The Mössbauer Effect - Experiment 28

In[1]:=
```
<< CurveFit`
```

CurveFit for Mathematica v7.x thru v10.x, Version 1.95, 1/2016

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In[2]:=
```
With[ {name = SystemDialogInput["FileOpen",
    {DataFileName, {"data files" -> {"*.dat", "*.mca"}, "all files" -> {"*"}}}]},
 If[ name =!= $Canceled,
  LoadFile[name]]
]
```

/home/yovan/Documents/Coursework/2_Smore_Year/2_Winter_2018/Ph6/Lab 6/Mossbauer_BadalYovan_2_20_2018.dat

Read 51 data points.

Lorentzian Fit

In[3]:=
```
LorentzianCFit[]
```

n = 51

$$y(\omega) = c \pm y_{max} \frac{\left(\frac{\gamma}{2}\right)^2}{(\omega - \omega_0)^2 + \left(\frac{\gamma}{2}\right)^2}$$

Fit of (x,y) (unweighted)

y_{max}= -53.2892	c= 208.59	
$\sigma_{y_{max}}$= 1.00673	σ_c= 0.721269	
ω_0= -0.20529	γ= 0.48465	
σ_{ω_0}= 0.00403277	σ_γ= 0.0171077	Std. deviation= 2.13998

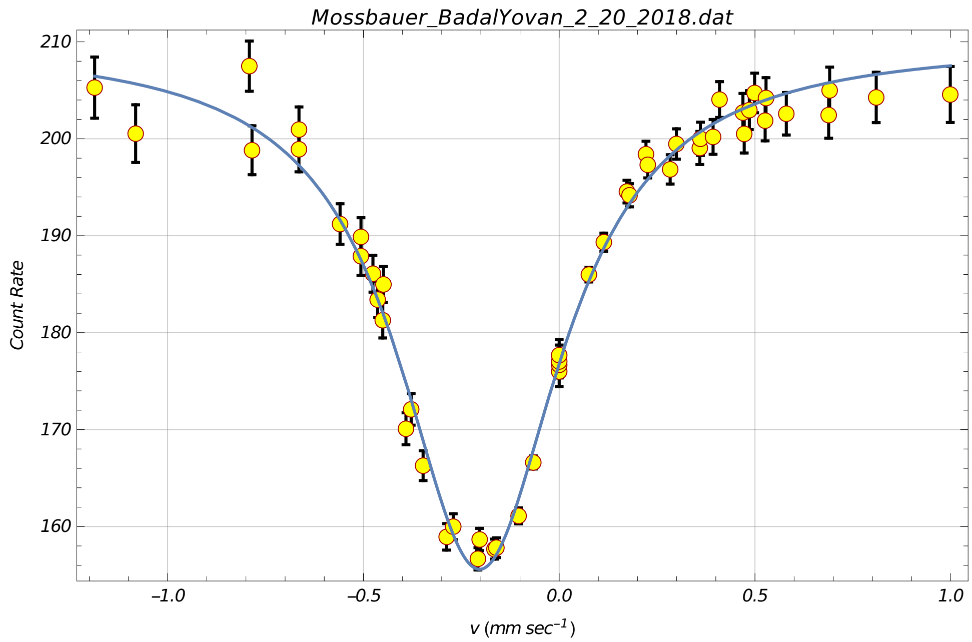
Fit of $(x, y \pm \sigma_y)$

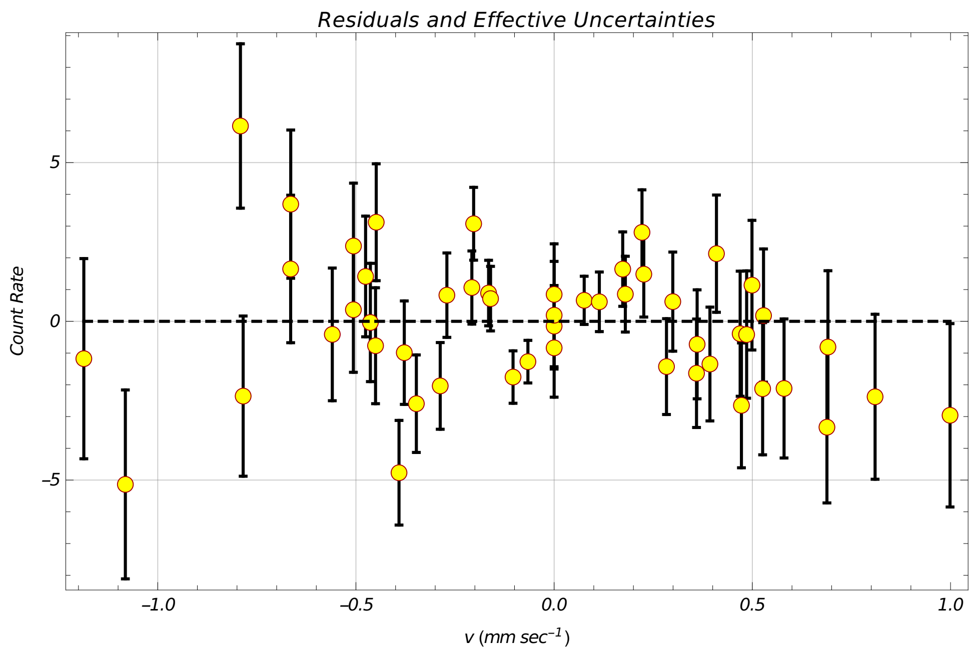
y_{max}= -54.2411	c= 209.833	
$\sigma_{y_{max}}$= 0.729878	σ_c= 0.692182	
ω_0= -0.203285	γ= 0.506767	
σ_{ω_0}= 0.00257381	σ_γ= 0.0124181	$\chi^2/(n-4)$ = 1.51873

