Tutorial 4.6 — Gamma Spectrum Analysis

Slide 1. Gamma Spectrum Analysis
In this module, we will apply the concepts that were discussed in Tutorial 4.1, “Interactions of Radiation with Matter.”

Slide 2. Learning Objectives
At the end of this module you should be able to:

- Describe how gamma spectrometers record signals resulting from the photoelectric effect, the Compton effect, and the pair production effect.
- Discuss how software parameters such as key line, peak centroid, energy tolerance, and FWHM are used to determine if a peak is “valid.”
- Identify the most common features and artifacts present in gamma spectra.
- List at least four factors that should be considered when attempting to identify an unidentified peak.

The key concepts to focus on in this module are:

- EPA Method 901.1 – “Gamma Emitting Radionuclides in Drinking Water” requires that all photopeaks in the gamma spectrum be identified.
- A “real” photopeak is characterized by a Compton edge and a Compton continuum preceding it.
- Coincidence sum peaks result from two gamma rays emitted by the same nucleus. Random sum peaks arise from different nuclei.
- Identifying low abundance gamma rays for the highest activity radionuclides found will require going to the decay schemes on NUDAT data base (http://www.nndc.bnl.gov/nuDat2/).

Slide 3. Gamma Ray Detectors – NaI(Tl)
There are three types of gamma ray detectors that are used for gamma ray analysis. The thallium doped sodium iodide crystal is actually a scintillation detector. The gamma ray transfers energy to the crystal through excitation of K-shell electrons via the photoelectric effect. These electrons migrate to the crystal’s ground state giving off photons in the Ultraviolet to Visible energy range. The crystal itself does not have a potential across it. The sodium iodide crystal is optically coupled to a photomultiplier tube. The photons from the de-excitation of the crystal are converted to an electronic pulse in the photomultiplier tube. The resultant pulse is proportional to the energy of the initial gamma ray. Sodium iodide detectors are operated at room temperature, are very rugged, relatively cheap and easy to operate, and they are not significantly affected by temperature or humidity. However they have limited ability to distinguish between gamma ray peaks that are closer together than about 80 keV.

Slide 4. Gamma Ray Detectors - HPGe
There are two types of germanium detectors. The older version was a lithium drifted crystal of purified germanium. It began to be phased out in the early 1980s when the production of high purity germanium became a more routine practice. The germanium

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detectors also detect gamma rays via the photoelectric effect, but these crystals are cooled to liquid nitrogen temperatures and have voltages applied to the crystals as high as 4,000 volts. In the germanium detectors the photoelectron is accelerated in the voltage field applied to the crystal and it ultimately produces a pulse at the detectors pre-amplifier that is proportional to the original gamma ray energy.

Older “jelly” detectors could not be warmed to room temperature, as the lithium would drift out of the crystal making the detector inoperable. Today most labs use high purity germanium, or HPGe, crystals where they can be warmed to room temperatures and then cooled back down again and operate as well as when they were first used. However, each electronic component of the HPGe system has a separate power source required so that we can achieve the exacting requirements needed for high resolution gamma ray analysis.

Slide 5. Comparing NaI(Tl) with HPGe Detectors
Compared to a sodium iodide detector the newer HPGe detectors are relatively expensive, more difficult to operate, require constant liquid nitrogen conditions to operate, and are sensitive to environmental conditions of the counting room. However, the big advantage of the HPGe is that it can resolve two gamma rays that are within 0.8 keV of each other. This is a significant advantage as many samples have naturally occurring decay products of uranium and thorium that have multiple gamma rays.

Finally a significant advantage of using an HPGe is that the sample can be analyzed directly for gamma emitting radionuclides, achieving detection limits as low as 1.0 pCi/L in aqueous samples. Later on in this tutorial we will be able to compare two spectra, one using a sodium iodide detector and one using an HPGe to see the differences in these two detector materials. The chart on the right summarizes the difference for these two detectors.

