CHM 3411 Problem Solving Session, 4-21-2018

Chapter 13: Electronic Spectroscopy

Topics

- Examples of excited states
  - O_2 singlet
- Potential energy surfaces for electronic states
- Franck-Condon principle/factor (for radiative transitions)
  - Vertical transition
- Examples of transitions
  - $\pi^* \leftarrow \pi$
  - $\pi^* \leftarrow n$
- Dissociation & Pre-dissociation
- Fluorescence & Phosphorescence
- Principle of lasers

Problem 13A.2

- Given: Vibrational wavenumber of O_2 molecule in electronic ground state is 1580 cm^{-1}, whereas that in the excited stat ($B^3\Sigma_u^-$), to which there is an allowed electronic transition, is 700 cm^{-1}. Separation in energy between the minima between PES's is 6175 eV.

- Determine: What is wavenumber of the lowest energy transition out of the the v=0 vibrational state of the electronic ground state to this excited state?
  - Helpful: 1 eV = 8065.5 cm^{-1} (treating both as energy units, which of course they are not really)

- Approach:
  - 1. Draw the PESs and label everything you know (from the problem)
  - 2. Draw a schematic absorption spectrum
  - 3. Add the vertical transition to your PES plot
  - 4. Now work on the problem

Problem 13A.3

Data given on board