Teaching FFT principles in the physical chemistry laboratory

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Teaching FFT Principles in the Physical Chemistry Laboratory

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Instruments and methods based on FFT (fast Fourier transform) principles are becoming increasingly common in chemistry, and there have been several expositions on various aspects of the subject (*1–9*). Nevertheless, because of the expense and complexity of commercial apparatus, few students have an opportunity to get hands-on experience with an instrument.

The result is that FFT concepts tend to remain an abstraction not easily grasped and certainly readily forgotten. In an attempt to remedy this situation, we have developed an experiment, based on the classic determination of the velocity of sound (v_s) in a gas, which uses simple and readily available equipment to exemplify some of the key concepts.

In the usual version of the experiment (*10, 11*), Kundt's tube, S is a speaker driven by a fixed frequency source (Fig. 1). The other end of the tube consists of a piston (P) that may be moved in or out until the resonance condition is met. Now, however, suppose that rather than a fixed-frequency sound source, we used one that *simultaneously* transmits a wide range of frequencies. By analogy to light, such a source may be regarded as a polychromatic or "white" source. Further suppose that the tube length is now fixed rather than variable. Then only certain wavelengths in the polychromatic source will be in resonance; other wavelengths will destructively interfere. If a small microphone is placed at P to detect the pressure fluctuations caused by the sound waves, then, as will be seen below, *the time record of the pressure variations contains the information necessary to extract the resonance frequencies*. The best known and most widely used method of transposing time domain data into the frequency domain is a process called Fourier transformation.

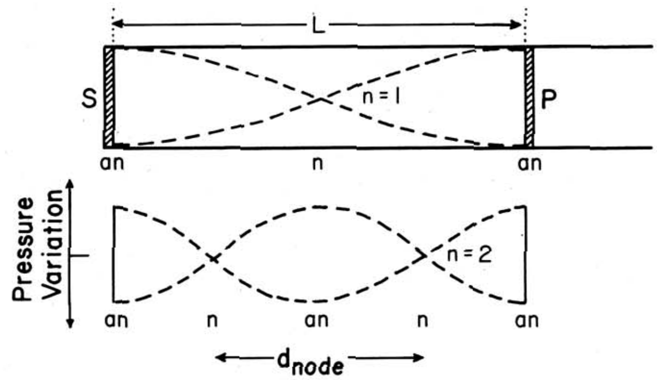

Figure 1. Standing waves in a tube of length *L*. The ends are regions of maximum pressure variation (antinodes).

General Principles

Although the propagation of sound waves and Fourier transformation are covered in many texts, a student's first incursion, especially into the latter area, can be formidable. In this section we summarize the salient theoretical features and hope to show that the underlying concepts for obtaining a discrete Fourier transform are in fact quite simple. Although perhaps mathematically less elegant, the reader will note that we make no recourse to imaginary notation.

Standing Waves in a Tube

Consider a long tube of length L closed at both ends and filled with a gas (Fig. 1). Sound waves traveling down the tube are reflected at the ends, and, if the wavelength (λ) of the waves is such that

$$L = n \cdot (\lambda/2) \tag{1}$$

with $n = 1, 2, 3, \ldots$, standing waves are established such that the ends are pressure antinodes (an). These antinodes are regions of maximum pressure oscillation (*12*). For $n = 1$ there is one pressure node (n) at the center of the tube at $L/2$, while for $n = 2$ there are two nodes at $L/4$ and $3L/4$, and so on. In the usual version of the Kundt's tube experiment, L is adjusted until eq 1 is satisfied, the distance between nodes or antinodes, d_{node}, is then measured yielding λ ($= 2 \cdot d_{node}$) and then v_s from

$$v_s = \nu \cdot \lambda \tag{2}$$

where ν is the frequency. In our version of the experiment S is now a "polychromatic" source and L is fixed. Only those source frequencies that satisfy both eqs 1 and 2 are in resonance, so that

$$\nu_{res}(n) = \frac{v_s}{2L} \cdot n \text{ with } n = 1, 2, \ldots \tag{3}$$

With the aid of FFT the values of the resonance frequencies, $\nu_{res}(n)$, are determined. A plot of $\nu_{res}(n)$ versus n then yields $v_s/2L$ and thus v_s.

