Part A. (40%) 選擇題、答對兩分，答錯不倒扣.

1. O_2 has a net spin angular momentum, so oxygen should be (1) paramagnetic (2) diamagnetic (3) neither.

2. The eigenvalue of a particle in a box is $n^2h^2 / 8mL^2$, where n is the quantum number and L is the length of the box, what is the energy that will excite the particle from the lowest level to the next one? (1) $h^2 / 8mL^2$ (2) $2h^2 / 8mL^2$ (3) $3h^2 / 8mL^2$ (4) $4h^2 / 8mL^2$

3. If the root mean square deviation of a particle in box is $L\sqrt{1-6/n^2\pi^2} / 2\sqrt{3}$, what is the corresponding classical root mean square deviation? (1) 0 (2) L (3) $L / 2\sqrt{3}$ (4) ∞.

4. What is the thermal energy at room temperature? (1) 0.6 kcal/mol (2) 1.2 kcal/mol (3) 4.8 kcal/mol (4) 9.6 kcal/mol.

5, The eigenvalues of a hermitian must be (1) positive (2) negative (3) real (4) complex.

6. The Boltzmann distribution of a particle with energy E is denoted by P, then $P \propto$ (1) $e^{E/kT}$ (2) $e^{-E/kT}$ (3) $e^{E^2/kT}$ (4) $e^{-E^2/kT}$

7. For light atoms with atom number $Z < 40$, what coupling scheme is usually used? (1) Russell-Saunders coupling scheme (2) j-j coupling scheme.

8. For atom with $L = 3, S = \frac{3}{2}, J = \frac{3}{2}$, the term symbol is (1) ${}^4D_{3/2}$ (2) ${}^{3/2}F_4$ (3) ${}^4F_{3/2}$

9. According to Hund's rule, the term with smaller multiplicity should be (1) more stable (2) less stable.

10 For a first order reaction, which of the following statements is correct (1) the half-life $\tau_{1/2}$ of a reactant is dependent on its initial concentration (2) the half-life $\tau_{1/2}$ of a reactant is independent of its initial concentration (3) the concentration of the reactant decays linearly with time.

11 What is the bond order of Ne_2? (1) 0 (2) 1 (3) 2.

12 What is steady-state approximation? (1) The concentrations of all intermediates are very small. (2) The rates of change of the concentrations of all intermediates are very small. (3) The concentrations of both reactant and product are "steady", i.e., unchanged.

13 If two nearby amino residues A and B have pKa values of 3.8 and 6.0, respectively, then it is reasonable to suppose that a proton can transfer (1) from A to B (2) from B to A (3) neither.

14. According to the assumptions of Transition State Theory, what happens to the fate of the particles that have crossed the transition state in the direction of products? (1) They cannot turn around and reform reactants. (2) They can turn around and reform reactants. (3) They will stay at the transition state forever.

15. What is the entropy of CO_2 at T=0? (1) 0(2) $R\ln 2$(3) $R\ln 3$. (R is the gas constant).

16. The diffusion-controlled limit sets for the enzymatic reactions (1) the upper limit (2) the lower limit (3) neither.

17. According to the variational principle, if an arbitrary wavefunction is used to calculate the energy, then the calculated energy is (1) never less than the true energy (2) always less than the true energy (3) always equal to the true energy.

18. A semiconductor is a substance with a conductivity that (1) increases as the temperature is raised (2) decreases as the temperature is raised (3) independent of the temperature.

19. According to the Born equation, the smaller the size of the ion, (1) the larger the solvation energy (2) the smaller the solvation energy (3) the solvation energy is independent of the size of the ion.

20. 1 cal = (1) 0.4184 j (2) 4.184 j (2) 41.84 j.

Part B. (24%) For the statements below, choose the word or words inside the parentheses that serve(s) to make a correct statement.

(1.) At 100°C, the equilibrium vapor pressure of water is 1 atm. Consider the process where 1 mol of water vapor at 1 atm pressure is reversible condensed to liquid water at 100°C by slowly removing heat into the surroundings. In this process the entropy of the system will (increase, remain unchanged, decrease). The entropy of the universe will (increase, remain unchanged, decrease).

(2.) According to the second law of thermodynamics, a spontaneous process, such as a balloon filled with hot gas cooling to the surroundings at constant pressure, will always occur (adiabatically, reversibly, irreversibly, without work done). The heat gained by the surroundings is just equal to the negative of the (internal energy change, enthalpy change, entropy change, Gibbs free energy change) of the system.

(3.) For the reaction A –> B, if at some stage $\Delta G > 0$, then the reaction (A -> B, B -> A, both, neither) is/are spontaneous.

(4.) The van't Hoff equation is an expression for the slope of a graph of the (free energy, equilibrium constant, heat capacity, enthalpy) plotted against the temperature.

(5.) ^{17}O has a nuclear spin (I) of 5/2, so its number of possible spin states is (3, 4, 5, 6). Outside a magnetic field, these spin states have (different, same) energy.

(6.) The gross selection rule for a molecular vibration is that the electric dipole moment of the molecule must change when the atoms are displaced. According to this rule, we can predict that (CO_2, NO, H_2O H_2, CH_4, N_2) have vibrational absorption spectra.

Part C. (36%)

1. (10%) Write down the electronic configurations of F_2^+ and F_2, predict and explain which one has a larger dissociation energy.

2. (6%) A pH meter is to be standardized with a pH 7 buffer. By accident, a student in the lab used a pH 8 standard buffer and the meter was adjusted to read pH 7. Then he measured his protein sample and the meter indicated that its pH is 5.7. What is the actual pH of the sample? What is the H^+ ion concentration at this actual pH?

3. (10%) A molecule has a spectral line at 3000 cm^{-1}.
   a.) What are its frequency and its wavelength? ($C=3 \times 10^{10}$ cm)
   b.) In what part of the spectrum is it located?

4. (10%) Standard Enthalpies of Formation at 298°K

Compound	ΔHf (kJ/mol)
CH_3OH (l)	-239
CO_2 (g)	-395
H_2O (l)	-286
H_2O (g)	-242

a.) Calculate the standard molar enthalpy for the combustion of liquid methanol(CH_3OH) to CO_2(g) and H_2O(l) at 298°K.

[Hint: first write a balanced equation for this reaction.]

b.) The liquid phase oxidation of methanol to formic acid (HCOOH) by O_2(g) at 298°K results in the evolution of 472 kJ of heat per mole of reaction at 1 atm. Calculate the standard enthalpy of formation of formic acid.