[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

#### Q.1 (a) Answer any four questions (1 mark each)

(4)

- (i) Predict the number of signals in the <sup>13</sup>C NMR spectrum of *o* dichlorobenzene
- (ii) Predict the number of signals in the <sup>1</sup>H NMR spectrum of hexan-3-one
- (iii) Draw structure of the ion responsible for the base peak in mass spectrum of n propanol
- (iv) Calculate the index of hydrogen deficiency for C<sub>8</sub>H<sub>7</sub>N
- (v) Give the coupling constant value for cis coupled protons for substituted alkene
- (vi) Arrange the following in increasing order of frequency for C=O stretch Aliphatic ketones,  $\alpha\beta$  unsaturated ketone,  $\alpha\beta$  unsaturated amide

## (b) Answer any eight questions

(2 Marks each)

(16)

(i) Predict UV λmax of

(ii) Predict UV λmax of

(iii) How will you distinguish between the following by <sup>1</sup>H NMR spectroscopy? Give distinguishing spectral data

(iv) How will you distinguish between the following compounds by IR spectroscopy? Give distinguishing spectral data

(v) How will you distinguish between the following by mass spectrometry? Give distinguishing spectral data

(vi) How will you distinguish between the following by <sup>13</sup>C NMR spectroscopy? Give distinguishing spectral data

$$H_3C$$
— $C$ — $CH_2$ — $CH_3$  and  $H_3C$ — $H_2C$ — $H_2C$ — $C$ — $H$ 

(vii) Depict one fragmentation pathway for 1-methylcyclohexene?

(viii) Predict ¹H NMR spectrum of the following giving δ value, splitting pattern and ratio of proton intensity. Do not give ranges.

$$H_3C$$
  $O$   $C$   $CH_3$   $CH_3$ 

(ix) A compound with molecular formula  $C_4H_6O_4$  gives only two  $^{13}C$  NMR signals while  $^{1}H$  NMR shows only one 2 signals, at and  $\delta 22$ . Deduce the structure and justify your answer

(x) Predict the IR spectrum of aniline.

#### Q.2 Answer any five questions (5x7 marks)

а

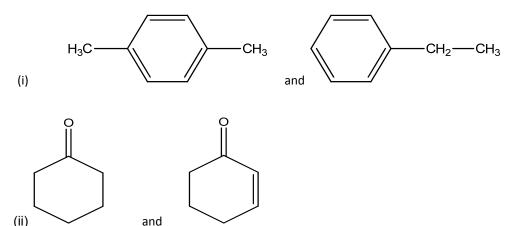
Predict IR spectrum, <sup>13</sup>C NMR and <sup>1</sup>H NMR spectrum of

$$N \underline{\hspace{1cm}} C - CH_2 - CH_2 - C - CH_3$$

**TURN OVER** 

35

b How will you distinguish between following compounds using spectral techniques? Give distinguishing spectral characteristics. If mass spectrometry is used, one fragmentation pathway must be depicted



Write all possible structures for compound with molecular formula  $C_4H_8O$  and whose IR spectrum shows a band at around 1720 cm<sup>-1</sup>. Predict <sup>13</sup>C NMR and <sup>1</sup>H NMR of each structure.

A compound with molecular weight 134 has a prominent band at 1693 cm<sup>-1</sup> in its IR spectrum. The  $^{1}$ H NMR spectrum shows two singlets in the ratio of 2:1 at  $\delta 8$  and  $\delta 10$ .  $^{13}$ C NMR spectrum gives 3 signals at  $\delta 130(d)$ , 139(s) and 191 (d). Mass spectrum shows m/z 134, 133, 105, 77, 51 and 29. Predict the structure and justify your answer. Depict how fragments 133 and 29 are formed.

A compound with molecular weight 156 shows IR bands at 3060, 2935, 2200 and 1600  $\,\mathrm{cm}^{-1}$ .

The <sup>1</sup>H NMR spectrum shows the following spectral characteristics

δ 7.3 s 40 squares

С

d

е

f

2.6 s 40 squares

The <sup>13</sup>C NMR spectrum shows the following signals

δ168 s, 136 s, 125 d, 30 t.

Deduce the structure and justify your answer.

A compound with molecular formula  $C_{10}H_{12}O_3$  has a prominent band at 1742 cm<sup>-1</sup> in its IR spectrum.

The <sup>1</sup>H NMR spectrum shows the following spectral characteristics

δ 7.9 dd 2H

6.9 dd 2H

4.0 q 2H

3.8 s 3H

1.4 t 3H

Predict the structure and justify your answer

4

g Predict the  $^{1}$ H NMR and mass spectrum of p methoxyisopropyl benzene. Depict two fragmentation pathways for the molecule, one involving fission and the other rearrangement

