

# Homework #2 – Numeric Computing

## Problem 1

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08/08/2025

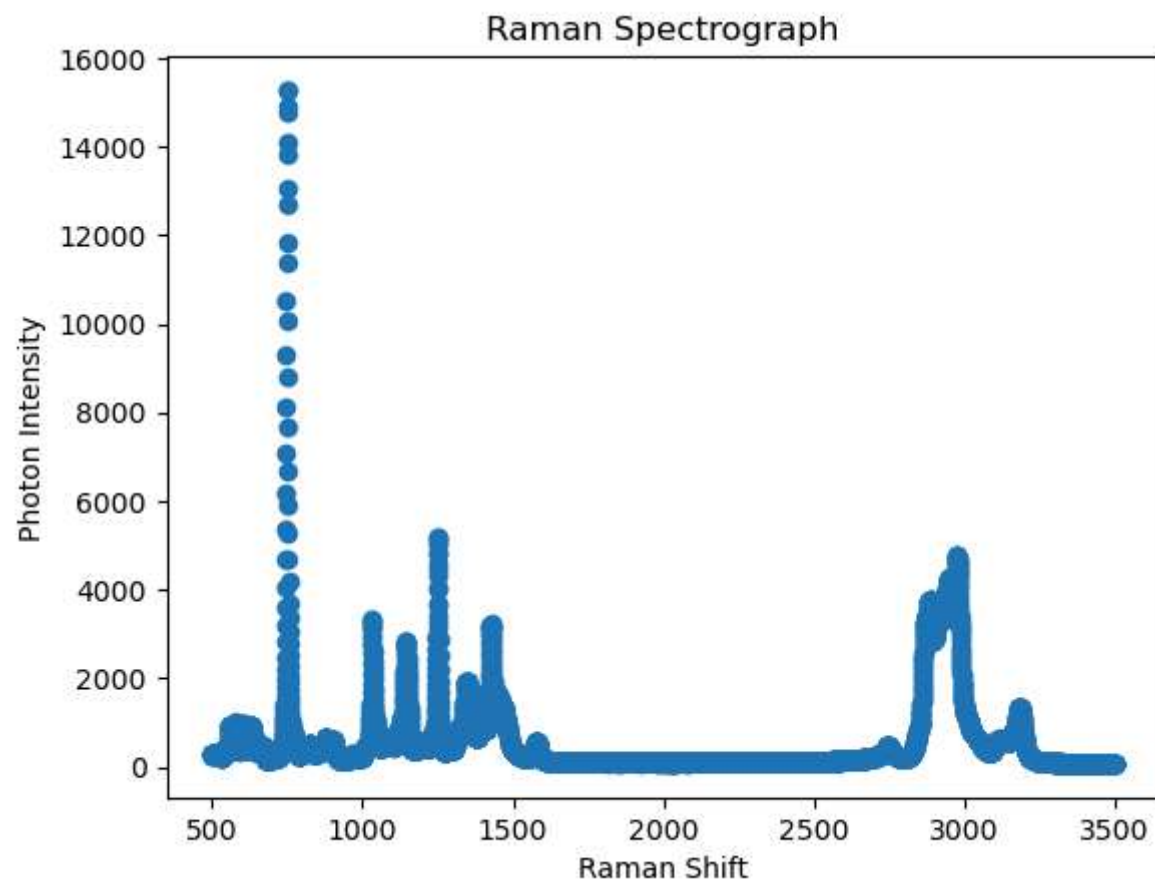
```
In [1]: # Imports
import numpy as np
import matplotlib.pyplot as plt
from scipy.signal import find_peaks
from scipy.interpolate import make_interp_spline
```

```
In [2]: # Constants
RAMAN_FILENAME = "../data/input/raman.txt"
CM_1 = "cm\u207B\u00B9"
```

```
In [3]: raman_data = np.loadtxt(RAMAN_FILENAME)
wavenumber = raman_data[:, 0]
intensity = raman_data[:, 1]

plt.figure()
plt.scatter(wavenumber, intensity)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
plt.figure()
```

```
Out[3]: <Figure size 640x480 with 0 Axes>
```



<Figure size 640x480 with 0 Axes>

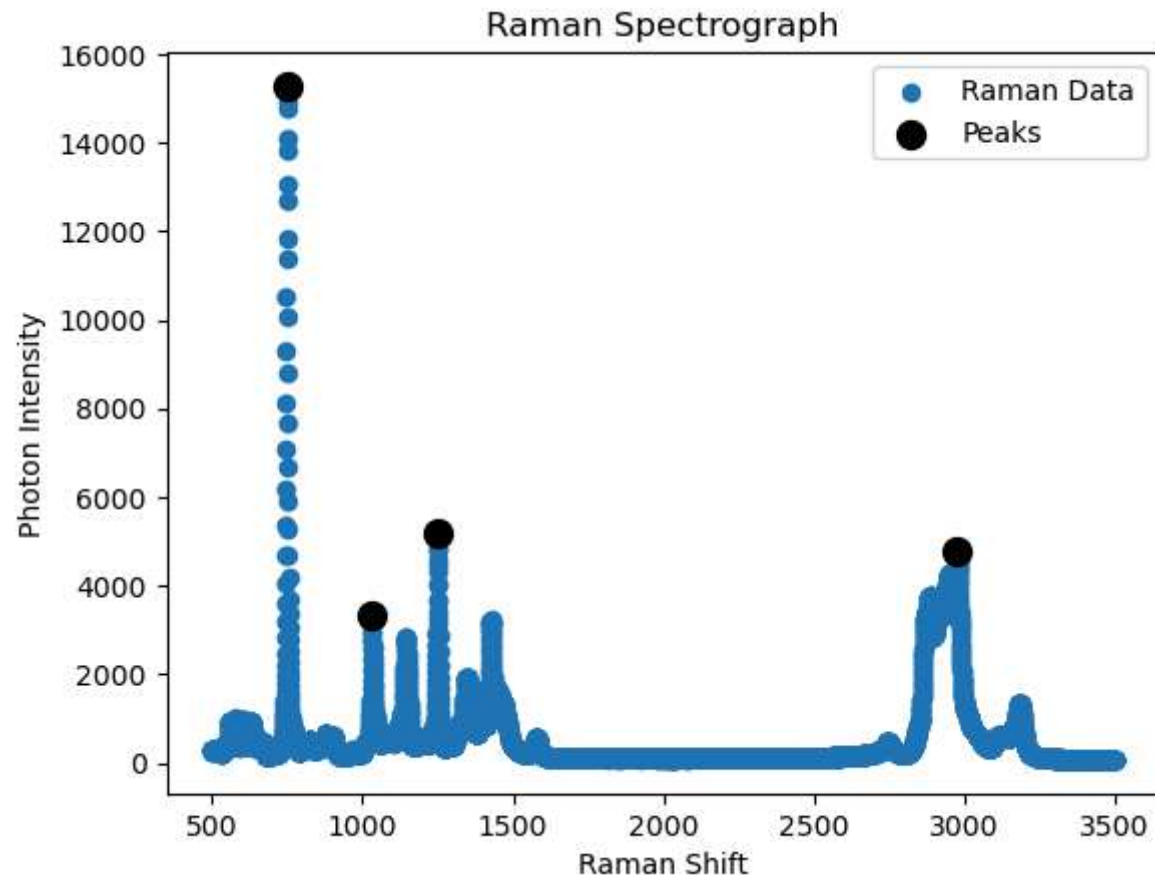
```
In [4]: min_height_of_peaks = 3000
horizontal_distance_bw_peaks = 500
peak_idx, _ = find_peaks(intensity, height=min_height_of_peaks, distance=horizontal_distance_bw_peaks)

wavenumber_peak = wavenumber[peak_idx]
intensity_peak = intensity[peak_idx]

plt.figure()
plt.scatter(wavenumber, intensity)
plt.scatter(wavenumber_peak, intensity_peak, c='k', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
```

```
plt.legend(["Raman Data", "Peaks"])
plt.savefig('raman_spectrograph.png', bbox_inches='tight')
plt.figure()
```