In[4]:=

```
LinearDifferencePlot[FrameLabel → {"v (mm sec⁻¹)", "Count Rate"}]
```

Out[4]=





$$y(\omega) = c \pm y_{max} \frac{\left(\frac{\gamma}{2}\right)^2}{(\omega-\omega_0)^2+\left(\frac{\gamma}{2}\right)^2}$$

y_{max} = -54.2411	c = 209.833	
$\sigma_{y_{max}}$ = 0.729878	σ_c = 0.692182	
ω_0 = -0.203285	γ = 0.506767	
σ_{ω_0} = 0.00257381	σ_γ = 0.0124181	$\chi^2/(n-4)$ = 1.51873

We observe that the data fits a Lorentzian distribution reasonably well ($\tilde{\chi}^2$ of 1.52), although it seems to have higher than expected residuals around the wings of the distribution.

At the center of the line, we observe a count rate decrease of ~26 % (the Lorentzian fit gives a differential peak of -54.2 and we graphically observe a baseline of ~205). We observe a relative isomeric shift of -0.203±0.003 mm sec^{-1}. Therefore in accordance with our pre-lab calculations, it is more likely that the emitter is embedded in Rh (theoretical relative isomeric shift of -0.199mm sec^{-1}) than in Pd (theoretical relative isomeric shift of -0.186 mm sec^{-1}.)

According to our pre-lab calculations, we expect a FWHM of 0.193 mm sec^{-1} for the Lorentzian. Instead, we observe the very different FWHM value of 0.507 mm sec^{-1}. This indicates that the absorption line may not be best described by a Lorentzian despite the good $\tilde{\chi}^2$. One possible cause for this may be the alloying in the stainless steel, causing significant deviations from the perfect crystal structure assumptions under which our theoretical expectation was derived. Now, we expect those deviations to be independent and random throughout the crystal, which could impart a Gaussian structure to our absorption line data. Therefore, we now attempt to fit a Gaussian to our data.

Gaussian Fit

```
(* We transform the data so we can use a Gaussian fit with an offset. *)
```

In[5]:=
```
xnew[ x_, y_ ] := x
ynew[ x_, y_ ] := -y
DataTransform[]
(* Use Undo[] if you don't like the results. *)
```

```
All 51 points transformed.
```

In[8]:=
```
GaussianCFit[]
```

n = 51

y(x) =

$$y_{max}\ \exp\left(\frac{-(x-\mu)^2}{2\,\mathrm{sigma}^2}\right) + c$$

Fit of (x,y) (unweighted)

