Lab 9: Spectroscopy

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In[2]:=
```
datafolder = NotebookDirectory[] <> "data/";
```

In[252]:=
```
numchannels[filename_] := ToExpression[
  StringSplit[StringSplit[Import[datafolder <> filename], "\n"][[12]]][[2]]]
counttime[filename_] := ToExpression[
  StringSplit[StringSplit[Import[datafolder <> filename], "\n"][[10]]][[1]]]
```

In[255]:=
```
numchannels["background2.spe"]
counttime["background2.spe"]
```

Out[255]= 1023

Out[256]= 600

In[152]:=
```
loaddata[filename_] := ToExpression[StringSplit[
    Import[datafolder <> filename], "\n"][[13 ;; numchannels[filename] + 12]]]
```

In[257]:=
```
bgcorrspec[filename_, bgfile_] :=
  loaddata[filename] / counttime[filename] - loaddata[bgfile] / counttime[bgfile];
```

In[312]:=
```
plotpairs[filename_, bgfile_] :=
 Multicolumn[Join[Range[0, 10, 10 / numchannels[filename]],
    bgcorrspec[filename, bgfile]], 2] // First
```

In[313]:=
```
plotspec[filename_, bgfile_] := ListPlot[plotpairs[filename, bgfile]]
```

In[40]:=
$$\text{gauss}[x\_, y\_, A\_, \text{mean}\_, \text{sigma}\_] := y + \frac{A}{\sqrt{2\pi\,\text{sigma}^2}} e^{\frac{-(x-\text{mean})^2}{2\,\text{sigma}^2}};$$

Assembled NaI (Tl) Detector : Setup and Spectral Analysis

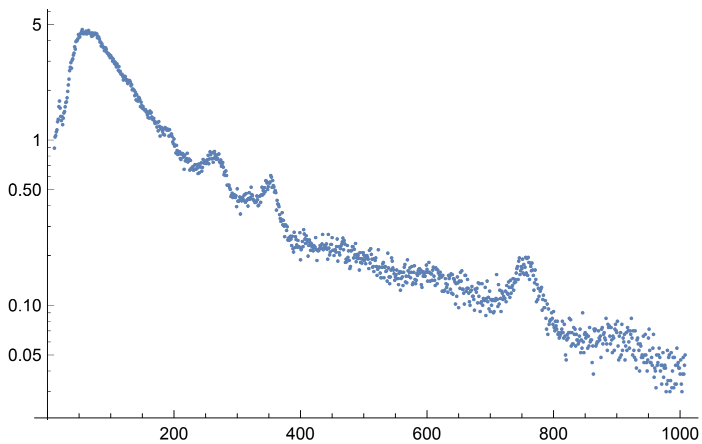
1. For each spectrum collected, determine the peak position by averaging over the peak. The answer should be in channel number.

Background

In[153]:=
```
file = "background2.Spe";
bgdata = loaddata[file];
bgtime = 600;
```

In[156]:=
```
ListLogPlot[bgdata / bgtime]
```

Out[156]=



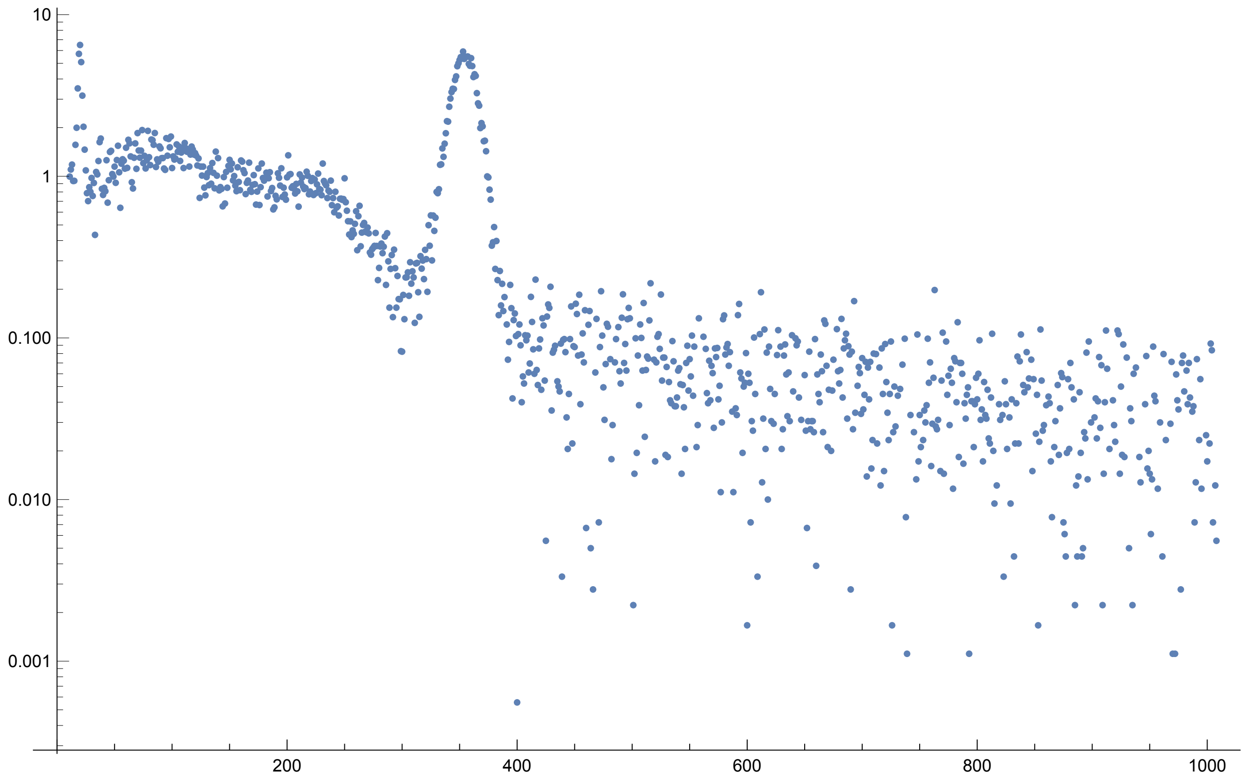
Cs-137

In[157]:=
```
file = "cs137part1-15.Spe";
data = loaddata[file];
time = 90;
pk = FindPeaks[data / time - bgdata / bgtime, 10, 10^-5, 1] // N
```

Out[160]=
```
{{20., 6.49389}, {82., 1.68833}, {201., 1.34833}, {353., 5.91222}}
```

In[161]:= ListLogPlot[data / time - bgdata / bgtime, ImageSize → Full]

Out[161]=



In[148]:= truecr = data / time - bgdata / bgtime;
Total[truecr[[300 ;; 400]] * Range[300, 400]] / Total[Range[300, 400]] // N

