BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

Make –up Test –2 (Open book)
Course Title :Chemistry I (CHEM UC141)

Date:
Time: 50 min

Total Marks:20
Weightage:20%

1.Answer all questions sequentially.
2.Show stepwise calculation indicating the units wherever it is required.
3.Only prescribed text book is allowed.

1.(i)The latent heat of vaporization of bromine is 29.2 kJ / mol at 59°C and 1 atm pressure. Calculate q, w and ΔU when 1 mole of bromine vaporizes.

(ii) Two moles of an ideal gas at 25° C expands isothermally and reversibly from an initial volume of 2 dm^3 to a final volume of 20 dm^3 against a pressure which is gradually reduced.Calculate q , w and ΔU.

(iii) Write the number of components, phases and evaluate the degrees of freedom for the following equilibrium.
(a)Two partially miscible liquids in the absence of vapour.
(b) $N_{2(g)} + 3H_2 \rightleftharpoons 2\ NH_{3(g)}$

(2.5 +2.5+2 M)

2. (i) Calculate the value of dT/dp for the water = ice system at 0°C. ΔH_f for water is 6007.8 $J.mol^{-1}$ ($1J = 9.87X10^{-3}dm^3$) atm;
molar volume of water = 18.00 cm^{-3}; of ice 19.63 cm^3.

(ii) Calculate the change in entropy accompanying heating of one mole of helium gas, assumed ideal, from a temperature of 298K to a temperature of 1000K at constant pressure.

(iii) Calculate the entropy change for vapourisation of water. Given enthalpy change for liquid water to steam at 100°C is 40.8KJ mol^{-1}

(2+2.5+2.5 M)

3. (i)Determine the enthalpy of the reaction,

$C_3H_8(g) + H_2(g) \longrightarrow C_2H_6(g) + CH_4(g)$

At 25 °C, using the given heat of combustion values under standard conditions.

Compound	ΔH^o (kJ/mol)
$H_2(g)$	-285.8
$CH_4(g)$	-890.0
$C_2H_6(g)$	-1560.0
C (graphite)	-393.5

The standard heat of formation of $C_3H_8(g)$ is -103.8 kJ/mol.

(ii) The heat of formation of MnO_2 and Al_2O_3 are -125 and -400 kcal respectively. Calculate the enthalpy change when 1 kg of Mn is formed by reaction of MnO_2 and Al.

(3+3 M)

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

COMPREHENSIVE EXAMINATION
Course Title :Chemistry- I (CHEM UC141)

Date: 4.01. 2006 **Total Marks:40**
Time:3 hours **Weightage:40%**

1.Answer all questions
2. Answer PART A, B and C in separate answer sheets.
2.Show stepwise calculation indicating the units wherever its required
3.Useful data : h = 6.626 x 10^{-34} J.sec ,c = 3 x 10^{10} cm/s,
m_e = 9.110 x 10^{-31} Kg,1ev = 1.602 X 10^{-19} C,R_H = 109677 cm^{-1}
R = 8.314 J/K/mol, F = 96500 C.

PART - A

1. (i) 0.440g of a substance dissolved in 22.2g of benzene lowered the freezing point of benzene by 0.567°C . Calculate the molecular mass of the substance (K_f = 5.12°C mol^{-1}).
(ii)Calculate the amount of O_2 (0.20 atm) dissolved in 1 dm^3 of water at 293 K. The Henry's law constant for O_2 is 4.58 x 10^4 atm at 293K.

[1.0 + 1.5 M]

2. (i) Draw the pH curve for the titration of CH_3COOH with NaOH and mark the specific points in the diagram.
(ii)Calculate the pH of the solution in which 21.2 ml of 0.22M HNO_3(aq)was added to 10.0 ml of 0.30M NaOH (aq)

[1.0 + 1.5 M]

3. (i)Sketch an electrochemical cell by combining a calomel electrode with a glass electrode. Using this how will you calculate the pH of an unknown solution ?
(ii)The cell

Zn | $ZnSO_4$ (M = 1) || $CuSO_4$ (M= 1) | Cu

was set up in a laboratory experiment . At 298 K standard reduction electrode potential of Zinc and Copper electrodes are − 0.763 V and + 0.337 V respectively. Calculate ΔG for the cell reaction and the equilibrium constant for the reactant.

[1.5 + 2.0 M]

4.(i)Mention the disadvantage of flow method in studying the kinetics of chemical reactions.

