

MANFRED BRATH, WS 2021/22

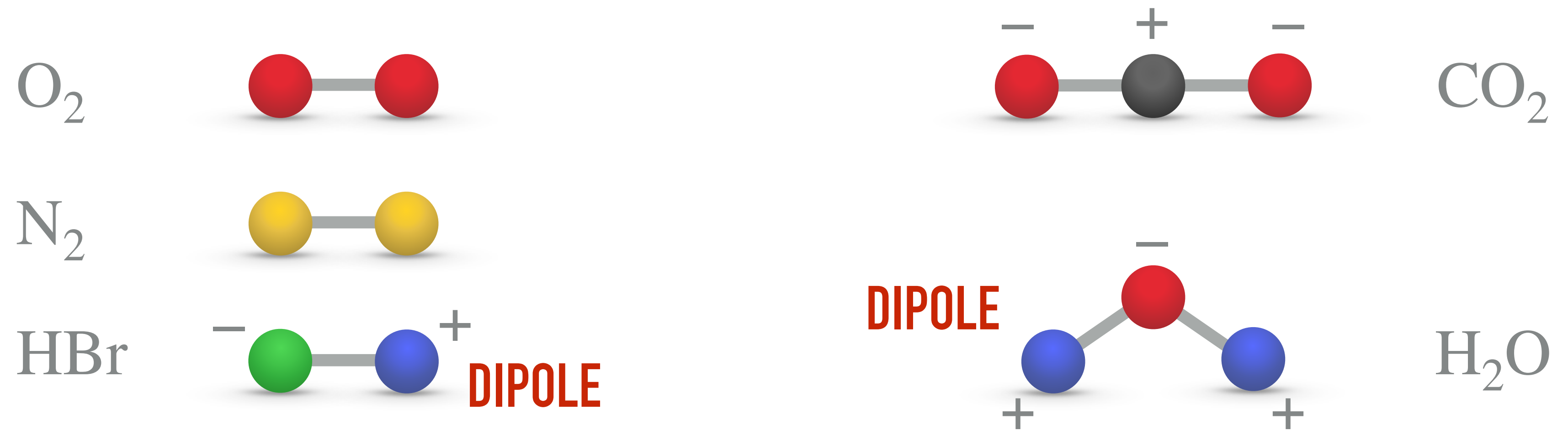
ADVANCED RADIATION AND REMOTE SENSING: ABSORPTION PROPERTIES OF THE ATMOSPHERE

MOLECULE SPECTRA

MOLECULE STRUCTURE

- ▶ This will be only a brief overview without going into any details.
- ▶ For those who interested in the details see
 - ▶ Haken, Hermann, und Hans Christoph Wolf. Molekülphysik Und Quantenchemie. Fünfte, völlig neubearbeitete und erweiterte Auflage. Springer-Verlag Berlin Heidelberg, 2006. <https://dx.doi.org/10.1007/3-540-30315-4>. (ebook/book, Stabi)
 - ▶ Demtröder, Wolfgang. Atoms, Molecules and Photons. Third edition. Springer, 2018. <https://dx.doi.org/10.1007/978-3-662-55523-1>. (ebook/book, Stabi)
 - ▶ or any other book about spectroscopy and molecular physics

MOLECULE STRUCTURE



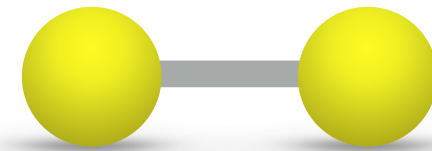
- ▶ Quantum mechanics and electrodynamics states that we need a dipole to interact with electromagnetic radiation.
 - ▶ Where do we have dipoles?

