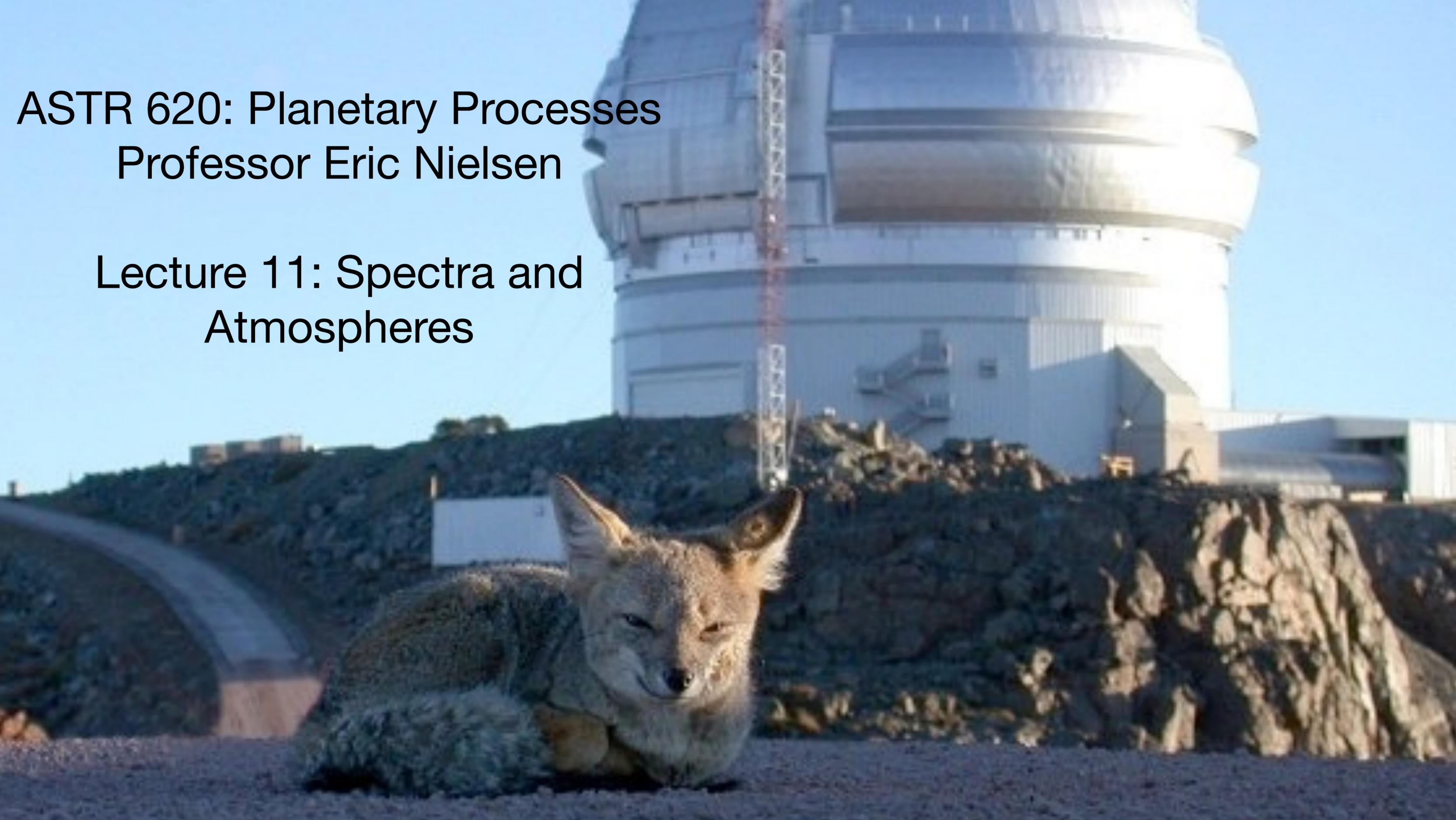


ASTR 620: Planetary Processes
Professor Eric Nielsen

Lecture 11: Spectra and
Atmospheres



Logistics

- Masks are encouraged
- No laptops, phones, or other electronic devices during class (I'll let you know in advance if we'll need laptops for an activity) **You may use a tablet to take notes if prefer, but please only use it for note-taking.**
- Remember to bring you response card to class
- Midterm in 9 days: Wednesday, October 5th (here in class)
- Homework 3 due Wednesday, September 28 at 11:59pm

Review of the last class

- How large is an atom?
 - (A) — $10^{-6}m$: 1 micron
 - (B) — $10^{-9}m$: 1 nanometer
 - (C) — $10^{-10}m$: 1 Angstrom
 - (D) — $10^{-12}m$: 1 picometer
 - (E) — $10^{-15}m$: 1 femtometer

Review of the last class

- How large is a nucleus?
 - (A) — $10^{-6}m$: 1 micron
 - (B) — $10^{-9}m$: 1 nanometer
 - (C) — $10^{-10}m$: 1 Angstrom
 - (D) — $10^{-12}m$: 1 picometer
 - (E) — $10^{-15}m$: 1 femtometer

Review of the last class

- Photon A is emitted when an electron in a hydrogen atom goes from level 4 to level 3. Photon B is emitted when that same electron goes from level 3 to level 2. Which photon has more energy, and what type of light is each photon?
 - (A) — Photon A has more energy, Photon A and B are both optical
 - (B) — Photon B has more energy, Photon A and B are both optical
 - (C) — Photon A has more energy, Photon A is optical, Photon B is infrared
 - (D) — Photon B has more energy, Photon A is infrared, Photon B is optical
 - (E) — Photon A has more energy, Photon A and Photon B are both infrared

Review of the last class

- Which correctly ranks transitions in molecules, from the highest energy transitions to the lowest energy transitions?
 - (A) — (highest) rotational, electron, vibrational (lowest)
 - (B) — (highest) vibrational, rotational, electron (lowest)
 - (C) — (highest) rotational, vibrational, electron (lowest)
 - (D) — (highest) electron, rotational, vibrational (lowest)
 - (E) — (highest) electron, vibrational, rotational (lowest)

Review of the last class

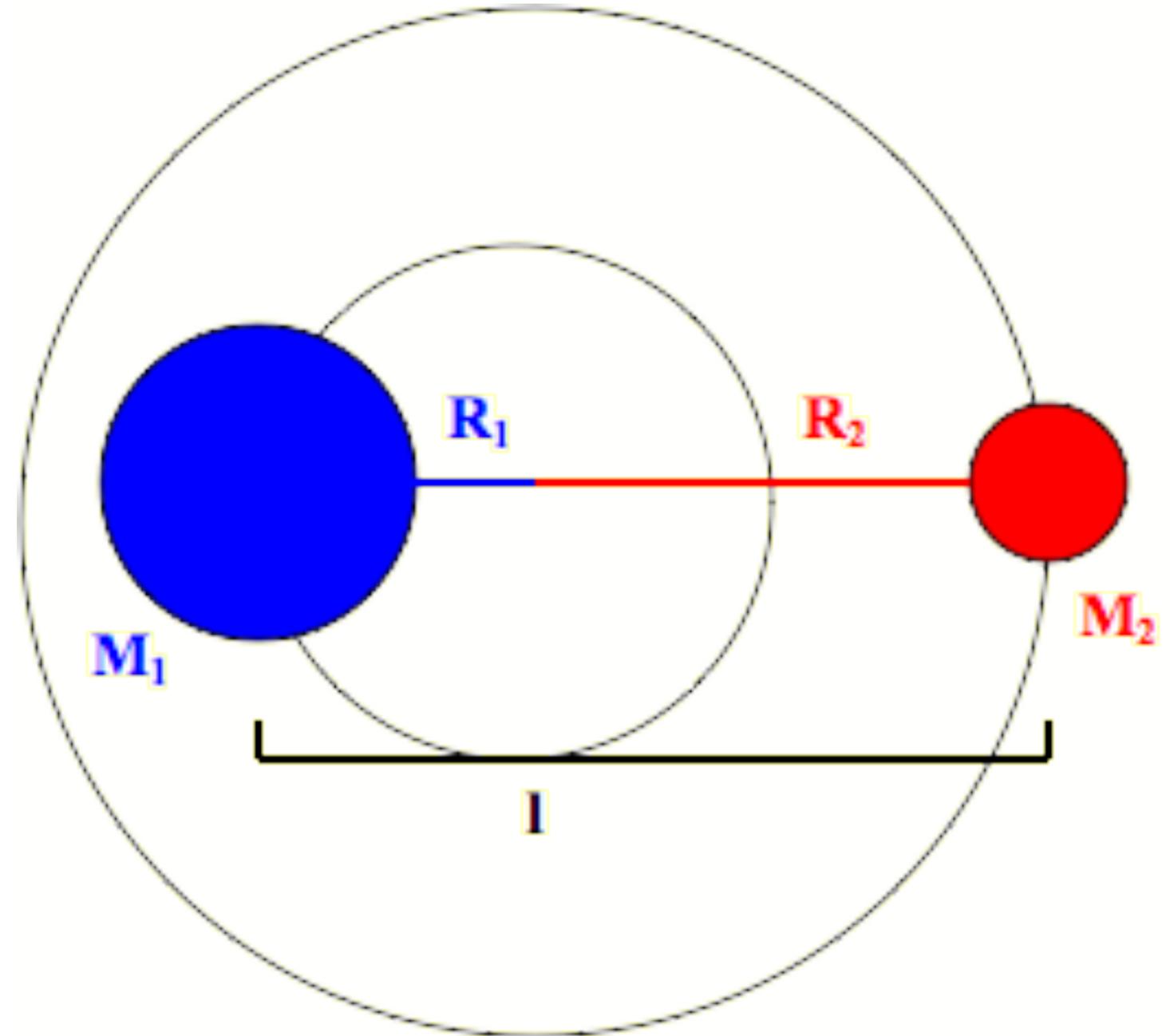
- Rotational emission lines are (mostly):
 - (A) — equally spaced in frequency, energy, wavenumber, and wavelength
 - (B) — equally spaced in frequency, energy, wavenumber
 - (C) — equally spaced in frequency, energy
 - (D) — equally spaced in energy
 - (E) — not equally spaced in any of these