### 3 Answer any 5 questions (5x4 marks)

a Distinguish between the following using a suitable spectral technique

$$CH_3$$
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 
 $CH_3$ 

- b Draw all possible structural isomers of C<sub>3</sub>H<sub>6</sub>O. Predict the number of signals in <sup>13</sup>C NMR of each isomer
- c A compound with molecular formula  $C_4H_8O_2$  has an IR band at 1150, a  $^1H$  NMR singlet at δ 3.95 and one signal at δ 66.5 in its  $^{13}C$  NMR spectrum. Predict its structure and justify your answer.
- A compound has m/z values of 112,114 and 116 in the molecular ion region of the mass spectrum. The  $^1$ H NMR spectrum has two doublets of equal intensity at  $\delta$  4.1 and 9.2. Deduce the structure and justify your answer.
- A compound with molecular weight 123 has following spectral characteristics  $^{1}\text{H NMR: }\delta$  8.1 (2H, m), 7.5 (3H, m) and it shows IR bands at 3030, 1600, 1550, 1500 cm  $^{-1}$ . Deduce its structure and justify your answer.
- f Predict the IR and <sup>13</sup>C NMR spectra for p- nitrobenzaldehyde
- g Depict two fragmentation pathways for pentan2-one, one involving fission and the other involving rearrangement

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# SPECTRAL CORRELATION TABLES

Chemical Shifts for Methylene Groups Attached to Two

	unctio	1	****	-	***************************************			1				-#	+ +-			10 1			+=		4 4	**
eour	j F	Q Ç	V	-B	ងុំ	, p	P	-8.	7	) JiO	, a	-0Fh	-00 = 0)R	-C(=0)R	-C(=0)Ph	-C(=0)OR	-C(=0)NR,	2	-NR.	-NHC = O)R	×	
-	1.44	1.90		450	13,00	8.47	3.57	3.43	3.20	3.70	3.40	J. F.	4.25	2,47		2.25	2.23		2.63	A	15)	2,
<del>.</del>	-CH, 1.17			2.55	1.91	1.84	3.23	3.03	2.52	3.26	3.06	3.93	3.83	2.40	2.54	2.25	2:29				2.67	
	-C=C	2.60	3.39	3.30	2.76	2.69	4,08	3.93	3.87	4.13	3.95 3.91	4.78	4.68	3.25	3.39	3.00	114	3.15			3.52	3
			1	13.50		1	4.09	3.90	10.01	1	1	1./.	1.71	1 31-2		-	-	1	3.30	1	1	+
		ϡ	3.11		2.88	2.81	4.20	4.00	3.49	4.28	4.03	4.90	4.80	3.37	3.51	3.22	3,26		3.24	3.97	3.67	
			,	3.17		3.50	4.50	4.35		S. D	4.70	4.91	5.08	3.55	.8.6	3.40		3.65	3.48			3.
			-Ph	3.93	3.29	3,22	4.61	4.41	3.90	4.58	4.44	5.31	5,21	3.78	3.92	3.63	3.66	3.78	3.65	4.34	4.04	3
				-CF,	2.63	2.58	3.97	3.76	3.26	4.01	3.80	4.67	4.57	3.12	3.28	2.99	3.03	3.12	3.01	3.71	3.41	3.
						. 7.5			3.56			- 1		. 1		1		1	1	1		Ť
				10.1.1	-CF,	2.51		3.70	3.19	3.93		4.60	4.54	3.07	3.21	2.92	2.96	3.07	2.94	3.64	3.34	3:
						~	4,99	-5.16	4.99		5.40				. ·	4.05	4.17	4.07	eno	30		
						-a	5.29	5.09 4.94	4,58	3,32	5.12	6.36	5.89	4.46	4.60	4.31 3.70	4.35 3.92	4.46	4.37	5.13	4.73	4.
						. ,	-Br	4.89	4.38	5.12	4.92	5.79	5.69	4.26	3.40	4.11	4.15	4.26	4.13	4.83	4.53	4.
									3.90	1.00	,					CART	3.65	3.65				T
							-	-1	3,37	4.61	4.41	5.16	5.06	3.75	3.89	3.60	3.64	3.75	3.62	4.32	4.02	3.
									-OH	4.35	\$.15	6.01	5.92	4.49	4.63	4,34	4.38	4.49	¥.35	\$.06	. 6.75	
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							. 5 . 4.			ÖR	4.95	5.82	5,72	4.29	4.43	4.22	4.18	4.29	4.15	4.94	4.64	4
			12.1	ud/file	2 1 M.Y		* 2 12	starij		15.3 (E)	OPh	660	6.59	5.16	5.30	5.09	4.45	5.16	5.03	5.86	(9)	
											V." [	0.07	0.37	4.42	3.30	3.09	4.03	3.16	3.03	3.60	5.56	3.
											-oc(=	O)R	6.46		5.20	4.91	4.95	5.10	4.92	5.63	5.37	5.0
													24 v.	3.60		3.37				4.10		_
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												:	-01=	OXPh	2 91	3.62	3.66	3.77	3.64	4.34	4.02	3.7
													<u> </u>	۱. ۳۰		3.35	3.00	3.77	3.17		7.02	3.
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CHARACTERISTIC DIFRARED ABSORPTIONS OF PUNCTIONAL GROUPS!

