Lecture 14, Feb 10, 2023

Molecular Spectroscopy

- Why does a molecule or atom absorb light?
  - The incoming photon is an electromagnetic wave, which moves the electron
  - This physically distorts the electron density and changes it into the shape of another stable configuration, e.g. 2s to 2p
- Spectroscopy measures emission wavelengths
  - The spectrum has a finite width which comes from the uncertainty principle, $\Delta E \Delta t \geq \dfrac{\hbar}{2}$ where Δt is the lifetime of the excitation
  - There is also a fundamental line resolution (distance between lines)
- Selection rules exist to determine whether transitions can take place – not all transitions happen
  - Transitions are either allowed (high probability) or forbidden (low probability)
  - Not a hard yes or no but probabilistic
- The dipole moment μ in an atom creates a potential difference when an electric field (photon) comes along $U = \mu E$
- The expectation value for the electric field to create a dipole moment via the mixing of electron distributions from the ground and excited states is only nonzero when we have a symmetry
  - Example: from an s orbital to p orbital involves a change in symmetry, so the transition is allowed (symmetry allowed); from 1s to 2s has no change in symmetry so it's not allowed (symmetry forbidden)
  - The change in l is always ± 1
  - There must be no spin multiplicity: $\Delta S = 0$