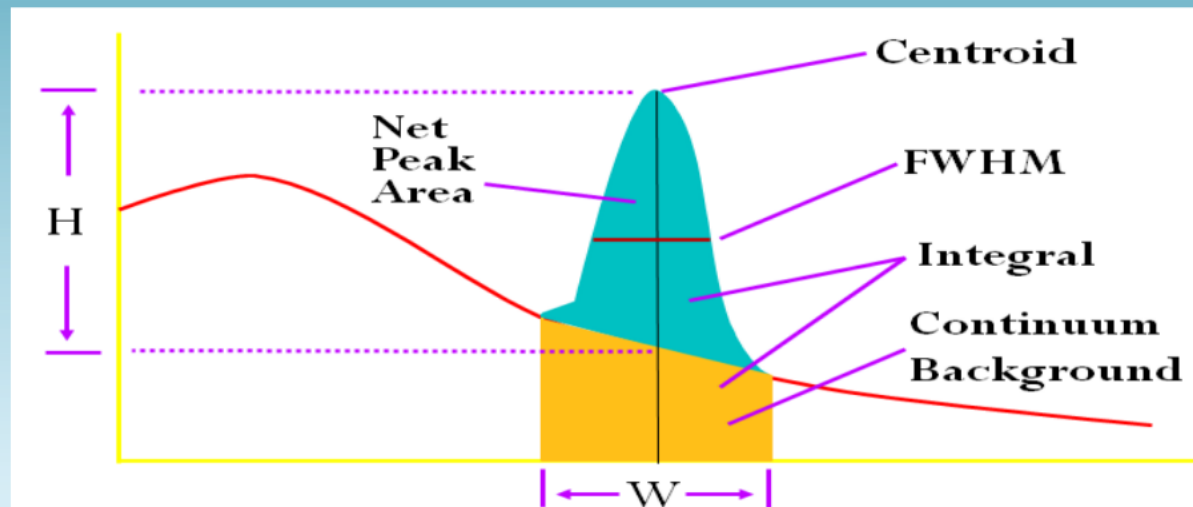
By determining the centroid channel location of two or more peaks of known gamma-ray energy E, a linear (first order) energy calibration function may be determined:

$$E = [\text{offset}] + [\text{slope} \cdot (\text{channel \#})]$$

$$\text{Energy} = 1.198\text{e-}01 \text{ keV} + 4.996\text{e-}01 \cdot \text{Ch} + 2.206\text{e-}07 \cdot \text{Ch}^2$$

Peak Shape Calibration

What do we mean by Peak Shape?