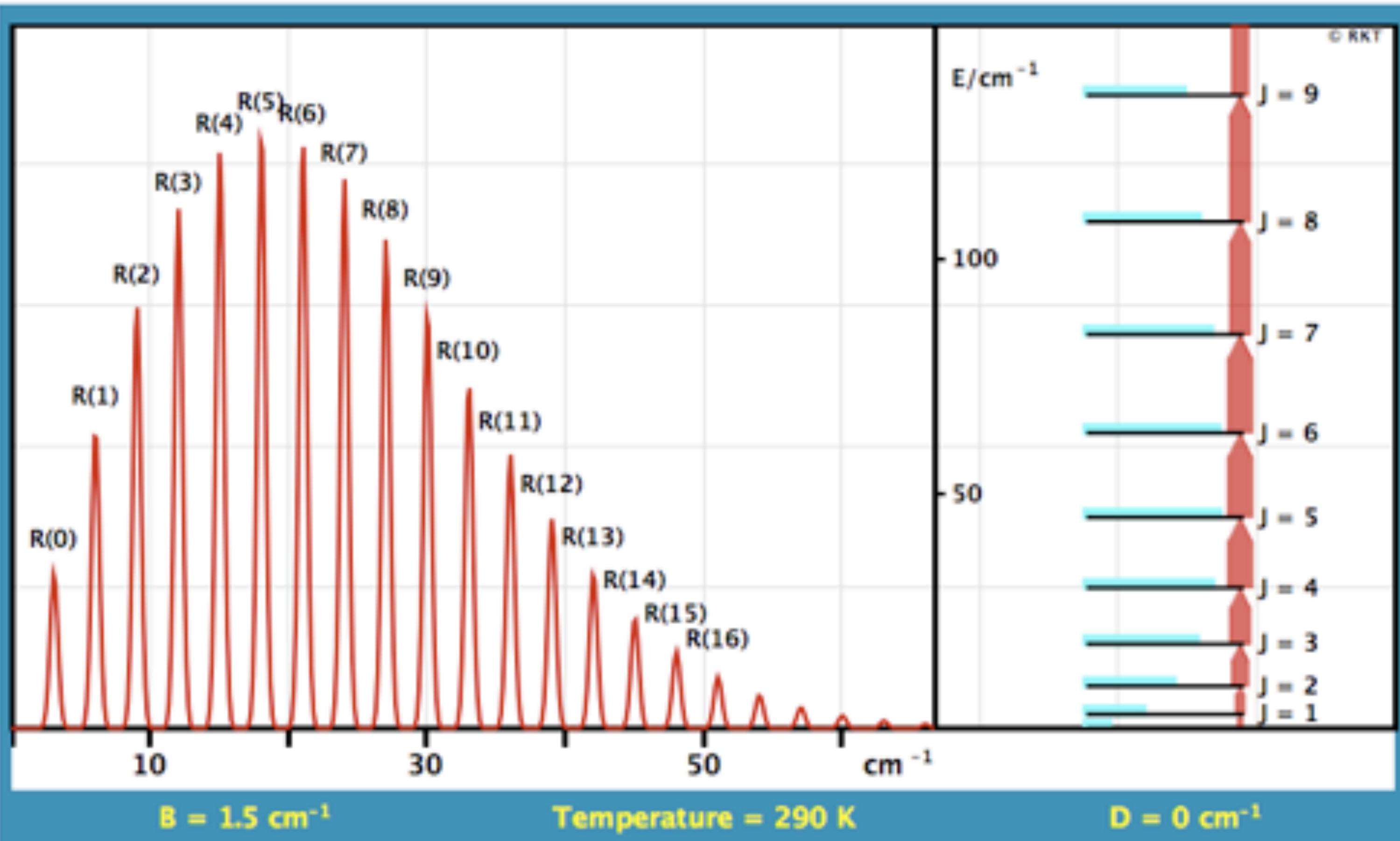
Rotational Temperature

- Pure rotational transitions are in the microwave
- The relative population of different rotational energy levels depends on temperature
- These closely-spaced energy levels allow us to extract temperature from the spectra
- Rotational level with the largest population is given by:

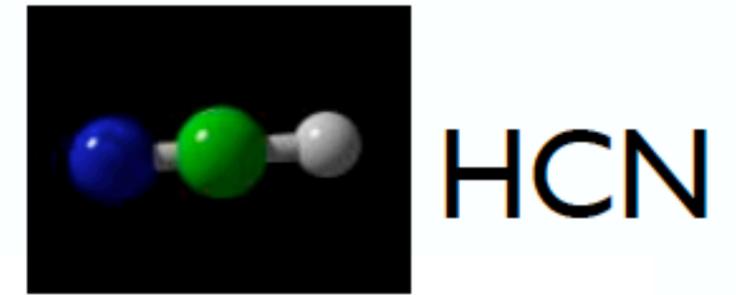
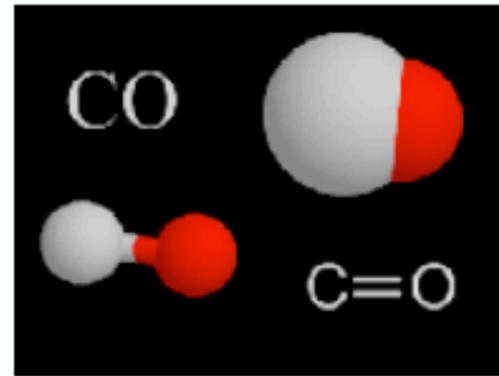
$$J = \left(\frac{kT}{2B} \right)^{\frac{1}{2}} - \frac{1}{2}$$

- k: Boltzmann constant with wavenumber units, $0.695 \text{ cm}^{-1} \text{ K}^{-1}$

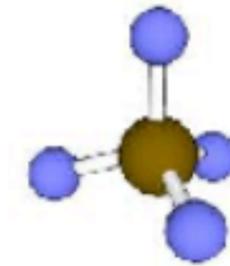
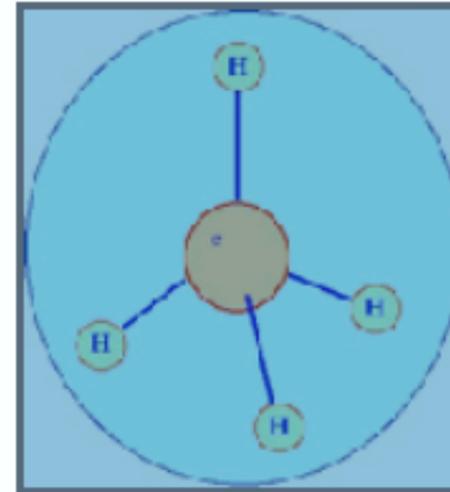




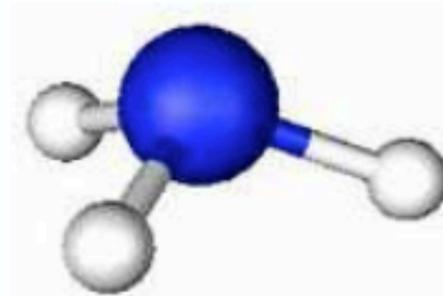
- linear molecule



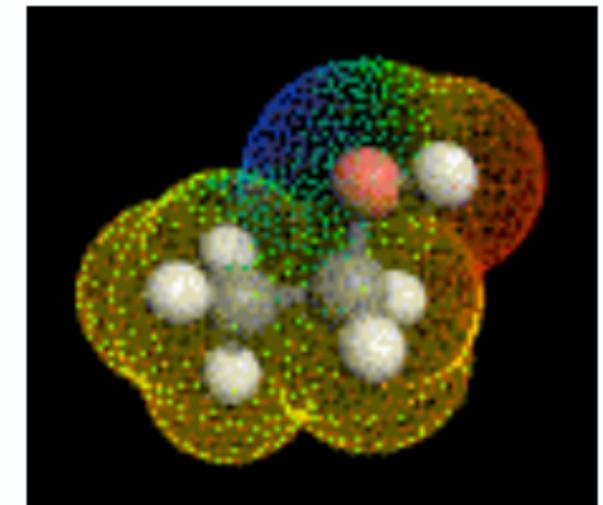
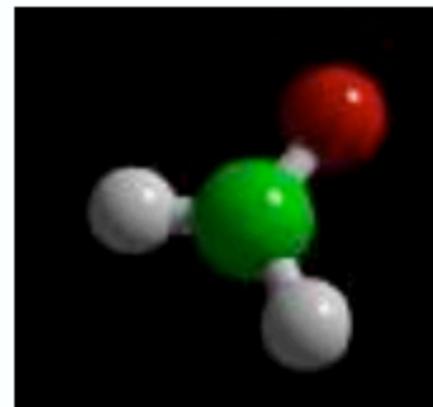
- spherical top



- symmetric top



- asymmetric top



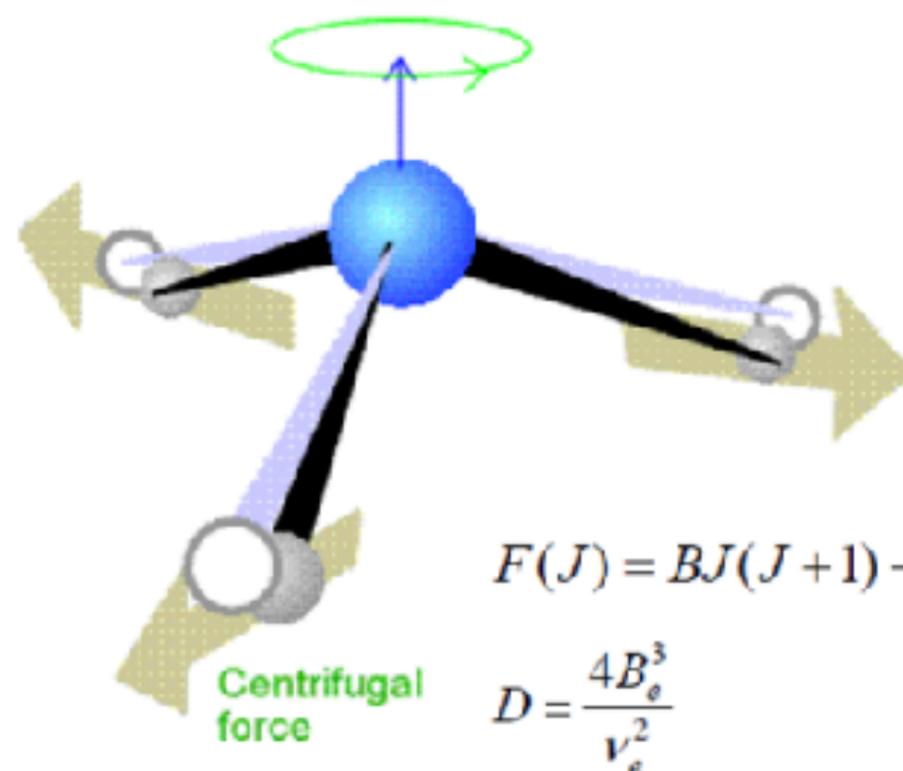
Molecules are *not* rigid rotors – their bonds stretch during rotation

As a result, the moment of inertia I change with J .

For real molecule, the rotational constant B depend on rotational quantum number J !

It is more convenient to treat centrifugal distortion as a perturbation to the rigid rotor terms.

In real rotational spectra the peaks are not perfectly equidistant: *centrifugal distortion* (D).



$$F(J) = BJ(J+1) - D[J(J+1)]^2$$

$$D = \frac{4B_e^3}{v_e^2}$$

- The effect of rotation on a molecule. The centrifugal force arising from rotation distorts the molecule, opening out bond angles and stretching bonds slightly. The effect is to increase the moment of inertia of the molecule and hence to decrease its rotational constant.

