

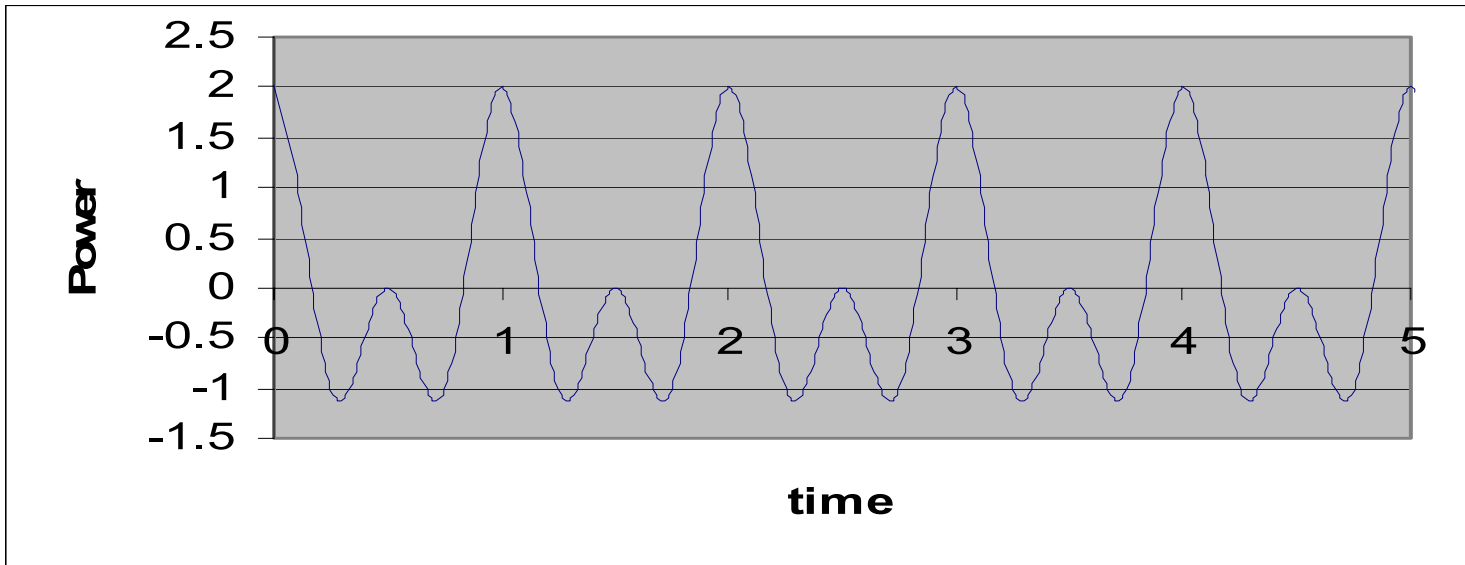
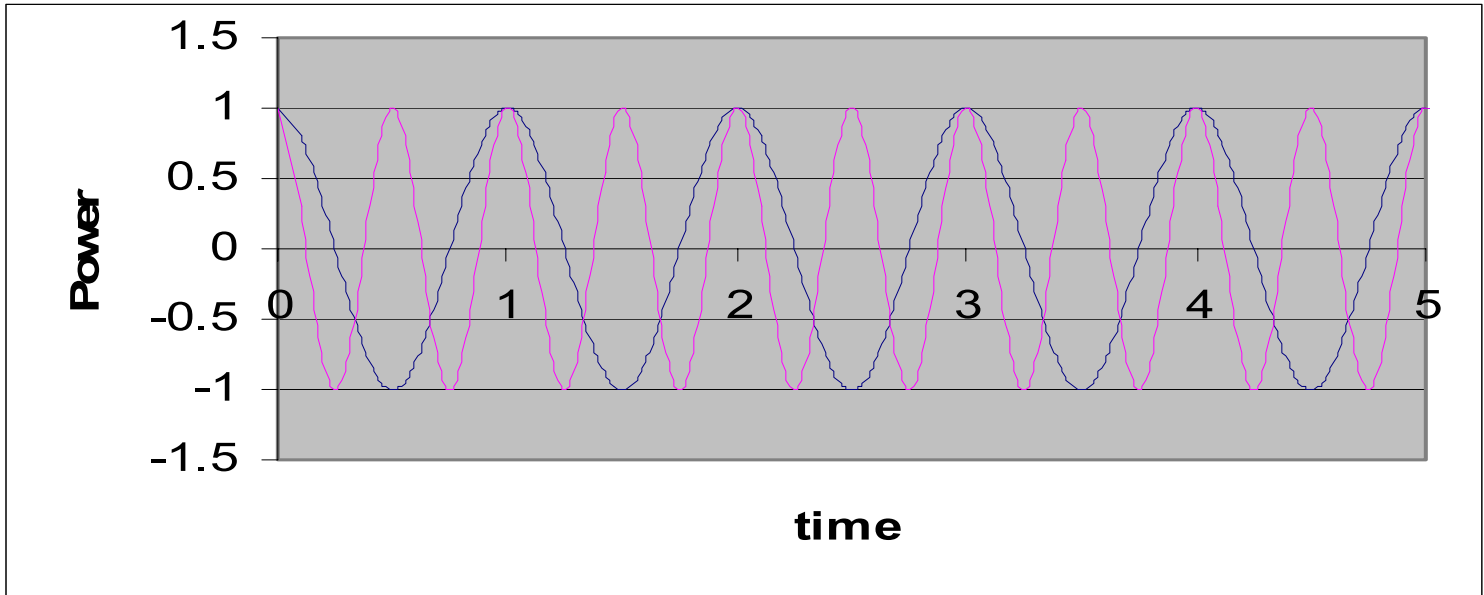
Fourier Transform

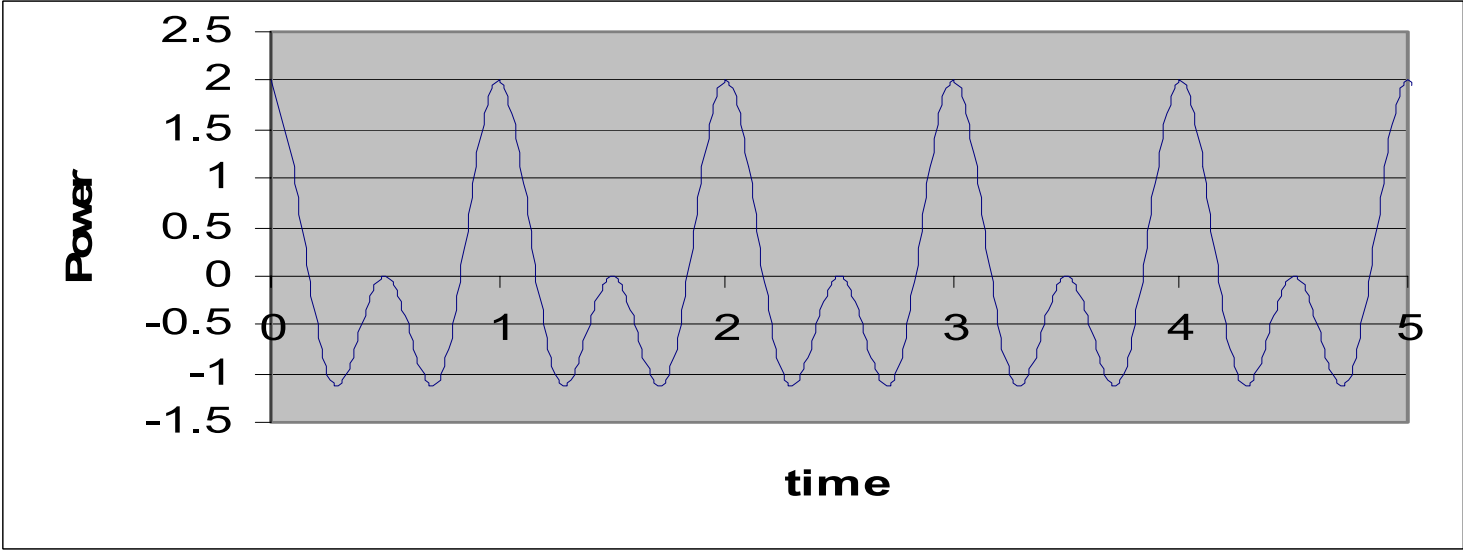
Why learn about Fourier Transform?

