# GS-2020 (Chemistry)

Full Name

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Roll No.

## TATA INSTITUTE OF FUNDAMENTAL RESEARCH

### Written Test in CHEMISTRY

# December 8<sup>th</sup>, 2019

Duration: Three hours (3 hours)

### Please read all instructions carefully before you attempt the questions.

- 1. Write your FULL NAME and ROLL NUMBER (see hall ticket) in block letters, both on this page and on your answer sheet (at the end of this booklet).
- This is a multiple-choice question paper with ONE section having a total of 40 questions. Each correct answer will get you 3 marks. Every wrong answer will get you -1 mark. Marks are not awarded or deducted when a question is not attempted. It is better not to answer a question if you are not sure.
- 3. Indicate your answers on the ANSWER SHEET by filling completely in the appropriate boxes. <u>Do not mark more than one box for any question</u>; this will be treated as an incorrect answer.
- 4. We advise you to first mark the correct answers in the QUESTION SHEET, and later transfer them to the ANSWER SHEET only when you are sure of your choice.
- 5. Rough work may be done on the back of the QUESTION SHEET. If needed, you may ask for extra rough sheets from an invigilator.
- 6. In answering the questions, please choose the option <u>that best describes</u> the solution to the problem.
- 7. Use of calculators is permitted in this subject test.

#### SOME USEFUL DATA

Avogadro number =  $6.02 \times 10^{23} \text{ mol}^{-1}$ RT/F = 0.0257 V at 25°C Faraday constant = 96500 C/mol Boltzmann constant  $k_B = 1.38 \times 10^{-23} \text{ J K}^{-1}$ Mass of an electron =  $9.109 \times 10^{-31} \text{ kg}$   $e = 1.6 \times 10^{-19} \text{ C}$ h = 6.626 \times 10^{-34} \text{ J s} c = 3 \times 10^8 \text{ m s}^{-1} R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}

- 1. Order of field effect of alkyl groups are tert-butyl > iso-propyl > ethyl > methyl. Which molecule among PhCH<sub>3</sub>, PhCH<sub>2</sub>CH<sub>3</sub>, PhCH(CH<sub>3</sub>)<sub>2</sub> and PhC(CH<sub>3</sub>)<sub>3</sub> has the highest dipole moment in gas phase.
  - A) PhCH<sub>3</sub>
  - B) PhCH<sub>2</sub>CH<sub>3</sub>
  - C) PhCH(CH<sub>3</sub>)<sub>2</sub>
  - $D) PhC(CH_3)_3$
- 2. Predict the product of the following reaction.



3. Predict the reagent for the following amine de-protection reaction.



4. The octanol-water partition coefficient (Log *P*) for the following amines are as shown below:



Which amine will have the highest solubility in water?



<mark>Ans: D</mark>

- 5. A flask contains 1 litre of growth medium (in which E. coli. bacteria are grown) with 180 gm of glucose as the only Carbon source for the bacteria. Provide a rough estimate of the number of E. coli. that can grow upto the final stage given
  - a. A bacterium contains  $\sim 3 \times 10^6$  protein molecules
  - b. An average protein has ~300 amino acids
  - c. Half of all glucose consumption goes to production
  - A) 10<sup>6</sup>

B) 3 x 10<sup>14</sup>

- C) 3 x 10<sup>16</sup>
- D) 2.5 x 10<sup>13</sup>

#### Answer: B

- 6. An optically transparent thin crystal shows a quadratic response to visible light, i.e. it scatters some of the light in a waveform that is square of the field of light that falls on it. If light of 500 nm wavelength falls on it, what are the wavelengths of the scattered light?
  - A) 500 nm and 750 nm
  - B) 500 nm and 250 nm
  - C) 500 nm and 1000 nm
  - D) 500 nm only
- 7. IR spectra of proteins have a peak in the 1600 1700 cm<sup>-1</sup> region, known as the "Amide I" region. This comes largely from the backbone C=O stretch vibration. Given the natural abundance of different isotopes, would occasionally find a backbone C=O at a different frequency? If so, what would be the next most common frequency, assuming that the "Amide I" has a peak exactly at 1650 cm<sup>-1</sup>?

