Absorption Spectroscopy

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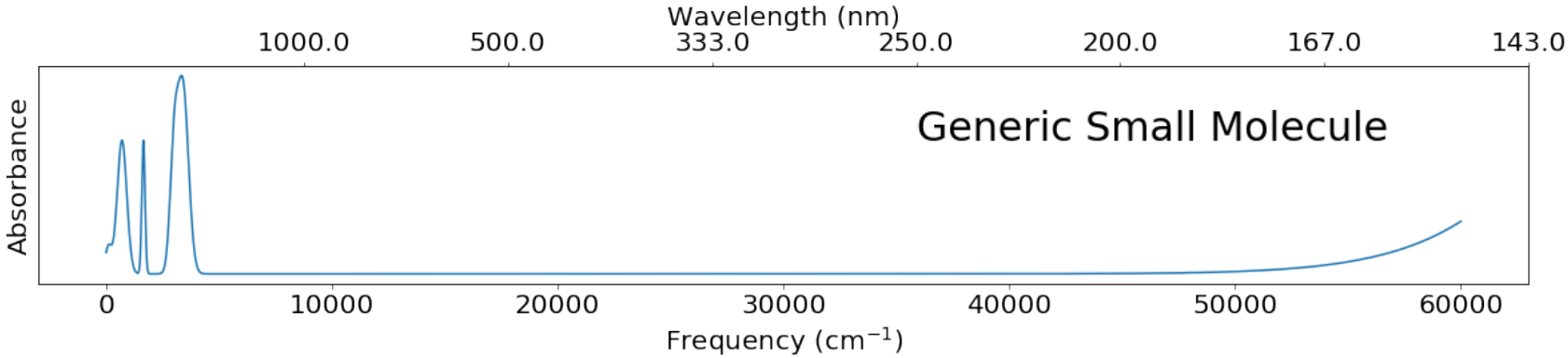
Last Time on CHM676...

Spectroscopic technique	Energy range of absorbed radiation (in wave numbers, cm^{-1})[a]	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 cm^{-1}	Molecular ionization and fragmentation	Molecular weights; modes of fragmentation (Sections 9-11 and 27-7)

[a]These ranges are not meant to be precise, but to give you a general idea of the energy changes involved. One wave number (cm^{-1}) is equivalent to 2.86 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%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

Molecular Absorption Basics



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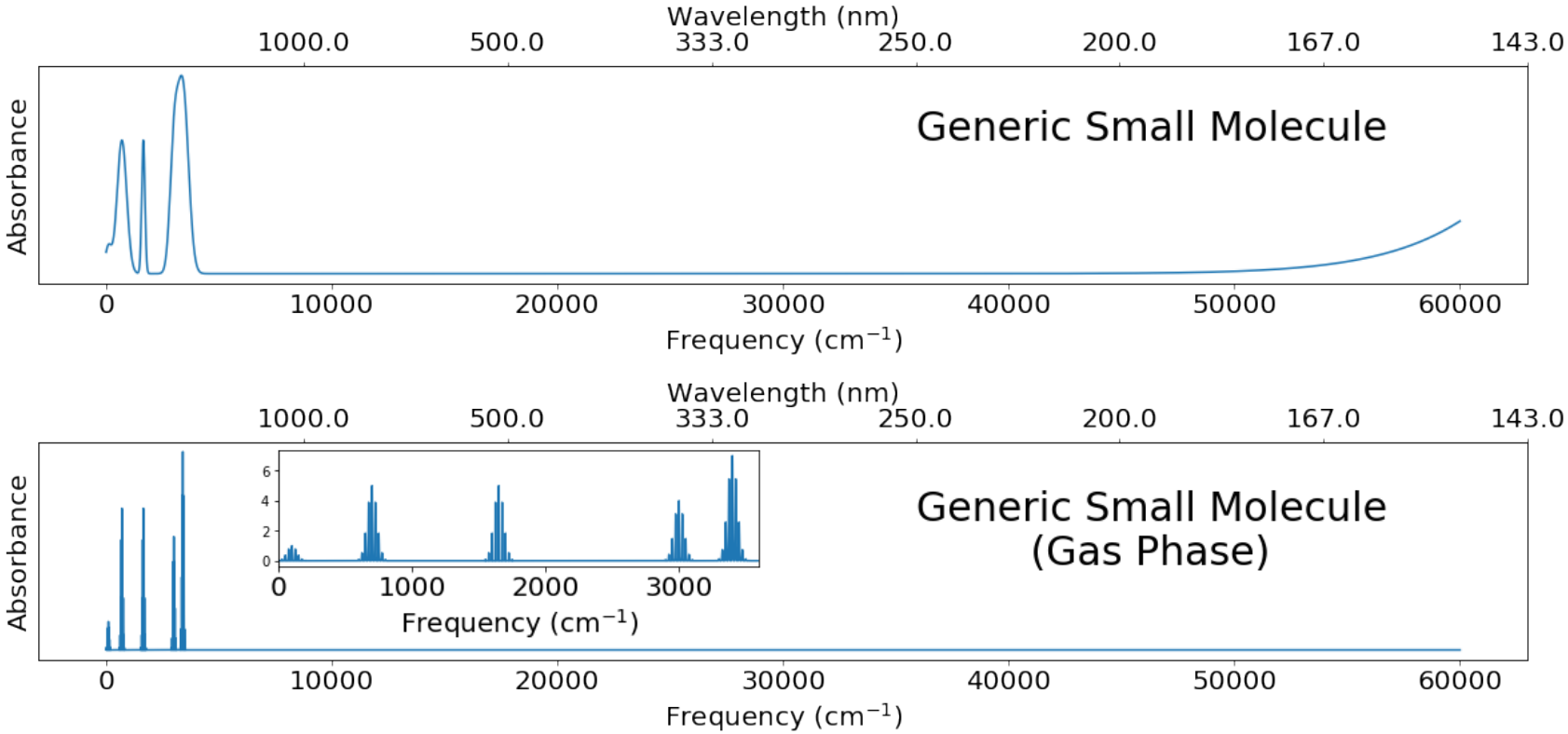