Out[4]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

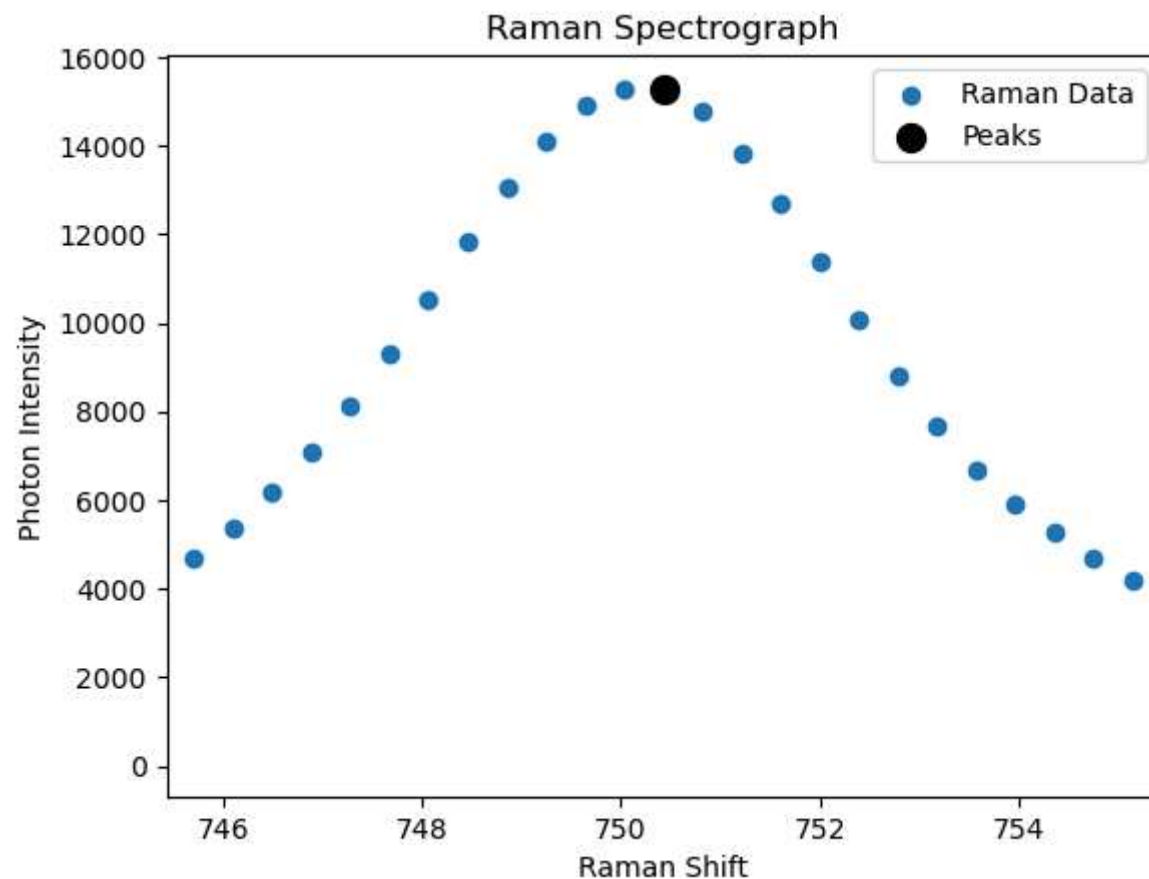
## Peak 1

```
In [5]: peak_1_idx = peak_idx[0]
n1 = 5

plt.figure()
```

```
plt.scatter(wavenumber, intensity)
plt.scatter(wavenumber[peak_1_idx], intensity[peak_1_idx], c='k', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
plt.legend(["Raman Data", "Peaks"])
plt.xlim(wavenumber[peak_1_idx] - n1, wavenumber[peak_1_idx] + n1)
plt.figure()
```

Out[5]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

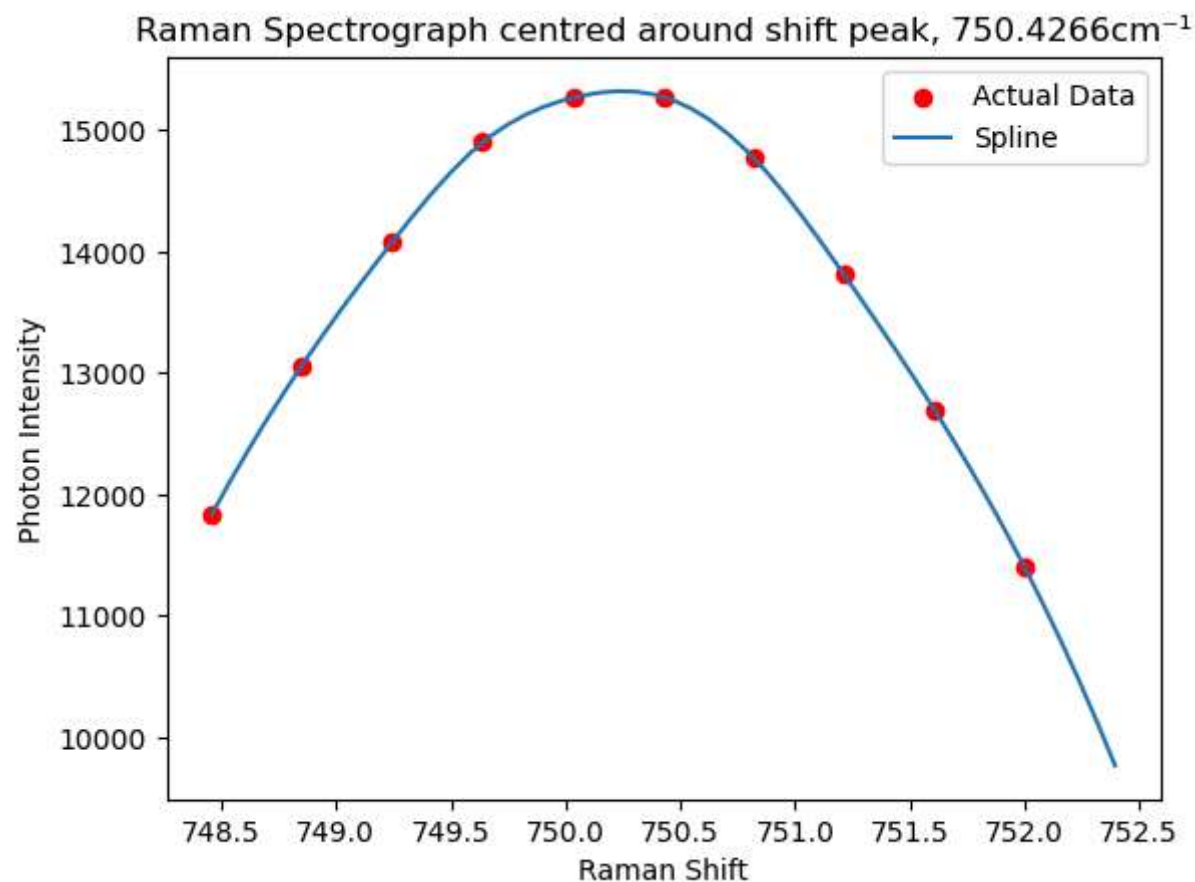
In [6]: `print(f"By experimentation, n1={n1} is a good width.")`