Vibrations

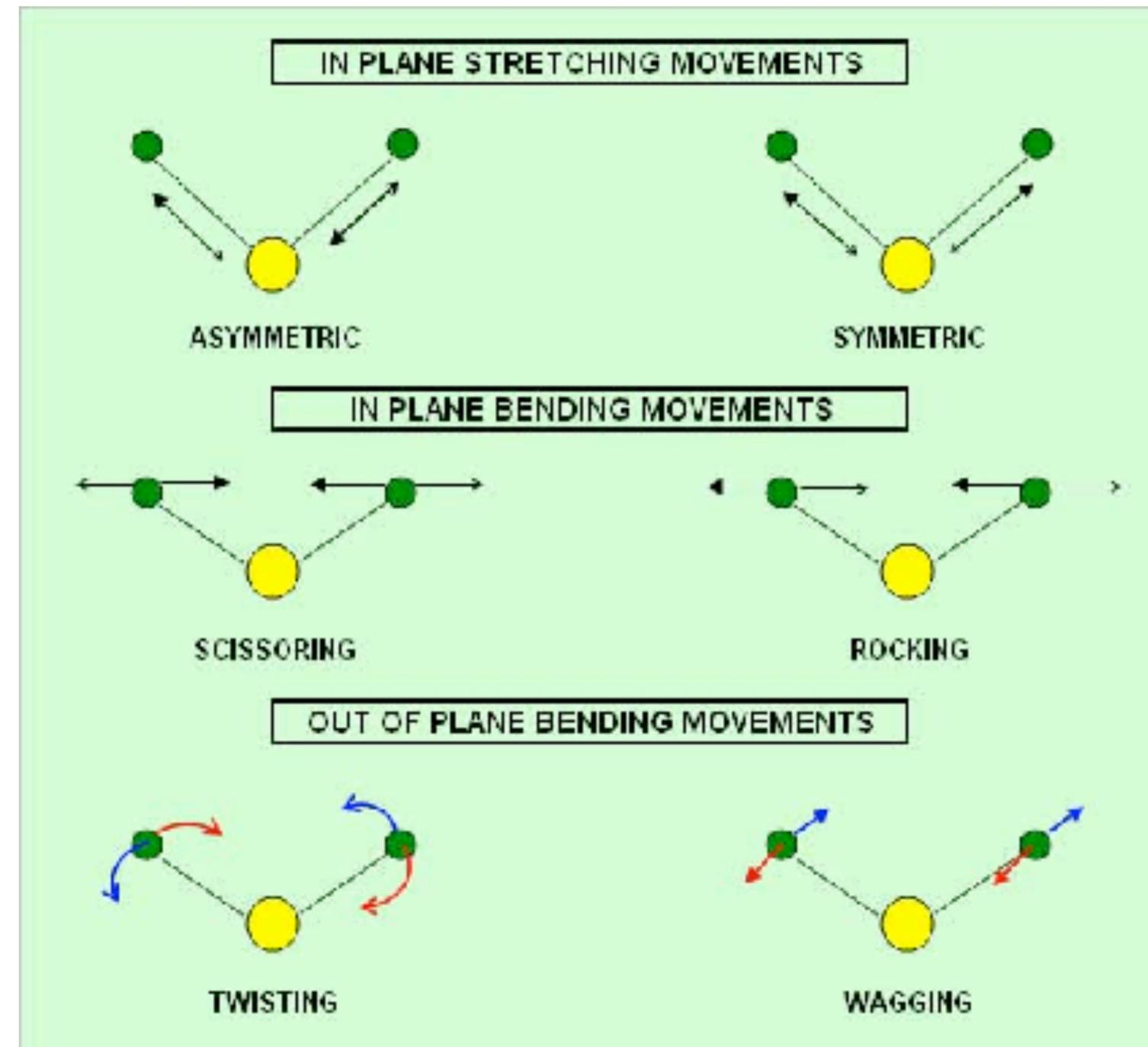
- Vibrations of molecules (relative positions of individual nuclei changing) are also quantized

- Energy levels for vibration given by:

$$E_\nu = \tilde{\nu} \left(\nu + \frac{1}{2} \right)$$

- ν : vibrational quantum number (0, 1, 2, ...)

- $\tilde{\nu}$: fundamental vibrational wavenumber



Vibrations

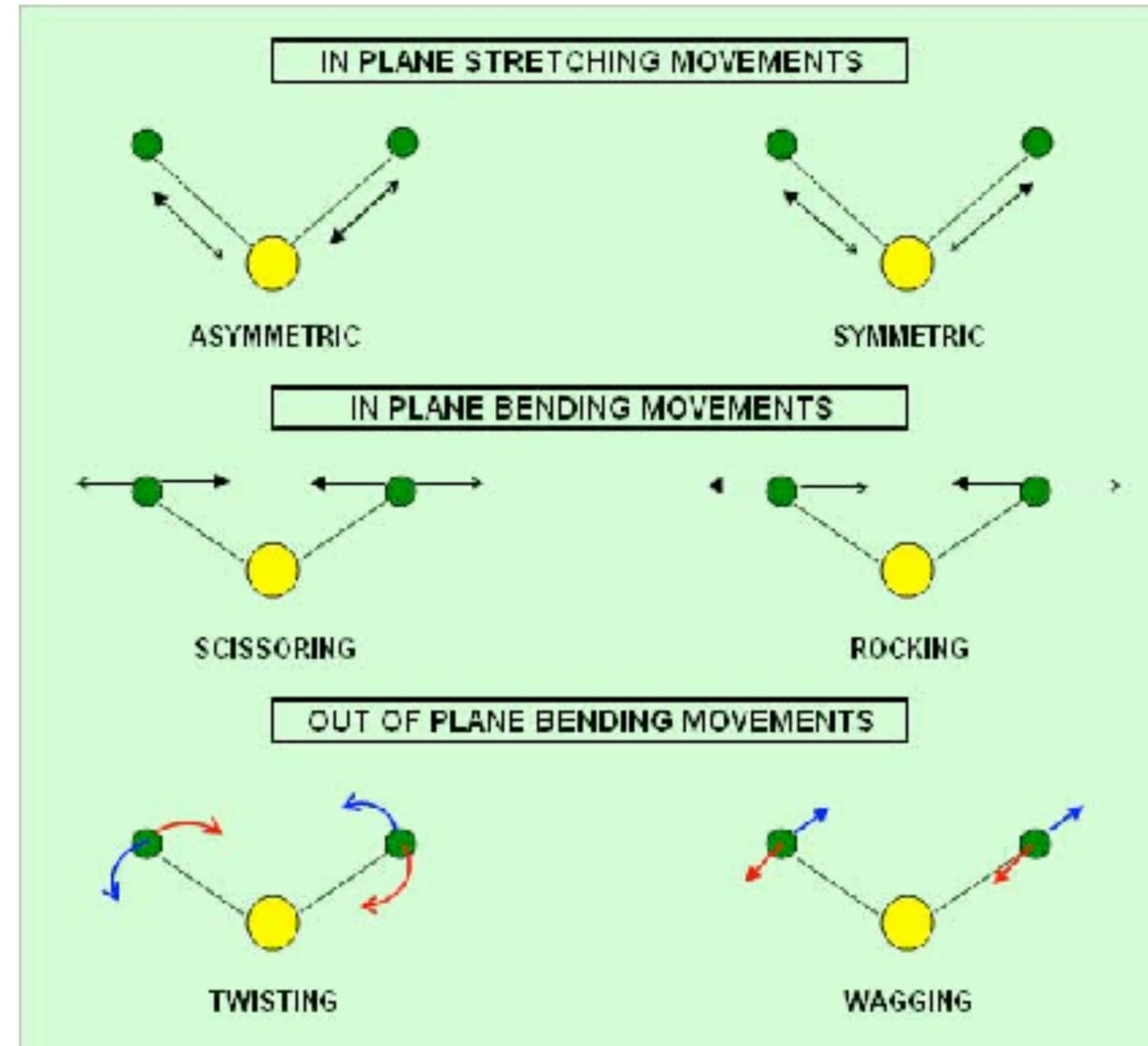
$$E_\nu = \tilde{\nu} \left(\nu + \frac{1}{2} \right)$$

$$\tilde{\nu} = \frac{1}{2\pi c} \sqrt{\frac{k}{\mu}}$$

• μ : reduced mass

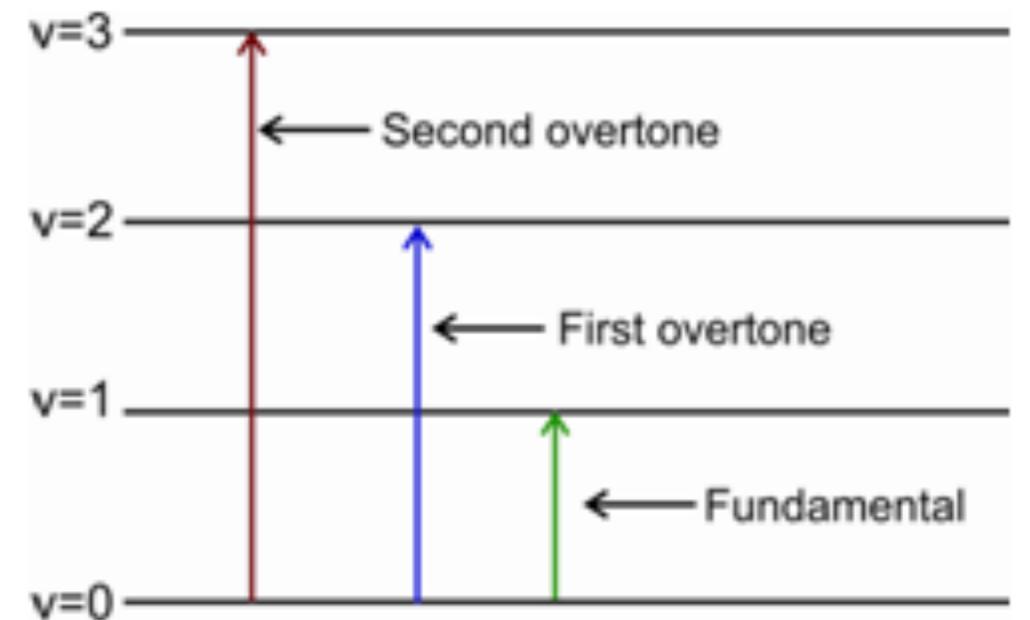
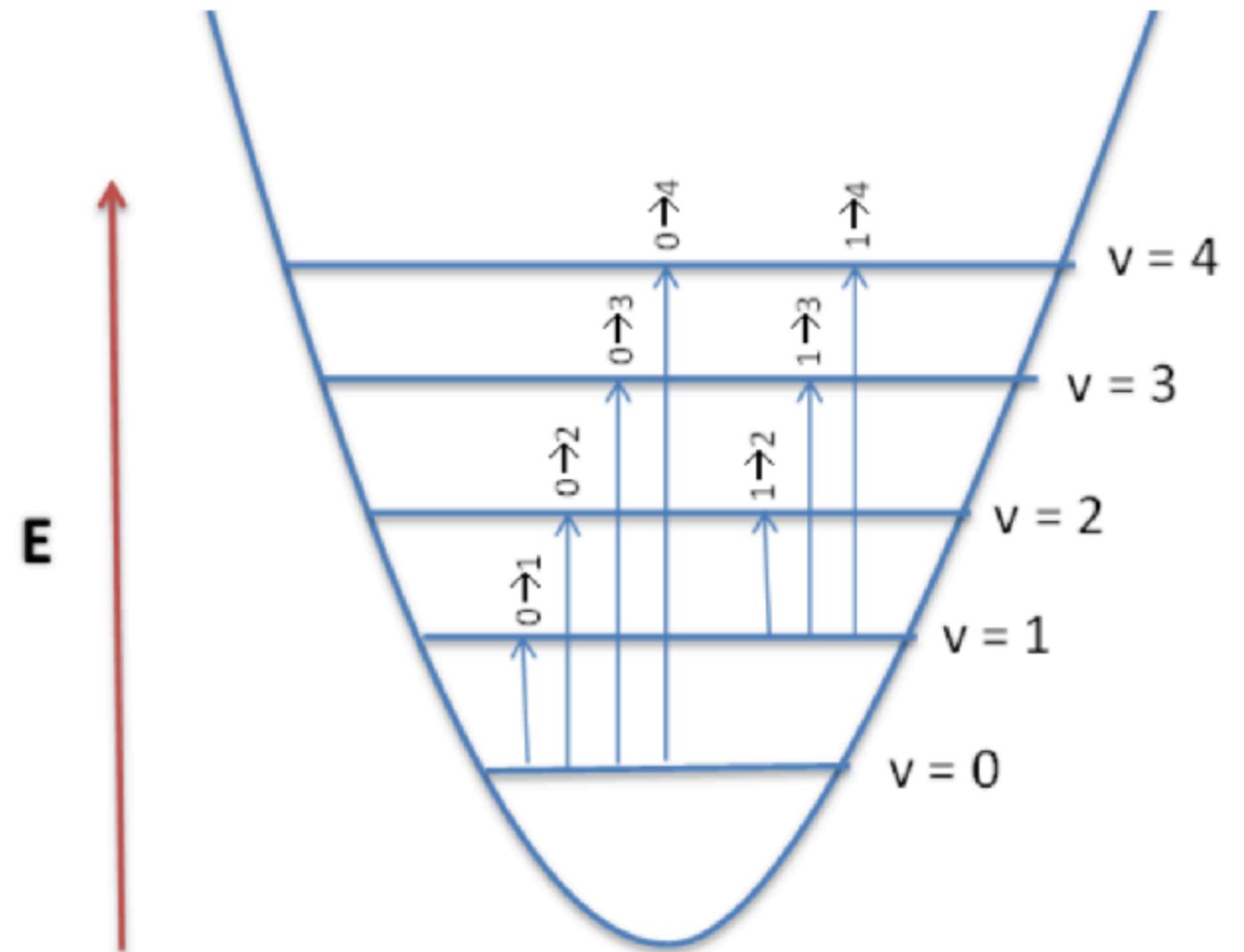
$$\left(\frac{1}{\mu} = \frac{1}{M_1} + \frac{1}{M_2} + \dots \right)$$

