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SCHOOL OF ADVANCED SCIENCES
B.Tech. – Semester- I
Continuous Assessment Test–I, Nov 2022

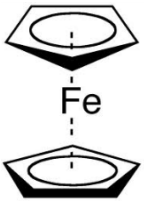
Course Code	BCHY101L	**Duration**	: 90 min.
Course name	Engineering Chemistry	**Max. Marks**	: 50
Semester	Fall 2022-2023	**Slot**	: B1+TB1
Faculty	Dr. S. Sumathi, Dr. M. Arunprasad, Dr. Jianping Hu, Dr. Amit Kuamr Tiwari, Dr. Madhumitha, Dr. Mausumi Goswami, Dr Sovan Roy, Dr. S. Senthilkumar	**Class No.**	5227, 5232, 5234, 5236, 5238, 5243, 5245, 7319

Q.No	Answer ALL the Questions (5 x 10 = 50 marks)	Max marks	CO	BL
1.	Comment on the stability, magnetic property of the following complexes with suitable diagram (a) $[CoF_6]^{3-}$ (b) $[Cr(CN)_6]^{3-}$ Stability (CFSE or EAN) – 2.5 marks x 2 examples = 5 marks Magentic Property (from diagram) – 2.5 marks x 2 examples = 5 marks $[CoF_6]^{3-}$ -- Weak field ligand – No pairing – paramagnetic – High spin complex- sp^3d^2 $[Cr(CN)_6]^{3-}$ -- Strong field ligand – Pairing of electrons – paramagnetic – d^2sp^3	10	CO1	BL2

2. a) Explain the structure of an organometallic compound which is used as a solid rocket propellant. 5+5 CO1 BL3

Ferrocene – 1 mark

Structure explanation – 4 marks



Mössbauer spectroscopy indicates that the iron center in ferrocene should be assigned the +2 oxidation state. Each cyclopentadienyl (Cp) ring should then be allocated a single negative charge. Thus ferrocene could be described as iron(II) bis(cyclopentadienide) $Fe^{2+}[C_5H_5^-]_2$.

The number of π-electrons on each ring is then six, which makes it aromatic according to Hückel's rule. These twelve π-electrons are then shared with the metal via covalent bonding. Since Fe^{2+} has six d-electrons, the complex attains an 18-electron configuration, which accounts for its stability. In modern notation, this sandwich structural model of the ferrocene molecule is denoted as $Fe(\eta^5\text{-}C_5H_5)_2$.

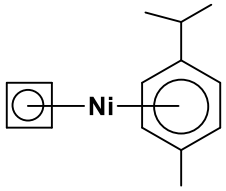
Crystallography reveals that the **cyclopentadienide rings are in staggered** conformation.

Hybridization: d^2sp^3

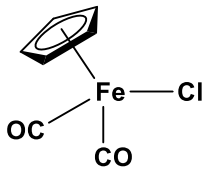
Magnetic Nature: Diamagnetic

b) Count the number of electrons in the following compounds and comment on their stability.

i)



ii)



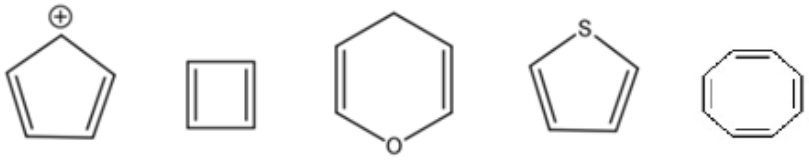
i) Nickel – oxidation state = 0
Group number – oxidn state = 10 -0 =10
No. of ligands from ligands = 4+6 = 10
Metal electrons + ligand electrons = 10+10 = 20 electrons – Not stable (2.5 marks)

ii) Iron – oxidation state = +2
Group number – oxidation state = 8-2 = d^6 electrons in metal
No. of electrons gained from ligands = 2+2+2+6 = 12

Metal electrons + ligand electrons = 6+12 =18 electrons - stable

3.	Label the following compounds appropriately as aromatic, non-aromatic or anti-aromatic with suitable justification:	10	CO1	BL4

