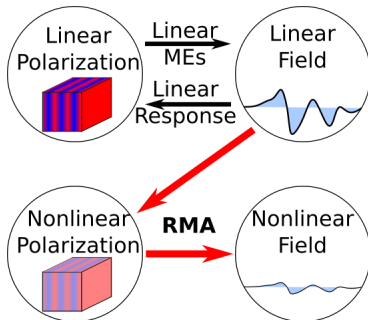


# Introduction to Spectroscopic Methods

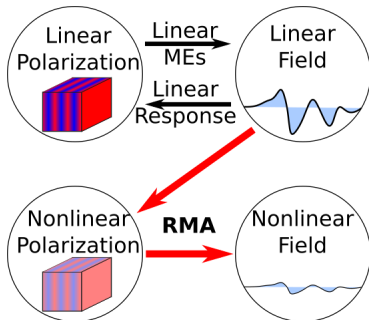
Mike Reppert

September 23, 2019

## Electrodynamics and Response Theory



## Electrodynamics and Response Theory



**Today:** Course Schedule + Intro to Methods

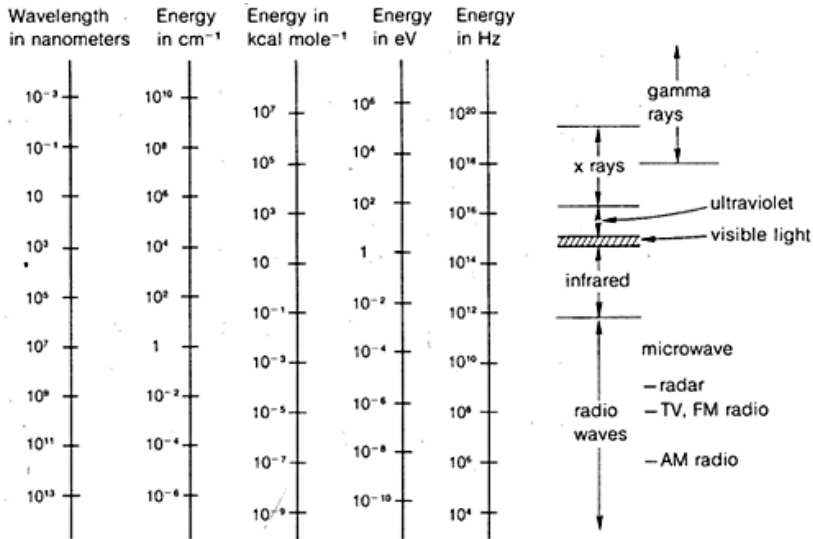
## Schedule:

<https://mreppert.github.io/education/chm676/schedule.pdf>

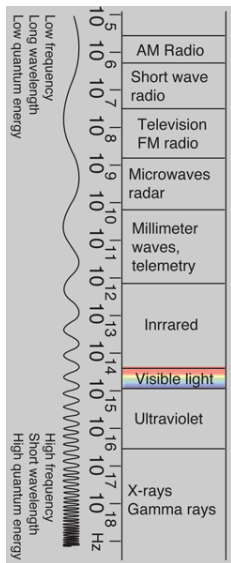
## Final Project:

<https://mreppert.github.io/education/chm676/project.pdf>

# Time and Frequency in Molecular Spectroscopy



[https://chem.libretexts.org/Bookshelves/Organic\\_Chemistry/Book%3A\\_Basic\\_Principles\\_of\\_Organic\\_Chemistry\\_\(Roberts\\_and\\_Caserio\)/09%3A\\_Separation%2C\\_Purification%2C\\_and\\_Identification\\_of\\_Organic\\_Compounds/9.03%3A\\_Why\\_Cannot\\_We\\_See\\_Molecules%3F](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Book%3A_Basic_Principles_of_Organic_Chemistry_(Roberts_and_Caserio)/09%3A_Separation%2C_Purification%2C_and_Identification_of_Organic_Compounds/9.03%3A_Why_Cannot_We_See_Molecules%3F)



<http://hyperphysics.phy-astr.gsu.edu/hbase/ems1.html>

# Time and Frequency in Molecular Spectroscopy

Spectroscopic technique	Energy range of absorbed radiation (in wave numbers, $\text{cm}^{-1}$ ) <sup>a</sup>	Type of excitation produced by absorbed radiation	Information obtained
Ion cyclotron resonance	$10^{-6}$ to $10^{-5}$	Excitation of ions moving in circular orbits in a magnetic field	Rates and equilibria for reactions of ions with neutral molecules in the gas phase (Section 27-8)
Nuclear magnetic resonance (nmr)	$10^{-4}$ to $10^{-2}$	Changes in nuclear spin orientations in a magnetic field	Chemical shifts and coupling constants; rapid reaction rates (Sections 9-10, 27-1, and 27-2)
Electron spin resonance (esr)	$10^{-2}$ to 1	Excitation of unpaired electron-spin orientations in a magnetic field	Electron distribution in radicals, electron-transfer reactions (Section 27-9)
Microwave	1 to 100	Rotational excitation	Spacings of rotational energy levels; bond distances and bond angles (Section 9-6)
Infrared (ir)	100 to 10,000	Rotational-vibrational excitation	Rotational and vibrational energy levels of molecules (Section 9-7)
Raman	100 to 4,000	Rotational-vibrational excitation	Rotational and vibrational energy levels of molecules (Section 9-8)
Visible	5,000 to 25,000	Electronic excitation accompanied by vibration-rotation changes	Electronic energy levels of molecules (Section 9-9)
Ultraviolet	25,000 to 50,000	Electronic excitation accompanied by vibration-rotation changes	Electronic energy levels of molecules (Sections 9-9 and 28-1)
Photoelectron	$10^5$ to $10^6$	Ejection of an electron from the valence or inner shell	Ionization energies of valence or inner-shell electrons of molecules (Section 27-5)
Mossbauer	$10^7$ to $10^9$	Excitation of atomic nuclei	Electric-field gradients at the nucleus produced by differences in bond types (Section 27-6)
Mass spectrometry	Excitation produced by electrons with energies of about $10^5 \text{ cm}^{-1}$	Molecular ionization and fragmentation	Molecular weights; modes of fragmentation (Sections 9-11 and 27-7)

<sup>a</sup>These ranges are not meant to be precise, but to give you a general idea of the energy changes involved. One wave number ( $\text{cm}^{-1}$ ) is equivalent to  $2.86 \text{ cal mole}^{-1}$ . Also see Figure 9-7 for comparison with other commonly used units of energy and wavelength.

[https://chem.libretexts.org/Bookshelves/Organic\\_Chemistry/Book%3ABasic\\_Principles\\_of\\_Organic\\_Chemistry\\_\(Roberts\\_and\\_Caserio\)/09%3ASeparation%2CPurification%2C\\_and\\_Identification\\_of\\_Organic\\_Compounds/9.03%3A\\_Why\\_Cannot\\_We\\_See\\_Molecules%3F](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Book%3ABasic_Principles_of_Organic_Chemistry_(Roberts_and_Caserio)/09%3ASeparation%2CPurification%2C_and_Identification_of_Organic_Compounds/9.03%3A_Why_Cannot_We_See_Molecules%3F)