		intensity strage cin				d Barre	The second	Kange cm
· · · · · · · · · · · · · · · · · · ·			-	Alkene, risubstituted, gem		- S	Ê	~1653
A. Elydrocarboa chromophore				Amene, trisubstituted		63-	E	~ 1669
1. C-H SIKETCHING		82 85		Aftene, tetrasubrituted		57	3	-1669
a. Allcane	3.38-3.51	000 000 000 000	2962-2853	Diene		99	3	1650
b. Alkene, monosubstituted (viayt)	.05	M (III)	3040-3010		Pod	25.	3	8
4	22	(B)	255-3075 2005-30075	b. Allyne, monosubstituted		4.67-4.76	E	2140-2100
Alkene, distribution, cis	3.29-3.32	(H)	3040-3010	Allyne, dirubatiuted		157	2	2260-2190
Alkene, disubstituted, mens	200	(H)	3040-3010	A News		W.	E	200
Alkene, disubstituted. gem	323-335	F (H)	2005-2007		Bud	Ť	E	100
Si granklikene, trisubstituted	329-337	100	3046-3010	d. Aromitie		200	2	\$
V. C. Alkyne	-3.03		C. C.	1977、1887、1897、1877、1877、1877、1877、1877、	  	11.9-	3	95
de Aromatic El Chester	~330	3				9	£ (	8 5
2 C-H BENDING	(a) + 12,5-12,4 \$ au	32.5 E. 13.50		THE STATE OF THE S	74	1	į	3 5
Constant Catherene und	7 43-2 78 -7.46	2000	. Pie	R. Carbonyl chromoshere			(m)	2
Altane - CH.	-	234	Tare 12.00	1. KETONE STRETCHING VIRKATIONS	1			
THE STREET AND THE COMPANY OF THE COMPANY	6.20-700	96		a. Saturated, acvelle	-6	*****	121	1716 1706
	411	20	120	b. Seturated, eyelie:	į.		}	
Alkane, fem-dimethyl	20-27-07-05	56	1365-1380	6-membered ring (and higher)		5.80-5.87	Ξ	1725-1705
	200 - 201 and 27.30-733	1 (F)	5967-8469	Fraembered ring		5.71-5.75	3	1750-1740
Alkane, tert-batyl	221-11.132	35	1395-1385	4-membered ring		197	3	-1775
	and ~7.33		200	c. e.b.Unsaturated, scyclic		5.94-601	3	1685-1665
b. Alkene, monosubstituted (vinyl)	10.05-10.15		536-366	d. e.f. Unsatutnied, cyclic.				
	202 317-5 310.93-11.05.	200	915-835	6-membered ring (and higher)	Q	40000	3	1685-1665
Margar and the same of the sam	90/T-40,7 bras	100	1430-1410	Control Statembered Ting	S .	5.80-5.85	\$	1725-1708
paralkene, disubstituted, cit	2 27 TO -1460	2000 C. 60 X	269	c. a.f., a.f. Unsaturated, reyelic	ž.	-109-66.5	3	1670-1663
Alkehe, disubstituted, trans	10.31-10.42	3	978-560			5.88-5.95	3	1700-1630
	2and 7.64-7.72	3	1310-1295	The state of the s		5.99-6.02	3	1670-1660
Alkene, disubstituted, gem	S. 11.17.18	8	855-685	h. e-Diketones		\$.78-5.85	3	1730-1710
and allegated in	and 7.04-7.09	100 - (E)	1420-1410	i. p. Diketones (enolic,)		6.10-6.50	Ξ	1640-1540
Alkene trisubstituted	11.90-12.66	3	\$40-790	j. I,4-Quinones	3	\$.92-6.02	Ξ	1690-1663
C. Alkyne D.	-15.9	3	97	k. Ketenes	1	14.65	Ξ	27.2
d. Aromatic, substitution type:1	(3)		;	2 ALDENYDES	9	3		·
five adjacent hydrogen atoms	-13(a)	ં (૪. ક)	1780	2. Carbonyl stretching vibrations	1	****		
Property Control of the Control of t	2 mmd -143	(X.S)	- 20	Saturated, all phatic	12.	5.75-5.81	3	1740-1720
four adjacent hydrogen atoms	٠	्र (४:४)	2750	e.B-Unsaturated, aliphatic		5.87-5.95	3	1705-1680
menthree adjacent hydrogen atoms	25.00-55.2	(W.m.)	27.0		F 12.	5.95-8.02	3	1680-1650
wordjacent hydrogen atoms	5.18-7.85 -120	(w.w)	-630	CACHE STANKER PROCESS IN TRANSPORT		5.83-5.90	Ξ	1715-1695
and a second hydrogen atom	jen day	(A. A.)	-880	b. C-H Stretching vibrations, two bands	17-84 -	3.43-335	1	2900-2820
3. CC. MULTIPLE BOND STRETCHING	3	00010000		Company of the Compan	and.	3.60-170	3	2775-2700
Alkene, nonconjugated	5.95-6.17	3	0031-0091	STER STRETCHING VIBRATIONS	÷.			
Alkene, monosubstituted (viayl)	and the second	3	1185	a. Saturated, acyclic		5.71-5.76	3	1750-1735
Alkene, disubstituted, cis.		(H	234	D. Saturaled, cyclic:				
Alkene, disabstituted, trans	CONTRACTOR OF THE PROPERTY OF	Œ	-1675	+lactooes (and larger rings)		271-174	Ξ	1750-1735
	-	-	The second second	1-18-00 acs			1	1700 1700

es abor those went hands in the reyfon 5.0-6.0 p. (2000-1970 cm.-1) region orbotistion type. See Fig. 3-30.