• k : bond force constant



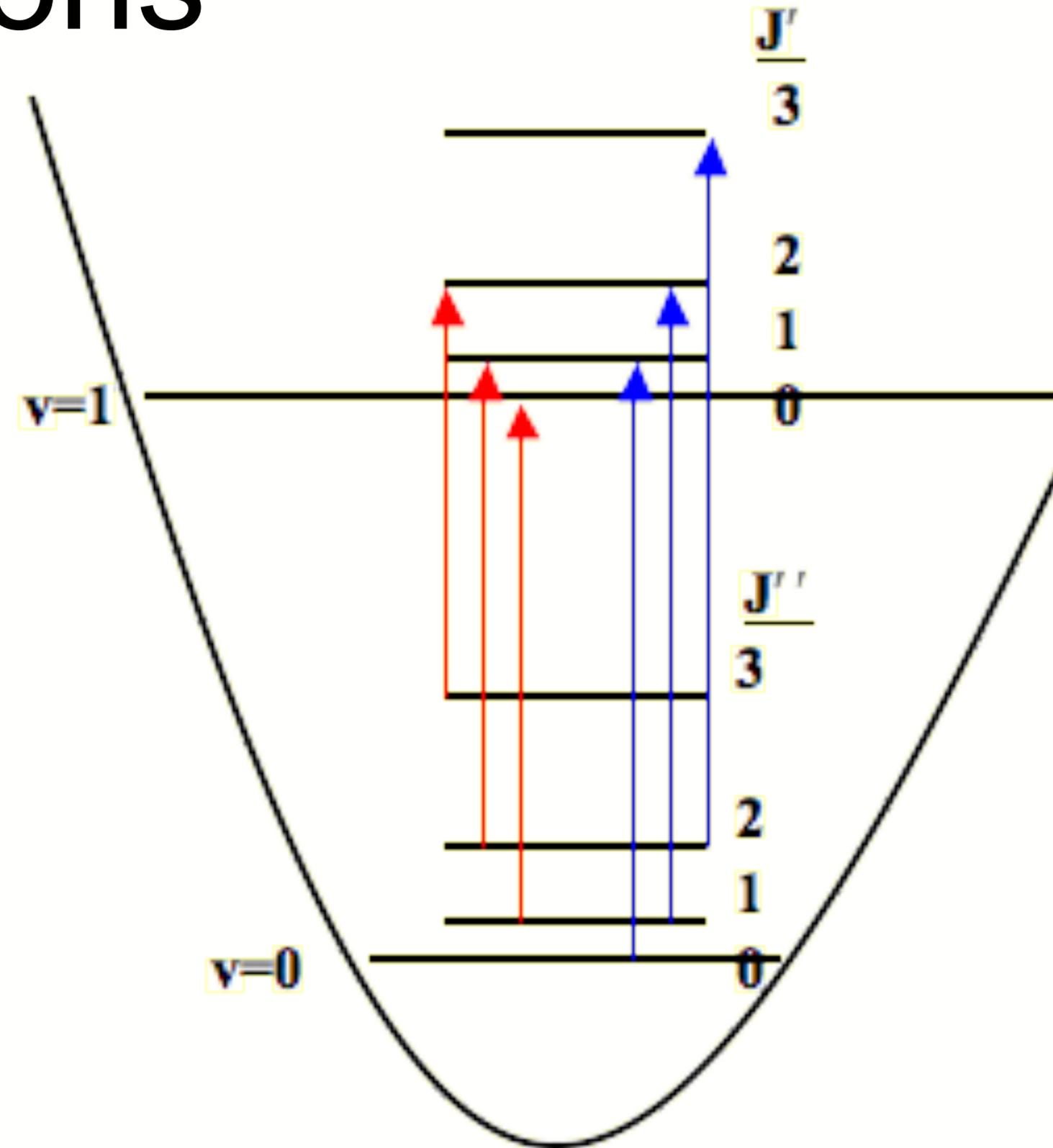
Vibrations

- $E_\nu = \tilde{\nu} \left(\nu + \frac{1}{2} \right)$
- Vibrational energy levels are evenly spaced
- There is a minimum (zero-point) energy (unlike rotation): $E_0 = \frac{1}{2} \tilde{\nu}$
- “Fundamental transition” from $\nu = 0$ to $\nu = 1$
- “Overtones” from $\nu = 0$ to $\nu = 2$ (or to 3, or to 4...)



RoVibrational Transitions

- Vibrational transition usually accompanied by rotational transition
 - A single photon is emitted (or absorbed) when a molecule changes its rotational state AND vibrational state at the same time
- rotational transitions are lower energy than vibrational transition
- Vibrational transition can jump multiple energy levels at once, but rotational can only move one energy level at a time ($\Delta J = \pm 1$)
 - (For some molecules, $\Delta J = 0$ is also allowed)

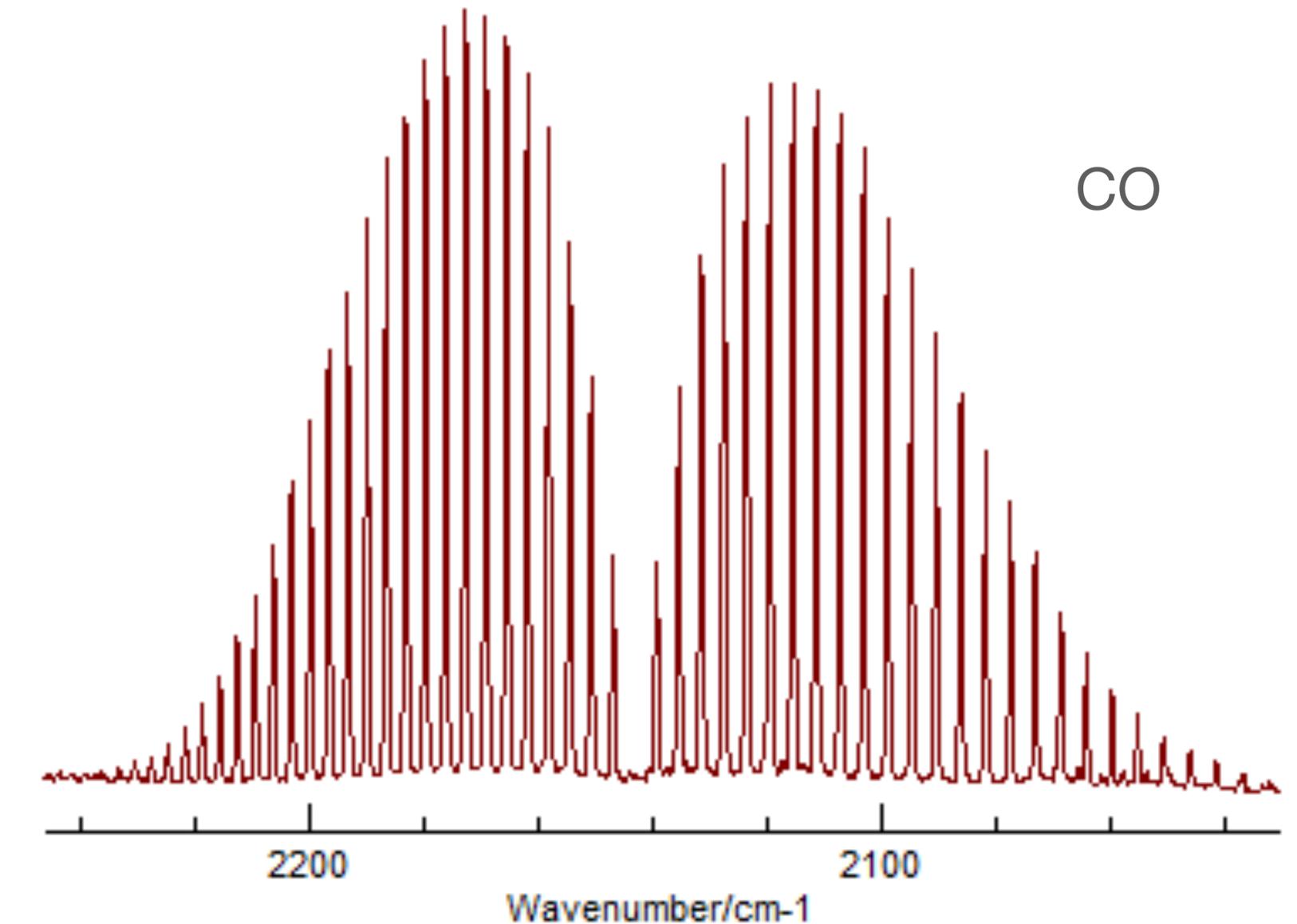


RoVibrational Transitions

- A single vibrational transition is marked by multiple lines, corresponding to various rotational transitions