By experimentation, n1=5 is a good width.

```
In [7]: wavenumber_around_peak1 = wavenumber[peak_1_idx - n1 : peak_1_idx + n1]
intensity_around_peak1 = intensity[peak_1_idx - n1 : peak_1_idx + n1]
f_1 = make_interp_spline(wavenumber_around_peak1, intensity_around_peak1)

x_points = np.linspace(wavenumber[peak_1_idx - n1], wavenumber[peak_1_idx + n1], 50)

plt.figure()
plt.scatter(wavenumber_around_peak1, intensity_around_peak1, c='r')
plt.plot(x_points, f_1(x_points))
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_1_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline"])
plt.show()
```

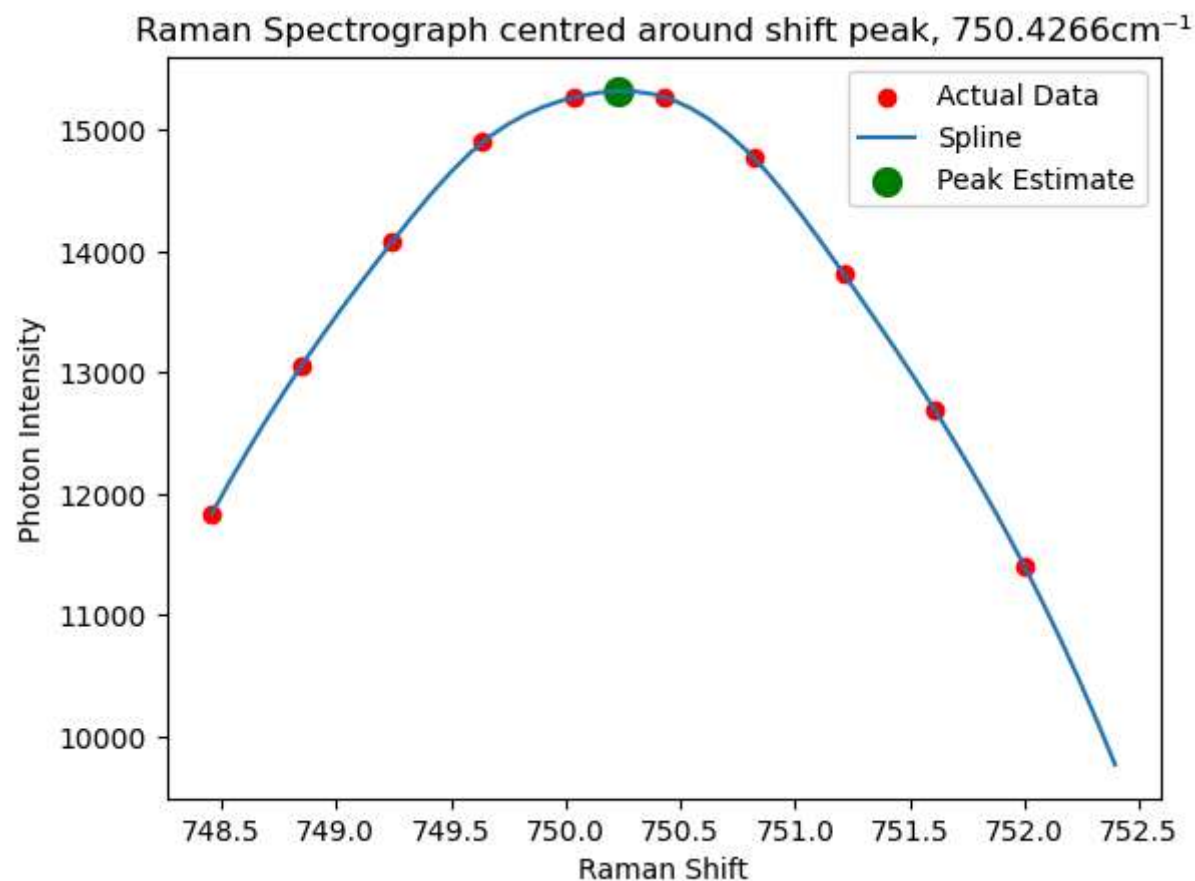


```
In [8]: dy_dx = np.gradient(f_1(x_points), x_points)
        zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

        wavenumber_peak1_estimate = x_points[zero_crossing][0]
        intensity_peak1_estimate = f_1(wavenumber_peak1_estimate)

        plt.figure()
        plt.scatter(wavenumber_around_peak1, intensity_around_peak1, c='r')
        plt.plot(x_points, f_1(x_points))
        plt.scatter(wavenumber_peak1_estimate, intensity_peak1_estimate, c='g', s=100)
        plt.xlabel("Raman Shift")
        plt.ylabel("Photon Intensity")
        plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_1_idx]:0.4f}{CM_1}")
        plt.legend(["Actual Data", "Spline", "Peak Estimate"])
```

```
plt.savefig('raman_spectrograph_peak1.png', bbox_inches='tight')  
plt.show()
```



```
In [9]: print(f"Estimated Spectral Peak 1 is of Intensity={intensity_peak1_estimate:0.4f} at Raman Shift={wavenumber_peak1_es
```