Out[149]= 1.61604

In[60]:= 201 / 353 * 662 // N

Out[60]= 376.946

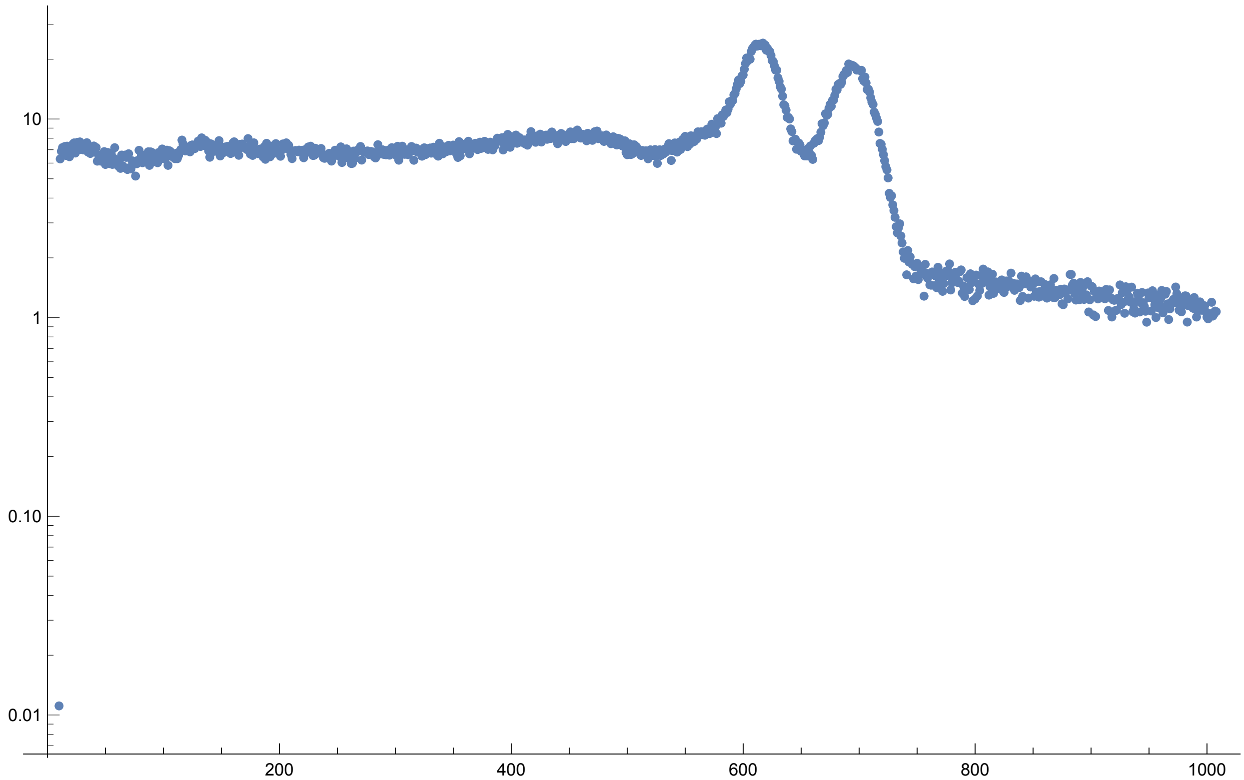
Co-60

In[162]:= file = "co60part1.Spe";
data = loaddata[file];
time = 90;
pk = FindPeaks[data / time - bgdata / bgtime, 5, 10^{-8}, 10] // N

Out[165]= {{617., 24.0922}, {693., 18.6911}}

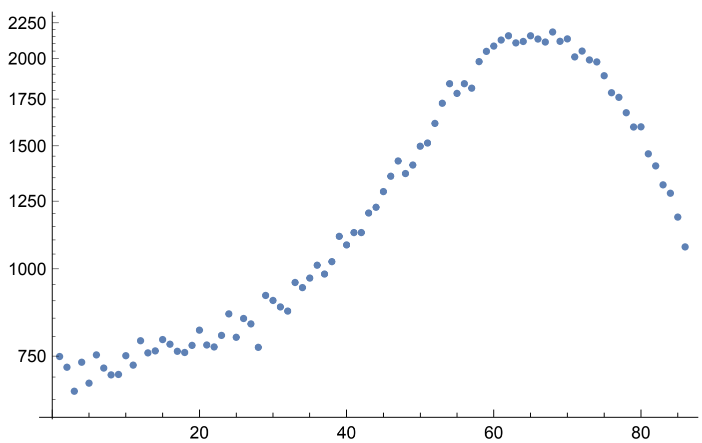
In[166]:= `ListLogPlot[data / time - bgdata / bgtime, ImageSize → Full]`

Out[166]=



In[39]:= `ListLogPlot[data[[550 ;; 635]]]`

Out[39]=



In[47]:= `NonlinearModelFit[Multicolumn[Join[Range[550, 633], data[[550 ;; 635]]], 2] // First, gauss[x, 42, A, m, s], {A, m, s}, x]`

NonlinearModelFit: Encountered a gradient that is effectively zero. The result returned may not be a minimum; it may be a maximum or a saddle point.

Out[47]= FittedModel[$42 + 0.398942\, e^{-0.5\,(-1.+x)^2}$]

From this attempt to fit a simple Gaussian to a pretty obvious peak, it seems that this approach needs some refinement. I was unable to get a convergent fit; this could be because of the low-resolution detector.

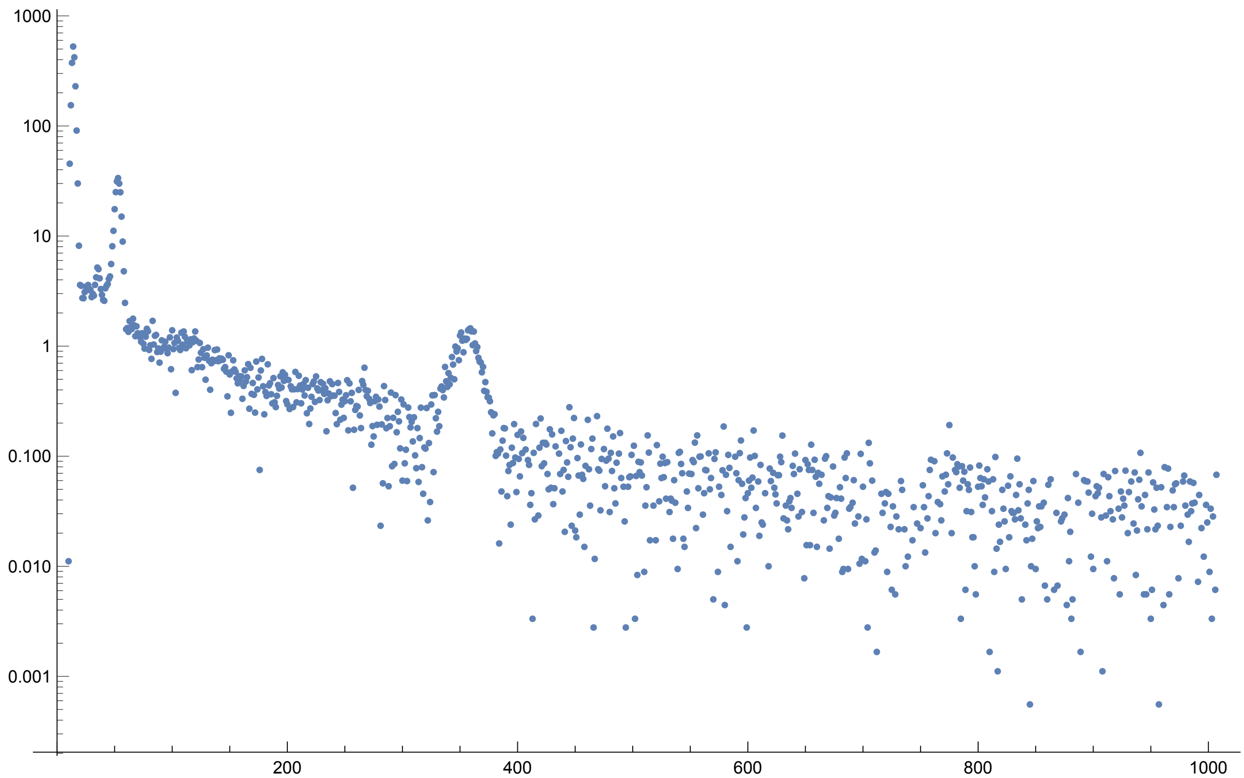
Cd-109

In[167]:=
```
file = "cd109part1.Spe";
data = loaddata[file];
time = 90;
pk = FindPeaks[data / time - bgdata / bgtime, 50, 10^-58, 400] // N
```