Single peaks have definite shape and predictable width

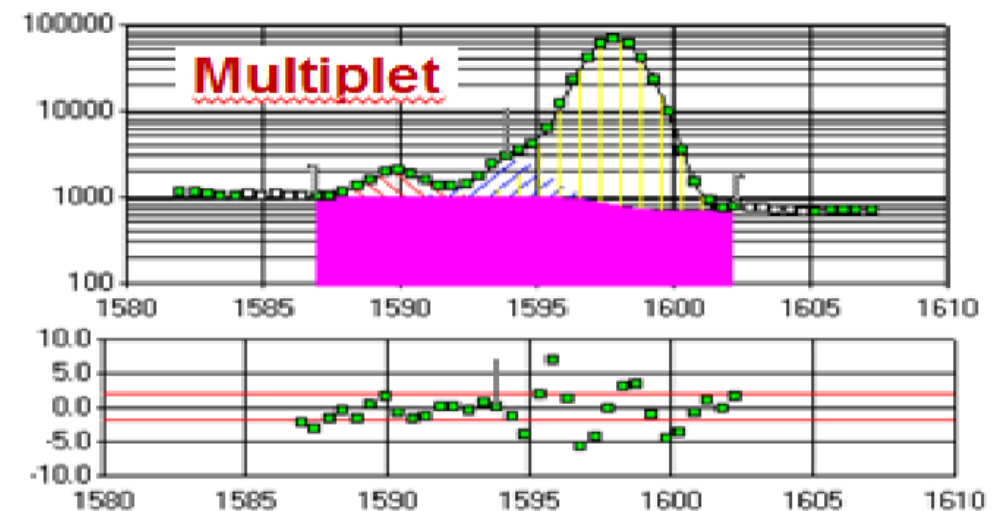
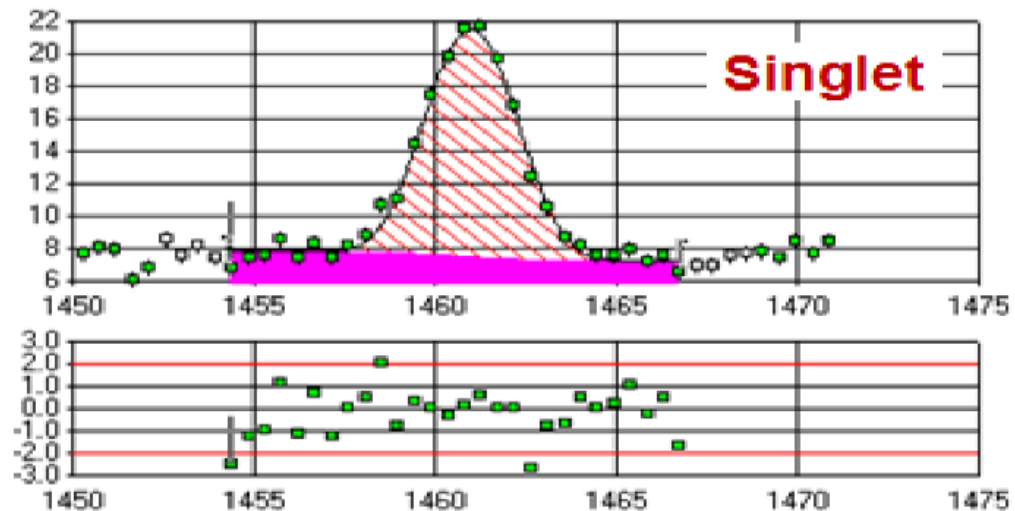
Knowing the expected peak shape as a function of energy will allow the software algorithms to give the best results.

