

Choose a correct answer to each question. Each correct answer is worth 2.5 points.

Question 1. How many electrons can be accommodated maximally in atomic $5d$ orbitals?

- A. 10
- B. 12
- C. 14
- D. 16
- E. 18

Question 2. Atomic configuration of the carbon atom in the ground state is $1s^2 2s^2 2p^2$. Which set of atomic terms corresponds to this configuration?

- A. $^4S^\circ$, $^2D^\circ$, and $^2P^\circ$
- B. 4S , 2D , and 2P
- C. $^1P^\circ$, $^1D^\circ$, and $^1S^\circ$
- D. 3P , 1D , and 1S
- E. 3P , 1D , and 3S

(Note: the small circle $^\circ$ denotes terms of odd parity.)

Question 3. An atomic term 4F in magnetic field splits into:

- A. four energy levels with $J = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}$
- B. five energy levels with $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}$
- C. four energy levels with $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$
- D. five energy levels with $J = \frac{3}{2}, \frac{5}{2}, \frac{7}{2}, \frac{9}{2}, \frac{11}{2}$
- E. none of the above

Question 4. Atomic configuration for vanadium with $Z = 23$ in the first excited state is:

- A. $[\text{Ar}] 3d^2 4s 4p$
- B. $[\text{Ar}] 3d^2 4s^2$
- C. $[\text{Ar}] 3d 4s^2 5s$
- D. $[\text{Ar}] 3d^3 4s$
- E. none of the above

Question 5. A hydrogenic orbital $11f_{xyz}$ can be characterized by:

- A. 3 radial nodal planes and 2 angular nodal planes
- B. 4 radial nodal planes and 3 angular nodal planes
- C. 5 radial nodal planes and 2 angular nodal planes
- D. 6 radial nodal planes and 3 angular nodal planes
- E. none of the above

Question 6. What is the unit of the Planck constant \hbar in the SI system?

- A. $N m^2 kg^{-2}$
- B. $J^{-1} C^2 m^{-1}$
- C. $J K^{-1} mol^{-1}$
- D. $m s^{-1}$
- E. none of the above

Question 7. The symmetry point group of the ethane molecule in its ground state is:

- A. C_{3v}
- B. D_{3v}
- C. C_{3h}
- D. D_{3h}
- E. D_{3d}

Question 8. The character table for the point group D_{4h} is given by

D_{4h}	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$		
A_{1g}	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		$x^2 - y^2$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	(R_x, R_y)	xy
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		(xz, yz)
E_g	2	0	-2	0	0	2	0	-2	0	0	z	
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	(x, y)	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0		

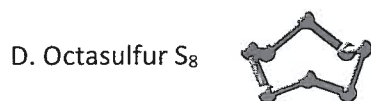
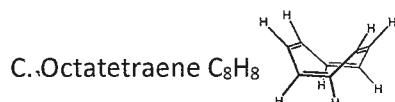
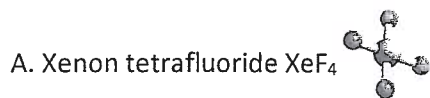
Which irreducible representations (irreps) correspond to modes that are Raman active for a molecule described by this point group?

- A. E_g and E_u
- B. A_g and E_g
- C. E_u and A_{2u}
- D. all *gerade* irreps
- E. none of the above answers is correct

Question 9. Using the character table for the point group D_{4h} given in the previous problem, find the decomposition of the reducible representation $E_u \times E_u$ into irreps.

- A. $E_u + E_u$
- B. $E_g + E_u$
- C. $E_g + E_g$
- D. $A_{1g} + A_{2g} + E_g$
- E. $A_{1g} + A_{2g} + B_{1g} + B_{2g}$

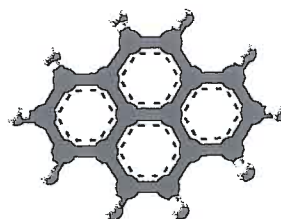
Question 10. Choose all the molecules below corresponding to the point group symmetry D_{4h} .



E. Two of the above answers are correct.

Question 11. How many distinct Kekulé structures can be written for pyrene?

- A. 5
- B. 6
- C. 7
- D. 8
- E. none of the above



Question 12. Assume that the energy levels of a single quantum particle in a harmonic well (i.e., harmonic oscillator) are given by the expression $E_n = n + \frac{1}{2}$. What are the three lowest distinct energy levels for four identical, non-interacting particles trapped in this well, assuming that the particles are fermions with spin $s = \frac{1}{2}$?