- FT-IR
- FT-NMR
- FT-MS

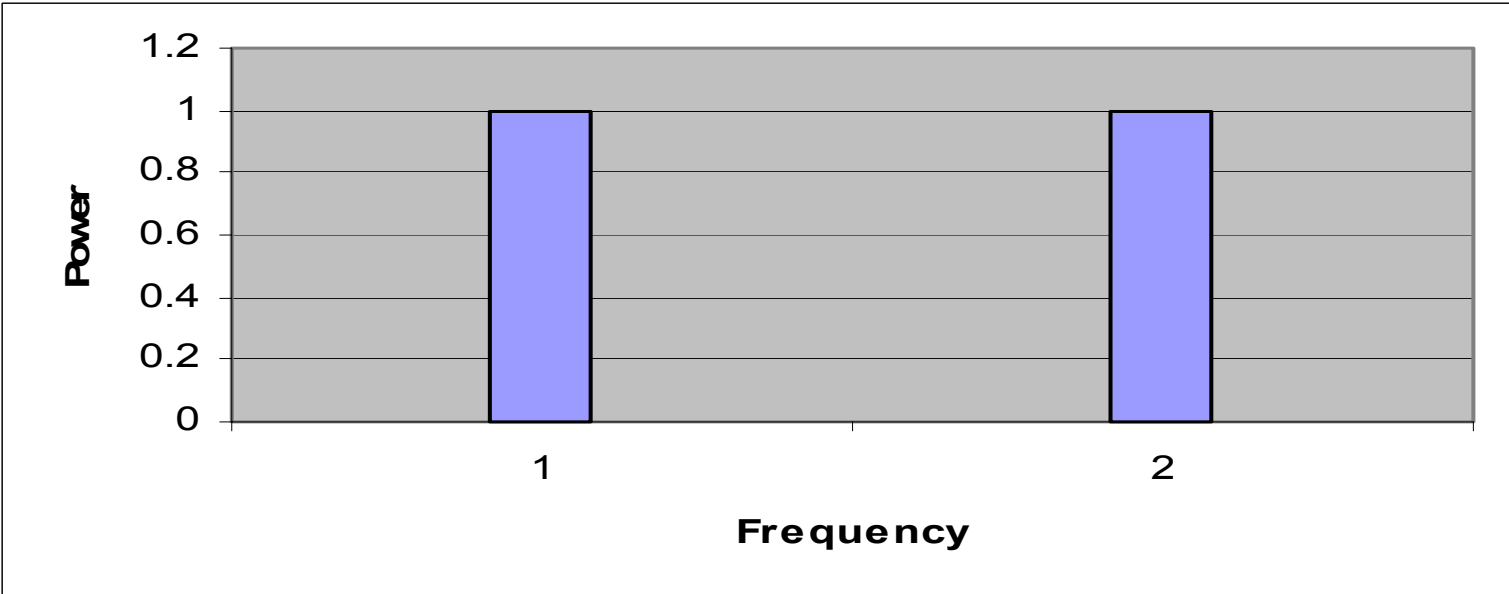
What is a Fourier Transform?

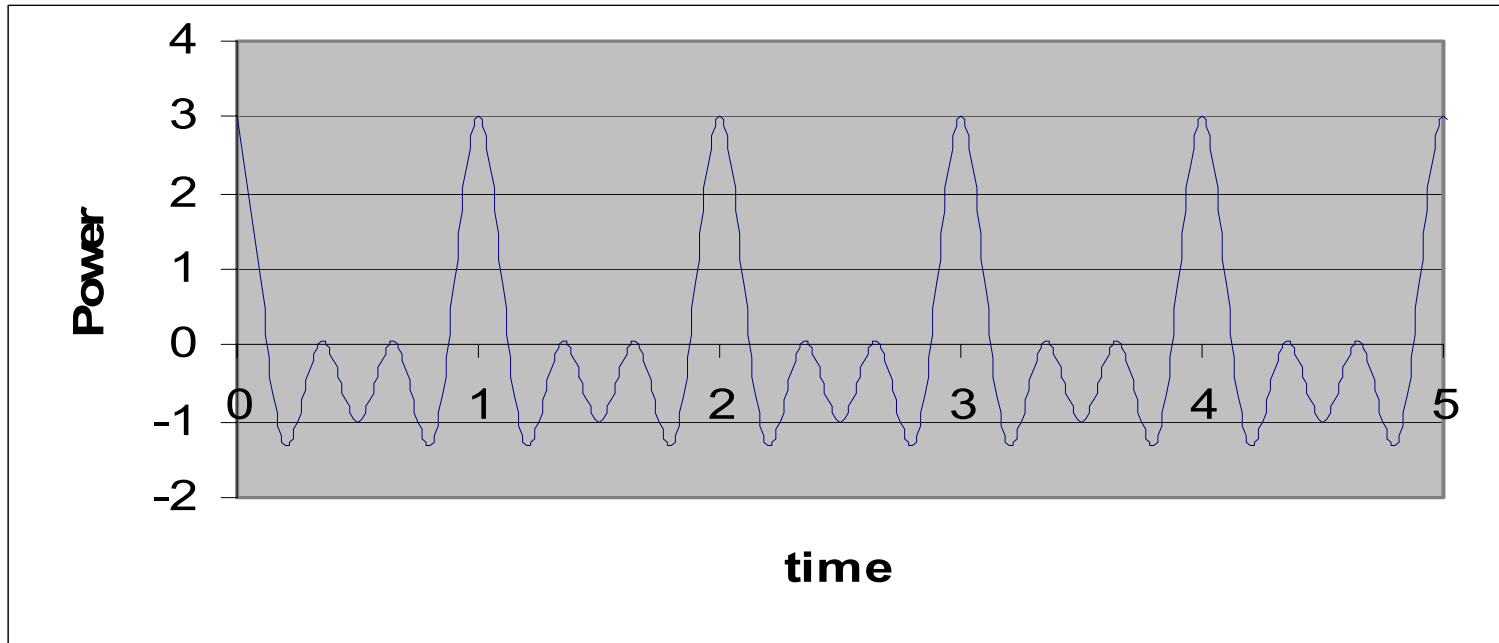
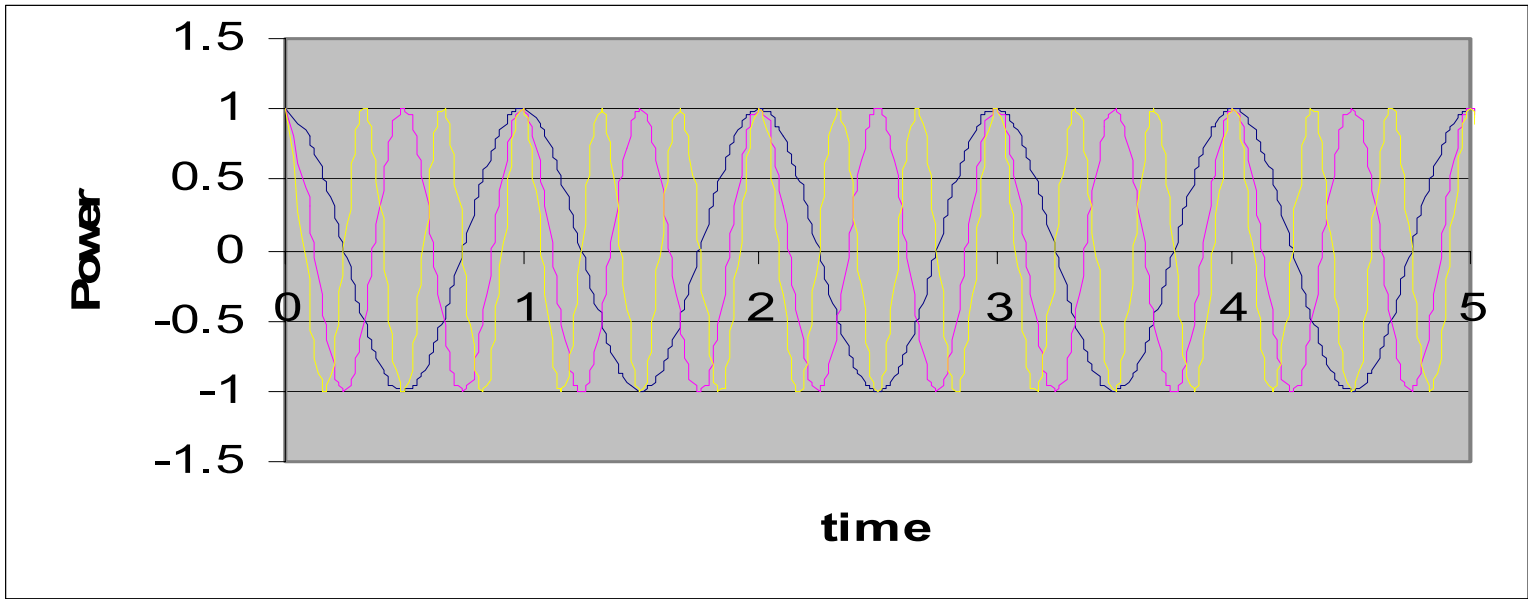
- For a sinusoidal signal, it allows you to convert from (to) the time domain to (from) frequency domain
- $P(t) \leftrightarrow P(\nu)$
$$P(t) = \int k \cos(2\pi\nu_x t)$$
- Implication: collect signal as a function of time, no dispersion as a function of frequency is needed

