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SPECTROSCOPY APPLICATIONS NOTE NUMBER 6

The Use of Fourier Transforms to Process Raman Data

The technique of laser Raman spectroscopy involves irradiation of a sample with coherent light and observation of Raman scattering at various frequencies, caused by vibrational energy transfers.[1] The very high background scattering from the monochromatic source itself often leads to drifting baselines which are sample dependent, as shown in Figure 1.

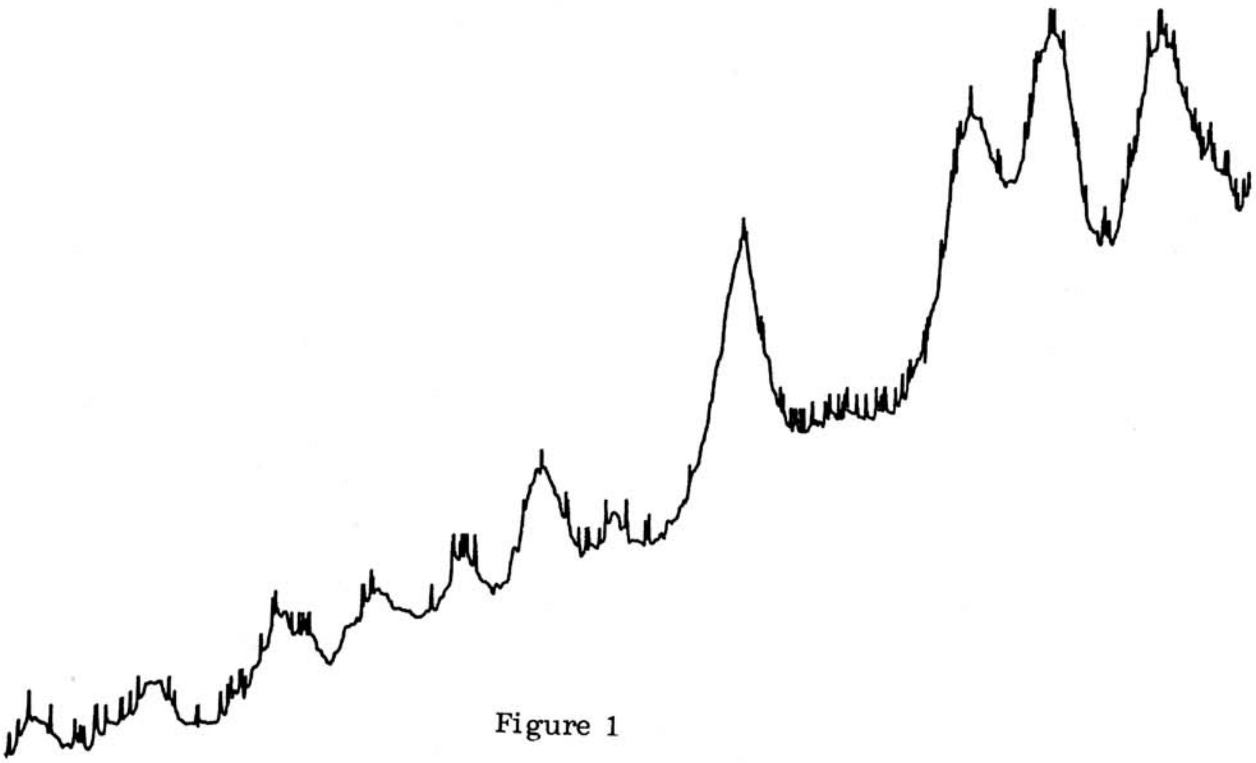

Figure 1

One of the most promising methods of leveling the baseline, so that spectra can be more conveniently analyzed and compared is through the application of a window function to the Fourier transform of the spectrum and then retransforming the resulting spectrum. Methods for data smoothing through application of window functions to the Fourier transform spectrum have been described by Horlick,[2] and Hayes, et. al.[3] Recently Bulkin[4] has proposed that the application of a trapezoidal window to the Fourier transform of a Raman spectrum can remove such baseline roll and enhace signal to noise to some extent.

