16

[Time: 3 Hours] [ Marks:75]

Please check whether you have got the right question paper.

N.B: (1) All questions are compulsory

- (2) Figures to the right indicate full marks
- (3) Answer all the sub-questions together and in order
- (4) Spectral correlation tables are allowed
- Q1) a) Answer any four (1 mark each)

Calculate the index of hydrogen deficiency for C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>

Predict the number of signals in the <sup>13</sup>C NMR of

iii Predict the number of signals in the <sup>1</sup>H NMR of Cl<sub>2</sub>CHCH<sub>2</sub>Br

iv Draw structure of the ion responsible for peak at m/z=46 in the mass spectrum of 2-butanol .

v Predict two characteristic IR frequencies of benzoic acid.

Name a simple spectroscopic technique which will help distinguish between

vi vi

Q.1) b) Answer any **eight** (two marks each)

i Predict the UV λmax for

ii Predict the UV λmax for

iii How will you distinguish between the following by <sup>13</sup>C NMR spectroscopy?

iv How will you distinguish between the following compounds by IR spectroscopy?

v How will you distinguish between the following by mass spectrometry?

$$H_3C$$
 $V$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
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- vi Depict two fragmentation pathways for 1-phenyl 1-propanone.
- vii Predict the  ${}^{1}$ H NMR spectrum of toluene giving  $\delta$  values, splitting pattern and ratio number of proton intensities.
- viii Distinguish the following by IR spectroscopy-

$$H_2 \stackrel{O}{\longrightarrow} H_2 \stackrel{O}{\longrightarrow} O - CH_3$$
 and  $H_3 \stackrel{O}{\longrightarrow} C \stackrel{O}{\longrightarrow} C \stackrel{C}{\longrightarrow} CH_3$ 

- ix In benzaldehyde, two of the ring protons have resonance at 7.87 ppm, and the other three have resonance in the range from 7.5 to 7.6 ppm. Explain.
- x Assign the vibrations for the following IR bands, 1550 and 1745 cm<sup>-1</sup>.
- Q.2 Answer any five questions  $(5 \times 7)$ 
  - a) Predict IR spectrum, <sup>13</sup>C NMR and <sup>1</sup>H NMR of –

$$N \equiv C - C \xrightarrow{H_2} O \xrightarrow{H_2} O - C \cdot CH_3$$

b) How will you distinguish between following compounds using any one spectral technique. Give distinguishing spectral characteristics. If mass spectrometry is used one fragmentation pathway has to be depicted.

$$CH_3$$
  $CH_3$   $CH_3$ 

$$H_3C$$
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 

c) A compound with molecular formula  $C_4H_8O_2$  has the following spectral data

IR: 2983, 1743, 1243 cm<sup>-1</sup>

i)

 $^{1}$ H NMR δ 4.3 (q), 2.1 (s), 1.2 (t)

Deduce the structure and depict one mass fragmentation pathway.

35

## Q.P. Code:21420

20

- d) An organic compound containing C, H and O, has molecular weight 150 and has characteristic IR bands at 1680, and 1250-1000 and  $^1$ H NMR at  $\delta$  7.8 (d, 2 sq),  $\delta$  7 (d, 2sq),  $\delta$  3.9 (s, 3sq),  $\delta$  2.6 (s, 3sq). The  $^{13}$  C-NMR shows 7 types of C at 200, 163, 131, 130, 114, 55 and 26 ppm. Predict its structure and justify your answer.
- e) Compound with molecular formula  $C_5H_{12}O$  has following spectral characteristics  $^1H$  NMR Shift ppm (splitting, Area): 2.4(s:D2O exchangeable,1sq), 1.4(q,2sq), 1.1(s, 6), 0.8(t,3sq) Deduce the structure and predict  $^{13}C$  NMR for the same.
- f) Predict the <sup>1</sup>H NMR and mass spectrum of the following compound

Depict two fragmentation pathways for the molecule one involving fission and the other rearrangement.

g) A compound, with formula  $C_5H_8O_4$ , shows strong absorption at 1734 cm<sup>-1</sup> and 1745. cm<sup>-1</sup>. Also it has several strong bands centering at about 1200 cm<sup>-1</sup> in the infrared spectrum. The <sup>1</sup>H NMR shows following characteristic signals.

 $^{1}$ H NMR  $\delta$  4.2 (q) , 3.4(s), 1.3(t) Draw its structure.

