MAY 2016 **P/ID 40129/PCHJ**

Time : Three hours Maximum : 100 marks

PART A — (10 × 2 = 20 marks)

Answer ALL questions.

1. What is meant by Born-Oppenheimer approximation?

2. Write the Huckel secular determinant for butadiene.

3. What is the relationship between forces and fluxes?

4. Calculate the ionic strength of 0.2 M $BaCl_2$ solution.

5. What types of molecules give vibrational spectra?

6. Write down selection rules for vibrational transition of anharmonic oscillator.

7. What is meant by spin-spin coupling?

8. How many kinds of protons are there in

   (a) $(CH_3)_2CHCH_2CH_3$

   (b) $C_6H_5CH_3$?

9. Give the values of L and S in the ^3D state.

10. State Franck-Condon principle.

PART B — (4 × 20 = 80 marks)

Answer ALL questions.

11. (a) (i) Outline the salient features of the HF-SCF theory for solving wave equation for many electron system. (10)

(ii) Set up the Huckel determinant for benzene and solve it for eigen function and eigen value. (10)

Or

(b) (i) Using the Variation method solve the Schrodinger wave equation for the ground state of helium atom. (10)

(ii) Discuss the R-S coupling. (10)

12. (a) (i) Discuss the electrokinetic effects. (10)

(ii) Explain the Guoy-Chapmann model of electrical double layer. (10)

Or

(b) (i) Discuss the Debye-Huckel theory of strong electrolytes. (10)

(ii) Discuss the Electrode-Electrolyte interface. (10)

13. (a) (i) What are P, Q and R branches of rotation, vibration spectrum? (10)

(ii) Explain with mathematical equations the type of pure rotational Raman spectrum expected for diatomic molecule. (10)

Or

(b) (i) Derive an expression for the frequency and wave number of lines in the rotational spectrum. (10)

(ii) Discuss the solvent effect on $\pi \rightarrow \pi^*$ transition and $n \rightarrow \pi^*$ transition in electronic spectra. (10)

14. (a) (i) What is meant by chemical shift? What are the factors which will affect the chemical shift? (10)

(ii) Discuss the applications of ^{31}P NMR spectroscopy. (10)

Or

(b) (i) Discuss the Fourier transformation resonance spectroscopy. (10)

(ii) Discuss the NMR simple AX and AMX type molecules. (10)

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