



BBX-2051

Seat No. _____

M. Sc. (Sem. - IV) Examination

March/April - 2014

Organic Chemistry : CHN - 701 (O)

Time : 3 Hours]

[Total Marks : 70

1 Answer any three : 14

- (a) Write a note on classification of natural carbohydrates. Give their examples.
- (b) Give the details of mutarotation.
- (c) What is prebiotic chemistry? Discuss the role of carbohydrates in the prebiotic system.
- (d) Give the classification and differences of nucleic acids. Give one method of synthesis of thymine.
- (e) Explain general methods of structure determination of nucleosides.
- (f) Describe properties and reactions of uric acid.

2 Answer any three : 14

- (a) Discuss the conformations of cyclopropane and its derivatives.
- (b) Draw and describe different conformers of 1,2,3,4,5,6 hexa chloro cyclo hexane. Which conformer(s) possess optical activity?

BBX-2051]

1

[Contd..

- 5 Answer any seven in brief : 14
- How can the conversion of oestrone into oestradiol be done ?
 - Explain the helical structure of DNA.
- 4 Answer any three : 14
- Explain the DQF ^1H - ^1H cosy spectra of iphenol
 - Discuss the ^1H - ^{13}C heteronuclear correlation spectrum.
 - Describe the TOCSY spectrum of β -lactose.
 - Write a note on NMR shift reagents
 - Write on any one of the following nuclear over hauser effect.
 - ^1H NMR NOE
 - ^{13}C NMR NOE
- 3 Answer any three : 14
- Give synthesis of progesterone from diosgenin
 - Give synthesis of cortisone.
 - Discuss the structure elucidation of oestrone
 - Describe the general biosynthesis of steroids.
 - Prove the structure of lanosterol
- 6 Give conformational analysis of cyclohexane-pentane and bicyclo (2,1,1) hexane
- Give conformational analysis of cyclohexanone and 2 bromo cyclohexanone
 - Discuss the conformational analysis of cyclohexane-1,2 dicarboxylic acid. Illustrate how chemical methods are useful for finding preferred conformation.

- (c) Give the definition of steroid
- (d) Draw one enantiomeric pair of 1,3 di methyl cyclohexane.
- (e) What are atrop isomers?
- (f) What is the meaning of correlation spectroscopy?
- (g) Give the full form of INADEQUATE. What is it?
- (h) What is spin decoupling?
- (i) Discuss the α alkyl ketone effect for cyclohexanone for methyl and isopropyl groups.
- (j) What is A-T and G-C pair in nucleic acids?



BBX-2052

Seat No. _____

M. Sc. (Sem. IV) Examination

April/May - 2014

CHN-701(I) Inorganic Chemistry : Paper - I

Time : 3 Hours]

[Total Marks : 70

Instruction : All questions carry equal marks.

1 Answer any two of the following questions : 14

- (1) Explain - Photochemical law.
- (2) Discuss the photo redox reactions.
- (3) Explain the major photochemical reactions of Cs (III) complexes.

2 Answer any two of the following questions : 14

- (1) Give the application of Mass Spectroscopy in inorganic chemistry.
- (2) How can one identify various isotopes in mass spectroscopy ?
- (3) Discuss the instrumental part of mass spectroscopy.

BBX-2052]

1

[Contd....

- 5 Answer any seven of the following questions : 14
- (1) Define Mass Spectroscopy.
 - (2) What is CMA ?
 - (3) Relaxation of Auger emission.
 - (4) What is absorbance and absorptivity ?
 - (5) What is quantum yield ?
 - (6) Give the full form of EXAFS and ESCA.
 - (7) Write the photochemical reaction of Mn^{+2} .
 - (8) What is fluorescence.
 - (9) Define stern volumes plots.
 - (10) Explain STM.
- 4 Answer the following questions : (any three) 14
- (1) Discuss the principle of AFM.
 - (2) Discuss the basic principle of Luminescence.
 - (3) Discuss the effect of pH on luminescence.
 - (4) Discuss the principle of STM.
- 3 Answer any three of the following questions : 14
- (1) Discuss application of AES.
 - (2) Discuss Instrument of AES.
 - (3) Discuss the Koopman's theorem.
 - (4) Draw the flow chart of EXAFS spectroscopy.



