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單選題，每題四分

1. Which of the following statement is correct for a particle in a box
   (A) the energy levels are equally spaced
   (B) wave functions of higher quantum numbers have less nodes
   (C) energy is proportional the quantum number
   (D) the average momentum is not zero
   (E) the lowest energy level has a nonzero energy called zero-point energy
2. The wave function of a particle moving on a circular ring is of the form $\Phi = Ne^{im\phi}$, where ϕ is the azimuth. The normalization constant N is
   (A) $\frac{1}{2}$ (B) $\frac{1}{2\pi}$ (C) $\frac{1}{\sqrt{2}}$ (D) $\frac{1}{\sqrt{2\pi}}$ (E) $\sqrt{2\pi}$
3. Which of the following function is the correct form for the He atom ground-state wave function that satisfy the Pauli Principle ($1S$ is the $1S$ spatial orbital; α and β are the spin functions; 1, 2 denotes the electron coordinates)
   (A) $[1S(1)1S(2)][\alpha(1)\beta(2)-\alpha(2)\beta(1)]$
   (B) $[1S(1)1S(2)][\alpha(1)\beta(2)+\alpha(2)\beta(1)]$
   (C) $[1S(1)1S(2)]\alpha(1)\alpha(2)$
   (D) $[1S(1)1S(2)]\beta(1)\beta(2)$
   (E) $[1S(1)1S(2)]\alpha(1)\beta(2)$
4. Given that the electronic configuration of the CN molecule is $\sigma(1s)^2\sigma^*(1s)^2\sigma(2s)^2\sigma^*(2s)^2\,\pi(2p)^4\sigma(2p)^1$, the term symbol of the CN ground state is
   (A) $^1\Sigma^+$ (B) $^2\Pi$ (C) $^2\Sigma^+$ (D) $^2\Delta$ (E) $^3\Sigma^+$
5. In quantum mechanics, the measurements of two different physical properties are represented by the operators $\hat{A}$ and $\hat{B}$. It is possible to measure precisely and simultaneously the values for both of these physical quantities only if the
   (A) eigenfunctions of $\hat{A}$ forms an orthornormal set and the eigenfunctions of $\hat{B}$ form an orthonormal set
   (B) eigenfunctions of both $\hat{A}$ and $\hat{B}$ can be normalized
   (C) eigenvalues for both $\hat{A}$ and $\hat{B}$ are real number
   (D) $\hat{A}$ and $\hat{B}$ are both Hermitian operators
   (E) $\hat{A}$ and $\hat{B}$ commute
6. Which of the following functions is a "well-behaved" (or acceptable) wave function
   (A) $\Psi(x) = ax^2$ (B) $\Psi(x) = e^{-ax^2}$ (C) $\Psi(x) = e^{-ax}$ (D) $\Psi(x) = e^{ax}$ (E) $\Psi(x) = \pm\cos x$
7. An electron in a $3d_0$ orbital has an angular momentum of magnitude
   (A) 0 (B) $\sqrt{2}\hbar$ (C) $\sqrt{6}\hbar$ (D) $\sqrt{3}\hbar$ (E) $2\hbar^2$

參考用

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8. A harmonic oscillator with a fundamental vibrational frequency ν is in a state described by a wave function $\Psi(x)=0.5\phi_0(x)+0.5\phi_1(x)+0.5\phi_2(x)+0.5\phi_3(x)$, where $\phi_0(x)$, $\phi_1(x)$, $\phi_2(x)$, $\phi_3(x)$ are eigenfunctions of the harmonic oscillator. The subscripts denote their vibrational quantum number (e.g. $\phi_2(x)$ is the eigenfunction for the v=2 level). The average energy associated with state Ψ is

(A) $\frac{7}{2}h\nu$ (B) $2h\nu$ (C) $\frac{1}{2}h\nu$ (D) $\frac{3}{2}h\nu$ (E) $4h\nu$

9. The hydrogen atomic wave functions can be expressed as $\Psi_{nlm}(r,\theta,\phi)=R_{nl}(r)Y_l^m(\theta,\phi)$.

$$R_{10}=2\left(\frac{1}{a_0}\right)^{3/2}e^{-r/a_0} \qquad R_{20}=\frac{1}{\sqrt{8}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0} \qquad R_{21}=\frac{1}{\sqrt{24}}\left(\frac{1}{a_0}\right)^{3/2}\frac{r}{a_0}e^{-r/2a_0}$$

$$Y_0^0=\left(\frac{1}{4\pi}\right)^{1/2} \qquad Y_1^0=\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta \qquad Y_1^1=\left(\frac{3}{8\pi}\right)^{1/2}(\sin\theta)e^{i\phi} \qquad Y_1^{-1}=\left(\frac{3}{8\pi}\right)^{1/2}(\sin\theta)e^{-i\phi}$$