Slide 6. The Importance of Peak Identification
Gamma ray spectra are much more complex than that of alpha or beta particles. Part of this is due to the fact that any gamma has the ability to interact with the detector crystal in one of three ways. As discussed in Module 4.1, these are the photoelectric effect the Compton effect and the pair production effect. EPA method 901.1 is used for detection of gamma emitting radionuclides in drinking water. This method requires that all gamma ray peaks in the spectrum be identified. The material we discuss in this module will provide the theoretical background for identifying the various sources of gamma rays and methods for “sleuthing” unknown peaks.

Slide 7. Typical Gamma Ray Spectrum
Shown on this slide is a gamma ray spectrum of a $^{60}$Co standard taken using an HPGe detector. There are at least 10 features of this gamma ray spectrum that you will be able to identify by the end of this module. The spectrum is a plot of total accumulated counts in a channel versus the channel number. The sample was counted for about 1,000 seconds. The energy range is about 50 to 2700 keV. In gamma ray spectrometry the area under the gamma ray peak is a direct measure of the activity of the radionuclide associated with that gamma ray.
Slide 8. Full Energy Peaks
The picture on this slide focuses on the energy range of the gamma ray spectrum for $^{60}$Co below 1,400 keV. Highlighted are the two gamma ray peaks that characterize the decay of $^{60}$Co. As you may recall from module 4.1 these two gamma rays at 1173 and 1332 keV are almost of exactly the same abundance factor. Each one of these is called a full energy peak, or FEP, since they correspond to an energy transition resulting from the $^{60}$Co decay. Each of these FEPs is a result of a gamma ray interacting with the detector via the photoelectric effect. Some radionuclides do not emit gamma rays upon decay, some emit only one or two, and some can emit hundreds. The greater the number of gamma rays that result from radioactive decay the more complicated the spectrum becomes.

Slide 9. Peak Characteristics – Key Line
One of the characteristics of the gamma ray software is to have an energy identified that is unique to a specific radionuclide. This is referred to as the “key line” function by some software manufacturers. The key line corresponds to a gamma ray that —

- Has the largest abundance,
- Has the least amount of interference from other gamma rays, or
- is sometimes neither and sometimes both.

This function does not always need to be selected. In those cases the software will determine the identity of the peak based on possible gamma ray energies in the library that are close to the measured energy (this is another preset function).

Slide 10. Peak Characteristics – Peak Centroid
The peak centroid is the mid-point of the gamma ray peak. It is determined by the peak search algorithm used in the software. The centroid will generally not be one of the discrete channels used to store information from the detector system, as the peak shape is a smoothed function.

Slide 11. Importance of the Peak Centroid
The centroid is used as the means for determining the energy of the gamma ray peak and also the full-width half-maximum, FWHM (to be discussed shortly).

The value of the centroid is compared to the gamma ray library to determine which radionuclides could correspond to this gamma ray energy.

The picture on this slide shows the location of the centroid for the 661.6 keV gamma ray for cesium-137.

Slide 12. Peak Characteristics – Full Width Half-Maximum
The FWHM is the difference in energy between the two points in the peak where we measure one-half the number of counts registered at the peak centroid. For a HPGe detector the value of the FWHM varies as a function of energy. During initial calibration of the detector the software will calculate a curve for the FWHM as a function of energy and use this when analyzing samples to assess whether a peak has a good shape.
The table at the right shows the expected FWHM for a certain detector at various energies. This was determined during the detector’s initial calibration. Once a sample count is completed, the software determines this among other parameters. It will take the energy of the peaks found, calculate a theoretical FWHM and compare this to the actual FWHM. If the measured value is a pre-selected value beyond the theoretical value, the software will flag the peak as having a poor shape. There may be several reasons for this:

- Temperature shift in the room.
- Humidity shift in the room.
- Spectral interference from a gamma ray that is very close in energy.

When a peak that is used to quantify a radionuclide has a suspect peak shape, the analyst must examine the spectrum and try to assess the reason for this. Some hints for how to do this are shown in this slide. In most cases, you will find that there is an environmental effect in the laboratory responsible for the poor peak shape. However, if there is no conclusive evidence that this was the cause, chemical separation may need to be performed for the analysis of that radionuclide to remove or mitigate the effect of the interfering radionuclides’ gamma ray.