A) 1613  $cm^{-1}$ 

- B) 1693 cm<sup>-1</sup>
- C) 1248  $cm^{-1}$

- D) No other frequency will be observed
- 8. An ideal gas obeys the gas law PV= nRT. However, real gases deviate from this, and their behavior can be described in

 $PV/nRT = 1 + B_PP + -----$ 

where  $B_P$  is the first virial coefficient in the expansion. Do you expect the  $B_P$  to be temperature dependent? If so, what would you expect the sign of  $B_P$  to be at low temperatures? (Near but above the critical point of condensation)

A) B<sub>P</sub> will be temperature independent

B) Negative

- C) Positive
- D) Can be either positive or negative
- 9. In a spherical polar coordinate system, a point A at (x, y, z) in the Cartesian coordinate system can be described by (r, θ, φ) where r, θ, and φ have their usual meaning. Expression for the volume of an infinitesimally small cube confined by dx, dy, and dz in terms of the spherical coordinate system is given by
  - A)  $dr d\theta d\phi$
  - B)  $rsin\theta dr d\theta d\phi$
  - C)  $r^2 sin^2 \theta dr d\theta d\phi$
  - D) r<sup>2</sup>sinθdrdθdø
- 10. The degeneracy of the energy level 12  $h^2/8 \text{ ma}^2$  of a particle in a three dimensional cube of length "a" is
  - A) 1
  - B) 3
  - C) 6
  - D) 12

- 11. Rotational energy of a diatomic molecule is given by  $E_{rot} = J(J + 1)hB_e$ , where  $E_{rot}$  is in Joules. If the rotational constant for H<sub>2</sub> molecule is given as  $B_e = 1.8324$  E+12 Hz, the rotational period of the H<sub>2</sub> molecule in J = 10 level will be
  - A)  $1.33 \times 10^{-19}$  sec B)  $5.0 \times 10^{-15}$  sec C)  $5.46 \times 10^{-13}$  sec D)  $7.39 \times 10^{-7}$  sec
- 12. For a Harmonic Oscillator in its ground state, i.e., v = 0 state, the energy is given by  $E = \frac{1}{2}hv$ , where v is the vibrational frequency. This is due to its
  - A) Kinetic energy
  - B) Potential energy
  - C) Sum of Kinetic and Potential energies
  - D) Heat of formation
- 13. The Standard reaction Gibbs energy ( $\Delta G^{\circ}$ ) for the ATP hydrolysis

 $ATP_{(aq)} \rightarrow ADP + P_{i(aq)}$  is -31 kJ/mol at 37°C.

In a typical bacterial cell, the concentration of ATP, ADP and  $P_i$  are 8 mmol  $L^{-1}$ , 1 mmol  $L^{-1}$  and 8 mmol  $L^{-1}$ , respectively. What is the reaction Gibbs energy under this condition?

A) -31 kJ mol<sup>-1</sup>
B) -49 kJ mol<sup>-1</sup>
C) -18 kJ mol<sup>-1</sup>
D) -13 kJ mol<sup>-1</sup>

- 14. The coefficient of compressibility of water at 293 K is  $4.9 \times 10^{-6}$  atm<sup>-1</sup> in the range 1 to 25 atm pressure. What will be the value of work involving the compression of 1 mol of liquid water from a pressure of 1 atm to 25 atm at 293 K in a reversible process.
  - A) 21.75 × 10<sup>-5</sup> atm dm<sup>3</sup>
    B) 0.2234 ×10<sup>-5</sup> atm dm<sup>3</sup>
    C) 225.223 × 10<sup>-5</sup> atm dm<sup>3</sup>
    D) 2.752 × 10<sup>-5</sup> atm dm<sup>3</sup>

15. For an ideal gas,  $\left(\frac{\partial H}{\partial P}\right)_{T}$  is equal to

A) V B) 0 C)  $\left(\frac{\partial V}{\partial T}\right)_P$ D)  $\left(\frac{\partial T}{\partial P}\right)_H$ 

- 16. The half-life for the decomposition of a substance dissolved in Chlorofom is 6 hours at 298K. How much of the substance will be left after a day if the initial weight of the dissolved substance is 160mg.
  - A) 40 mg
  - B) 160 mg

C) 10 mg

D) 27 mg

- 17. If 1.50 g of H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> · 2H<sub>2</sub>O were heated to drive off the water of hydration, how much anhydrous H<sub>2</sub>C<sub>2</sub>O<sub>4</sub> would remain?
  - A) 0.34 g
  - B) 0.92 g
  - C) 1.07 g
  - D) 1.50 g

B)

18. How many absorption peaks will the following compound have in its <sup>13</sup>C-NMR spectrum?



- 19. An organic compound is estimated through Dumas method and was found to evolve 6 moles of CO<sub>2</sub>, 4 moles of H<sub>2</sub>O and 1 mole of N<sub>2</sub> gas. The formula of the compound is:
  - $C_{12}H_8N$ A)
  - B)  $C_{12}H_8N_2$
  - C)  $C_6H_8N$
  - D)  $C_6H_8N_2$

- 20. Which of the following belongs to the same symmetry group as NH<sub>3</sub>?
  - A) BF<sub>3</sub>
  - B) CH<sub>4</sub>
  - C) CH<sub>3</sub>OH

D) CHCl<sub>3</sub>

- 21. Within a circle of radius 'b', four largest possible identical circles of radius 'a' are fit such that they do not cross each other. What is the ratio a/b?
  - A) ½
  - B) 1/(1+sqrt(2))
  - C) 2/(1+sqrt(2))
  - D) 1/2(1+sqrt(2))
- 22. Beer's law for electromagnetic radiation absorption through a medium can be expressed as:

 $I = I_0 \exp(-\alpha L)$ 

Where,  $\alpha$  is the absorption coefficient, L is the path length through the medium,  $I_0$  is the incident intensity and I is the transmitted intensity.