If an electron of a hydrogen atom is in the $2p_z$ orbital, what is the *probability density* of finding that electron at $r=a_0$? (a_0: Bohr radius)

(A) $\frac{e^{-1}}{8a_0^3}$ (B) $\frac{e^{-1}}{24a_0^3}$ (C) $\frac{e^{-1}}{8a_0}$ (D) $\frac{e^{-1}}{24a_0}$ (E) $\frac{e^{-1}}{24a_0^3}\left(\frac{3}{4\pi}\cos^2\theta\right)$

10. The line spacing in the rotational-vibrational spectrum of a rigid rotor molecule with rotational constant $\tilde{B}$ is

(A) $\tilde{B}J(J+1)$ (B) $J^2\tilde{B}$ (C) $2\tilde{B}$ (D) $(2J+1)\tilde{B}$ (E) $\tilde{B}$

11. Given that the ground-state ionization potential of the hydrogen atom is 13.6 eV, how much energy in eV is required to remove an electron from the 3*d* orbital in a hydrogen atom?
(A) 1.5 eV (B) 3.4 eV (C) 4.5 eV (D) 27.2 eV (E) 40.8 eV

12. An enzyme catalyzed reaction proceeds via the Michaelis-Menten mechanism

$$\mathrm{E+R} \xrightarrow{k_1} \mathrm{E\cdot R}$$
$$\mathrm{E\cdot R} \xrightarrow{k_{-1}} \mathrm{E+R}$$
$$\mathrm{E\cdot R} \xrightarrow{k_2} \mathrm{E+Product}$$

E stands for the enzyme, R the reactant and P the product. If the initial enzyme concentration is $[E]_0$ and the E·R complex is unstable such that the steady-state approximation is applied, then the rate of the reaction ($d[P]/dt$) is

(A) $\frac{k_1[\mathrm{E}]_0[\mathrm{R}]}{k_{-1}+k_2}$ (B) $\frac{k_1k_2[\mathrm{E}]_0[\mathrm{R}]}{k_{-1}+k_2}$ (C) $\frac{k_1k_2[\mathrm{E}]_0[\mathrm{R}]}{k_{-1}+k_2+k_1[\mathrm{R}]}$ (D) $k_2[\mathrm{E}]_0$ (E) $k_1k_2[\mathrm{E}]_0$

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13. A molecule is excited from the singlet ground state (S_0) to its first singlet electronically excited state (S_1) by absorbing a photon. The excited molecules decay through the following parallel mechanism:

$$S_1 \xrightarrow{k_f} S_0 + h\nu \quad \text{(fluorescence)}$$
$$S_1 \xrightarrow{k_{ISC}} T_1 \quad \text{(intersystem crossing)}$$
$$S_1 \xrightarrow{k_{IC}} S_0 \quad \text{(internal conversion)}$$

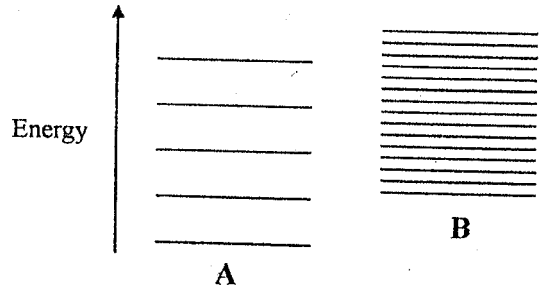
the fluorescence quantum yield Φ_f is

(A) $\frac{k_f}{k_f + k_{ISC} + k_{IC}}$ (B) $\frac{1}{k_f + k_{ISC} + k_{IC}}$ (C) $\frac{1}{k_f}$ (D) $k_f + k_{ISC} + k_{IC}$ (E) $k_f \cdot k_{ISC} \cdot k_{IC}$

14. Consider a reversible isomerization reaction A ⇆ B with a forward rate constant k_f and a backward rate constant k_b. If the initial concentration of A is $[A]_0$ and the initial concentration of B is zero, then the equilibrium concentration of B is

(A) $\frac{k_b}{k_f}[A]_0$ (B) $\frac{k_f}{k_b}[A]_0$ (C) $\frac{k_b}{k_f + k_b}[A]_0$ (D) $\frac{k_f}{k_f + k_b}[A]_0$ (E) $(k_f - k_b)[A]_0$

