Example CHEM 4448 Final Examination.
The multiple choice answers have not been included.

1) In general, a wavefunction with zero nodes will have a lower kinetic energy than a wavefunction with many nodes.

2) Increasing the mass of the particle in a quantum mechanical model will lower the energy level spacing.

3) The kinetic energy of a wave function is proportional to the curvature of the wave function.

4) Which of these would yield the energy of Y_n?

5) The intensity of an absorbance transition is proportional to what?

6) What are the direct absorption and emission selection rules for the principle quantum number?

7) What are the selection rules for the angular momentum quantum number?

8) The "forbidden" **emission** transition from the triplet P state to the singlet S in Helium is called:

9) Which atom exhibits two half-filled subshells in its ground state electron configuration?

10) Refer to the Octahedral Character Table. What is the Mullikan symmetry notation for the p orbitals?

11) Refer to the Octahedral Direct Product Table. What is the result of the direct product of T_{1u} and T_{2g}?

12) What is the point group, and the HCO angle value in formaldehyde (CH_2O)?

13) What is the point group, of the gas phase methyl cation (CH_3^+)?

14) What is the point group of 1,2,3-trichlorobenzene?

15) What is the symmetry set-up of the transition dipole moment for the allowed vibrational transition for the asymmetric stretch in water?

16) What is the symmetry set-up of the transition dipole moment for the allowed vibrational transition for the symmetric stretch in ammonia?

17) How many rotational degrees of freedom does a linear molecule possess?

18) Formic acid (HCOOH) will have _____vibrational degrees of freedom.

19) Centrifugal distortion causes _____.

20) What is the spacing between the rovibrational lines in the infrared spectrum?

21) What is the spacing between the rovibrational lines in the Raman spectrum?

22) Which second row diatomic ion has the shortest bond length?

23) The _____Factor accounts for the thermal population of excited energy states..

24) Picture in your mind a Jablonski diagram. A radiative transfer from S_1 to S_0 is _____.

25) The multiplicity of the methyl protons (CH3) on 2-propanol is _____.

26) The multiplicity of the central proton (CH) on 2-propanol is _____.

27) The multiplicity of the hydroxyl proton (OH) on 2-propanol is _____.

28) Why are NMR spectra reported in terms of chemical shift?

29) If the rotational constant of $^{1}H^{37}Cl$ is 9.9 +/- 0.2 cm^{-1}, what is the bond length?

30) If the rotational constant of $^{1}H^{37}Cl$ is 9.9 +/- 0.2 cm^{-1}, what is the uncertainty in bond length?

31) (9%) Gallium nitride (GaN) is an important species in LEDs. Draw the MO diagram of GaN. (Ignore the filled 3d shell for simplicity.) Label the atom energy levels, the MO energy levels, populate the atomic orbitals with valence electrons, and the MOs with electrons. Label the HOMO and LUMO. Calculate the bond order, and the number of valence-band XPS peaks that would be seen in this species.