- A. 1, 2, and 3
- B. 2, 3, and 4
- C. 3, 4, and 5
- D. 4, 5, and 6
- E. none of the above

Question 13. Like Question 12, but assume now that the particles are bosons with spin $s = 0$.

- A. 1, 2, and 3
- B. 2, 3, and 4
- C. 3, 4, and 5
- D. 4, 5, and 6
- E. none of the above

Question 14. The quantity defined as $\langle w \rangle = \int \Psi^* \hat{w} \Psi d\tau$ corresponds to

- A. the eigenvalue of the operator \hat{w} in the eigenstate Ψ
- B. the expectation value of the operator \hat{w} for the state Ψ
- C. the mean absolute value of the operator \hat{w} for the state Ψ
- D. the variation of the operator \hat{w} for the state Ψ
- E. none of the above

Question 15. The radial wave function of a hydrogenic orbital consists of a normalization factor, exponential factor, centrifugal factor, and a polynomial. This polynomial belongs to the family of:

- A. Hermite polynomials
- B. Legendre polynomials
- C. associated Legendre polynomials
- D. associated Laguerre polynomials
- E. none of the above

Question 16. For a molecule classified as a spherical rotor, the components of the moment of inertia $\vec{I} = [I_x, I_y, I_z]$ satisfy the following relationships:

- A. $I_x = I_y < I_z$
- B. $I_x = I_y > I_z$
- C. $I_x > I_y > I_z$
- D. $I_x = I_y = I_z = 0$
- E. none of the above answers is correct

Question 17. The effective mass associated with the molecular vibration in a diatomic molecule AB is given by the following equation:

- A. $m_{\text{eff}} = m_A + m_B$
- B. $m_{\text{eff}} = \frac{m_A + m_B}{2}$
- C. $m_{\text{eff}} = \frac{m_A + m_B}{m_A m_B}$
- D. $m_{\text{eff}} = \frac{m_A m_B}{m_A + m_B}$
- E. none of the above answers is correct

Question 18. Methane CH_4 has $3N - 6 = 9$ vibrational degrees of freedom but shows only four distinct fundamental vibrational transitions because:

- A. the remaining vibrational degrees of freedom are IR inactive
- B. the remaining vibrational degrees of freedom are Raman inactive
- C. the remaining vibrational degrees of freedom are IR and Raman inactive
- D. high symmetry of methane suppresses the remaining transitions
- E. high symmetry of methane causes degeneracies of vibrational energy levels

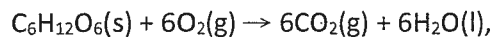
Question 19. A typical frequency range for the C–H stretching vibration is:

- A. 3500 – 3600 cm^{-1}
- B. 2900 – 3100 cm^{-1}
- C. 2100 – 2400 cm^{-1}
- D. 1500 – 1800 cm^{-1}
- E. 900 – 1100 cm^{-1}

Question 20. A water molecule has three vibrational fundamental modes: ν_{sym} – symmetric stretching of the O–H bonds, ν_{asym} – antisymmetric stretching of the O–H bonds, and ν_{bend} – scissoring bending of the H–O–H angle. The three experimentally observed vibrational fundamental levels are: ν_1 at 1595 cm^{-1} , ν_2 at 3657 cm^{-1} , and ν_3 at 3756 cm^{-1} . The correct assignment of these modes is:

- A. $\nu_{\text{sym}} = \nu_1$, $\nu_{\text{asym}} = \nu_2$, and $\nu_{\text{bend}} = \nu_3$
- B. $\nu_{\text{asym}} = \nu_1$, $\nu_{\text{sym}} = \nu_2$, and $\nu_{\text{bend}} = \nu_3$
- C. $\nu_{\text{sym}} = \nu_1$, $\nu_{\text{bend}} = \nu_2$, and $\nu_{\text{asym}} = \nu_3$
- D. $\nu_{\text{asym}} = \nu_1$, $\nu_{\text{bend}} = \nu_2$, and $\nu_{\text{sym}} = \nu_3$
- E. $\nu_{\text{bend}} = \nu_1$, $\nu_{\text{sym}} = \nu_2$, and $\nu_{\text{asym}} = \nu_3$

Question 21. When 1.00 mol glucose is oxidized to carbon dioxide and water in a rigid box according to the equation



calorimetric measurements give $\Delta U = -2808 \text{ kJ}$ and $\Delta S = +180 \text{ JK}^{-1}$ at 27°C. How much energy change can be extracted as work?

