

BS-101A		Chemistry					
L	T	P	Credit	Major Test	Minor Test	Total	Time
3	1	-	4	75	25	100	3h
Purpose	To familiarize the students with basic and applied concept in chemistry						
CO1	An insight into the atomic and molecular structure						
CO2	Analytical techniques used in identification of molecules						
CO3	To understand Periodic properties						
CO4	To understand the spatial arrangement of molecules						
CO5	To understand <b>Basic concepts of thermodynamics and its applications.</b>						
CO6	To familiarize with basic chemical reactions and synthesis of common drugs.						

### UNIT - I

Atomic and molecular structure (10 lectures)

Molecular orbitals of diatomic molecules ( $N_2$ ,  $O_2$ ,  $CO$ ) Equations for atomic and molecular orbitals. Energy level diagrams of diatomics. Pi-molecular orbitals of butadiene and benzene and aromaticity. Crystal field theory and energy level diagrams of  $[Co(NH_3)_6]$ ,  $[Ni(CO)_4]$ ,  $[PtCl_2(NH_3)_2]$  and magnetic properties of metal complexes. Band structure of solids and the role of doping on band structures.

### UNIT - II

Spectroscopic techniques and applications (8 lectures)

Principles of spectroscopy and selection rules. Electronic spectroscopy(basic concept). Fluorescence and its applications in medicine. Vibrational and rotational spectroscopy of diatomic molecules. Applications. Basic concepts of Nuclear magnetic resonance and magnetic resonance imaging, Diffraction and scattering.

### UNIT - III

Use of free energy in chemical equilibria (4 lectures)

Thermodynamic functions: energy, entropy and free energy. Estimations of entropy and free energies. Free energy and emf. Cell potentials, the Nernst equation and applications.

Periodic properties (4 Lectures)

Effective nuclear charge, penetration of orbitals, variations of s, p, d and f orbital energies of atoms in the periodic table, electronic configurations, atomic and ionic sizes, ionization energies, electron affinity and

electronegativity, polarizability, oxidation states, coordination numbers and geometries, hard soft acids and bases, molecular geometries ( $\text{H}_2\text{O}$ ,  $\text{NH}_3$ ,  $\text{PCl}_5$ ,  $\text{SF}_6$ ,  $\text{CCl}_4$ ,  $\text{Pt}(\text{NH}_3)_2\text{Cl}_2$ )

#### UNIT - IV

Stereochemistry (6 lectures)

Representations of 3 dimensional structures, structural isomers and stereoisomers, configurations and symmetry and chirality, enantiomers, diastereomers, optical activity, absolute configurations and conformational analysis.

Organic reactions and synthesis of a drug molecule (4 lectures)

Introduction to reactions involving substitution, addition, elimination, oxidation, reduction, cyclization and ring openings. Synthesis of a commonly used drug molecule (paracetamol and Aspirin)

Suggested Books:

- 1) University chemistry, by B. M. Mahan, Pearson Education
- 2) Chemistry: Principles and Applications, by M. J. Sienko and R. A. Plane
- 3) Fundamentals of Molecular Spectroscopy, by C. N. Banwell
- 4) Engineering Chemistry (NPTEL Web-book), by B. L. Tembe, Kamaluddin and M. S. Krishnan
- 5) Physical Chemistry, by P. W. Atkins
- 6) Organic Chemistry: Structure and Function by K. P. C. Vollhardt and N. E. Schore, 5th Edition  
<http://bcs.whfreeman.com/vollhardtschore5e/default.asp>

Note: The paper setter will set the paper as per the question paper templates provided.

## ACADEMIC CALENDER

### LECTURES TOPICS

L- 3      T- 1

<b>Unit -I</b>	Atomic and molecular structure
<b>Lect. No.</b>	<b>Topics to be covered</b>
L1	Molecular orbitals of diatomic molecules (N <sub>2</sub> , O <sub>2</sub> , CO)
L2	Equations for atomic and molecular orbitals.
L3	Energy level diagrams of diatomics.
L4	Pi-molecular orbitals of butadiene aromaticity.
L5	Pi-molecular orbitals of benzene
L6	Aromaticity and Huckel Rule
L7	Crystal field theory, Postulates
L8	Energy level diagrams of [Co(NH <sub>3</sub> ) <sub>6</sub> ], [Ni(CO) <sub>4</sub> ], [PtCl <sub>2</sub> (NH <sub>3</sub> ) <sub>2</sub> ]
L9	Magnetic properties of metal complexes
L10	Band structure of solids
L11	The role of doping on band structures.
<b>Unit -II</b>	Spectroscopic techniques and applications
L 12	Principles of spectroscopy
L 13	selection rules
L 14	Electronic spectroscopy(basic concept).
L15	Fluorescence
L 16	Applications of fluorescence in medicine
L 17	Vibrational spectroscopy of diatomic molecules
L18	Rotational spectroscopy of diatomic molecules
L 19	Applications of Vibrational spectroscopy and Rotational spectroscopy
L20	Basic concepts of Nuclear magnetic resonance
L 21	Magnetic resonance imaging,
L 22	Diffraction
L 23	scattering.