Q.3) Answer any five questions (4 marks each)

a) Distinguish between the following compounds using suitable spectral techniques



b) Identify the compound with molecular formula C<sub>10</sub>H<sub>14</sub> showing following spectral information

1H NMR	7.2 (4H, s), 2.6(2H,q),1.25(3H, t)
13C NMR	141,127, 28, 15

- c) How will you distinguish between cis and trans isomers of CH<sub>3</sub>CH=CHCOOH.
- d) Draw the structure a compound having molecular weight 116, which meet the following (i)  $^{1}$ HNMR data-  $\delta$  11 (1H, s),  $\delta$  2.6 (4H, t),  $\delta$  2.12 (3H, s)

(ii) IR: 3333-2850, 2965, 1715, 1200 cm<sup>-1</sup>

e) Predict IR, <sup>13</sup>CNMR spectra for 3-Methylbutanamide.



- f) A compound with molecular formula  $C_8H_8O$  show <sup>1</sup>H NMR signals at  $\delta$  8.1 (t), 7.2(s), 2.6(d) ppm. The IR bands are seen at 1720, 2800-2710 and 1600-1500 cm<sup>-1</sup>. Identify the structure and justify.
- g) Depict the fragmentation pathways in mass spectroscopy one by fission and another by rearrangement for heptanal.

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SPECTRAL CORRELATION TABLES
Chemical Shifts for Methylene Groups Attached to Two
loups (Y-OH2-Z)

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	-c-c	2,87	2.99	3.40	2,76	2.65	4.08	3,88	3.37	4.13	3.91	4,78	4.68	3,25	3.39	3.10	3.74	3.25	3.13	1	1,52	
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	and 5.56-5.71 (4)	1600-1750		21.15	Œ).	227
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ARACTERISTIC INFRARED AREORPHONS OF FUNCTIONAL GROUPS

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. a.A. Unsatutated compounds	£1.0~70.0	Ξ.	2001-2001	- se approximately		C
C NEX - Statesting Vibrations,			2000 2907 5			
azo compounds	6.14-6.35	Ξ	0701960			
dN=C=N-Siretching vibrations.	•	į			-	
dimindes.	Z. Ž.	į	2155-2130			
- M. Stellehing wibrations, atides	4.63-4.72	<u>9</u>	2160-2120			
	and 7.46-1.48		1340-1180			
			1			

		 9
ኒ ኒ	:	

