Final Exam, Chem 311, 120 minutes, Dr. H. Guo, Dec. 17, 2008

You are allowed to bring a two page sheet containing equations and a calculator

I. Answer the following multiple choice questions (5 pts each), choose one answer only!

1. Which of the following phenomena is **not** a quantum effect?
A. Zero-point energy.
B. Quantized energy.
C. Quantized angular momentum.
D. Tunneling.
E. Energy conservation.

2. What is the spin multiplicity of the ground electronic state of a Na atom?
A. 0.
B. 1.
C. 2.
D. 3.
E. 4.

3. For an electron restricted to a two-dimensional rectangular well, how many quantum numbers does it have?
A. 0.
B. 1.
C. 2.
D. 3.
E. 4.

4. The term "interstate crossing" is used for
A. a transition from an excited singlet state to another singlet state.
B. a transition from the ground singlet state to an excited singlet state.
C. a transition from an excited singlet state to an excited triplet state.
D. a transition from an excited triplet state to an excited singlet state.
E. a transition from an excited triplet state to the ground singlet state.

5. Which of the following conditions is appropriate for a symmetric rotor?
A. $I_x=I_y=I_z$.
B. $I_x=I_y\neq I_z$.
C. $I_x\neq I_y\neq I_z$.
D. $I_x=I_y$, $I_z=0$.
E. none of the above.

6. The probability for finding a particle at a point (x,y,z) in a three-dimensional space is given by

A. $\Psi(x, y, z)$

B. $|\Psi(x, y, z)|^2$

C. $\Psi(x, y, z)dxdydz$

D. $|\Psi(x, y, z)|^2 dxdydz$

E. $\int|\Psi(x, y, z)|^2 dxdydz$

7. Which of the following approximations assumes the separation of electronic and nuclear motions ?

A. The Born-Oppenheimer approximation.

B. The Hund's rule.

C. Heisenberg's uncertainty principle.

D. The Hartree-Fock approximation.

E. The Hückel approximation.

8. How many vibrational quantum numbers does the molecule CH_4 have?

A. 5.

B. 9.

C. 10.

D. 12.

E. 15.

9. What point group does the molecule CO_2 belong to?

A. C_i.

B. C_s.

C. $D_{\infty h}$.

D. $C_{\infty v}$.

E. C_{2v}.

10. Which of the following molecules has **no** rotational spectrum?

A. NH_3.

B. HCl.

C. N_2.

D. H_2O.

E. NO.

II. Solve the following simple problems

11. (10 pts) An electron is trapped in a one-dimensional well, which has a length of 1.5 nm. Calculate the photon wavelength needed to excite the electron from the ground state to the first excited state.

12. (10 pts) An atom has an electronic configuration corresponding to ^4D. Determine all possible *J* values and write the all the term symbols.

13. (10 pts) Electrons ejected from a metal by a 346 nm light are detected to have a velocity of 1.3×10^5 m/s. Calculate the work function of the metal in eV.

14. (10 pts) An electron is measured to have a speed of 1.5×10^5 m/s with an uncertainty of 0.5×10^5 m/s. Calculate the uncertainty of its position.

15. (10pts) A proton is accelerated to a speed of 2.3×10^3 m/s. Calculate its de Broglie wavelength in nm.

16. (10 pts) Prove that the linear combinations $p_x \pm ip_y$ are eigenfunctions of the angular momentum operator $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$ and calculate the corresponding eigenvalues.

($p_x = f(r)\sin\theta\cos\phi$, $p_y = f(r)\sin\theta\sin\phi$)

III. Solve the following more complicated problems

17. (15 pts) Determine if the following integral of H_2O is zero based on the symmetry of the molecule. The character table is attached in the back of the test.

$$I = \int \Psi(a_1) x \Psi(b_2) d\tau$$

in which $\Psi(a_1)$ and $\Psi(b_2)$ are molecular orbitals of H_2O belonging to the A_1 and B_2 irreducible representations of the C_{2v} group.

Character table for C_{2v} point group

	E	**C_2 (z)**	**σ_v(xz)**	**σ_v(yz)**	**linear, rotations**	**quadratic**
A_1	1	1	1	1	z	x^2, y^2, z^2
A_2	1	1	-1	-1	R_z	xy
B_1	1	-1	1	-1	x, R_y	xz
B_2	1	-1	-1	1	y, R_x	yz

18. (15 pts) Draw the molecular orbital energy level diagram for O_2. Calculate the bond order and the spin multiplicity of the molecule. Sketch the shapes of the HOMO and LUMO. Derive the electronic configuration for O_2^- and O_2^+ and compare their relative stability.

19. (20 pts) The IR spectrum of HBr is dominated by a strong line at 2649 cm^{-1}. Determine the force constant and zero-point energy of this molecule, assuming it can be approximated by a harmonic oscillator. If the hydrogen is replaced by deuterium, what will be the transition frequency in cm^{-1} for DBr?

20. (20 pts) The microwave spectrum of $H^{35}Cl$ consists of equally spaced lines separated by 21.2 cm^{-1}. Calculate the rotational constant and the moment of inertia of the molecule and determine its bond length. Explain the quantization of the rotational angular momentum by drawing the vector model for the J=2 state.

21. (20 pts) A spectral line in the Balmer (2→*n*) series of the hydrogen atom was detected at 15233 cm^{-1}. Find out the principle quantum number (*n*) of the state into which electron made the transition. If the electron is further excited to the vacuum by a 256 nm photon, what will be the kinetic energy of the free electron? (R_H=109677 cm^{-1})