Roll No. : .....

Total No. of Questions : **11**] [Total No. of Printed Pages : **3**

BPF–2205

M.Sc. (Final) Examination, 2022

CHEMISTRY

Paper - IX (B)

Group–C **(CH–508)**

(Computational Chemistry)

*Time : **3** Hours*] [*Maximum Marks : **75***

Section–A **(Marks : 2 × 10 = 20)**

Note :– Answer all *ten* questions (Answer limit **50** words). Each question carries **2** marks.

Section–B **(Marks : 5 × 5 = 25)**

Note :– Answer all *five* questions. Each question has internal choice (Answer limit **200** words). Each question carries **5** marks.

Section–C **(Marks : 10 × 3 = 30)**

Note :– Answer any *three* questions out of five (Answer limit **500** words). Each question carries **10** marks.

Section–A 2 each

1. Attempt all *ten* questions. Answer should not exceed **50** words in each question :

   (i) Define Jacobi method for eigenvalues.

   (ii) What is Newton–Cotes Formulae ?

(iii) What do you know about CHARAM ?

(iv) What is QUANTA ?

(v) Define pH Titration.

(vi) What is Radioactive Decay ?

(vii) Define Slateer–Condon rules.

(viii) Define Gaussian basis sets.

(ix) What is ZDO Approximation ?

(x) Describe treatment of CNDO theory.

Section–B 5 each

Note :– Answer all *five* questions. Each question has internal choice. Answer limit **200** words.

2. Describe about Newton–Raphson method.

Or

Describe differential equation of solutions by Taylor Series.

3. What is benefits of AMBER software package in Quantum Chemistry ?

Or

Give a short note on MOPAC.

4. Describe evaluation of Lattice energy and ionic radii from experimental data.

Or

Discuss linear regression.

5. Describe Born–Oppenheimer Approximation.

Or

Discuss Hartree-Fock equation.

6. Discuss PPP treatment.

Or

Discuss treatment of INDO theory.

Section–C

10 each

Note :– Attempt any *three* questions out of five. Answer limit **500** words.

7. Explain about advanced programming features of FORTRAN/C.

8. Explain software package 'GAUSSIAN and GAMESS'.

9. Explain about elementary structural features such as bond length, bond angle and dihedral angle of molecules extracted from Cambridge data base.

10. Explain MC-SCF method.

11. Explain derivation of Hohenberg-Kohn theorem.