3550-3450

(v. sh) (s. b)

(v. sh) 3650-3590

(v. sh) 3570-3450 (w. b) 3200-2500

sh = sharp,

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1350 1350 1350 1350 1345 1345

SS (EEEEE)

1620-1530

CHARACTERISTIC INFRARED ABSORPTIONS OF FUNCTIONAL GROUPS

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CTERISTIC INFRARED ABSORPTIONS OF FUNCTIONAL GROUPS

Intensity Range cm-1

1750-1700

0.1780-1770 - 1.580 - 1.1840 - 1.740-1650 - 1.740-1650 - 1.710

333333333 SSSS

	200 am	2000	dnoiD	Konge #
The state of the s	7 × 1 0 × 1			
	Ŕ		Cyclic, y-lactams, fused to another	
vinyi ester type and a second		1800-1770	ring, dilute solution	5.71-5.88
a R-unsaturated and aryl	5.78-5.82	1730-1717	Cyclic, B-lactams, dilute solution	5.68-5.78
a, 8-unsaturated 6-lactone	5.78-5.82 (\$)	1730±171	Ovelie, 8-lactams, fused to another	
2,B-unsaturated y-lactone	5.68-5.75	1750-1740	citals solution	37 6 67 5
8,7-unsaturated 7-lactone	~5.56 (\$)	~1\$00	in the second second second	
d. o-Ketoesters		0521-35Z1	I I I I was madical formant based at	70.07
6-Keinesters (enolis)		SYL	Oreas, cycle, e-incinocred nng	20.10
	1	0001	Oreas, cyclic, 3-membered ring	~5.81
	(\$)	1/80-1/40	Urethanes	5.75-5.92
CARBOXYLICACIDS	e de la constante de la consta		Imides, acyclic	~5.85
a. Cartonyl stretching vibrations:				2nd ~ 5.88
saturated aliphatic	5.80-5.88	1725-1700	Inides cyclic 6-membered ma	
a.B-unsaturated aliphatic	5.83-5.92	-		20.0
	į	_	O STEEL STEEL	
h Hudrorul etretching Thomdad		(a)	לושומכאי כאכווכי מיש-תוציותו שוכםי	
מאמנסאלו אתפוכוווונף (סטותכת),			o-membered nng	`
several bands	er	7.00-2500		and ~5.99
c. Carboxylate anion stretching	6.21-6.45	1610-1550	Imides, cyclic, 5-membered ring	~ 5.65
	(s) (s) 1.15-7.69	1400-1300	Complete State of the Complete	23d ~5.88
ANHYDRIDE STRETCHING	7.5 -0234	· 公子	Imisles, eyelie, a.B-unsaturated	
VIBRATIONS	- A	100 mm (200 mm)	S-membered ring	95,7
Carmated sacuration of the sacrates	5.41-5.56	1850-1800		28 3 Per
		1790_174h	T N I	
The state of the passesses of the state of t	CA 2-CA 2	1870 1780	Design Continue Manuals	70 6
מים-סיומים שונה שונה של זי שר לרחר		170-170	ו וווואוץ, זוכב ואס סחוסי	200
Consequence of the second blood of the second of	073 573	0031 0031	The state of the s	
c. Saturated, S-memorica inig	6 6 6 7 1	1900 1750	ramay, bonded, two cands	•
and the second s		001-001	The second of t	C1.C1
d. a.fUnsaturated, 5-membered ring	3.41-5.50	1837–1881	Secondary, free; one hand	~2.92
	and 5.47-5.62 (s)	1830-1760	Secondary, bonded; one band	3.0-3.2
ACYL HALIDE STRETCHING			c. N-H Bending vibrations	
VIBRATIONS		10 m	Primary amides, dilute solution	6.17-6.29
a. Acyl fluorides	-5.41	~;\$30	Secondary amides, dilute solution	6.45-6.62
b. Acyl chlorides	~5.57 (S)	~1795	C. Miscellaneous chromophoric groups	
c. Acyl bromides and particises seed	~5.53	~1810	-1. ALCOHOLS AND PHENOLS	
a 6-Unsaturated and arvi	5.61-5.72	1780-1750	a. O—H Stretching vibrations	
	and 5.72-5.82 (m)		Free Off Hand Service Services	274-279
September 1998 Company Control of the Control of th	\$ 10		bobased mesosbyd virginialization	9
	Santa a	10.00	And the state of t	
r. coci.	e e	0701	(Change on dilding)	20,000
g. COBrz	(5) /5%	1878	single hindge compounds	7.82-2.90
1. AMIDES	!		polymeric association	2.94-3.13
a. Carbonyl stretching vibrations	entancement of the second of the second of the second of	A STATE OF THE PROPERTY OF THE PERSON OF THE	Intramolecularly hydrogen bonded	•
Primary, solid and concentrated	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	THE WORLD WINDOWS	(no change on dilution)	
colution	~6.06	~1650	single bridge compaunds	2.80-2.90
Primary dilute solution		~1690	chelate compounds	3.1-4.0
Secondary solid and concentrated	FREE COST OF TANKS OF THE PROPERTY OF THE PROP		는 100 100 100 100 100 100 100 100 100 10	75 STS 1 - 2000/2003 in 19
	5.95-5.14 (s)	1630-1630	breviations: s = strong, m = medium, w	= weak, v = vanible, b = bread, st
Secondary dilute solution	,		- = approximately	
Territory solid and all colutions		:		
Cyclic Alactame dilute solution				
Configuration of the column				
Cyclic, Y-lactams, dilute solution				

