Term symbols for molecules

Syntax: \( ^{2S+1}|M_L| \)

\[
M_L = \sum m_l, \quad S = \sum s
\]

\[
m_l = 0 \ (\sigma \text{ from } s \text{ or } p_z \text{ orbitals}),
\]

\[
m_l = \pm 1 \ (\pi \text{ from } p_x, p_y \text{-orbitals})
\]

- Simplified by the selection rules
  - no electron with same quantum number set!!
Spectroscopy

• Absorption/Emission of energy in the form of a wave-particle duality
  – happens at UV-vis and IR-wavelengths
  – most often involves the ground state
    Boltzmann distribution

• Drives Chemistry in the Atmosphere!
  – solar input is converted to
    • higher chemical potential (entropy $\rightarrow$ radicals)
    • higher kinetic energy
Some ground rules

• an “electronic transition” describes a change of the electron configuration of an atom or molecule, usually cause by UV-vis light
  – transitions usually occur between “S₀” and “S₁”

• a “ro-vibrational transition” describes a change of the quantum mechanical “sub-states” of rotation or vibration, usually caused by visible or IR-light
Boltzmann distribution

\[ \frac{N_i}{N_j} = \exp\left(-\frac{(E_i - E_j)}{kT}\right) \]

from Atkinson: Physical Chemistry
from Boeker and van Grondelle: Environmental Physics

Solar Spectrum

Transmittance (\%)
Oxygen electronic states

from Finlayson-Pitts and Pitts: Chemistry of the upper and lower Atmosphere
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1968.

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