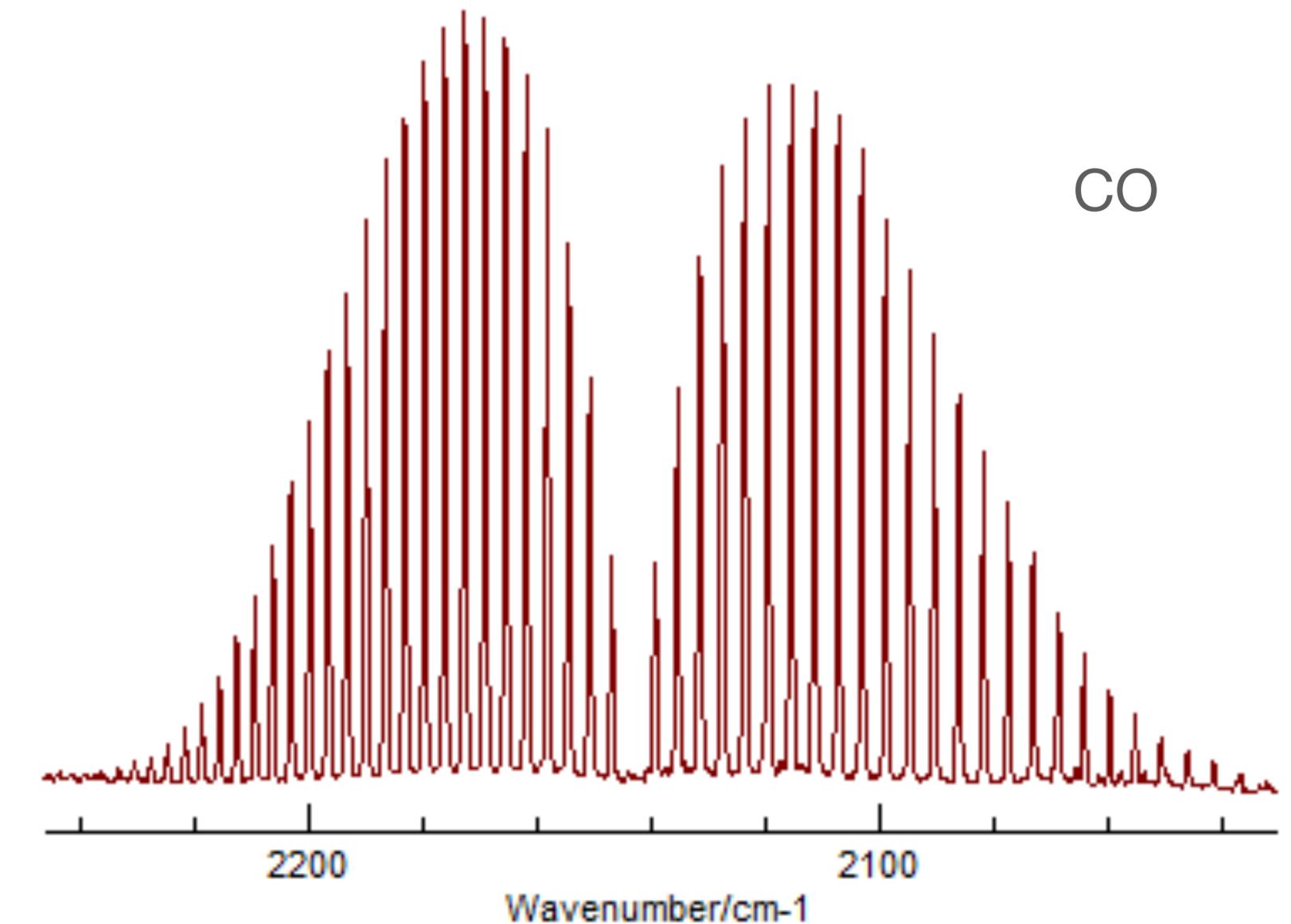
$$E_{\nu,r} = \tilde{\nu} \left(\nu + \frac{1}{2} \right) + BJ(J + 1)$$

- (Remember B is much smaller — lower energy — than $\tilde{\nu}$)



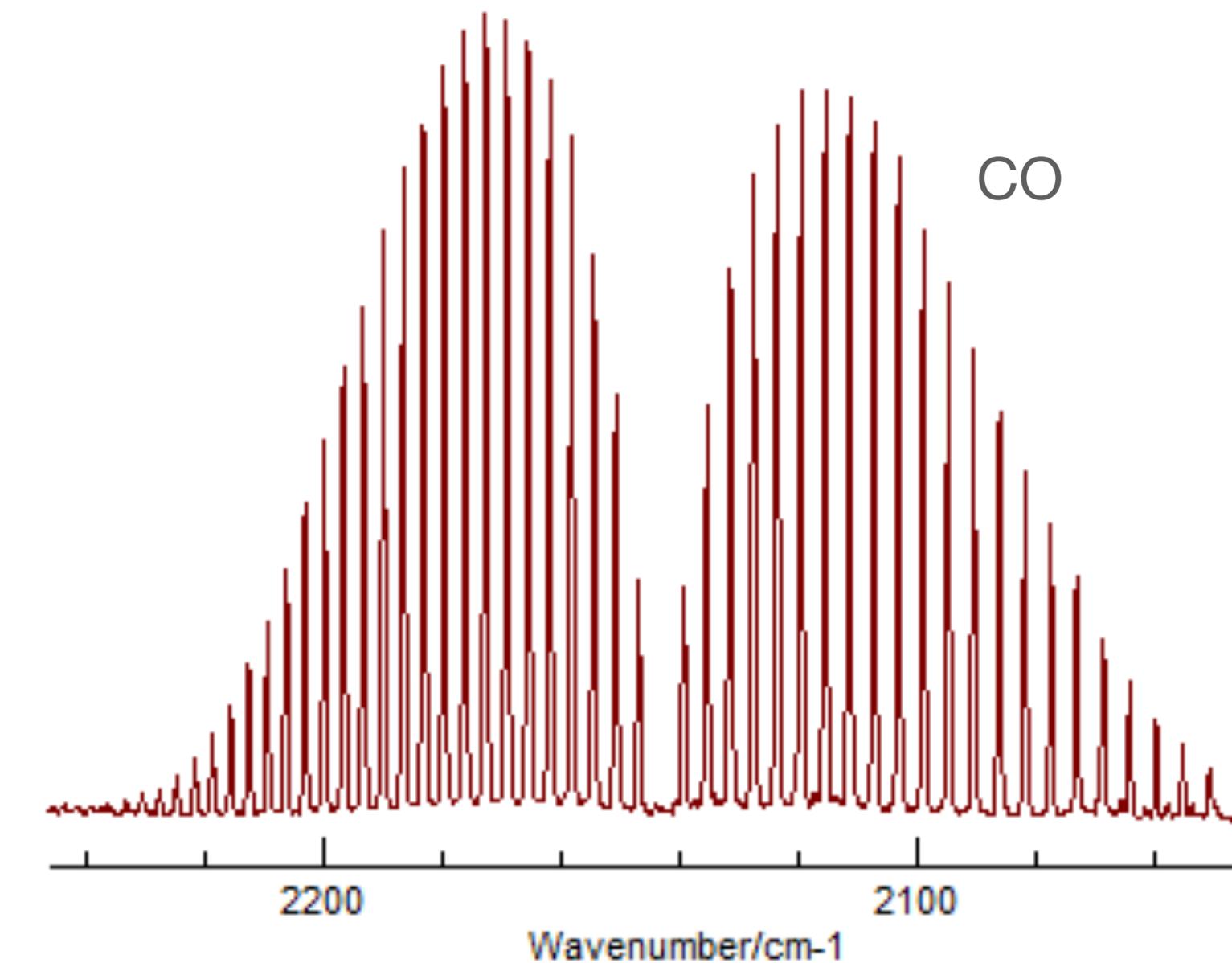
RoVibrational Transitions

- $E_{\nu,r} = \tilde{\nu} \left(\nu + \frac{1}{2} \right) + BJ(J + 1)$
- “R-branch”: Transitions where the molecule moves to a higher energy level in both vibration and rotation (or lower in both)
- “P-branch”: Transitions where the molecules move to a higher rotational energy and a lower vibrational energy (or lower+higher)
- R-branch has higher energy transition than P branch



Response Card Question

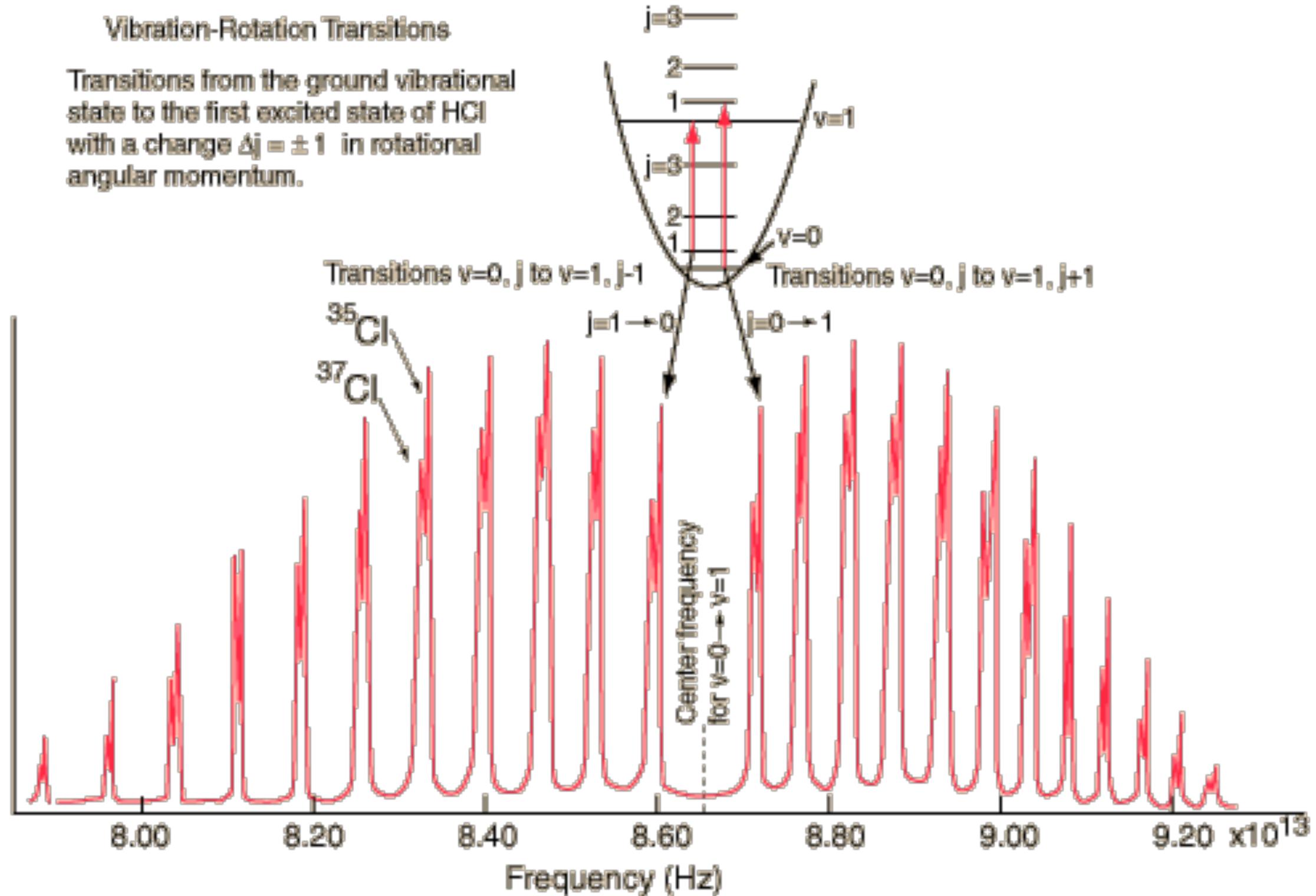
- “R-branch”: Transitions where the molecule moves to a higher energy level in both vibration and rotation (or lower in both)
- “P-branch”: Transitions where the molecule moves to a higher rotational energy and a lower vibrational energy (or lower+higher)
- Which is the P-branch?
 - (A) — The one on the left
 - (B) — The one on the right



