BITS PILANI, DUBAI CAMPUS

I YEAR FIRST SEMESTER, 2012-2013

COMPREHENSIVE EXAMINATION-CLOSED BOOK

Course Title: General Chemistry **Course No: CHEM F111**

Date: 31.12.2012 **Total Marks: 80**

Time: 3Hrs **Weightage: 40%**

1. **Answer all questions sequentially. (Part-A, B and should be answered separately)**
2. **Show stepwise calculation indicating the units wherever it is required**
3. **Useful data: 1 eV=1.602x10^{-19}C, h = 6.626 x 10^{-34} J.s, c = 3 x 10^{10} cm/s, R_H = 109677 cm^{-1}, R=8.314 J/K/mol Mass of electron = 9.1x 10^{-31} kg, Mass of hydrogen = 1.67x10^{-27} kg, Atomic number of H =1, He=2, C=6, N= 7, O= 8, Cl = 17, Fe=26, Co=27, Cr=24, Br = 35.**

PART-A

1. (i) Write the significance of Z^2 in the calculation of permitted energies of hydrogenic atoms.

   (ii) Draw the MO diagram of NO molecule. Write the MO configuration, calculate the bond order and find out its magnetic behavior.

   (iii) Account for the formation of overtone bands. **[2 + 4 + 3M]**

2. (i) The force constant of HI bond, where H oscillates towards and away from the stationary I atom, is 316 Nm $^{-1}$. Find the vibrational frequency of the HI molecule.

   (ii) Which of the molecules are infrared active: O_2, CO_2 .HCl, N_2O. Justify your answer.

   (iii) Account for the formation of broad peaks in Electronic spectroscopy. **[4 +2 +3 M]**

3. (i) Mention the conditions for the maximum reversible expansion work in a system.

   (ii) How fast would a particle of mass 5 mg need to travel to have a momentum same as that of a photon of wavelength 350 nm?

   (iii) Calculate the enthalpy of combustion of ethanol at 25^{0}C and 1 atm. pressure. The $\Delta_f H^0$ values for $CO_{2(g)}$, $H_2O_{(l)}$ and $C_2H_5OH_{(l)}$ are -393.5, -285.9 and -277.7 kJ/mol respectively. **[3 +3 + 3 M]**

PART-B

(i) Using Valence bond theory, predict the state of hybridization of the central metal showing the electronic configuration, geometry, magnetic behavior of the complex **$[Co(CN)_6]^{3-}$** .

(ii) Give reasons for the fact that octahedral complexes are more stable and more common than tetrahedral complexes.

(iii) Using CFT, draw the CFsplitting diagram showing the distribution of electrons, predict the geometry and calculate CFSE for the complex **$[Fe(H_2O)_6]^{2+}$**.

(iv) Explain the Jahn-Teller effect in octahedral complexes of Cr^{2+}.

(v) Draw the structure of EDTA indicating the donor atoms. Also write any two applications of EDTA as a chelating agent.

[4+2+4+4+4M]

2. (i) Write the structure of all optical isomers of $[Co(en)_2Cl_2]^+$.

(ii) Write the principle involved in quenching method used for studying the rate of chemical reactions.

(iii) The gas-phase reaction between methane and diatomic sulphur is given by the equation

$$CH_4(g) + 2S_2(g) \rightarrow CS_2(g) + 2H_2S(g)$$

At 500°C, the rate constant for this reaction is 1.1 $dm^3\ mol^{-1}\ s^{-1}$ and at 625°C the rate constant is 6.4 $dm^3\ mol^{-1}\ s^{-1}$. Calculate E_a for this reaction.

(iv) Calculate the equilibrium constant of the reaction

$$Cu^{2+}(aq) + 4\ NH_3(aq) \rightleftharpoons Cu(NH_3)_4{}^{2+}{}_{(aq)}$$

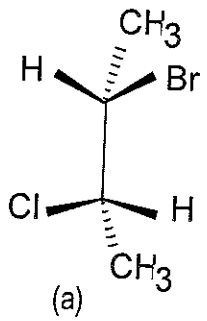
at 25°C given that $\Delta_r G° = -76.0\ kJ\ mol^{-1}$

[3+2+2+2M]

PART-C

1. (i) With the help of potential energy diagram, discuss the stability of various conformers of n-butane.

(ii) Find out the relationship between the given stereo isomers as enantiomers/ diastereomers/identical.