The spectra shown in this note were obtained from a SPEX 1401 laser Raman spectrometer scanning at 50 cm^{-1}/min and processed using a Nicolet LAB-80 data system. Each spectrum consisted of 2048 data points and was Fourier transformed along with a block of 2048 zeroes to produce intermediate results as shown in Figure 2.

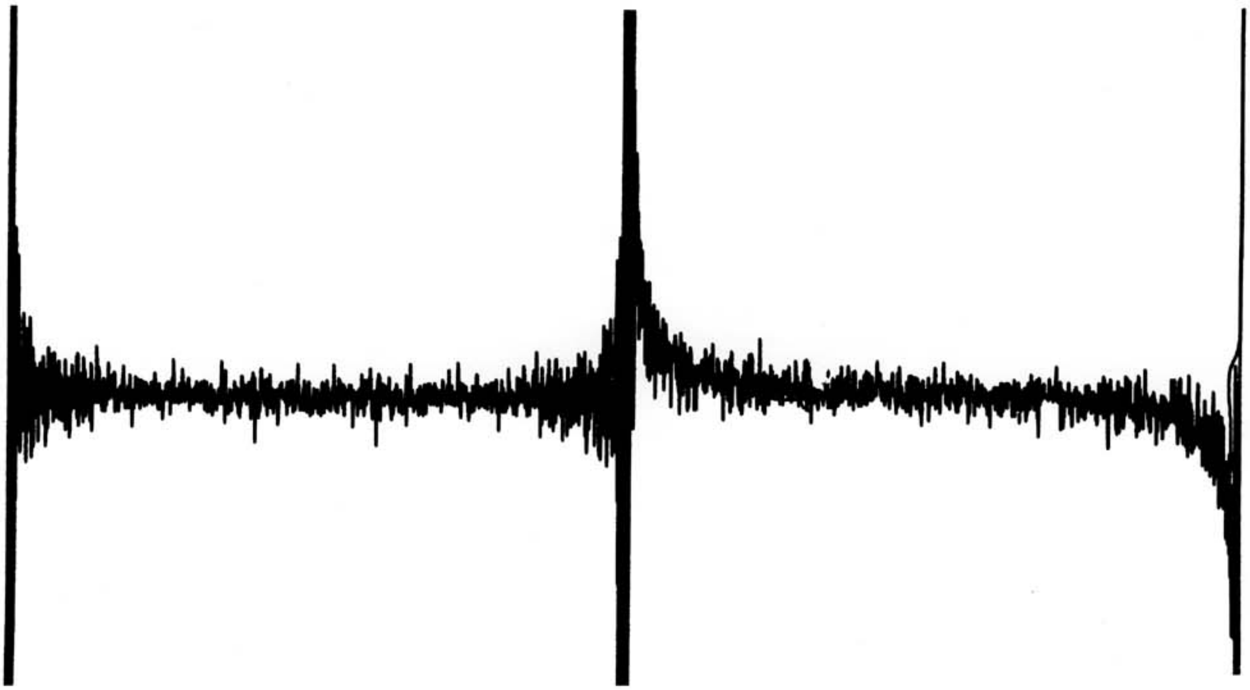

Figure 2

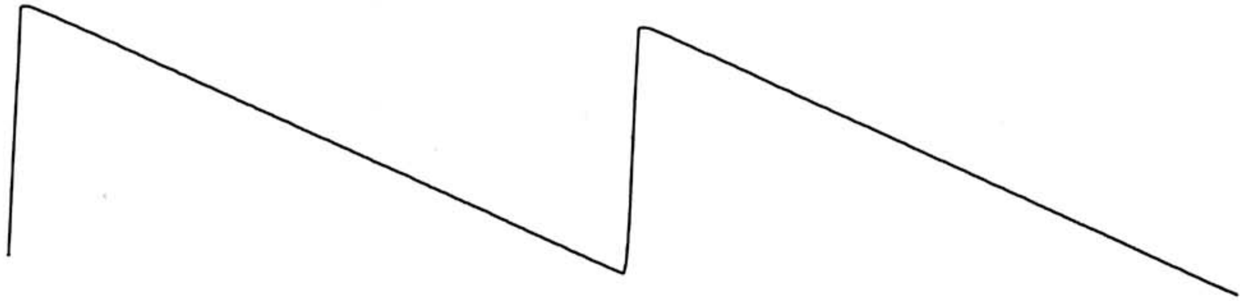

Figure 3

This Fourier transformed spectrum consists of a 2048 point set of real and a 2048 point set of imaginary Fourier coefficients. It was multiplied by a trapezoidal function which had a rising diagonal over the first 15 addresses and a falling diagonal over the last 2038 addresses. In other words, points 1 through 15 were multiplied by i/15 and points 10 - 2048 by (2048-i)/2048. This function was applied to both the real and imaginary portions of the spectrum as shown in Figure 3.

The spectrum was then transformed back into the frequency domain and plotted as shown in Figure 4. The spectrum is of 2-carboxy-2'-hydroxy-5'-sulfoformazylbenzene (zincon) at 4.81 x 10^{-4} M, buffered at pH 8.75, from 900 - 1335 cm^{-1}.