BBX-2061

Seat No. _____

M. Sc. (Sem. - IV) Examination

April/May - 2014

CHN - 702 (P) : Physical Chemistry

Time : 3 Hours] [Total Marks : 70

1 Give answer any two : 14

(i) Explain the resonance effect may be generated by a substituent on a reaction site.

(ii) Write a short note : Transition state theory.

(iii) Discuss the Hammond Postulate.

(iv) Explain the Taft model.

2 Give answer any two : 14

(i) What is the condition of the Proton in solution ?

(ii) Derive the equation

$$v = \left[C \cdot \frac{h}{kT} \cdot e^{-\Delta G^\ddagger / RT} \right] \cdot e^{-z \cdot F \cdot \Delta \phi / RT}$$

(iii) Calculate the ionic mobilities of K⁺ and OH⁻ ions at infinite dilution.

$$\lambda_{K^+}^\circ = 73.65 \times 10^{-4} \text{ S m}^2 \text{ mol}^{-1}$$

$$\lambda_{OH^-}^\circ = 197.6 \times 10^{-4} \text{ S m}^2 \text{ mol}^{-1}$$

(iv) Write a short note : Fused-oxide systems in Metallurgy.

BBX-2061]

1

[Contd...

- 3 Give answers any two :
- (i) Discuss the following parameters of scales based on spectroscopic properties
 - (A) S-parameter
 - (B) $X_B \cdot X_R$ Scales
 - (C) Er-Parameter
 - (ii) Explain the qualitative understanding of solvent solute effect on reactivity.
 - (iii) Write a short note : Multiparameter solvation analysis.
 - (iv) Write a use of solvation scales in mechanistic studies.
- 14
- 4 Give answers any two :
- (i) Derive the polarography wave equation.
 - (ii) How chronopotentiometry is different from ordinary potentiometry ?
 - (iii) Why the cyclic voltammetry is highly applicable for redox titration ?
 - (iv) Write basic principle, instrumentation and application of Amperometry.
- 14
- 5 Give answer any seven :
- (i) Discuss the existence of the H_3O^+ from the point of view of Proton Mobility.
 - (ii) Explain the relationships between empirical solvation scales.
 - (iii) Explain the heat capacity of activation.
 - (iv) Explain the LFER.
 - (v) Explain the importance of DME.
 - (vi) Write the basic principle of capillary electrophoresis.
 - (vii) Explain the electricity storage density.
 - (viii) Explain the effects of solvation on reaction rates.
 - (ix) Explain the principles of reactivity.
 - (x) Write an application of cyclic voltammetry.



BBX-2059

Seat No. _____

M. Sc. (Sem. IV) Examination

April/May - 2014

CHN-702(O) Organic Chemistry : Paper - II

Time : 3 Hours]

[Total Marks : 70

Instruction : All questions carry equal marks.

1 Answer any three :

- (1) Give the name of various processes of distillation of petroleum and give an account on any one.
- (2) Write a note on C_2 chemicals.
- (3) Write a note on polyester fibers.
- (4) Give an account on Aromatic Chemicals
- (5) Explain the process of refining of crude oil

2

Answer any three :

- (1) Write a note on classification of paints and give their examples
- (2) Write a note on manufacture of varnish.
- (3) What are propellants?
- (4) What are military explosives?
- (5) Write a note on toxic chemical agents.

3

Answer any three :

- (1) What are Resins? Give production and uses of polymethyl methacrylate.
- (2) Give the difference of Nylon6 and Nylon6,6. Give the manufacture and uses of Nylon6,6.
- (3) Give a detail account of co-polymers of ethylene
- (4) Explain cross linking in polymer with illustrations.