1070-1030 1160-1140 1130-1300 1230-1150 1430-1350 1185-1165 1130-1340 1130-1340 1130-1340 1130-1340 1210-1150 1210-1150

800-600 800-600 800-500

Intensity Range cm-1

1570-1500 1370-1300 1570-1550 1380-1370 1550-1600 1300-1250 1600-1500 1680-1650

CHARACTERISTIC INFRARED ANSORPTIONS OF FUNCTIONAL GROUPS

<b>√</b> 0	CILMANCTERISTIC INFRARED ABSORETIONS OF FUNCTIONAL GROUPS!  Compounds:  aromatic  aromatic  aliphatic  b. C—NO, Nitrates  and 730-7.70  aliphatic  c. O—NO, Nitrates  and 726-6.05  d. O—NO, Nitrites  and 7.26-7.20  and 7.26-6.05  and 7.26-6.05  c. C—B  c. C—B  c. C—B  d. C—I  s. SULFUR COMPOUNDS  c. C—B  d. C—I  s. SULFUR COMPOUNDS	Intensity Ra 10
Orcup   Sange # Intensity Range cm-1	ENISTIC INFRARED ABSORETIONS OF PLYCHONAL GROUPS    Group  Group  C—NO <sub>2</sub> , Mitro compounds;  aliphatic  aliphatic  aliphatic  Alicas compounds  C—NO <sub>2</sub> , Nitrates  ALOGEN COMPOUNDS, C—X  RETCHING VIBRATIONS  C—F  C—F  C—F  C—B  C—B  C—B  C—B  C—B	
## Bending and C.—O streiching  ## alcohols	C-NO, Nitros compounds  C-NO,	
1000	C-NO <sub>2</sub> , Nitros compounds:  C-NO <sub>2</sub> , Nitros compounds:  C-NO <sub>2</sub> , Nitros compounds:  C-NO <sub>2</sub> , Nitros compounds  C-NO <sub>2</sub> , Nitros compounds  C-NO <sub>3</sub> , Nitros compounds  C-NO <sub>4</sub> , Nitros compounds  C-NO <sub>5</sub> , Nitros compounds  C-NO <sub>6</sub> , Nitros compounds  C-NO <sub>7</sub> , Nitros co	
ary alcohols and 7,4-7.9 (s) 1350-1260  ary alcohols and 7,4-7.9 (s) 1350-1260  ary alcohols and 7,1-7.6 (s) 1410-1310  s and 7,1-7.6 (s) 1410-1310  and 2,2-4.303 (m) 3,400-3300  alts  bending vibrations  and 2,2-4.303 (m) 3,400-3300  and 3,2-3.3 (s) 1600-1575  and 4,5-4.50 (s) 1360-1300  and 6,5-6.29 (s-m) 1650-1300  and 6,5-6.29 (s-m) 1650-1300  and 6,5-6.30 (s) 1360-1310  and 6,5-6.30 (s) 1360-1310  and 6,5-6.30 (s) 1360-1310  and 7,1-7.6 (m) 2260-2240  includes  bending vibrations  and -2,4-4 (m) 2260-2240  includes  bending vibrations  and -7,1 (m) 2260-2240  includes  and -7,1 (m	ENISTIC INFARED ABSORUTIONS OF PLYCTIONAL GROUPS    Group  Group  C—NO <sub>2</sub> , Mitro compounds;  aliphatic  Alipha	
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ary alcohols  ary alcohols  s  sleabhols  s  and 71-76  s) 1350-1260  -8.3  s) 1410-1310  s  structuling vibrations  y, free; two bands  and 71-76  s) 1410-1310  310-1300  310-1300  310-300  3	and and and	
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Stretching vibrations  Stretching vibrations  Stretching vibrations  Stretching vibrations  Stretching vibrations  saits	Da Da	
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Stretching vibrations	Pur Pur	
Stretching vibrations  Stretching vibrations  Stretching vibrations  y, free; two bands  and -2.4 (m) -3400  186-3.02 (m) 3500-3310  2ats  ant -2.4 (m) 3400-3300  2ats  Bending vibrations  6.05-6.29 (s-m) 1650-1590  6.00-6.45 (w) 1650-1590  6.14-1.58 (s) 1600-1575  and -6.67 (s) 1360-1210  11tic, primary  7.46-8.00 (s) 1340-1290  11tic, tertiary  1.20-1020	pur pur	
Stretching vibrations  Stretching vibrations  3, free; two bands  and -2.84 (m) -3400  any, free; one band  2, 84-3.02 (m) 3500-3310  2, 84-3.03 (m) 3400-3300  2, 84-3.03 (m) 3400-3300  2, 84-3.03 (m) 3410-3000  3, 2-3.3 (m) 3130-3000  3, 2-3.3 (m) 3130-3000  3, 2-3.3 (m) 3130-3000  6, 66-6.29 (s-m) 1650-1590  6, 66-6.45 (w) 1650-1590  6, 66-6.45 (w) 1650-1590  6, 1360-1510  1, 44-5.00 (s) 1340-1290  1, 136-1500  1, 136-1500  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1020  1, 150-1040  1, 150-1040	pur pur	
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4.40-4.40 (m) 22.13-2240 tretching vibrations mas) /, (m) 1220-2070 sunds) /, (m) 1690-1640	sulfonamides 8.48-5.77	(S)
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C=N— Stretching vibrations (imines, oximes) Alkyl compounds 5.92-6.10 (v) 1670-1640		
(imines, oximes) 1, 5 Alkyl compounds 2		
3.92-6.10 (v) 1690-1640	#SI ~ pue	9 6
mpounds 6.02-6.14 (v) 1660-1630	f Abbreviations: s = strong, m = medium, w = weak, v = variable, b = broad, sh = sharp,	and sh = sharp
2008	roximately	. 27
6.14-6.35 (v) 1630-1575		
resident vibrations		
(s) (t) Type Tree Tree Tree Tree Tree Tree Tree Tr		
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HC-C-CH; 1093 Frotons Frotons Frotons HC-F; 155 HC-NR; 105 145 170 Cyclopropane HC-C-NR; 105 145 170 Cyclopropane HC-C-CR; 100 135 170 Cyclopropane HC-C-CR; 110 135 170 Cyclopropane HC-C-CR; 110 135 170 Cyclopropane HC-C-CR; 110 110 115 170 Cyclopropane HC-C-CR; 110 110 115 170 Cyclopropane HC-C-CR; 110 115 170 Cyclopropane HC-C-CR; 115 170 Cyclopropane HC-C-CR; 115 170 170 Cyclopropane HC-C-CR; 115 170 170 170 170 Cyclopropane HC-C-CR; 115 170 170 170 170 170 170 170 170 170 170		Methylene	Methine	Substituent Group	Protons	Protons	icne int	Proton
HE-C-CR; 109 1.45 1.70 Cyclopropa; 1.70 Cyclopropa; 2.45 1.70 Cycl	stituent Group P	Protons	Preton	HC-F	4.25	4.50		4.80
HC-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-	-C-CH <sub>2</sub>	1.20	1.55	HC-NO <sub>2</sub>	4.30	<b>4.3</b>	A Company of the Comp	7.00
Head-Color   House		1.35	1.70	Cyclobutane		2.45		\$4.5 6.70
HC-C(C=0)NR,   110   120   1	C  NB 41	1.55	1.95	Cyclopentane		1.61		4
HC-C-(C=O)NR;   1.10   1.50	-C-NH(C=O)R	1.50	1.80	Cyclohexane		1.54		8
HC-C(C=0)AR 1.15 1.35 1.90 Substituent Group Proton Shift Substituent Group Proton Shift HC-C(C=0)AR 1.15 1.35 1.90 HC-CAR 1.25 1.90 HC-CAR 1.25 1.90 HC-CAR 1.25 HC-CAR 1.25 1.90 HC-CAR 1.25 HC-CAR 1.25 1.90 HC-CAR 1.25 HC	-C-(C=0)NR;	1.50	1.80	Cycloneptane				
