Homework #2 – Numeric Computing

Problem 1

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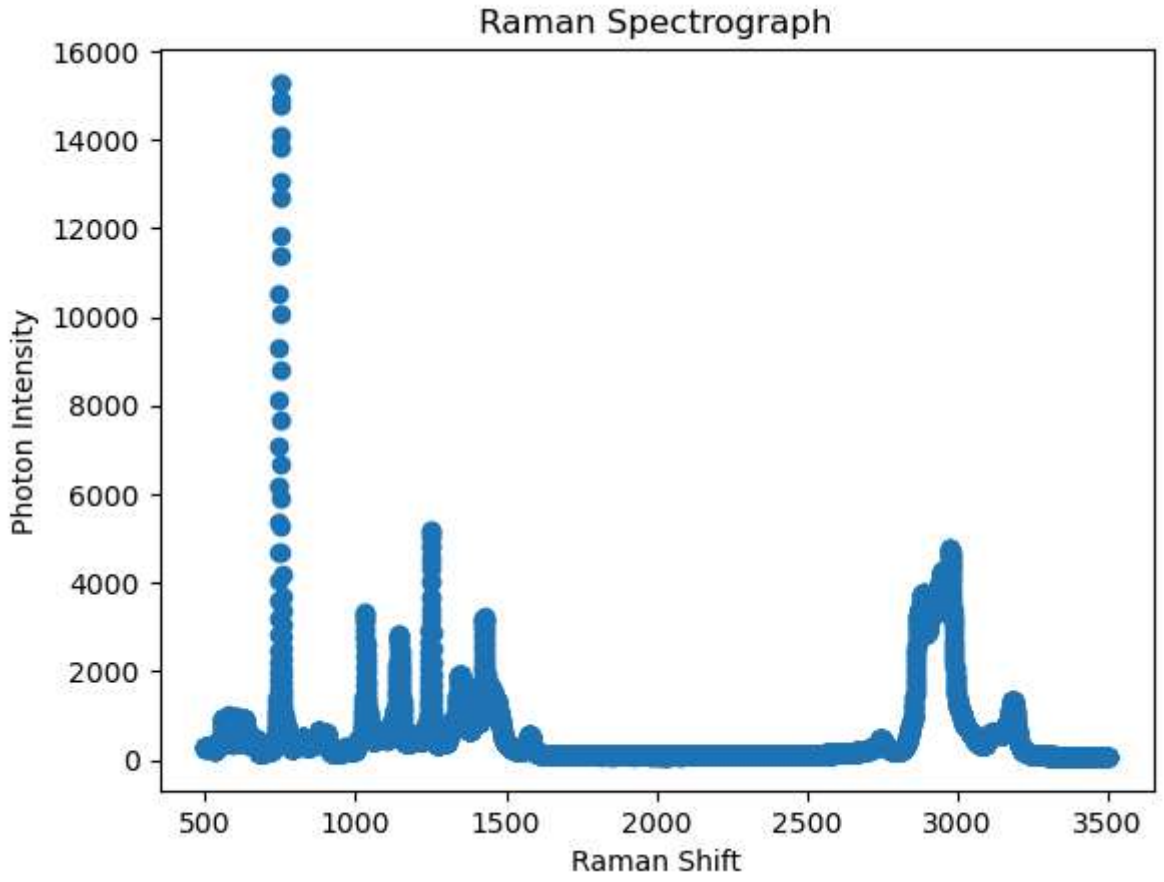
In [2]:
```
# Imports
import numpy as np
import matplotlib.pyplot as plt
from scipy.signal import find_peaks
from scipy.interpolate import make_interp_spline
```

In [3]:
```
# Constants
RAMAN_FILENAME = "../data/input/raman.txt"
CM_1 = "cm\u207B\u00B9"
```

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



<Figure size 640x480 with 0 Axes>

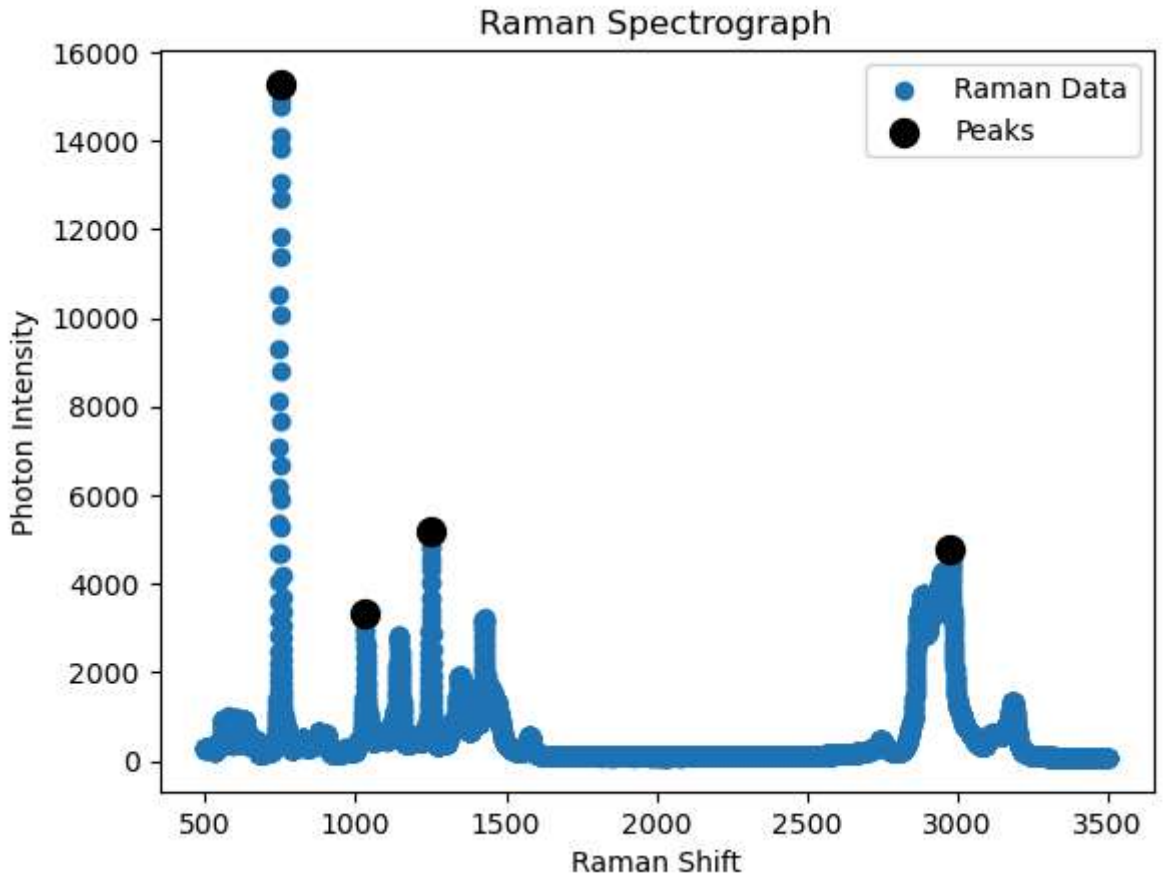
In [5]:
```
min_height_of_peaks = 3000
horizontal_distance_bw_peaks = 500
peak_idx, _ = find_peaks(intensity, height=min_height_of_peaks, distance=horizontal_distance_bw_peaks)

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.figure()
```

