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GBX-1602-03 Seat No._____

M. Sc. (Sem. II) Examination

April/May - 2017

CHN-504(A) & (B) : Chemistry : Paper - XI

(A) Spectroscopy

(B) Computers For Chemists

Time : 2 Hours] [Total Marks : 50

(A) Spectroscopy

1 Answer any five of the following : 20

(a) Explain P and Q branches in rotational vibrational spectra.

(b) Write a note on metal-ligand vibrations.

(c) Give an account on force constant and bond strength using vibrational spectroscopy.

(d) What is Born-Oppenheimer approximation ? Explain its use.

(e) Discuss applications of coherent anti-stokes Raman scattering.

(f) Explain : Stark effect.

(g) Give the principle and applications of Raman spectroscopy.

2 Answer any five of the following : 20

(a) Write a note on ^{31}P NMR.

(b) Discuss the factors affecting Geminal spin-spin coupling in ^{1}H–NMR.

(c) Give an account on ^{19}F NMR with applications.

(d) Discuss the factors affecting the chemical shift in ^{13}C NMR.

(e) Give the instrumental details of NMR spectroscopy.

(f) Distinguish between chemical shift equivalence and magnetic equivalence.

(g) Explain ABC and AMX system.

3 Answer any five questions in brief : 10

(a) What is Morse potential energy diagram ?

(b) Distinguish between stokes and anti stokes lines.

(c) What are overtones and hot bands?

(d) What is the difference between chemical shift and spin–spin coupling ?

(e) How does the rotational energy decrease ?

(f) Why water cannot be used as a solvent in IR spectroscopy ?

(g) Explain and draw ^{1}H-NMR spectrum of 2-Bromo butanoic acid.

(h) What is noise decoupled spectra ?

(i) What are shift reagents ?

(B) Computers For Chemists

1 Write any four : **20**

(1) What is memory ? Explain types of memories in brief.

(2) Discuss about "C" language features.

(3) What is LOGICAL variables ? Explain its uses.

(4) Describe the difference between function and procedure.

(5) What is operator ? Explain all operators with example.

2 Write any four : **20**

(1) Write down solution for Vandar Waals equation.

(2) What is Mat-Lab ? Explain any one application of Mat-Lab.

(3) Explain linear simultaneous equations to solve secular equation within Huckel theory.

(4) What is Mat-Lab ? Explain any one application of Mat-Lab.

(5) Explain elementary structural features such as bond lengths and bond angles.

3 Write any five : 10

(1) Any three name of I/O devices.

(2) Use of Header/Footer in MS Word.

(3) Short key for format painter and paint.

(4) Short key for Save and copy.

(5) Name of formula for antilog.

(6) Difference between FORTRAN and BASIC language.
