SUBJECT CODE: 11CH/PC/RM14

REG. NO._____

COURSE: MAJOR
PAPER: RESEARCH IN METHODOLOGY
TIME: 1h   30 min   **MAX MARKS : 50**

PART A (THEORY)
SECTION – A
Answer all the Questions   (10X 2 = 20)

1.   Mention any two secondary sources used in chemical literature

2. What is meant by science citation index

3. Give any two uses of foot notes in thesis writing

4. Define the term patent .Give any one use of patent

5. What is the purpose of bibliography in thesis writing

6. Give any two polynomials used in chemistry

7. Give the steps involved in determining sine of a number in radiance.

8. Give any two advantages of energy minimization technique

9..   How are computers useful in chemistry? Give one example each for use of software
       and Hardware?

10 . . Name the developer of the following force fields.

   a. GEM   b. NEMO

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SECTION-B

<u>Answer any Five Questions</u>   (5X 6 = 30)

11. Explain the different force fields involved in molecular modeling.

12. Explain primary sources with two examples

13. Give any three parts of the table in scientific writing.The given table shows fractional data . give the correct foramt

.81
.76
1.,31

14.Give the guidelines for the use of abbreviations and symbols in thesis writng. Give two symbals used in scientific reports

15. .Explain Scifinder and Science direct

16. Give the advantages of chemical abstracts. Give any two journals with high impact

factor

17. Expand the following terms MM2, CCF, MM4 ,PFF, SIBFA

18. Explain any two types of charts with one example each

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PART B (PRACTICAL)

1. The following results were obtained for the analysis of Copper in a sample (5*2=10)

Volumetrically. 23.3, 28.4, 26.3, 17.4, 22.4, 29.2, 25.4

Answer **any five** of the following:

   i.   Mean
   ii.   Deviation
   iii.   Absolute error
   iv.   Standard deviation
   v.   Variance
   vi.   Relative deviation in %
   vii.   Median

Answer any Five Questions   (6X 5 = 30)

1. Draw the structure of the given compound in Chem draw, convert to 3D and anlyse important bond
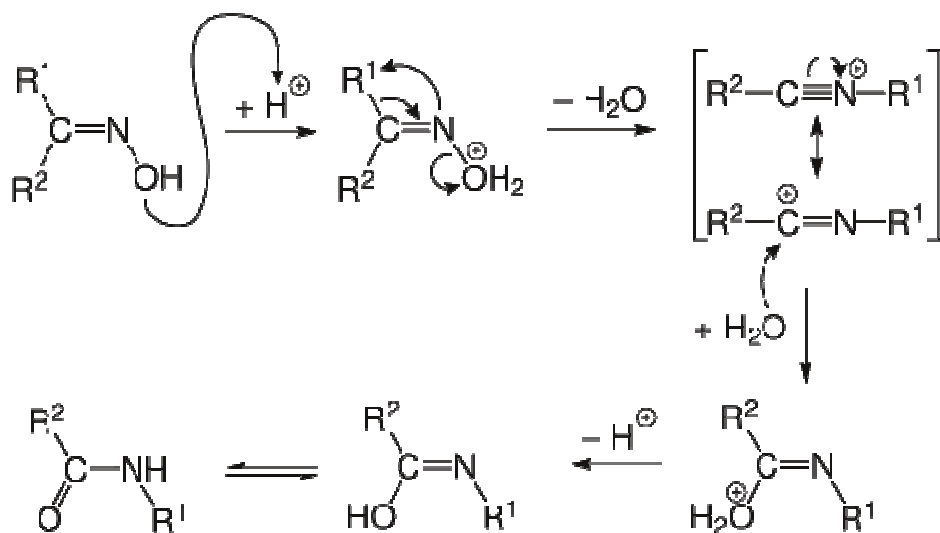   lengths and dihedral angles?

o- CH_3- C_6H_4 -p-C_6H_4 –CH_2 -C_6H_4 –m-COOH
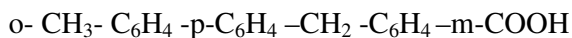
2.   Compare the bond distances of (i) O-H , (ii)C-O in Phenol and isopropylalcohol

3. Calculate the amount of work done by 2moles of an ideal gas at 300K in reversible
     isothermal expansion from V_1= 1.0 L to V_2=10 L ?

        Use W= -2.303 nRT log (V_2/V_1)
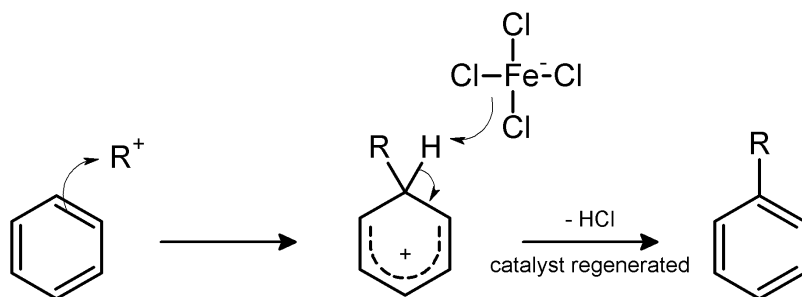
4 .Draw the following using Chemdraw
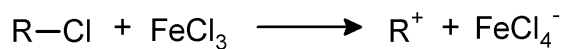

5.a) Draw the 3D structure of p –nitro phenol.[2]

b) Draw a histogram of the following data using EXCEL [3]

Data	%Fein steel
1	55
2	65
3	71.5
4	43
5	78.5

6. Draw the following mechanism using Chemdraw:
   (i)

$$R{-}Cl + FeCl_3 \longrightarrow R^+ + FeCl_4^-$$

- HCl

catalyst regenerated

7. From the following density and pressure data for SO_2 at 273.15K, calculate the limiting value of $(\rho / P)_0$ and the molecular mass of SO_2 ?

P, Bar	1.000	0.500	0.100	0.010	0.001	0.0001
ρ / P	2.8884	2.8545	2.8275	2.8214	2.8210	2.8210

Plot (ρ / P) Vs P and find (ρ / P) at P=0 which is limiting value of $(\rho / P)_0$ .R=8.314 $JK^{-1}mol^{-1}$. Find M using the formula, M= $(\rho / P)_0$ x RT

Answer any one question (1*10=10)
1. Draw Intensities of A, B, C Vs 2theta values in the same graph sheet and compare?

2theta	A	B	C
0.85	76	74	36
0.9	83	65	35
0.95	95	64	34
1	125	82	25
1.05	169	78	28
1.1	196	97	22
1.15	244	154	27
1.2	317	198	20
1.25	395	229	28
1.3	473	291	12
1.35	526	276	19
1.44	509	293	23
1.45	463	280	26
1.5	354	274	23
1.55	283	223	27
1.6	227	200	22
1.65	173	181	24
1.7	139	150	36
1.75	127	157	32
1.8	126	142	56
1.85	107	142	48
1.9	103	124	33
1.95	91	122	43
2	88	120	51
2.05	84	105	42
2.1	66	103	28
2.15	62	104	39
2.2	75	107	30
2.25	77	97	43
2.3	65	102	37
2.35	74	92	32

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2. a) A particle moves in a one dimension box of length a = 24nm. Plot a graph of   a. ψ = $\sqrt{2}/a$ Sin $n\pi x/a$ vs different values of x. for n = 1, 2   b. ψ^2 vs different values of x. for n = 1, 2

b) Determine the spectral data (H-NMR and C13 NMR) for the following:

i. Bezoic Acid
ii Benzophenone   [5+5]