M. Sc. Physics Examination, 2022

(3rd Year, 2nd Semester)

Atomic, Molecular and Optical Physics

Paper – 413

Time : Two hours   Full Marks : 40

Answer *any four* questions.

1. a) What is 'LCAO' approximation? What are the necessary conditions to be satisfied by the contributing atomic orbitals to generate an effective molecular orbital?

   b) From molecular orbital theory, obtain the expressions for normalized wavefunctions associated with the bonding and antibonding orbitals of H_2^+ molecule. Hence deduce the expression of their corresponding energy eigen values in terms of Coulomb, Exchange and Overlap integrals. What are the physical significances of bonding and antibonding orbitals?   1+2+2+4+1

2. a) What information you need to form Déslandres table? Why is it so useful in molecular spectroscopy?

   b) Discuss in brief the gain-guided and index-guided semiconductor double heterostructure laser.

   c) Discuss the selection rules for electronic transitions.
                                        3+4+3

[Turn over

3. a) Obtain the expressions for the '*S*' and '*O*' branches associated with the rotational fine structures in the vibrational Raman spectrum of a simple diatomic molecule in gas phase. Comment on the relative intensities of Raman lines belonging to the above referred '*S*' and '*O*' branches.

   b) For H_2 molecule, the spacing between the '*S*'-branch lines in the Raman spectrum is 243.2 cm^{-1}. Estimate the bond length of the molecule.   3+3+1+3

4. a) Discuss the basic principle of holography.

   b) In the rotational fine structure of electronic vibration spectra, in certain molecules the band head appears at the violet side of the spectrum and in some molecules it appears at the red side – Explain.

   c) Discuss the role of Franck-Condon principle in connection with intensity of vibrational electronic spectral lines.   4+3+3

5. a) What do you mean by the terms 'symmetry element' and 'symmetry operation' in the context of molecular symmetry.

   b) How many symmetry elements are present in a H_2O molecule? What is its point group? Establish its character table. [Consequences of the 'Great Orthogonality Theorem' may be used without formal

deduction]. Hence show from atomic displacement diagrams that both the 'symmetric stretching' and '*in-plane bending*' modes of H_2O molecule are represented by 'A_1' irreducible representation. Are these vibrations polarized in the Raman spectrum of H_2O molecule?   2+1+1+3+2+1

6. a) Deduce the expression for the difference of *Band head* and *Band origin* in connection with Fortrat parabolae. Also mention its significance.

   b) Explain the lasing action that takes place in neodymium lasers with the help of necessary energy level diagram.

   c) Briefly discuss the applications of holography.
          3+4+3