It will also allow the software to best estimate the presence of a peak

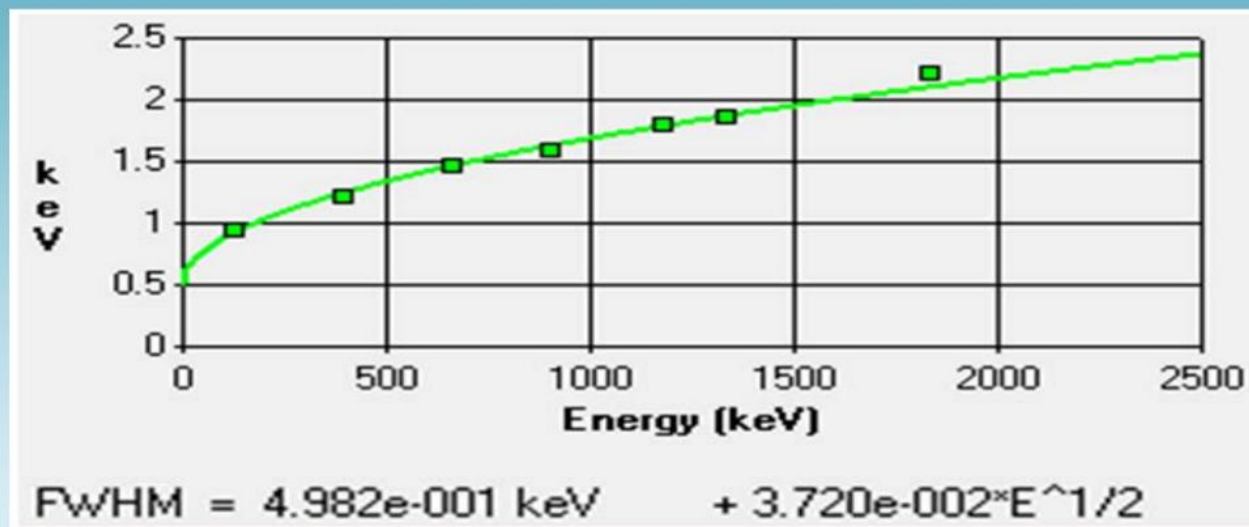
Peak Shape Calibration

Aids in optimizing “Peak Fitting” for single peaks or multiple overlapping peaks

Necessary for the estimation of detection limits



Peak Shape Calibration



- Many software settings can be optimized using “Number of FWHM’s”
- Allows a different setting as a function of energy...
- Examples:
 - Energy Tolerances (“x must be less than 1.5 FWHM units from y”)
 - Region of Interest “sizes” (# of FWHM between two regions)
 - Number of channels to consider in the continuum.

Nuclide Library

Nuclide Library Description: Typical mixed gamma source

Nuclide Name	Half-Life (Seconds)	Energy (keV)	Energy Uncert. (keV)	Yield (%)	Yield Uncert. (Abs.+/-)
CO-57	2.3406E+07	122.063*	0.000	85.5100	0.1800
		136.476	0.000	10.6000	0.1800
CO-60	1.6634E+08	1173.216	0.000	100.0000	0.0000
		1332.486*	0.000	100.0000	0.0000
SR-85	5.6022E+06	513.990*	0.000	99.2700	0.0220
Y-88	9.2102E+06	898.021	0.000	93.4000	0.4000
		1836.010*	0.000	99.3800	0.0200
CD-109	4.0090E+07	88.032*	0.000	3.7200	0.1100
SN-113	9.9446E+06	391.688*	0.000	64.9000	0.7000
CS-137	9.5207E+08	661.650*	0.000	85.1200	0.2300
CE-139	1.1894E+07	165.850*	0.000	80.3500	0.0800
HG-203	4.0262E+06	279.190*	0.000	77.3000	0.8000

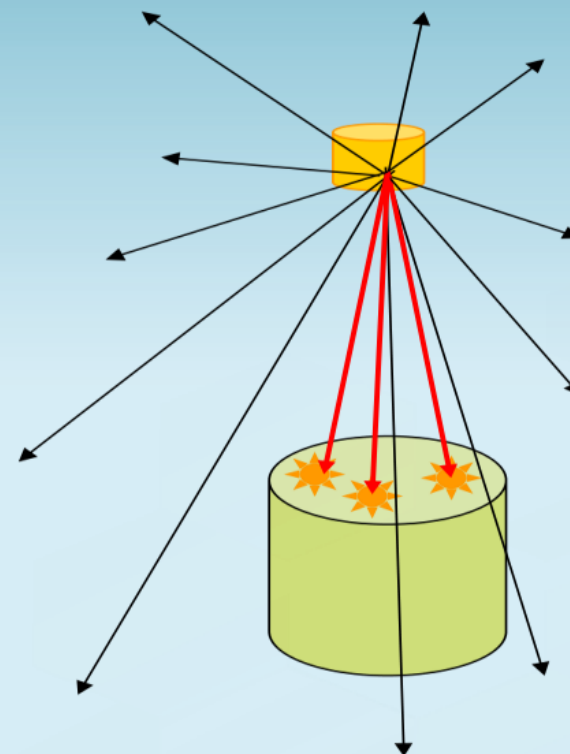
* = key line

What is Efficiency?