BBX-2059]

1

[Contd....

- Answer any three :
- (1) Discuss the small scale manufacture of writing ink.
 - (2) Discuss the small scale manufacture of Agarbittis and phenyl dis-infectant.
 - (3) Write small scale manufacture of naphthalene balls and wax candles.
 - (4) How can you remove different stains from clothes
 - (5) Discuss the small scale manufacture of safety matches.
- Answer any seven :
- (1) What is cordite? Explain
 - (2) What is gun powder?
 - (3) What are the uses of Teflon
 - (4) Give one example of cyclization reaction to prepare a polymer
 - (5) Give the differences of thermo plastic and thermo setting.
 - (6) What are live polymers?
 - (7) What is kieselghur and gumtragacanth ?
 - (8) Give the structure and industrial uses of cumine and di iso butylene.
 - (9) Write the names of different classes of coal
 - (10) What is coke own gas and how light oil can be prepared on it.
 - (11) Name any three pigments having blue color.
 - (12) Which are different types of detergants?



BBX-2060

Seat No. _____

M. Sc. (Sem. IV) Examination

March / April - 2014

CHN-702(D) : Inorganic Chemistry : Paper-II

Time : 3 Hours]

[Total Marks : 70

Instruction : All questions carry equal marks.

1 Answer any two of the following questions : 14

(i) Write a short note on Boron Nitride.

(ii) Explain the compounds of substituted

Borazines.

(ii) Discuss the Boro Phosphate glass.

2 Answer any two of the following questions : 14

(i) Discuss the uses of Inorganic Polymers.

(ii) Explain the synthesis of co-ordination polymers.

(iii) Give the difference between Organic and

Inorganic Polymers.

BBX-2060]

1

[Contd....

- 3 Answer any two of the following questions : 14
- (i) Give the applications of IR spectra for the establishment of stereochemistry of different compounds of various co-ordination numbers.
 - (ii) Explain the Bonding and Electronic Structure of the compounds of co-ordination number 9 according to stereochemistry.
 - (iii) Discuss the stereochemistry of the compounds of co-ordination number-2.
- 4 Answer any two of the following questions : 14
- (i) Prove the structures of B_5H_9 and $B_{10}H_{14}$ by using balance equation.
 - (ii) Explain the bridge Structure of B_2H_6 (Diborane).
 - (iii) Discuss the synthesis of various Boranes.
- 5 Answer any seven of the following questions : 14
- (i) Define Boroxine.
 - (ii) Give the definition of Chelate Polymers.
 - (iii) Why Boron Hydrides are electron deficient compounds?
 - (iv) What is silicon resin?
 - (v) Give the structure of B_4H_{10} and $B_{10}H_{14}$.
 - (vi) What is unusual co-ordination number?

-
- (vii) Draw the structure of Boron nitride.
- (viii) Give two uses of Borophosphate glass.
- (ix) Why BH_3 does not exist?
- (x) Why Boron shows similarity with silicon?



BBX-2067-68-69-70-71 Seat No. _____

M. Sc. (Sem. - IV) Examination

April/May - 2014

(1) CHN - 703 (O) : Chemistry : Paper - III

(CC) (Organic)

(2) CHN - 703 (I) : Inorganic Chemistry

(Corrosion)

(3) CHN - 703 (P) : Physical Chemistry :

Paper - I

(4) CHN - 703 (I) : Inorganic Chemistry :

Paper - II

(5) CHN - 703 (I) : Inorganic Chemistry :

Paper - III

(Corrosion) (New Course)

Time : 3 Hours] [Total Marks : 70

(1) CHN - 703 (O) : Chemistry : Paper - III

(Organic)

Instructions : (1) All questions are compulsory. (2) Digits of the right indicate full marks (3) Start a new question from a new page.

1 (a) Answer any three of the following questions: 9

(1) Explain the life cycles of malarial parasites. (2) Give synthesis of 8-aminoquinolines and 9-aminoquinolines.