The energy tolerance is a user selected value that tells the software how far from the library listed value you will accept the identity of a gamma ray peak. For example the library has the gamma ray energy for $^{137}\text{Cs}$ listed as 661.6 keV. You the user have selected an energy tolerance of 0.5 keV. A sample has a peak centroid measured at 660.9 keV. Based on the selected energy tolerance the lowest energy the software thinks that cesium-137 can have is 661.1 keV. It will not identify this peak as Cs-137. This makes the process of checking your library and ensuring the correct energy listed very important function.

Keep in mind that the peak centroid will shift due to minor fluctuations in temperature, humidity, line voltage, and background radiation from other radionuclides. Thus when the user selects a delta keV preset value it should be based somewhat on the experience with the instrument at hand and the type of samples being measured.

The user is allowed to select an energy tolerance for the gamma ray spectrum analysis of energies. The energy tolerance is the maximum amount that the measured energy of a gamma ray can be different from the library value to have the software decide that it belongs to a particular radionuclide. Energy tolerance values are usually in the range of 0.8 to 2.0 keV. The higher the activity of the sample the larger the number of counts in a gamma ray peak and thus the easier it will be for the software to determine the peak centroid and the energy. For high activity samples the energy tolerance should be on the lower end towards 0.8 keV. For environmental samples where there are few counts in the peak the energy tolerance should be set wider, like at 2.0 keV. If the measured gamma ray energy falls outside the energy tolerance of any gamma ray listed in the library, it will
call the peak unidentified. The user then needs to be a sleuth, and determine the true identity of the peak.

Slide 16. Peak Characteristics – Peak Area
The gamma spectrometer software has a peak search algorithm that locates the peak centroid, determines the shape of the peak based on the FWHM, and then calculates the area under the peak. Theoretically, gamma rays are monoergic, that is, a gamma ray has only one energy. This would mean that all the counts for a single gamma ray would ideally come in one channel. However, due to electronic voltage, temperature, and humidity variations and the imperfect response of the crystal, the FEP gamma ray events are spread out over several channels.

Slide 17. Calculating the Peak Area
The peak area is directly proportional to the number of radioactive decays of the radionuclide whose gamma ray this is, and thus proportional to the activity. Gamma ray spectrometry is different from gas proportional counting or liquid scintillation in that the software determines where the peak ends coincide with the background. Then it takes the average of several channels above and below the peak that are in the background, multiplies the average by the number of channels in the peak and subtracts the background from the total area. Notice in the diagram that the background is the average of the high and low energy side backgrounds drawn through the base of the peak.

Slide 18. Artifacts in Gamma Ray Spectrometry
The several different ways that gamma rays interact with the detector crystal and the surrounding shielding allows us to observe some very distinct features in the gamma ray spectrum. These features are listed here as:

- Compton continuum.
- Compton edge.
- Backscatter peak.
- Single and double escape peaks.
- Coincidence and random sum peaks.
- Annihilation peak, X-ray, and Bremsstrahlung background radiation.

These features, coupled with multiple gamma rays being possible from multiple radionuclides, can create a very complicated spectrum. The next few slides explain how to distinguish artifacts from real gamma rays.

Slide 19. Compton Continuums
Recall from Tutorial 4.1 that the Compton effect occurs when only part of the incident gamma ray energy is transferred to an electron. There is a minimum energy that this interaction can occur with for each gamma ray. This means that if the interaction occurs within the detector, the liberated electron can have a finite, maximum energy based on the incident gamma ray energy. All other interactions will yield electrons that are lower in energy and this forms what is called the Compton continuum. The Compton continuum for the lower energy of the two $^{60}$Co gamma rays shown is highlighted in green.
Slide 20. Example of a Compton Continuum
Note that although the green highlighted area is associated with the 1.17 MeV gamma ray that the 1.33 MeV gamma ray will also have a Compton continuum that tails off to lower energies. Each true gamma ray emitted from a nucleus will have a Compton continuum associated with it.

Slide 21. The Compton Edge
The Compton edge appears in the gamma ray spectrum as a sharp drop in the background at an energy below the full energy gamma ray peak. The formula to calculate where the edge for each gamma ray occurs is shown on this slide. The calculation for the minimum scattered gamma ray energy is identified on the next slide. The edge to the Compton peak is angled slightly towards higher energy due to the background radiation associated with the spectrum.

