Exercises in Organic Structure Determination

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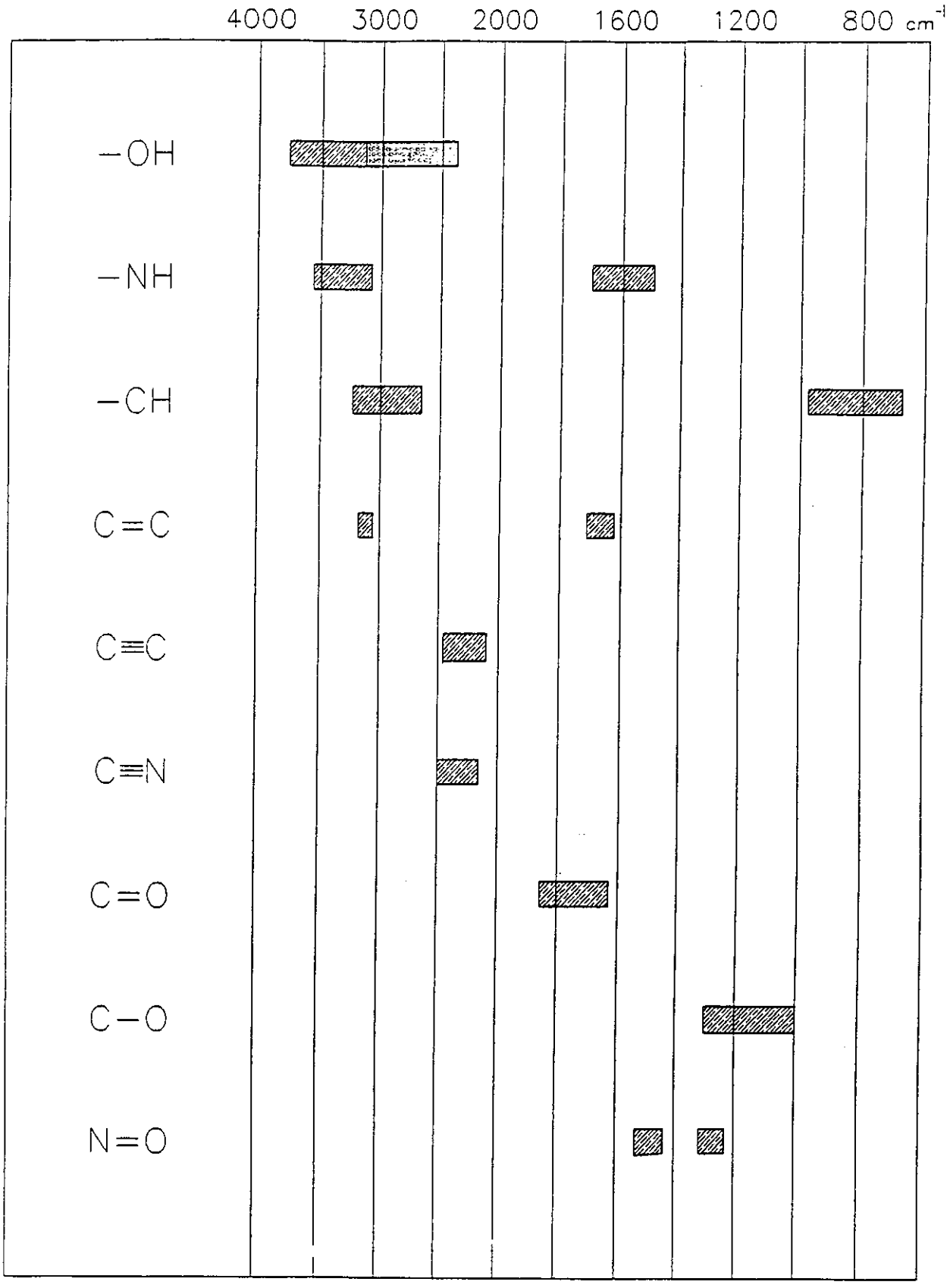
Common Infrared Absorbtion Ranges



Introduction:

This book is intended to be used in conjunction with a reference book, although we have included several tables for convenience. We have attempted to rank the accompanying problems in order of increasing difficulty although this a very subjective ranking. We have attempted to incorporate examples with elements other than C, H, N and O. We have included problems which contain I, Br, Cl, F, P, S, Si, Sn, Fe, Cr, Hg, Mo, and Rh. To this end we have included some standard unknowns as well as some organometallic compounds, research samples, natural products, and two polymer samples. We have not included the same information for every problem in part because we could not obtain the information and also because we felt that when one sits down to do a real world spectral problem one does not always start with the same amount of information.

Generally each problem includes a mass spectra and/or a high resolution mass spectra of the parent peak (exact mass), an infrared spectrum with the conditions of the collection, a ^{1}H NMR spectra and a ^{13}C NMR spectra. For some problems 2D NMR spectra are given.

Elemental analyses are included for many of the problems. In many cases the problems contain redundant information to provide experience in some of the newer NMR techniques.

The infrared spectra were collected on either a Mattson Cygnus25 FT Infrared spectrometer or a Perkin Elmer 710B Infrared spectrometer. The method of sample preparation is noted in each case. Table I illustrates the general spectral regions for some common organic functional groups.

Many of the mass spectra were obtained from the Wiley Registry of Mass Spectral Data. The others were collected on various Mass Spectrometers. The exact masses were calculated from the chemical formula.

All NMR spectra were recorded on General Electric QE300 FT NMR spectrometer. The ^{1}H NMR spectra were obtained at 300.2 MHz. The ^{13}C NMR spectra were obtained at 75.49 MHz. Table II shows some typical ^{1}H NMR shifts of organic compounds. Multiplicities of the ^{13}C NMR peaks are given through either off resonance decoupled spectra or an APT experiment.

