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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: $2 \times 10 = 20$)

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

Section–B (Marks: $5 \times 5 = 25$)

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

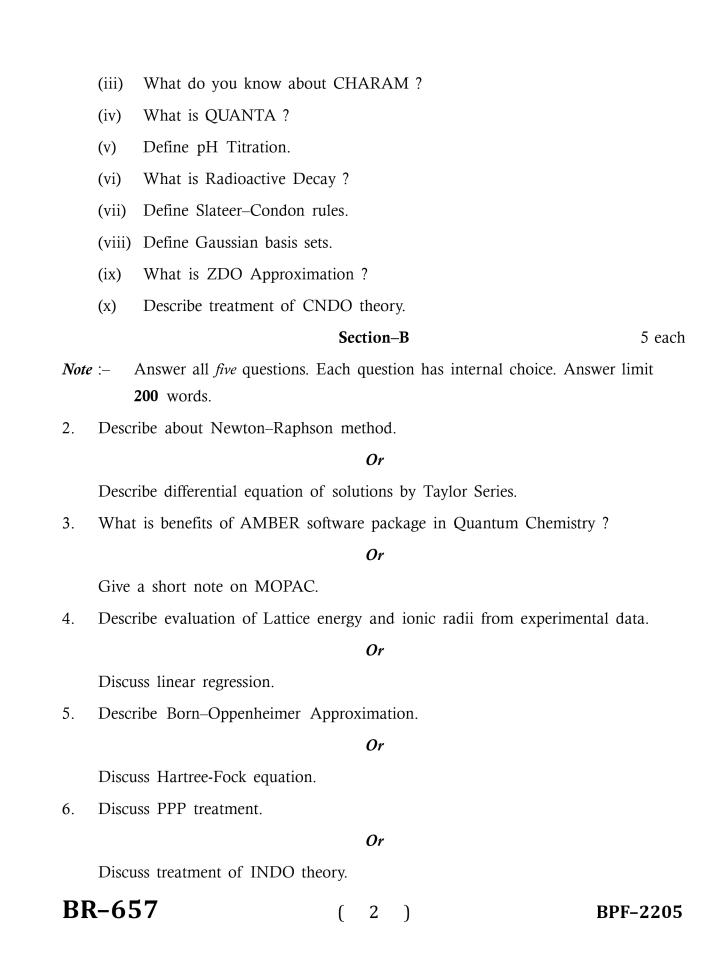
Section–C (Marks: $10 \times 3 = 30$)

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?

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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.