(ii)The gas phase reaction between CH_4 and diatomic sulphur (S_2) is given by the equation

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

At 550°C the rate constant for this reaction is 1.1 litre mol^{-1} sec and at 625°C the rate constant is 6.4 litre mol^{-1} sec .Calculate E_a for this reaction.

[0.5 + 1.5 M]

5.(i)Mention the criterion for successful collisions of the reactant species in the case of bimolecular gas –phase reactions.

(ii)Derive the rate law of unimolecular gas phase reactions using Lindemann mechanism.

[1.0 + 2.5 M]

Part-B

1.(i)At temperature T, the endothermic reaction A ------>B proceeds almost to completion. Why ΔS is +ve?

(ii)Mention the temperature & pressure corresponding to triple point & critical point in the phase diagram of CO_2

[1.0+1.0 M]

2. Calculate (a) q (b) w (c)ΔU for the reversible adiabatic expansion of 1 mole of an ideal gas (C_v = 3/2R) from 5.0 to 25.0 litres. The initial temperature is 27°C.

[3.0 M]

3. Consider a class room of dimensions 5x10x3 m^3 at temperature 20°C and pressure 1 atm. There are 50 people in the room, each losing energy at the average of 150 watt. Assuming that the walls, ceiling, floor and furniture perfectly insulated and none of them absorbing heat, how much time will be needed for rising the temperature of air in the room to body temperature, i.e.,37°C. For air C_p = 7/2 R. Loss of air to the outside as the temperature rises may be neglected.

[2.5 M]

4.Calculate the

(i) entropy change in 400 kg of water at 55°C when 75 J heat flows out of it into surroundings at 20°C

(ii)What is the entropy change in the surrounding (iii) What is the total entropy change in the universe due to this process? Assume the temperature remains constant.

[2.5M]

5. Determine the enthalpy change for

$C_3H_{8(g)} + H_{2(g)} \longrightarrow C_2H_{6(g)} + CH_{4(g)}$

At 25° C using heat of combustion values under standard conditions.

Compounds	$H_{2(g)}$	$CH_{4(g)}$	$C_2H_{6(g)}$	C (graphite)
ΔH° in kJ/mol	-285.8	-890.0	-1560.0	-393.5

The standard heat of formation of $C_3H_{8(g)}$ is -103.8kJ mol^{-1}

[3.0 M]

PART-C

1.(i) An FM radio transmitter broadcasts at 98.4 MHz with a power of 45 kW. How many photons does it generate per second?

(ii) An electron is confined in a one dimensional box of length 2 Å. Calculate its zero-point energy.

[1.5 + 1.0 M]

2. (i) Calculate the wave length of radiation emitted for the electronic transition from infinity to stationary state of the hydrogen atom.

(ii) Is the combination of quantum numbers,

$n = 2, l = 2, m = 1, s = ½,$

allowed or not? Explain.

[1.5 + 1.0 M]

3. (i) Draw the Molecular orbital energy level diagram for B_2 clearly labeling all the orbitals, showing electronic arrangements in the molecular orbitals. Determine the bond order and the magnetic behavior.

(ii) Ethylene is a planar molecule while acetylene is a linear molecule. Why?

[2.5 + 1.0 M]

4. (i) A 1 % solution of a dye transmitted 60 % of the light in a cell of 1.0 cm thickness. Find the percentage of light transmitted by a 2 % solution of the same dye in the same cell.

(ii) Calculate the rotational constant of $^{1}H_{2}$. Use R_e (H_2) = 74 pm.

[2.0 +2.5M]

****

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

Test –2 (Open book)
Course Title :Chemistry I (CHEM UC141)

Date: 18.12.2005 **Total Marks:20**
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 is allowed.

1.(i)For combustion of heptane in a constant volume calorimeter $q_v = -4800$ kJ at 298 K. Calculate the change in enthalpy of the process at 298 K.

(ii)One mole of oxygen at 300 K expands isothermally from 3 atmospheres to 1 atmosphere .Assuming that oxygen behaves ideally calculate w , if the expansion is (a) reversible and (b) single step against a constant pressure of 1 atmosphere.

(iii)Write the number of components, phases and evaluate the degrees of freedom for the following equilibrium
(a) A gas in equilibrium with its solution in liquid.
(b) $I_{2\,(s)} \rightleftharpoons I_{2(v)}$

(2+3.5+1.5 M)

2.(i)1 mole of an ideal gas at 25°C is subjected to expand reversibly ten times of its initial volume. Calculate the change in entropy of expansion.