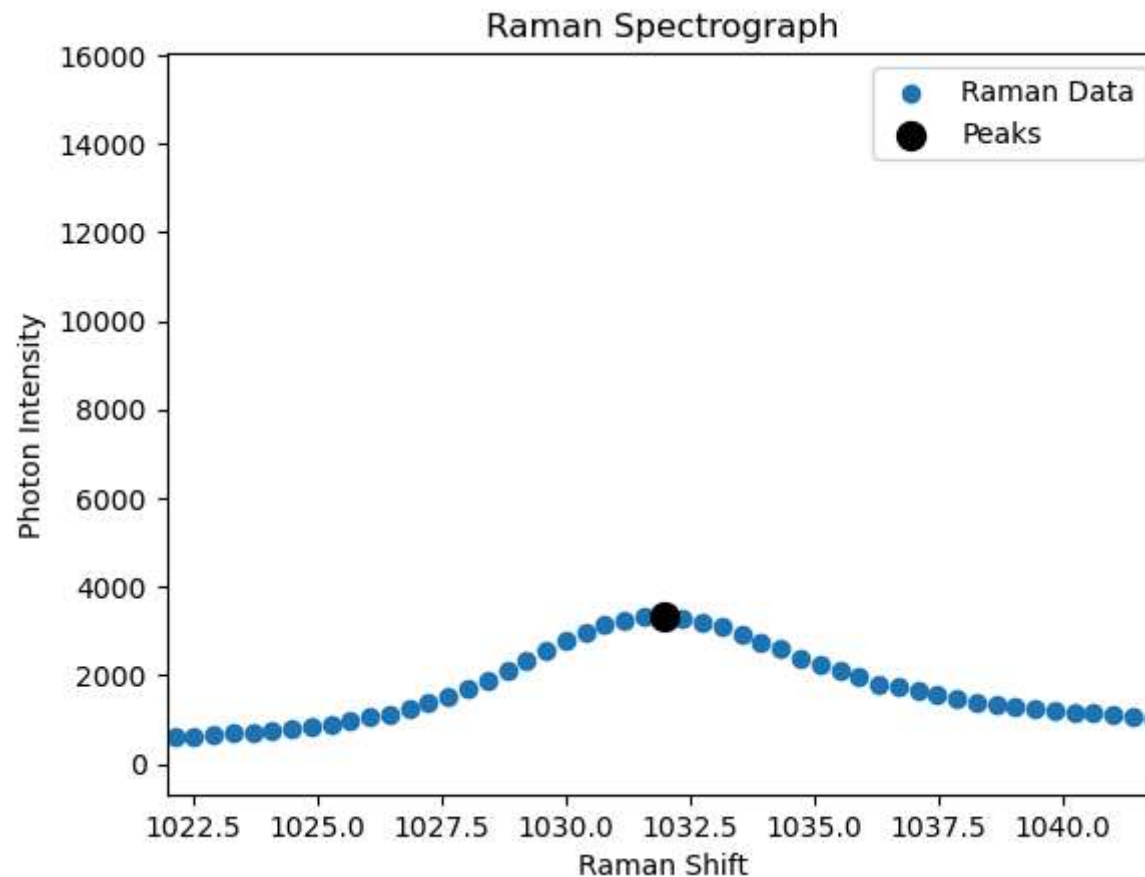
Estimated Spectral Peak 1 is of Intensity=15322.6535 at Raman Shift= $750.2257\text{cm}^{-1}$

## Peak 2

```
In [10]: peak_2_idx = peak_idx[1]  
n2 = 10  
  
plt.figure()
```

```
plt.scatter(wavenumber, intensity)
plt.scatter(wavenumber[peak_2_idx], intensity[peak_2_idx], c='k', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
plt.legend(["Raman Data", "Peaks"])
plt.xlim(wavenumber[peak_2_idx] - n2, wavenumber[peak_2_idx] + n2)
plt.figure()
```

Out[10]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

```
In [11]: print(f"By experimentation, n2={n2} is a good width.")
```

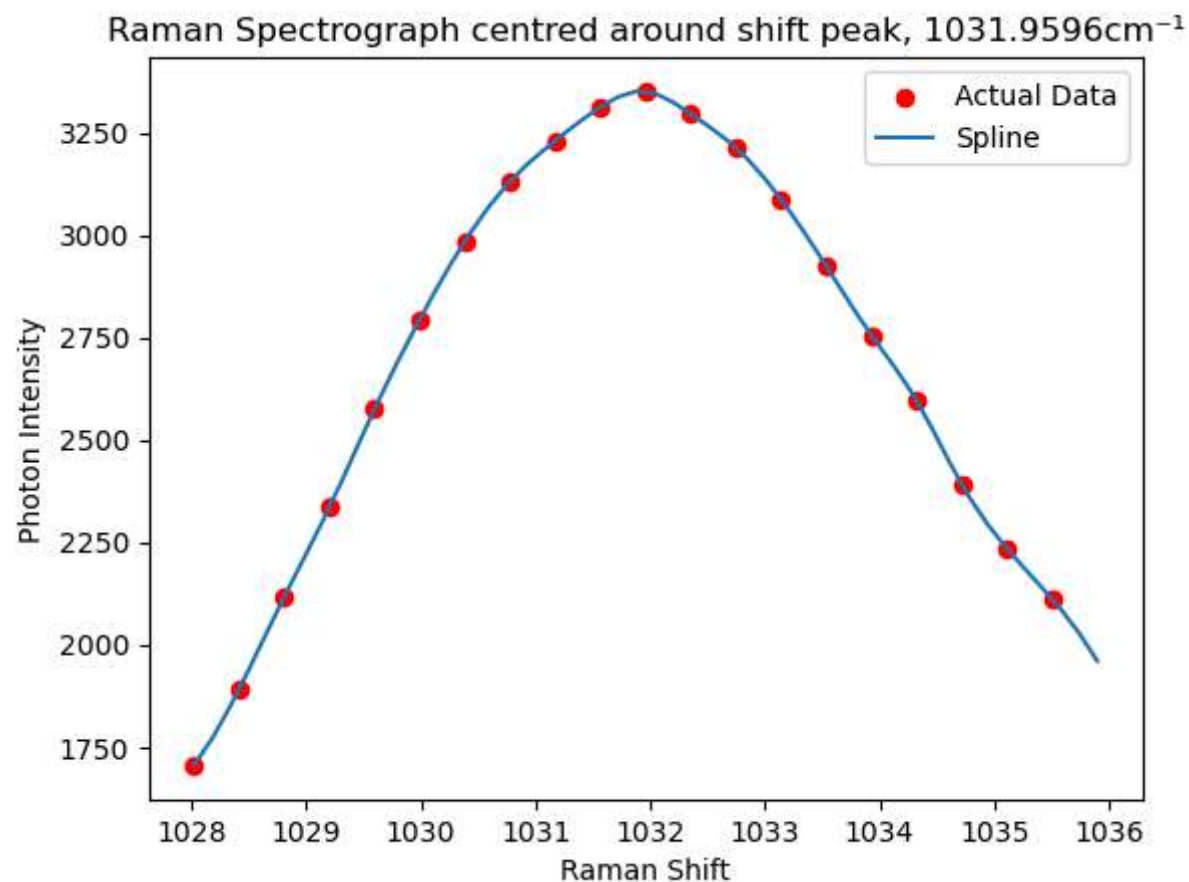
By experimentation, n2=10 is a good width.



```
In [12]: wavenumber_around_peak2 = wavenumber[peak_2_idx - n2 : peak_2_idx + n2]
intensity_around_peak2 = intensity[peak_2_idx - n2 : peak_2_idx + n2]
f_2 = make_interp_spline(wavenumber_around_peak2, intensity_around_peak2)

x_points = np.linspace(wavenumber[peak_2_idx - n2], wavenumber[peak_2_idx + n2], 50)

plt.figure()
plt.scatter(wavenumber_around_peak2, intensity_around_peak2, c='r')
plt.plot(x_points, f_2(x_points))
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_2_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline"])
plt.show()
```