Fourier Transformation

(a) *The Fourier Series*. It is well known (*1, 13*) that, subject to a few conditions known as the *Dirichlet criteria*, a periodic function or signal, $S(t)$, can be represented by a Fourier series

$$S(t) = a_0 + \sum_{k=1}^{\infty} \{a_k \cdot \cos(2\pi k \nu_1 t) + b_k \cdot \sin(2\pi k \nu_1 t)\} \tag{4}$$

The period (T) of the signal equals $1/\nu_1$, the reciprocal of the fundamental frequency. The other spectral components (or lines) of the signal are overtones occurring with spacing $\Delta\nu = \nu_1$ at $\nu_k = k \cdot \nu_1$ ($k = 2, 3, \ldots$). The Fourier coefficients (a_k, b_k) associated with the spectral lines are the amplitudes of the various cosine and sine components. The coefficient a_0 is the coefficient associated with the zero-frequency (dc) component.

Since $\sin(\theta_1 + \theta_2) = \sin\theta_1 \cdot \cos\theta_2 + \cos\theta_1 \cdot \sin\theta_2$, eq 4 can be rewritten more compactly as

$$S(t) = a_0 + \sum_{k=1}^{\infty} A_k \cdot \sin(2\pi k\nu_1 t + \delta_k) \tag{5}$$

where δ_k is a phase angle such that

$$a_k = A_k \cdot \sin\delta_k \tag{6}$$

and

$$b_k = A_k \cdot \cos\delta_k \tag{7}$$

with $A_k = \sqrt{(a_k^2 + b_k^2)}$. By virtue of orthogonality relationships Fourier coefficients can be obtained from

$$a_k = (2/T)\int_0^T S(t)\cos(2\pi k\nu_1 t)\mathrm{d}t \tag{8}$$

and

$$b_k = (2/T)\int_0^T S(t)\sin(2\pi k\nu_1 t)\mathrm{d}t \tag{9}$$

Knowing a_k and b_k and using eqs 6 and 7, A_k and δ_k can then be obtained, permitting representation of the original time-dependent signal in the frequency domain. Figures 2a and b show schematically such a transformation for a repetitive signal with period T. The first spectral line occurs at frequency $1/T$ and the others with spacing $1/T$. Notice that the spectral lines continue indefinitely.

(b) *Discrete Fourier Analysis* (*1, 2*). We now examine the more realistic situation in which discrete data from a nonrepetitive signal is gathered during a finite time interval. When a signal is sampled at time intervals Δt using an analogue-to-digital (A/D) converter, a finite number of samples (N) is taken during a finite record time (T_R) with $T_R = N \cdot \Delta t$, Figure 2c. Although in reality we do not know what happens to the signal before or after this observation time, the Fourier transform procedure implicitly assumes that the signal is periodic with period T_R. As we have seen from Figures 2a and b, this implied periodic time will control not only the lowest frequency $\nu_1 = 1/T_R$ but also the spacing, $\Delta\nu = 1/T_R$, between the discrete frequencies corresponding to the spectral lines. The sampling frequency ν_{samp}, equal to the reciprocal of the time between data samples (Δt), controls the highest frequency component (ν_{max}) in the Fourier series, Figure 2d. This can be seen as follows. If N equally spaced data samples are gathered in the time domain, then $N/2$ frequencies with equal spacing $\Delta\nu$ are generated in the frequency domain. Only half as many spectral lines are generated as there are time samples because each frequency actually contains two bits of data—amplitude and phase. Thus $\nu_{max} = N/2 \cdot \Delta\nu = (N/2) \cdot (1/T_R) = \frac{1}{2}\nu_{samp}$. This maximum frequency is often called the Nyquist frequency ($\nu_{NQ} = \nu_{max}$).

In Figure 2a we have a continuous signal that corresponds to a sampling interval (Δt) of zero. Thus ν_{samp} (and hence ν_{max}) are infinite so that the spectral lines of the Fourier transform (FT) in Figure 2b continue indefinitely. Sampling of a continuous signal, as is shown in Figure 2c, yields a discrete Fourier transform (DFT), Figure 2d, which is an approximation to the Fourier transform of the continuous signal in that the DFT cannot yield spectral lines above $\frac{1}{2}\nu_{samp}$.