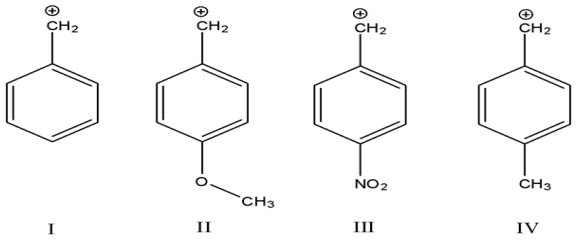
Aromatic or anti or non – 1 mark for each compound (5 marks)
Justification – 1 mark for each compounds (5 marks)



A B C D E

A = Antiaromatic (4 pi electrons)
B = Antiaromatic (4 pi electrons)
C = Nonaromatic (sp3 carbon)
D = Aromatic (6 pi electrons)
E = Nonaromatic (non planar)

4. a) Arrange the following carbocations in the decreasing order of stability and explain the reason: 5+5 CO1 BL3



I II III IV

i) Arrangement in decreasing order (higher stable to lower stable) – 1mark

ii) II>IV>I>III (4 marks with reason)

Electron releasing substituent increases the stability. The stability of carbocation is dependent on the nature and position of the substituent. Electron withdrawing substituent decreases the stability of carbocation.

When methoxy group attached at paraposition of CH2+ it behaves like Electron releasing group

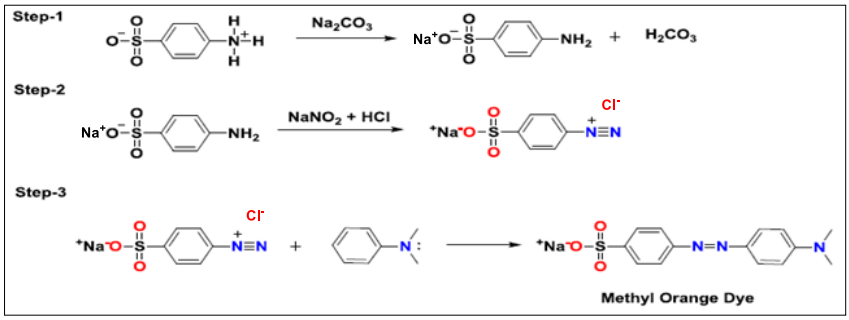
A methoxy substituent actually impacts the ring electronics via two competing effects. The oxygen's lone pair is well-placed to delocalize and increase electron density within the ring's conjugated system. This allows delocalization to better stabilize positive charges. So the methoxy is electron-donating from a resonance perspective. On the other hand, because oxygen is quite electronegative, the methoxy group is electron-withdrawing in an inductive sense via the σσ bonds

As a rule of thumb, if the atom that is attached to the benzene ring is surrounded by more electronegative atoms, the group withdraws electron from the ring. (-NO2, -C=O, -CN, -COOH). And, if the atom directly attached to the ring is surrounded by less electronegative ones, the group donates electron (-NH2, -OR, -OH, -R, etc.)

b) Explain the preparation and important steps involved in the

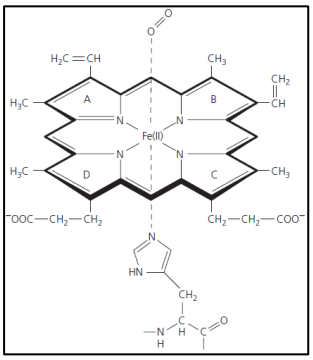
synthesis of an azo dye.

