

Roll No :

Total No. of Questions : 11]

[Total No. of Printed Pages : 3

SP-684

M.Sc. (Final) Examination, 2021

CHEMISTRY

Paper - IX (B) Group-C

CH-508

(Computational Chemistry)

Time : 1½ Hours]

[Maximum Marks : 75

Section-A

(Marks : 2 × 10 = 20)

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

(खण्ड-अ)

(अंक : 2 × 10 = 20)

नोट :- सभी दस प्रश्नों के उत्तर दीजिए (उत्तर-सीमा 50 शब्द)। प्रत्येक प्रश्न 2 अंक का है।

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.

(खण्ड-ब)

(अंक : 5 × 5 = 25)

नोट :- सभी पाँच प्रश्नों के उत्तर दीजिए। प्रत्येक प्रश्न में विकल्प का चयन कीजिए (उत्तर-सीमा 200 शब्द)। प्रत्येक प्रश्न 5 अंक का है।

Section-C

(Marks : 10 × 3 = 30)

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

(खण्ड-स)

(अंक : 10 × 3 = 30)

नोट :- पाँच में से किन्हीं तीन प्रश्नों के उत्तर दीजिए। (उत्तर-सीमा 500 शब्द)। प्रत्येक प्रश्न 10 अंक का है।

BI-325

(1)

SP-684 P.T.O.

Section–A

2 each

1. Attempt all *ten* question. Answers should not exceed **50** words in each question.
- (i) Define Gaussian-elimination.
 - (ii) Define Jacobi method for eigen values.
 - (iii) What is Dynamic packages ?
 - (iv) What do you know about AMBER ?
 - (v) Describe Numerical Integration.
 - (vi) What do you understand by Evaluation of lattice energy ?
 - (vii) Define Gaussian basis sets.
 - (viii) Define Born-Oppenheimer approximations.
 - (ix) What is PPP treatment ?
 - (x) Describe treatment of INDO theory.

Section–B

5 each

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

2. Describe about Newton-Cotes formulae.

Or

What is Pivoting Strategy ?

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

Or

Give a short note on CHARMM modeling software.

4. Discuss linear regression.

Or

Describe linear simultaneous equations to solve secular equations with in the Huckel theory.

5. Explain Slater-Codon rule.

Or

Discuss Koopmans and Brillouin theories.

6. Discuss ZDO approximation.

Or

Discuss treatment of CNDO theory.

Section–C

10 each

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

7. Explain about advanced programming features of FORTRAN/C.
8. Explain basic ideas on structure activity relating drug and catalysis design.
9. Explain about elementary structural features such as bond length, bond angle and dihedral angles of molecules extracted from Cambridge data base.
10. Explain about configuration interaction.
11. Explain about treatment of chemical concepts with the density functional theory.