MOLECULE STRUCTURE

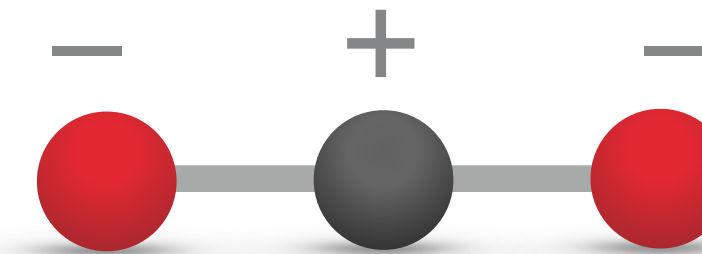
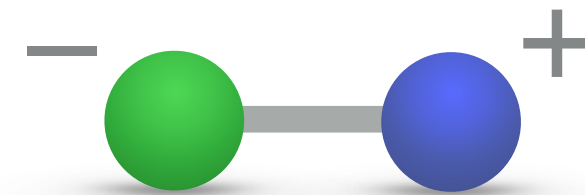
O₂



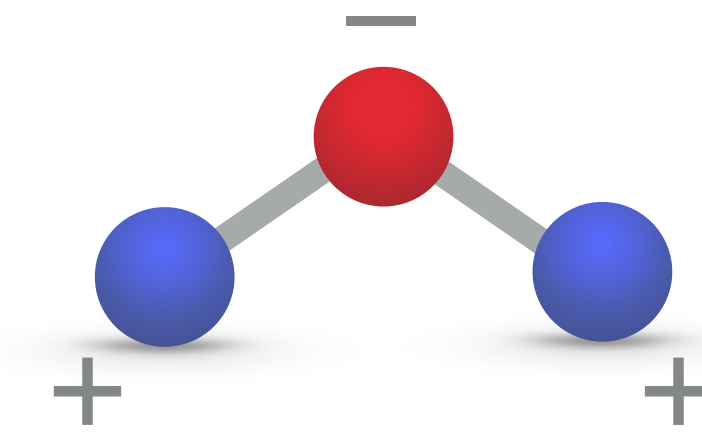
N₂



HBr



CO₂



H₂O

- ▶ A dipole is not enough. What else do we need?
- ▶ We need a periodically moving dipole.
- ▶ Two ways: Rotation and Vibration

MOLECULE STRUCTURE

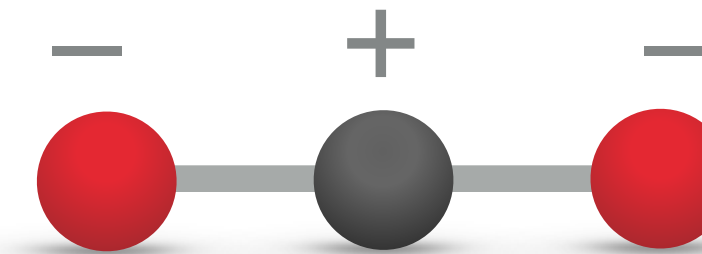
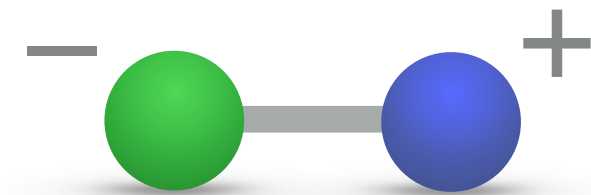
O₂



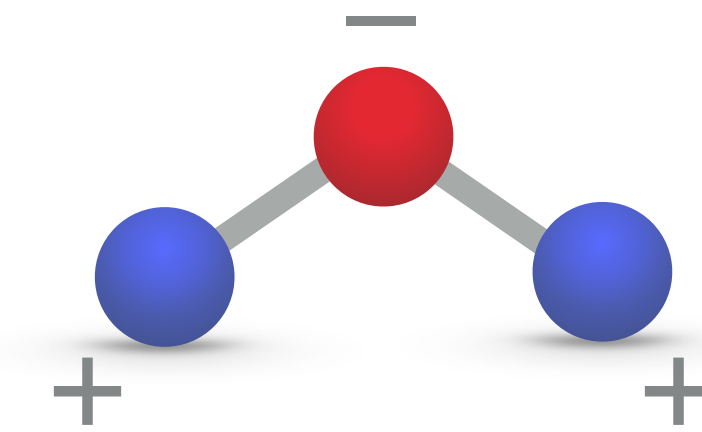
N₂



HBr



CO₂



H₂O

- What takes more energy into account rotation or vibration?

$$E_{rot} < E_{vib} < E_{el}$$

ENERGY-FREQUENCY RELATIONS

- ▶ Energy E and frequency ν differ only by the Planck constant h .