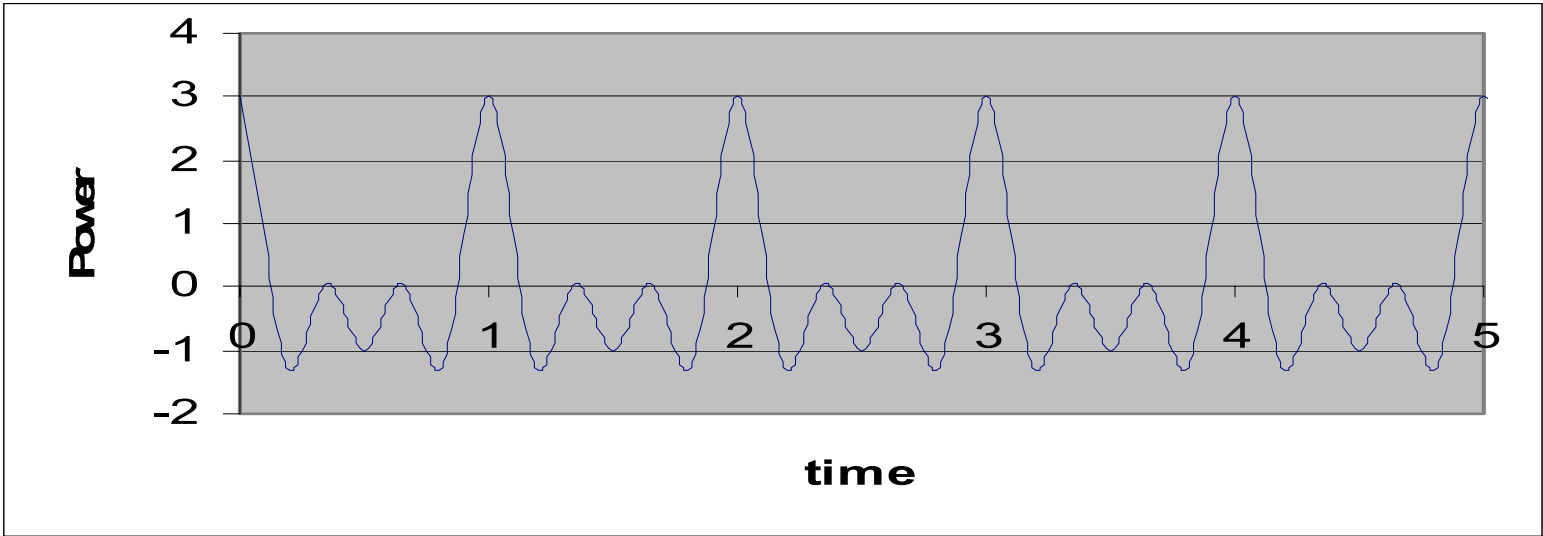




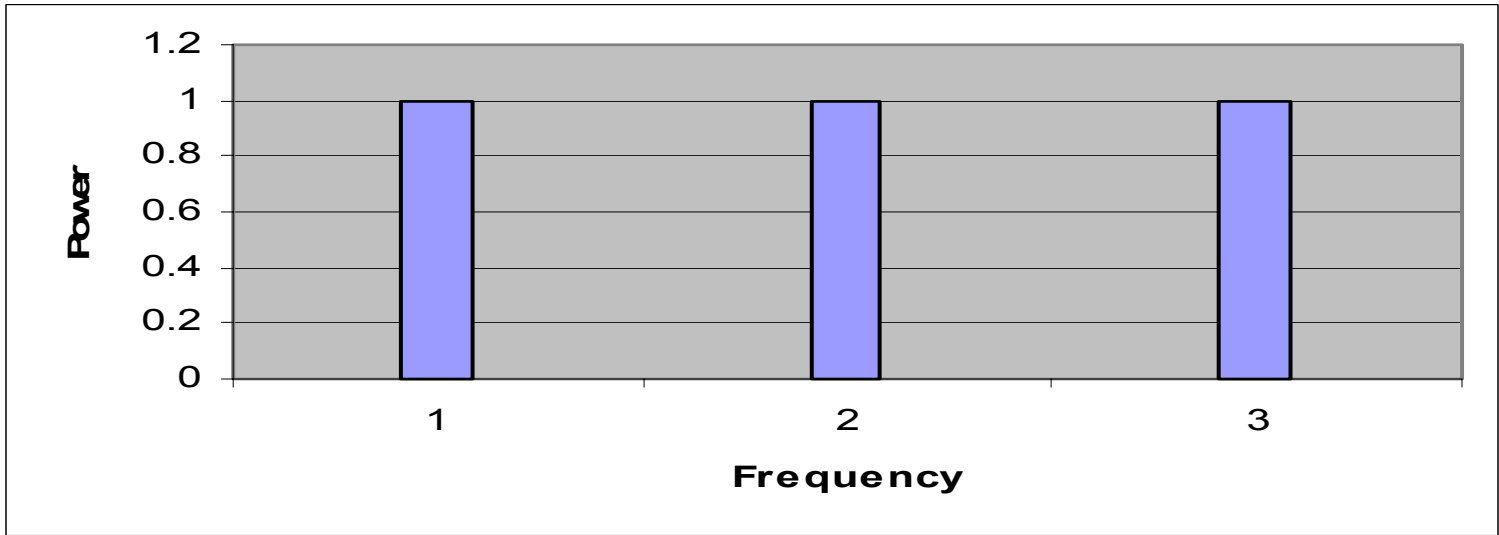
FT
↓

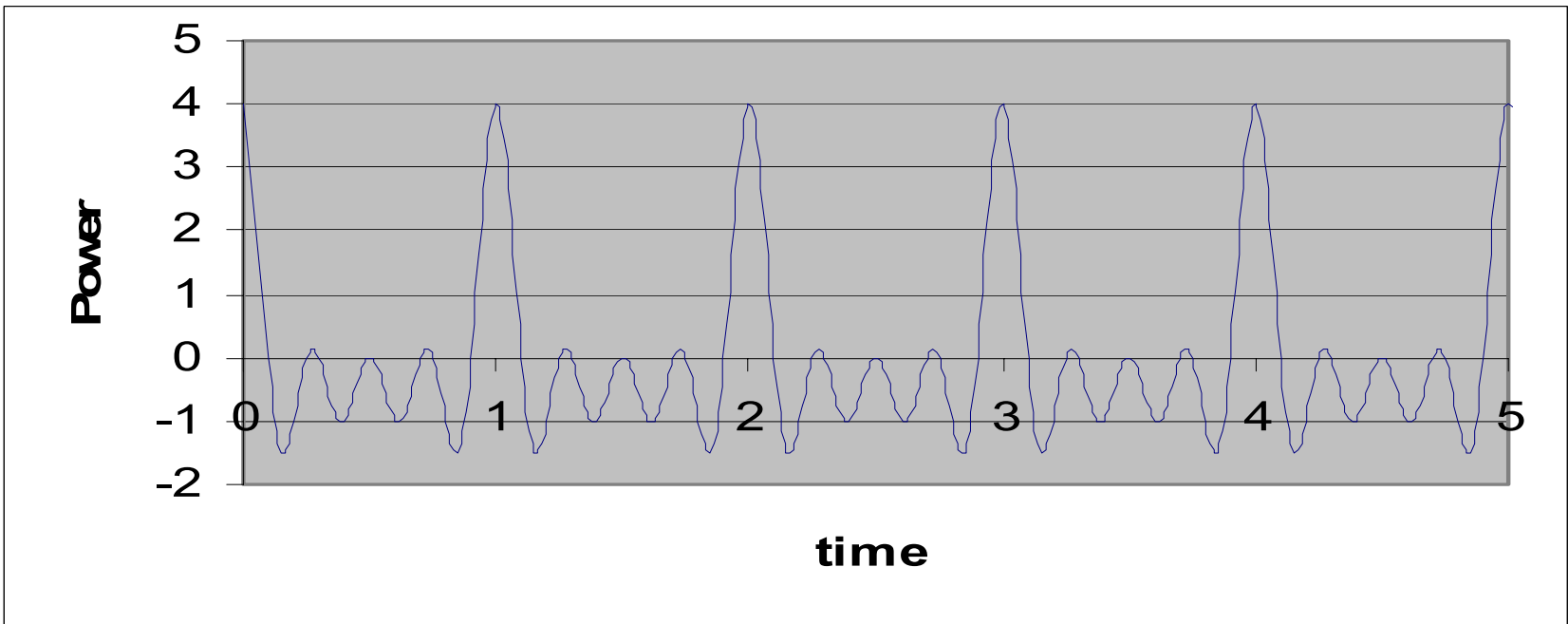
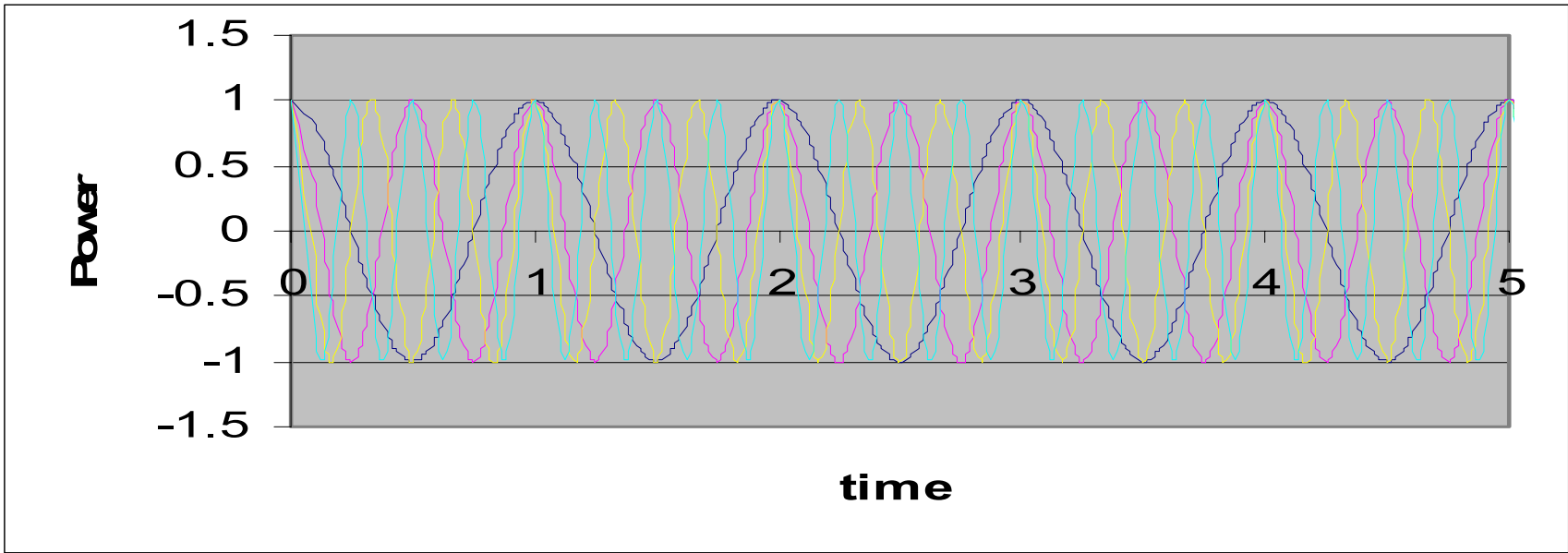