Out[170]= {{14., 526.591}}

In[171]:=
```
ListLogPlot[data / time - bgdata / bgtime, ImageSize → Full]
```

Out[171]=



Ba-133

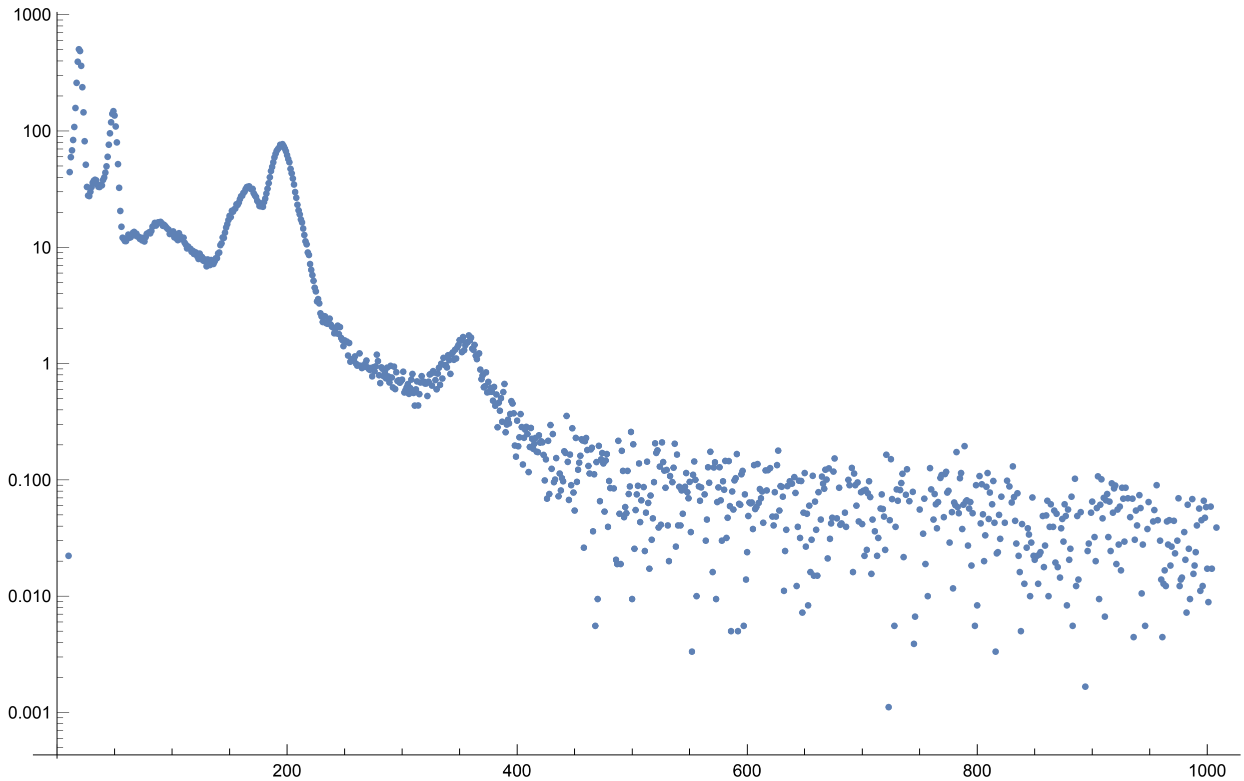
In[172]:=
```
file = "ba133part1.Spe";
data = loaddata[file];
time = 90;
pk = FindPeaks[data / time - bgdata / bgtime, 10, 10^-85, 8]
```

Out[175]= $\left\{\left\{19, \frac{302507}{600}\right\}, \left\{90, \frac{14881}{900}\right\}, \left\{196, \frac{138641}{1800}\right\}\right\}$

In[176]:=

```
ListLogPlot[data / time - bgdata / bgtime, ImageSize → Full]
```

Out[176]=



In[72]:=

```
200 / 353 * 662 // N
```

Out[72]= 375.071

2. Make a properly formatted table in Mathematica listing the source, the emission energy, and the peak position determined from step one.

In[79]:=

```
td = {
   {"Ba-133", 384, 196},
   {"Cd-109", 88.04, 14},
   {"Co-60", 1173, 617},
   {"Co-60", 1332, 693},
   {"Cs-137", 661.7, 353}
  };
```

In[80]:=
```
TableForm[td, TableHeadings → {None, {"Isotope", "Eγ (keV)", "Peak Channel"}}]
```

Out[80]//TableForm=

Isotope	E_γ (keV)	Peak Channel
Ba-133	384	196
Cd-109	88.04	14
Co-60	1173	617
Co-60	1332	693
Cs-137	661.7	353

3. From the data within the table, conduct a first order polynomial fit on the data to find the voltage to energy conversion.

In[94]:=
```
peakfitdata = td[[ ;; , 2 ;; 3]]
firstorder = LinearModelFit[peakfitdata, {1, x}, x]
```

Out[94]= {{384, 196}, {88.04, 14}, {1173, 617}, {1332, 693}, {661.7, 353}}

Out[95]= FittedModel[$-20.0162+0.542243\,x$]

4. Now try a second order polynomial.

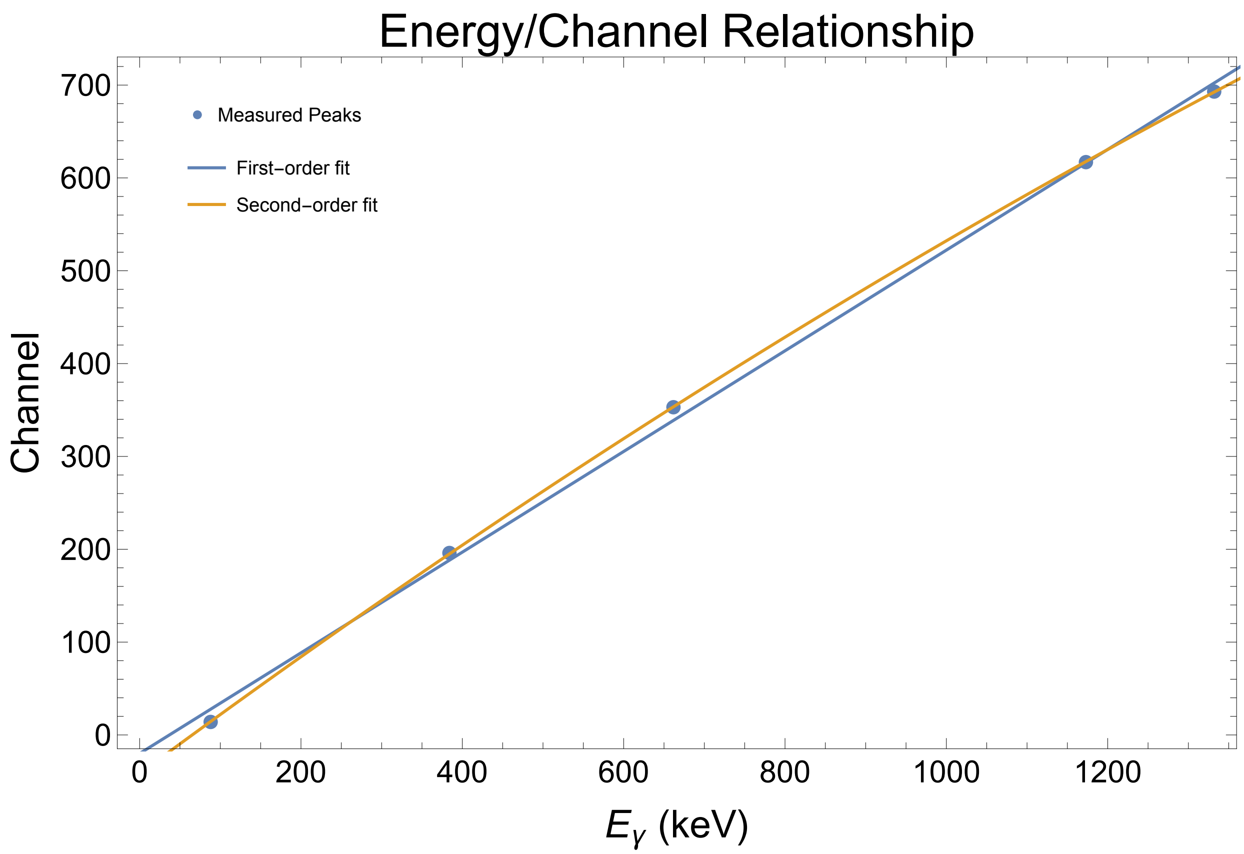
In[83]:=
```
secondorder = LinearModelFit[peakfitdata, {1, x, x^2}, x]
```

Out[83]= FittedModel[$-41.5701+0.642314\,x-0.0000684871\,x^2$]

5. Plot the data (channel number vs. energy) along with the first and second order polynomial fits on the same, properly formatted, plot.

In[111]:=
```
lp = ListPlot[peakfitdata, ImageSize → Full, Frame → True,
   FrameLabel → {Style["Eγ (keV)", 20], Style["Channel", 20]},
   PlotLabel → Style["Energy/Channel Relationship", 24], PlotLegends →
    Placed[{"Measured Peaks"}, {0.15, 0.85}], FrameTicksStyle → Directive[16]];
fp = Plot[{firstorder[x], secondorder[x]}, {x, 0, 1400},
   PlotLegends → Placed[{"First-order fit", "Second-order fit"}, {0.15, 0.85}]];
Show[
 lp,
 fp]
```

Out[113]=



6. In a text-style cell, discuss whether the first order or second order polynomial fit better describes the data and why. Further discuss how non-proportional the NaI(Tl) detector is.