$$E = h\nu$$

- ▶ In quantum mechanics a different version is often used.

$$E = \hbar\omega = \frac{h}{2\pi}2\pi\nu$$

TYPICAL SPECTRAL QUANTITIES, UNITS AND ORDER OF MAGNITUDE

Microwave (MW) Frequency ν $\mathcal{O}(100 \text{ GHz})$

Infrared (IR) Wavenumber $\tilde{\nu}$ $\mathcal{O}(1000 \text{ cm}^{-1})$

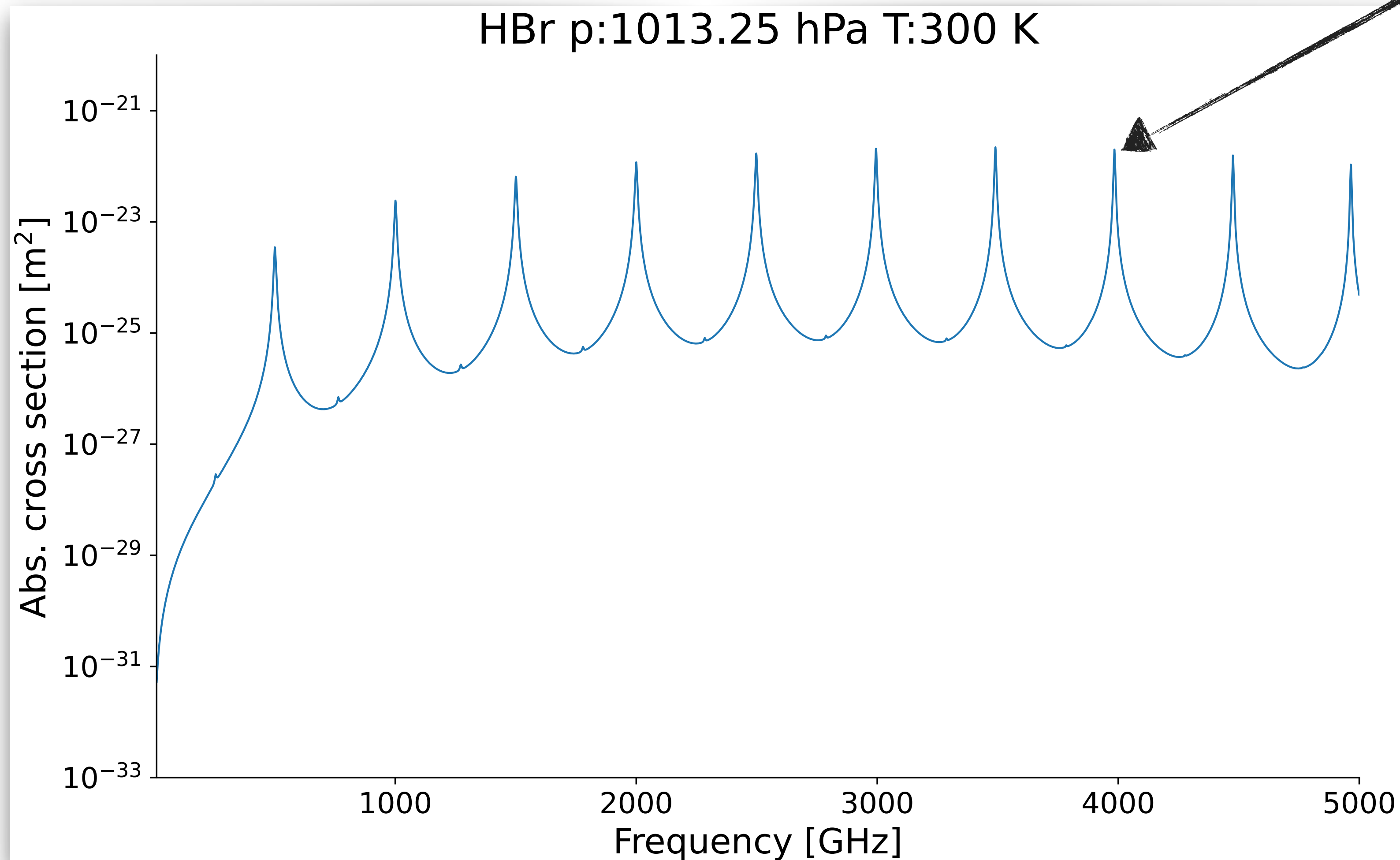
Wavelength λ $\mathcal{O}(15 \mu\text{m})$