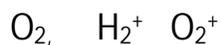
<b>Unit -III</b>	Use of free energy in chemical equilibria
L 24	Thermodynamic functions: energy, entropy and free energy
L 25	Estimations of entropy
L26	Estimations of free energy
L 27	Free energy and emf.
L 28	Cell potentials, the Nernst equation and applications.
L29	The Nernst equation and applications.
<b>UNIT- III</b>	Periodic properties
L30	Effective nuclear charge,
L 31	penetration of orbitals
L 32	variations of s, p, d and f orbital energies of atoms in the periodic table
L 33	Variations in electronic configurations
L 34	Variations in atomic and ionic sizes, ionization energies,
L 35	Variations in electron affinity and electronegativity
L 36	Variations in polarizability, oxidation states, coordination numbers and geometries
L 37	hard soft acids and bases
L 38	Molecular geometries (H <sub>2</sub> O, NH <sub>3</sub> , PCl <sub>5</sub> , SF <sub>6</sub> , CCl <sub>4</sub> , Pt(NH <sub>3</sub> ) <sub>2</sub> Cl <sub>2</sub> )

<b>Unit IV</b>	Stereochemistry
L39	Representations of 3 dimensional structures
L 40	structural isomers and stereoisomers
L 41	configurations and symmetry
L 42	chirality, enantiomers and its Properties
L 43	Diastereomers and its properties
L 44	optical activity, absolute configurations
L 45	conformational analysis.

<b>Unit IV</b>	Organic reactions and synthesis of a drug molecule
L 46	Introduction to reactions involving substitution reactions
L 47	Elimination reactions and its mechanism
L 48	Addition, cyclization and ring openings reactions
L 49	Oxidation and reduction, reactions and its mechanism
L 50	Synthesis of a commonly used drug molecule (paracetamol and Aspirin)

## Tutorial sheet 1

Q1. With the help of M.O theory predict which of the following species is diamagnetic ?

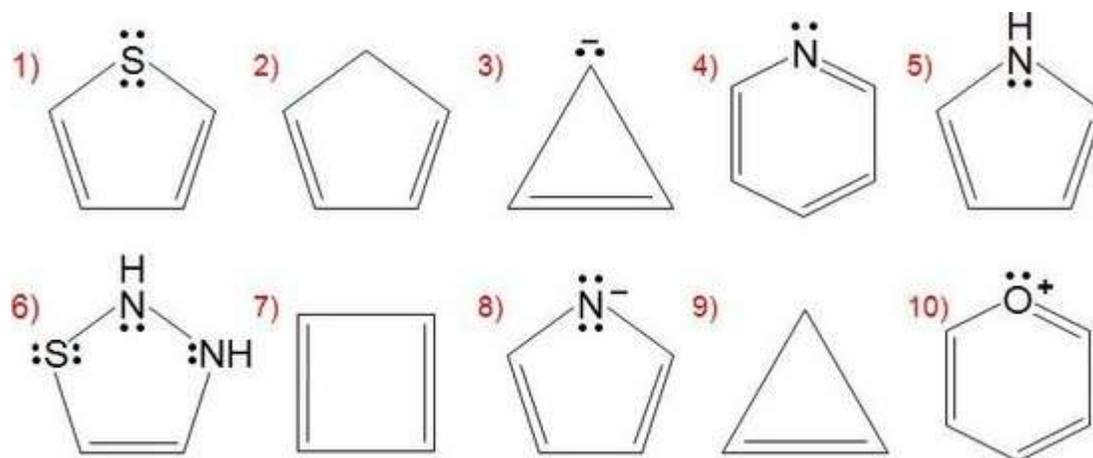


Q2. Arrange  $O_2$ ,  $O_2^+$   $O_2^-$   $O_2^{2-}$  in increasing order of bond length?

Q3. Draw the MO Diagram for CO and calculate its B.O?

Q4. Write a short note on conjugation in 1,3 butadiene?

Q 5. Predict whether the following compounds are aromatic or antiaromatic on the basis of Huckel rule?



Q6. Explain crystal field theory for octahedral complexes and draw CFT diagram for  $[Co(NH_3)_6]$ ?