RoVib Transitions

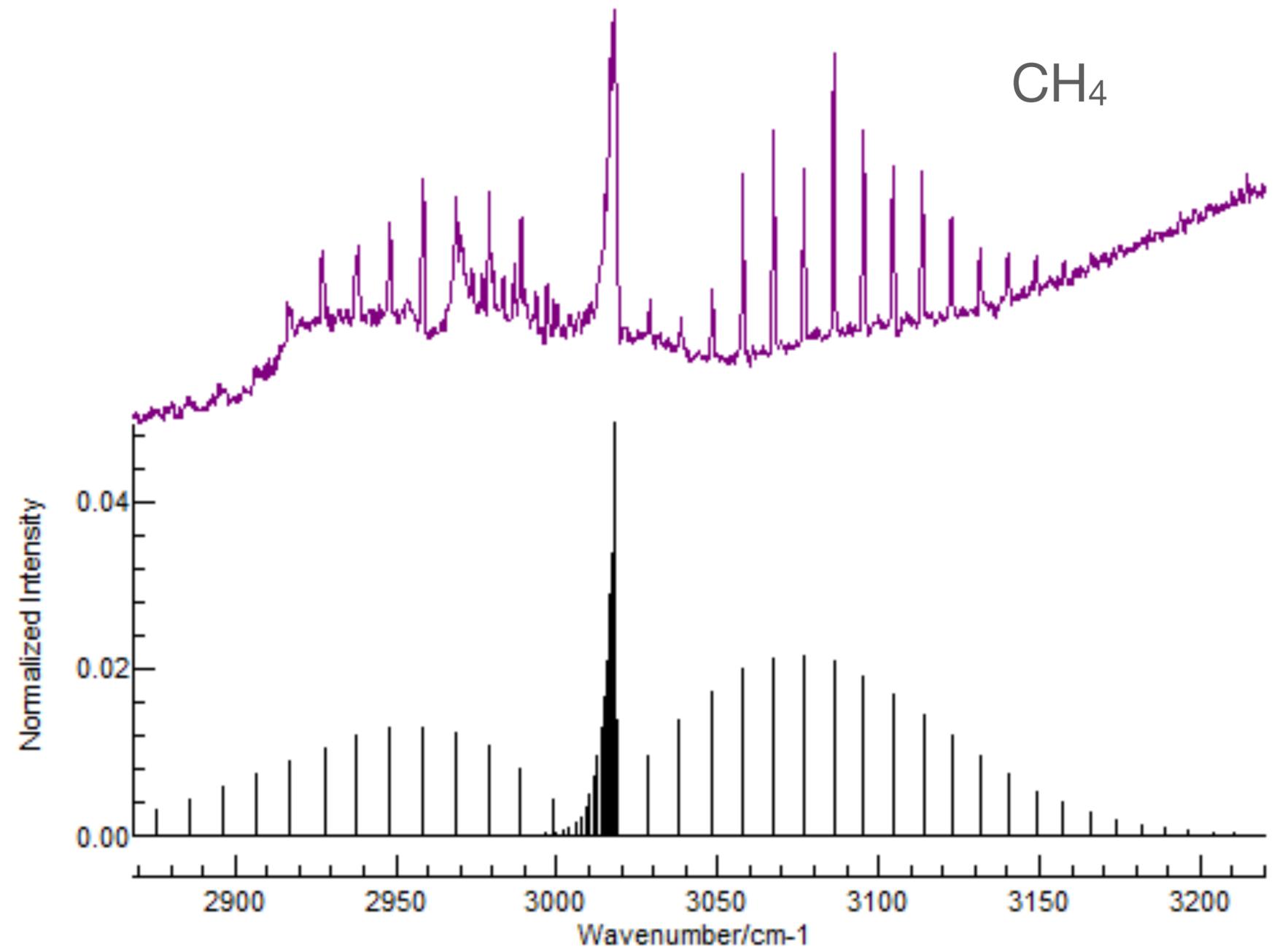
Vibration-Rotation Transitions

Transitions from the ground vibrational state to the first excited state of HCl with a change $\Delta j = \pm 1$ in rotational angular momentum.



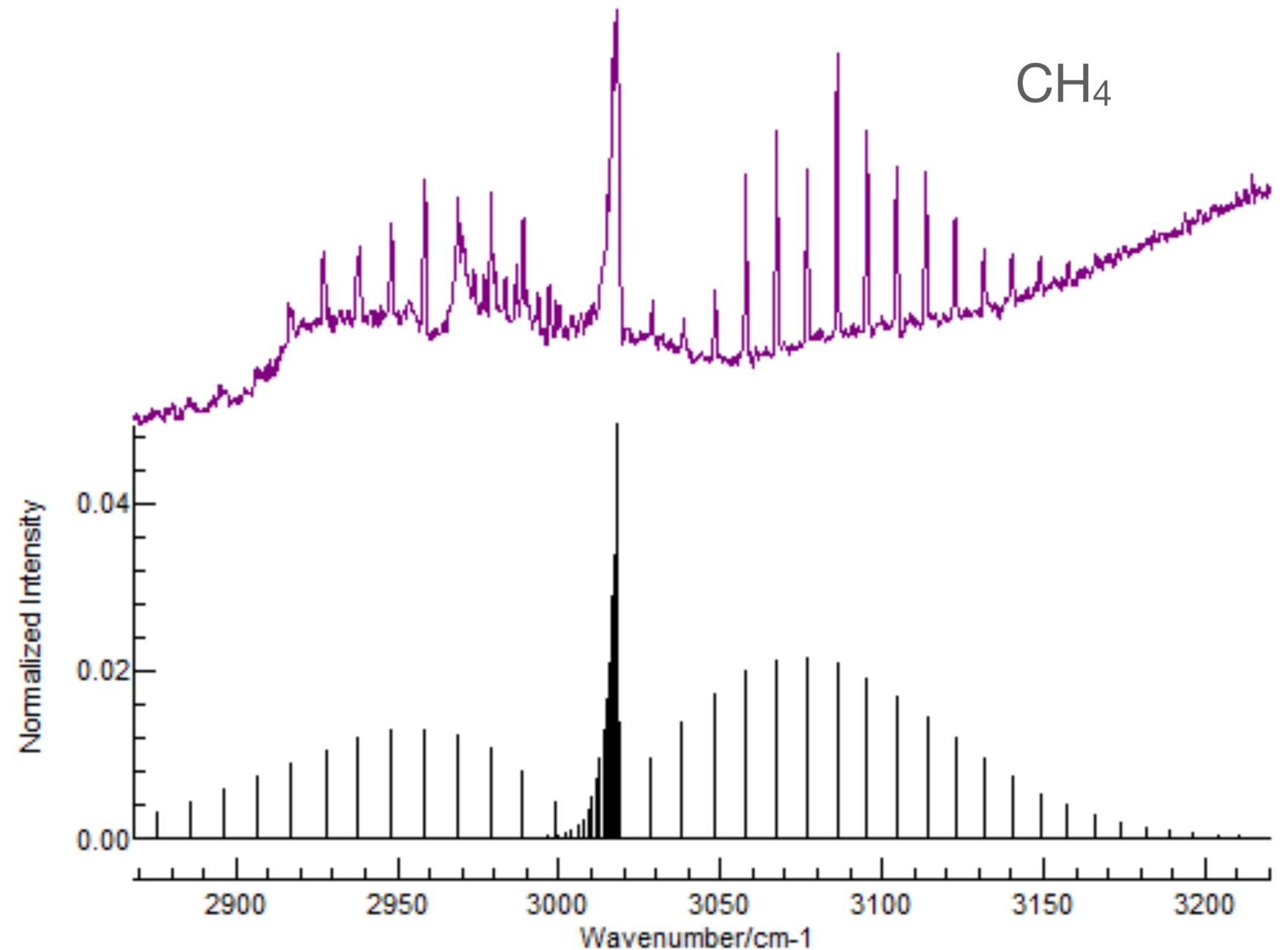
Q Branch

- Some molecules have possible transitions at $\Delta J = \pm 1, 0$
- “Q Branch” is vibrational transitions where the rotational energy state does not change
 - Multiple lines from an electron changing states
 - Or from degenerate vibrational modes

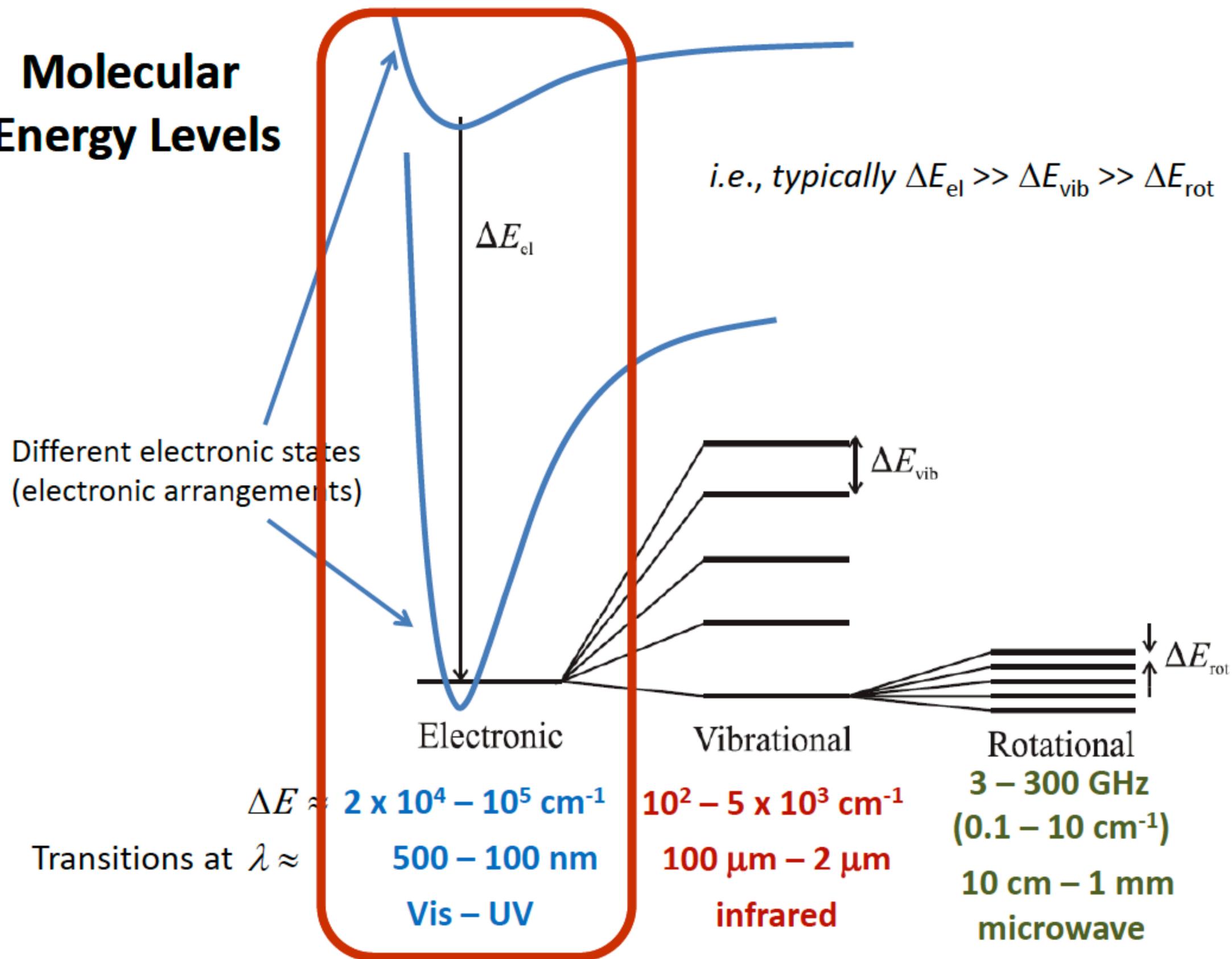


Electronic Transitions

- Not generally important for molecules
 - Any collision or photon energetic enough to move an electron between energy levels will typically dissociate (destroy) the molecule

