Chem360 Final Exam Practice

Mission:

More practice to get in the groove
(“getting groovy, baby”)

1. Resonance (caffeine)
2. VOMELDs (O_2 and BrNNCN)
3. IR-active modes (HCCH)
4. Write out operators (V for HO, H for elementary problems and Fe^{2+} and CH_4)
5. Energy level transition math (Phyllis the Photon)
6. Probability for being in a range
7. <r> and r_{mp}

Other tips:
--know your terminology (orthogonal, superposition, eigenfunction, rovibronic, …
--know your energy level diagrams
--lots of little things, e.g. uncertainty = standard deviation = SQRT of variance

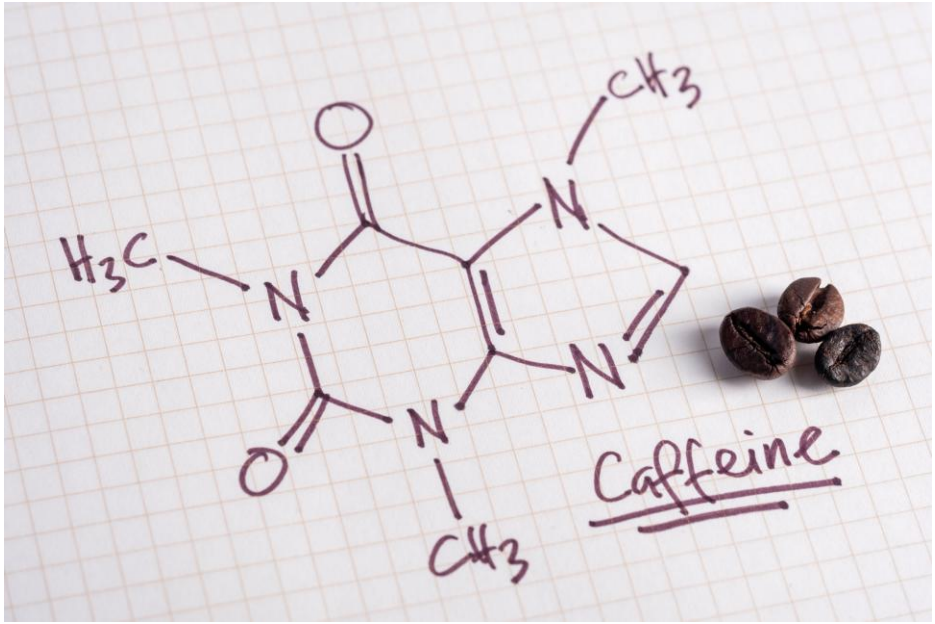
Exam rules:
--No bunnyhugs/hoodies! (new rule ~2023)
--No food/drink except water in clear labelless plastic bottles
--calculator inspection
--show university ID (gym rules)

1. Caffeine resonance

In the caffeine molecule, all four N's are sp^2-hybridized.

(a) How many occupied σ_{NB} and π_{NB} molecular orbitals are in the molecule?