Consider an absorbing medium with two energy levels spaced by  $600 \text{ cm}^{-1}$ . On this medium, when monochromatic infrared radiation on resonance is made incident, which of the following statement(s) holds true?

- A) Light absorption will increase with increasing the temperature of the absorbing medium
- B) Beer's law is valid only for ultraviolet-visible part of the spectrum and is invalid in the infrared spectral region
- C) Light absorption will decrease with increasing temperature of the absorbing medium
- D) Light absorption not change with the temperature of the absorbing medium

- 23. In the case of Eigenstates of a particle in a box with infinite walls, which of the following statements is true about the wavefunction  $(\psi(r))$ , its first  $(\psi'(r) = d\psi(r)/dr)$  and second derivatives  $(\psi''(r) = d^2\psi(r)/dr^2)$ ?
  - A) All three quantities are continuous everywhere
  - B)  $\psi(r)$ ,  $\psi'(r)$  are continuous but not  $\psi''(r)$ .
  - C)  $\psi(r)$  is continuous everywhere, but discontinuous at the boundaries of the box.
  - D)  $\psi(r)$  is continuous everywhere,  $\psi'(r)$  and  $\psi''(r)$  are continuous everywhere except at the boundaries.
- 24. The nitrogen mustard Chlorambucil is an anti-cancer drug. Predict the product obtained when Chlorambucil interacts with the DNA base pair AT shown below under physiological conditions.







D)



25. An isolated water molecule has  $C_{2v}$  symmetry, however water clusters can have symmetries other than  $C_{2v}$ . What are the symmetries of the following three water clusters?



A) All of them have  $C_{2v}$  symmetry

B) i)  $C_{2v}$  ii)  $D_{2h}$  iii)  $C_s$ 

- C) i)  $C_s$  ii)  $D_{2h}$  iii)  $C_s$
- D) i)  $C_{2v}$  ii)  $D_{2h}$  iii)  $C_{2v}$
- 26. Among the following, which molecule will have the smallest spacing between vibrational levels? (superscripts denote the nuclear mass of the atoms)
  - A) <sup>1</sup>H<sup>35</sup>Cl
  - B) <sup>1</sup>H<sup>37</sup>Cl
  - C) <sup>2</sup>H<sup>37</sup>Cl
  - D) <sup>2</sup>H<sup>35</sup>Cl
- 27. A complex of Chromium (3+) in aqueous hydrochloric acid, was found to exist in two geometric isomeric forms. A white precipitate was formed on addition of equimolar amount of AgNO<sub>3</sub> solution to the complex. The structure of the complex is:

A)  $[CrCl_3(H_2O)_3]$ 

- $B) [CrCl_2(H_2O)_4]Cl$
- C)  $[CrCl(H_2O)_5]Cl_2$
- D)  $[Cr(H_2O)_6]Cl_3$

28. Compound 2 and compound 1 were mixed in a 1:4 molar ratio. The mixture was subjected to an ammonium molybdate test for phosphate estimation. The result of the molybdate test yielded a phosphate concentration of 36.0 mM for the mixture. What are the concentrations of compound 1 and compound 2 in the mixture?



- A) Compound 1: 30 mM Compound 2: 6 mM
- B) Compound 1: 24 mM Compound 2: 6 mM
- C) Compound 1: 28.8 mM Compound 2: 7.2 mM
- D) Compound **1**: 24 mM Compound **2**: 12 mM
- 29. Methyl groups in the following compounds are



- A) diastereotopic (I), enantiotopic (II), diastereotopic (III)
- B) enantiotopic (I), enantiotopic (II), enantiotopic (III)
- C) diastereotopic (I), neither enantiotopic nor diastereotopic (II), diastereotopic (III)
- D) enantiotopic (I), neither enantiotopic nor diastereotopic (II), enantiotopic (III)