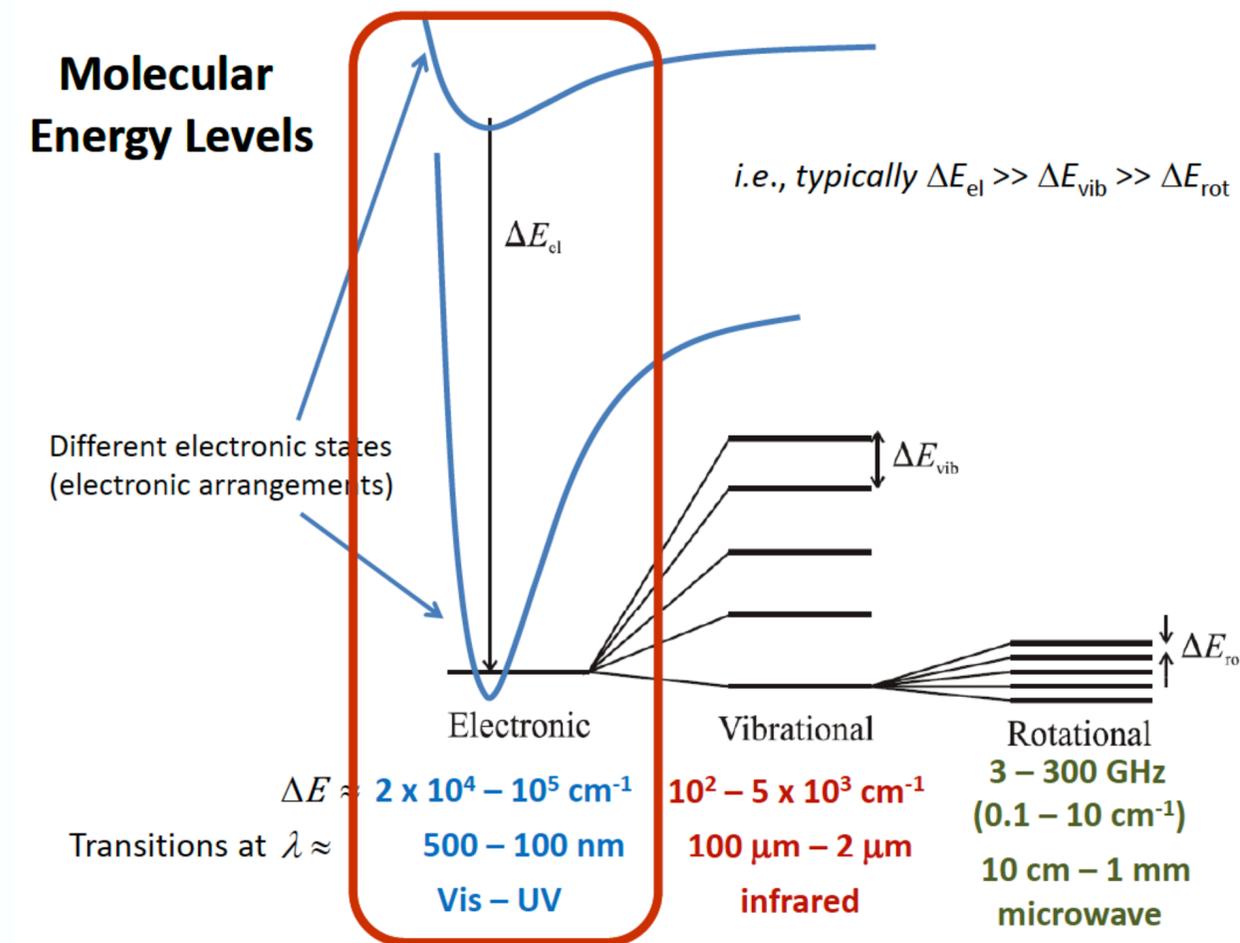


Molecular Energy Levels



Order of Magnitude: RoVibrational Transitions

- The resolution of a spectrograph is given by $R = \frac{\lambda}{\Delta\lambda}$
- Some near-infrared spectrographs:
 - Gemini/GPI: $R \sim 50$
 - APO/Triplespec: $R \sim 5000$
 - Keck/NIRSPEC $R \sim 25000$
- Suppose we want to resolve the individual rotational lines of a molecule with a vibrational line at 2 microns, and rotational transition of 1 cm^{-1}
- (1) What is the energy difference (ΔE_v) of this vibrational line, in inverse centimeters?
- (2) What is the wavelength difference between a line with no rotational transition (ΔE_v) and one with both a vibrational and rotational transition ($\Delta E_v + \Delta E_r$)?
- (3) What resolution would you need to resolve these lines?
- (4) Which of the above instruments (if any) could resolve these lines?



Order of Magnitude: RoVibrational Transitions

- (1) What is the energy difference (ΔE_v) of this vibrational line, in inverse centimeters?
- 2 microns is $2 \times 10^{-4} \text{ cm}$, and we just need to invert that to get wavenumber:

$$\omega_n = \frac{1}{2 \times 10^{-4} \text{ cm}} = 0.5 \times 10^4 \text{ cm}^{-1} = 5 \times 10^3 \text{ cm}^{-1}$$

- (2) What is the wavelength difference between a line with no rotational transition (ΔE_v) and one with both a vibrational and rotational transition ($\Delta E_v + \Delta E_r$)?
- We already know the wavelength of the no rotational transition case, it's 2 microns.
- The wavelength of the combined line will be:

$$\lambda = \frac{1}{\Delta E_v + \Delta E_r}$$

Order of Magnitude: RoVibrational Transitions

- So the wavelength difference will be:

$$\Delta\lambda = \frac{1}{\Delta E_v + \Delta E_r} - \frac{1}{\Delta E_v}$$

- Let's get a common denominator and simplify a bit:

$$\Delta\lambda = \frac{\Delta E_v - \Delta E_v - \Delta E_r}{\Delta E_v(\Delta E_v + \Delta E_r)} = -\frac{\Delta E_r}{\Delta E_v(\Delta E_v + \Delta E_r)}$$

- Plugging in numbers:

$$\Delta\lambda = -\frac{\Delta E_r}{\Delta E_v(\Delta E_v + \Delta E_r)} = \frac{(1\text{cm}^{-1})}{(5 \times 10^3 \text{cm}^{-1})(5 \times 10^3 \text{cm}^{-1} + 1\text{cm}^{-1})} = \frac{1}{25 \times 10^6 \text{cm}^{-1}} = 0.04 \times 10^{-6} \text{cm}$$

$$\Delta\lambda = 4 \times 10^{-8} \text{cm} = 4 \times 10^{-4} \mu\text{m}$$

Order of Magnitude: RoVibrational Transitions

- (2) What resolution would you need to resolve these lines?

- We just need to divide lambda by delta lambda:

- $$R = \frac{\lambda}{\Delta\lambda} = \frac{2\mu m}{4 \times 10^{-4} \mu m} = 0.5 \times 10^4 = 5000 \text{ (at a minimum)}$$

- (3) Which of the above instruments (if any) could resolve these lines?

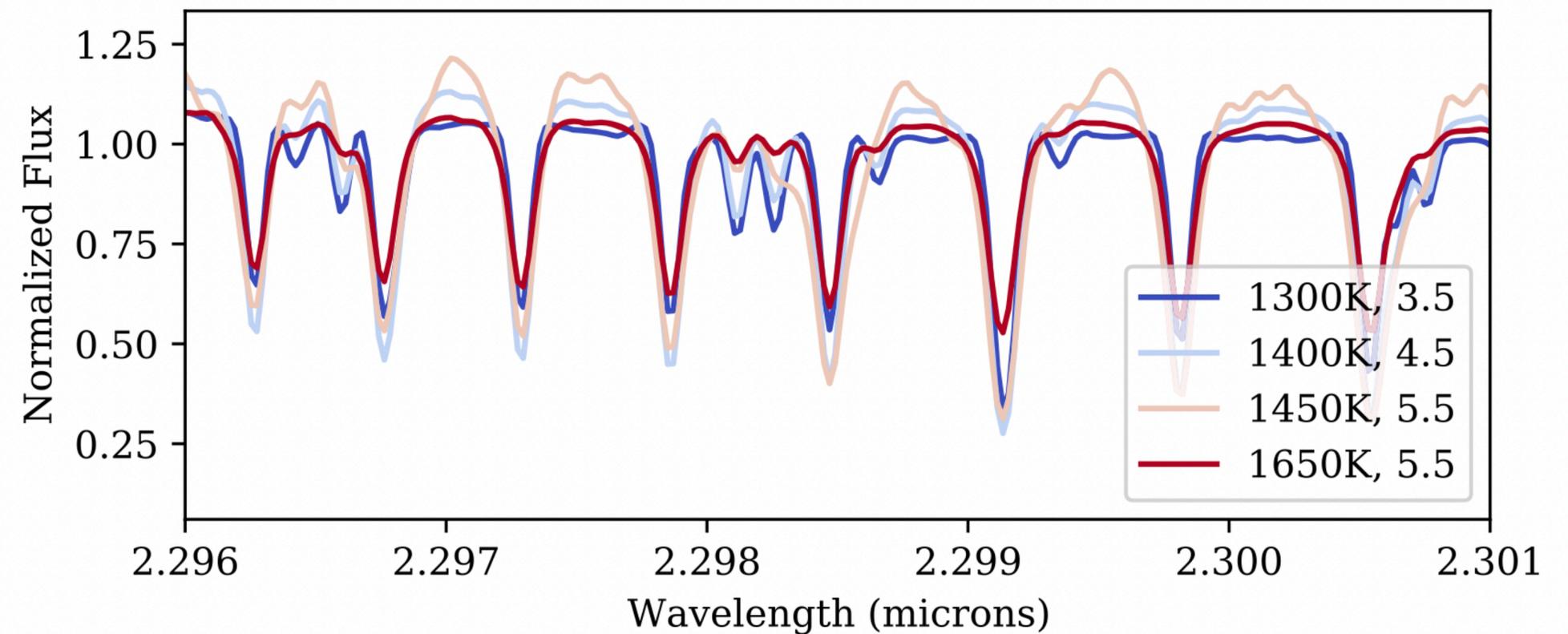
- GPI is too low resolution, Triplespec could just barely do it, NIRSPEC could do it comfortably.