(3) Write a note on antiameobic drugs. (4) Write a brief account on antifungal drugs.

(b) Answer any one of the following questions 5 (1) How drugs are classified? Write note on antitubercular drugs.

(2) Write a note on antileprotic drugs.

BBX-2067-68-69-70-71] 1 [Contd...

2 (a) Attempt any three questions from the following : 9

(1) Give an account of antidepressant drugs.

(2) What are anti-anxiety drugs?

(3) What are sedatives? Explain their chemical structure and activity.

(4) Give the structures of antipsychotics.

(b) Attempt any one of the following questions 5

(1) Write a note on anticonvulsants.

(2) How anesthetics are classified? Give an account on general anesthetics.

3 Answer any two of the following questions: 14

(1) Give the synthesis of any two diuretics.

(2) Write a note on cardiac drugs.

(3) Name the different drugs acting on Renal system with their mode of action.

4 Answer any two of the following questions: 14

(1) Define and classify antidiabetics with one example of each.

(2) Write a note on hypertensive drugs.

(3) Define and classify types of cancer. Write a note on anticancer drugs.

5 Answer any seven of the following questions. 14

- (1) Give the structure of diaminopyrimidines and mention effective functional group.
- (2) Define chemotherapeutic drugs.
- (3) What are Psychopharmacological agents?
- (4) Draw structures of any two gaseous general anesthetics.

(5) Give synthesis of any one antileprotic drug.

(6) What are calcium channel blockers?

(7) Explain life cycle of virus.

(8) Write full forms of AIDS and HIV.

(9) Give the structure of Nitrogen mustards and mention effective functional groups.

(10) Compare the structure of PAS (Pamino Salicylic Acid) and PABA (a-aminobenzoic acid) according to their functional groups.

(2) CHN - 703 (I) : Inorganic Chemistry

1 Answer any two:

- (1) Discuss the effect of pH on corrosion.
- (2) Discuss the corrosion of varieties of Iron steel.
- (3) Describe the effect of dissolved oxygen on corrosion.
- (4) Write a short note on "Heat treatment".

BBX-2067-68-69-70-71]

3

[Contd...

2 Answer any two:

(1) Discuss the theories of Passivity and Mechanism of Passivation.

(2) Explain the theory of Vapor-phase Inhibitors.

(3) Discuss the Application of Passivators.

(4) Write a short note on "Packing inhibitors".

3 Answer any two:

(1) Write a short note on: "Methods of cathodic protection"

(2) Discuss about sacrificial anode.

(3) Write a short note on Anodic protection.

(4) Explain the theory of cathodic protection.

Answer any two :

4 (1) Discuss the methods of application of coating

(2) Explain the classification of cation.

(3) Write a note on Incejel.

(4) Discuss the Alloying on Monel Metal.



5 Answer any two:

(1) Discuss the Aqueous environment affecting on the corrosion of steel.

(2) Write short note on "slushing compound"

(3) Discuss the alloying for corrosion resistance on Hastalloy.

(4) Explain the organic cation for corrosion resistance.

Instruction : Figures to the right indicate full marks.

- 1 (a) Answer any two of the following : 10
- (i) What is meant by retrosynthetic analysis ?
 - (ii) Explain synthetic equivalent with example.
 - (iii) What is reversal polarity ? Discuss the use of 1,3-dithiones as umpolung reagent.
 - (iv) Discuss the protection of amine giving suitable example.
 - (v) Discuss the use of cyclic and acyclic acetals and ketals for protecting carbonyl group.
- (b) Answer any two of the following : 6
- (i) Give an account of cyclisation reactions.
 - (ii) Giving example discuss any two methods for protecting carboxyl group.
 - (iii) How would you involve FGI to convert nitro group to keto group ?
 - (iv) Explain chemoselectivity in two group C-X disconnection.
- (c) Answer any two of the following : 4
- (i) What is stereoelectronic effect ?
 - (ii) Give names of protecting groups for mono alcohols 1,2 and 1,3-diols.
 - (iii) Discuss intramolecular and intermolecular reaction giving suitable example.
 - (iv) Give application of aliphatic nitro group in organic synthesis.