The elemental analyses were calculated from the formula with oxygen done by difference. Analyses for Cl and Br were intentionally omitted since these are readily identified by their isotopic distribution patterns in the mass spectrum. The relative peak areas for proton NMR data is provided by either integration or the areas are typed in. The ^{13}C NMR broad band spectra were collected until it was determined that all carbons were accounted for, although, there are some cases of concidental overlap. The off-resonance spectra are offset

plotted in most instances, in several cases the results of the off-resonance spectra have been labeled with the broad band decoupled spectra as q (quartet, CH_3), t (triplet, CH_2), d (doublet, CH), or s (singlet, C). The APT (attached proton test) spectra are offset above the broad band spectra; a negative indicating an odd number of hydrogens attached (CH_3 or CH), a positive peak indicating an even number of hydrogens (CH_2 or C). In some spectra the APT results are not plotted, but given labels, u or d (up, positive; down, negative) with the accompanying broad band decoupled spectrum. In general, one can infer whether a positive peak is a CH_2 or C by the intensity; the quaternary carbon generally being much less intense. The methyl can be distinguished from the methine by the chemical shift; the methyl resonance usually being upfield of the methine. Generally any negative peaks below 60 ppm will necessarily be methines. Selected problems have 2-DNMR spectra attached. We have chosen to include only two of the many types of 2-D NMR experiments, the homo and hetero COSY.

Suggested Readings

Spectrometric Indentification of Organic Compounds, 5th ed., M. Silverstein, G.C. Bassler, and T.C. Morril, John Wiley and Sons, New York, NY, 1991

Modern NMR Techniques for Chemistry Research, A.E. Derome, Pergamon Press, Elmsford, NY, 1987.

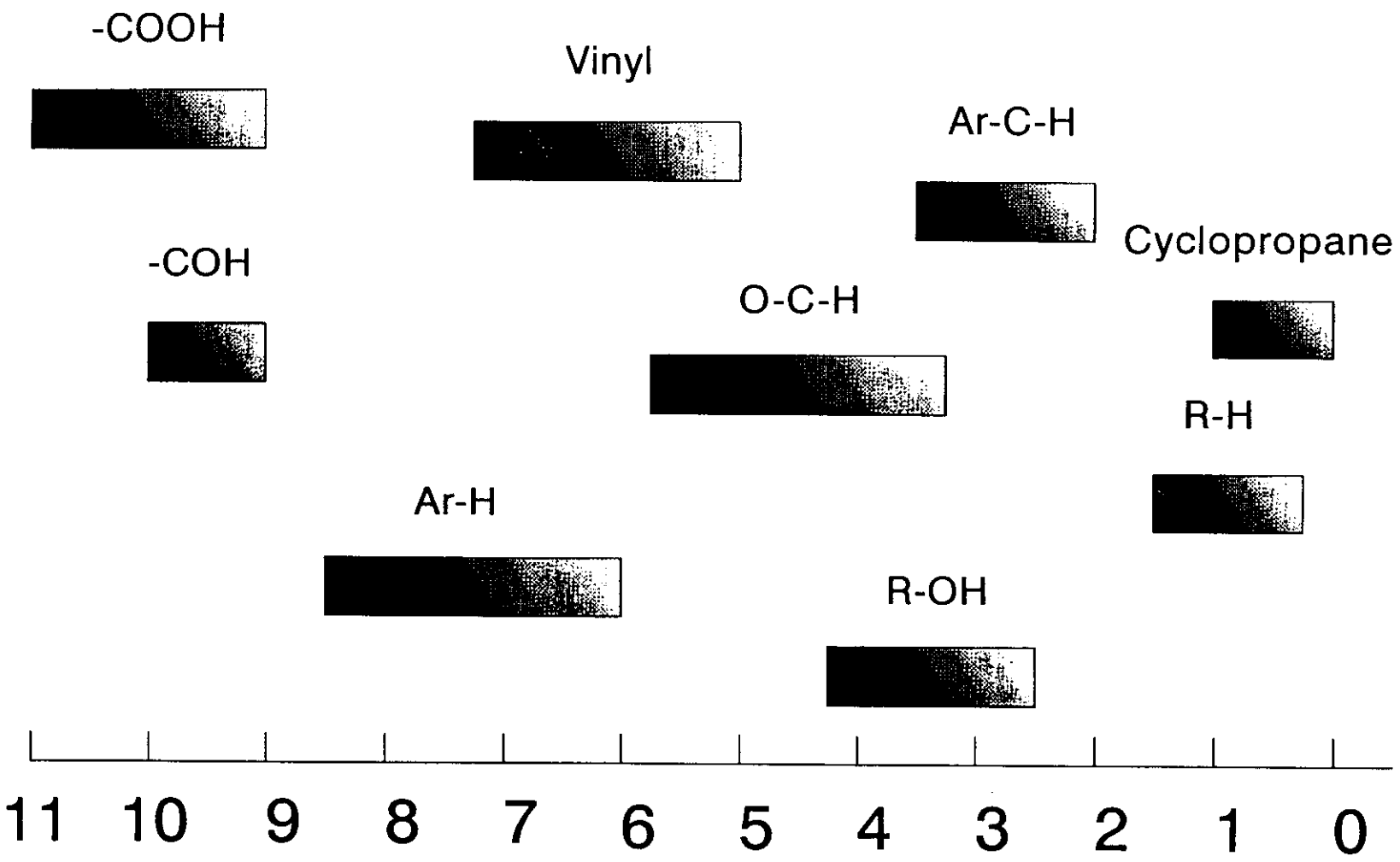
Interpretation of Mass Spectra, 3rd ed., F.W. McLaffety, University Science books, Mill Valley, CA, 1980

References

Tables of Spectral Data for Structure Determination of Organic Compounds, E. Pretsch, J. Seibl, W. Simon, and T. Clerc, Springer-Verlag, Berlin, 1983