15. Consider a reversible reaction A ⇆ B for which the energy levels of the reactant and products are shown below. The degeneracy of each level is unity (g=1 for all levels). Which of the following statement is correct about the equilibrium of the reaction



(A) A predominates at any temperature
(B) B predominates at any temperature
(C) A predominates at low temperature, B at high temperature
(D) B predominates at low temperature, A at high temperature
(E) The reaction equilibrium is temperature independent

16. Consider the following half-reactions and voltages.

$2H^+_{(aq)} + 2e^- \rightarrow H_{2(g)}$ $E^\circ = 0.0$ V
$Li^+_{(aq)} + 1e^- \rightarrow Li_{(s)}$ $E^\circ = -3.05$ V

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$O_{2(g)} + 4H^+_{(aq)} + 4e^- \rightarrow 2H_2O(l)$　　$E^\circ = 1.23$ V

$F_{2(g)} + 2e^- \rightarrow 2F^-_{(aq)}$　　$E^\circ = 2.87$ V

What is the product produced at the cathode when a current is passed through an aqueous solution of LiF?

(A) lithium　(B) fluorine　(C) hydrogen　(D) oxygen　(E) none of the above

17. Which of the followings is a zero order reaction?

(A) Thermal isomerization of cis-stilbene to trans-stilbene

(B) enzyme oxidation of glucose to gluconic acid

(C) decay of radioactivity of ^{60}Co

(D) decay of triplet excited C_{60} to ground state

(E) none of the above

18. Which of the following equations is not correct?

(A) $dG = Vdp - SdT$　(B) $\varepsilon = \varepsilon^\circ - (nF/RT)\ln(Q)$　(C) $(\partial S/\partial P)_T = -(\partial V/\partial T)_p$

(D) $dP/dT = \Delta H_m/T\,\Delta V_m$.　(E) none of the above.

19. A chemical reaction will always be spontaneous when

(A) $\Delta H<0$ and $\Delta S<0$　(B) $\Delta H>0$ and $\Delta S>0$　(C) $\Delta G>0$　(D) $\Delta H<0$ and $\Delta S>0$

(E) none of the above.

20. Given that

$2Hg + SO_4^{2-} \rightarrow Hg_2SO_4 + 2e^-$　　$E^\circ = -0.6125$ V

$Fe^{2+} + 2e^- \rightarrow Fe$　　$E^\circ = -0.447$ V

Consider the cell $Hg(l)|Hg_2SO_4(s)|FeSO_4(aq, a = 0.0100)|Fe(s)$. What is the cell potential at 25 ℃?

(A) 1.08 V　(B) 1.18 V　(C) 1.30 V　(D) 1.50 V　(E) 1.72 V

21. What is the ionic strength of 0.05 M Na_2SO_4 (in a unit of mol kg^{-1})?

(A) 0.05　(B) 0.10　(C) 0.15　(D) 0.20　(E) 0.25

22. Which of the following statements is incorrect?

(A) The Debye-Huckel limiting law predicts that at a highly diluted condition, the natural log of the activity coefficient, $\ln \gamma_\pm$, of an electrolyte is proportional to the square root of the ionic strength.

(B) The Nernst equation predict that the reduction potential of an metal ion, M, is

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proportional to ratio, $-\log\frac{[Ox]}{[\mathrm{Re}\,d]}$

(C) The partial pressure of a real solution follows the Raoult's law.

(D) The Clapeyron equation is equal to $\frac{dP}{dT}=\frac{\Delta S_m}{\Delta V_m}$

(E) none of the above

23. Which of the following statements is incorrect?

(A) In the Joule-Thomson experiment, there is no heat exchange between the system and the surroundings.

(B) The Joule-Thomson experiment is under an isoenthalpy condition.

(C) For any ideal gas, the Joule-Thomson coefficient $\mu_{J\text{-}T}$ is always zero.

(D) The Joule-Thomson coefficient $\mu_{J\text{-}T} = [dP/dT]_H$.

(E) none of the above

24. What is the maximum work that can be done by a reversible heat engine operating between 500 and 200 K if 1000 J is absorbed at 500 K?

(A) 500 J (B) 600 J (C) 700 J (D) 800 J (E) 900 J

25. For water, $\Delta H_{vaporization}$ is 40.65 kJ mol^{-1}, and the normal boiling point is 373.15 K. What is the boiling point for water on the top of a mountain of height 5500 m, where the normal barometric pressure is 380 Torr.

(A) 350.3 K (B) 368.1 K (C) 383.5 K (D) 247.2 K (E) 354.4 K