

## 物理常數

$$\begin{array}{lll}
 h = 6.626 \times 10^{-34} \text{ J}\cdot\text{s} & e = 1.602 \times 10^{-19} \text{ C} & m_e = 9.109 \times 10^{-31} \text{ kg} \\
 c = 2.998 \times 10^8 \text{ m s}^{-1} & 4\pi\epsilon_0 = 1.113 \times 10^{-10} \text{ J}^{-1} \text{ C}^2 \text{ m}^{-1} & 1 \text{ cal} = 4.184 \text{ J} \\
 L = 6.022 \times 10^{23} \text{ mol}^{-1} & k_B = 1.381 \times 10^{-23} \text{ J K}^{-1} & \text{amu} = 1.66054 \times 10^{-27} \text{ kg}
 \end{array}$$

## 單選題 (每題四分，共一百分)

- Comparing the following energies in magnitude (1) ionization energy of H atom (2) ionization energy of He atom (3) vibrational zero-point energy of  $\text{CH}_4$  (4) hydrogen bonding in water dimer (5) average rotational energy of benzene at room temperature  
(A) (2) > (1) > (3) > (5) > (4) (B) (2) > (1) > (3) > (4) > (5) (C) (1) > (2) > (3) > (5) > (4)  
(D) (2) > (1) > (5) > (3) > (4) (E) (2) > (3) > (1) > (4) > (5)
- What is the molar heat capacity of the copper metal at room temperatures? (A) 8.314 J/K (B) 20.8 J/K (C) 4.185 J/K (D) 25.0 J/K (E) 0.0 J/K
- Which of the following molecule is paramagnetic?  
(A)  $\text{B}_2$  (B)  $\text{C}_2$  (C)  $\text{N}_2$  (D)  $\text{NO}^+$  (E)  $\text{LiF}$ .
- The vibrational frequency of  $\text{O}_2$  molecule is  $1580 \text{ cm}^{-1}$ . The force constant of the O=O chemical bond is:  
(A) 509 N/m (B) 120 N/m (C) 253 N/m (D) 1664 N/m (E) 1177 N/m
- Following the above question, what is the separation between the vibrational ground state and the first excited state of the  $\text{O}_2$  molecule?  
(A) 4.5 kcal/mol (B) 1.3 kcal/mol (C) 2.3 kcal/mol (D) 0.7 kcal/mol (E) 9 kcal/mol
- Which of the following molecule can easily be identified by an IR spectrometer?  
(A)  $\text{F}_2$  (B)  $\text{H}_2$  (C)  $\text{CO}$  (D)  $\text{He}_2$  (E)  $\text{C}_2$
- What is the ground-state term symbol for the oxygen atom?  
(A)  $^2P_{1/2}$  (B)  $^2P_{3/2}$  (C)  $^1P_1$  (D)  $^1S_0$  (E)  $^3P_2$
- Which of the following is an eigenfunction of 1-D harmonic oscillator? ( $c$  is a constant)  
(A)  $x^2$  (B)  $e^{-cx}$  (C)  $\sin cx$  (D)  $e^{-cx^2}$  (E)  $xe^{-cx}$
- What is the de Broglie wavelength of an electron moving at a speed of  $1.0 \times 10^6 \text{ m s}^{-1}$ .  
(A) 4.1 Å (B) 7.3 Å (C) 22 Å (D) 4100 Å (E) 0.65 Å