In[115]:=
```
firstorder["RSquared"]
```

Out[115]= 0.998333

In[116]:=
```
secondorder["RSquared"]
```

Out[116]=
```
0.999993
```

It is visually apparent that the second order polynomial is a better fit for the data than the first order polynomial. This is to be expected as first-order fits are a subset of second-order fits. Some nonlinearity is expected, and this is compounded by the inaccuracy of the detector. That said, the first order fit is still very good, indicating that the response of this detector is still essentially linear.

7. Using the best fit to the data, convert the spectrum from counts vs. channel number to counts vs. energy for the Cs-137 spectrum.

In[130]:=
```
file = "cs137part1-15.Spe";
data = loaddata[file];
time = 90;
chtoe = LinearModelFit[
  Multicolumn[Join[peakfitdata[[ ;; , 2]], peakfitdata[[ ;; , 1]]], 2] // First,
  {1, x, x^2}, x]
```

Out[133]= FittedModel[$66.4153 + 1.54\,x + 0.000412287\,x^2$]

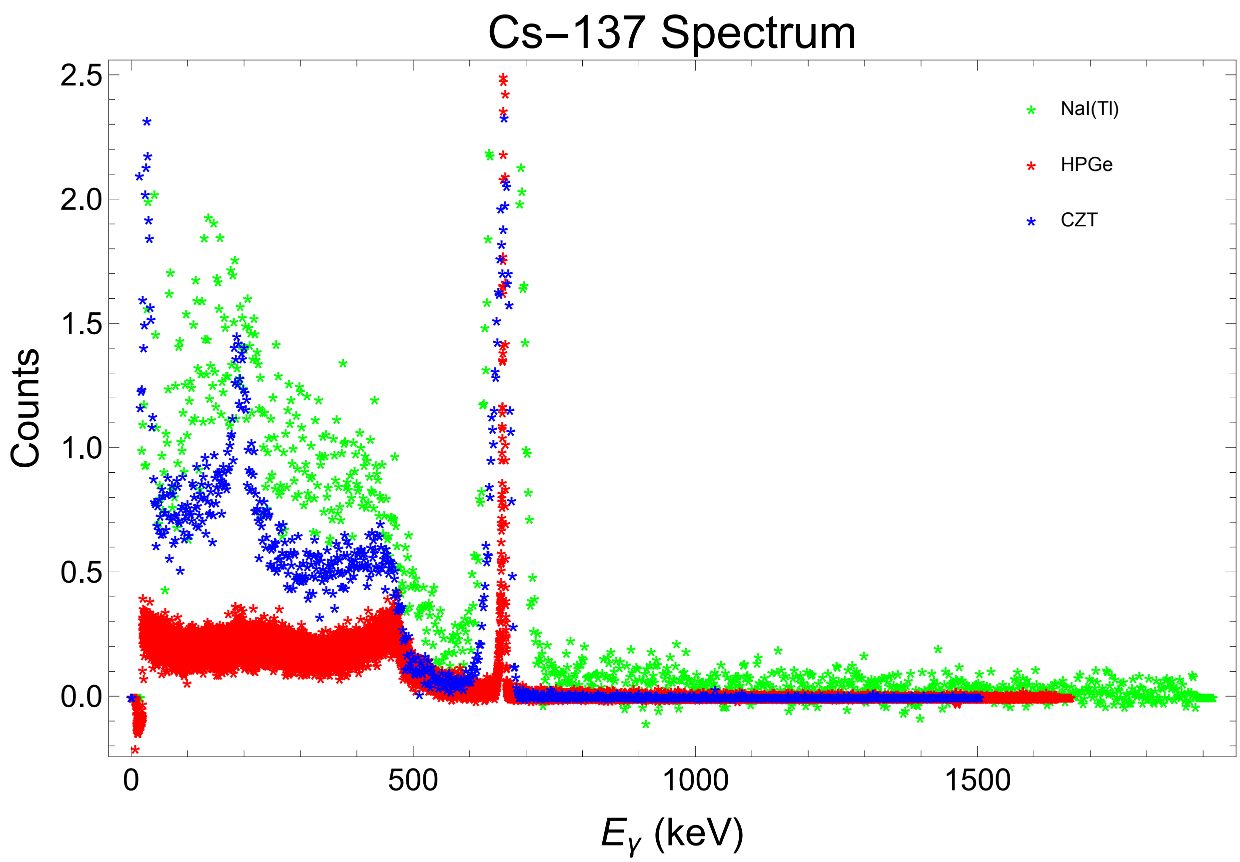
In[135]:=
```
energies = Table[chtoe[x], {x, Length[data]}];
```

8. Plot the Cs-137 energy spectrum against the HPGe and CZT Cs-137 energy spectra.

In[457]:=
```
naiplotdata =
  Multicolumn[Join[plotpairs["cs137part1-15.Spe", "Background2.Spe"][[ ;; , 1]] *
      662 / (10 / 2^10 * 353),
     plotpairs["cs137part1-15.Spe", "Background2.Spe"][[ ;; , 2]]], 2] // First;
naiplot = ListPlot[naiplotdata, Frame → True, FrameLabel →
    {Style["Eγ (keV)", 20], Style["Counts", 20]}, FrameTicksStyle → Directive[16],
   ImageSize → Full, PlotLabel → Style["Cs-137 Spectrum", 24],
   PlotStyle → Green, PlotLegends → Placed[{"NaI(Tl)"}, {0.85, 0.85}],
   PlotMarkers → Style["*", Medium]];
hpgeplot = ListPlot[Multicolumn[Join[plotpairs["Cs137.Spe", "bkg.Spe"][[ ;; , 1]] *
       662 / (10 / 2^14 * 6510), plotpairs["Cs137.Spe", "bkg.Spe"][[ ;; , 2]]], 2] //
    First, PlotStyle → Red, PlotLegends → Placed[{"HPGe"}, {0.85, 0.85}],
   PlotMarkers → Style["*", Medium]];
numchannels["Cs_137_120sec.Spe"]
cztplot = ListPlot[Multicolumn[
     Join[plotpairs["Cs_137_120sec.Spe", "Background_600sec.Spe"][[ ;; , 1]] *
       662 / (10 / 2^10 * 450), plotpairs["Cs_137_120sec.Spe",
        "Background_600sec.Spe"][[ ;; , 2]]], 2] // First,
   PlotStyle → Blue, PlotLegends → Placed[{"CZT"}, {0.85, 0.85}],
   PlotMarkers → Style["*", Medium]];
Show[naiplot, hpgeplot, cztplot]
```

Out[460]=
```
1023
```

Out[462]=



As expected, the HPGe

9. Below the plot, and in a text-style cell, discuss what you see on the plot in step 8. Describe the shape of each spectra and the resolution of each.

Here's what I see: the HPGe detector has the best resolution available, and its spectrum features narrow peaks at the energies corresponding to the Cesium spectrum--most notably 662 keV. Coming next in the lineup is another semiconductor detector--CZT, or cadmium zinc telluride. The CZT has a larger band gap (1.2-2.2 eV) than the HPGe crystals, meaning that its resolution is lower. This causes the peaks to undergo a gaussian broadening--making them harder to match to a specific energy and potentially overlapping nearby spectral peaks. Finally, the NaI(Tl) curve shown above has the worst resolution of the three. Distinguishing between even well-separated peaks (e.g. Co-60) becomes more difficult, or (in the case of Ba-133) impossible (see plot above). NaI(Tl) detectors do have the advantage of size, however--they can be grown very large, increasing their intrinsic efficiency.

The Need for a Preamplifier

1. For each spectrum collected with and without the preamplifier in the pulse processing chain, determined

the full energy peak position in channel number units.