- A. -2808 kJ
- B. -2815 kJ
- C. -2862 kJ
- D. -10258 kJ
- E. -57200 kJ

Question 22. Free expansion of the ideal gas of n mol occurred at temperature T , and the volume changed from V_i to V_f . The work arising from the change in the volume is calculated with

- A. difference in the volume ($V_f - V_i$), and temperature T
- B. ratio of the volume (V_f / V_i), and temperature T
- C. molar amount n , and temperature T
- D. difference in the volume ($V_f - V_i$), molar amount n , and temperature T
- E. none of the above answers is correct

Question 23. The heat capacity at constant volume (C_V) and at constant pressure (C_P) are given as $C_V = \left(\frac{\partial U}{\partial T}\right)_V$ and $C_P = \left(\frac{\partial H}{\partial T}\right)_P$, respectively. For 1 mol of the ideal gas, there is a relationship that

- A. $C_P - C_V = 0$
- B. $C_P - C_V = 1$
- C. $C_P - C_V = R$
- D. $\frac{C_P}{C_V} = \frac{3}{2}$
- E. $\frac{C_P}{C_V} = \frac{5}{2}$

Question 24. The enthalpy change ΔH accompanying the formation of 1.00 mol $\text{NH}_3(\text{g})$ from its elements at 300 K is -46.1 kJ. What is the change in the internal energy ΔU ?

- A. -43.6 kJ
- B. -41.1 kJ
- C. -46.1 kJ
- D. -45.1 kJ
- E. $+46.1$ kJ

Question 25. Calculate the enthalpy of formation of ethylene from the heat of combustion in Table.

- A. 25.5 kJ mol $^{-1}$
- B. 51 kJ mol $^{-1}$
- C. 337 kJ mol $^{-1}$
- D. 445 kJ mol $^{-1}$
- E. 731 kJ mol $^{-1}$

compound	chemical formula	$-\Delta H_c^\circ$ /kJ mol $^{-1}$
carbon	C	394.0
hydrogen	H $_2$	286.0
ethylene	CH $_2$ =CH $_2$	1411.0

Question 26. Calculate the entropy S of 1.00 mol carbon monoxide in the crystal at 0 K. (Note: $\ln 2 = 0.7$)

- A. 0.0 J K $^{-1}$
- B. 9.7×10^{-23} J K $^{-1}$
- C. 0.7 J K $^{-1}$
- D. 5.8 J K $^{-1}$
- E. 11.9 J K $^{-1}$

Question 27. Volume of 0.5-mol ideal gas increased from 1 L to 1.414 L isothermally. What is the change in entropy?

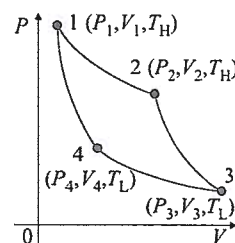
- A. 0.0 J K $^{-1}$
- B. 2.4×10^{-24} J K $^{-1}$
- C. 1.45 J K $^{-1}$
- D. 2.9 J K $^{-1}$
- E. 5.8 J K $^{-1}$

Question 28. Calculate the freezing point depression of a 250-cm³ glass of H₂O upon dissolving 18 g of glucose (MW = 180). The cryoscopic constant of H₂O is 2.0 K kg mol⁻¹.

- A. 0.0008 K
- B. 0.014 K
- C. 0.12 K
- D. 0.8 K
- E. 2.0 K

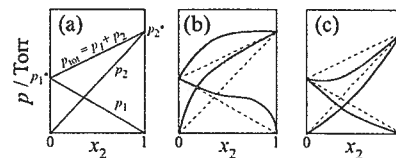
Question 29. Choose wrong description about the Carnot cycle of an ideal gas (Figure).

- A. 1 → 2 and 3 → 4 are the isothermal processes.
- B. 2 → 3 and 4 → 1 are the adiabatic processes.
- C. $\frac{V_4}{V_3}$ is equal to $\frac{V_1}{V_2}$.
- D. Work in one cycle is a function of T_H , T_L , V_1 , and V_2 .
- E. This cycle is always reversible.



Question 30. Figures show a relationship between the mole fraction of component 2 (x_2) and vapor pressure of the components 1 (p_1) and 2 (p_2), and the total pressure (p_{tot}).

Choose a proper description about the figures.