2 (a) Answer any two of the following : 10

(i) Discuss regioselectivity in Michael addition reaction.

(ii) Explain the disconnection approach to α,β -unsaturated carbonyl compounds.

(iii) Give the retrosynthesis of camphor.

(iv) Discuss the use of acetylene in organic synthesis.

(b) Answer any two of the following : 6

(i) Discuss retrosynthesis of cortisone.

(ii) Discuss disconnection approach to Diels Alder reaction.

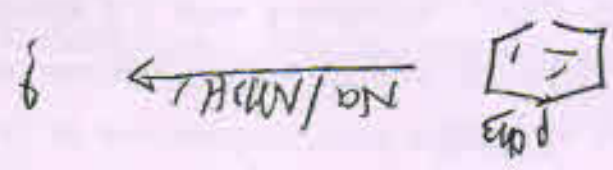
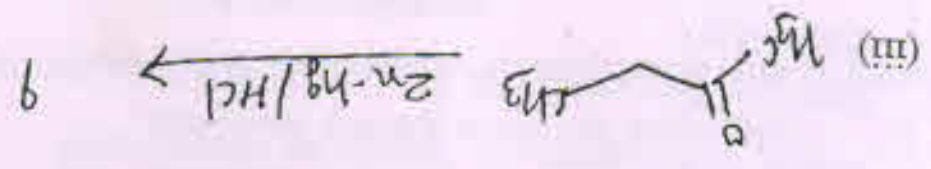
(iii) Illustrate a synthetic reaction using ketene as an intermediate.

(iv) Discuss the application of Bishler-Napieraski reaction in synthesis of heterocycles.

(c) Answer any two of the following : 4

(i) How oxirane is synthesized ? Explain giving one example.

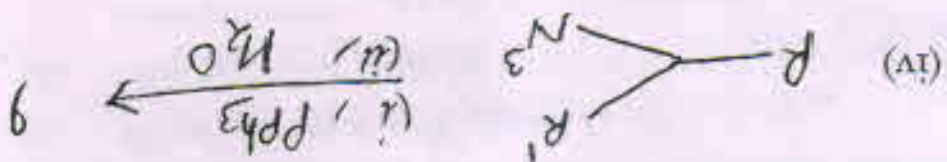
(ii) Give the end product with mechanism.



- 1 Answer any two in detail : 10
- (a) Give an account on applications of ferrous and nonferrous alloys.
 (b) Describe refractory materials w.r.t. their production.
 (c) Discuss properties of various steels.
 (d) Enlist uses of different glasses.

(3) CHN - 704 (C) : Chemistry Of Materials

- 3 Answer any five of the following : 10
- (i) Give one use of FMOC and THP.
 (ii) Give two examples of illogical electrophile.
 (iii) Give one application of Trityl group.
 (iv) Give examples of internal Claisen condensation.
 (v) How can you convert alcohol in to alkyl halide ?
 (vi) Give structure of equivalent synthon for CH_3CO^+ .
 (vii) Give application of Grignard reagent in disconnection of carboxylic acid.
 (viii) What is Frankland reagent.
 (ix) Write name of BOC and CB2 protecting group.
 (x) Discuss N-oxide as protecting group.