10. Which of the following is *not* a correct approximation to the electronic wavefunction for the excited helium atom  $1s^1 2s^1$ ?
- (A)  $[1s(1)2s(2) + 1s(2)2s(1)] [\alpha(1)\beta(2) - \alpha(2)\beta(1)]$   
(B)  $[1s(1)2s(2) - 1s(2)2s(1)] \alpha(1)\alpha(2)$   
(C)  $[1s(1)2s(2) + 1s(2)2s(1)] [\alpha(1)\beta(2) + \alpha(2)\beta(1)]$   
(D)  $[1s(1)2s(2) - 1s(2)2s(1)] \beta(1)\beta(2)$   
(E)  $[1s(1)2s(2) - 1s(2)2s(1)] [\alpha(1)\beta(2) + \alpha(2)\beta(1)]$
11. Which of the following molecule *does not* have a pure rotational spectrum?  
(A)  $H_2O$  (B) HF (C)  $NF_3$  (D)  $C_6H_6$  (E) HCOH
12. What is the degree of degeneracy for the second-lowest energy level of a particle of mass  $m$  in a three-dimensional cube of length  $a$ ?  
(A) 3 (B) 4 (C) 6 (D) 2 (E) 1
13. Which of the person in the following list is involved in the development of relativistic quantum mechanics?  
(A) Bohr (B) Dirac (C) Heisenberg (D) Lewis (E) Hamilton
14. The Sun has approximately a blackbody spectrum with  $\lambda_{\max} = 500$  nm. From the Wein displacement law  $\lambda_{\max} T \cong hc/5k$ , the surface temperature of Sun is:  
(A) 10000 K (B) 15000 K (C) 20000 K (D) 4000 K (E) 6000 K
15. Which one of the following is *not* a consequence of the Pauli principle?  
(A) two electrons in a orbital must have opposite spin.  
(B) wavefunction must be antisymmetric with respect to interchange of two electrons  
(C) singlet and triplet states have different energies for helium  $1s^1 2s^1$  excited state.  
(D) electrons must have 1/2 spin quantum number  
(E) periodic properties of chemical elements
16. How many nodes are there in the  $4d$  radial function of a hydrogen-like atom?  
(A) 0 (B) 1 (C) 2 (D) 3 (E) 4
17. Which of the following properties can be determined precisely at the same time in a hydrogen atom?  
(A) kinetic and potential energies of the electron  
(B) total energy and the magnitude of the orbital angular momentum  
(C) position and moment of the electron  
(D) all three components of the orbital angular momentum  
(E) all three components of the spin angular momentum

18. What is the delocalization energy of cyclobutadiene predicted by the Hückel theory?  
(A)  $\beta$  (B)  $2\beta$  (C) 0 (D)  $1.73\beta$  (E)  $2.0\beta$
19. The small energy difference between the  $^3P_0$  and  $^3P_2$  terms of the oxygen atom in the ground-state electron configuration is due to  
(A) spin-orbital interaction  
(B) uncertainty principle  
(C) Pauli exclusion principle  
(D) Born-Oppenheimer approximation  
(E) atomic selection rules
20. The ground-state term symbol for the electron configuration  $3d^9$  is:  
(A)  $^1S$  (B)  $^2G$  (C)  $^2D$  (D)  $^2P$  (E)  $^4F$
21. The first ionization energy of He is 24.6 eV. What is the total electronic energy of the He atom?  
(A)  $-24.6$  eV (B)  $-38.4$  eV (C)  $-48.6$  eV (D)  $-73.8$  eV (E)  $-79.0$  eV
22. Which of the following statement is incorrect  
(A) quantum mechanical operators are linear  
(B) Hermitian operator must have real eigenvalues  
(C) all eigenfunctions of a hermitian operator form a complete set  
(D) the eigenvalues of a hermitian operator are quantized  
(E) the spin angular momentum operator has no classical analog
23. The spherical harmonic  $Y_{2,1}$  is an eigenfunction of the angular momentum square operator ( $L^2$ ) in 3D with eigenvalues of  
(A)  $2\hbar^2$  (B)  $6\hbar^2$  (C)  $4\hbar^2$  (D)  $1\hbar^2$  (E)  $0\hbar^2$
24. What is the ground-state molecular term symbol of the  $C_2$  molecule?  
(A)  $^1\Sigma_g$  (B)  $^1\Sigma_u$  (C)  $^3\Sigma_g$  (D)  $^3\Sigma_u$  (E)  $^1\Delta_g$
25. The work function of potassium metal is 2.2 eV. What is the threshold wavelength to produce the photoelectric effect?  
(A) 250 nm (B) 375 nm (C) 427 nm (D) 509 nm (E) 564 nm