HC-C-ON (C-O)(C-O)(R and NR <sub>2</sub> ) 1.15 1.55 1.50 1.50 HC-C-O) (C-O)(R and NR <sub>2</sub> ) 1.15 1.55 1.50 1.50 HC-C-O) (C-O)(R and NR <sub>2</sub> ) 1.15 1.55 1.50 HC-C-O) 1.15 1.50 1.50 HC-C-O) 1.15 1.50 1.50 HC-C-O(R and NR <sub>2</sub> ) 1.25 1.50 1.50 HC-C-O) 1.50 HC-C-O) 1.50 1.50 1.50 HC-C-O) 1.50 1.50 1.50 1.50 HC-C-O) 1.50 1.50 1.50 1.50 HC-C-O) 1.50 1.50 1.50 1.50 ILS HC-C-O) 1.50 1.50 ILS HC-C-O) 1.50 1.50 ILS HC-C-O) 1.50 ILS HC	-C-(C=O)OR	1.55	1.90	Substituent Group	Proton Shift	Substituent (	2	Proton Shift
HCC-C-CSEC 1.20 HCC-C-C-CSEC 1.20 HCC-C-C-CSEC 1.20 HCC-C-C-CSEC 1.20 HCC-C-CSEC 1.20 HCC-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C-C	-C-Ar -C-Oli (and OR)	1.55	1.80	НС≡СН	2.35	H0-C=	0	10-12
HCC-C-SN   1.33   1.60   1.90   HCO-R   HCC-C-OAT   HCC-OAT   HCC-C-OAT   HC	-C-C=CR	1.50	1.80	HC=C-C=C	2.75	HO-NO		4.5-6.5
CC-CO(C=C)R   1.30   1.55   1.20   1.60   1.80	C-SR 1	1.60	2.00 1.90	HAI CONTRACT	7.20	HO-R		0.5-4.5
HCCCCSSI HCCCCNST HCCCNST HCCNST HCNST HCCNST H	-C-0Ar -C-0(C=0)R	1.55	2.00	HCO-R	9.4-10.0	HS-R		1-2
HC-C−O(C=O)CF <sub>3</sub> 1.40 1.75 HC-C−O(C=O)CF <sub>3</sub> 1.40 1.65 HC-C−C(C=O)CF <sub>4</sub> 1.55 HC-C−C(C=O)CF <sub>4</sub> 1.55 HC-C−C(C=O)Ar 1.65 HC-C−CH <sub>3</sub> 1.80 1.85 HC-C−CH <sub>3</sub> 1.80 1.80 1.85 HC-C−CH <sub>3</sub> 1.80 1.80 1.80 HC-CH <sub>3</sub> 1.90 1.80 1.80 1.80 HC-CCH <sub>3</sub> 1.90 1.30 1.50 HC-CCH <sub>3</sub> 1.90 1.30 1.50 HC-CCH <sub>3</sub> 1.90 1.90 1.30 1.50 HC-CCH <sub>3</sub> 1.90 1.90 1.90 1.90 1.90 1.90 1.90 1.90	-C-SH -C-(S=0)F, and -SO,R	1.60	1,65	HO-N=C(oxime)	9-12	HN-R		0.5-5
HCCCO(C=O)Ar 1.55 HCCCO(C=O)Ar 1.65 HCCC-B; HCCCB; HCCCB; HCCCCB; HCCCCCB; HCCCCCC 1.60 HCCCCCC 1.60 HCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCCC 1.70 HCCCCCCC 1.70 HCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 HCCCCCC 1.70 H	-C-NR3 ·1	1.75	2.05		,	- 1885 - 1886 - 1886		
HCC-Br HCC-CH,		1.80	1.95					
1.60   2.05   2.80	HC-C-Br	1.85	1.50	C	nemical Shifts (Valu	es given on the ô sca	le, relative to	TMS.)
2.05 2.10 2.10 2.10 2.30 2.55 C=C≤ C=C C=O C=O C=O C=O C=O C=O C=O C=O C=O	C C =0)0R (and NR <sub>3</sub> )	2.08 2.20 2.25	2.80	Substituent Group	Primary Carbon	Secondary Carbon	to	
Column   C		. 2.30	3.00 2.55	<b>I).</b>		25 10 45	30 to 60	35 to 70
C=00       2.20       2.40       C=N       20 to 45       40 to 60       50 to 70       65 to 70         and NR2)       2.25       2.45       2.85       C=Halide       37 to 35       -10 to 45       40 to 55       55 to 10       60       10 to 13       15 to 14       15 to 15       15 to 15       15 to 15       165 to 15       165 to 15       165 to 15       165 to 15       160 to 15       160 to 15       160 to 15       160 to	HC(C=O)R 2.10	2.35	2.65	0/0/	40 to 60	40 to 70	60 to 75	70 to 85
2.35 2.70 2.35 2.70 2.40 2.70 2.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.40 2.70 3.60 2.60 2.60 2.60 2.70 3.05 2.70 3.40 Alkynes 110 to 150 Carbonates 150 to Car	AT (and NR.)	2.40	) (	C-S	20 to 45 10 to 30		50 to 70	65 to 75 55 to 70
Lr       2.40       3.10       3.60       Alkynes       70 to 100       Isocyanides       130 to         R and -(SO)R       2.60       3.05       3.60       Alkenes       110 to 150       Carbonates       150 to         R and -(SO)R       2.60       3.05       3.40       4.10       C-qubstituted       125 to 145       Ureas       155 to         2.95       3.10       3.60       Heteroaromatics       115 to 140       Ureas       150 to         2.95       3.35       3.85       C-α       135 to 155       Esters, Anhydrides       165 to         3.05       3.45       4.05       Cyanates       105 to 135       Acids, Acyl chlorides       160 to         3.50       3.65       4.10       3.60       Isocyanates       110 to 130       Aldehydes       175 to         -0)R       3.60       4.00       4.60       Cyanates       120 to 140       Ketones       175 to	−SSR −(C=O)Ar	2.70	3 40	C-Halide	-37 to 35 (I) (CI)	(C) (C)	-	(1) (CI)
R and -(SO)R       2.60       3.05       Auxenes       110 to 130       Carbonates       130 to 130       Carbonates         2.70       3.40       4.10       C-substituted       125 to 145       Ureas       155 to         2.95       3.10       3.60       Heteroaromatics       115 to 140       Thioureas       155 to         2.95       3.35       3.85       Cα       135 to 155       Esters, Anhydrides       165 to         3.05       3.45       4.05       Cyanates       105 to 120       Amides       150 to         3.00       3.50       3.75       4.05       Isocyanates       110 to 120       Aldehydes       175 to         =O)R       3.60       4.00       4.60       Cyanides       120 to 140       Ketones       175 to	Total the year the St.	3.10	3 60	Alkynes	70 to 100	Isocyanides	Section 10 Section 10	
C=O)R 2.95 3.10 3.60 Heteroaromatics 115 to 145 Ureas 150 to 2.95 3.35 3.85 C-\alpha 135 to 155 to 1	$-SO_2R$ and $-(SO)R$	3.05		Aromatics	. 110 to 135	Oximes		
C=O)R  2.95  3.35  3.85  C-α  135 to 155  C-α  135 to 155  Esters, Anhydrides 150 to and -OR  3.20  3.40  3.60  3.75  4.05  Cyanates 115 to 135  Esters, Anhydrides 160 to Anides 160 to Acids, Acyl chlorides 175 to 3.80  4.00  4.00  4.00  4.00  4.00  Cyanides 110 to 130  Ketones 175 to		3.10	3.60	C-substituted	125 to 145	Ureas		8
and -OR 3.20 3.40 3.60 Cyanates 105 to 120 Amides 160 to 3.50 3.75 4.05 Isocyanates 115 to 135 Acids, Acyl chlorides 160 to 3.60 3.65 4.10 4.95 Thiocyanates 110 to 120 Aldehydes 175 to 3.80 4.00 4.60 Cyanates 120 to 140 Ketones 175 to 110 to 130		3.35	3.85	C-a		Esters, Anhyo	frides	6 6
=0)R 3.50 3.75 4.05 Indices 110 to 120 Adenydes 175 =0)R 150 3.65 4.10 4.95 Thiocyanates 110 to 120 Adenydes 175 3.80 4.00 4.60 Cyanides 110 to 120 Ketones 175	and -OR	3.40	3.60	Cyanates	105 to 120	Amides		160 to 180
3.80 4.00 4.60 Isothiocyanates 120 to 140 Ketones 175	=0)R	.3.75 4.10	4.05	Thiocyanates	110 to 120	Aldehydes	Morraes	175 to 205
	•	4.00	4.60	Isothiocyanates Cyanides	120 to 140	Ketones		õ