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



<Figure size 640x480 with 0 Axes>

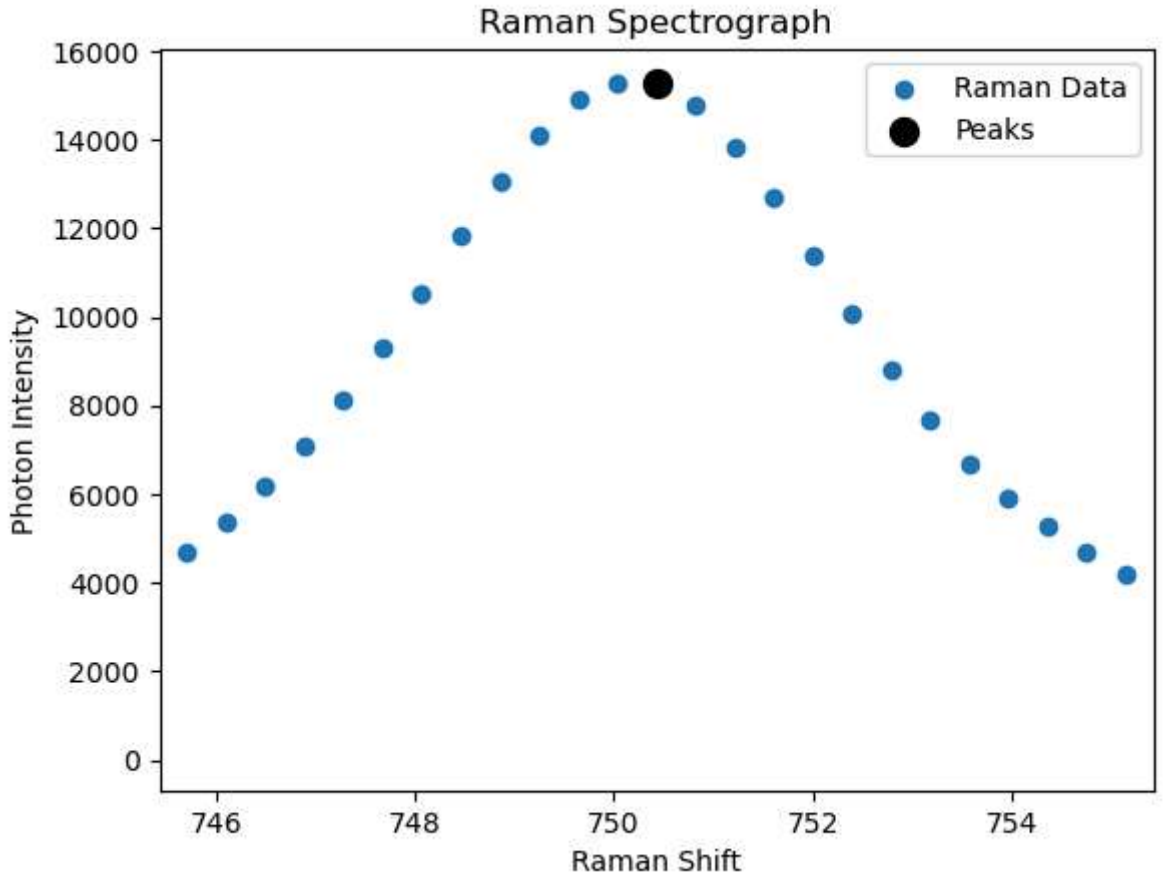
Peak 1

In [6]:
```
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[6]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

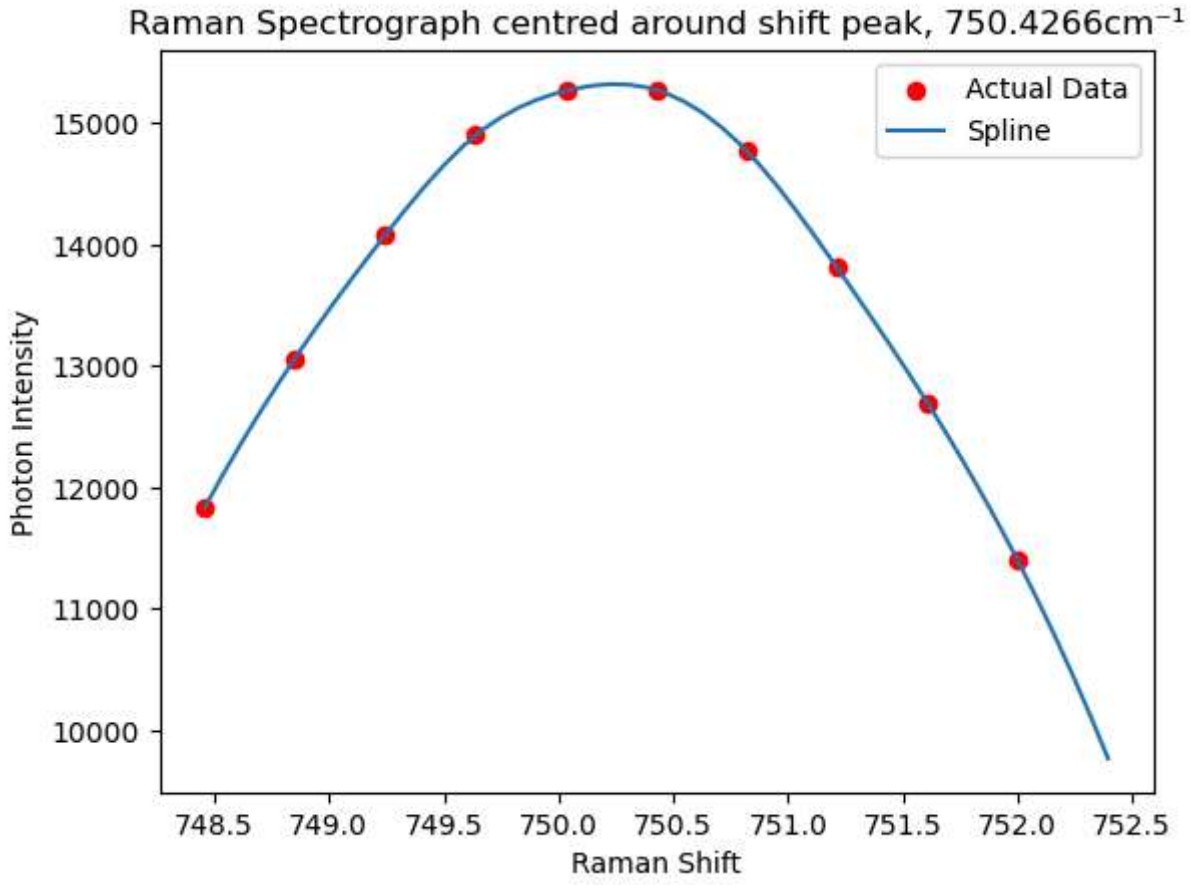
In [7]:
```
print(f"By experimentation, n1={n1} is a good width.")
```

By experimentation, n1=5 is a good width.

In [8]:
```
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()
```

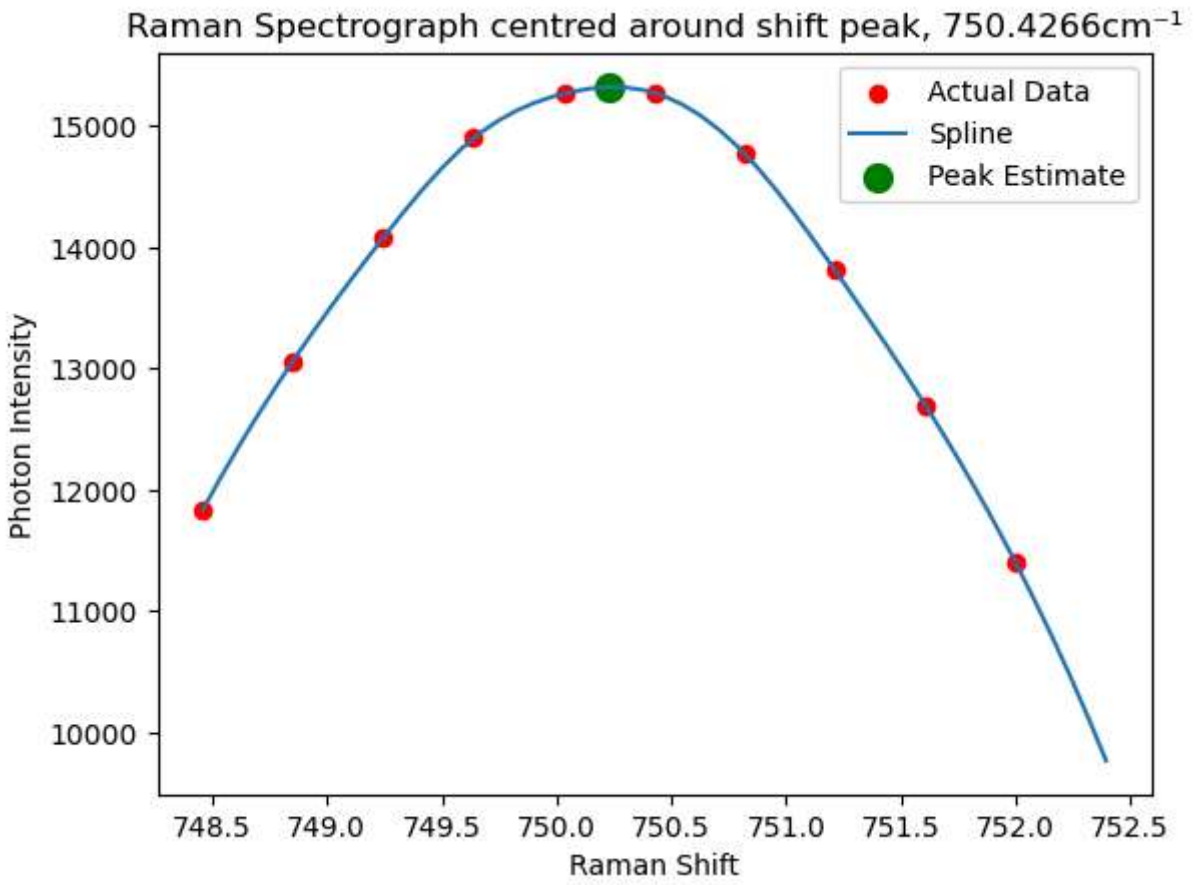


In [9]:
```
dy_dx = np.gradient(f_1(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