Break

05:00

Molecular spectra: high resolution

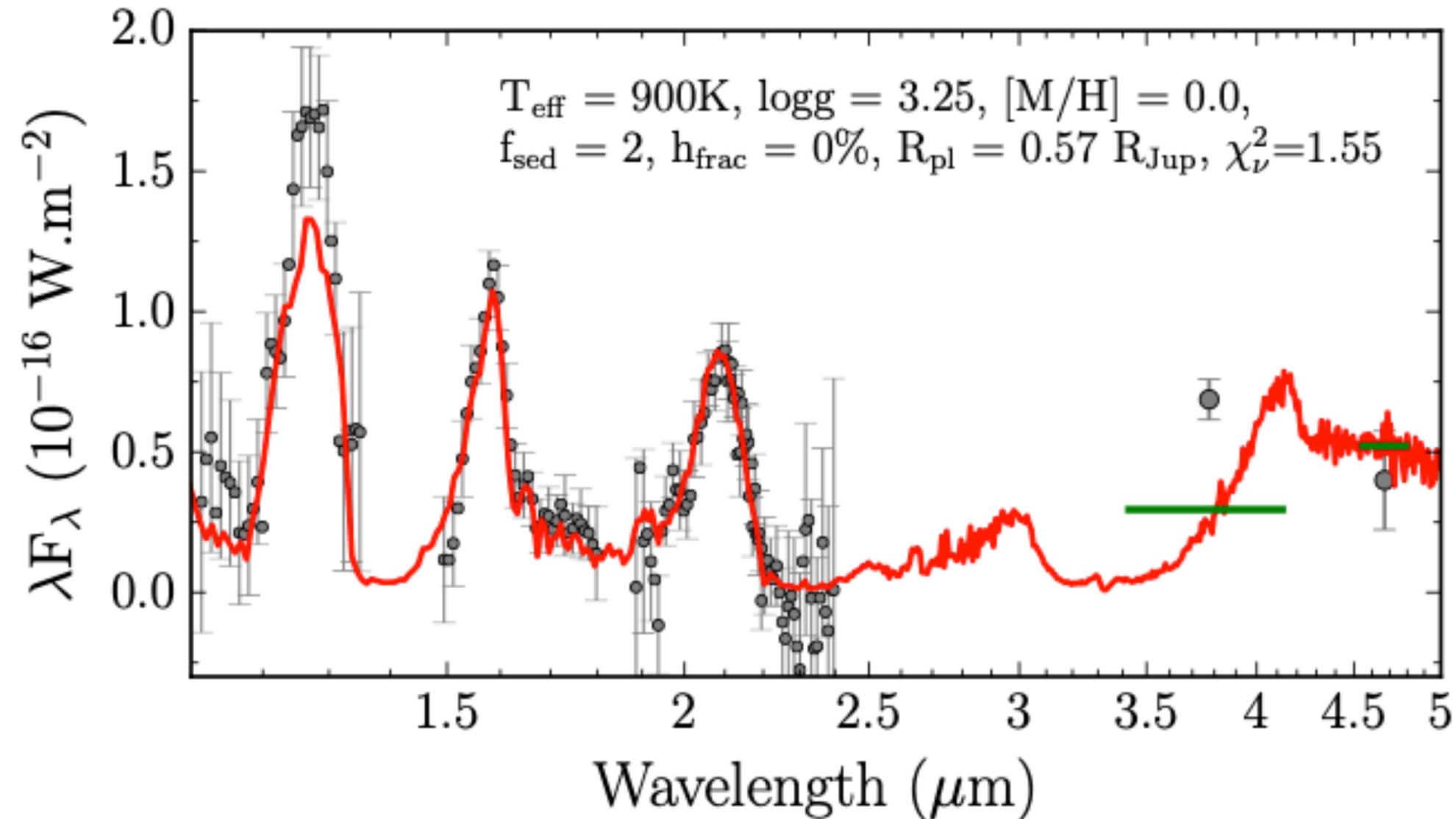
- Each molecule contributes hundreds of closely-spaced lines
- At high resolution, these individual lines can be resolved



Wang et al. 2021

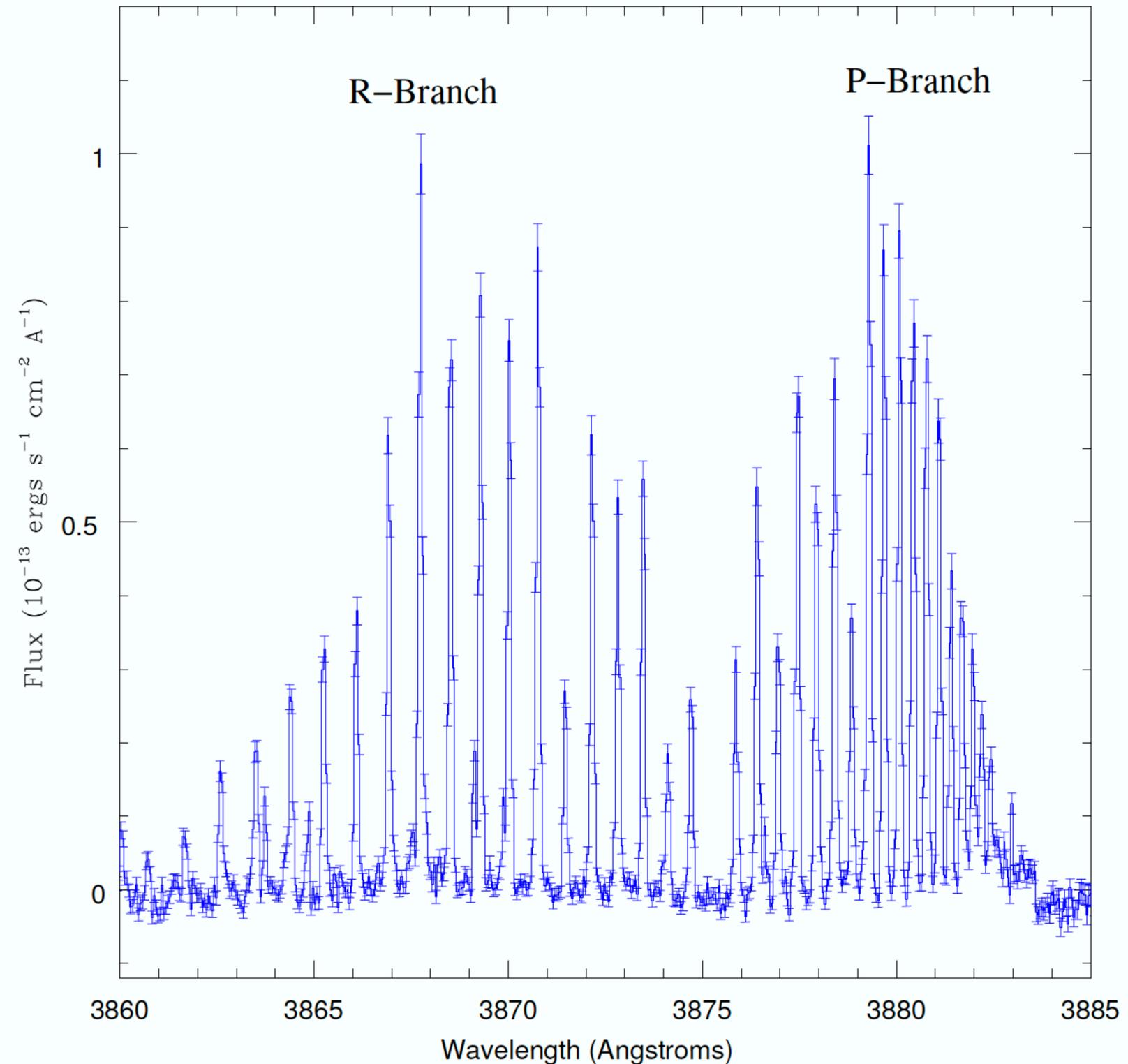
Molecular spectra: low resolution

- At low resolution, multiple lines blend together to form wide, deep “molecular absorption bands”
- 51 Eri: water, methane are dominant absorbers

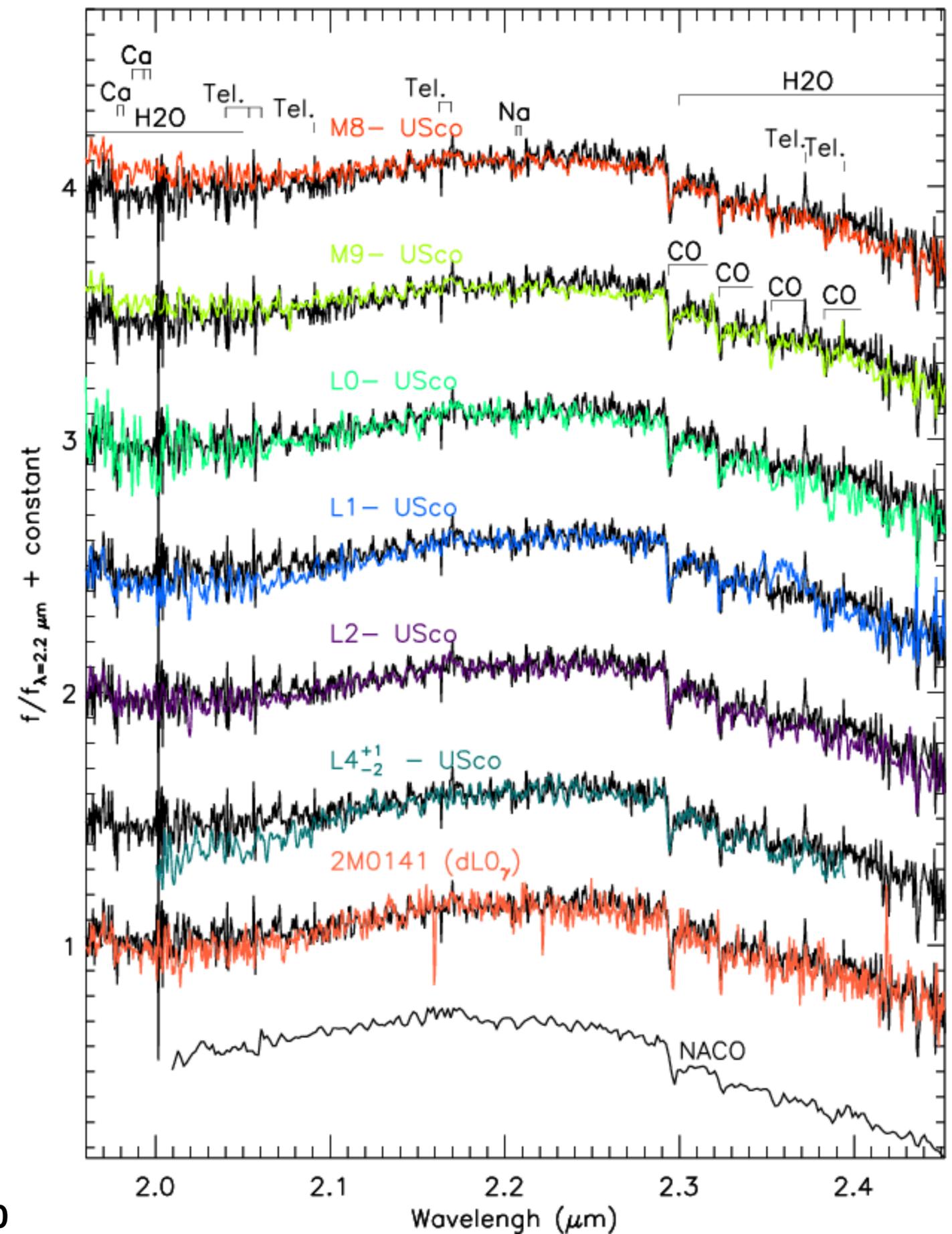


Molecular spectra: Band heads

- Because of a centrifugal distortion, and interactions between vibrational and rotational states, lines in the P branch bunch up, and lines in the R branch spread out
- This creates a “band head” (where the lines begin) to the blue



Molecular spectra: Band heads



For next time

- Reading: de Pater & Lissaeuer Chaper 3, section 3.2.2
- Homework 3 due Wednesday, September 28 at 11:59pm