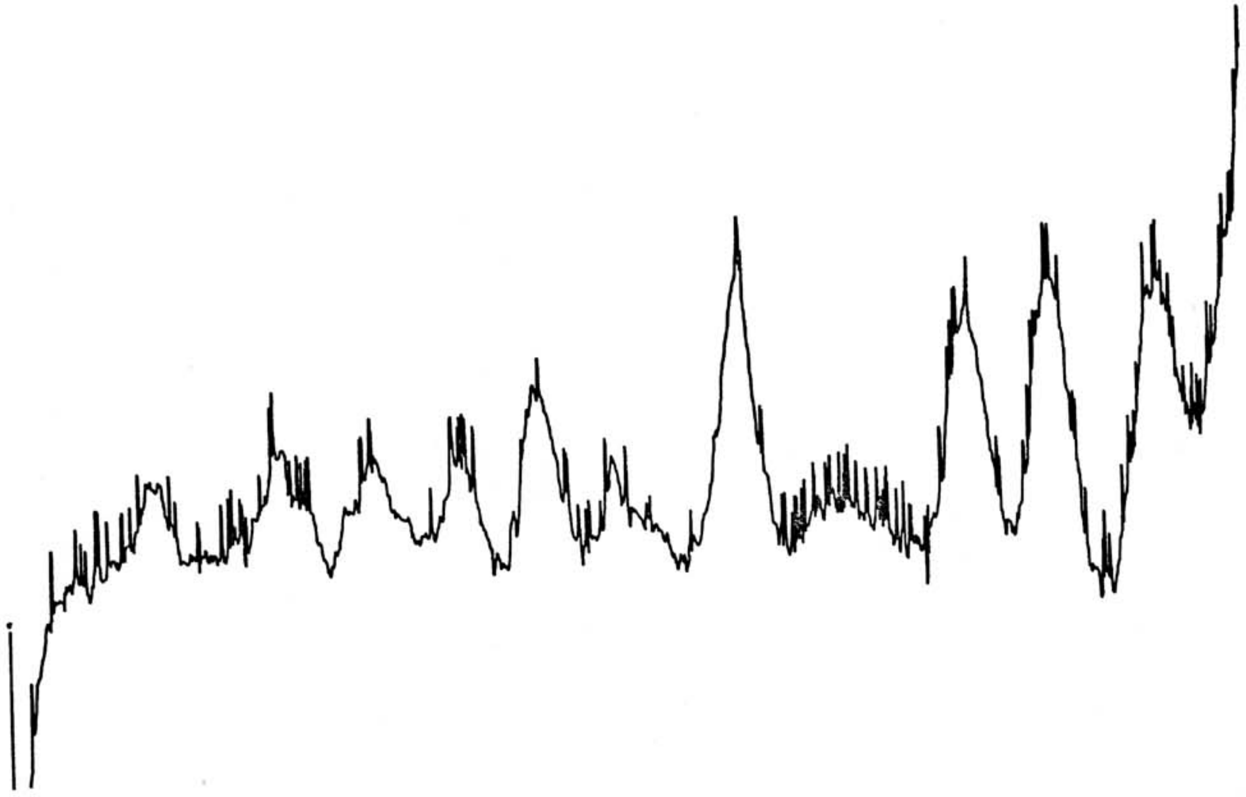

Figure 4

Similarly, Figure 5 shows the same sample, zincon, from 1300-1735 cm^{-1}, and Figure 6 shows a more dilute solution of zincon (4.7 x 10^{-5} M) complexed with liver alcohol dehydrogenase (1.3 x 10^{-4} M), also buffered at pH 8.75. A detailed analysis of the chemistry of this complexation is the subject of a paper in press.[5]

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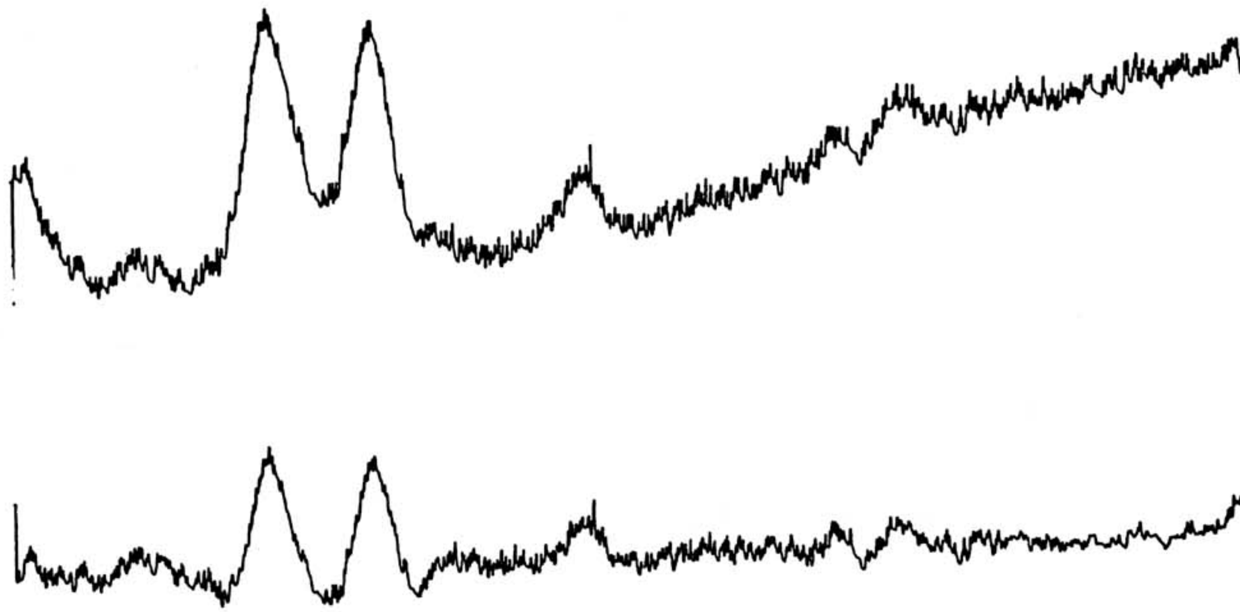