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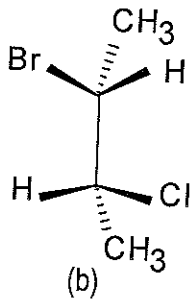

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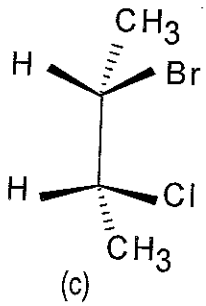

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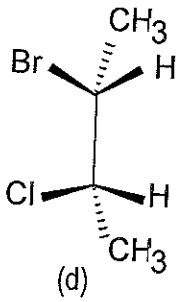


(d)

(iii) Reaction of 1-bromobutane with sodium methoxide produces 1-methoxy butane –suggest a mechanism for the reaction.

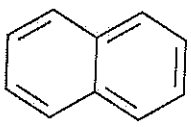
[5+4+4M]

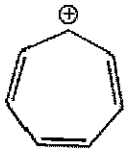
2. (i) Solvolysis of 2-bromo-3-methyl butane gives 2-methyl-2-butene and 2-methyl-1-butene. On the basis of Zaitsev's rule identify and justify the formation of major product.

(ii) Write the reaction mechanism for the addition of water to cyclohexene.

(iii) Identify whether the given below compounds are aromatic or non aromatic based on Huckel's rule of aromaticity. Justify your answer.

[4+5+4M]


(a)



(b)

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BITS PILANI, DUBAI CAMPUS
I YEAR FIRST SEMESTER, 2012-2013
TEST-II-OPEN BOOK

Course Title: General Chemistry **Course No: CHEM F111**
Date: 18.11.2012 **Total Marks: 40**
Time: 50 Min **Weightage: 20%**

1. Answer all questions sequentially.
2. Show stepwise calculation indicating the units wherever it is required.
3. Only prescribed text book and original hand written class notes are allowed.

1. Find the possible number of vibrational absorption bands in the IR spectra of the following compounds
   (a) HCN (b) Aniline
2. Assume that O-H group in an alcohol can be considered as isolated from the rest of the molecule. Calculate the vibrational frequency of the bond assuming the force constant of the bond as 516 Nm^{-1}
3. A sample of gas is compressed by an average pressure of 0.50 atm so as to decrease its volume from 400cm^3 to 200 cm^3. During the process 8.00 J of heat flows out to surroundings. Calculate the change in internal energy of the system.

[6+5+4M]

4. The heat of combustion of naphthalene $C_{10}H_8(s)$ is – 123 .25 kcal .If the heat of formation of $CO_2(g)$ and H_2O (l) are −97.0 and −68.4 kcal respectively. Calculate the heat of formation of naphthalene .
5. A sample of aluminium of mass 1.25 Kg is cooled at constant pressure from 300K to 260K. Calculate the energy that must be removed as heat and the change in entropy of the sample. The molar heat capacity of aluminium is 24.35 J/K/mol.
6. Calculate ΔG for the following reaction at 25°C .Predict whether the reaction is spontaneous or not .

   $NH_{3(g)} + HCl_{(g)} \rightarrow NH_4Cl_{(s)}$
   $\Delta H = -176.0$ kJ $\Delta S = -284.8$ J/K

[7+4+4M]

7. The molar extinction coefficient of an organic compound is 12,000 L $mol^{-1}cm^{-1}$ and the compound absorbs at 290 nm with $I/I_0 = 0.43$. Calculate the minimum concentration of the solution that can be detected in a cell of path length 2 cm.
8. Aniline is colourless but in tetracyanoethylene, aniline is deep blue in colour. Explain.
9. List all possible electronic transitions for the following compounds.
   (a) CH_3Cl (b) 1,3 – butadiene.