Visible Wavelength λ $\mathcal{O}(500 \text{ nm})$

$$\tilde{\nu} = \frac{\nu}{c_0}$$

$$\lambda = \frac{c}{\nu}$$

ROTATION SPECTRA



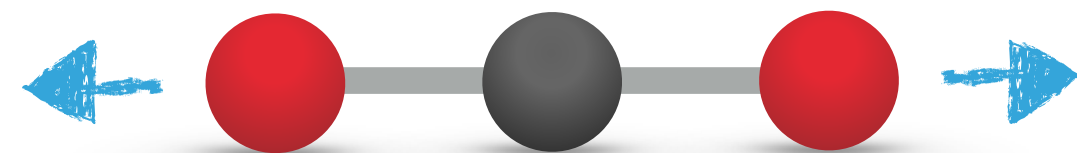
Transition from one state to another **not** the rotational state

- ▶ Spectrum consists several discrete lines.
- ▶ Rotational states are discrete (quantised).

VIBRATION

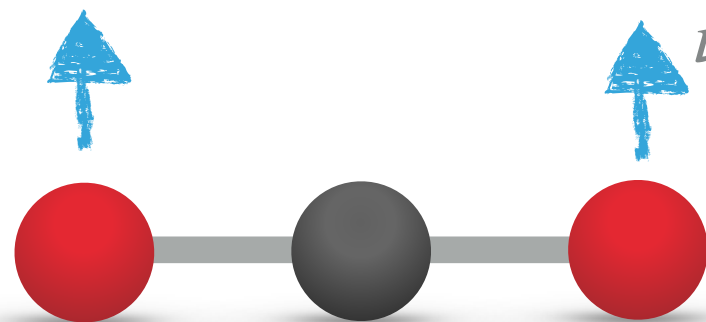


$\tilde{\nu}_1 = 1330 \text{ cm}^{-1}$



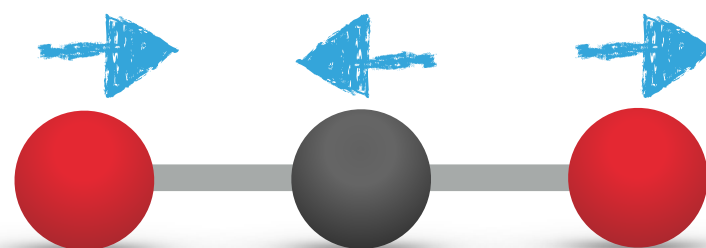
DIPOLE

$\tilde{\nu}_2 = 667 \text{ cm}^{-1}$

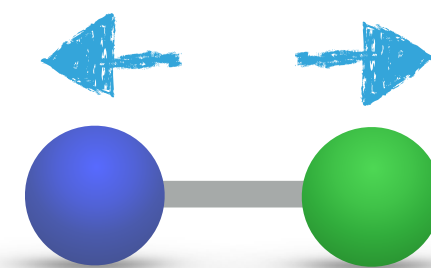


DIPOLE

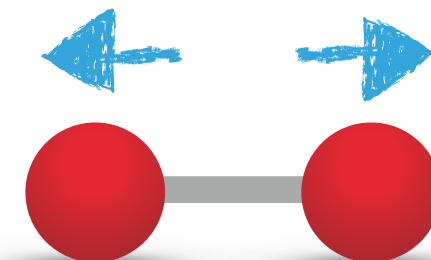
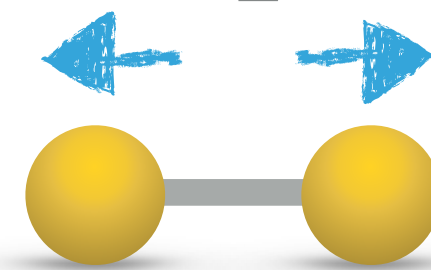
$\tilde{\nu}_3 = 2350 \text{ cm}^{-1}$