(ii)Calculate the free energy change (ΔG) which occurs when 1 mole of an ideal gas expands reversibly and isothermally at 37°C from an initial volume of 55 dm^3 to 1000dm^3 .

(iii)The vapour pressure of water at 100°C is 760mm. What will be the vapour pressure at 95°C? The heat of vapourisation of water in this temperature range is 41.27 kJ per mole.

(2.5+2 +2.5 M)

P.T.O

3. (i) Calculate the standard enthalpy of hydrogenation of cyclohexene to cyclohexane given that the standard enthalpy of combustion of cyclohexene is –2782 kJ mol^{-1} and of cyclohexane is –2923 kJ mol^{-1}. The enthalpy of formation of liquid water is –286 kJ mol^{-1}.

(ii)The enthalpy of sublimation of calcium at 25 °C is 178.2 kJ mol^{-1}. How much energy (at constant temperature and pressure) must be supplied as heat to 16.00g of solid calcium to produce plasma (an ionic gas) composed of Ca^{2+} ions and electrons? The first and second ionization enthalpies of Ca(g) are +590 kJ mol^{-1} and +1150 kJ mol^{-1}.

(iii) How is 'dry ice' formed?

(iv) Why liquid carbon dioxide does not exist at normal conditions?

(2+2+1+1M)

****

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

Name of the student :
ID No & Sec :

MAKE-UP QUIZ -2 (Closed Book)

Course Title :Chemistry I **Course No:CHEMUC141**
Date: 1.12.2005 **Total Marks:20**
Time:30 min **Weightage:10%**

1. For multiple choice questions tick and underline the correct answer.
2.Overwriting will be taken as a wrong answer.
3.Question paper contains 4 pages.

(1M x 20= 20M)

1.The parallel band of Q branch in the vibration rotation spectra of _____ molecule will be missing.
(a)H_2O (b)SO_2 (c) NO (d)HCl

2.Why are pure rotational spectra studied only in the gaseous state of atoms and molecules?

3.How many fundamental vibrational frequencies are expected for benzene molecule ?

4.Sketch the IR active modes of CO_2 molecule.

5.Why lasers are used as the radiation sources in Raman Spectrometers ?

6.The energy levels of a symmetric rotor determined by quantum numbers J and K are found to be _____.

7.Give any two consequences of anharmonicity in the case of a molecule undergoing vibrational transitions.

8.Write the expression for Hooke's Law.

9. Write the wavelength region of I.R. spectra.

10. No two compounds except _____ can have identical I.R Spectrum.

11. Which of the following are microwave active?
(i) HCl (ii) N_2 (iii) NO (iv) CO (v) C_2H_4 (vi) HBr (vii) CH_4 (Viii) Cl_2

12. CO_2 present in atmosphere contribute to Green House effect while N_2 and O_2 do not – Why?

13. In IR spectra free O-H_{str} absorption is observed at 3600cm^{-1} . At what frequency region you will get an absorption peak / band for inter molecularly H-bonded O-H_{str}?

14. . A _____ is used to generate radiation in the mid-infrared.

15. Mention one application of resonance Raman spectroscopy.

16. All spherical rotors are rotationally Raman _____

17. Write the Franck-Condon principle.

18. The Doppler width increases with temperature. Therefore, to obtain spectra of maximum sharpness, it is best to work with _____

19. In Raman spectroscopy, the incident radiation is _____ by the molecules.

20. Name any two chromophores.

****

A

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

Name of the student :
ID No & Sec :

QUIZ -2 (Closed Book)

Course Title :Chemistry I **Course No:CHEMUC141**
Date: 22.11.2005 **Total Marks:20**
Time:30 min **Weightage:10%**

1. For multiple choice questions tick and underline the correct answer.
2.Overwriting will be taken as a wrong answer.
3.Question paper contains 4 pages.

(1M x 20= 20M)

1.Which of the following relationship is correct regarding molecular energy levels?
(a) E(electronic) > E(vibrational) > E(rotational)
(b) E(rotational) > E(vibrational) > E(electronic)
(c) E(electronic) > E(rotational) > E(vibrational)
(d) E(vibrational)> E(electronic) > E(rotational)

2.The selection rule of the transition in rotational energy levels in the Raman spectrum is
(a) $\Delta J = \pm 1$ (b) $\Delta J = +1$ (c) $\Delta J = +2$ (d) $\Delta J = \pm 2$

3.First overtone in the IR spectra corresponds to
(a) $\Delta v = \pm 1$ (b) $\Delta v = \pm 2$ (c) $\Delta v = \pm 3$ (d) $\Delta v = \pm 4$

4.The separation between lines in the P and R branches of a vibrational transition is
(a) 3B (b) 4B (c) 2B (d) 5B

5.List all the electronic transitions possible for CH_3Cl

6.Which of the following molecules will show a pure rotational spectrum?

