b) Using the Great Orthogonality Theorem prove that the Vectors whose components are the characters of two different Irreducible Representations are orthogonal. 3

9. Mention the Schoenflies Symbol of Cube. Identify all symmetry operations and the Stereogram. Why cube is a Platonic Solid ? 5

10. a) Defive Projection Operation assuming a set of orthonormal functions. $2\frac{1}{2}$

b) Find out the SALCs for hydrogen 1s orbitals in H_2O. $2\frac{1}{2}$

M. Sc. Chemistry Examination, 2019

(1st Semester)

Theoretical Chemistry

Paper - I

Time : Two hours Full Marks : 50

(25 marks for each unit)

Use a separate answerscript for each unit.

UNIT - 1011

1. Answer ***any two*** : 3×2

a) Prove that a projection operator, $\hat{P}_i = |\phi_i><\phi_i|$ is a hermitian operator.

b) Determine the eigenvalue of the commutator $[\hat{p}, \hat{q}]$, where $\hat{p}$ and $\hat{q}$ represent the momentum and co-ordinate operators.

c) Show that the spherical harmonics $Y_{l,\, m_l}(\theta, \phi)$ are eigenfunctions of $(\widehat{l_x 2} + \widehat{l_y 2})$. Evaluate the eigenvalues.

2. What are stationary states ? Show that a quantum mechanical system which does not experience any time-dependent external force, the wavefunction $\psi(x, t)$ remains stationary. 7

3. Answer ***any one*** : 6

a) A step-up angular momentum operator $(\hat{l}_+)$ is defined as follows.

$$\hat{l}_+ Y_{l,m_l} = C\, Y_{l,m_l+1}$$

Using the properties of angular momentum operators and spherical harmonics, find out the expression of C in terms of quantum numbers l and m_l.

b) Find out the expressions of quantum mechanical average values of x^2 and p_x^2 for the first excited state of one dimensional Harmonic Oscillator and show that it supports Heisenberg Uncertainty principle.

4. a) Construct the singlet excited state wavefunction of $He(1s^1 2s^1)$ in the form of a Slater Determinant. $1\frac{1}{2}$

b) Apply ladder operators for the spin of an electron to construct Pauli spin matrices : $\mathbf{S}_x$ and $\mathbf{S}_y$. 2

c) For n numbers of indistinguishable microscopic particles, it is required that the wavefunctions must be either symmetric or antisymmetric with respect to every possible interchange of two particles - Justify the statement. $2\frac{1}{2}$

UNIT - 1012

Answer ***any five*** questions

5. a) 'Wave functions serve as bases of irreducible representation' - prove it considering three sets of p-wave functions of central nitrogen atom in NH_3 $2\frac{1}{2}$

b) Prove that the representation of a direct product Γ_{AB}, will contain the totally symmetric representation only if the irreducible Γ_A = the irreducible Γ_B. $2\frac{1}{2}$

6. a) Prove that $a_i = 1/h[\Sigma\chi(R)\chi_i(R)]$ (symbols have usual meanings). 3

b) In NH_3 molecule all three σ_vs are equivalent whereas in H_2O molecule, two σ_vs are different. - Explain 2

7. a) What is meant by character of a Representation ? Why is it preferred to describe a Representation than the matrices constituting the Representation ? 3

b) Find out the matrix Representation for $C_3(Z)$ symmetry element. 2

8. a) State the Great Orthogonality Theorem and meaning of the symbols. 2