Slide 22. Calculating the Location of the Compton Edge
The equation on this slide identifies how to calculate the location of the Compton edge. This can be very useful when attempting to identify why another gamma ray has an unusually large FWHM. Although there may be no way to avoid such an interference without chemical separation, the analysts will know that the results of the analysis will be biased due to the change in background due to the Compton edge.

One other note about Compton edges: If a peak is due to a random sum event, it cannot have a Compton peak, because the random sum peak is an artifact of the detection system.

Slide 23. What is Backscatter?
When the Compton effect occurs in a medium other than the detector, some of the gammas may be deflected through an angle that is 180° to the original gamma ray path. This turns out to be the gamma ray with the minimum energy when interaction occurs by Compton effect. Since samples are placed in proximity to the detector there is a probability that this deflected gamma will strike the detector. If this gamma interacts with the detector via the photoelectric effect, it will cause a signal that is not related to any individual radionuclide.

Slide 24. The Backscatter Peak
In the diagram to the right we see an example of a backscatter peak highlighted in green. Note that it’s shape is the reverse of the Compton edge, as its minimum energy is in the range of about 200–250 keV. This is because many different gamma rays contribute to its appearance. The Compton effect only becomes of significance above about 140 keV, so that the scattered gamma minimum is about 90 keV. The effects of the detector casing made of aluminum shields some of these lower energy backscattered gamma rays giving the backscatter peak an odd shape.

Slide 25. Pair Production and Annihilation-Review
Recall that one of the mechanisms for gamma rays interacting with matter is by the pair production effect. The incident gamma ray must have greater than 1.022 MeV of energy
for this to occur since a positron and electron are formed, both of which have the rest mass equivalent energy of 0.511 MeV.

Also remember that positrons have a very short life, undergoing annihilation with an electron within picoseconds of their formation. When annihilation occurs two 0.511 MeV gamma rays are formed.

**Slide 26. Escape Peaks (Slide 1 of 2)**

A germanium detector has a high voltage applied to it so that when gamma rays interact via the photoelectric effect the electrons produced will migrate in the electric field to ultimately yield a signal. When pair production occurs inside a gamma ray detector, the electron formed immediately begins to migrate in the electric field as does the positron. Thus the energy associated with the incident gamma ray is now split between these two particles. As the electron is migrating the positron undergoes annihilation. Keep in mind that the kinetic energy of the positron begins to radiate as very low energy photons as it approaches its annihilation with an electron. These low energy photons interact with the detector via the photoelectric effect producing additional electrons. When the positron annihilates it produces two 0.511 MeV gamma rays. If one of these gamma rays interacts with the detector to yield a photoelectron, it will likely be counted with all the other electrons that have been formed in this process as a single pulse. Since all of the initial gamma ray energy is recorded except the 0.511 MeV gamma that “escaped” the detector without interacting, a peak in the gamma ray spectrum appears. This peak is exactly 0.511 MeV less than the original gamma ray energy, and is called a single escape peak.

**Slide 27. Escape Peaks (Slide 2 of 2)**

What happens if both of the annihilation 0.511 MeV photons do not interact with the detector? Then there will be a separate peak that is exactly 1.022 MeV less than the full energy peak energy.

The spectrum on the right shows the single escape and double escape peak for the 1.332 MeV gamma ray of $^{60}$Co. Note how small they both are compared to the $^{60}$Co peak. Also note that there is no detectable single or double escape peaks for the 1.173 MeV peak. This is because the pair production effect increases exponentially as a function of energy above 1.022 MeV, and it is just too rare an event for the lower energy peak to produce these artifacts. Of the two artifacts it is more likely to see the double escape peak based on the greater probability that both 0.511 MeV gamma rays will escape the active detector area.

