國立中正大學104學年度學士班三年級轉學生招生考試試題學系別:化學暨生物化學系 科目:物理化學(量子化學)

第2節

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物理常數

 $\begin{array}{lll} h = 6.626 \times 10^{-34} \; J.s & e = 1.602 \times 10^{-19} \; C & m_e = 9.109 \times 10^{-31} \; kg \\ c = 2.998 \times 10^8 \; m \; s^{-1} & 4\pi\epsilon_0 = 1.113 \times 10^{-10} \; J^{-1} \; C^2 \; m^{-1} & 1 \; cal = 4.184 \; J \\ L = 6.022 \times 10^{23} \; mol^{-1} & k_B = 1.381 \times 10^{-23} \; J \; K^{-1} & amu = 1.66054 \times 10^{-27} \; kg \\ 1 \; eV = 23.06 \; kcal/mol & 1 \; k_B = 1.381 \times 10^{-23} \; J \; K^{-1} & amu = 1.66054 \times 10^{-27} \; kg \\ \end{array}$

單選題(每題四分,共一百分)

- A 100-W sodium-vapor lamp emits yellow light of wavelength 590 nm. The number of photons emitted per second is:
 (A) 1.2 × 10⁵ (B) 3.0 × 10²⁰ (C) 7.2 × 10¹⁶ (D) 5.1 × 10²³ (E) 9.5 × 10²⁷
- 2. What is the de Broglie wavelength of a beam of free electrons with 100 eV kinetic energy. (A) 1.6×10^{-22} m (B) 2.3×10^{-11} m (C) 9.0×10^{-5} m (D) 7.7×10^{-8} m (E) 5.5×10^{-18} m
- 3. Which of the following molecule is not paramagnetic in its electronic ground-state? (A) B_2 (B) O_2 (C) OH (D) NO (E) C_2 .
- The vibrational frequency of H₂ molecule is 4400 cm⁻¹. The force constant of the H-H chemical bond is:
 (A) 310 N/m (B) 125 N/m (C) 570 N/m (D) 1664 N/m (E) 86 N/m
- 5. Following the above question, what is the vibrational zero-point energy of the H₂ molecule? (A) 0.8 kcal/mol (B) 1.6 kcal/mol (C) 3.2 kcal/mol (D) 6.3 kcal/mol (E) 12.6 kcal/mol
- 6. Following the above question, what is the vibrational frequency of D_2 molecule? (A) 2200 cm^{-1} (B) 3100 cm^{-1} (C) 4400 cm^{-1} (D) 1100 cm^{-1} (E) 550 cm^{-1}
- 7. Which of the following gas-phase molecule can't readily be identified by an IR spectrometer? (A) HF (B) NH₃ (C) CO (D) HCN (E) F₂
- 8. What is the ground-state term symbol for the chlorine atom? (A) $^2P_{5/2}$ (B) $^2P_{3/2}$ (C) $^4P_{1/2}$ (D) 1S_0 (E) 3P_0
- 9. Which of the following is an eigenfunction of particle in a 1-D box of length L $(0 \le x \le L)$? (A) $L\pi x^2$ (B) $e^{-cx/L}$ (C) $\sin(2\pi x/L)$ (D) $e^{-c(x/L)^2}$ (E) $\cos(\pi x/L)$

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- 10. Which of the following property is *not* a requirement for a wavefunction of electrons?

 (A) periodic (B) continuous (C) single-valued (D) finite at large distance (E) antisymmetric
- 11. Which of the following is a correct approximation to the electronic wavefunction for the excited helium atom 1s¹2s¹?
 - (A) $[1s(1)2s(2)][\alpha(1)\beta(2) \alpha(2)\beta(1)]$
 - (B) $[1s(1)2s(2) 1s(2)2s(1)] \alpha(1)\alpha(2)$
 - (C) $[1s(1)2s(2) + 1s(2)2s(1)] \alpha(1)\beta(2)$
 - (D) $[1s(1)2s(2) 1s(2)2s(1)] [\alpha(1)\beta(2) \alpha(2)\beta(1)]$
 - (E) $[1s(1)2s(2)][\alpha(1)\beta(2) \alpha(2)\beta(1)]$
- 12. Which of the following molecule *does not* have a pure rotational spectrum? (A) CH₃OH (B) HI (C) NH₃ (D) CH₄ (E) HCN
- 13. Neglect the spin-orbital coupling, what is the degrees of degeneracy for the ground-state carbon atom (³P)?