- 2 Answer any two in detail : 10
- (a) What is photolithography ?
- (b) Distinguish clearly between nematic and smectic mesophases.
- (c) Which are chemical methods of preparation of thin films ?
- (d) Discuss lyotropic phases in liquid crystals.
- 3 Answer any two in detail : 10
- (a) Give an account on conducting polymers.
- (b) Write a note on superionic conductors.
- (c) What are perovskites ?
- (d) Discuss crystallinity in polymers.
- (e) Classify ionic conductors.
- 4 Answer any two in detail : 10
- (a) Give an account on transistor materials.
- (b) Write a note on organic superconductors.
- (c) Describe optical properties of solid state devices.
- (d) Explain magnetism of organic materials.
- 5 Answer any ten in brief. 10
- (a) Give any two examples of low melting alloys.
- (b) What is glass transition temperature ?
- (c) Define a gel.
- (d) What is dielectric susceptibility ?
- (e) What is ferro electricity ?
- (f) What is interstitial (Frenkel) jump ?
- (g) Define super conductivity.
- (h) Define a capacitor.
- (i) What is rectifier ?
- (j) What is molecular hyper polarisability ?
- (k) What is lyotropic phase ?
- (l) Name any three glass modifiers.
- (m) What is MOCVD ?



BBX-2074-75-76-77-78-R Seat No. _____

M. Sc. (Sem. - IV) Examination

April/May - 2014

(1) CHN - 704 (A) : Organometallic Chemistry

(Elective)

(2) CHN - 704 (B) : Organic Synthesis :

Paper - II

(Elective)

(3) CHN - 704 (C) : Chemistry Of Materials

(4) CHN - 704 (D) : Computational Chemistry

(Elective)

(5) CHN - 704 (E) : Advanced Quantum

Chemistry

(Elective)

Time : 2 Hours]

[Total Marks : 50

(1) CHN - 704 (A) : Organometallic Chemistry

1 (A) Attempt any two of the following : 10

(i) Discuss the methods of preparation and

synthetic applications of organocopper

compounds.

(ii) Define : Organometallic compounds. Give its

classification based on metal-carbon bond in

detail.

(iii) Write down the methods of preparation,

structure and bonding in Zeise's salt.

(iv) Discuss the preparation, structure and bonding

in transition metal alkynes complexes.

BBX-2074-75-76-77-78]

1

[Contd...

- (b) Attempt any two of the following : 4
- (i) Explain why the transition metal aryl compounds are more stable than the corresponding alkyl compounds ?
- (ii) Differentiate the characteristic between Fischer carbene complexes and Schrock carbene complexes.
- (iii) Give the valence electron counts for the following species. Which one obeys the 18-electron rule ?
- (a) $\left[\text{Ni}(\eta^3\text{-C}_3\text{H}_5)_2 \right]$
- (b) $\left(\eta^5\text{-C}_5\text{H}_5 \right)_2 \text{TiCl}_2$
- (c) $\left[\text{MnCH}_3(\text{CO})_5 \right]$
- (iv) Define : Transition metal hydrides. How are they characterized ?
- (c) Attempt any two of the following : 4
- (i) How will you distinguish between dihydrogen and dihydride complexes ?
- (ii) Distinguish between carbyne and alkylidene complexes.
- (iii) Write down synthesis and applications of Tebbe's reagent.
- (iv) Define the following terms with appropriate examples :
- (A) Oxidative-addition reaction
- (b) Insertion reaction

2 (A) Attempt any two of the following : 10

(i) Write down the mechanism of polymerization

of propene catalyzed by Ziegler-Natta catalyst.

(ii) Discuss the catalytic mechanism of

hydroformylation of alkene using $\text{Co}_2(\text{CO})_8$ as

a catalyst.

(iii) Discuss the structure and bonding in transition

metal hydrides with bridging H-atom.

(iv) What are fluxional organometallic

compounds ? Discuss the fluxionality in

η^3 -allyl complexes.

(b) Attempt any two of the following : 6

(i) Define the following terms with appropriate

illustrations :

(A) Catalytic cycle

(b) Homogeneous catalysis

(c) Wilkinson's catalyst

(ii) What is ZSM-5 ? How methanol can be

transformed into gasoline using ZSM-5 as a

catalyst.

(iii) Discuss structure and bonding in

cyclobutadiene complexes.

(iv) Show that the Mannich and nitration reaction

with ferrocene.

OR

2 (A) Attempt any two of the following : 4

(i) Discuss in brief : Structure and bonding in

bisbenzene chromium compound.