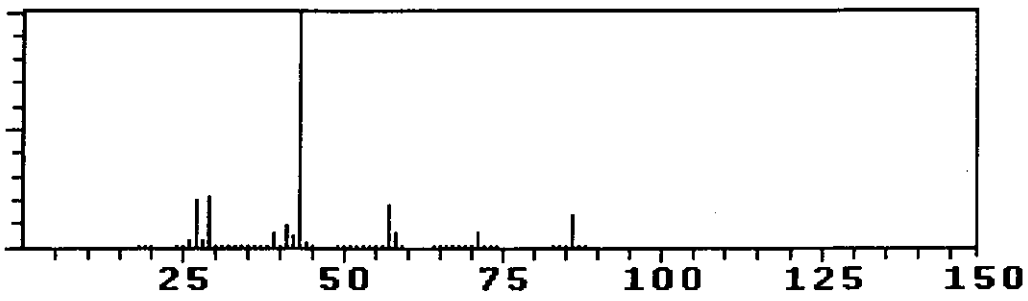
Infrared Absorption Spectroscopy, 2nd ed., K. Nakanishi, P.H., Solomon, Holden-Day, Oakland, CA, 1977

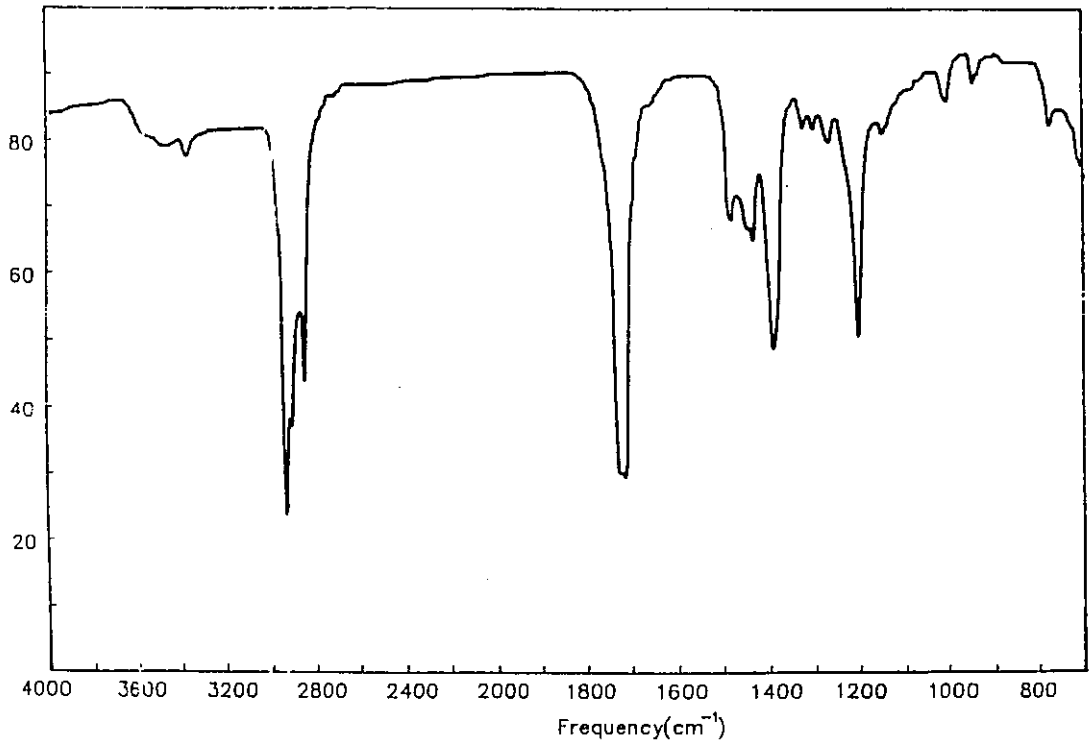
Common ^{1}H NMR Chemical Shifts

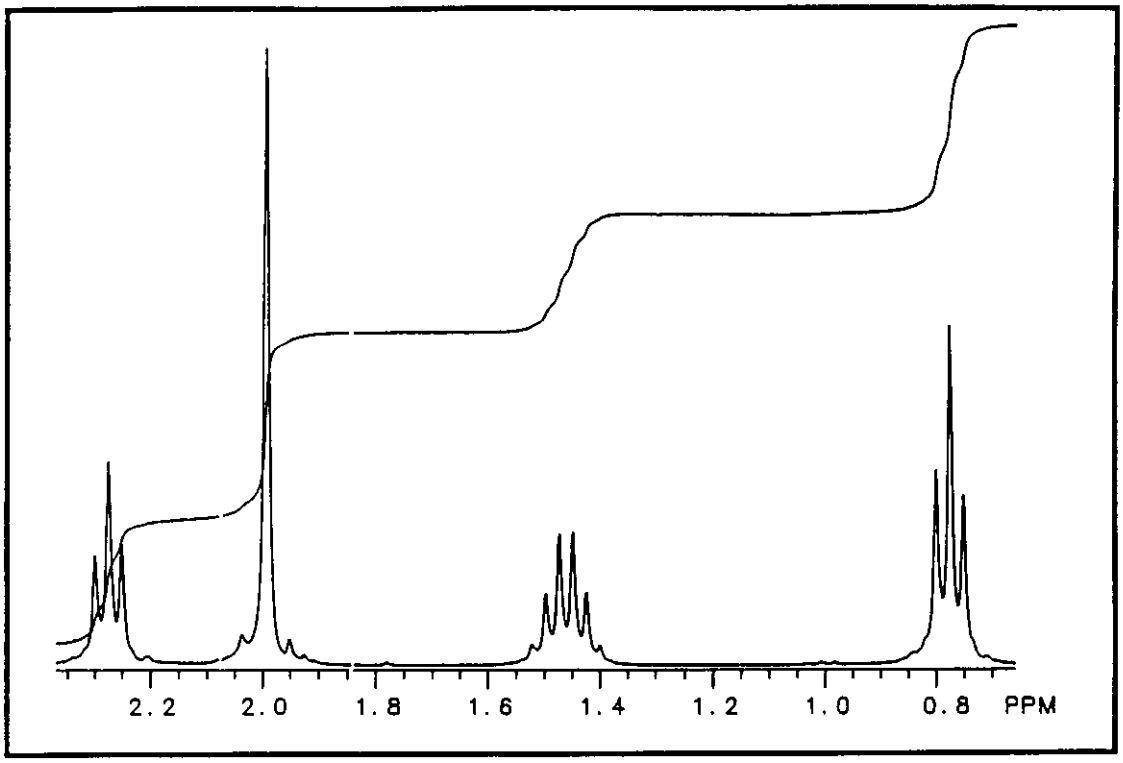


Problem 1