- ▶ **General definition for radiation detection applications: efficiency is the relationship between the observation rate of a radiation event and the emission rate of that radiation from a calibration source or a sample**
- ▶ **Absolutely necessary to calculate activity**

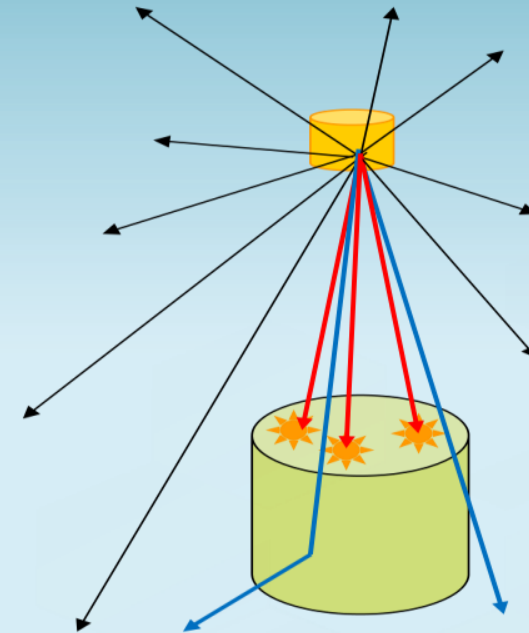
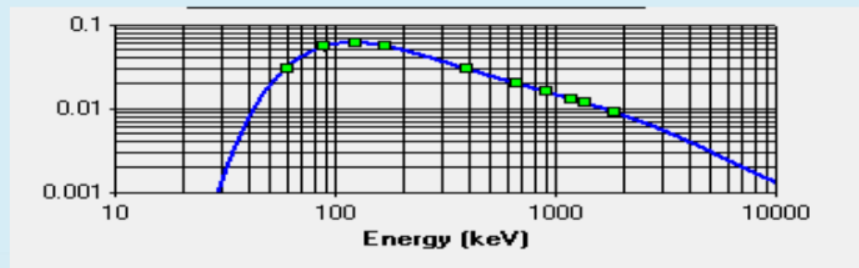
$$A_E = \frac{N_E}{\varepsilon_E \times t \times \gamma_E \times e^{-\lambda t_2}}$$

- ▶ **For gamma spectroscopy measurements, we will define and calculate “full-energy peak efficiency”, aka “peak” or “absolute” efficiency**
- ▶ **We can also define (but rarely calculate):**
 - “Geometric” efficiency
 - “Intrinsic” efficiency
 - “Total” efficiency



What is Full Energy Peak Efficiency

- ▶ Some (typically most) gamma rays emitted by the source or sample will not intercept the detector
- ▶ Of the gamma rays that do intercept the detector, some will not produce a count in the “full-energy” spectral peak
- ▶ The probability that an emitted gamma ray will deposit all of its energy in the detector (produce a count in the full-energy peak) is the “**full-energy peak efficiency**”
- ▶ Unless otherwise stated, the term “efficiency” will hereafter refer to “full-energy peak efficiency”, which is dependent upon the source/sample-to-detector **geometry** and the **energy** of the gamma ray



Certificate

Certificate Description: Canberra Spectrum 2 certificate

Certificate Title: Canberra Spectrum 2 Certificate

Quantity : 1.00 units

Assay date : 9/1/1978 6:00:00 AM

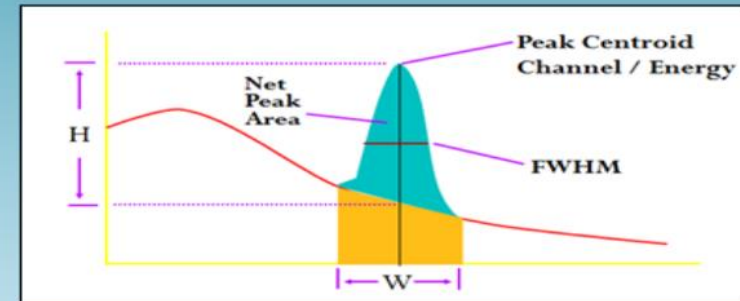
Original Certificate:

Date of Decayed Emission Rate: 9/23/2021 8:49:55 AM

Nuclide Name	Half-Life (Days)	Energy (keV)	Emission Rate /S/Unit	Emission Rate % Uncert	Decayed Emis. Rate /S/Unit
CD-109	4.6390E+02	88.0370*	514.3	4.10	3.1995E-08
CO-57	2.7240E+02	122.0630	917.7	2.20	3.8151E-15
CE-139	1.3770E+02	165.8530	551.4	4.00	2.2790E-32
HG-203	4.6620E+01	279.1880	1738.5	2.50	0.0000E+00
SN-113	1.1500E+02	391.6880	1651.4	4.80	1.1755E-38
SR-85	6.4850E+01	513.9960	2751.6	3.00	0.0000E+00
CS-137	1.0957E+04	661.6379	1424.1	3.00	5.2655E+02
Y-88	1.0666E+02	898.0210	10231.0	4.00	1.1755E-38
CO-60	1.9252E+03	1173.2080	3626.1	0.90	1.2593E+01
CO-60	1.9252E+03	1332.4640	3629.3	0.90	1.2604E+01
Y-88	1.0666E+02	1836.0140*	10699.0	3.00	1.1755E-38

Efficiency Value Calculation

Efficiency at a specific energy = E is traditionally determined **based on the measured net peak area for a spectral peak at energy = E, after counting a standardized source with known gamma-ray emission rate at energy = E**



$$\text{Efficiency (E)} = \frac{\text{Net counts in calibration peak at energy = E}}{\text{Total gammas with energy = E emitted from source}}$$

Efficiency may also be **determined** by **mathematical modeling methods** (e.g., using Canberra's ISOCS and LabSOCS software applications)

LabSOCS – Simplified Marinelli Beaker Template

Edit dimensions - Simplified Marinelli Beaker

Description:

Comment:

Units: ☒ mm ☐ cm ☐ m ☐ in ☐ ft

Specify sample by its: ☒ Dimensions ☐ Volume ☐ Weight

No.	Description	d.1	d.2	d.3	d.4	Material	Density	Volume, ml
1	Container	0	0	0	0		0	
2	Source	0					0	
3	Source - Detector	0						

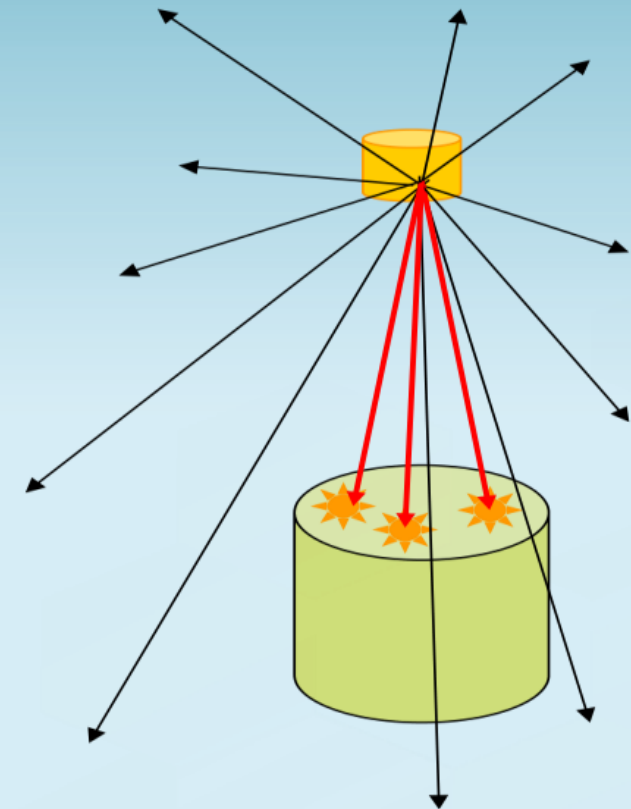
Simplified Marinelli Beaker

The diagram shows a cross-section of a Marinelli beaker. The dimensions are: 1.2 (top width), 3.1 (left height), 1.4 (inner width), 1.3 (inner height), 2.1 (right height), and 1.1 (bottom width).