Substituent Group   Netholy   Neth										•	Proton
100   120			. /	etbyl	Methylene	Methine	Substituent Group	Frotons			
100   145   170	Sucantinent	croup	-:[	otons	rotons	Proton	HC.F	4.25	4,50		4.80
100   1.45   1.70   Cyclopropine   2.45   1.50	HC-C-CH,		<b>.</b>	. 95	1.20	55.1.	HC-NO2	4,30	\$6.4		4,60
1,00   1,35   1,70   Cyclopatrays   1,45   1,45   1,45   1,15   1,10	HC-C-NR			.05	1.45	1.70	Cyclopropane		0.20		0,40
1.00   1.55   1.95   Cyclobrates   1.50   1.50     1.10   1.10   1.10     1.10   1.10     1.10   1.10   1.10     1.10	HC-C-C-		<b>-</b>	8,	1.35	1.70	Cyclobutane		2.45	· 4:	
1.00   1.30	10-10-10-10-10-10-10-10-10-10-10-10-10-1		·	.05	1.55	1.95	Cyclopentane				. :
1.00   1.00	がとしている。	בר ליכול		2.5	1.50		Cyclohexane		1,50		1.80
1.15   1.25   1.20		SNR.	<b>:</b> -	2.5	05.1	2	Cycloheptane		A 11.25	(§) · ·	
1.15   1.75	HO-O-OH	0)Ar	•	, v.	25.	200		4.14	-	Ì	100
1.15	HC-C-(C=	0)OR		. 15	92.1	06.1	Substituent Croup	Proton Shift			ליסוסם איווו
1.20   1.50   1.50   1.75	HC-C-A	•	÷	.15	1.55	1.80	110-000	36.6	O-C CIT		21
1.20   1.50	HC-C-OH	(and OR)	-	.20	1.50	1.75		7 6			
1.25	HC-C-CH	×		.20	1.50	1.80	これという	37.6	HOLA		4 S-6 S
123   1.56   1.50   1100-R	HO-O-OH	7		25.	, ,1.65	2.00	A TAN		) C	•	2 7 0
1.30	HC-C-SR			7.5	1.60	06.1	Q-02H	2	H		2.8-3.6
1.50	HG-C-OA		-	.30 0.	1.55	5.00	2 P	0 4-10 0	HALB		1-2
1.50	HC-C-O(C	=0)R	ا پيد	9	1.60	1.80	HCO-Ar	9.7-10.5	HNIA	<u>.</u>	φ,
F. and - SOp R.   1.35   1.70   1.75   1.9	HC-C-SH	:	-	30	1.60	1,65	A LINE CHANGE				V .
1,40	HC-C-(S=	O) F. and	_	.35	1.70	۲	Carling Carling	71.7	W-Wit		
O)CF <sub>3</sub> . 156 1155 1165 1176 1185 1186 1197 1186 1197 1187 1187 1187 1187 1187 1187 1187	HC-C-NR		=	. <del>4</del> 0	1.75	2.05	 				<b>:</b>
1.55   1.56   1.55   1.56   1.55	) 	=0)CF3	<del>-</del>	04.	1.65		:			<u>د</u> .	. •
1.65 1.75 1.85 1.90			نس	.55	1.80	1.95			<b>:: •</b>		•
1.50 1.85 1.90 1.50 1.54 1.54 1.55 1.90 1.59 1.50 1.50 1.50 1.50 1.50 1.50 1.50 1.50	)0-0-0H	=0)Ar	<b>–</b>	.65	1.75	1.85					
1.50   1.50   1.50   1.50     1.60   2.20   2.20   2.20   2.20   2.20     1.70   2.20   2.20   2.20     2.20   2.20   2.20   2.20     2.20   2.20   2.20   2.20     2.31   2.32   2.35   2.65     2.40   2.40   2.40   2.40     2.40   2.40   2.40   2.40     2.40   2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40   2.40     2.40   2.40	HC-C-Br	•	÷ (		1.85	1.90	17.40	Camifred Chiftee (Val)	Salana American con the American	T of estima	נאאני
(and NR <sub>3</sub> )         1.50         2.05         2.80         Substituent Group         Frimary         Secondary         Tertury           2.05         2.25         2.50         Substituent Group         Garbon         Carbon		÷	o .	. 061	5.30	1.50	J	nemice de la merita de	ices given on the o seate,	Television 10 1	, ('Cu
Rand NRs.)         1.70         2.20         2.80         Substituent Group         Carbon         Carbon         Carbon           2.00         2.25         2.50         Alkener         -20 to 30         25 to 45         30 pc 60           2.10         2.25         2.45         2.65         C-C         40 to 60         40 to 70         60 to 75           2.10         2.25         2.45         2.90         C-N         20 to 60         40 to 65         40 to 65           2.10         2.25         2.46         2.90         C-N         10 to 60         50 to 70         60 to 73           2.20         2.25         2.46         2.90         C-N         10 to 60         25 to 45         40 to 65           2.22         2.46         2.83         C-Halide         -31 to 65         50 to 65         50 to 65           2.25         2.70         3.40         Alkynes         10 to 100         Incorpanites         10 to 100         Incorpanites           2.40         3.10         3.60         Alkynes         110 to 135         Oxines           2.50         3.10         3.40         4.00         60         Incorpanites         Incorpanites           2.70         3.40<	いしてい		<b>~</b> ∙•••	09.	2.05	<u>.</u>		Primery		reject	Gustemany
Canon Charles   Canon Charle			:	.70	2.20	2.80	Substituent Group	Carbon		rhon	
2.05 2.55 3.00 Alkanes 2.10 2.35 2.65 C=C 2.10 2.35 C=C 2.10 10.35 C=C 2.10	HC-(CHO)	OR (and NE	_	0.0	2,25	2.50	droin impires	Caroon		· incorr	HOOT TAKE
2.10 2.35 C=C	HC-SX		• ``	.05	2,55	3.00	Alkaner				• •
2.10 2.35 2.65 C=O 40 to 60 40 to 70 60 to 72 2.15 2.45 2.90 C=N 20 to 45 40 to 60 70 60 to 73 2.25 2.45 2.90 C=N 20 to 45 40 to 60 70 60 to 73 2.25 2.45 2.90 C=S 10 to 30 2.50 4	200		ri (	0	. 2.30.	2,55	\! \! !	-20 to 30.		110.60	15 to 70
184). 2.65 2.64 2.65 2.66 2.66 30 to 70  184). 2.22 2.40 2.85 2.85 C.—S 10 to 30 25 to 45 40 to 55 2.25 2.40 2.85 C.—S 10 to 30 25 to 45 40 to 55 2.25 2.45 2.85 C.—S 10 to 30 25 to 45 40 to 55 2.25 2.40 2.70 3.40 Alkynes 70 to 100 Isocyanides 1.0 (I) (CI) (II) (CI) (C			7 (	٥,	N. 17	2.65	/   0	40 to 60	••	10 75	70 to 85