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



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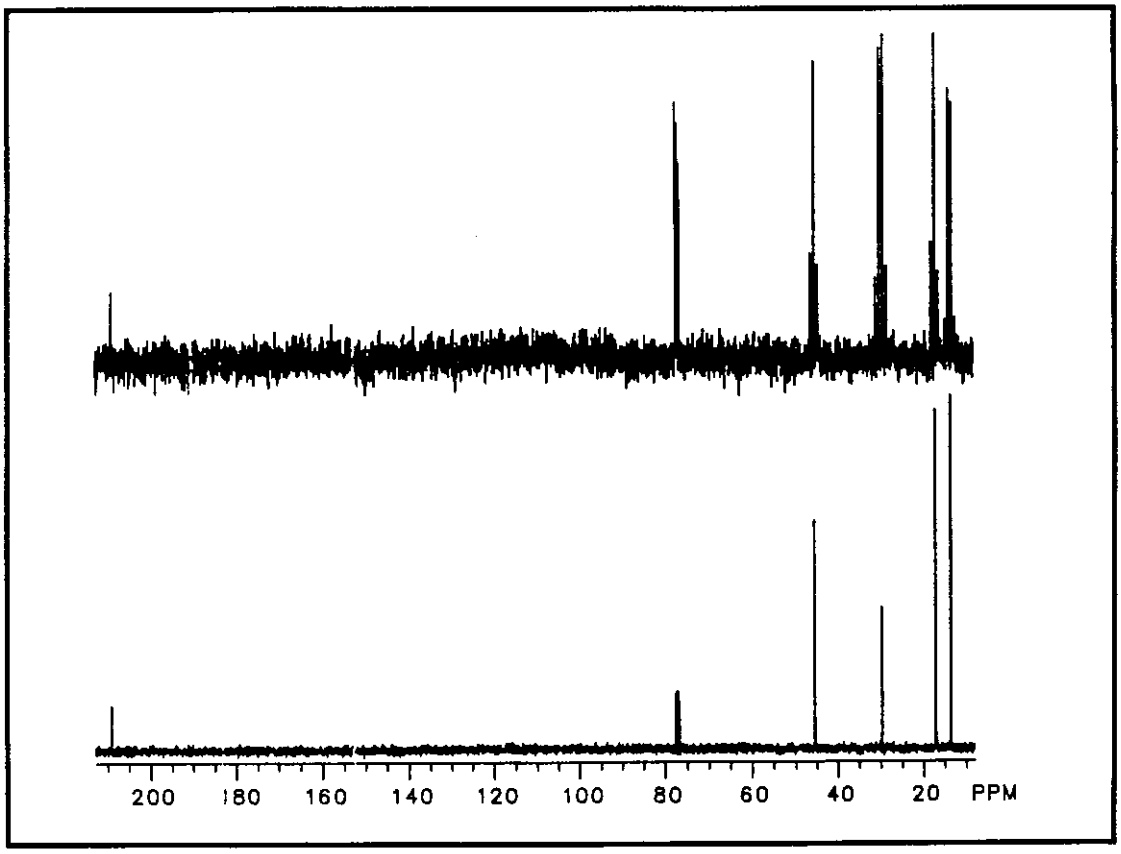
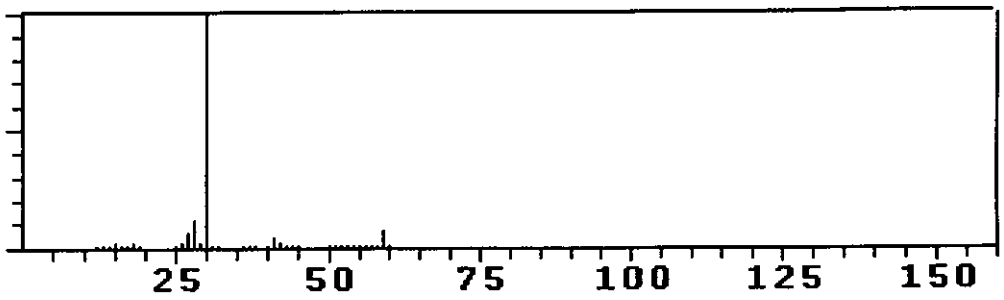
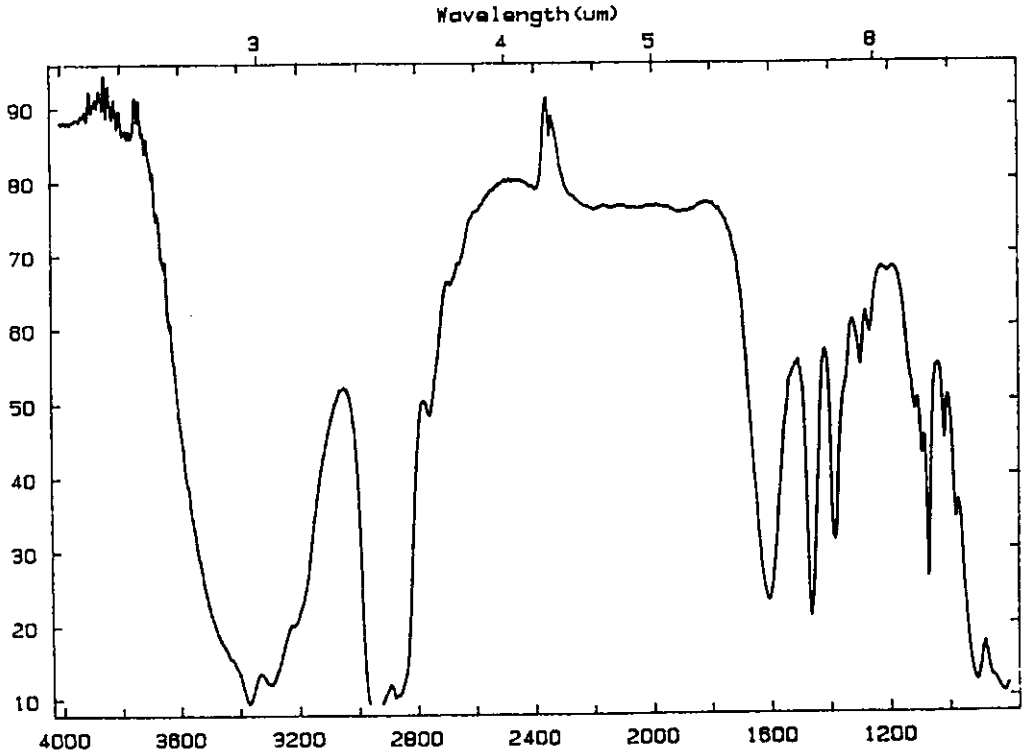
2.0
1.8
1.6
1.4
1.2
1.0
0.8
PPM

