

『物理化學』，單選題 25 題，每題 4 分，總分 100 分

1. Comparing the following energies in magnitude (1) ionization energy of H atom (2) bond energy of O₂ molecule (3) vibrational zero-point energy of H₂O (4) hydrogen bonding in water dimer (5) lowest electronic excited state energy of benzene
(A) (2) > (1) > (3) > (5) > (4) (B) (5) > (1) > (2) > (4) > (3) (C) (1) > (2) > (3) > (5) > (4)
(D) (1) > (2) > (5) > (3) > (4) (E) (2) > (5) > (1) > (4) > (3)
2. What is the molar heat capacity of the copper metal at temperatures very close to the absolute zero? (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
3. Which of the following molecule has the highest bond order?
(A) Li₂ (B) CN⁺ (C) O₂⁻ (D) NO⁺ (E) C₂.
4. A sodium lamp emits yellow light at 550 nm. What is the frequency of the yellow light?
(speed of light = 2.998×10^8 m)
(A) 5.45×10^{14} s⁻¹ (B) 5.45×10^{11} s⁻¹ (C) 1.65×10^2 s⁻¹ (D) 1.65×10^5 s⁻¹ (E) 1.82×10^6 s⁻¹
5. What is the ground-state term symbol for the carbon atom?
(A) ²P_{1/2} (B) ²P_{3/2} (C) ³P₀ (D) ¹S₀ (E) ³P₂
6. The fundamental frequency of hydrogen molecule is 4159 cm⁻¹. What is the force constant of the H-H bond? (1 amu = 1.66×10^{-27} kg)
(A) 509 N/m (B) 2080 N/m (C) 320 N/m (D) 1006 N/m (E) 254 N/m
7. Following the above question, what is the vibrational zero-point energy of the H₂ molecule?
(A) 12 kcal/mol (B) 5.9 kcal/mol (C) 3 kcal/mol (D) 2 kcal/mol (E) 24.4 kcal/mol
8. What is the de Broglie wavelength of an α-particle moving at a speed of 1.5×10^7 m s⁻¹.
(A) 0.0023 cm (B) 2.7×10^{-7} m (C) 6.6×10^{-12} m (D) 6.7×10^{-15} m (E) 3.6×10^{-17} m
(Planck constant = 6.626×10^{-34} J s)

9. Which of the following is a correct approximation to the electronic wavefunction for helium atom?
- (A) $1s(1)1s(2) [\alpha(1)\beta(2) - \alpha(2)\beta(1)]$
(B) $1s(1)1s(2) \alpha(1)\alpha(2)$
(C) $1s(1)1s(2) \alpha(1)\beta(2)$
(D) $1s(1)2s(2) \alpha(1)\alpha(2)$
(E) $1s(1)2s(2) \alpha(1)\beta(2)$
10. Which of the following molecules has a pure rotational spectrum?
- (A) CH_4
(B) NH_3
(C) BF_3
(D) C_6H_6
(E) CO_2
11. What is the second-lowest energy level of a particle of mass m in a one-dimensional box of length a ?
- (A) $h^2/8ma$ (B) $h^2/2ma^2$ (C) $h^2/8ma^2$ (D) $h^2/4ma^2$ (E) $3h^2/8ma$
12. Which of the person in the following list is not involved in the development of quantum mechanics?
- (A) Bohr (B) Rutherford (C) Einstein (D) Dirac (E) Boltzmann
13. Sirius, one of the hottest known star, has approximately a blackbody spectrum with $\lambda_{\max} = 260 \text{ nm}$. From the Wein displacement law $\lambda_{\max} T \cong hc/5k$, the surface temperature of Sirius is: ($k = 1.381 \times 10^{-23} \text{ J/K}$)
- (A) 11000 K (B) 15000 K (C) 20000 K (D) 6000 K (E) 3000 K
14. The Pauli principle states that
- (A) two electrons in a molecule must have opposite spin.
(B) two bosons expel each other in an atom
(C) wave function must be anti-symmetric with respect to the exchange of two identical fermions.
(D) terms with higher spin multiplicity are lower in energy
(E) electrons most have half-integer spin quantum numbers
15. The classical electromagnetic theory failed to account for the experimental results of the blackbody radiation because:
- (A) it used Boltzmann distribution
(B) it failed to take electron spin into account
(C) it treated radiation as waves
(D) it assumed continuous energy distribution for vibration
(E) it did not take the photoelectric effect into consideration
16. Which of the following is not a requirement for a wavefunction?
- (A) single-valued (B) continuous (C) continuous first derivative (D) finite (E) symmetric

17. Which of the following systems has evenly-spaced energy levels?
(A) harmonic oscillator (B) particle in a box (C) rotation in 2-D (D) hydrogen atom (E) hydrogen molecule.
18. What is the number of degenerate wavefunctions for a hydrogen atom (including spin)
(A) n (B) $2n$ (C) $2l + 1$ (D) $2n^2$ (E) $l(l + 1)$
19. The energy difference between the 3P_0 and 3P_2 terms of the oxygen atom in the ground-state electron configuration is:
(A) 0.03 eV (B) 0.3 eV (C) 3eV (D) 13 eV (E) 30 eV
20. The ground-state term symbol for the electron configuration $3d^2$ is:
(A) 1S (B) 1G (C) 1D (D) 3P (E) 3F
21. Which of the following is not necessary information to perform an a quantum chemical calculation?
(A) charge (B) molecular structure (C) bond order (D) multiplicity (E) basis sets
22. Which of the following is not a property of quantum mechanical operators:
(A) must commute with the total energy operator
(B) must have real eigenvalues
(C) must be hermitian
(D) must be linear
(E) any experimental observation must correspond to an eigenvalue
23. The spherical harmonics are not eigenfunctions of the hamiltonian of
(A) rotation in 2-D (B) rotation in 3-D (C) hydrogen molecular ion (D) hydrogen atom (E) the square of the orbital angular momentum
24. What is the ground-state molecular term symbol of the oxygen molecule?
(A) $^1\Sigma_g$ (B) $^1\Sigma_u$ (C) $^3\Sigma_g$ (D) $^3\Sigma_u$ (E) $^1\Delta_g$
25. Which of the following molecule is paramagnetic?
(A) O_3 (B) B_2 (C) CO (D) HF (E) C_2