(ii) What are the limitations of 18-electron rule ?

(iii) What are the disadvantages of HCo(CO)_4 used as a catalyst in the hydroformylation of alkenes?

(iv) Differentiate between singlet carbene and triplet carbene.

3 Answer the following questions briefly : 10

(i) What do you mean by hapticity?

(ii) How could the complex $\text{Cr(CO)}_3(\text{C}_6\text{H}_5)_2$ attain the 18-electron configuration?

(iii) Write down the structure of $\text{Al}_2(\text{CH}_3)_6$ and give the nature of bonding in it.

(iv) In what conditions transition metal alkyls can be stable?

(v) Define: Hydrogenation reaction with suitable example.

(vi) Write down the structure of HMn(CO)_5 compound.

(vii) Give the name of catalyst used by Monsanto acetic acid synthesis.

(viii) What do you mean by activation energy?

(ix) Draw the structure of $\text{Fe}_2(\text{CO})_9$ compound.

(x) How can the fluxionality behaviour of organometallic compounds be detected with the help of ^1H NMR spectroscopy?

Instruction : Attempt all questions.

1 Answer any four of the following : $4 \times 5 = 20$

- (A) Explain Newton-Raphson in solving polynomial equations.
- (B) Discuss the role of Gauss-Seidel method in solving linear simultaneous equation.
- (C) How eigen values are calculated using Jacobi and Householder method ? Explain it.
- (D) Write a note on Taylor series.
- (E) Explain the Role of Newton Cotes formulae in error analysis.
- (F) Discuss Polynomial wiggle problem and its role in interpolation.
- (G) Explain Pivoting strategy.

2 Answer any two of the following : $2 \times 8 = 16$

- (A) Ab initio calculation packages
- (B) Gaussian
- (C) Amber
- (D) ASAR

3 (A) Discuss the role of networking in chemical research. $1 \times 4 = 4$

OR

(A) How networking improves the standard of research in sciences. Comment on it. Attempt five from the following : $5 \times 2 = 10$

(i) Bisection

(ii) Errors

(iii) Hermite interpolation

(iv) Runge Kutta method

(v) Games

(vi) Any exercise done by you using MOPAC

(vii) Simulation programming

(viii) Advanced level scientific software package

(ix) Convergence

(5) CHN - 704 (E) : Advanced Quantum

Chemistry

1 Answer any three questions from the following : 20

(i) For Born Oppenheimer approximation, prove

$$\text{that } H_N(R) \Psi_N(R) = E_T \Psi_N(R)$$

(ii) Calculate the value of matrix elements F_{rs} by applying CGJ Roothan's method.

(iii) Calculate the total electronic energy for H_2O molecule which includes the value of Configuration Interaction.

(iv) Explain Slater-Condon rule.

(v) Discuss MC-SCF method.

(i) Explain Hohenberg-Kohn's two theorems.

(ii) By applying Kohn-Sham equation, obtain the value of exchange-correlation potential, $V_{xc}(r)$.

(iii) Explain Zero Differential Overlap.

(iv) Explain the use of the MM2 modeling software in quantum mechanics.

(v) Explain the use of the Gaussian software in quantum mechanics.

3 Answer any five questions from the following : 10

(i) The complete Schrodinger equation covers both the nuclear and electronic motions. True or False.

(ii) The Roothan used which approximation for MOs to obtain algebraic equations from the HF integro differential equations.

(iii) Hohenberg and Kohn justified the use of which parameter as the basis variable in determining the electronic energy ?

2 Answer any three questions from the following : 20

- (iv) In INDO, for $\mu_A = \mu_B$, what is the value of $S_{\mu_A \mu_B}$?
- (v) In CNDO, for the evaluation of HFR matrix elements $F_{\mu\nu}$ involves which two parameters?
- (vi) What is the formula of Gaussian function at a point centered around an atom?
- (vii) Hartree involved which term to the Schrodinger equation for many electron atoms?
- (viii) Who discovered the Gaussian software first?
-