Type	J. cps	Турс	J, cps
H <sub>2</sub> +	280	C=CH-CH=C	9-13
CHit	12.4	H-C≡C-H†	9.1
H	12-15	CH-C≡C-H	10 <b>2+3</b> 18
H	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	H \$	in an Alice
CH-CI	, 9	CH-C	1-3
of the control of the control			y grin
-c-(-¢-)¢-	~0	`c=c'''	
н і н	<b>押报表</b> (		6-8
CH1CH2-X	6.5-7.5	Ö	
CH4			0-6-9
CHW	5.5-7.0	()	m- 1-3
CH,			p-0-1
	a,a 5-10		4.4.4.20
H-C-C-11	a.c 2-4		aft 0.6-1.0
Drain de la sec	c.c 2-4		an 1.3-1.8
, 11	The second second		/s/r 3.2-3.8
C=C	0.5-3	Egyptical Prof. Stories	REFERENCE
`H .			aff 2.0-2.6
11	7-12		aff: 1.5-2.2
C=C	No. of the Control of	· · · · · · · · · · · · · · · · · · ·	an' 1.8-2.3
11		15 2 <b>4 1</b> 6 22.0	BB 28-4.0
C=CL	13-18		
	market are 100 ft &	and party and the party of	aff 4.6-5.8
Н			aff 1.0-1.8
C=C	4-10	3	αα' 2.1-1 -##' 3.0-4.3
	43.47.	-0.00 Delta -0.00	8 8 7 7
C-11	All g. Toley Sg.	and the state of t	αβ 4.9-5.7
· · · · · · · · · · · · · · · · · · ·	·· ' ''" <sup>j</sup> 0.5-2.5	a consistency of the	ay 1.6-2.0
н	. and 11	$\bigcirc$	"/ 0.7 1.1
	and the second of the second o		nn' (1.2-0.5
н. с-и	-0 /2 5		By 7.2-8.5
C=C		and ald	BB 1.4-1.9