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.show()
```



In [10]:
```
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=750.2257cm⁻¹
```

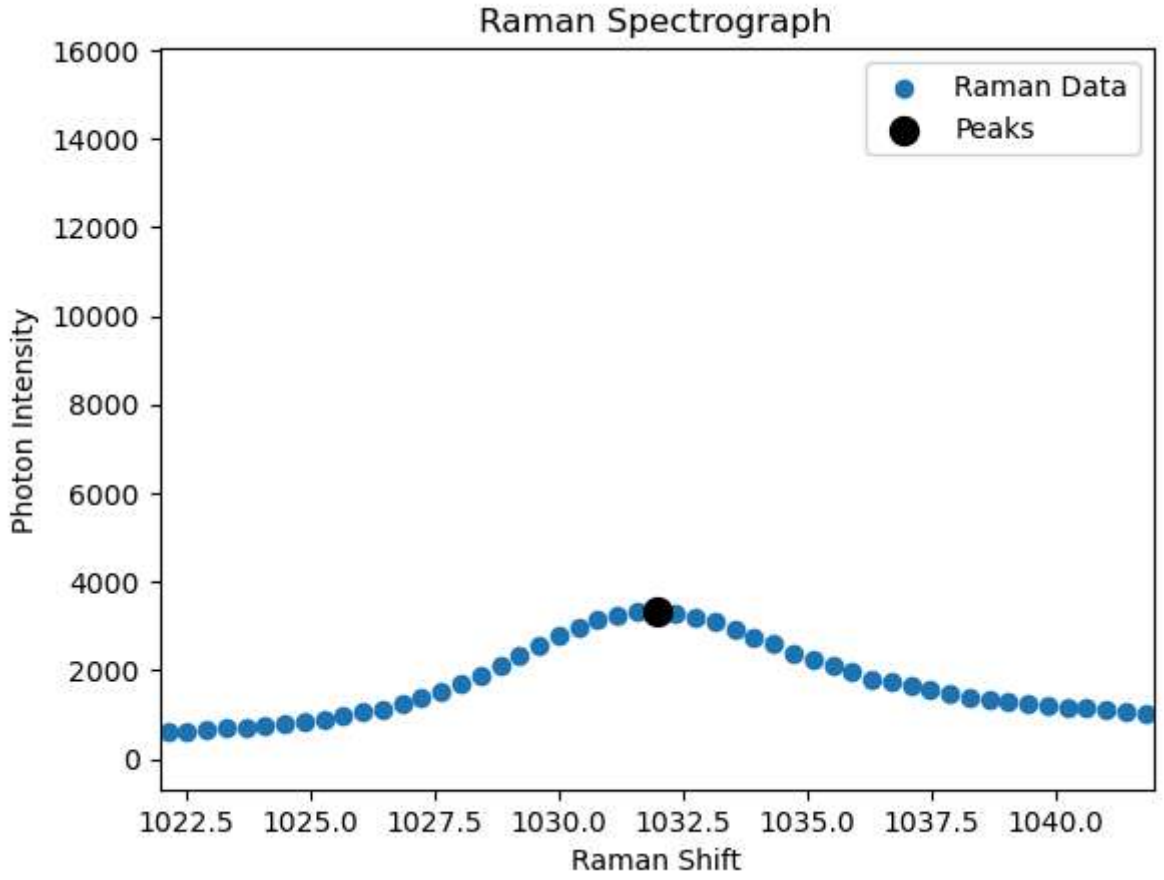
Peak 2

In [11]:
```
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[11]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

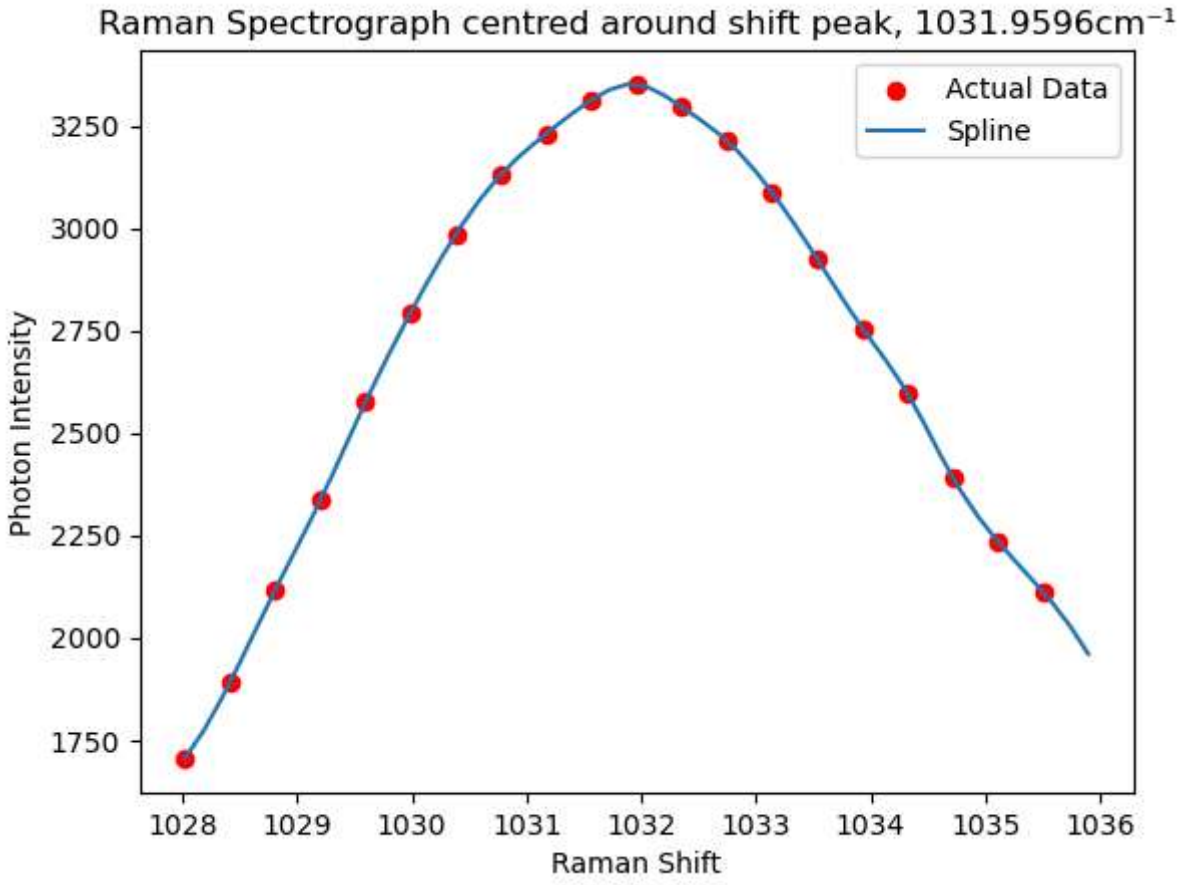
In [12]:
```
print(f"By experimentation, n2={n2} is a good width.")
```

By experimentation, n2=10 is a good width.