Figure 5

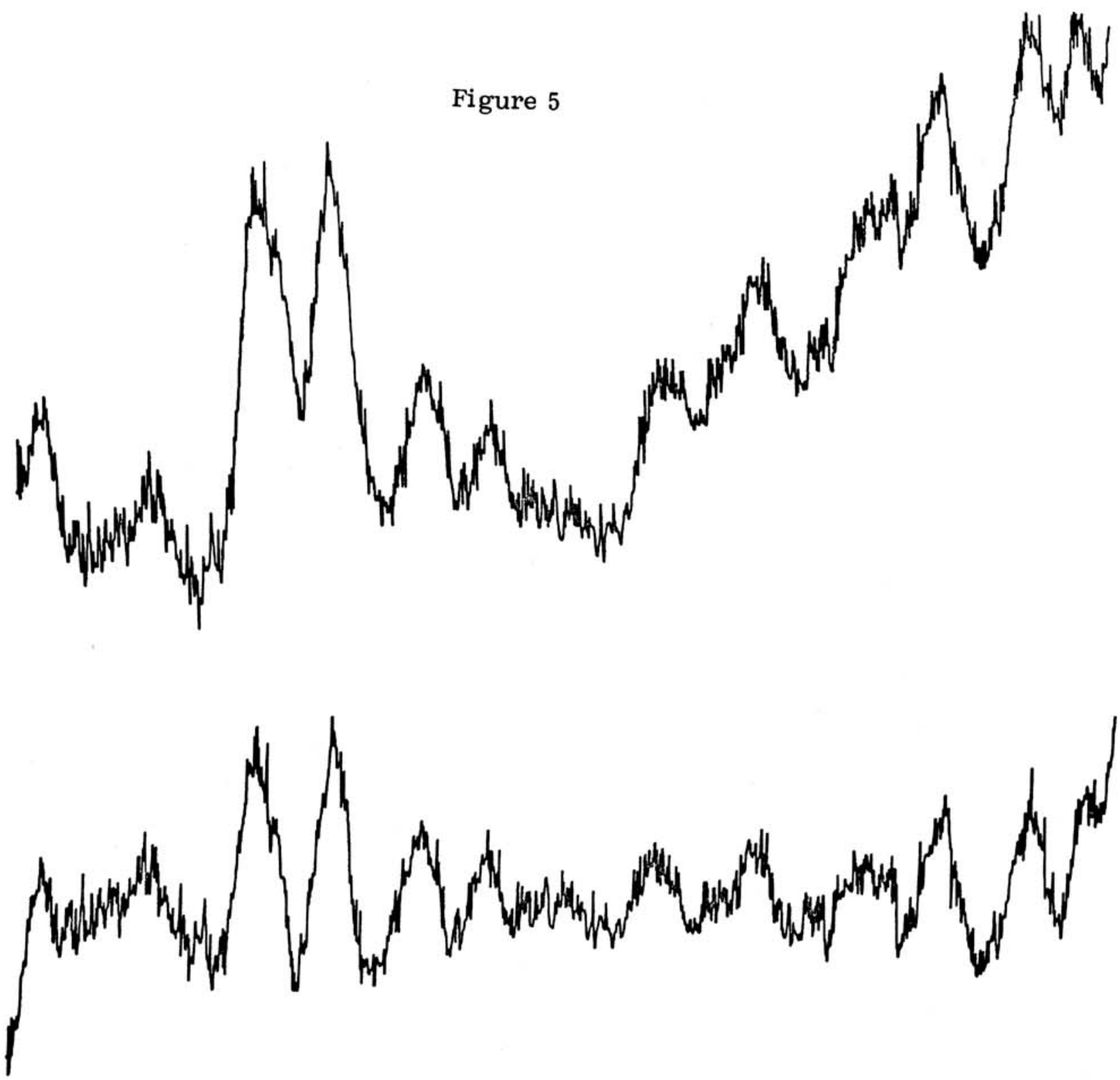

Figure 6

References

1. See for example G. Eglinton "Infrared and Raman Spectroscopy," in Physical Methods in Organic Chemistry, J.C.P. Schwarz, editor, Holden-Day, (1964).

2. G. Horlick, Anal. Chem, 44, 943 (1972).

3. J. W. Hayes, D. E. Glover, D. E. Smith and M. W. Overton, Anal. Chem. 45, 277 (1973).

4. Bernard Bulkin, Hunter College, private communication.

5. James T. McFarland, Richard L. Petersen and Kenneth L. Watters, "Resonance Raman Investigation of an Enzyme-Inhibitor Complex," in press.