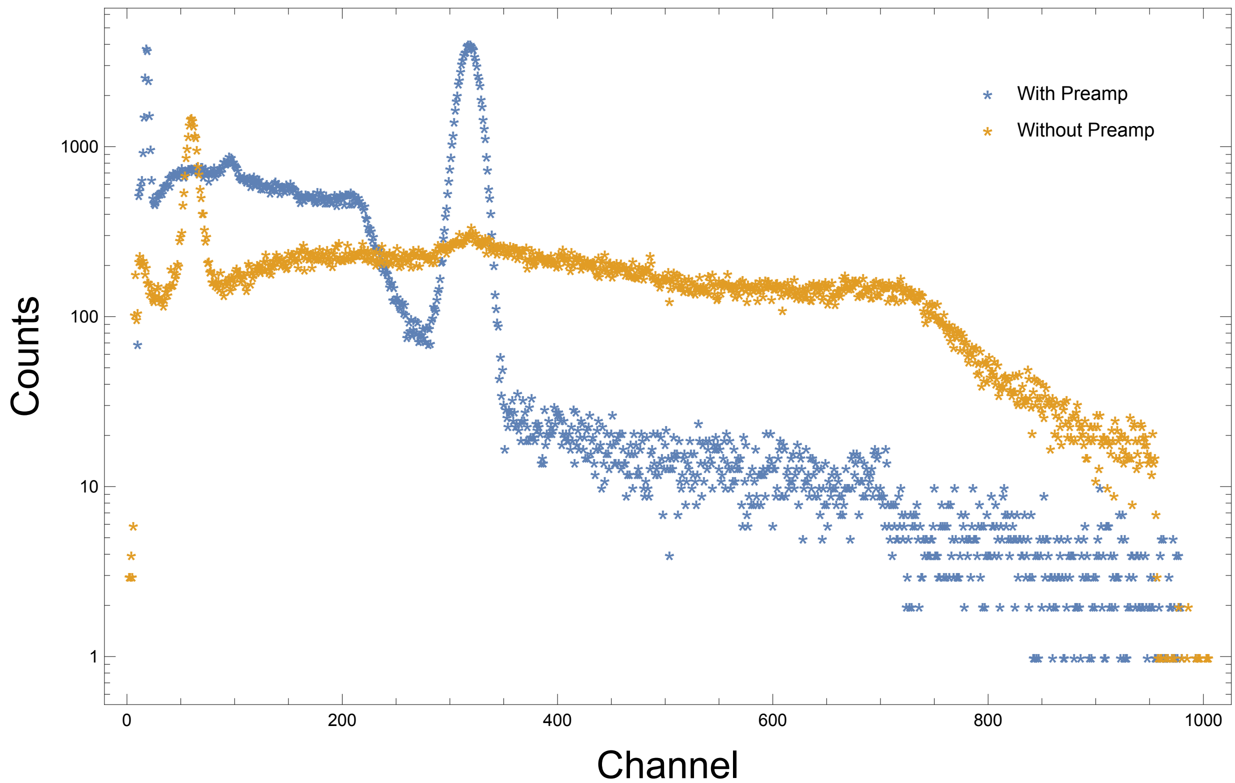
a. **Note:** The peak may drift away for larger shaping time constants, and may even disappear. If this happens, label it as “Not Present”.

In[192]:=
```
filenames = {
   "Amp05.Spe",
"Amp1.Spe",
"Amp10.Spe",
"Amp2.Spe",
"Amp3.Spe",
"Amp6.Spe",
"PreAmp-05.Spe",
"PreAmp-1.Spe",
"PreAmp-10.Spe",
"PreAmp-2.Spe",
"PreAmp-3.Spe",
"PreAmp-6.Spe"
  };
```

Shaping time = 0.5μs

In[246]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-05.Spe", "Amp05.Spe"}], ImageSize → Full,
 PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
 PlotMarkers → Style["*", Medium], Frame → True,
 FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[246]=



In[212]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-05.Spe", "Amp05.Spe"}}]
```

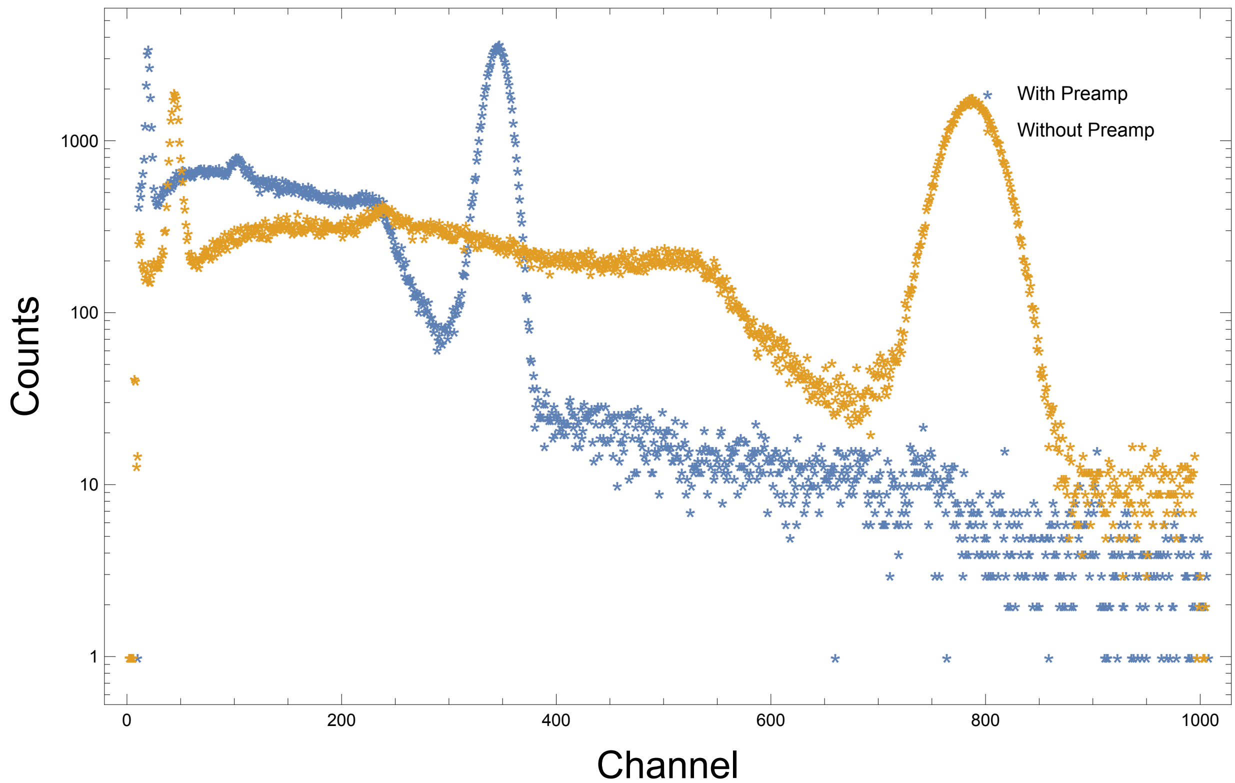
Out[212]= {{{18, 3854}, {319, 4076}}, {{60, 1506}}}

The peak for the preamp is at channel 319; for the Amp there is no obvious peak on scale.

Shaping time = 1 μs

In[247]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-1.Spe", "Amp1.Spe"}], ImageSize → Full,
  PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
  PlotMarkers → Style["*", Medium], Frame → True,
  FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[247]=



In[218]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-1.Spe", "Amp1.Spe"}}]
```