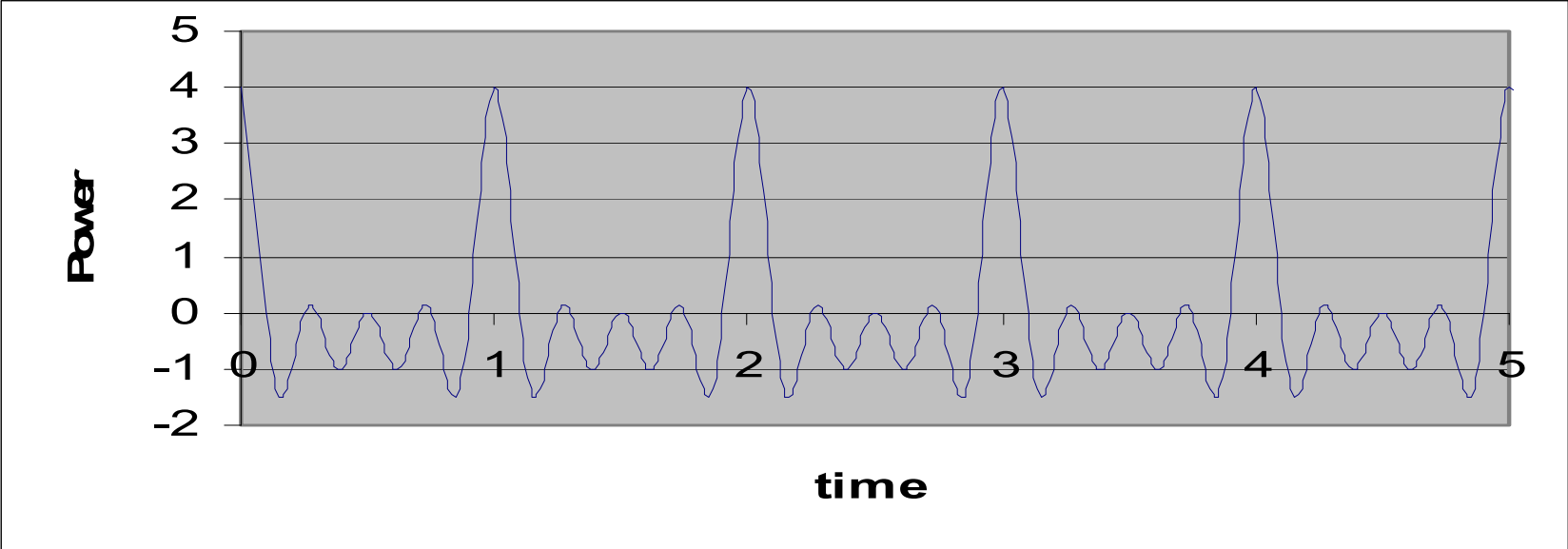




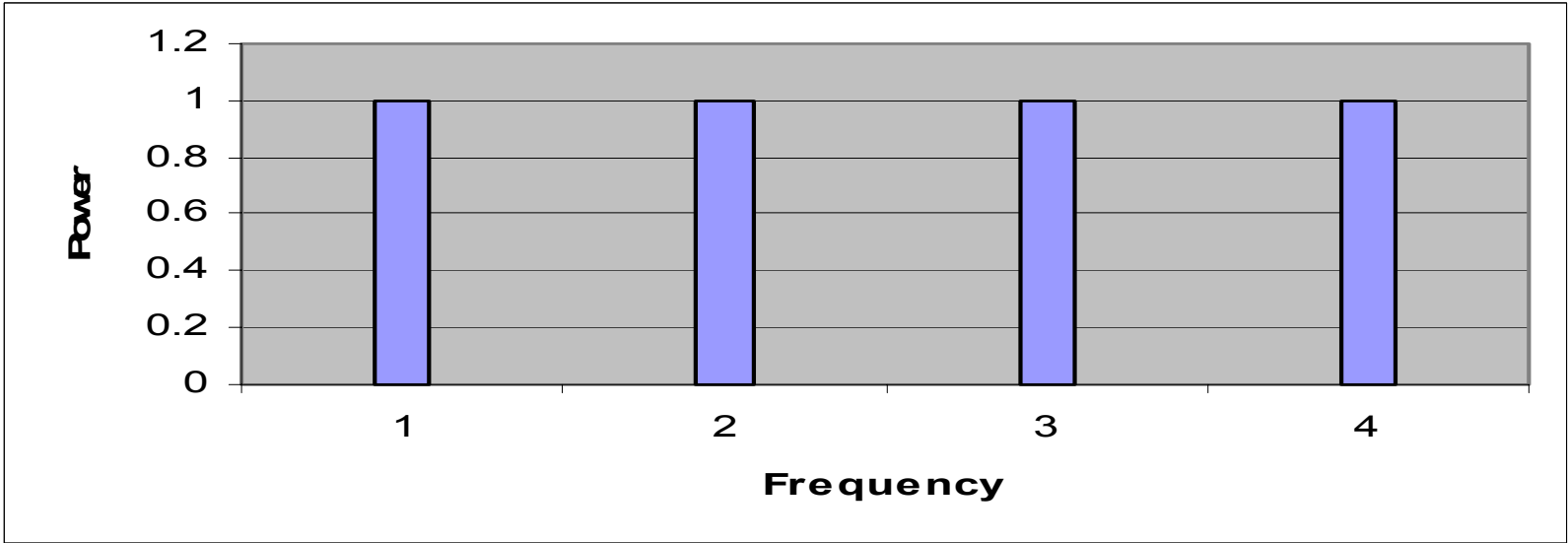
FT
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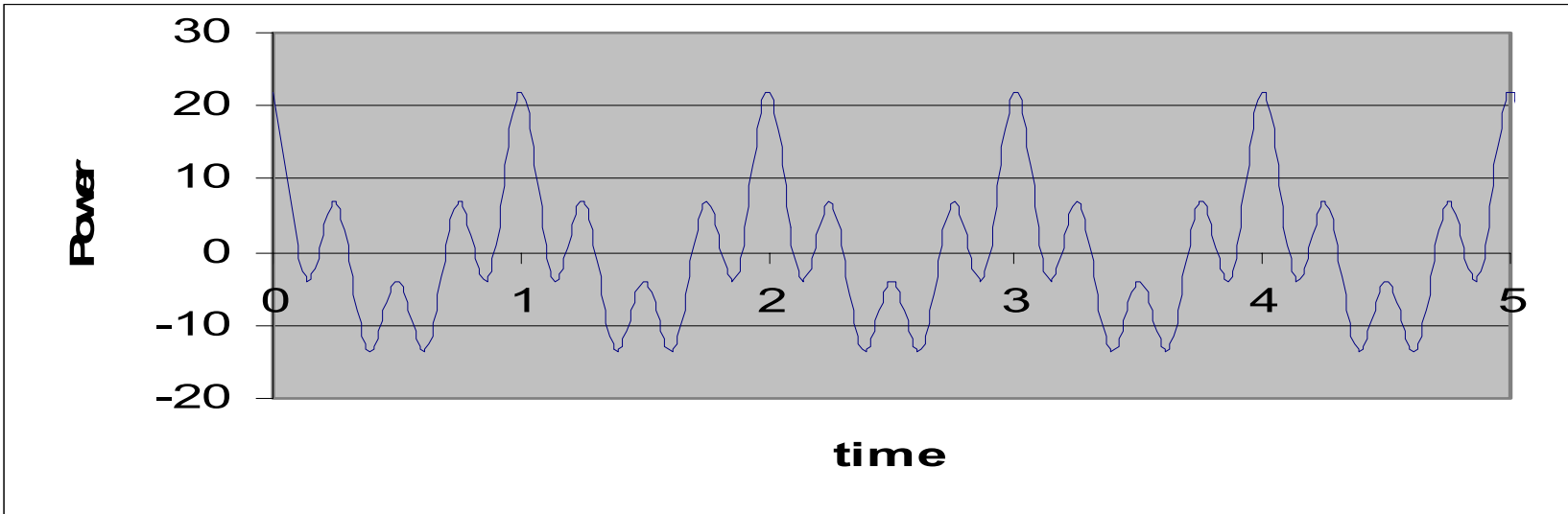