**Slide 28. Summation Peaks: Coincidence Sum Peaks**

A coincidence sum peak occurs when a radionuclide has two energy levels that decay to another state in rapid succession. For reasons beyond the scope of this tutorial, it is possible that both the gamma rays strike the detector simultaneously making it appear to the detector as a single event and recording the energy as the sum of the two. In the case of $^{60}$Co, the 2.505 MeV state undergoes de-excitation to the 1.1732 MeV state, and then from there to the ground state. Additionally a very small percentage of the time the 2.505 MeV state goes directly to ground state. For $^{60}$Co the 2.505 MeV gamma results from
both a direct transition as well as coincidence sum effect. Because it has a direct transition the 2.505 MeV peak has a Compton edge. However there are some radionuclides that do not have such a direct transition. Their coincidence sum peaks would not have a Compton edge associated with it.

Slide 29. Summation Peaks: Random Sum Peaks
The coincidence sum peak results from transitions in one atom. A random sum peak occurs when two different gamma rays, likely from two different radionuclides randomly strike the detector at the same time. Again the detector will record the sum of the two energies as one. A random sum peak will not have a Compton edge.

Neither the efficiency curve for the detector nor the software can accurately compensate for coincidence sum effects. The best way to resolve this issue is to move the sample farther away from the detector and count it for a longer period of time. The exact reasoning for this working is beyond the scope of this tutorial.

Slide 30. Annihilation Peaks, X-rays and Bremsstrahlung
The annihilation peak is due either to a radionuclide that decays by positron emission or the pair production effect occurring outside the detector and the resultant 0.511 MeV annihilation photon interacting with the detector via the photoelectric effect. This will often be a feature of the gamma ray spectrum.

When a gamma ray interacts with the lead shielding around the detector via the photoelectric effect, lead X-rays are produced. These X-rays can strike the detector giving rise to a signal at about 72 keV. In the previous gamma-ray spectrum for $^{60}$Co the lead X-rays can be seen as a very small peak at the very low end of the energy range.

Many radionuclides decay by negatron emission. The Bremsstrahlung radiation that results will be low in energy and will be detected by the HPGe detector. However since it varies with negatron energy and the nucleus of interaction there is no specific peak—just general background counts.

Slide 31. NaI(Tl) vs HPGe Spectra
Shown on this slide are two spectra of $^{60}$Co. The one on the left used a NaI(Tl) detector and the one on the right a HPGe detector. The left spectrum has the 1173 and 1332 peaks for cobalt separated at the baseline by one channel. The FWHM of these peaks is about 80 keV. For the right hand spectrum counted using a HPGe detector the separation between these same two peaks is 159 channels and the FWHM of these peaks are about 1.5 keV. It is easy to see from the comparison of these two spectra that the NaI(Tl) detector would never be able to resolve other gamma rays if they were between the two $^{60}$Co peaks.

Slide 32. Peak Identity
EPA Method 901.1 requires that when a drinking water sample is analyzed for gamma emitting radionuclides that all gamma rays peaks identified by the software be matched to a known radionuclide. When we have naturally occurring radionuclides such as lead or
bismuth, there can be many gamma rays, some of them with abundances of less than 1%. Ensure that any peaks in the unidentified list are matched to a known radionuclide and that they can be quantitated to ensure that the maximum contaminant levels are not exceeded.

Slide 33. How to Identify an Unidentified Peak
This is where the gamma ray spectrometrist becomes a sleuth. We have discussed many different types of artifacts that can occur in the spectra routinely. We also now know that the instrument is sensitive to environmental conditions and thus energy shifts can occur causing erroneous or no identification of gamma rays. Listed here are some tools that you can use to narrow down the list of usual suspects.

Slide 34. Still Unidentified?
Sometimes a literature search for low abundance gamma energies is required. The NUDAT data base is the most complete and accepted compilation of gamma ray energies for all radionuclides.

If you are still stumped, determining the half life of the radionuclide by performing multiple counts will help nail down the identity. Some tips on how to do this are noted on this slide.

Slide 35. Conclusion
Gamma spectrometry is very different form other forms of radioactivity analysis. You have been exposed to the basics of how to examine a gamma-ray spectrum. It requires practice to get good at it. So you should review some gamma-ray spectra and their associated printouts and verify that you can:

- Compare the software results to the spectrum and identify FEPs and artifactual peaks on a gamma spectrum.
- Show with which gamma rays single- and double-escape peaks are associated.
- Identify most unidentified peaks using a variety of data and resources.