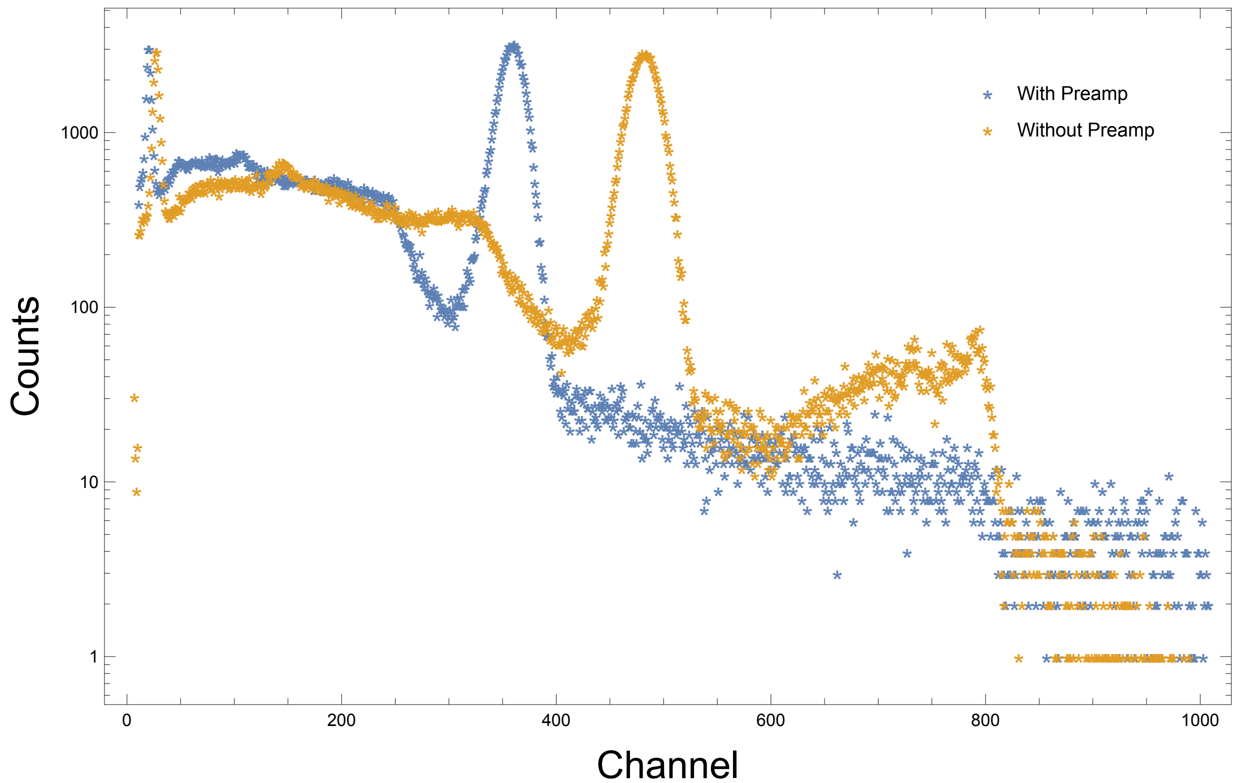
Out[218]=
```
{{{20, 3472}, {347, 3706}}, {{44, 1937}, {788, 1810}}}
```

The peak for the preamp is at channel 347; for the Amp it is at 788.

Shaping time = 2μs

In[248]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-2.Spe", "Amp2.Spe"}], ImageSize → Full,
 PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
 PlotMarkers → Style["*", Medium], Frame → True,
 FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[248]=



In[220]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-2.Spe", "Amp2.Spe"}}]
```

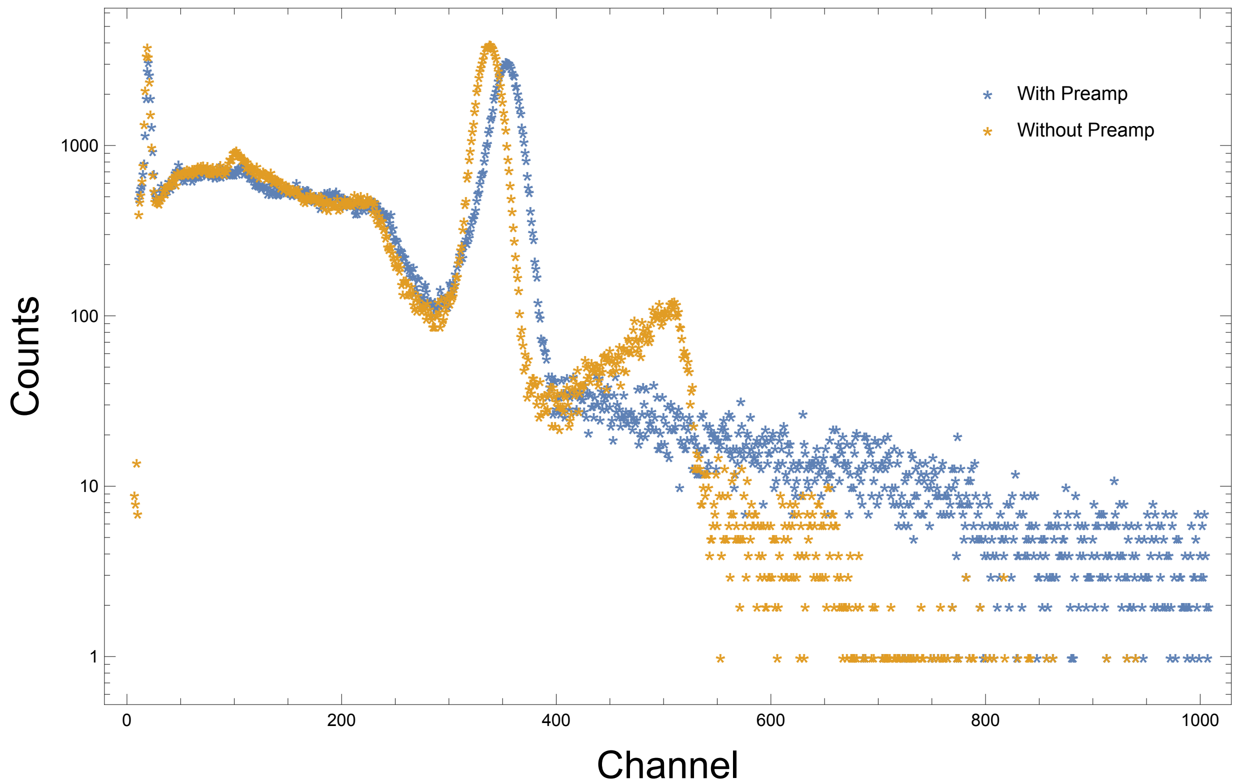
Out[220]=
```
{{{20, 3057}, {361, 3258}}, {{28, 2952}, {484, 2874}}}
```

The peak for the preamp is at channel 361; for the Amp it is at 484.

Shaping time = 3μs

In[249]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-3.Spe", "Amp3.Spe"}], ImageSize → Full,
 PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
 PlotMarkers → Style["*", Medium], Frame → True,
 FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[249]=



In[221]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-3.Spe", "Amp3.Spe"}}]
```

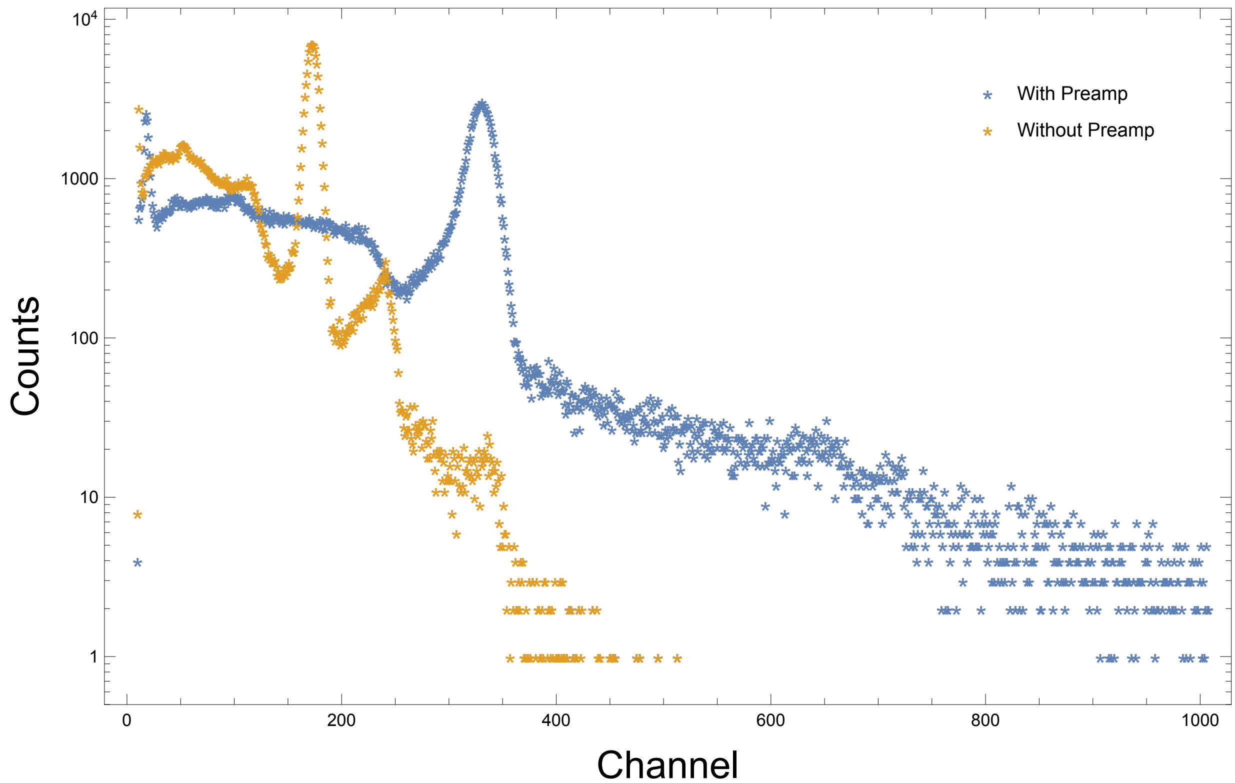
Out[221]= {{{20, 3138}, {353, 3149}}, {{19, 3846}, {338, 3999}}}

The peak for the preamp is at channel 353; for the Amp it is at 338.