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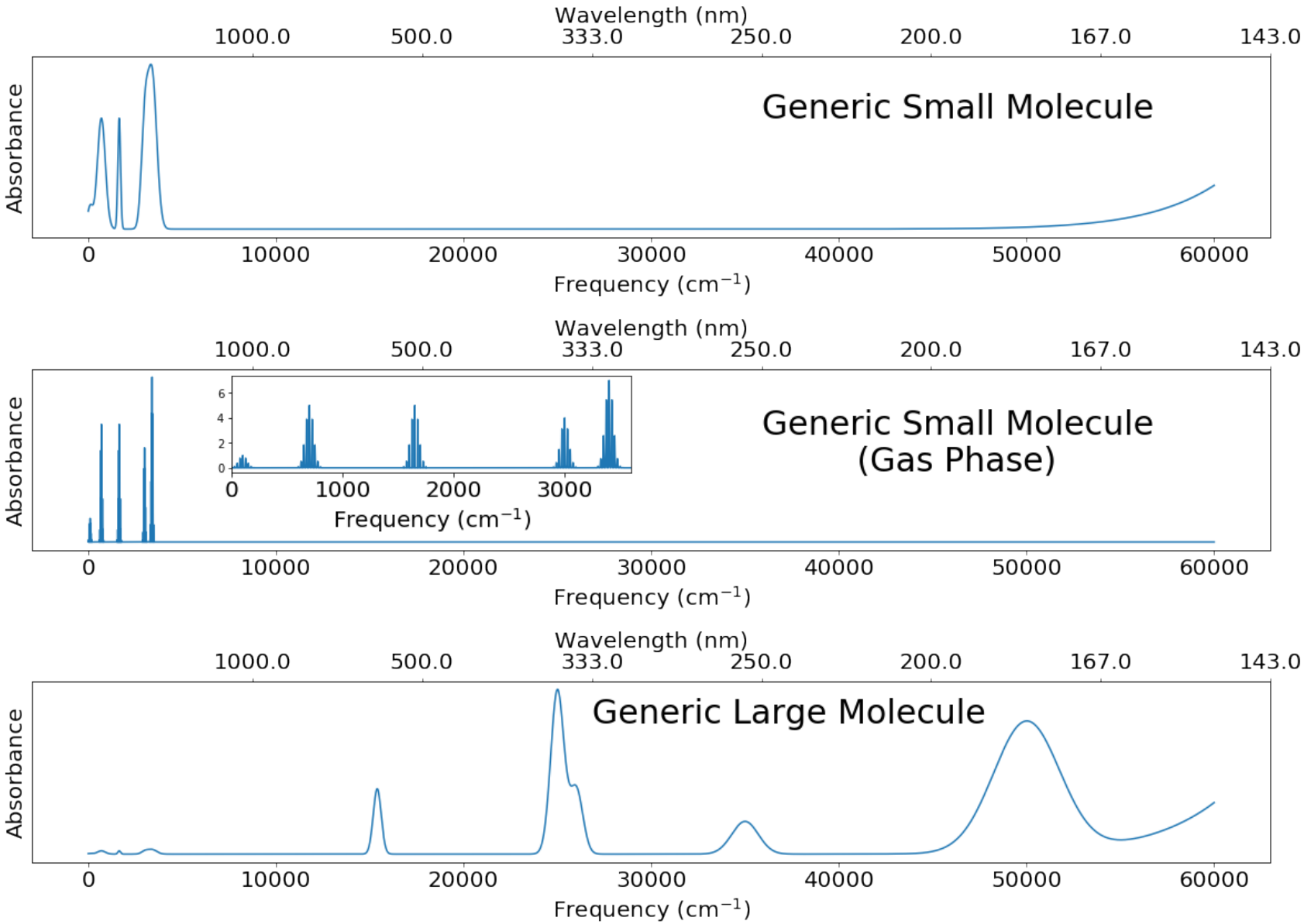

IR Spectroscopy

Frequency Range: 10 - 12,500 cm^{-1}

Molecular motion involved:

IR Spectroscopy

Frequency Range: 10 - 12,500 cm^{-1}

Molecular motion involved: Vibrations

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Examples: `https://webbook.nist.gov/chemistry/`

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Applications:

- Analytical chemistry: identification (chemical fingerprints)
- Chemical structure determination (functional groups)
- Protein structure determination (Amide I)

UV/Vis Spectroscopy

Frequency Range: 12,500 - 10^6 cm^{-1}

UV/Vis Spectroscopy

Frequency Range: 12,500 - 10^6 cm^{-1}

Molecular Motion involved:

UV/Vis Spectroscopy

Frequency Range: 12,500 - 10^6 cm^{-1}

Molecular Motion involved: Electronic transitions

UV/Vis Spectroscopy

Frequency Range: 12,500 - 10^6 cm^{-1}

Molecular Motion involved: Electronic transitions

Applications:

- Physical Chem: Electronic structure (energy levels)
- Analytical Chem: concentration
- Biochem: biomolecular assays

Spectrum Basics

Frequency vs. Angular Frequency:

Frequency/Wavelength Conversion:

Frequency vs. Energy:

Spectrum Basics

Frequency vs. Angular Frequency:

$$\omega = 2\pi\nu$$

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Frequency vs. Energy:

$$E = \hbar\omega = h\nu$$