2.55 2.40 2.40 2.85 C.—S. 10 to 30 25 to 4.5 40 to 55 2.50 2.50 2.50 2.50 2.50 2.50 2.50 2			4 6		2.45	2.90	2	20 to 45		10 70	65 to 75
2.55 2.45 2.85 C-Halide -71, 635 -10 to 45 30 to 65 2.40 2.70 3.40 Alkynes (D. (CI)			4 0	77	2.40	•	. v	10 to 30		10.55	. 55 to 70
Columbrater	としている。	. ( E V V )	4.6	97	2.45	2,85	Chitalide	-17 to 35	:	16 65	85 to 75
-(SO)R 2.60 3.10 3.60 Alkynes 70 to 100 Isocyanides 1	HO   ()		, ,	, <del>,</del>	2.70				-	đ	<del>(</del> C)
-(SO)R.         2.60         Alkynes         70 to 100         Isocyanides           -(SO)R.         2.60         3.60         Alkenes         10 io 150         Carbonates           2.70         3.40         4.70         Carbonatics         110 io 150         Carbonates           2.70         3.40         4.70         Carbonatics         110 io 150         Carbonates           1.70         3.40         4.70         Carbonatics         110 io 135         Oxines           1.8         2.95         3.10         3.60         Heteroacomatics         115 to 145         Thiouress           1.8         3.75         4.60         Ioocyanates         10 io 155         Esters, Anhydrides           1.0         3.50         3.75         4.05         Thiocyanates         110 to 120         Aidehydes           1.0         4.00         4.00         4.00         Cyanides         10 to 130         Ketones	HC-SAT	!			7.7	36.0					
-(50)R   2.60   3.00   Alkenes   110 to 150   Carbonates   110 to 150   Carbonates   110 to 150   Carbonates   110 to 150   Carbonates   12.50   3.40   4.10   4.25   3.10   3.60   Heteroaronatics   115 to 140   Thiouress   13.50   3.45   4.55   4.50   4.50   4.50   Thiocyanates   115 to 135   Acids, Acyl chlorides   13.50   3.50   4.10   4.50   Thiocyanates   110 to 120   Aldehydes   120 to 140   Ketones   120 to 130   Ketones   120 to 130   Ketones   120 to 130   Ketones   120 to 130   Ketones   13.80   4.50   4	HC-NRAL	· ·		2 5		7.0	Alkynes	70 to 100	Isocyanides		130 to 150
2.70         3.40         4.10         Asymatics         4.10 to 135         Oximes         1           2.95         3.10         3.60         Hetroaromatics         115 to 145         Ureas           2.95         3.10         3.60         Hetroaromatics         115 to 145         Ureas           2.95         3.35         3.45         4.05         C-a         13 to 155         Esters, Anhydrides         1           OR         3.20         3.45         4.05         Cyantes         105 to 120         Amides         1           OR         3.50         3.75         4.05         Thocyantes         115 to 135         Acids, Acyl chlorides         1           3.65         4.10         4.95         Isothiocyantes         120 to 120         Aldehydes         1           7         4.00         4.60         Cyanides         10 to 130         Ketones         1	HC-SO-R	and -(50)R			. 30 5	.00.	Alkenes	110 to 150	Carbonates		150 to 160
C-substituted   125 to 145   Ureas   1	HC-B			25	7 000	्	Aromatics	. 1.to to 135	Oximes		155 to 165
Retroacomatics   115 to 140   Thlouress   13	HC-NR:	;		56	, r	2.5	Caubstituted	125 to 145	Ureas		150 to 170
3.05 3.45 4.05 Cyanates 135 to 155 Esters, Anhydrides 1 3.20 3.40 3.60 Lisocyanates 115 to 120 Anides 1 3.50 3.75 4.05 Thiocyanates 110 to 120 Aldehydes 1.50 4.00 4.00 4.00 Cyanides 110 to 130 Ketones 1.50 0.09 110 to 130 Ketones 1.50 0.09 110 to 130 11	HC-NH(C-	O)R	7	95		00.0	Heterogromatics	115 to 140	Thiourers		165 to 185
OR 3.20 3.40 Cyanates 105 to 120 Amides 1 3.50 3.50 3.40 Locyanates 115 to 135 Acids, Acyl chlorides 1 3.50 3.50 4.10 4.95 Explisiocyanates 120 to 140 Ketones 1 4.00 4.20 Cyanides 120 to 130 Ketones 1 3.80 4.20 5.05 Cyanides 110 to 130	HC	•	. ~	0.0		600	8	135 to 155	Esters, Anhydric	les	150 to 175
3.50 3.75 4.05 Isocyánates 115 to 135 Acids, Acyl chlorides 1 3.50 4.10 4.50 Isothiocyánates 120 to 140 Ketones 1 3.80 4.20 5.05 Cyanides 110 to 130	HC-OH and	1-OR		20	i w	200	Cyanates .	105 to 120	- Yuldes	•	160 to 180
3:65 4:10 4.55 Thiocyanates 110 to 120 Aldehydes 1 1.50 to 140 Ketones 1 10 to 130 Ketones 1 1.50 to 140 Ketones 1 1.50 to 140 Ketones 1 1.50 to 130 Ketones 1 1.50 Ketones 1 1	HC-NH,		. m	So	3.75	200.7	Isocyanates	115 to 135	Acids, Acyl chlo	rides	160 to 185
3.80 4.00 4.60 Fotblocyantes 120 to 140 Ketones 1 3.80 4.20 5.05 Cyanides: 110 to 130	HC-0(0-1)	),R	m	.65	0	\$ **	Thiocyanates	110 to 120	Aldehydes		175 to 205
3.80 4:20 5.05 Cyanides	HC-OAs	•	ฑ์	80	4,00	4.60	Isothiocyanates	120 to 140	Ketones		175 to 225
	JHC-O(CHC	))Ar	m	08.	4:20	50.5	Cyanides	110 to 130		•	٠.