We still have to cast eqs 8 and 9 in forms suitable for digital analysis. Replacing t by $n \cdot \Delta t$, ν_1 by $1/N \cdot \Delta t (= 1/T_R)$ and $\mathrm{d}t/T$ by $\Delta t/N \cdot \Delta t$ we obtain

$$a_k = 2/N \cdot \sum_{n=0}^{N-1} S(n)\cos(2\pi kn/N) \tag{10}$$

and

$$b_k = 2/N \cdot \sum_{n=0}^{N-1} S(n)\sin(2\pi kn/N) \tag{11}$$

where $S(n)$ are the signals obtained at times $t(n) = n \cdot \Delta t$. These equations allow numerical determination of the a_k and b_k coefficients. Equations 6 and 7 can then be used to obtain the amplitudes (A_k) and phases (δ_k) associated with the various $\nu_k = k/T_R$ for $k = 1, 2, \ldots, N/2$.

The fast Fourier transform (FFT) is simply a procedure for carrying out a DFT efficiently. Most FFT's require N time samples where N equals 2 raised to some integral power, e.g., 512 or 1024. In our case we used a modified version of the program described in ref *1*.

(c) *Aliasing and the Nyquist Theorem.* Clearly if we wish to include all the frequencies contained in our signal, the maximum signal frequency ($\nu_{sig,max}$) should be less than or equal to the highest frequency we can get from the FFT, i.e., ν_{NQ}. In fact Nyquist's theorem (*1, 2, 6*) states that the sampling frequency should be at least twice the highest frequency in the signal to be analyzed. However, suppose that we are not careful enough and that our signal source contains frequencies ν_1, ν_2, ν_3, and ν_4, one of which (ν_4) lies above ν_{NQ}, Figure 3. Then, when the FFT is carried out, an alias frequency is generated at ν_4' as if ν_4 had been reflected about a line at ν_{NQ}; in general $\nu_n + \nu_n' = 2 \cdot \nu_{NQ} = \nu_{samp}$. A simple example of aliasing is when we have a single frequency and sample at exactly this frequency, then, as can be seen from Figure 4, sampling would lead us to conclude erroneously that we have a dc signal. Thus, if our source contains frequencies that lie above $\frac{1}{2}\nu_{samp}$, we should take care to insert a filter, commonly called an anti-alias filter, to remove frequencies in this region.

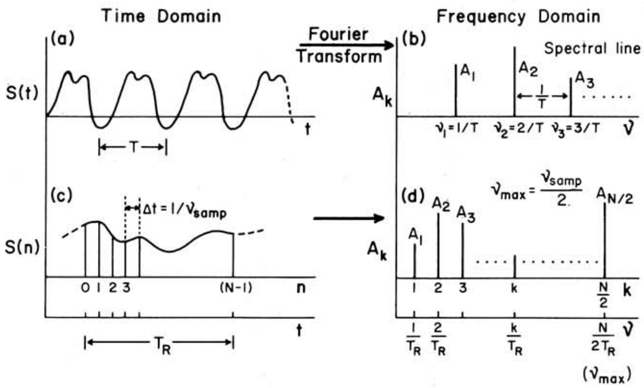

Figure 2. Schematic representation of Fourier transformation of signals from the time to frequency domain.

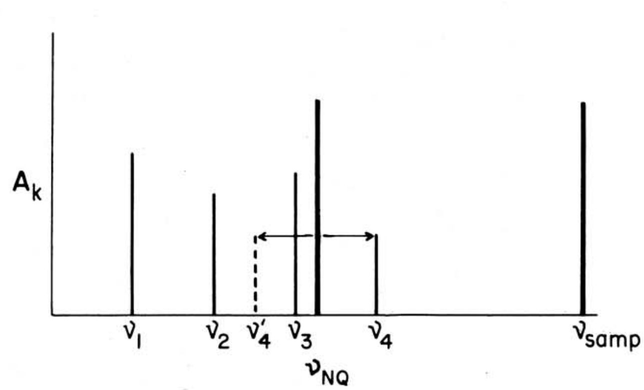

Figure 3. How a frequency ν_4 greater than the Nyquist frequency ($\nu_{NQ} = \nu_{samp}/2$) generates an alias at ν_4'.

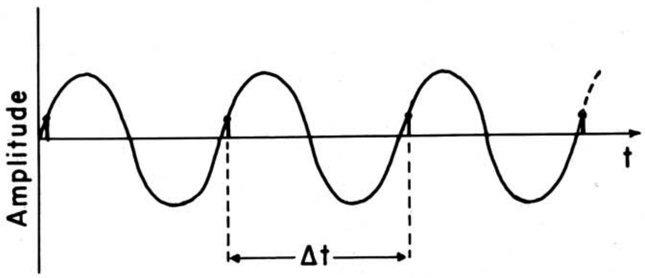

Figure 4. An example of aliasing when the sampling time (Δt) and the period (T) are the same. Sampling gives a constant signal and so generates an alias at $\nu' = 0$.