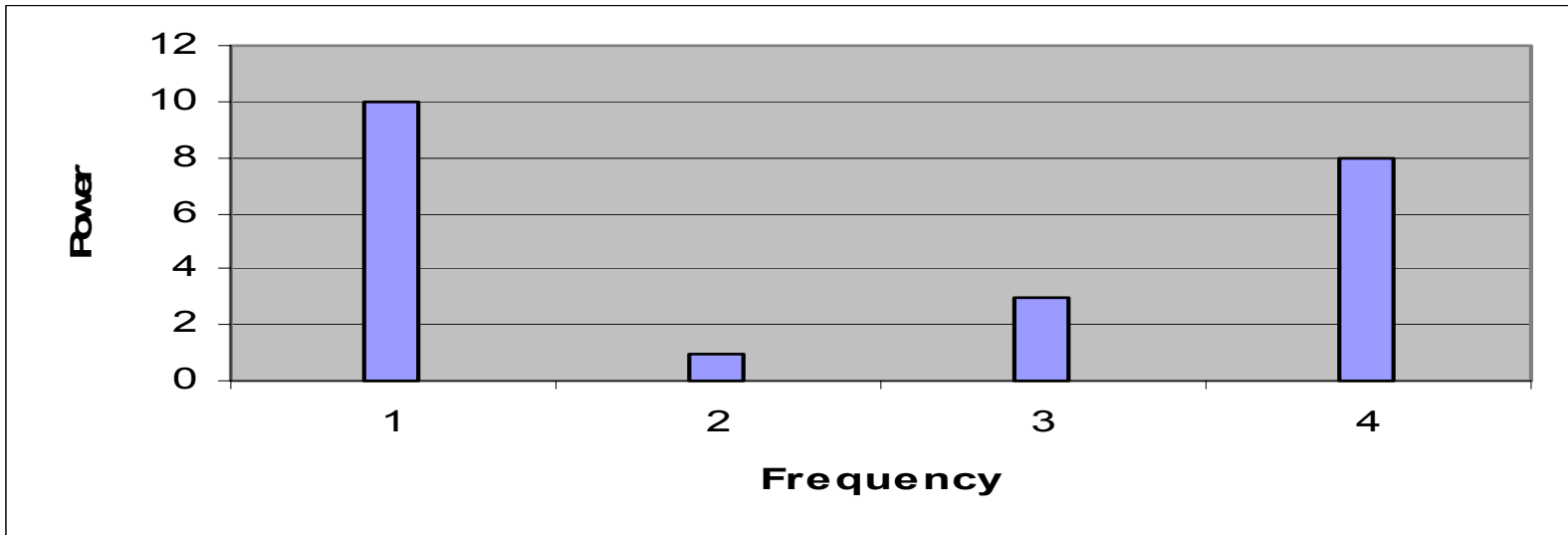


FT
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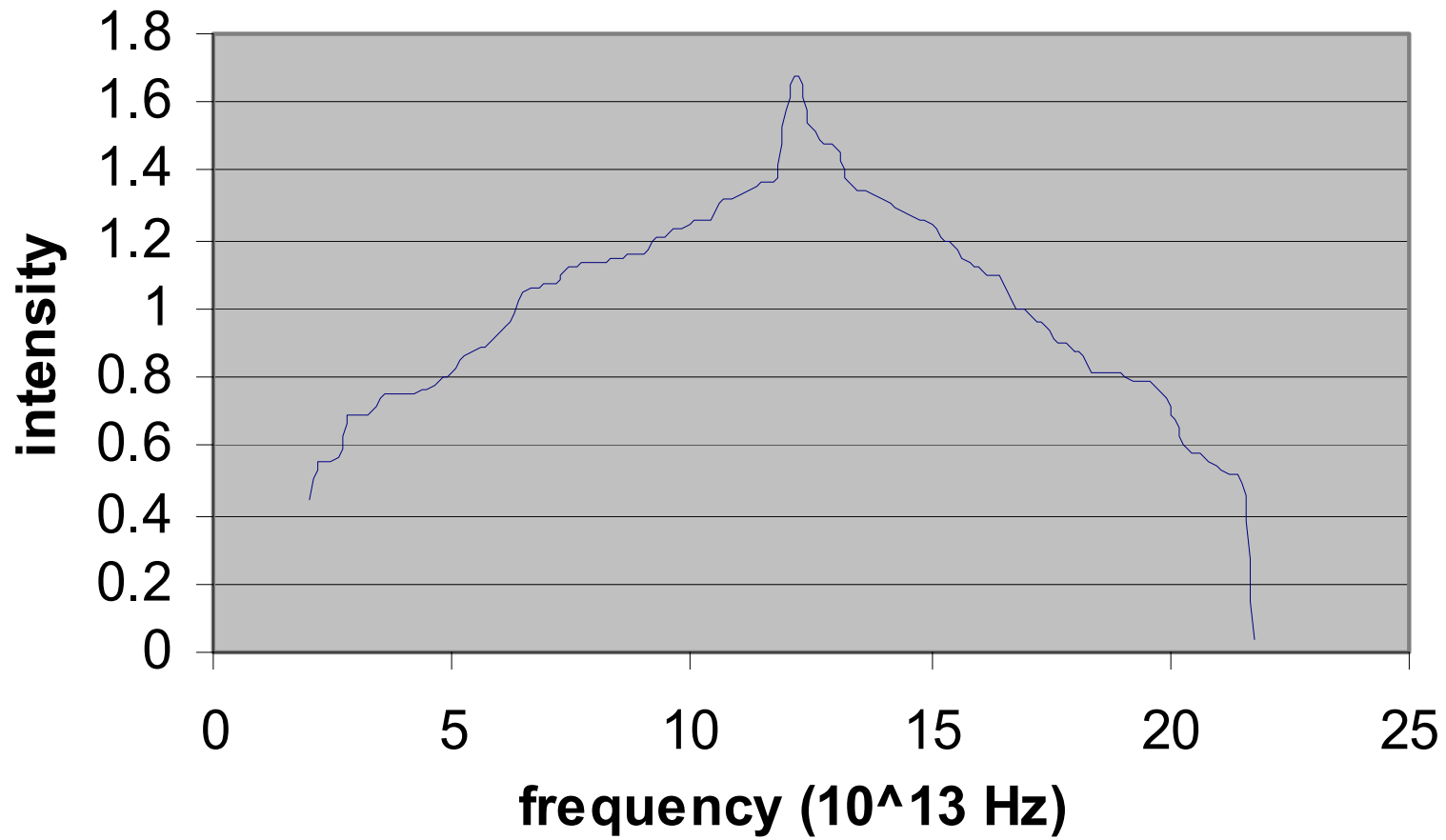