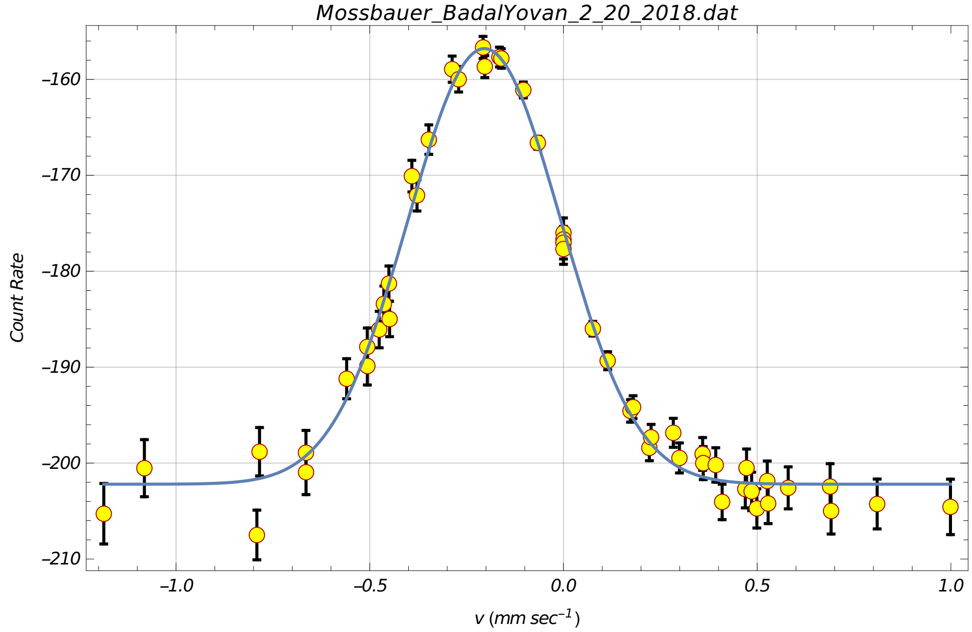
y_{max}= 45.7057	c= −202.699	
$\sigma_{y_{max}}$= 0.774196	σ_c= 0.436531	
μ= −0.204306	sigma= 0.198951	
σ_μ= 0.00334971	σ_{sigma}= 0.00446511	Std. deviation= 1.87357

Fit of $(x, y \pm \sigma_y)$

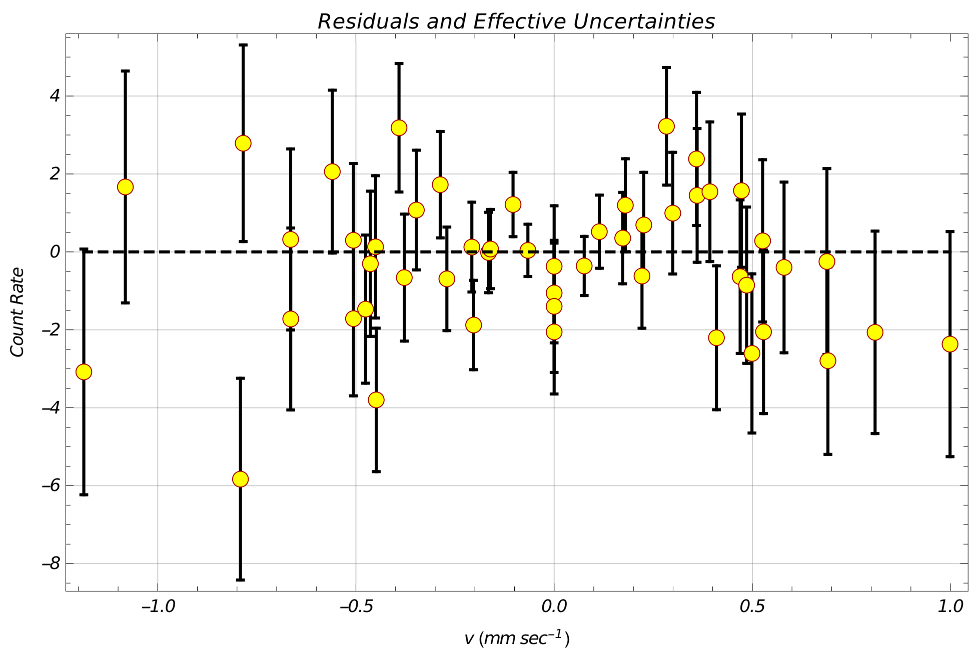
y_{max}= 45.4106	c= −202.199	
$\sigma_{y_{max}}$= 0.572426	σ_c= 0.47459	
μ= −0.204099	sigma= 0.197143	
σ_μ= 0.00249411	σ_{sigma}= 0.00351981	$\chi^2/(n-4)$= 1.00177

In[9]:=

```
LinearDifferencePlot[FrameLabel → {"v (mm sec^-1)", "Count Rate"}]
```



Out[9]=



$$y(x) = y_{max} \exp\left(\frac{-(x-\mu)^2}{2\,\mathrm{sigma}^2}\right) + c$$

y_{max} = 45.4106	c = -202.199	
$\sigma_{y_{max}}$ = 0.572426	σ_c = 0.47459	
μ = -0.204099	sigma = 0.197143	
σ_μ = 0.00249411	σ_{sigma} = 0.00351981	$\chi^2/(n-4)$ = 1.00177

We observe a better $\tilde{\chi}^2$ for the Gaussian fit (1.002) than for the Lorentzian fit! This indicates that the alloying does in fact impart a Gaussian structure to our absorption line data. Here we obtain a FWHM of 2.36σ = 0.465±0.007 mm sec^{-1}. This is still much greater than our theoretical expectation (as we would expect if additional uncertainty was added to the distribution via Gaussian-distributed deviations from the theoretical distribution), but still lower than the FWHM obtained using the Lorentzian fit.