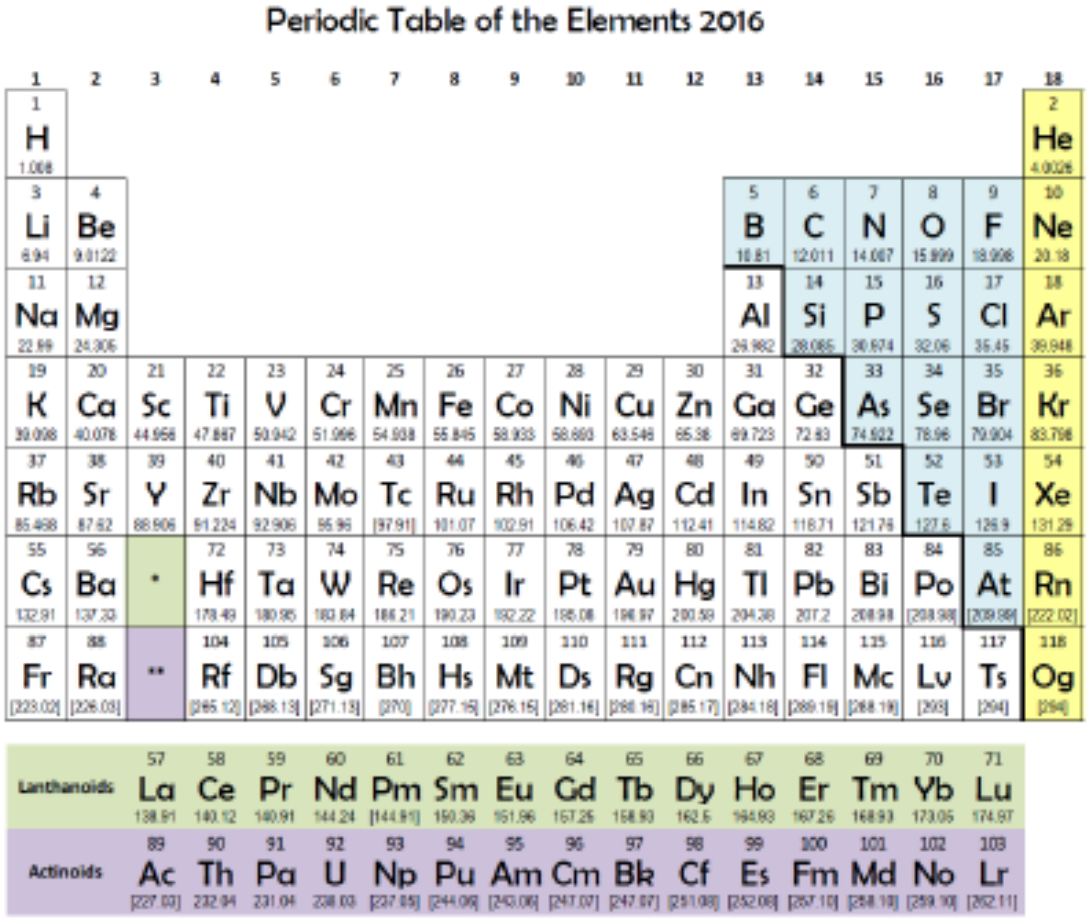
(b) Explain each π_{NB} by showing an appropriate secondary Lewis structure with formal charge separation (put the negative charge on an O atom).



2. VOMELD for O_2 and BrNNCN

(a) Sketch the VOMELD for O_2 molecule and predict its HOMO

(b) Sketch the total-molecule VOMELD for BrNNCN (the three central atoms are each 2-coordinate)



3. IR-active modes of HCCH

The molecule HCCH has 7 normal modes of vibration:

CC str,
sym CH str,
antisym CH str,
sym HCC bend xz plane,
antisym HCC bend xz plane,
sym HCC bend yz plane,
antisym HCC bend yz plane

(a) How many of these would be IR active? (Hint: sketching out the modes may help)

(b) If no overtone or combination bands are present, how many distinct peaks would you expect to see in the ordinary (low-resolution) IR spectrum?

4. Write out operators (V for HO, H for elementary problems and Fe^{2+} and CH_4)

Write out the operators for:

(a) $\hat{V}$ for particle in a box

(b) $\hat{V}$ for harmonic oscillator

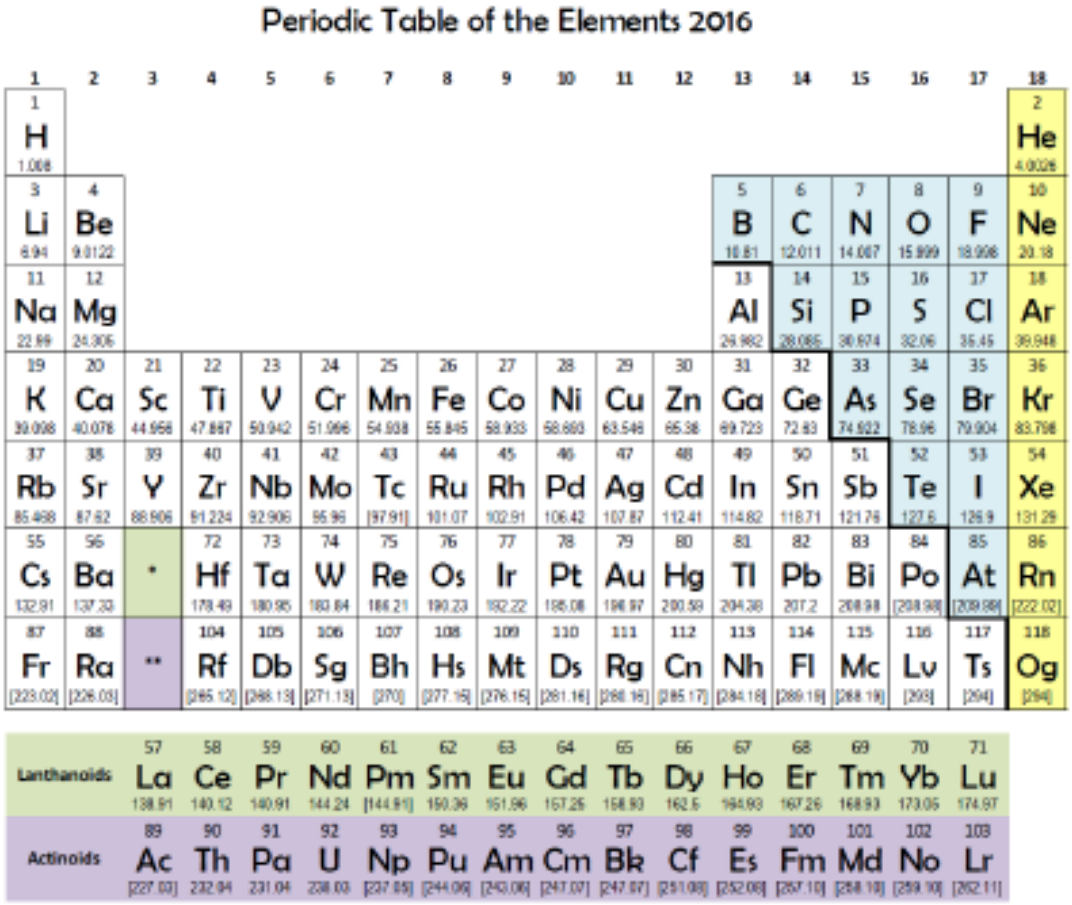
(c) $\hat{H}$ for particle in a box

(d) $\hat{H}$ for one-body harmonic oscillator

(e) $\hat{H}$ for two-body 2D rigid rotor

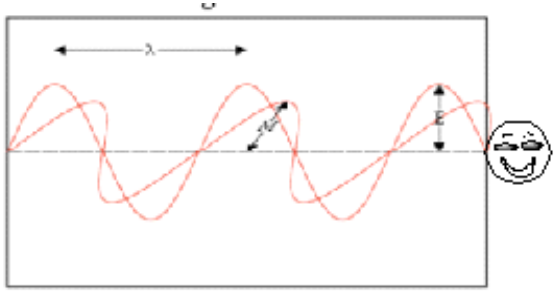
(f) $\hat{H}_{elec}$ for Fe^{2+} atom

(g) $\hat{H}_{elec}$ for CH_4 molecule



5. Phyllis the Photon (energy level transition math)

Phyllis the Photon has an energy of 7.5×10^{-19} J.



a) Determine her frequency, wavenumber, wavelength, and momentum.
b) She can boost the energy of a neutron from its n=2 to its n=6 state if the neutron is a particle-in-a-1D box with no forces. Determine the length of the 1D box.
c) She can boost the energy of an oscillating neutron from its n=1 to its n=2 state if the neutron is a one-body harmonic oscillator. Determine the force constant k.
d) She can kick out a photoelectron from a metal of work function $\Phi = 4.4 \times 10^{-19}$ J. Determine the speed of the photoelectron.

6. Probability for being in a range

Consider a particle in a box in its n=2 state.

(a) How many internal nodes does its wavefunction have?

(b) Calculate the probability that the particle is in the middle third of its range at any given moment.

7. <r> and r_{mp}

Calculate <r> and r_{mp} for the excited Be^{3+} ion having its only electron up in a 3d orbital.