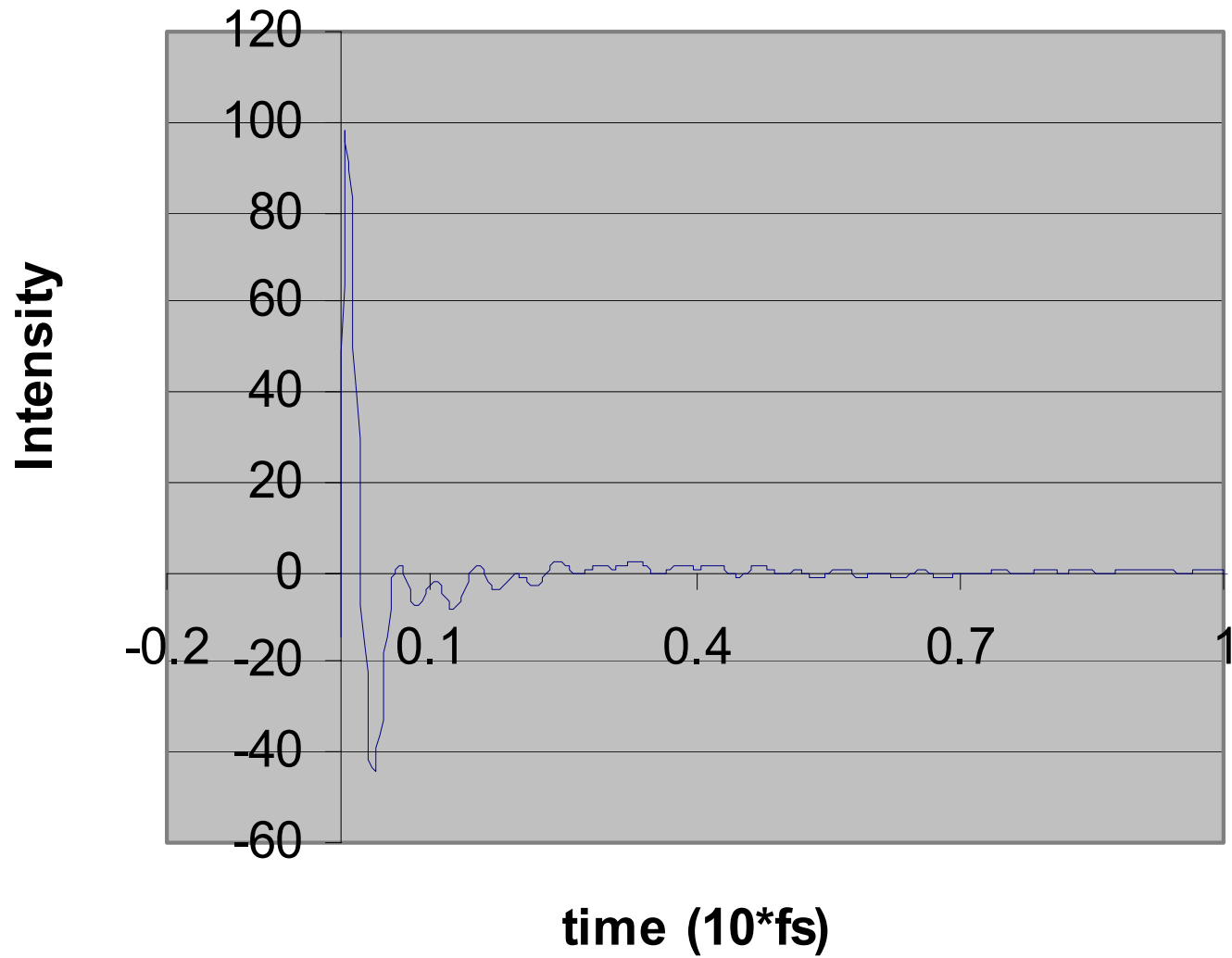
FT
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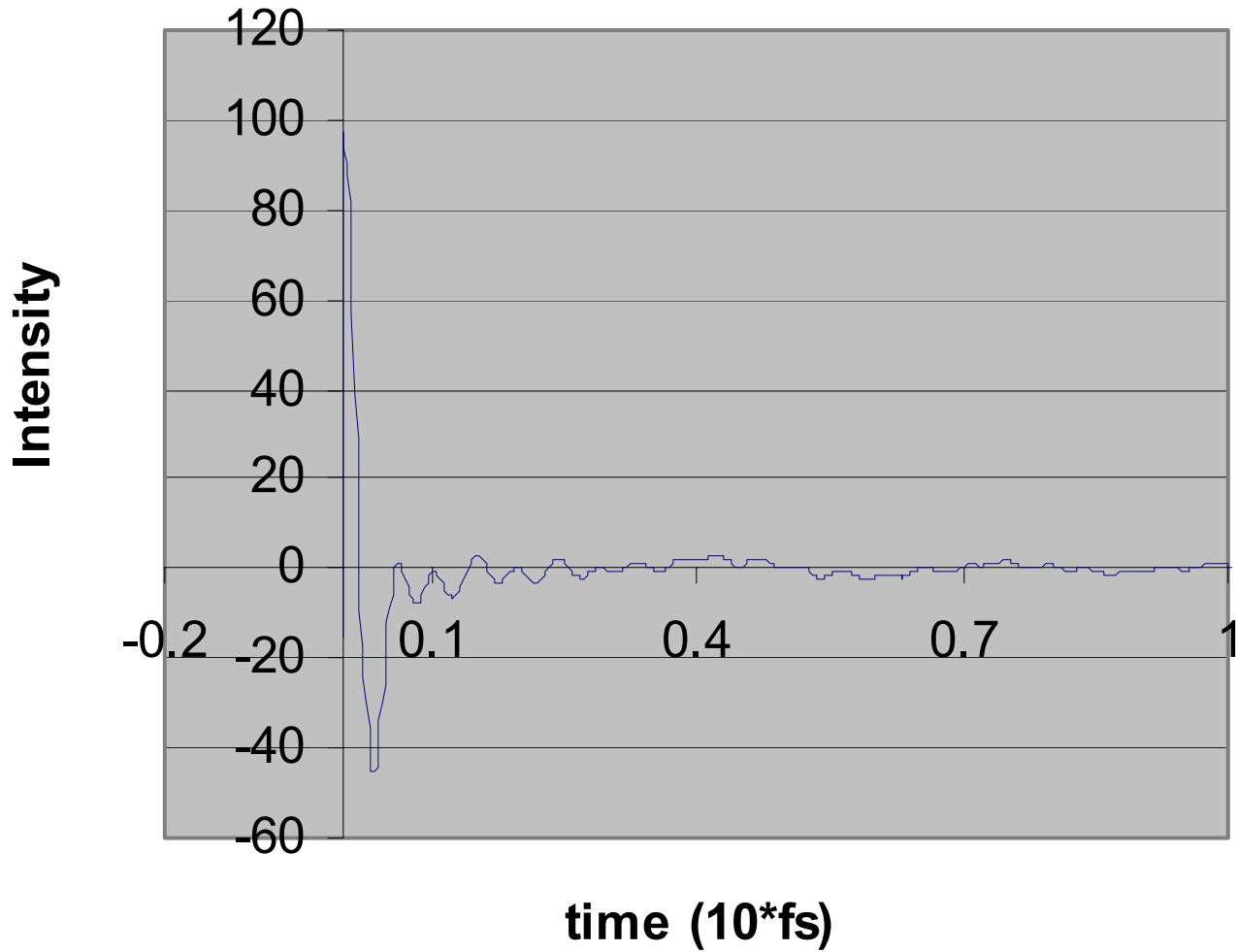
Free Induction Decay (FID)

- A Continuous range of frequencies gives a free induction decay due to destructive interferences
- A continuous range of frequencies will never all be in-phase again