Conjugated dienes & Trienes, Solvent: Ethanol

Conjugated dienes of Triches, borr	
Parent value for Butadiene system	217 nm
or acyclic conjugated diene	
Acyclic triene	245 nm
Homoannular conjugated diene	253 nm
Hetroannular conjugated diene	215 nm
Increment for	each substituents
Alkyl substituents or ring residue	5 nm
Exocyclic double bond	5 nm
Double bond extending conjugation	30 nm
Auxochrome	
-OR	+6 nm
-SR	+30 nm
-Cl, -Br	+5 nm
NR <sub>2</sub>	+60 nm
-OCOCH <sub>3</sub>	0

Woodward Fieser rules for aB-unsaturated carbonyl compounds:-

Woodward Fies	ser rides for ab-uns	aturated card	onyi compounds
a) Parent value	S		
αβ-unsaturated a	cyclic or six	215 nm	est to the second
membered keton	e ·	. 44 4	
αβ-unsaturated	five membered ring	202 nm	
ketone		51 / A	1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
αβ-unsaturated	aldehyde	207 nm	
b)Increments	1997	57.75	A STATE OF THE STA
i) Each alkyl su	bstituents or ring r	esidue	
At a position		10 nm	
At β position		12 nm	
At gamma and h	igher position	18 nm	
ii) Each exocycl	ic double bond	5 nm	, g. 40 g
iii) Double bond		30 nm	
conjugation			
iv) Homoannula	r conjugated	39 nm	
diene	•		
Auxochromes	Positio	ns	
	α	β	gamma
-OH	35	30	50
-OR	35	30	17
-SR	-	85	
-OCOCH <sub>3</sub>	6	6	6
-Cl	15	12	
-Br	25	30	
-NR <sub>2</sub>	4	.95	