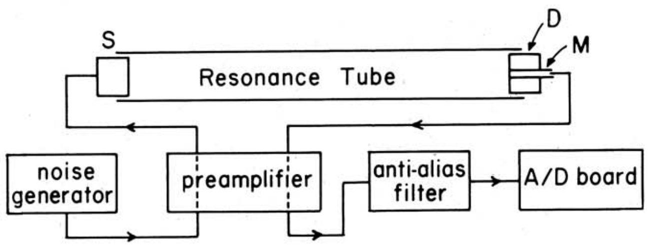

Figure 5. A block diagram of the FFT apparatus for determining the velocity of sound.

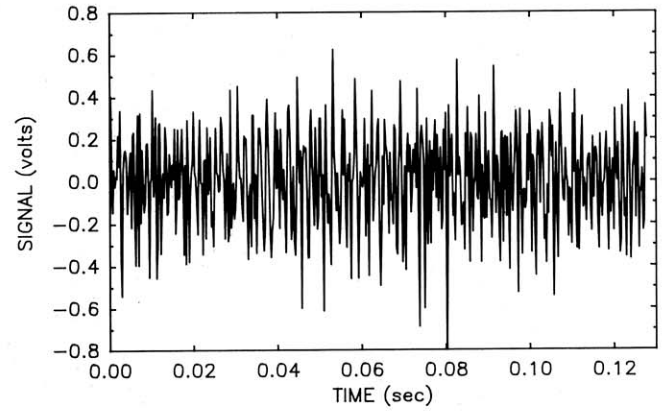

Figure 6. The time record of 512 data values sampled every 250 μs. The gas is dry air at 23.3 °C.

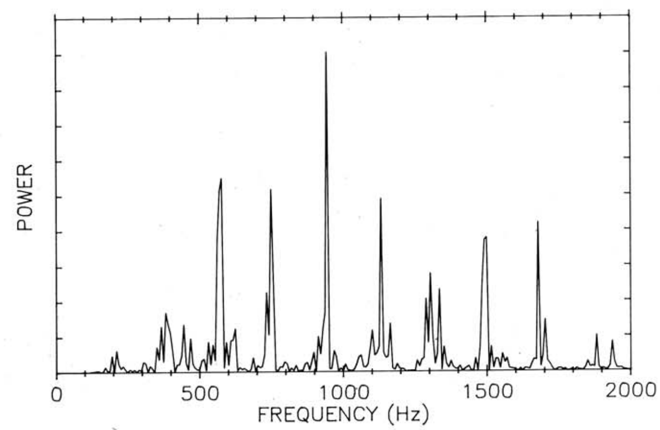

Figure 7. Fourier transform of the data in Figure 6. Since Δt = 250 μs, $\nu_{NQ} = \Delta t/2$ = 2.0 kHz.

Before proceeding we should also clarify a common misconception, namely that the Nyquist theorem means that only two data points are required to establish a frequency. Since N samples are collected during a time T_R, N samples span one period of the fundamental frequency ($\nu_1 = 1/T_R$). In the same way, $N/2$ samples span one period of the first overtone ($\nu_2 = 2/T_R$), but the samples are gathered for two periods. Finally, for the highest overtone with frequency $(N/2) \cdot (1/T_R)$, although only two samples are gathered in one period, we actually sample for $N/2$ periods to obtain a "composite sketch" of that frequency component. The Nyquist limit answers the question, "where does our ability to trade off points per period for number of periods sampled end?" The answer is when we have two or fewer points per period in our time record.