(A) 9 (B) 6 (C) 4 (D) 3 (E) 2

- 14. Which of the following persons first proposed correct theories of photoelectric effects and material waves, respectively? (They both won the Nobel Prize for their work.)
 (A) Hertz, Bohr (B) Born, Dirac (C) Einstein, Heisenberg (D) Einstein, de Broglie
 (E) Millikan, de Broglie
- 15. Sirius, one of the hottest known star, has a blackbody spectrum with $\lambda_{\text{max}} = 260$ nm. From the Wein's displacement law λ_{max} $T \cong hc/5k$, the surface temperature of Sirius is: (A) 32000 K (B) 24000 K (C) 18000 K (D) 15000 K (E) 11000 K
- 16. The lowest-energy Balmer line in hydrogen atomic spectrum is due to which electron transition?

 (1) 2 (P) 2 (P) 2 (P) 2 (P) 3 (

(A) $2s \rightarrow 1s$ (B) $3s \rightarrow 2s$ (C) $3p \rightarrow 2s$ (D) $3d \rightarrow 2s$ (E) $3p \rightarrow 1s$

- 17. How many nodes are there in the 4p radial function of a hydrogen-like atom? (A) 4 (B) 3 (C) 2 (D) 1 (E) 0
- 18. What is the delocalization energy of 1,3-butadiene predicted by the Hückel theory? (A) 1.48 β (B) 0.48 β (C) 0 (D) 2 β (E) 0.618 β
- 19. The energy difference between the 3P_0 and 3P_2 terms of the oxygen atom in the ground-state electron configuration is mostly like to be: (A) 2.2 eV (B) 0.03 eV (C) 0.5 eV (D) 13.6 eV (E) 22.5 eV

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- 20. The ground-state term symbol for the electron configuration $3d^5$ is: (A) 6 S (B) 4 G (C) 2 F (D) 2 P (E) 1 S
- 21. The total electronic energy (relative to free electrons and nucleus) of the He atom is -79.0 eV. What is the first ionization energy of the He atom?

 (A) 13.6 eV (B) 54.4 eV (C) 27.2 eV (D) 3.4 eV (E) 24.6 eV
- 22. Which of the following statement is incorrect (A) quantum mechanical operators are Hermitian
 - (B) the wavefunction must be real and continuous
 - (C) all eigenfunctions of a Hermitian operator form a complete set
 - (D) the eigenfunctions of a Hermitian operator with different eigenvalues are orthogonal
 - (E) the wavefunctions of an atom can also be the eigenfunctions of the square of total spin angular momentum operator
- 23. The sphereical harmonic $Y_{3,-1}$ is an eigenfunction of the angular momentum square operator (L^2) with the eigenvalue of (A) 3 \hbar^2 (B) 12 \hbar^2 (C) 4 \hbar^2 (D) 6 \hbar^2 (E) 9 \hbar^2
 - (A) $3 h^2$ (B) $12 h^2$ (C) $4 h^2$ (D) $0 h^2$ (E) $9 h^2$
- 24. What is the ground-state molecular term symbol of the O_2 molecule? (A) $^1\Sigma g$ (B) $^1\Sigma u$ (C) $^3\Pi$ (D) $^3\Sigma g$ (E) $^1\Delta g$
- 25. The separation between the two lowest rotational levels of $^{12}C^{32}S$ is 3.246×10^{-23} J. What
 - is the C=S bond distance? (A) 1.71 Å (B) 2.10 Å (C) 1.38 Å (D) 2.51 Å (E) 1.54 Å