Shaping time = 6μs

In[250]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-6.Spe", "Amp6.Spe"}], ImageSize → Full,
 PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
 PlotMarkers → Style["*", Medium], Frame → True,
 FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[250]=



In[224]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-6.Spe", "Amp6.Spe"}}]
```

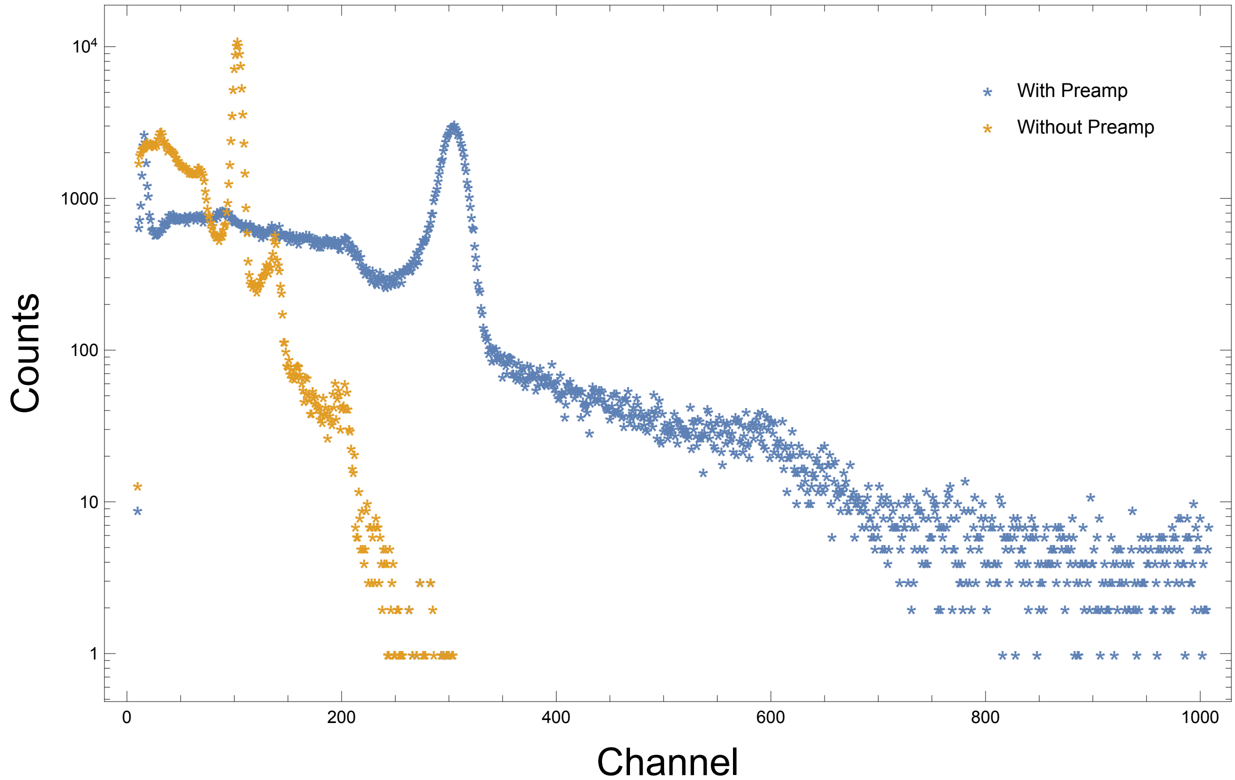
Out[224]= {{{18, 2603}, {331, 3071}}, {{53, 1679}, {172, 7106}}}

The peak for the preamp is at channel 331; for the Amp it is at 172.

Shaping time = 10μs

In[251]:=
```
ListLogPlot[Map[loaddata, {"PreAmp-10.Spe", "Amp10.Spe"}], ImageSize → Full,
 PlotLegends → Placed[{"With Preamp", "Without Preamp"}, {0.85, 0.85}],
 PlotMarkers → Style["*", Medium], Frame → True,
 FrameLabel → {Style["Channel", 20], Style["Counts", 20]}]
```

Out[251]=



In[226]:=
```
Table[FindPeaks[loaddata[f], 10, 10^-5, 1500], {f, {"PreAmp-10.Spe", "Amp10.Spe"}}]
```

Out[226]=
```
{{{16, 2696}, {305, 3131}}, {{32, 2827}, {103, 11078}}}
```

The peak for the preamp is at channel 305; for the Amp it is at 103.

2. Make a properly formatted table in Mathematica that includes the shaping time, peak position with preamp, and peak position without preamp.

In[233]:=
```
headers = {"Shaping Time (μs)", "Preamp Peak Channel", "Amp Peak Channel"};
td = {
   {0.5, 319, "NA"},
   {1, 347, 788},
   {2, 361, 484},
   {3, 353, 338},
   {6, 331, 172},
   {10, 305, 103}
  };
TableForm[td, TableHeadings → {None, headers}]
```

Out[235]//TableForm=

Shaping Time (μs)	Preamp Peak Channel	Amp Peak Channel
0.5	319	NA
1	347	788
2	361	484
3	353	338
6	331	172
10	305	103

3. Investigating the data contained within the table, discuss the trends observed with and without the preamplifier present in a text-style cell. Theorize the origin of the differences between the two datasets, [sic] and further comment on why the use of a preamplifier is necessary.

The detectors we use do not integrate voltage; instead they collect charge. The preamplifier's role is to convert these current pulses into a voltage, but this voltage takes the form of a slowly decaying, quasi-square wave pulse. The amplifier then takes this voltage and converts it into a quasi-gaussian pulse with amplitude equal to the charge collected in the detector by acting as a crude differentiator.