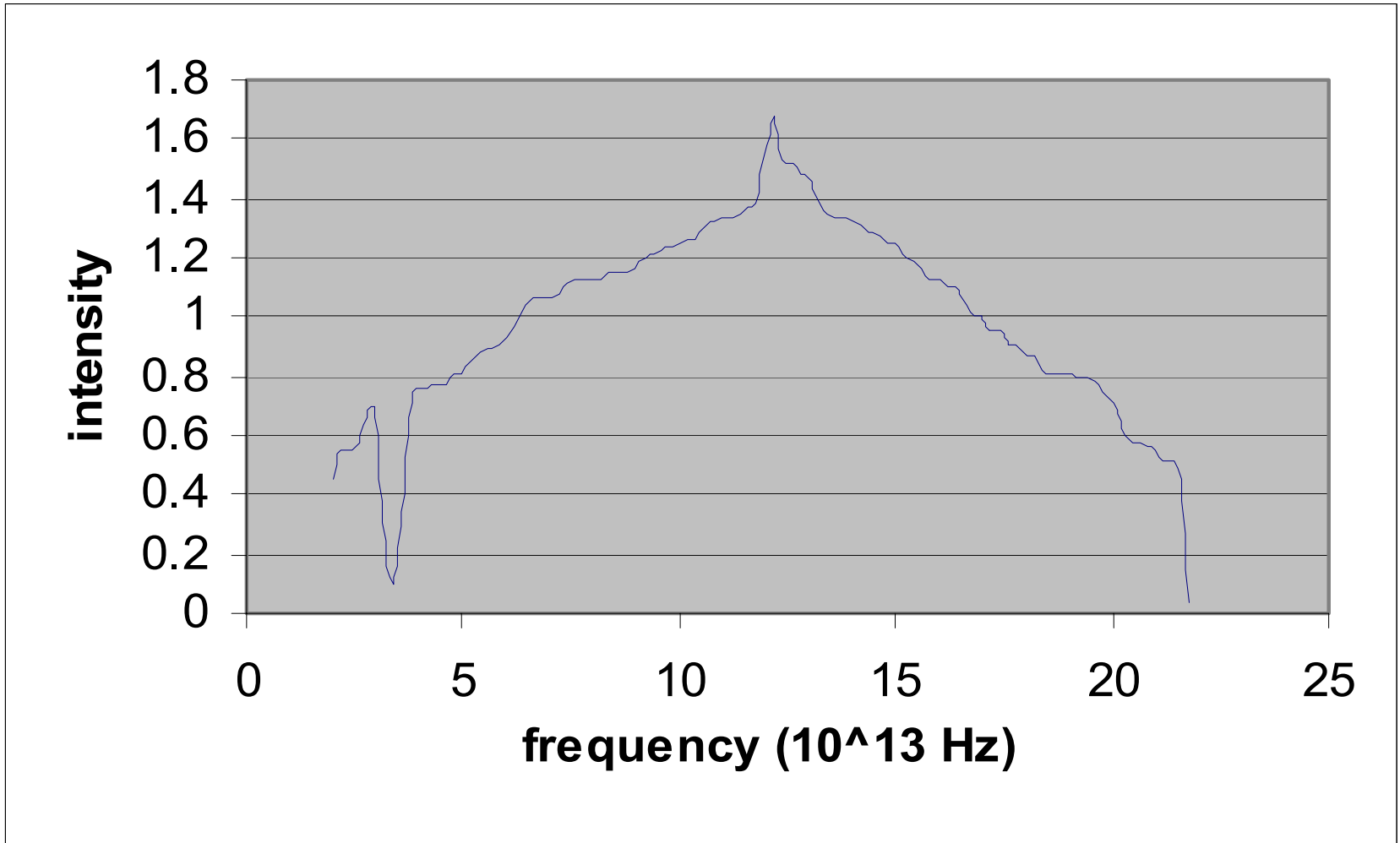




Sample FID



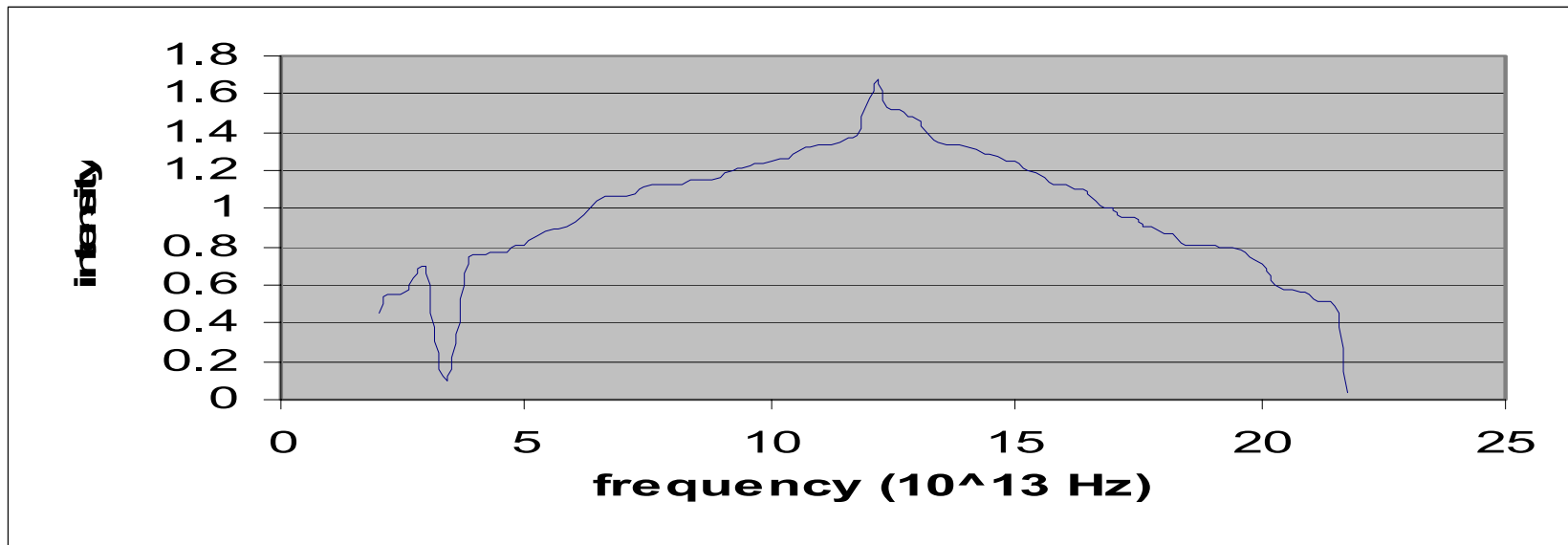
Sample



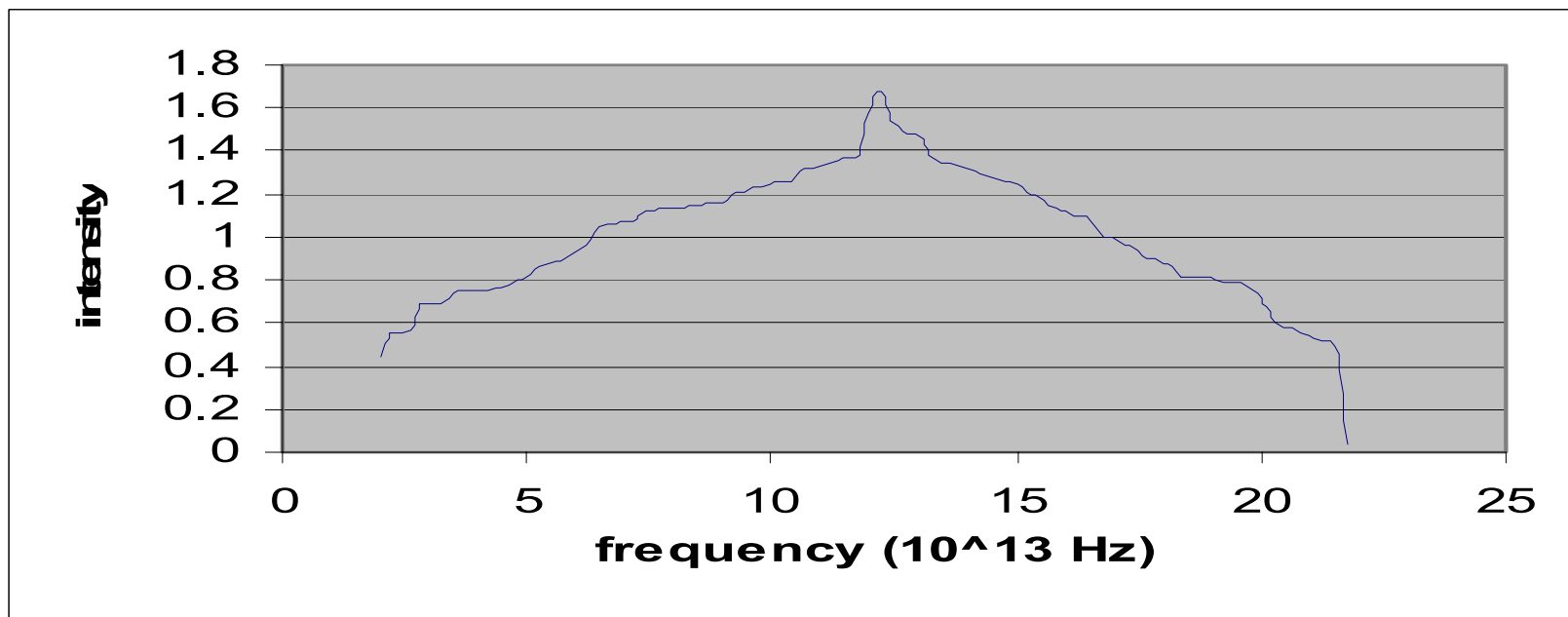
Calculating the FT-IR Spectra

- $\%T = 100 \cdot (P/P_0)$ at each frequency
- Plot $\%T$ vs. frequency
- Actually most often we plot $\% T$ vs wavenumber (λ^{-1} or ν/c) in cm^{-1}