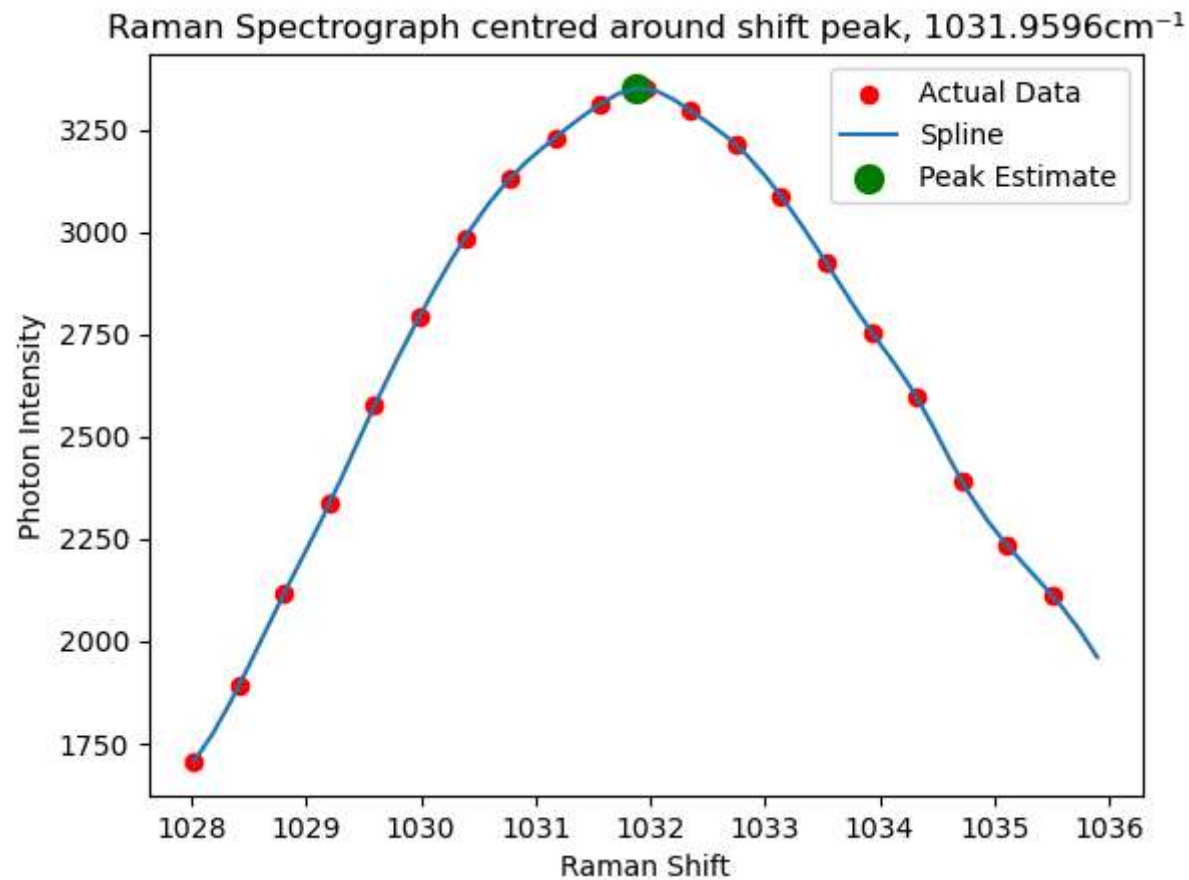


```
In [13]: dy_dx = np.gradient(f_2(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

wavenumber_peak2_estimate = x_points[zero_crossing][0]
intensity_peak2_estimate = f_2(wavenumber_peak2_estimate)

plt.figure()
plt.scatter(wavenumber_around_peak2, intensity_around_peak2, c='r')
plt.plot(x_points, f_2(x_points))
plt.scatter(wavenumber_peak2_estimate, intensity_peak2_estimate, c='g', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_2_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline", "Peak Estimate"])
```

```
plt.savefig('raman_spectrograph_peak2.png', bbox_inches='tight')  
plt.show()
```



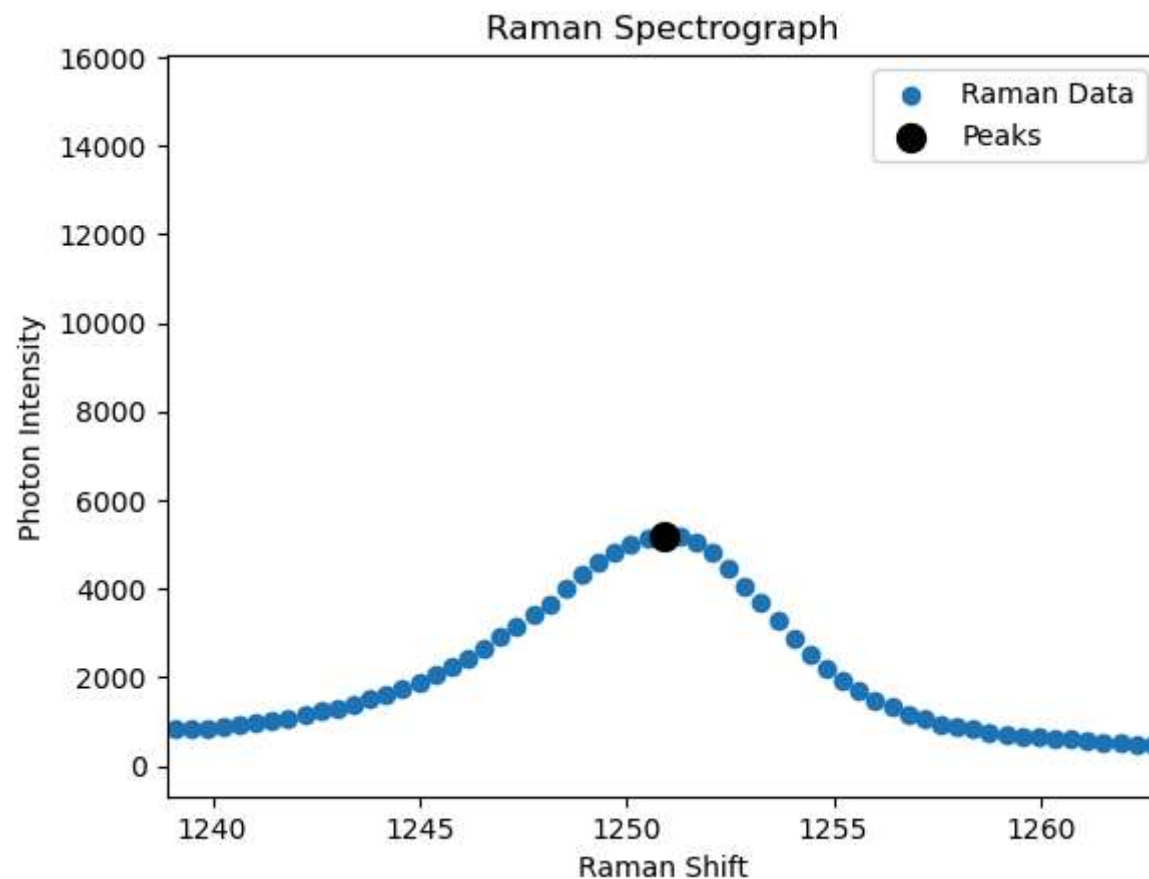
```
In [14]: print(f"Estimated Spectral Peak 2 is of Intensity={intensity_peak2_estimate:0.4f} at Raman Shift={wavenumber_peak2_es  
Estimated Spectral Peak 2 is of Intensity=3351.3739 at Raman Shift=1031.8792cm-1
```