30. Which one of the following compounds has largest dipole moment?



- 31. How many normal modes does the CS<sub>2</sub> molecule have? How many of them can be observed using IR spectroscopy?
  - A) 3 modes, 2 can be observed
  - B) 6 modes, 5 can be observed
  - C) 4 modes, 3 can be observed
  - D) 3 modes, 3 can be observed
- 32. Light excitation of a molecule promotes an electron from a state  $\phi_a(x, y, z)$  to  $\phi_b(x, y, z)$ , where x, y, z are spatial coordinates with respect to the molecular centre of mass. The change in the spatial position x of the electron can be calculated as:
  - A)  $\int_{-\infty}^{\infty} \phi_b^*(x, y, z) x \phi_b(x, y, z) dx dy dz \int_{-\infty}^{\infty} \phi_a^*(x, y, z) x \phi_a(x, y, z) dx dy dz$
  - B)  $\int_{-\infty}^{\infty} \phi_b^{*}(x, y, z) x \phi_b(x, y, z) dx \int_{-\infty}^{\infty} \phi_a^{*}(x, y, z) x \phi_a(x, y, z) dx$
  - C)  $\int_{-\infty}^{\infty} \phi_b^*(x, y, z) \phi_b(x, y, z) dx \int_{-\infty}^{\infty} \phi_a^*(x, y, z) x \phi_a(x, y, z) dx$
  - D)  $\int_{-\infty}^{\infty} \phi_b^{*}(x, y, z) \phi_b(x, y, z) dxdydz \int_{-\infty}^{\infty} \phi_a^{*}(x, y, z) \phi_a(x, y, z) dx$

33. A protein sequence in solution at temperature T folds from a denatured extended state to its native state. Under which of the following conditions on changes in enthalpy (ΔH) and entropy (ΔS) should such a transition be NOT favorable?

 $\mathbf{A}) \ \mathbf{0} > \Delta \mathbf{H} > \mathbf{T} \Delta \mathbf{S}$ 

B)  $\Delta H < 0 < T \Delta S$ 

C)  $0 > T\Delta S > \Delta H$ 

D)  $\Delta H = 0$  and  $T\Delta S > 0$ 

- 34. A particle is thermally diffusing on a 1-dimensional harmonic potential given by  $V(x) = \frac{1}{2}kx^2$ , A where k is the spring constant and x is the position of the particle. The equilibrium probability P(x) of finding the particle at a position x follows:
  - A)  $P(x) \propto x^2$
  - B)  $P(x) \propto x$
  - C)  $P(x) \propto \exp(-Ax^2)$ , where A is a constant
  - D)  $P(x) \propto \exp(-Ax)$ , where A is a constant
- 35. Which reaction has the greatest increase in entropy?
  - A)  $C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$
  - B)  $H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$
  - C)  $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$
  - D)  $C_2H_4(g) + H_2(g) \rightarrow C_2H_6(g)$

- 36. A scalar coupling (<sup>2</sup>J<sub>1H-1H</sub>) constant for a doublet in compound X is measured as 5.0 Hz on a 500 MHz NMR spectrometer. Which of the following statements is incorrect?
  - A) The difference  $\Delta\delta$  for the two components of the doublet depends on the field strength of the spectrometer.
  - B) For this doublet, the coupling constant measured in Hz depends on the field strength of the spectrometer.
  - C) For this doublet, the coupling constant is 5.0 Hz when the spectrum of X is recorded on a 250 MHz NMR spectrometer
  - D) The difference  $\Delta\delta$  for the two components of this doublet is 0.05ppm when measured on a 100MHz spectrometer.
- 37. What is the last digit of  $3^{4798}$ ?
  - A) 3
  - <mark>B) 9</mark>
  - C) 1
  - D) 7
- 38. In a face centered arrangement of A and B atoms. Where A atoms are at the corners of the unit cell and B atoms are at the face centers. For each unit cell, one A atom is missing from a corner position and one B atom is missing from one face position. The simplest formula of the resulting compound will be:
  - A)  $A_{14}B_{40}$
  - $B) A_7B_{20}$
  - C)  $A_{1-x}B_{3-x}$
  - D)  $AB_2$

- 39. Iron, Cobalt and Nickel are three known elements that display ferromagnetism. Which of the following statements is true about ferromagnets:
  - A) In the presence of a magnetic field, the unpaired spins of a ferromagnet all align with the external field. Then in the absence of the external magnetic field, these spins then revert back immediately to their original state.
  - B) The origin of magnetism in a ferromagnet arises from randomly arranged paired spins in a lattice.
  - C) A ferromagnetic material is weaker (in its attraction to an external magnetic field) than a paramagnetic material
  - D) None of the above.

D.

40. The major product formed in the following reaction is



## The following question does NOT carry any marks and is given to collect information only:

- 41) How much time did you take to complete this chemistry exam?
  - A) Less than 1 hour
  - B) Between 1 to 2 hours
  - C) Between 2 to 3 hours
  - D) Insufficient time was given