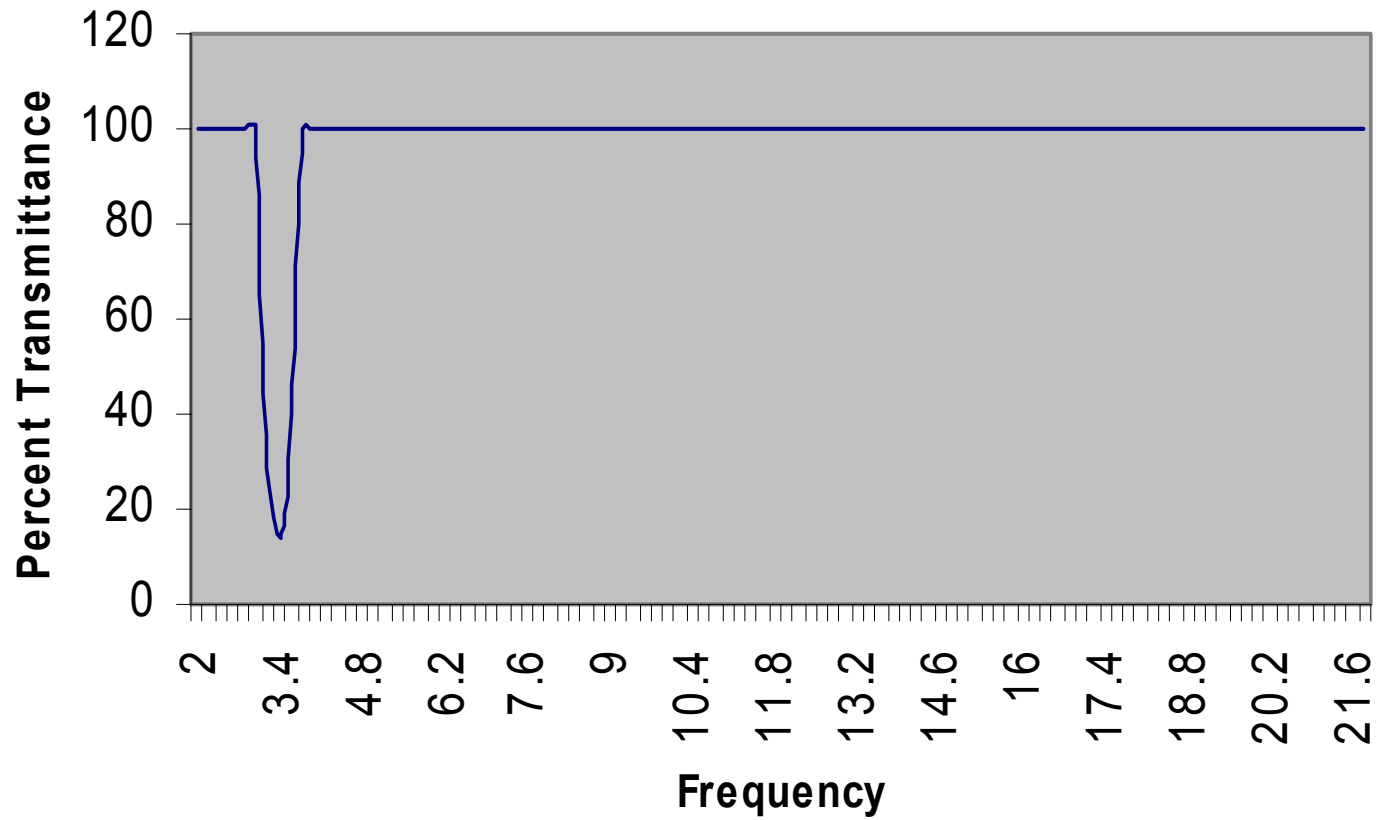
Sample



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FT-IR Spectrum



Fourier Transform-Infrared Spectroscopy

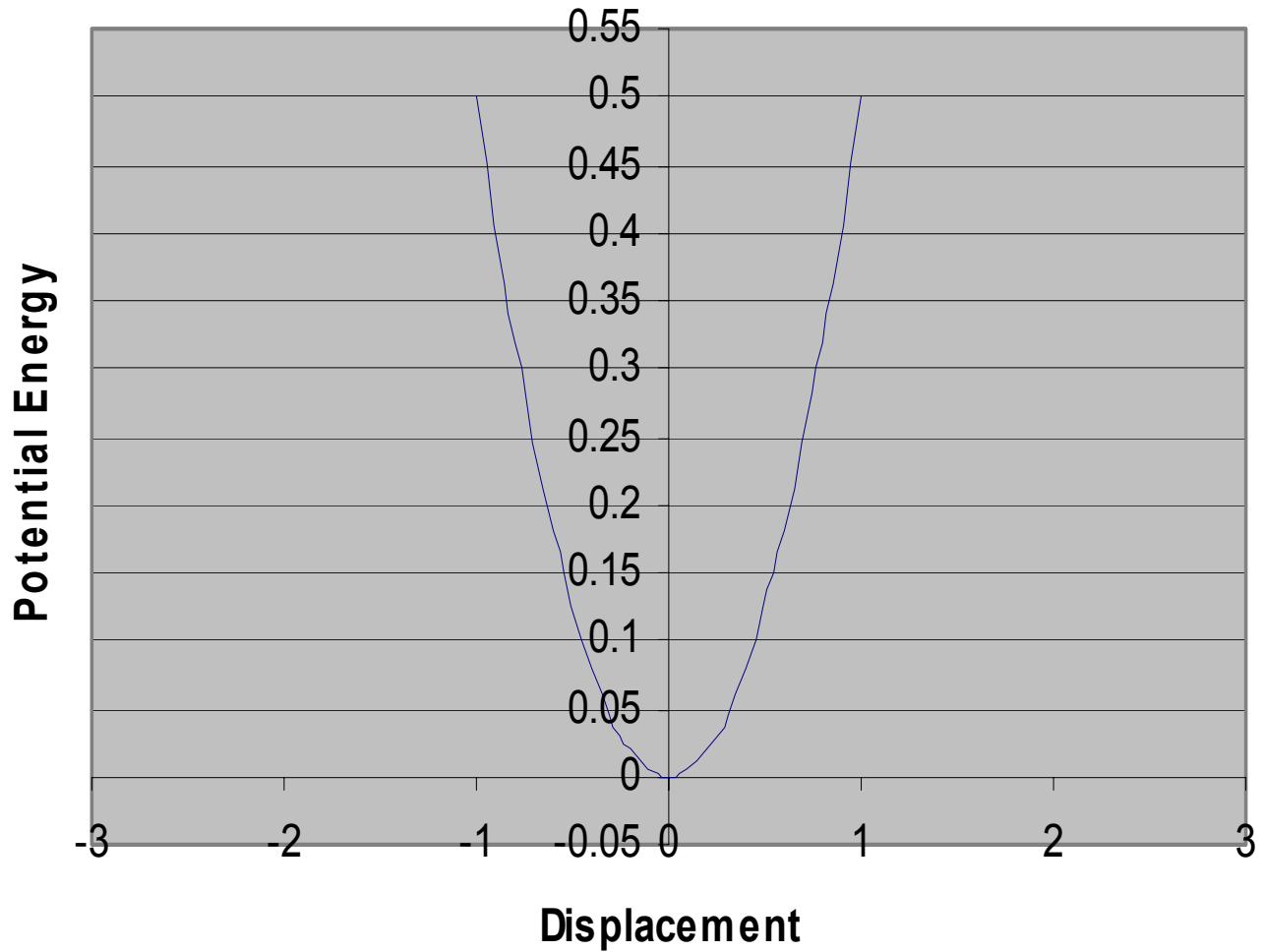
FT-IR

Probing molecular vibrations

- Harmonic oscillator – $\Delta E = h\nu = (h/2\pi)(k/\mu)^{1/2}$
- Selection rules
- $3N-6$ ($3N-5$ for linear molecules)
- Must undergo a change in dipole moment to be active
- Anharmonic oscillator
 - Overtones
 - Sums and differences

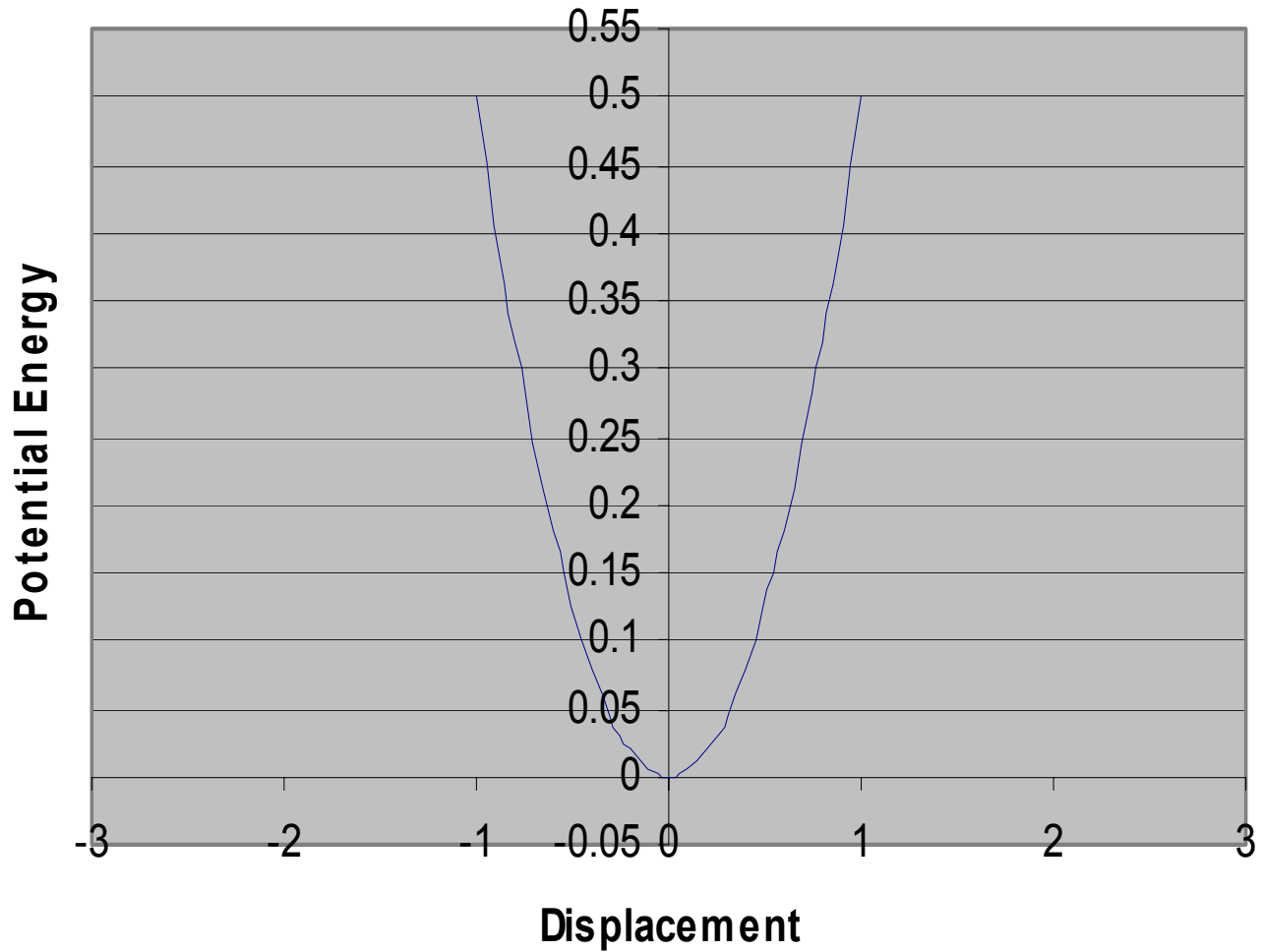
Harmonic oscillator

- $PE = \frac{1}{2} ky^2$
- Classical treatment of molecular vibrations
 $\Delta E = h\nu = (h/2\pi)(k/\mu)^{1/2}$



Quantum Treatment

- $\Delta E = (n + \frac{1}{2}) h/2\pi (k/\mu)^{1/2}$
 - Quantization
 - Ground vibrational level



Anharmonic oscillator

- Selection Rules, $\Delta v = \pm 1$
- Total number of vibrations in a molecule
 - $3N-6$ ($3N-5$ for linear molecules), N = number of atoms in the molecule
 - Example; CH_2OH , 9 independent vibrations

Complications

- Overtones; Δv between energy levels decrease at higher energies and $\Delta n = 2$ or 3 is possible
- Sums and differences
- Coupling- influenced by neighbors
- Must have Change in Dipole Moment to be IR active
 - O=C=O

Functional Group Analysis

- Vibrational energy depends on the type of atoms bonded together and the bond order
- As a result different functional groups give unique absorption stretches
- IR spectra tells you whether you have an alcohol or and aldehyde
- Correlation Chart (pg 412-413)