



2018 19 EVEN 18CYB101J CLA1 AK FN

Chemistry (SRM Institute of Science and Technology)



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**DEPARTMENT OF CHEMISTRY**  
**Faculty of Engineering and Technology**  
**SRMIST, Kattankulathur**  
**CLA –I Answer Key**

Program: B. Tech

Semester: II

Subject/Code: Chemistry/18CYB101J

Date : 09.02.2019

Time : 8.00-8.50am

Max Marks: 25 marks

**Part-A 3x4=12Marks****Answer any THREE Questions**

1. Write a note on angular wave function for hydrogen atom.

The angular parts of the wave function depend only on direction ( $\Phi$  and  $\Theta$ ) are independent of the value of principle quantum number ( $n$ ) and the distance from the radius ( $r$ ). Thus,  $A^2$  is the probability of finding an electron at a given direction  $\Phi$  and  $\Theta$  at any distance from the nucleus to infinity. They depend primarily on the values of  $l$ . For  $l = 0$ , i.e.  $s$  orbitals, the angular wave function is constant and independent of the angles  $\theta$  and  $\Phi$ . Therefore, this function will provide a sphere. Angular functions for some orbitals, [3 marks]

$s$ orbital	$p_z$ orbital	$d_{z^2}$
$\Theta\Phi = (1/4\pi)^{1/2}$	$\Theta\Phi = (3/4\pi)^{1/2} \cos\theta$	$\Theta\Phi = (5/16\pi)^{1/2} (3 \cos^2\theta - 1)$

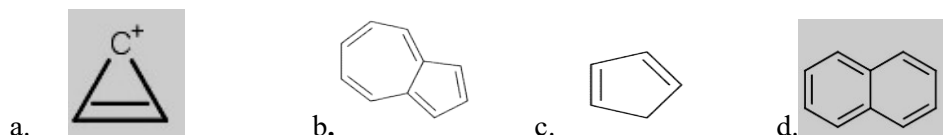
[1 mark]

2. Differentiate bonding and anti-bonding molecular orbital.

Any four of the following: [4 x1= 4marks]

S.No	Bonding Molecular Orbitals	Anti-bonding Molecular Orbitals
1.	They are a type of molecular orbitals that are involved in the formation of a chemical bond.	They are orbitals containing electrons outside the region between two atomic nuclei.
2.	Here the electron density in bonding molecular orbitals is higher	Here it is low
3.	The energy of bonding molecular orbital is lower comparatively.	The energy of antibonding molecular orbital is higher comparatively.
4.	Electrons in the bonding molecular orbital contribute to the formation of a bond.	The electrons in anti-bonding molecular orbitals do not contribute to the formation of the bond.
5.	The stability of bonding molecular orbitals is comparatively higher.	The stability of bonding molecular orbitals is comparatively lower.

3. Identify aromatic, non-aromatic and anti-aromatic compounds using Huckel's rule from the following:



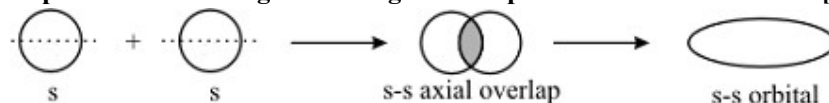
a. **Aromatic** [N.B: With  $n = 0$ , the Hückel value is 2. It has two pi electrons, hence only one double bond. It is an exception to the rule of conjugation; It is aromatic.]

b. **aromatic** c. **Non-aromatic** d. **aromatic**

4. Briefly explain the overlap of s-s orbitals taking an example.

**Overlapping between s-s orbital's of two similar or dissimilar atoms is known as s-s overlapping and forms a single covalent bond.** [1 mark]

**Explanation with diagram taking an example** [3 marks]



**Part-B**

**1x13=13Marks**

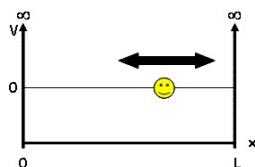
5. a. Solve Eigen value and Eigen function using Schrodinger equation for 1-D box.

[10 marks]

b. Write a note on the features of Molecular orbital theory.

[3 marks]

a. **Derivation using Schrodinger equation for solving Eigen value and function with diagram.** [9+1=10marks]



b. Any Three features.