In [13]:
```
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()
```

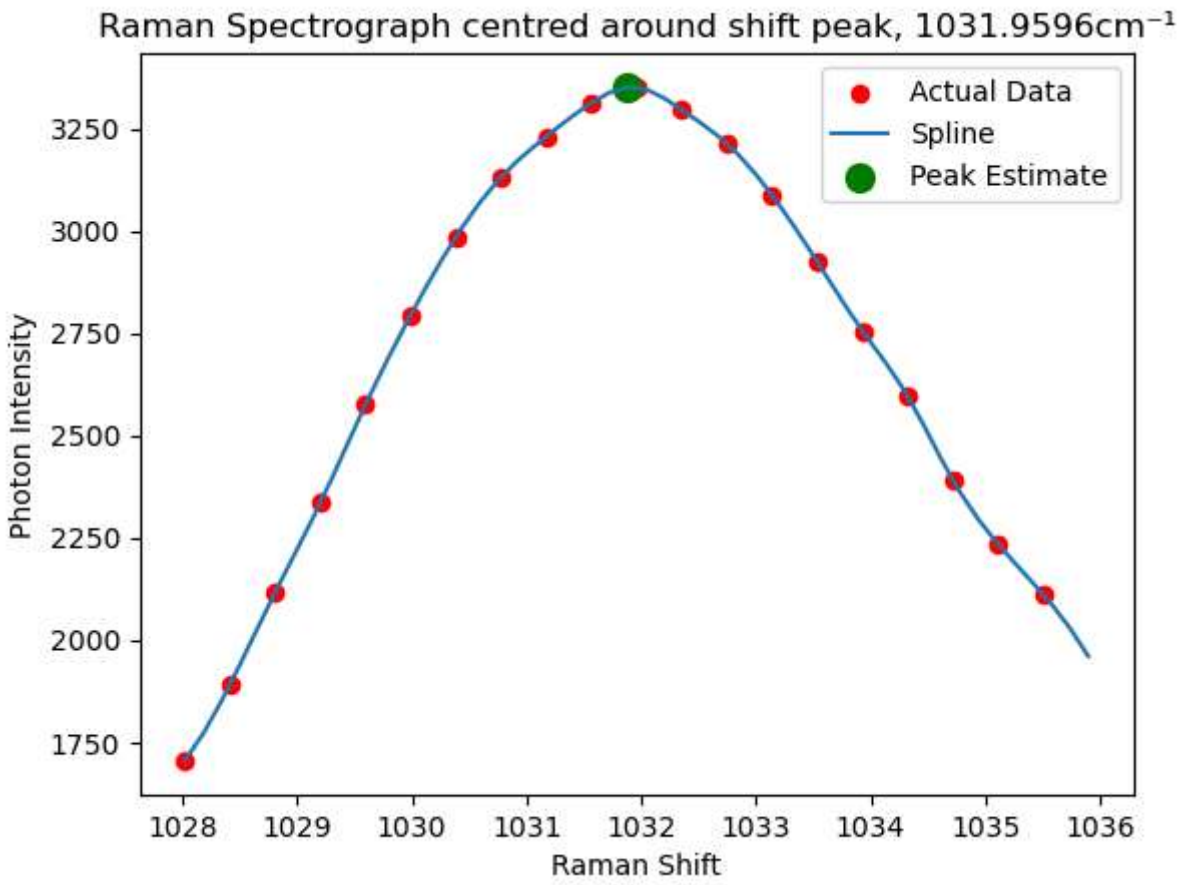


In [14]:
```
dy_dx = np.gradient(f_2(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

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.show()
```