$\tilde{\nu} = 2558 \text{ cm}^{-1}$

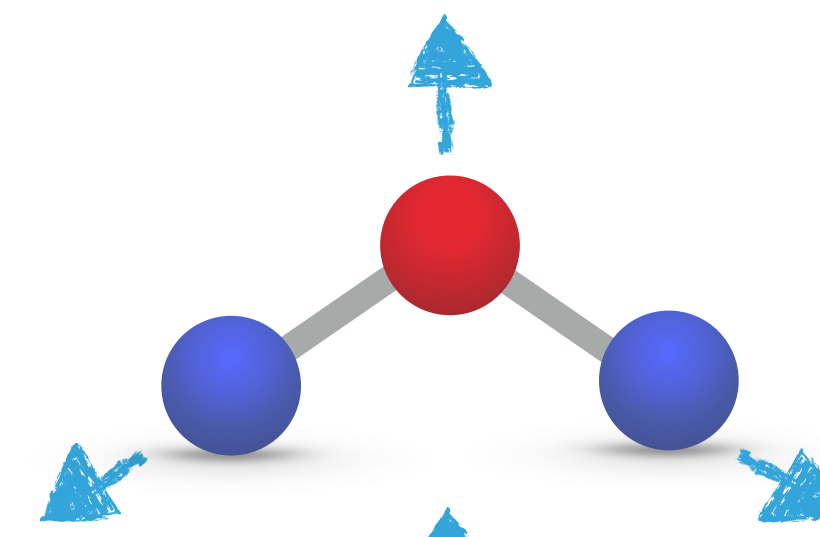


DIPOLE



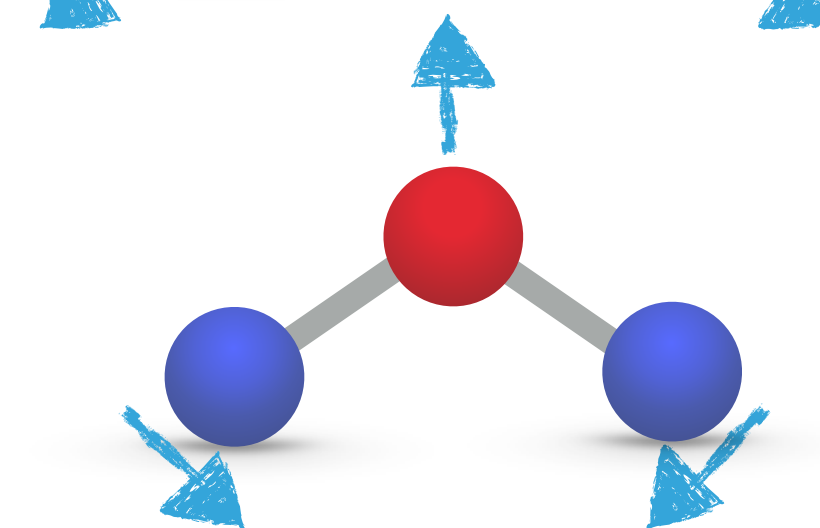
$\tilde{\nu}_1 = 3652 \text{ cm}^{-1}$

DIPOLE



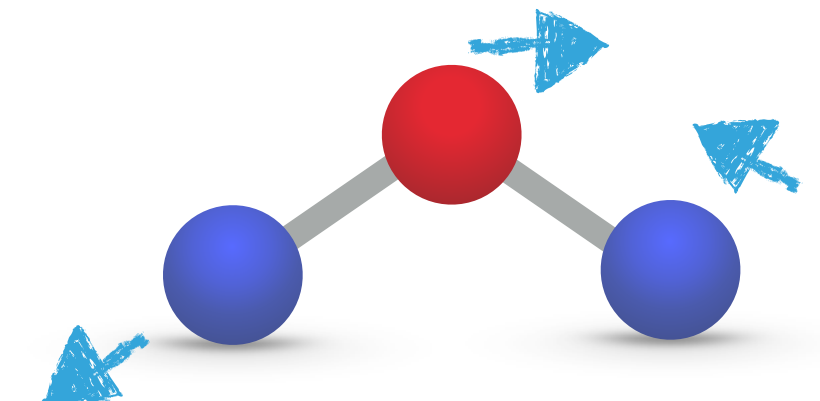
$\tilde{\nu}_2 = 1595 \text{ cm}^{-1}$

DIPOLE