Methyl orange (1 + 4 marks) = 5 marks



5. a) Explain the structure of hemoglobin and role of distal histidine in detail. 5+5 CO1 BL2

Structure – 1 mark

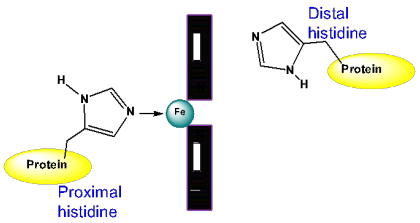


Explanation – 3 marks

- The organic component of the heme group—the protoporphyrin—is made up of four pyrrole rings (A, B, C & D) linked by methine bridges to form a tetrapyrrole ring. Four methyl groups, two vinyl groups, and two proprionate side chains are attached.
- The iron atom at the center of the protoporphyrin is bonded to the four pyrrole atoms.
- Under normal conditions the iron is in the ferrous (Fe^{2+}) oxidation state. The iron atom can form two additional bonds, one on each side of the heme plane, called the fifth and sixth coordination sites.
- The fifth coordination site is covalently bound by the imidazole side chain of the globin chain (the "proximal histidine," α87 and β92).
- The sixth coordination site of the iron ion can bind O_2 or other gaseous ligands (CO, NO,
- CN^-, and H_2S

Role of distal histidine - 1 mark

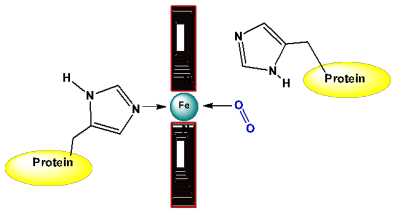
- Makes O_2 to bind in a bent fashion and makes it difficult for CO to bind in a linear fashion.



Fe^{2+} $t_{2g}^4e_g^2$, HIgh spin, radius 92 pm

Paramagnetic

Fe 42 pm outside porphyrin plane



Fe^{3+} $t_{2g}^5e_g^0$, Low spin, radius 75 pm

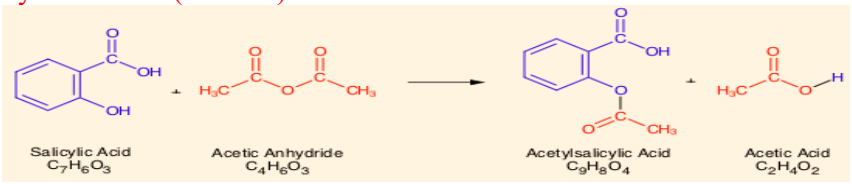
Diamagnetic

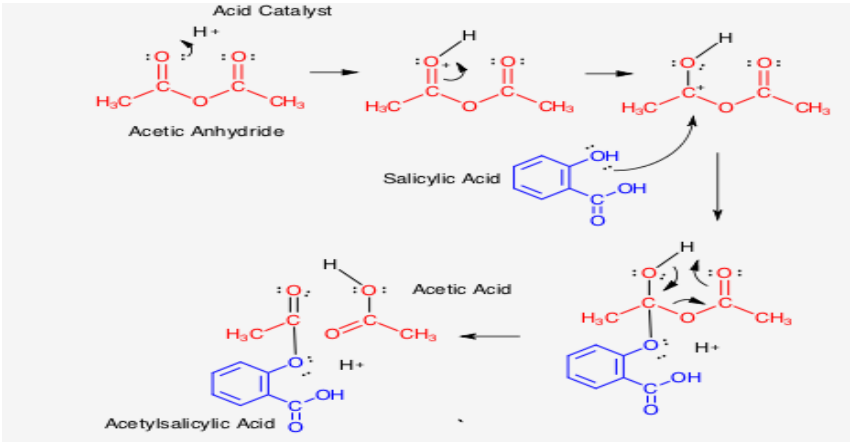
Fe fits inside the porphyrin plane

b) Identify the antipyretic drug which smells like vinegar and explain the synthesis of the drug with any two applications.

Aspirin (1 mark)

Synthesis (2 marks)





Applications (2 marks)

- Used as an inhibitor of cyclooxygenase, in the treatment of different types of headaches and to prevent venous and arterial thrombosis.
- Useful as an anti-inflammatory agent for long-term as well as acute inflammation; gained a reputation for treating cardiovascular and cancer.
- It is a first-line treatment for the fever and joint-pain symptoms of acute rheumatic fever and Kawasaki disease.
- Similarly, used as an intermediate and raw material in producing other medicines or chemical compounds like 4-hydroxycoumarin.