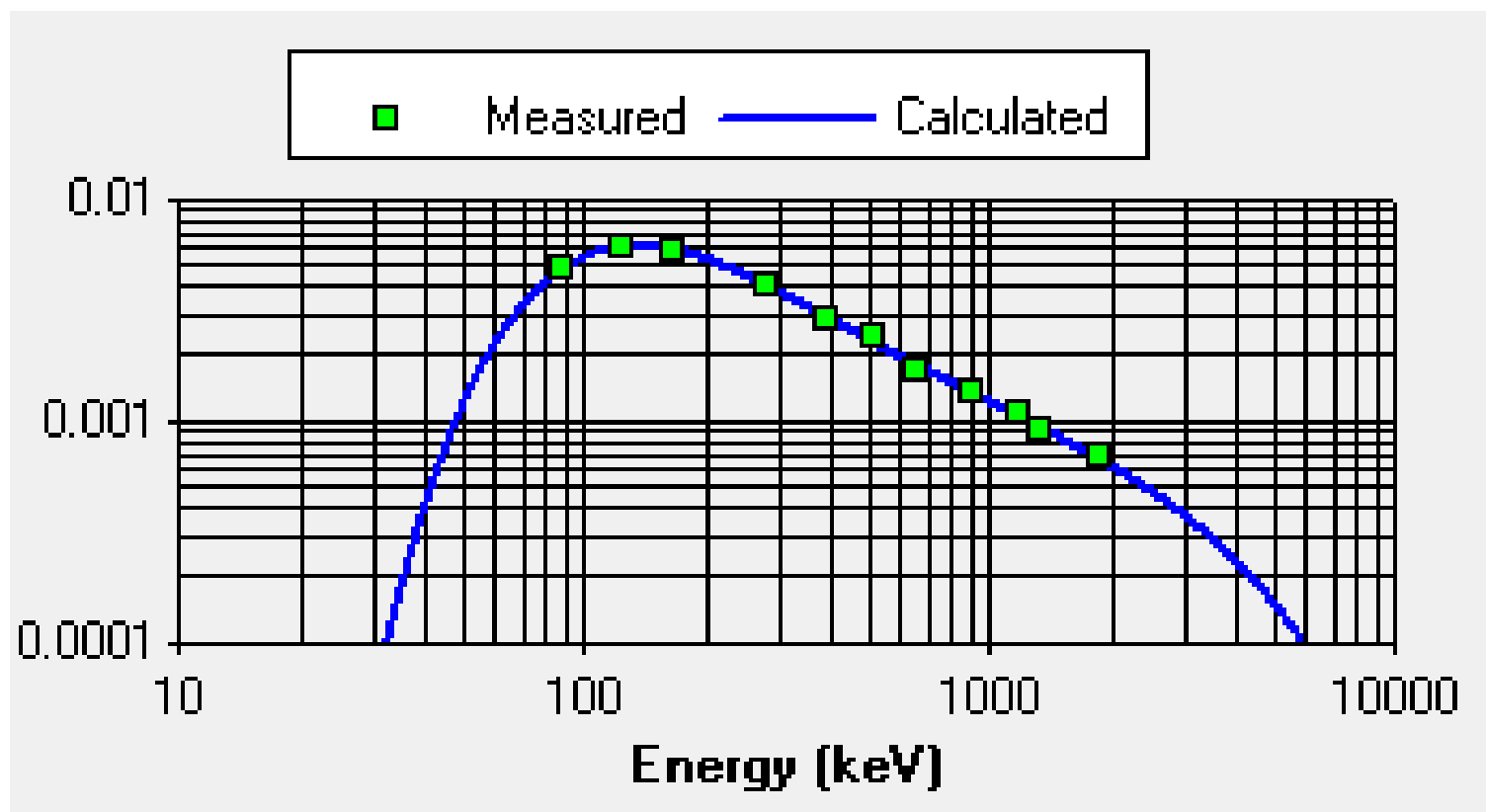
Geometry Related Factors that Affect Efficiency