H_2, CO , HCl , H_2 (liquid) ,NH_4Cl (s)

7.Sketch the vibrational modes of water molecule .

8.Mention the names of different types of bending vibrations.

9.Find out the number of theoretical vibrational absorption bands for the molecule $CH_2 = CH_2$.

10.Write the exclusion rule for IR and Raman spectra.

11. Source of microwave radiation is
(a) Globar (b)tungsten-iodine lamp (c)klystron (d)xenon in quartz

12. Give any 2 detector used in modern spectrometers.

13. Write the expression for the width of a spectral line at half its maximum height

14. When a rigid molecule changes its rotational quantum number from J to J+1 in an absorption, the change in rotational energy of the molecule is given by _____.

15. Tetrahedral and Octahedral molecules are rotationally Raman _____.

16. Vibrational transitions are always accompanied by _____ transitions

17. Write the expression for Beer-Lambert law.

18.Mention any one application of Circular Dichroism spectra.

19.Name any two charge-transfer donors.

20.Absorption spectrum in UV region results from
(a) electronic excitation (b) increase in vibration
(c) decrease in rotational energy (d) increase in P.E.

****

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2004-2005

MAKE UP TEST- 1 (closed book)

Course Title :Chemistry-I **Course No:CHEM UC141**
Date: **Total Marks:20**
Time: 50 min **Weightage:20%**

1.Answer all questions
2.Show stepwise calculation indicating the units wherever it is required
3.Useful data:h = 6.626 x 10^{-34}J.sec, c = 2.998 x 10^{8} m/sec ,
R_H = 109677 cm^{-1}

4.Atomic numbers:P(15) ,S(16)

1.(i)Draw the Molecular Orbital energy diagram for NO molecule clearly labeling all the orbitals and showing the electronic arrangements in the molecular orbitals.Write the MO configuration of NO molecule and calculate the bond order.

(ii) Draw the shapes of $\pi^*(2p_y)$ and $\sigma(2p_z)$ molecular orbitals.

(iii)Predict the hybrid state of the central atom of the following species

(a) $POCl_3$ (b)SO_3

(4+2+1M)

2.(i)Write the mathematical form of a 1s orbital for a hydrogen atom.

(ii) Light of wavelength 12818 Å is emitted when the electron of a hydrogen atom drops from 5^{th} to 3^{rd} quantum level. Find the wavelength of the photon emitted when electron falls from 3^{rd} to ground level.

(iii)State the orbital degeneracy of the levels in the hydrogen atom that have energy
(a) $-1/9\ hcR_H$ (b) $-1/49\ hcR_H$

(2+2+2M)

3.(i) Among o-hydroxybenzaldehyde and p-hydroxybenzaldehyde which is more soluble in water and why?

(ii)Why is LiCl is more covalent than KCl ?

(iii) Mention the conditions for effective combination of atomic orbitals.

(iv)Why does N_2 have greater dissociation energy than N_2^+ whereas O_2 has lower dissociation energy than O_2^+ ?

(2+1+2+2M)

****

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

TEST- 1 (Closed book)

Course Title :Chemistry-I **Course No:CHEM UC141**
Date:10.11.2005 **Total Marks:20**
Time: 50 min **Weightage:20%**

1.Answer all questions
2.Show stepwise calculation indicating the units wherever it is required
3.Useful data : h =6.626 x 10^{-34} J sec,c = 2.998 x 10^{8} m/sec,
R_H = 109677 cm^{-1}
4.Atomic numbers:I(53),Cu(29),Ca(20),P(15)
5.Question paper has 2 pages

1.(i)Write the mathematical form of a $2p_z$ orbital.

(ii)Give the selection rules of hydrogenic atoms.

(iii)Calculate the ratio of wavelength of first spectral lines of Lyman and Balmer series of hydrogen spectrum.

(2+1+3 M)

2.(i) Which of the following substance will have higher boiling point . Justify your answer.
o-nitrophenol or p-nitrophenol

(ii)The "Humphreys Series" is another group of lines in the spectrum of atomic hydrogen .It begins at 12368 nm and has been traced to 3281 nm. At what wavelength would you expect the longest wavelength transition of the Humphreys series to occur in He^+ ?