Voigt Fit

In[10]:=
```
Undo[]
```

```
Mossbauer_BadalYovan_2_20_2018.dat
```

```
n = 51
```

In[21]:=
```
(* We define a scaling of the Voigt distribution
 with an offset and fit the PDF using FitAnyFunction.nb *)
```

In[22]:=
```
p[fwhm_, sig_, median_, x_, k_, c_] :=
 k * PDF[VoigtDistribution[fwhm / 2, sig], x - median] + c

FitData[
  (* The expression defining the function *) p[fwhm, sig, median, x, k, c],
 (* The symbol for the variable in the expression *) x,
 (* A list of the parameters in the function to fit *) {fwhm, sig , median , k, c},
 (* A list of starting values for the parameters *) {0.15, 0.1 , -0.2 , -30, 200}
]
```

n = 51

p = 5

$$f[x] = c + \frac{k\left(e^{\frac{\left(\frac{fwhm}{2} - i\,(-median+x)\right)^2}{2\,sig^2}}\,\text{Erfc}\left[\frac{\frac{fwhm}{2} - i\,(-median+x)}{\sqrt{2}\,sig}\right] + e^{\frac{\left(\frac{fwhm}{2} + i\,(-median+x)\right)^2}{2\,sig^2}}\,\text{Erfc}\left[\frac{\frac{fwhm}{2} + i\,(-median+x)}{\sqrt{2}\,sig}\right]\right)}{2\sqrt{2\pi}\,sig}$$

***Fit of* (*x*,*y*) (*unweighted*):**

fwhm	=	0.198558	±	0.0745072
sig	=	0.150831	±	0.0207717
median	=	−0.20488	±	0.00318979
k	=	−28.872	±	2.65881
c	=	204.837	±	0.979996

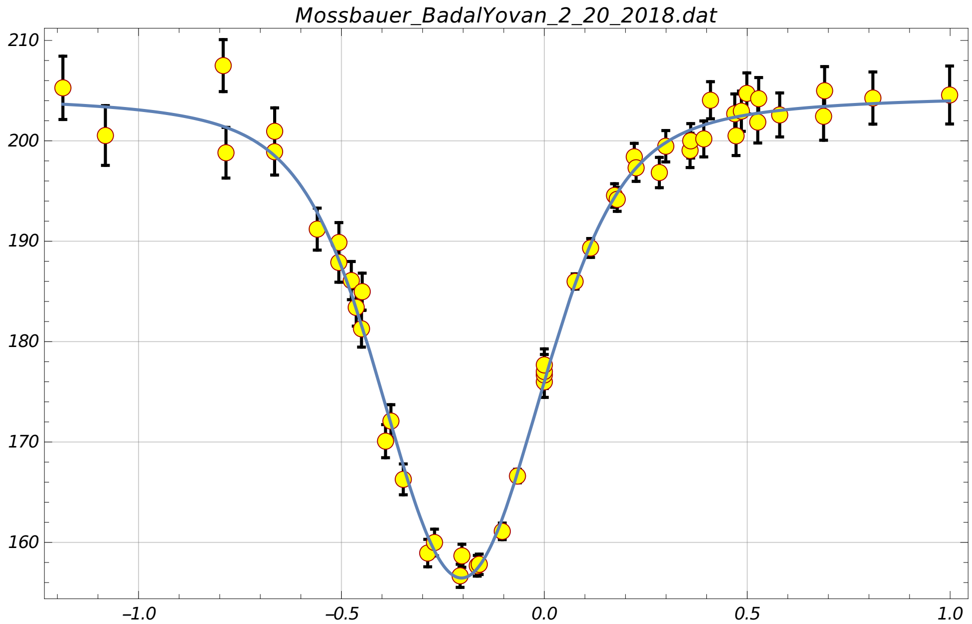
Std. Deviation = 1.77417

***Fit of* (x,$y \pm \sigma_y$):**

fwhm	=	0.188553	±	0.0789763
sig	=	0.154429	±	0.0203498
median	=	−0.204115	±	0.00250897
k	=	−28.564	±	2.96976
c	=	204.6	±	1.20602

$$\frac{\chi^2}{n-p} = 0.907407 + 0.\,i$$

{fwhm → 0.188553, sig → 0.154429, median → −0.204115, k → −28.564, c → 204.6}



We observe that the Voigtfit is by far the best fit we have for our data, with a FWHM of 0.189±0.007 mm sec^{-1} which is within error of the expected value for the FHWM. Therefore the data is most likely to be Voigt-distributed.

```
(* Note:
 I haven't been able to get CurveFit to plot the residuals for some reason,
it simply aborts when I send the command *)
```