Experimental

A block diagram of the apparatus is shown in Figure 5. Since noise encompasses all frequencies, a noise generator is a suitable broad-band sound source. Such generators are readily available or can be easily constructed by amplifying the noise across a diode junction (*14*). Even a detuned FM radio with the antenna removed can act as a source. If necessary, the noise signal can be amplified by a simple audio preamplifier (Radio Shack SA10) before it is used to drive a small speaker (S) mounted at one end of the resonance tube (T), which is simply a 1-m glass tube (i.d. = 48 mm). We have found that the speaker in a conventional telephone receiver works well. Such speakers have a response up to about 5 kHz, which is adequate for this experiment, see Figure 9 below. A small electret microphone (M) (Radio Shack 33-1052) is a suitable detector for the pressure fluctuations. It should be mounted in a disc (D) made of some hard material such as Lucite that acts as a reflective surface for the sound waves. This assembly is installed at the opposite end of the tube from the speaker. If gases other than air are to be used, the tube should be provided with inlet and outlet ports for adding gases and the apparatus made reasonably leak tight. In our case, since the diameters of S and D were comparable to the i.d. of the glass resonance tube, we found that carefully applied electrical tape worked well and allowed ready disassembly of the apparatus. The microphone signal is fed via the second channel of the preamplifier and an anti-alias filter to the A/D board (Data Translations DT2801) in the IBM/PC computer. Ideally the filter should pass all frequencies up to the Nyquist limit (ν_{NQ}) and none above that. Specifically designed commercial filters are readily available, but a filter that falls off well enough for the experiment can easily be constructed from readily available components (*14, 15*). We constructed a third-order low-pass active filter with a 3-dB cutoff frequency at 2 kHz. This filter had the following transmittances at 2, 3, 4, and 5 kHz—0.71, 0.25, 0.13, 0.06. Most of the A/D board manufacturers provide sample programs for digital data acquisition; there are also commercial packages. As mentioned above we used a slightly modified version of the FFT program given in ref *1* for the transformation of this digitally acquired data. Using a compiled Basic program (Microsoft Basic v. 4.0), our smallest sampling time was 73 μs, which corresponds to a sampling frequency of 13.7 kHz.

The FFT software together with the A/D board and the PC compose a spectrum analyzer, which will be found in many physics laboratories. Such an item can be useful in setting up the equipment.

Results and Discussion

A typical time record is shown in Figure 6. Five hundred twelve data points were gathered with a sampling time (Δt) = 250 μs so that T_R = 128 ms. The FFT is shown in Figure 7,

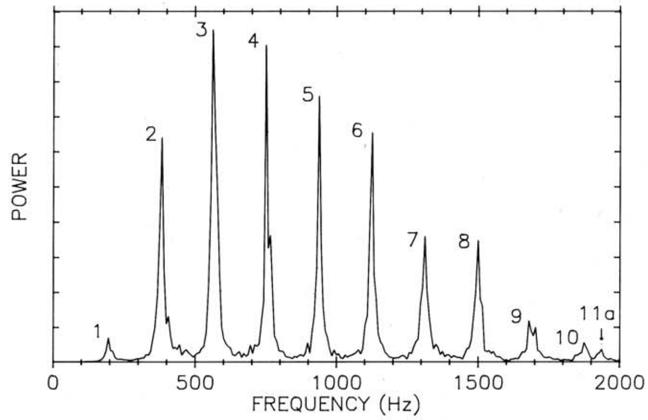

Figure 8. The result of averaging a spectrum like that in Figure 7 10 times. The peak labeled 1 is the fundamental, 2 is the first overtone, and so on. Peak 11 occurs above the Nyquist limit and shows up as the alias labeled 11a.

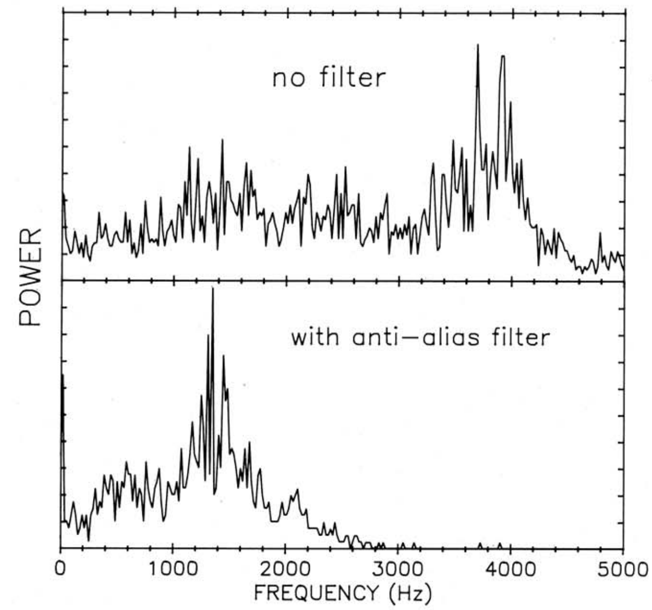

Figure 9. Power spectrum of the source in the absence and presence of the anti-alias filter. Notice that frequencies above 2 kHz are still present accounting for the alias peak in Figure 8.

while the very beneficial effect of carrying out 10 iterations and averaging is displayed in Figure 8. Notice that we have chosen to display the results as a power, rather than amplitude, spectrum where power(ν) is proportional to amp(ν)^2. This is a common practice in FFT experimentation to make peaks stand out somewhat more sharply from the background and small unwanted peaks. For example, an alias peak that is 10% of a real peak on an amplitude scale is only 1% of the real peak on a power scale. Also notice that frequencies not in resonance do indeed destructively interfere and so have negligible power components.