[3 marks]

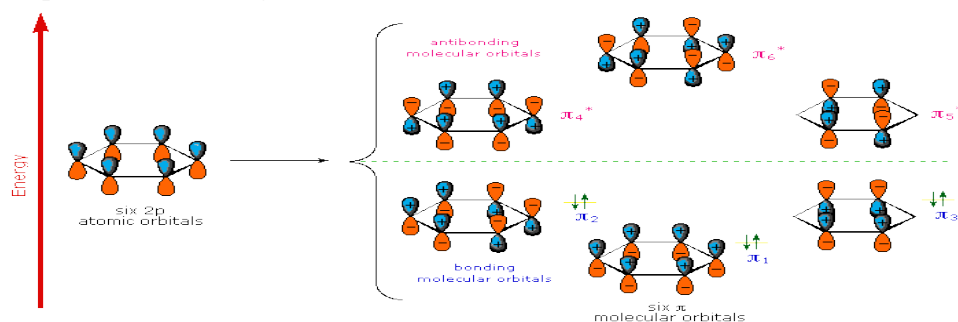
(OR)

6. Explain in detail the structure and molecular orbital picture of Benzene.

[13 marks]

**Explanation with diagram**

**[10+3=13 marks]**



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**Part-A            3x4=12Marks**

**Answer any THREE Questions**

1. What is Linear Combination of Atomic Orbitals (LCAO)? Give the wave function equations for the formation of molecular orbital by the combination of atomic orbitals?

A linear combination of atomic orbitals, or LCAO, is a quantum superposition of atomic orbitals and a technique for calculating molecular orbitals in quantum chemistry. [2 marks]

$$\psi_{(AB)} = N(c_1\psi_{(A)} + c_2\psi_{(B)})$$

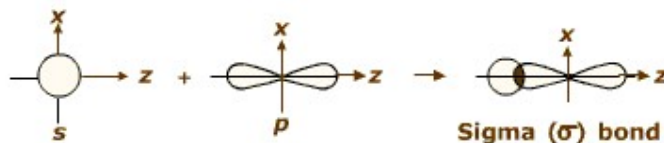
[2 marks]

Where  $\psi(A)$ ,  $\psi(B)$  are the wave function of atomic orbitals A and B and  $\psi(AB)$  is the wave function of molecular orbitals of the molecule AB. N, the normalization constant chosen to get the probability of finding an electron in a space is unity and  $c_1$  and  $c_2$  are constants for energy.

2. What is Huckel's rule for aromaticity? Explain with an example.  
 Huckel's rule states that, if a cyclic, planar molecule has  $4n+2 \pi$  electrons ( $n=0$  or any positive integer), and also fully conjugated it is considered to be aromatic. [2 marks]

Explanation taking an example. [2 marks]

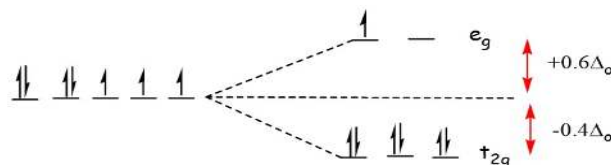
3. Explain the overlap of s-p orbitals with an example.  
 Overlapping between s- and p-orbital's is known as s-p overlapping forming sigma bond.



[2 marks]

Explanation taking an example. [2 marks]

4. Calculate **CFSE** in terms of **Dq** for low spin octahedral complexes having **d<sup>7</sup>** configuration.



Normally, there are two paired electrons in degeneracy state. But in the presence of strong field, the low spin complex has only one unpaired electron in  $e_g$  level, as one electron from  $e_g$  level would have paired with  $t_{2g}$  single electron. Hence only one pairing has occurred. [2 marks]

$$\text{CFSE} = (-0.4 \times 6) + (0.6 \times 1) + 1P$$

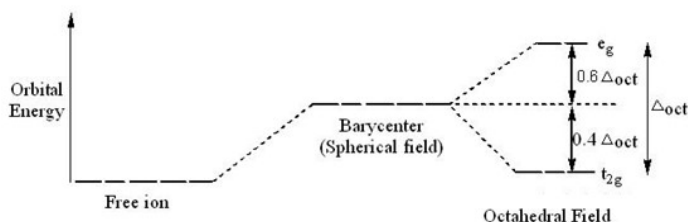
$$= -1.8 \Delta_o + 1P \text{ (or) in terms of } Dq \text{ it is } -18 Dq + 1P$$

[2 marks]

### Part-B

1x13=13Marks

5. a. Discuss on crystal field splitting of octahedral complexes with suitable diagram. [10 marks]  
 b. Differentiate anti-aromatic and non-aromatic compounds with an example for each. [3 marks]  
 a. Explanation with a diagram. [8+2=10 marks]



- b. Any two differences with an example for each.

[1.5x2=3 marks]

(OR)

6. a. Explain Heisenberg uncertainty principle. [5 marks]  
 b. Discuss on the salient features of crystal field theory. [8 marks]  
 a. The Heisenberg uncertainty principle states that, it's impossible to determine simultaneously with high precision for both momentum and position for a subatomic particle like electron. The product of the uncertainties in the position and the momentum of a particle equals  $h/(4\pi)$  or more.  
 $\Delta x \cdot \Delta p \geq h/(4\pi)$ ;  $\Delta x$  = uncertainty in position and  $\Delta p$  is uncertainty in momentum. [2 marks]

Explanation.

[3 marks]

- b. Salient features - Any four points.

[4x2 = 8 marks]