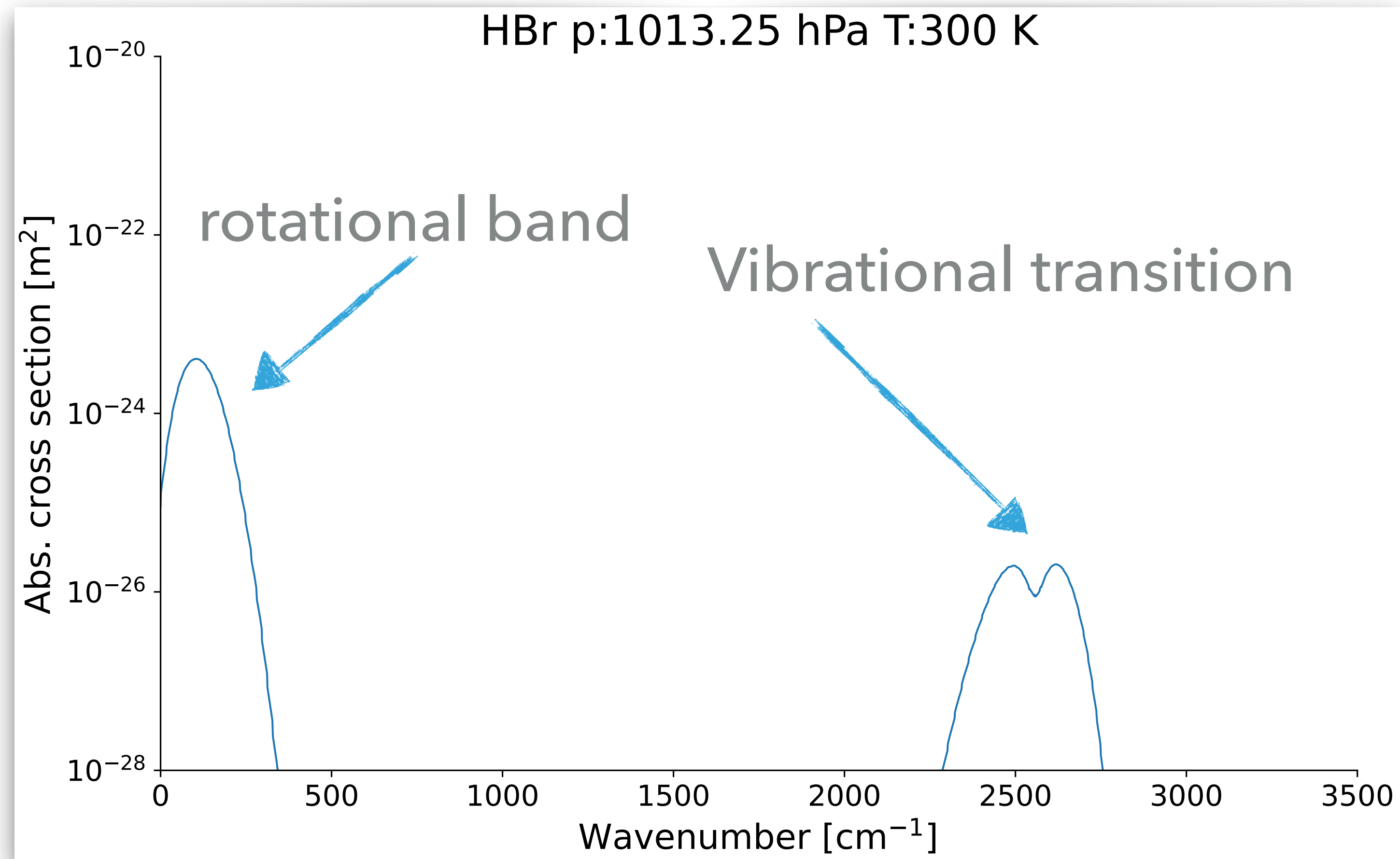
$\tilde{\nu}_3 = 3756 \text{ cm}^{-1}$

DIPOLE



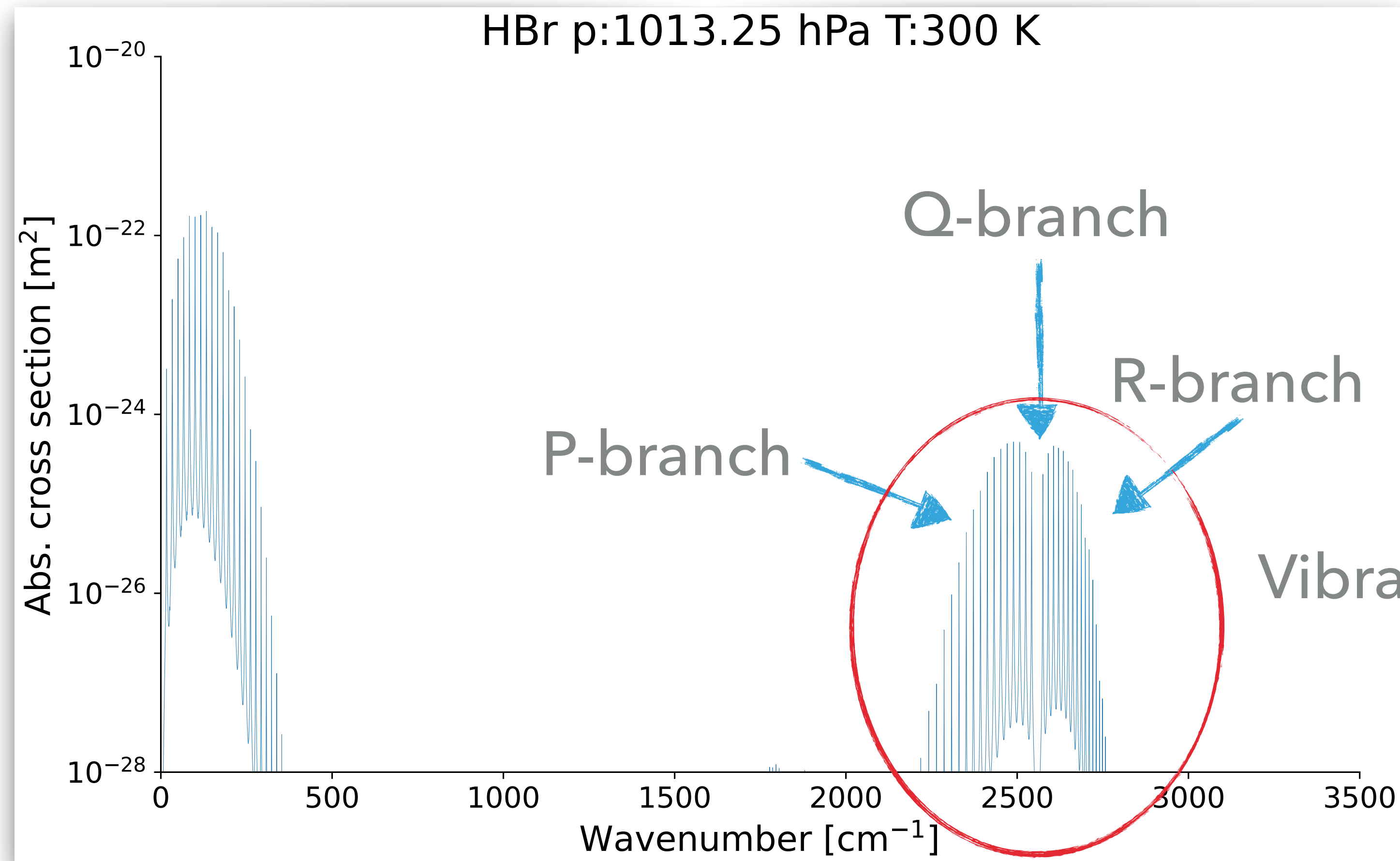
- Which of these vibrational modes induce a changing dipole?

VIBRATION (LOW-RES)



- ▶ Vibrational transitions occur at 10 to 100 times larger energy levels than rotational transitions.
- ▶ Vibrational transitions are also quantised.

VIBRATION (HI-RES)



- ▶ Vibrational transitions in general never occur alone but are coupled with simultaneous rotational transitions.
- ▶ CO₂ is one of the exclusions.

SWITCH TO EXERCISE 1