Since our filter did not fall off sufficiently sharply above ν_{NQ}, an alias peak (indicated 11a) can be seen. If the experiment is repeated without the filter, alias peaks become more prominent and so can be readily distinguished. If the alias peaks fall too close to the true resonances, they can be shifted by varying the sampling frequency which changes ν_{NQ}. A spectrum of the noise source can be obtained by sampling the speaker output in the absence of the resonance tube. This is shown in Figure 9, where it will be seen that some frequencies above 2 kHz do get past the filter accounting for the alias peak 11a in Figure 8.

The values of the resonance maxima are easily determined by examining a tabular output of the data displayed in Figure 8. A plot of the resonance maxima versus n yields a straight line with slope $187.4 \pm 0.4\ s^{-1}$. Using this value and $L = 916.9$ mm, gives $v_s = 343.6 \pm 0.7$ m/s (see eq 3), which compares very favorably with the accepted value (345.0 m/s) for the speed of sound in dry air at 296 K. Six sets of independent experiments taken over a period of weeks gave $v_s = 343.3 \pm 1.1$ m/s; the slightly larger error probably reflects the fact that in each experiment a new value of L was used. Indeed the technique is sufficiently precise so that the small difference in the velocity of sound in such similar gases as nitrogen (347.8 m/s) and oxygen (328.9 m/s) can be measured, so that the traditional experiment of measuring heat capacity ratios γ ($v_s = (RT_\gamma/M)^{1/2}$) of different gases can be carried out with excellent accuracy.

More significantly, through the experiment the student learns about important characteristics of FFT; these include:

(1) Primary data in the time domain (Fig. 6) may look hopelessly complex, but nevertheless they yield simple interpretable data when transferred into the frequency domain (Figs. 7 and 8).

(2) The experiment can be performed by using a frequency generator to scan through the frequencies sequentially and observing the amplitude of the signals on an oscilloscope. This corresponds to the usual way of taking a spectrum. However, a FFT spectrometer is inherently more efficient than a conventional scanning instrument because the sample is irradiated with all frequencies simultaneously. This allows a FFT spectrum to be recorded in a shorter time than a conventional spectrum—an advantage commonly referred to as the Fellgett advantage (*3*, *6*). Because of rapid data acquisition, averaging over many runs becomes quite feasible, especially since the data are gathered digitally and are already in the computer. The resulting improvement in signal-to-noise ratio often results in enhanced sensitivity. The 512 data points in Figure 7 were gathered in 128 ms. Carrying out the actual Fourier transformation may be slower. In our case, using a simple IBM/PC equipped with a math coprocessor chip and using a compiled Basic program, an individual FFT took 14 s.

(3) In a conventional spectrometer excitation radiation is generally selected by instrumental elements such as slits and a monochromator that limit the energy throughput. In a FFT instrument there can be a large energy throughput because such elements are absent. This advantage is usually referred to as the Jacquinot advantage (*3*, *6*).

(4) In a FFT experiment both the lowest frequency and the frequency resolution are controlled by the time of record (T_R), while the highest frequency (ν_{NQ}) is controlled by the sampling frequency (ν_{samp}).

(5) In an FFT experiment care has to be taken so that the sampling frequency is at least twice as great as the highest frequency in the source otherwise alias resonances may appear.

(6) An FFT spectrometer is a multiplex device in that a single signal channel and detector simultaneously handle all frequencies.

Besides these points the experiment provides a good pedagogic forum for exemplifying: (a) the properties of noise, (b) A/D methods, (c) regression analysis, (d) data averaging, (e) constructive and destructive interference of waves, and (f) boundary conditions. Although the establishment of standing waves defined by boundary conditions is important both practically (e.g., lasers) and theoretically (e.g., quantum mechanics), chemistry students are rarely exposed to a practical example.

Those wishing detailed information about the equipment, including circuits and programs, may obtain this by writing directly to the authors.

Acknowledgment

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