In [15]:
```
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
```

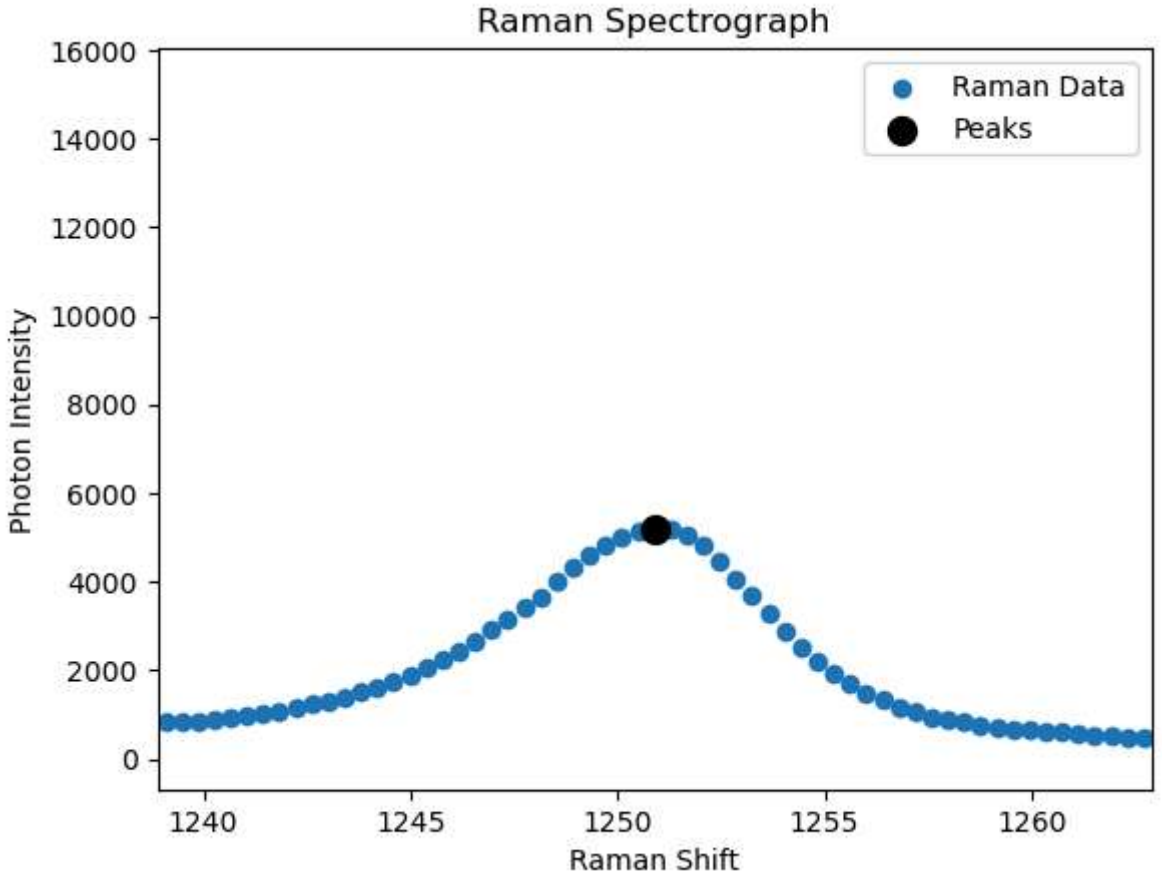
Peak 3

In [16]:
```
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[16]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

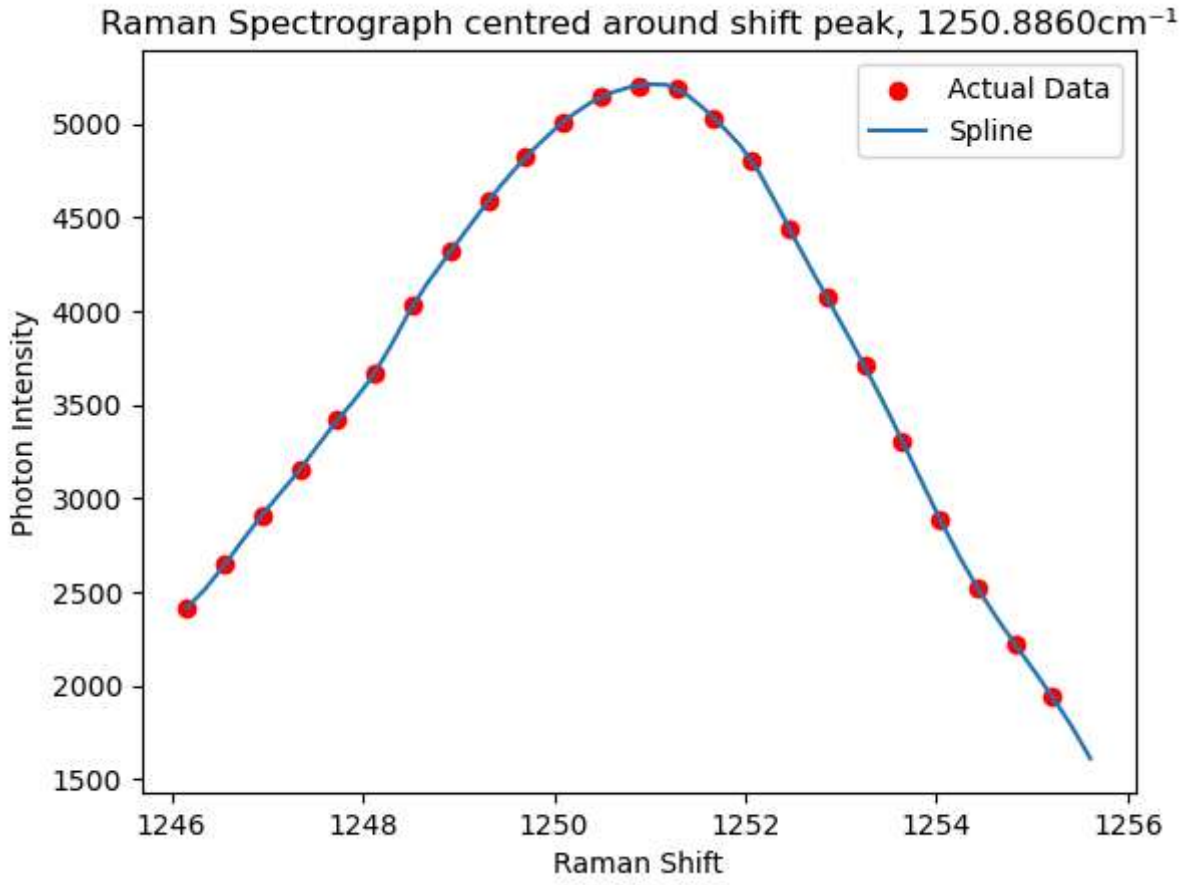
In [17]:
```
print(f"By experimentation, n3={n3} is a good width.")
```

By experimentation, n3=12 is a good width.

In [18]:
```
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()
```

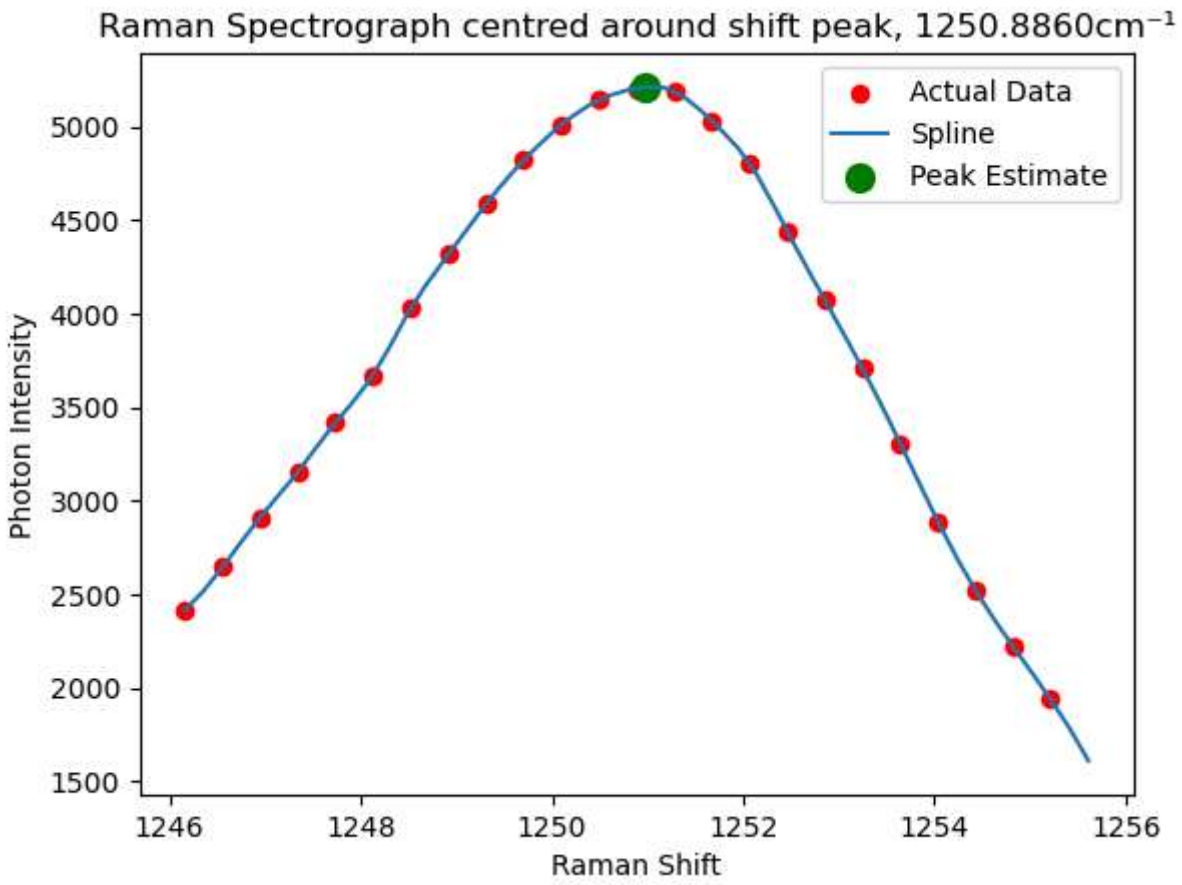


In [19]:
```
dy_dx = np.gradient(f_3(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