[3+3+4M]

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BITS PILANI, DUBAI CAMPUS
I YEAR FIRST SEMESTER, 2012-2013
TEST-I-CLOSED BOOK

Course Title: General Chemistry **Course No: CHEM F111**
Date: 30.09.2012 **Total Marks: 50**
Time: 50 Min **Weightage: 25%**

1. Answer all questions sequentially.
2. Show stepwise calculation indicating the units wherever it is required
3. Useful data: 1 eV=1.602x10^{-19}C, h = 6.626 x 10^{-34} J.sec, c = 3 x 10^{10} cm/s, R_H = 109677 cm^{-1}
Mass of electron =9.1x 10^{-31} kg, Atomic Numbers of H =1, He= 2

1. (i) List the three crucial experiments that were able to prove the failure of classical mechanics and the success of quantum theory.
   (ii) Write Bohr Frequency relation and define the terms
   (iii) The work function for rubidium is 2.10 eV. Calculate the kinetic energy and speed of electron ejected by the light of wavelength 430nm.
   (iv) Calculate the probability that an electron will be found between x= 0.2nm and 0.3 nm in a box of length 10nm when its wave function $\Psi = (2/L)^{1/2}\sin(2\pi x/L)$.
   (v) Write time dependent Schrodinger equation for a single particle of mass **m** moving with energy **E** in one dimension and define the terms in the equation.

[3+2+5+4+3M]

2. (i) Calculate the uncertainty in position if the electron has a speed of 500 m s^{-1} with an uncertainty of 0.02%.
   (ii) Mention any two conditions for quantum mechanical tunnelling.
   (iii) Write an expression for the energy level E, when n = 6 for a particle in one dimensional box subjected to translational motion and sketch the shape of the wave function.
   (iv) Calculate the zero-point energy of a harmonic oscillator consisting of a particle of mass 2.33 × 10^{-26} kg and force constant 155 N/m.

[5+2+5+5M]

3. (i) The frequency of one of the lines in the Paschen series of the spectrum of the atomic hydrogen is ~~4.8214x10^{15}~~ Hz. Find the principal quantum number of the upper state in the transition. 2.9244x10^{14}
   (ii) Calculate the allowed energy levels of He^+ with n=3
   (iii) Mention the number of orbitals in a shell with n=4 and write their designations.
   (iv) What do you mean by the term selection rules in Spectroscopy ? Mention the selection rules for hydrogenic atoms.

[5+3+4+4M]

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B

BITS PILANI, DUBAI CAMPUS

I YEAR FIRST SEMESTER, 2012-2013

QUIZ-II-CLOSED BOOK

Date: 04.12.2012

Course Title: General Chemistry | Course No: CHEM F111 | Time: 20 Min

Total Marks: 14 | Answer all questions | Weightage: 7%

Name: | I.D.No. | Sec:

1. The equilibrium constant for the isomerization of cis-2-pentene to trans-2-pentene is K = 3.0 at 500 K. Calculate the standard reaction Gibbs energy for the isomerization. (R=8.314J/K/mol) (3M)

2. Draw the general form of an Arrhenius plot and indicate clearly the Arrhenius parameters. (2M)

Mention the significances of the solid – liquid transition temperature. (3M)

4. Give an example for pseudo first order reaction. (1M)

5. Mention the experimental technique that has been widely used to study the kinetics of enzyme action. **(1M)**

6. Write Arrhenius equation showing the temperature dependence of rate constant and define the terms in it. **(2M)**

7. Write the rate expression for the gas phase oxidation of NO giving NO_2 (third order form) **(2M)**

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BITS PILANI, DUBAI CAMPUS

A

I YEAR FIRST SEMESTER, 2012-2013

QUIZ-I-CLOSED BOOK

Course Title: General Chemistry Course No: CHEM F111 **Date: 23.10.2012**

Total Marks: 16 Weightage: 8% **Time: 20 Min**

Answer all questions

1. Draw a molecular potential energy curve showing the dependence of molecular energy on inter nuclear distance **(2M)**

2. Write the (unnormalized) wave function for the two electrons in hydrogen molecule **(2M)**

3. Predict the state of hybridization for the central atom in SO_2 (atomic number of O=8,S=16,) **(2M)**

4. The value of electron affinity of argon is negative. Justify. **(2M)**

5. Why the atomic radius of carbon is lower than that of boron? (atomic number of B=5,C=6,) **(1M)**

6. Write the order of energies of orbitals in the M shell of a titanium atom.(Atomic number of Ti= 22) **(1M)**

7. Calculate the bond order in Ne_2 and state whether the molecule exists or not. (atomic number of Ne=10) **(2M)**

8. Schematically represent the overlap for the formation of $\pi^*(2p_y)$ antibonding molecular orbital. **(2M)**

9. Which can be expected to have the higher bond dissociation energy NO^- or NO^+ ? Justify your answer through bond order calculation. **(2M)**

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