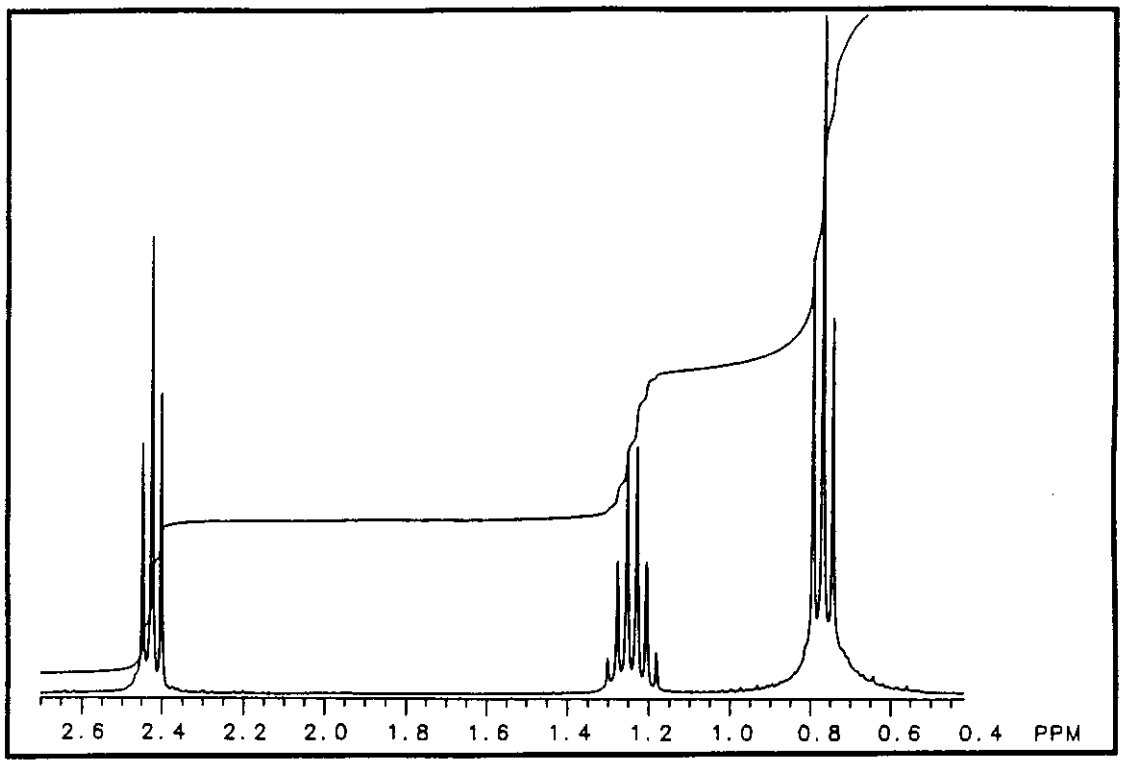

200
180
160
140
120
100
80
60
40
20
PPM

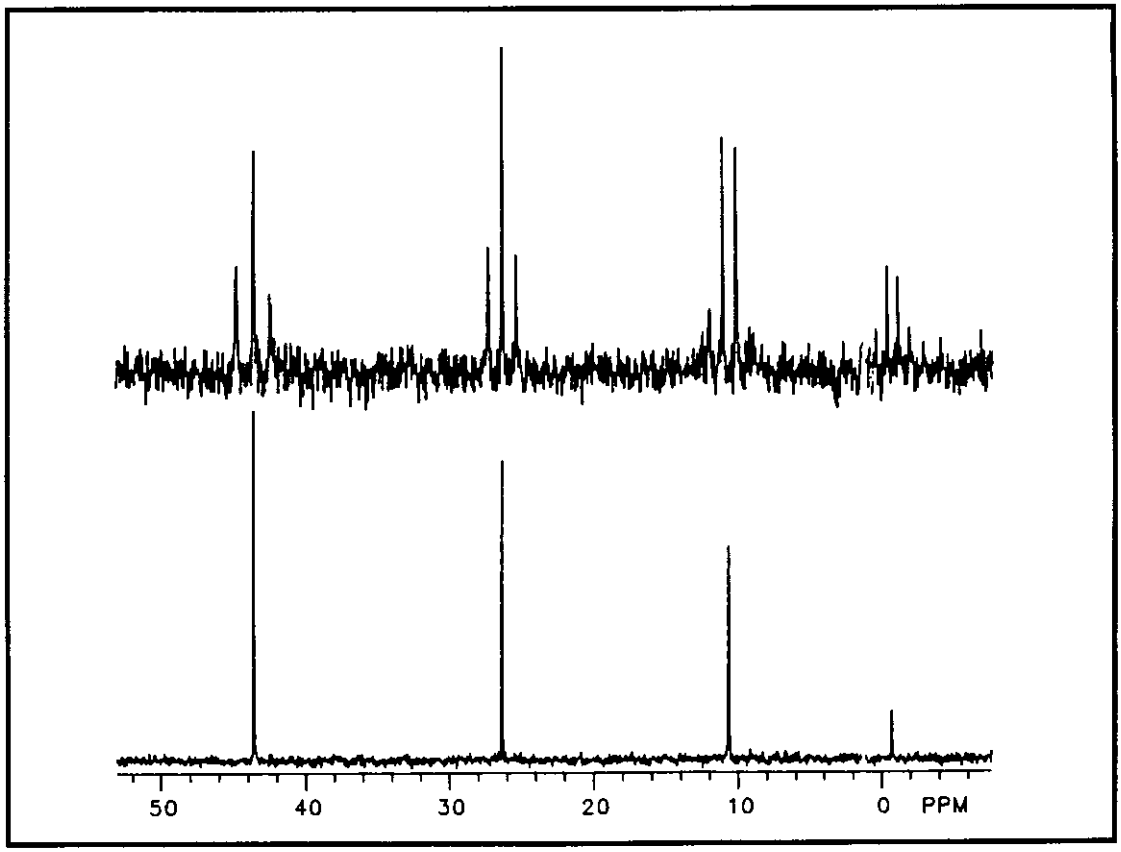
Problem 2

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