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.show()
```



In [20]:
```
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⁻¹
```

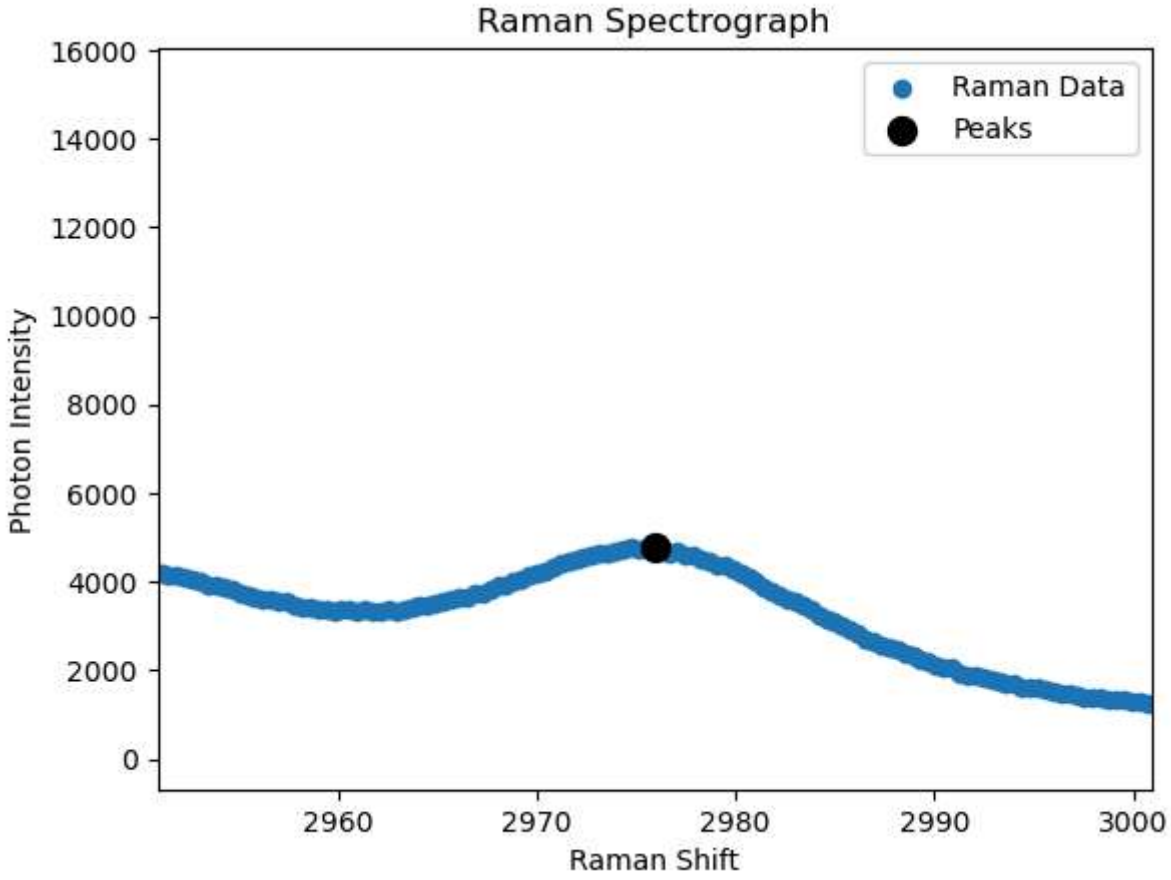
Peak 4

In [34]:
```
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[34]: <Figure size 640x480 with 0 Axes>