(iii)How many electrons are possible in all shells with n+l = 5?

(iv)Write the expression for the electronegativity difference ($\Delta\chi$) for the diatomic molecule A—B based on Pauling scale clearly writing the expression for the extra bond energy ΔE.

(v)State giving reason which cation will exert greater polarizing power Cu^+ or Ca^{2+}

(2+2+1+1+1M)

P.T.O

3.(i)Label the molecular orbitals formed by the following combinations of atomic orbitals

(a) 2s+2s (b) $2p_x - 2p_x$

(ii)Draw the Molecular Orbital energy diagram for N_2 molecule clearly labeling all the orbitals and showing the electronic arrangements in the molecular orbitals. Write the MO configuration of nitrogen molecule and calculate the bond order.

(iii)Write the hybridization state of the central atom of the following species.

(a) ICl^- (b) PO_4^{3-}

(iv) Of the species $O_2, O_2^{2-}, O_2^+, O_2^-$ which would have the maximum bond strength ?

(1+4+1+1M)

****

BITS PILANI -DUBAI CAMPUS,KNOWLEDGE VILLAGE ,DUBAI
I YEAR FIRST SEMESTER,2005-2006

Name of the student :
ID No & Sec :

QUIZ (Closed Book)

Course Title :Chemistry I **Course No:CHEMUC141**
Date: 27.09.2005 **Total Marks:20**
Time:30 min **Weightage:10%**

1. For multiple choice questions tick and underline the correct answer.
2. Overwriting will be taken as a wrong answer.
3. Useful data :Planck's constant $h=6.626 \times 10^{-34}$ J sec, $1ev = 1.602 \times 10^{-19}$ J, $c = 2.998 \times 10^{8}$m/sec, Mass of electron = 9.110×10^{-31} Kg. $R_H = 109677\ cm^{-1}$

(1M x 20= 20M)

1. With the increasing principal quantum number, the energy difference between adjacent energy levels in H atom
(a) increases (b) decreases (c) remains constant (d) decreases for low values of Z and increases for higher values of Z.

2. If the uncertainty in position of electron is zero ,the uncertainty in its momentum would be
(a) zero (b) $h/2\pi$ (c) $h/4\pi$ (d) infinity

3 What is the distance (in pm) for the maximum radial density of the 1s orbital in the hydrogen atom?

4. The wavelength of a spectral line for an electronic transition is inversely related to
a)number of electrons undergone transition (b) the nuclear charge of the atom (c) the velocity of an electron undergoing transition (d) the difference in the energy levels involved in the transition.

5. If the energy of the photoelectrons emitted from a metal is twice the workfunction ,by what factor must the frequency of the incident radiation be increased to double the energy of the photoelectrons ?
(a) 2/3 (b) 3/2 (c) 5/3 (d) 3/5

6. What is the wavelength of a 1keV electron?
(a) 0.4Å (b) 0.04Å (c) 4Å (d) 4 nm

7. Schematically represent the energy levels of a particle that can move in a circular path.

8. The wave character of an electron was verified by _____

9. The zero point energy for a particle of mass m confined in an one dimensional box of length L is E = _____.

10. The radial part of wave function depends on the quantum numbers _____ and independent of _____.

11. Mention any two applications of the " Scanning Tunnelling Microscopy" technique.

12. For an electron in a hydrogen atom the wavefunction Ψ is proportional to $\exp^{-r/a_0}$ where a_0 is the Bohr radius. What is the ratio of the probability of finding the electron at the nucleus to the probability of finding it at a_0
(a) e (b) e^2 (c) $1/e^2$ (d) zero.

13. The average distance of an electron from the nucleus of a hydrogenic atom of atomic number Z is _____.

14. Assume that a new material developed could be used as a filament at 3700° C instead of 3000° C . By what factor would the power output of a lamp that used the new material increase?

15. Mention the boundary conditions for a particle that undergoes harmonic motion.

16. What is the lowest value of n that allows the g subshell to exist?

17. The energy of an electron in the first Bohr orbit of H atom is – 13.6eV. The possible energy value(s) of the excited state(s) for electrons in Bohr orbits of hydrogen is (are)
(a) –3.4eV (b) –4.2eV (c) –6.8eV (d) + 6.8eV

18. What experimental evidence requires that the emission of energy by an atom must be quantized?

19. Justify how Planck's result account quantitatively for the Wien's law.

20. The wavelength of the first line of Balmer series of H atom is 6581 Å . Calculate the wavelength of the second line of the series .

****