► For gamma spectroscopy measurements, “geometric”, “intrinsic”, “total” and “full-energy peak” efficiency will vary with changes in:

- Distance between source/sample and detector
- Offset of source/sample from detector axis
- Source/sample container dimensions
- Source/sample matrix characteristics
 - Chemical composition
 - Density
 - Fill height / mass / volume
- Detector crystal size and shape
- Detector end-cap material(s) and dimensions
- “Dead layer” on surfaces of detector crystal
- Other absorber materials located between the source/sample and detector end-cap



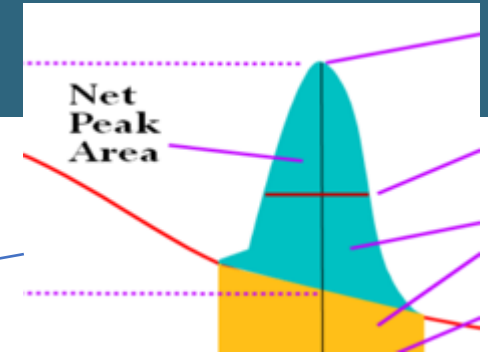
Efficiency Curve Example



Datasource: C:\GENIE2K\CAMFILES\NBSSTD.CNF

$$\ln(\text{Eff}) = -1.680e+02 + 1.127e+02 \ln(E) - 2.998e+01 \ln(E)^2 + 3.828e+00 \ln(E)^3 - 2.335e-01 \ln(E)^4 + 5.312e-03 \ln(E)^5$$

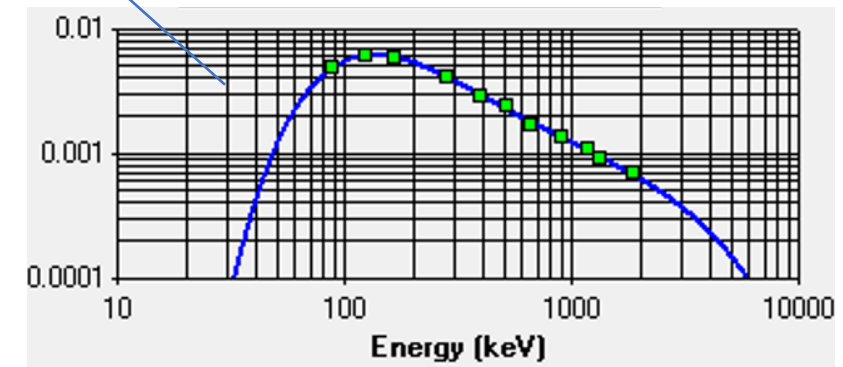
Putting it All Together



(Net Peak Area)

$$\text{Line Activity (Bq)} = \frac{(\text{Net Peak Area})}{(\text{Live Time}) * (\text{Nuclide Line Intensity}) * (\text{Efficiency at E}) * (\text{Decay Correction}) * (\text{Sample Quantity})}$$

Nuclide Name	Half-Life (Seconds)	Energy (keV)	Energy Uncert. (keV)	Yield (%)
CO-57	2.3406E+07	122.063*	0.000	85.5100
		136.476	0.000	10.6000
CO-60	1.6634E+08	1173.216	0.000	100.0000



Mirion Courses Available

- GP201 - Fundamentals of Gamma Spectroscopy
- GP301 - Applied Principles of Gamma Spectroscopy
- SU601 Interpretation of Gamma Spectroscopy Results