<Figure size 640x480 with 0 Axes>

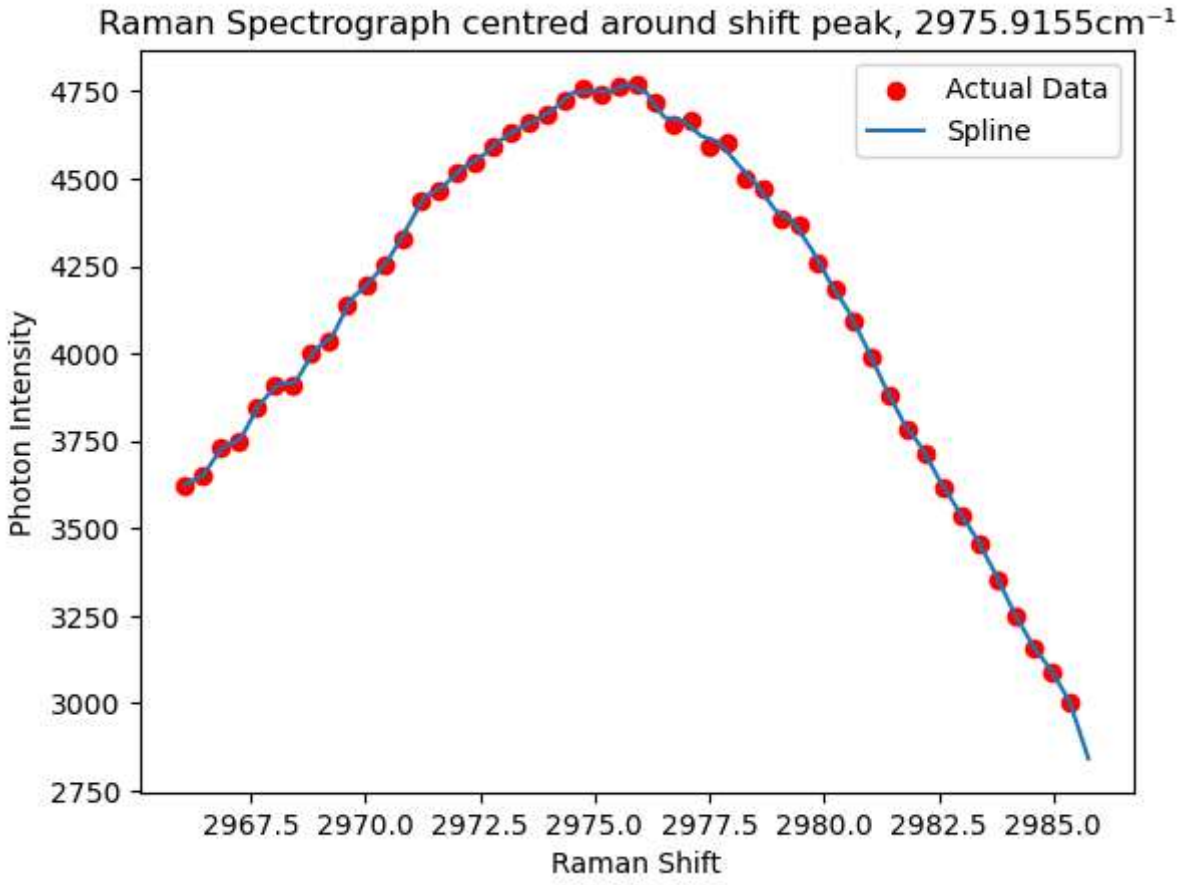
In [35]:
```
print(f"By experimentation, n4={n4} is a good width.")
```

By experimentation, n4=25 is a good width.

In [36]:
```
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()
```

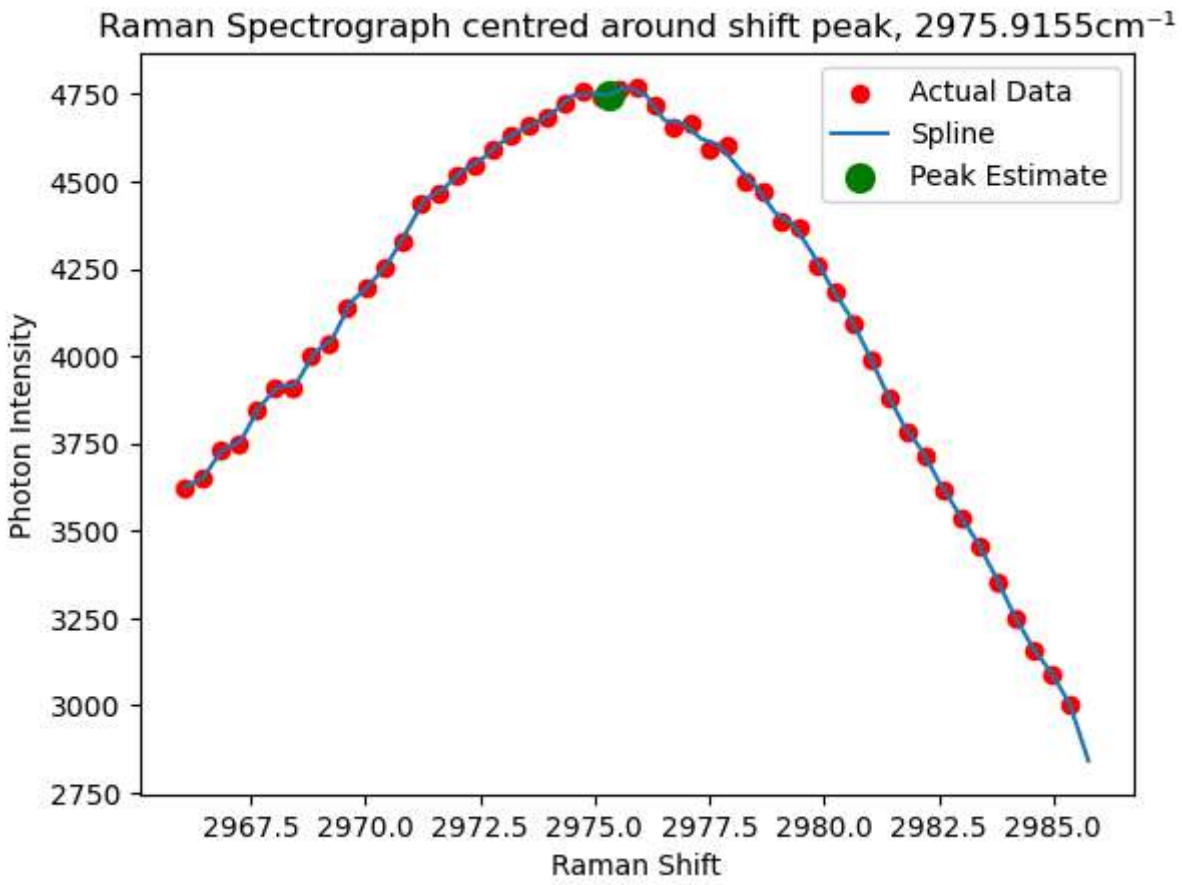


In [37]:
```
dy_dx = np.gradient(f_4(x_points), x_points)
zero_crossing = np.where(np.diff(np.sign(dy_dx)))[0]

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.show()
```



In [38]:
```
print(f"Estimated Spectral Peak 4 is of Intensity={intensity_peak4_estimate:0.4f} at Raman Shift={wavenumber_peak4_es
```

```
Estimated Spectral Peak 4 is of Intensity=4748.0016 at Raman Shift=2975.3129cm⁻¹
```

In [39]:
```
print(wavenumber_peak1_estimate)
print(wavenumber_peak2_estimate)
print(wavenumber_peak3_estimate)
print(wavenumber_peak4_estimate)
```

```
750.2256771428571
1031.8792428571428
1250.982379591837
2975.3128714285717
```