Without the preamplifier, changing the shaping time of the amplifier causes it to collect charge over a different period of time. If that time is shorter, then a smaller voltage builds up in the output signal, which the MCA sees as a lower energy channel. With the preamplifier in line, this effect does not occur. We see this happening

Integral Pulse Height Spectrum

1. Make a 2D list of data of LLD (x-value) and counts (y-value).

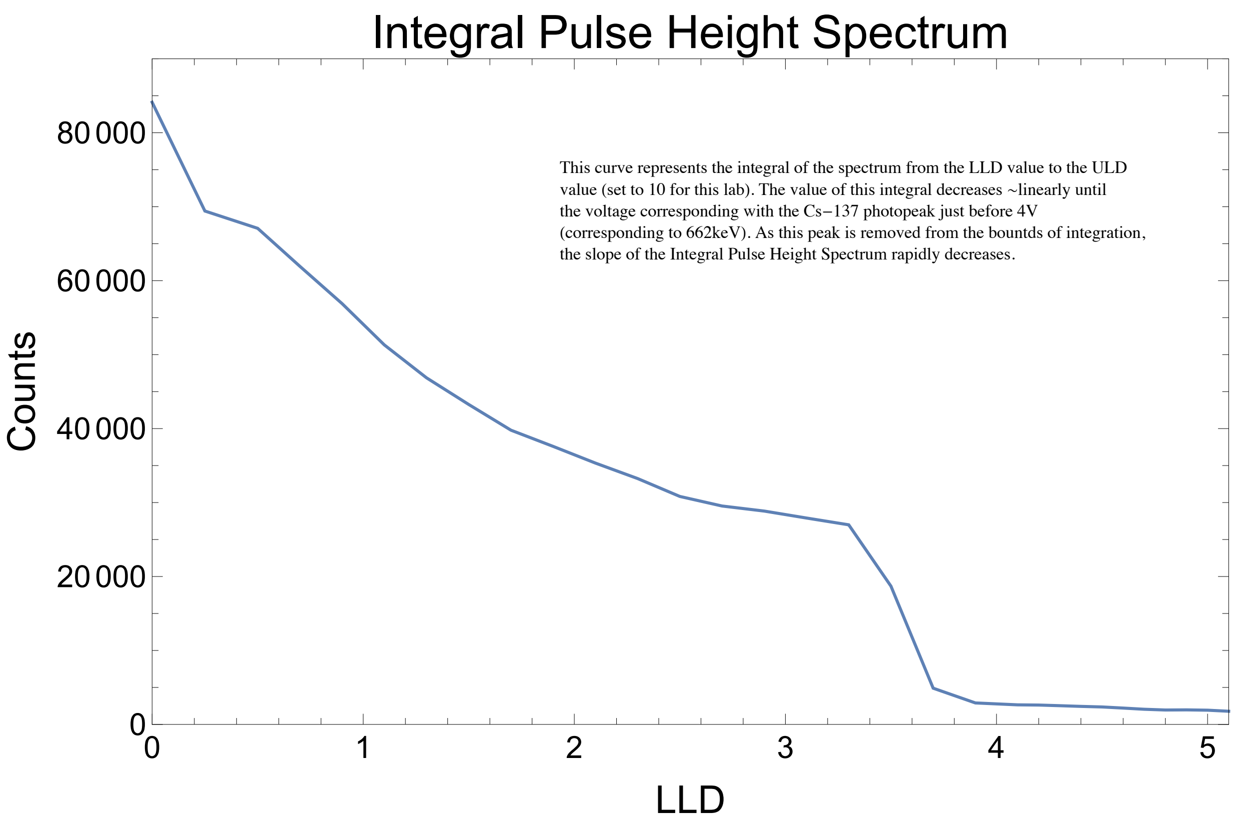
In[471]:=
```
iphsdata =
  Multicolumn[Join[{0, 0.25, 0.50, 0.7, 0.9, 1.1, 1.3, 1.5, 1.7, 1.9, 2.1, 2.3, 2.5,
      2.7, 2.9, 3.1, 3.3, 3.5, 3.7, 3.9, 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8, 4.9,
      5.0, 5.1}, {84 125, 69 417, 67 078, 61 940, 56 896, 51 316, 46 862, 43 257, 39 783,
      37 589, 35 336, 33 244, 30 825, 29 532, 28 846, 27 907, 26 990, 18 696, 4899, 2905,
      2648, 2619, 2532, 2439, 2361, 2211, 2051, 1951, 1967, 1924, 1782}], 2] // First;
```

2. Change the collected Cs-137 spectra in the first part of the lab from counts vs. channel number to counts vs. voltage.

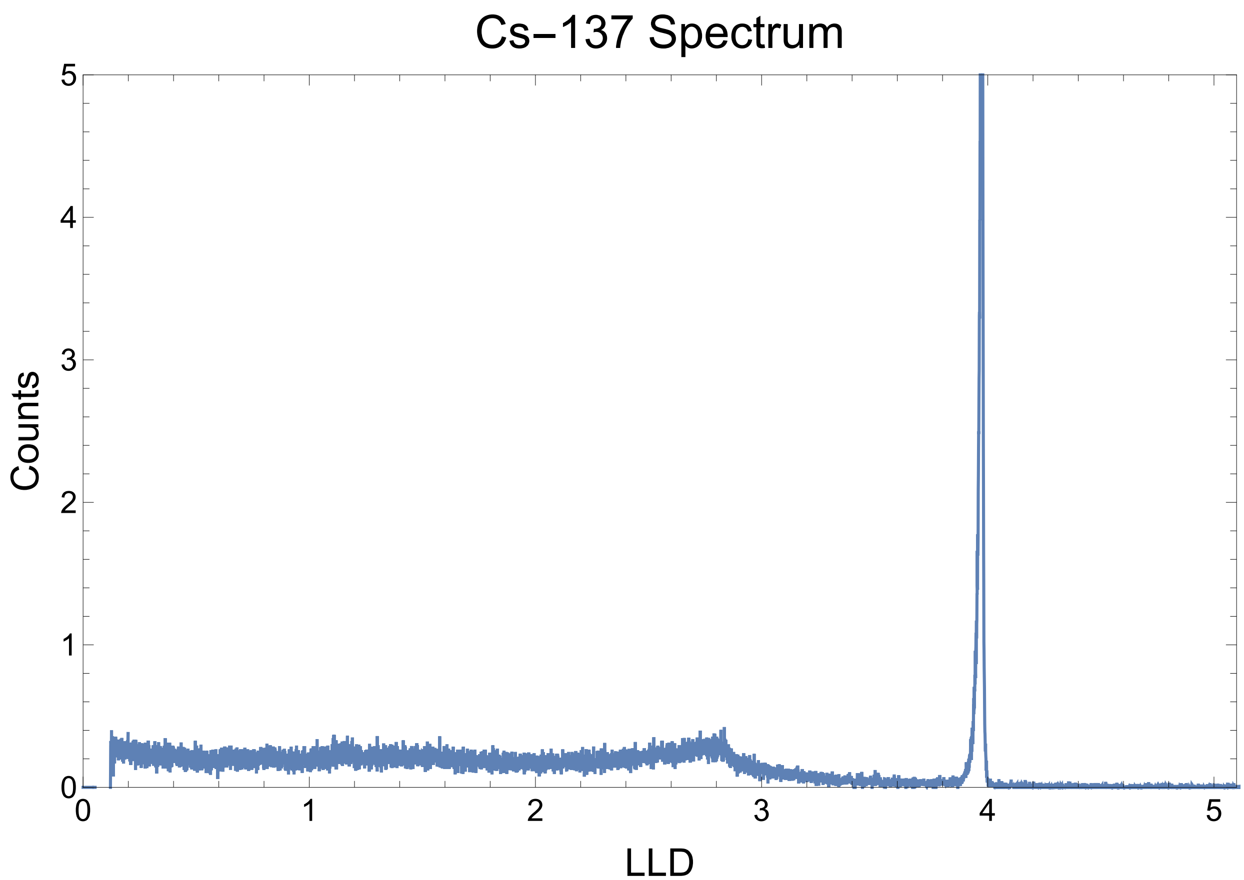
3. Plot the 2D list of data, which is a crude integral pulse height spectrum, against the quality differential pulse height spectrum.

a. You may try and connect the dots between data points using the “Interpolation” option in Mathematica for graphing purposes so it is easier to compare the two spectra.

In[507]:=
```
ihpsplot = ListPlot[iphsdata, Joined → True,
  Frame → True, FrameLabel → {Style["LLD", 20], Style["Counts", 20]},
  FrameTicksStyle → Directive[16],
  PlotLabel → Style["Integral Pulse Height Spectrum", 24],
  ImageSize → Full, PlotRange → {{0, 5.1}, {0, 90 000}}]
cs137plot = ListPlot[plotpairs["Cs137.Spe", "bkg.Spe"], Joined → True,
  Frame → True, FrameLabel → {Style["LLD", 20], Style["Counts", 20]},
  FrameTicksStyle → Directive[16], PlotLabel → Style["Cs-137 Spectrum", 24],
  ImageSize → Full, PlotRange → {{0, 5.1}, {0, 5}}]
```


Integral Pulse Height Spectrum
Counts
LLD
0
20 000
40 000
60 000
80 000
0
1
2
3
4
5
This curve represents the integral of the spectrum from the LLD value to the ULD value (set to 10 for this lab). The value of this integral decreases ~linearly until the voltage corresponding with the Cs−137 photopeak just before 4V (corresponding to 662keV). As this peak is removed from the bountds of integration, the slope of the Integral Pulse Height Spectrum rapidly decreases.

Out[508]=



4. Using the drawing tools, correlate the shape of each spectra with each other.