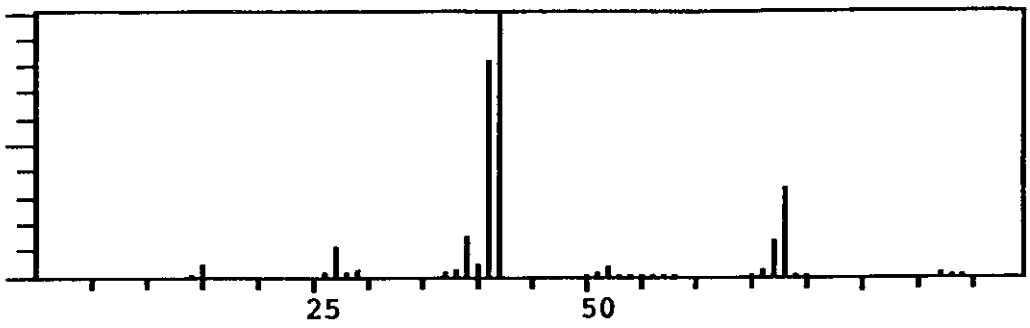


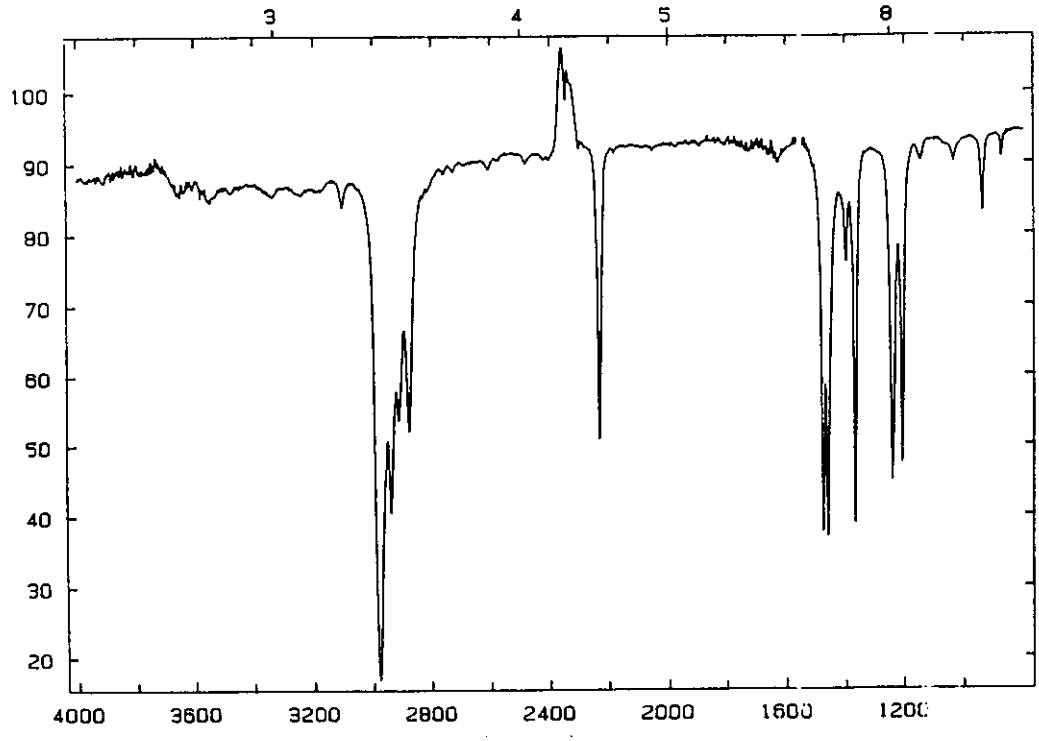

2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
PPM

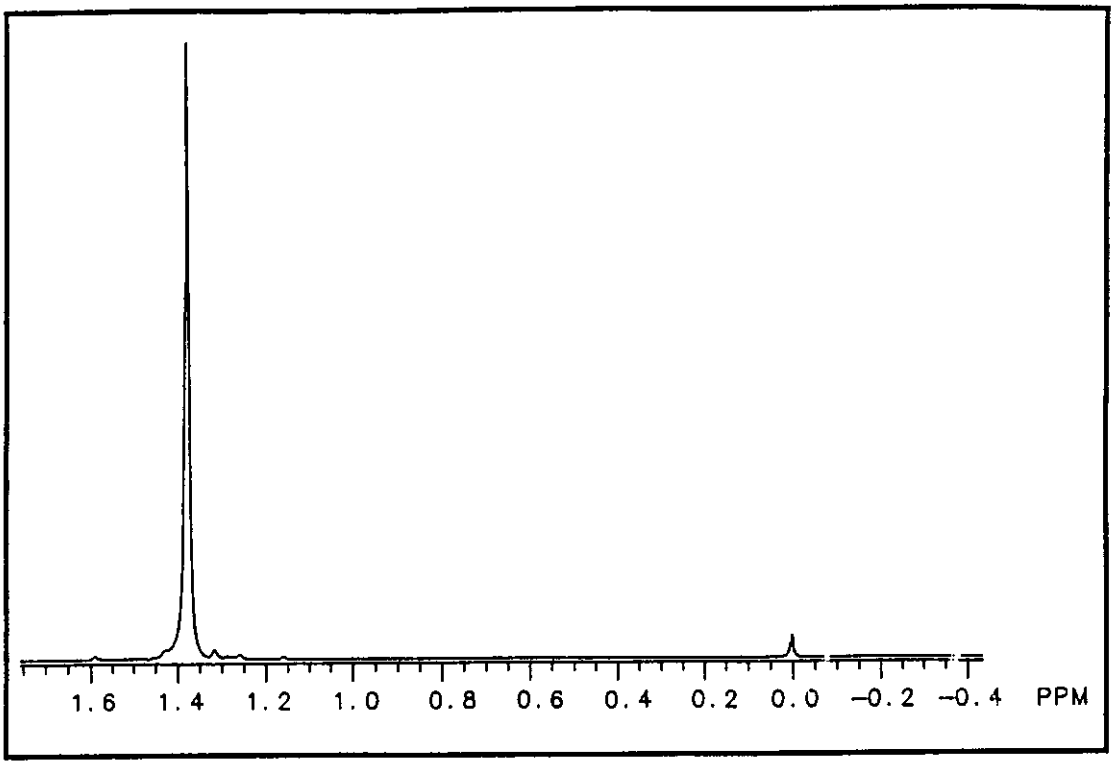