TURN OVER

## SPIN-SPIN COUPLING CONSTANTS

Type	J. cps	Турс	J, cps
Hit	280	C-CH-CH-C	9-13
CHA	12.4	H-C=C-H+	9.1
E H	12-15	CII-C≡C-II	2-3-
્રિંધ		Н	
CH-CII	2 9	CH-C	1-3
-C-1-C-1C-	,	, It	
H	~0	C=C II	6-8
CHT-CH2-X	6.5-7.5	. <u>Ç</u>	
CH₁ CH₩	\$ 5 <b>9</b> A		a- 6-9
CH.	5.5-7.0		m- 1-3
	a.a 5-10	~	p=0-1
H-C-C-11	a.c 2-4		aB 1.6-2.0
ZN: A	c.c 2-4		a/r 0.6-1.0
11		8	ida" 1.3-1.8 /// 3.2-3.8
CE C	0,5-3	•	
и ји .		$\bigcirc$	7/12.012.6
CEC .	712	1.	alt 1.5-2.2 aa 1.8-2.3
11		, <b>t</b> i	BB 2:8-4:0
<b>6</b> =0,	13~18		01660
H,			aft4.6-5.8 = aft,1.0-1.8
C=C	4-10	3	an' 2.1-1.3
		•	- <del>111-3</del> -0-4.2
16-11	a Bash ( `		a 8 4.9-5.7
(tel Carrier	0.5- <del>2.5</del> والمالية	•	ay 1.6-2.6
- <b>H</b>	and the state of t		nn 0.2-0.5
H. , C-!I	-4	W. Company	By 7.2=8.5
C=C	•		HF 1.4-1.9

TURN OVER

	•				
Conjugated diene	s & Trienes, Solv	ent: Ethanol			
Parent value for Bu	itadiene system	217 nm			
or acyclic conjugat					
Acyclic triene		245 nm	The second second		
Homoannular conj	ugated diene	253 nm			
Hetroannular conju		215 nm			
		each substituents			
Alkyl substituents	or ring residue	5 nm			
Exocyclic double l		5 nm	` `		
Double bond exter		30 nm	13.		
	Auxochrome				
-OR		+6 nm			
-SR		+30 nm			
-Cl, -Br	*	+5 nm .			
NR <sub>2</sub>	•	+60 nm			
-OCOCH <sub>3</sub>		0			
	r rules for aB-un	saturated carbonyl	compounds:-		
a) Parent values					
αβ-unsaturated ac	velic or six	215 nm			
membered ketone	•		•		
αβ-unsaturated fi		202 nm	:		
ketone					
αβ-unsaturated al	ldehyde	207 nm			
b)Increments		***			
i) Each alkyl sub	stituents or ring	residue			
At a position	•	10 nm <sub>2 g</sub> 5.22			
At β position	, pr	12 nm			
At gamma and his	cher position	18 nm			
ii) Each exocyclic double bond		·   5 nm			
iii) Double bond extending		30 nm			
conjugation					
'iv) Homoannulai	iv) Homoannular conjugated		39 nm		
diene					
Auxochromes	Positi				
	α	<u>β</u>	gamma		
-OH	35	30	50		
-OR	35	30	17		
-SR	1	85			
-OCOCH3	6	6	6		
- <u>Cl</u>	15	12			
-Br	25	30	••		