## Peak 3

```
In [15]: peak_3_idx = peak_idx[2]  
n3 = 12  
  
plt.figure()
```

```
plt.scatter(wavenumber, intensity)
plt.scatter(wavenumber[peak_3_idx], intensity[peak_3_idx], c='k', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
plt.legend(["Raman Data", "Peaks"])
plt.xlim(wavenumber[peak_3_idx] - n3, wavenumber[peak_3_idx] + n3)
plt.figure()
```

Out[15]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

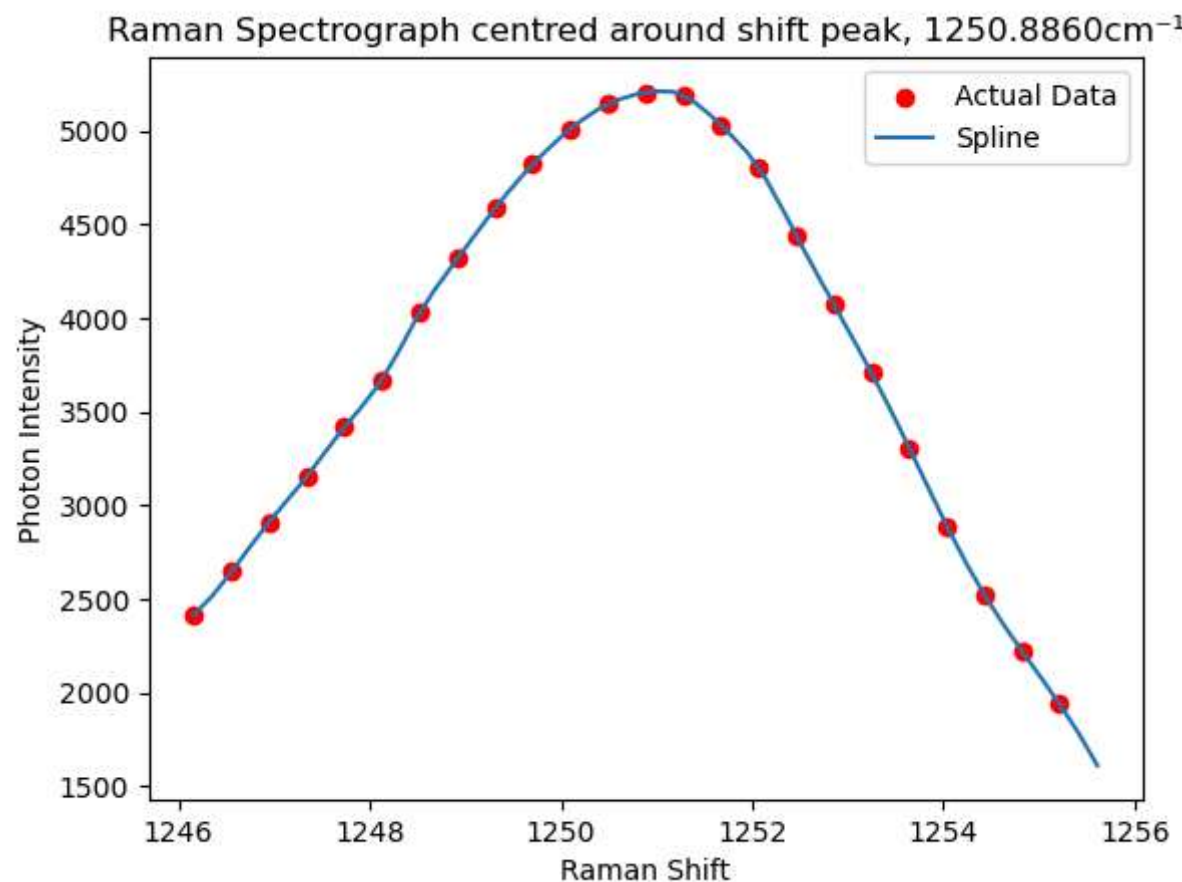
In [16]: `print(f"By experimentation, n3={n3} is a good width.")`

By experimentation, n3=12 is a good width.

```
In [17]: wavenumber_around_peak3 = wavenumber[peak_3_idx - n3 : peak_3_idx + n3]
intensity_around_peak3 = intensity[peak_3_idx - n3 : peak_3_idx + n3]
f_3 = make_interp_spline(wavenumber_around_peak3, intensity_around_peak3)

x_points = np.linspace(wavenumber[peak_3_idx - n3], wavenumber[peak_3_idx + n3], 50)

plt.figure()
plt.scatter(wavenumber_around_peak3, intensity_around_peak3, c='r')
plt.plot(x_points, f_3(x_points))
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_3_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline"])
plt.show()
```

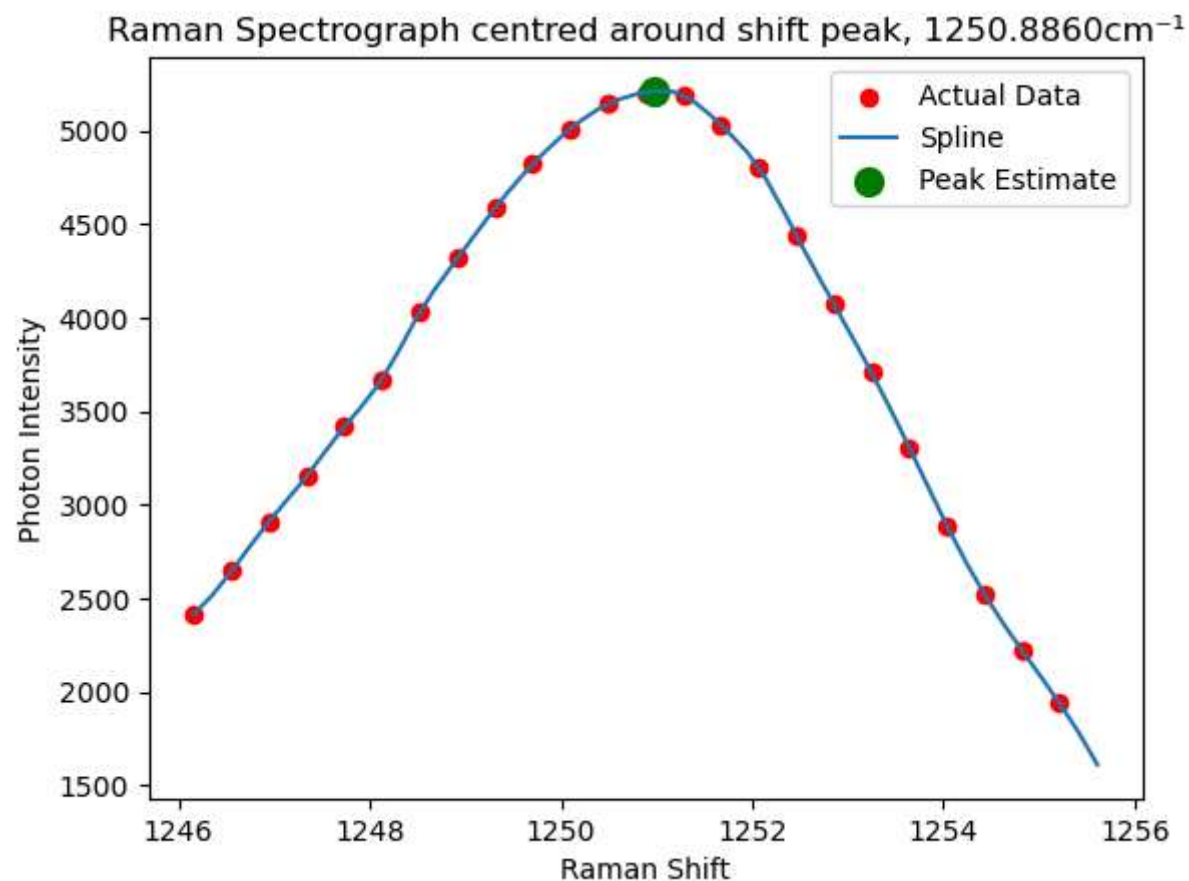


```
In [18]: dy_dx = np.gradient(f_3(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

wavenumber_peak3_estimate = x_points[zero_crossing][0]
intensity_peak3_estimate = f_3(wavenumber_peak3_estimate)

plt.figure()
plt.scatter(wavenumber_around_peak3, intensity_around_peak3, c='r')
plt.plot(x_points, f_3(x_points))
plt.scatter(wavenumber_peak3_estimate, intensity_peak3_estimate, c='g', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_3_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline", "Peak Estimate"])
```

```
plt.savefig('raman_spectrograph_peak3.png', bbox_inches='tight')  
plt.show()
```



```
In [19]: print(f"Estimated Spectral Peak 3 is of Intensity={intensity_peak3_estimate:0.4f} at Raman Shift={wavenumber_peak3_es
```