50
40
30
20
10
0
PPM

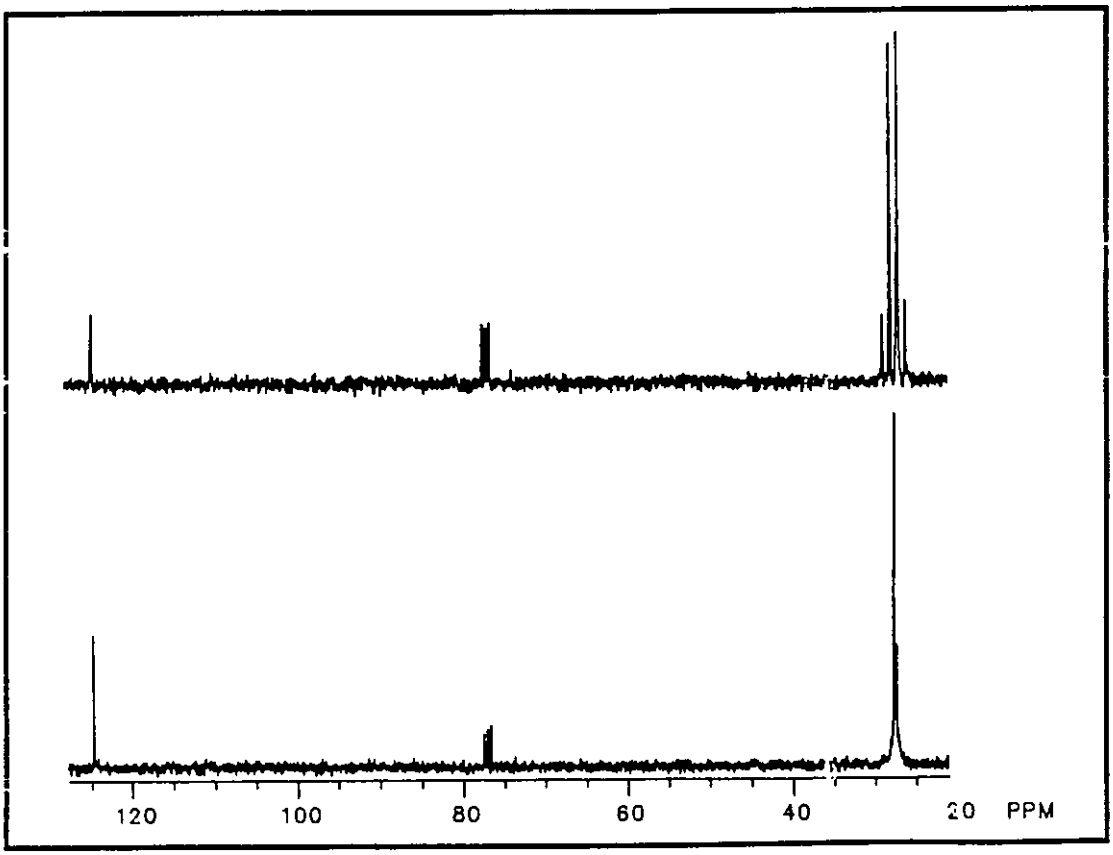
Problem 3

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



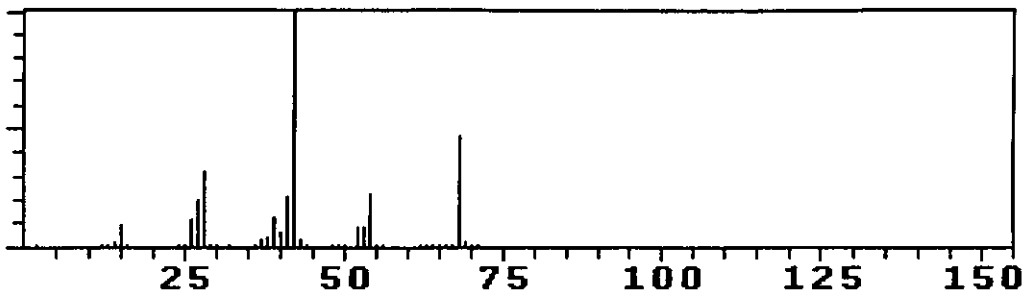


