

Roll No. :

Total No. of Questions : 11]

[Total No. of Printed Pages : 3

BFMS-429

M.Sc. (Final) Examination, 2023

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.

BRI-741

(1)

BFMS-429 P.T.O.

Section–A

1. (i) Define Jacobi methods for eigen values.
- (ii) Define Interpolation.
- (iii) What do you know about AMBER ?
- (iv) On which approximation GAUSSIAN is based ?
- (v) What do you mean by radioactive decay ?
- (vi) What do you mean by lattice energy ?
- (vii) On which principle CI method is based ?
- (viii) Define Born-Oppenheimer approximations.
- (ix) Describe treatment of INDO theory.
- (x) What is EHT treatment ?

Section–B

2. Define Gauss-Jordan method for LSE.

Or

What is Pivoting Strategy ?

3. What benefits of CHARAM software package in Quantum Chemistry ?

Or

Give a short note on QUANTA.

4. Explain Linear simultaneous equation.

Or

Discuss numerical Integration.

5. Explain Koopmans Theory.

Or

Describe Slater-Codon rule.

6. Explain ZDO approximation.

Or

Write a short note on AMI.

Section-C

7. Write a short note on solution of simple differential equation by Runge-Kutta method.

8. Explain software package 'MM2 and MOPAC'. 5+5=10

9. Explain Computer Application on Chemistry.

10. Explain the following :

(i) Hartree-Fock theory

(ii) Gaussian basis sets 5+5=10

11. Write short notes on the following :

(i) Derivation of Hohenberg-Kohn theorem

(ii) Kohn Sham formulation 7+3=10