Estimated Spectral Peak 3 is of Intensity=5210.1585 at Raman Shift=1250.9824cm<sup>-1</sup>

## Peak 4

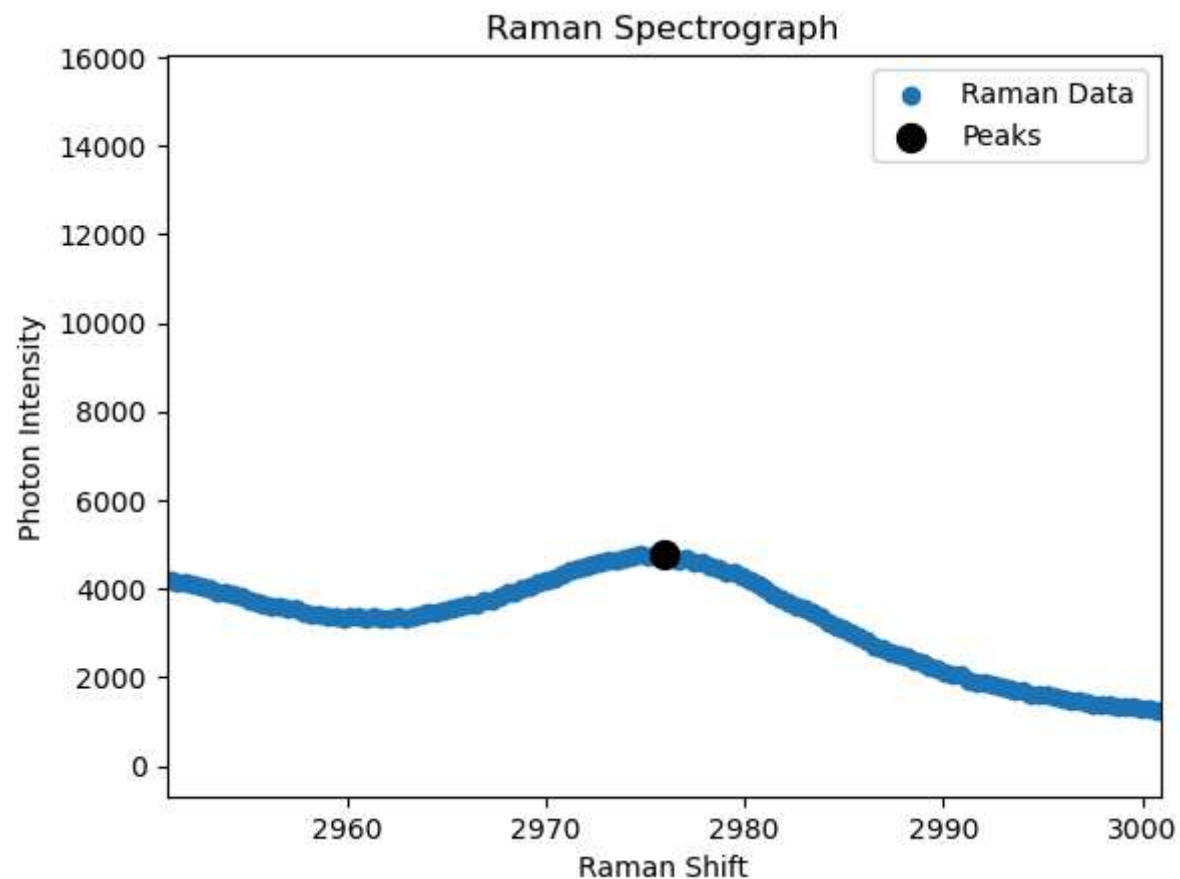
```
In [20]: peak_4_idx = peak_idx[3]
```

```
n4 = 25
```

```
plt.figure()
```

```
plt.scatter(wavenumber, intensity)
plt.scatter(wavenumber[peak_4_idx], intensity[peak_4_idx], c='k', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title("Raman Spectrograph")
plt.legend(["Raman Data", "Peaks"])
plt.xlim(wavenumber[peak_4_idx] - n4, wavenumber[peak_4_idx] + n4)
plt.figure()
```

Out[20]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

```
In [21]: print(f"By experimentation, n4={n4} is a good width.")
```