Q7. What is meant by doping and why germanium doped with antimony is called an n-type semiconductor?

Q8. Draw CFSE diagram for  $Ni(CO)_4$

## Tutorial sheet 2

Q1. write a short note on MRI and its important applications in medicine?

Q2. Which of the following compounds will show only single peak in NMR?

(a)  $\text{CH}_3\text{CH}_3$  (b)  $\text{CH}_3\text{CH}_2\text{CH}_3$  (c)  $\text{C}_6\text{H}_5\text{CH}_3$  (d)  $\text{CH}_2=\text{CH}_2$

Q3. Write a short note on Principal of U.V Spectroscopy and its applications ?

Q4. What do you understand by Bathochromic shift and Hypsochromic shift ?

Q5. What do understand by Chemical Shift in NMR ,Explain?

Q6. What is Fluorescence and what are its applications in medicine?

Q7. Write a short note on selection rules of Spectroscopy?

### Tutorial sheet 3

Q1. Explain that noble gases has highest ionization energy?

Q2. Explain why electron affinity of N is lower than that of P?

Q3. What are the postulates of VSEPR theory and explain the structures of H<sub>2</sub>O and NH<sub>3</sub>?

Q4. What are the factors affecting Electronegativity ?

Q 5 Write a short note on HSAB concept?

Q6. Calculate EAN for 3d electrons of Cr ?

Q7. Define Polarizability?

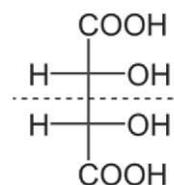
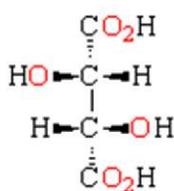
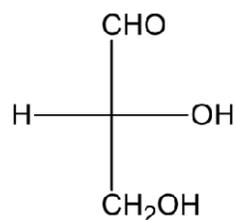
### Tutorial 4

Q1. Write a short note on functional isomerism with example?

Q2. What are enantiomers explain also write its properties?

Q3. Write a short note on Elimination Reactions and its mechanism?

Q.4. Determine R and S nomenclature?



Q5. Draw all the conformations of n-butane?

Q6 Explain Nucleophilic substitution reactions?

Q7 Write the synthesis of Aspirin and also write its important uses?

Q8. What do you mean by Chirality, Explain?

Total Pages : 3

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31037

CHEMISTRY

Paper : BS-101A

Time : Three Hours]

[Maximum Marks : 75

Note : Attempt any *five* questions, selecting at least *one* question from each unit. All questions carry equal marks.

**UNIT-I**

1. (a) Draw the molecular orbital energy level diagram for CO and N<sub>2</sub> molecules. Also find out the bond order in each case. 10
- (b) Define orbital and differentiate between  $\sigma$  and  $\pi$  molecular orbitals. 5
2. (a) What is crystal field stabilization energy. How is it calculated in tetrahedral, octahedral and square planar fields of ligands. 6
- (b) Write spectrochemical series and explain its importance. 3
- (c) What do you mean by aromaticity. Explain Huckel rule of aromaticity with examples. 6

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## UNIT-II

3. (a) What is absorption spectra ? Explain the following in respect of UV-visible spectroscopy.
- Bathochromic shift, Hyperchromic shift  
Hypsochromic shift, Hypochromic shift. (2+8)
- (b) Explain stretching and bending vibrations with respect to IR spectroscopy. 5
4. (a) On what principle NMR spectroscopy is based ? What type of nuclei show NMR spectra. Explain. 5
- (b) Explain chemical shift, shielding and deshielding in NMR spectroscopy. 3
- (c) Write a short note on MRI. 4
- (d) What are selection rules in spectroscopy? 3

## UNIT-III

5. (a) Explain the terms internal energy and enthalpy in thermodynamics. (2+2)
- (b) What is the physical significance of entropy? 3
- (c) Explain the term polarization, polarizability and polarising power. What is the significance of polarization? 5
- (d) Write a short note on hard and soft acids. 3
6. (a) Explain the following periodic properties in detail.
- (i) Ionization energy.
- (ii) Electro negativity. (5+5)

- (b) What is meant by effective nuclear charge. Write Slater rules for finding out effective nuclear charge. 5

#### UNIT-IV

7. What is isomerism ? Explain all.
- (a) The different types of structural isomers with example in each case. 10
- (b) What is drug ? How is aspirin synthesised ? What is the use of aspirin ? 5
8. Write short notes on the following :
- (a) Elimination reactions.
- (b) Enantiomerism.
- (c) CIP rules for writing absolute configuration. (5×3=15)
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