- A. p_2 / p_2^* equals x_2 in (a). This relationship is known as Henry's law for ideal solutions.
- B. Positive deviation in (b) is due to attractive interaction between the two components.
- C. Negative deviation in (c) is due to attractive interaction between the two components.
- D. Total pressure p_{tot} is not always equal to the sum of p_1 and p_2 .
- E. CCl₄, CHCl₃, CH₂Cl₂, and CH₃Cl are the representative ideal liquids.

Question 31. Calculate the maximum efficiency of a reversible heat engine working between a hot source (500 K) and a cold sink of (300 K).

- A. 0.40
- B. 0.60
- C. 0.67
- D. 1.50
- E. 1.67

Question 32. What is the unit of the gas constant R in the SI system?

- A. $N m^2 kg^{-2}$
- B. $J^{-1} C^2 m^{-1}$
- C. $J K^{-1} mol^{-1}$
- D. $m s^{-1}$
- E. none of the above

Question 33. NH_3 is in a box (2.00 m^3 , 15.0 atm at 27°C). A catalyst decomposed it to N_2 and H_2 at 327°C and reached equilibrium. The pressure is 50.0 atm . What is the degree of dissociation of NH_3 ?

- A. 0.49
- B. 0.56
- C. 0.66
- D. 0.70
- E. 0.77

Question 34. Vapor pressure of certain liquid is 500 Torr at 380 K and 1000 Torr at 400 K . Calculate the molar enthalpy of vaporization around 390 K .

- A. 11 kJ mol^{-1}
- B. 22 kJ mol^{-1}
- C. 33 kJ mol^{-1}
- D. 44 kJ mol^{-1}
- E. 55 kJ mol^{-1}

Question 35. The change in the Gibbs free energy of a certain constant-pressure process was given as $\Delta G / \text{J} = -85.4 + 36.5(T/\text{K})$. Calculate the value of ΔS in this process.

- A. -85.4
- B. $+85.4$
- C. -36.5
- D. $+36.5$
- E. None of the values listed above

Question 36. Calculate the change in chemical potential of an ideal gas that is compressed isothermally from 1.8 atm to 3.6 atm at 27°C .

- A. 0.7 J mol^{-1}
- B. 157 J mol^{-1}
- C. -157 J mol^{-1}
- D. 1745 J mol^{-1}
- E. -1745 J mol^{-1}

Question 37. Choose wrong description.

- A. " kJ mol^{-1} " is the unit of enthalpy.
- B. Change in Gibbs energy equals the maximum work that system do at constant pressure.
- C. Change in Internal energy is sum of the work done on a system and the heat supplied to it.
- D. Work and heat are state functions. They depends only on the property of the system.
- E. Difference between the enthalpy and the internal energy is PV .

Question 38. At 90°C, the vapor pressure of toluene is 400 Torr and that of o-xylene is 150 Torr. What is the composition of the liquid mixture (i.e., toluene : o-xylene) that boils at 90°C when the pressure is 380 Torr?

- A. 0.73 : 0.27
- B. 0.80 : 0.20
- C. 0.88 : 0.12
- D. 0.92 : 0.08
- E. 0.96 : 0.04

Question 39. The vapor pressure of a 500-g sample of benzene (C_6H_6 ; MW=78) was 400 Torr at 60°C, but it fell to 385 Torr when 20.0 g of an involatile organic compound was dissolved in it. Calculate the molar mass of the compound.

- A. 72
- B. 74
- C. 76
- D. 78
- E. 80

Question 40. There are three battery cells; (a) $Zn|Zn^{2+}||H^+|H_2$ (1 atm), Pt, (b) $Sn|Sn^{2+}||Ag^+|Ag$, (c) $Zn|Zn^{2+}||Cu^{2+}|Cu$. Sort the electromotive force of each cell at 298 K (refer Table and regard that the activity coefficient of each species is 1.0) from large to small.

- A. (a) > (b) > (c)
- B. (a) > (c) > (b)
- C. (c) > (a) > (b)
- D. (b) > (c) > (a)
- E. (c) > (b) > (a)

Standard potentials at 298 K

Couple	E° / V
$Ag^+ + e^- = Ag$	+ 0.80
$Cu^{2+} + 2e^- = Cu$	+ 0.34
$2H^+ + 2e^- = H_2$	0
$Sn^{2+} + 2e^- = Sn$	- 0.14
$Zn^{2+} + 2e^- = Zn$	- 0.76