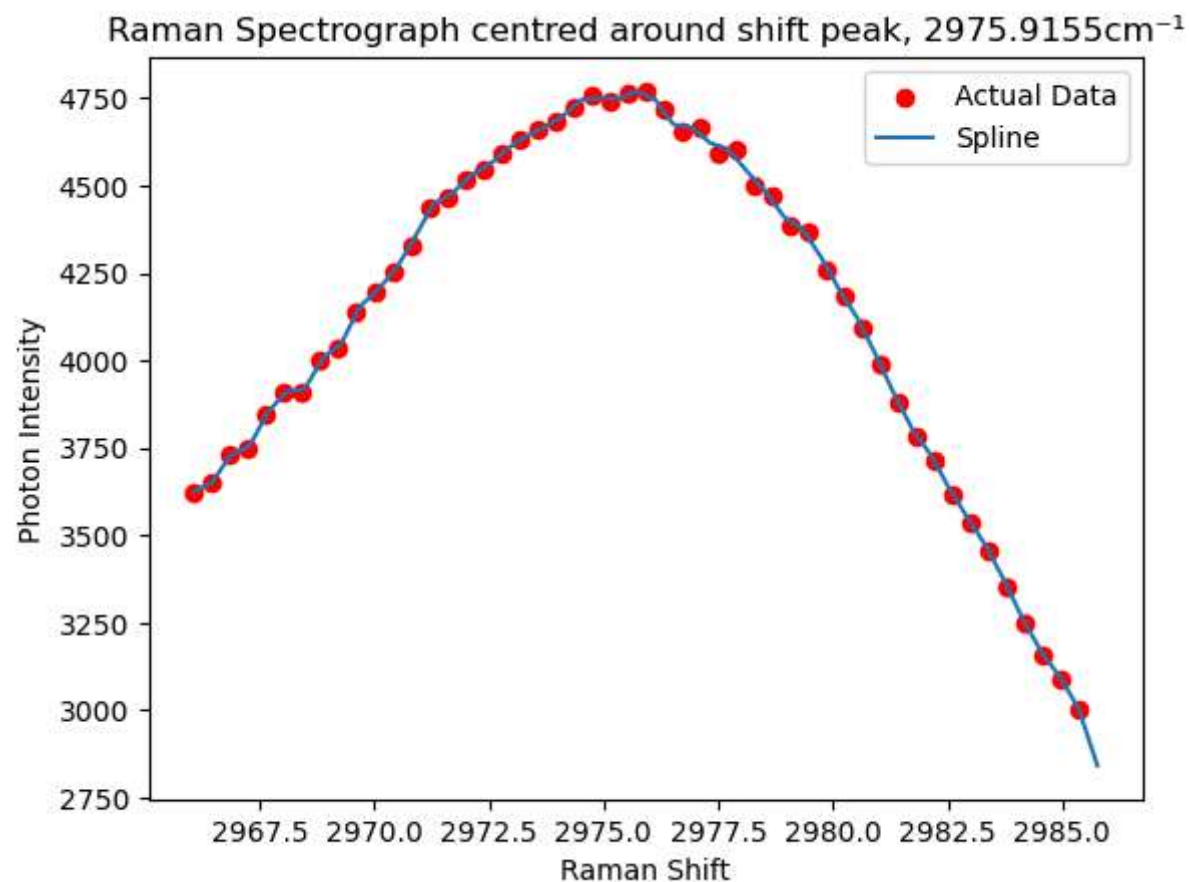
By experimentation, n4=25 is a good width.



```
In [22]: wavenumber_around_peak4 = wavenumber[peak_4_idx - n4 : peak_4_idx + n4]
intensity_around_peak4 = intensity[peak_4_idx - n4 : peak_4_idx + n4]
f_4 = make_interp_spline(wavenumber_around_peak4, intensity_around_peak4)

x_points = np.linspace(wavenumber[peak_4_idx - n4], wavenumber[peak_4_idx + n4], 50)

plt.figure()
plt.scatter(wavenumber_around_peak4, intensity_around_peak4, c='r')
plt.plot(x_points, f_4(x_points))
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_4_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline"])
plt.show()
```

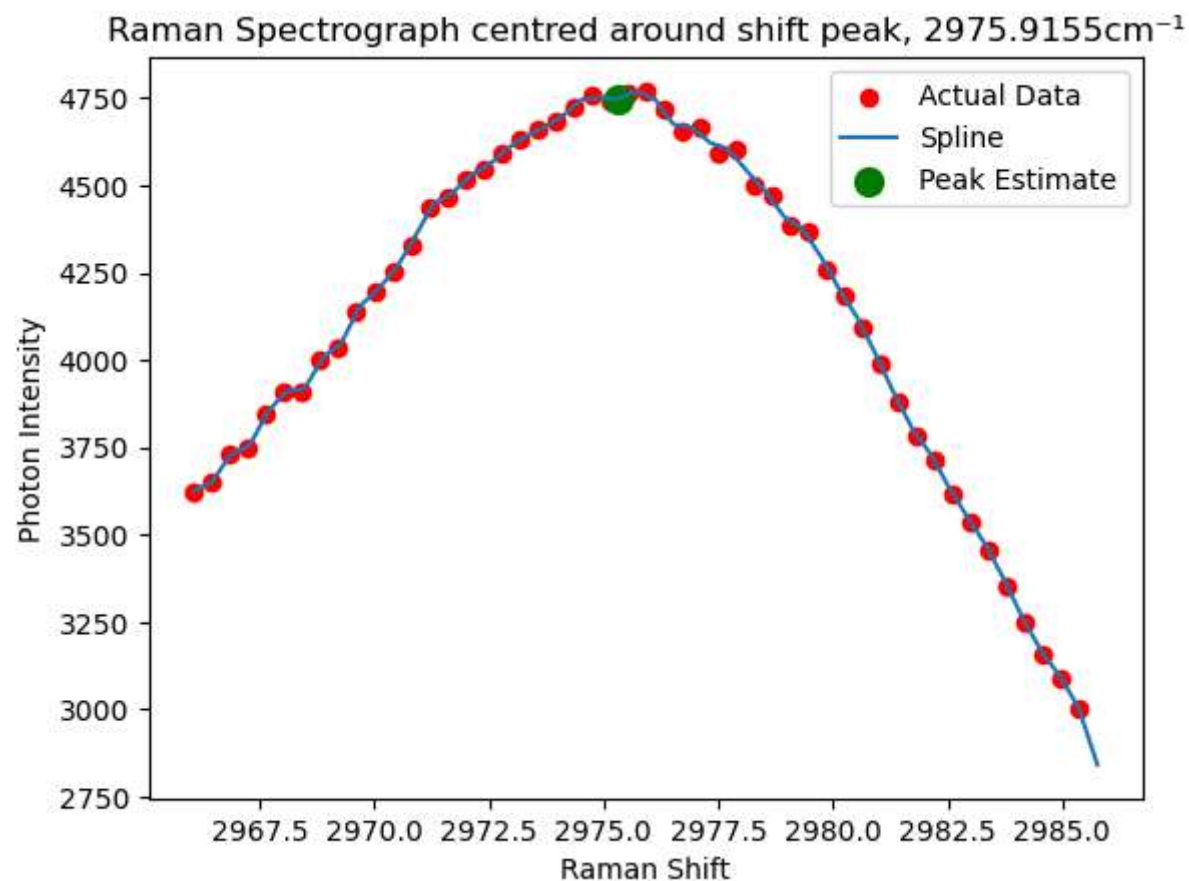


```
In [23]: dy_dx = np.gradient(f_4(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

wavenumber_peak4_estimate = x_points[zero_crossing][0]
intensity_peak4_estimate = f_4(wavenumber_peak4_estimate)

plt.figure()
plt.scatter(wavenumber_around_peak4, intensity_around_peak4, c='r')
plt.plot(x_points, f_4(x_points))
plt.scatter(wavenumber_peak4_estimate, intensity_peak4_estimate, c='g', s=100)
plt.xlabel("Raman Shift")
plt.ylabel("Photon Intensity")
plt.title(f"Raman Spectrograph centred around shift peak, {wavenumber[peak_4_idx]:0.4f}{CM_1}")
plt.legend(["Actual Data", "Spline", "Peak Estimate"])
```

```
plt.savefig('raman_spectrograph_peak4.png', bbox_inches='tight')  
plt.show()
```



```
In [24]: print(f"Estimated Spectral Peak 4 is of Intensity={intensity_peak4_estimate:0.4f} at Raman Shift={wavenumber_peak4_estimate:0.4f}")
```

Estimated Spectral Peak 4 is of Intensity=4748.0016 at Raman Shift=2975.3129cm<sup>-1</sup>

```
In [25]: print(wavenumber_peak1_estimate)  
print(wavenumber_peak2_estimate)  
print(wavenumber_peak3_estimate)  
print(wavenumber_peak4_estimate)
```

750.2256771428571  
1031.8792428571428  
1250.982379591837  
2975.3128714285717