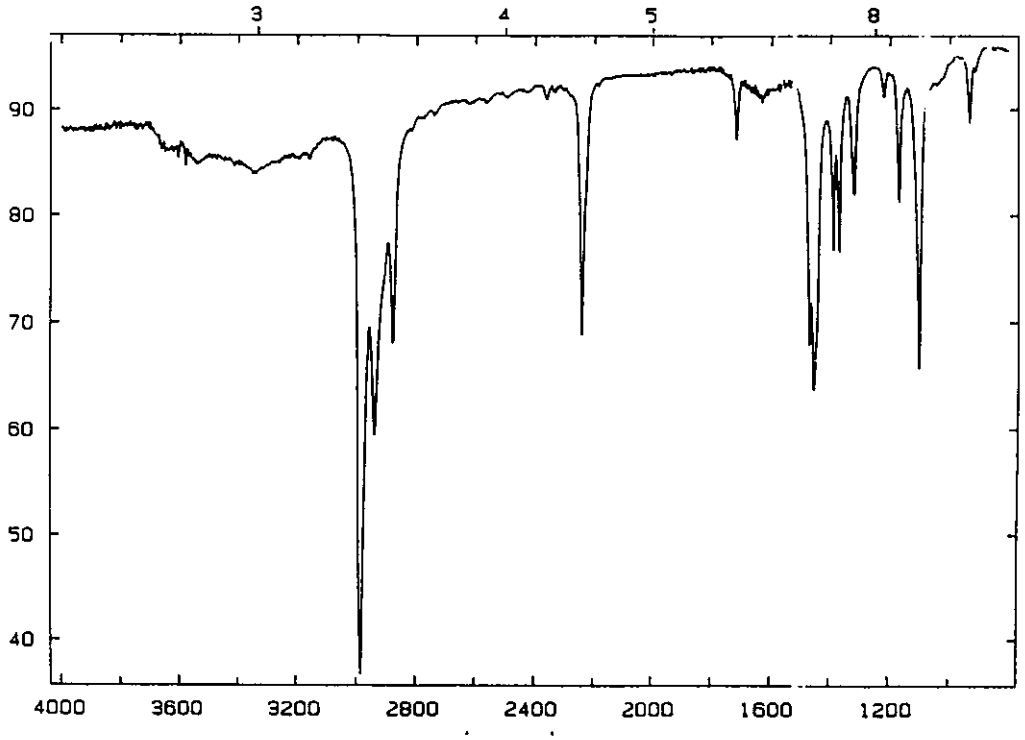

1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
PPM

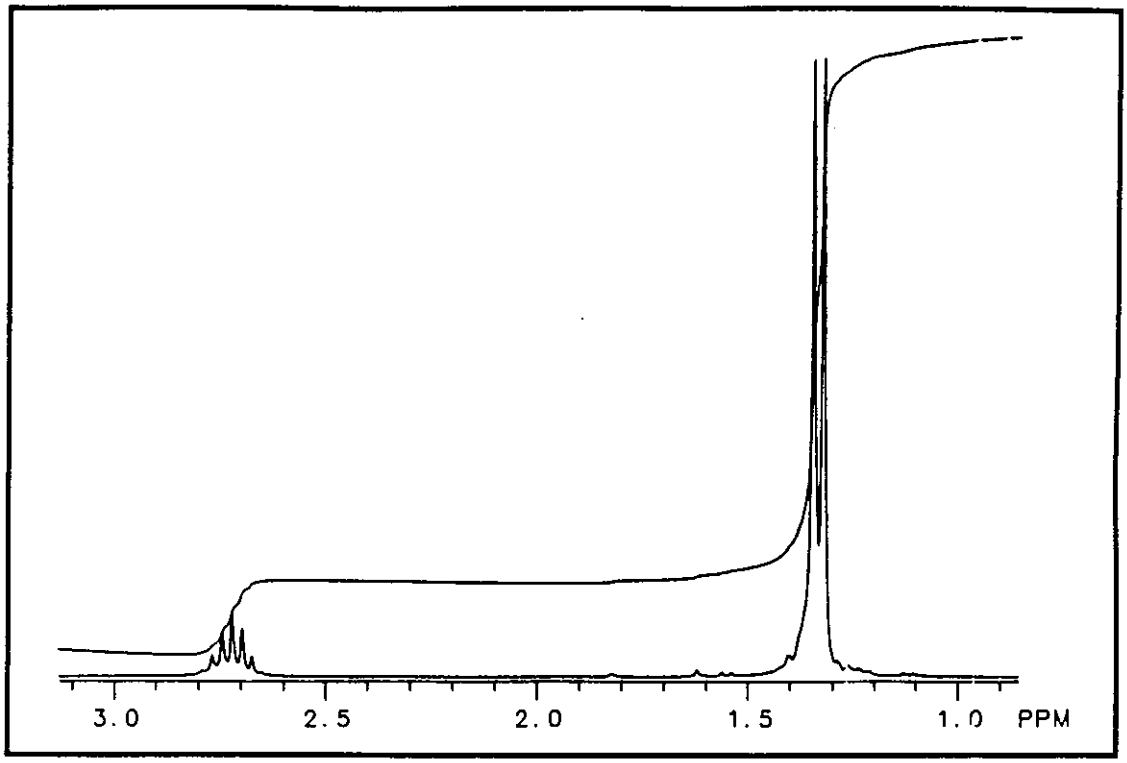

120
100
80
60
40
20
PPM

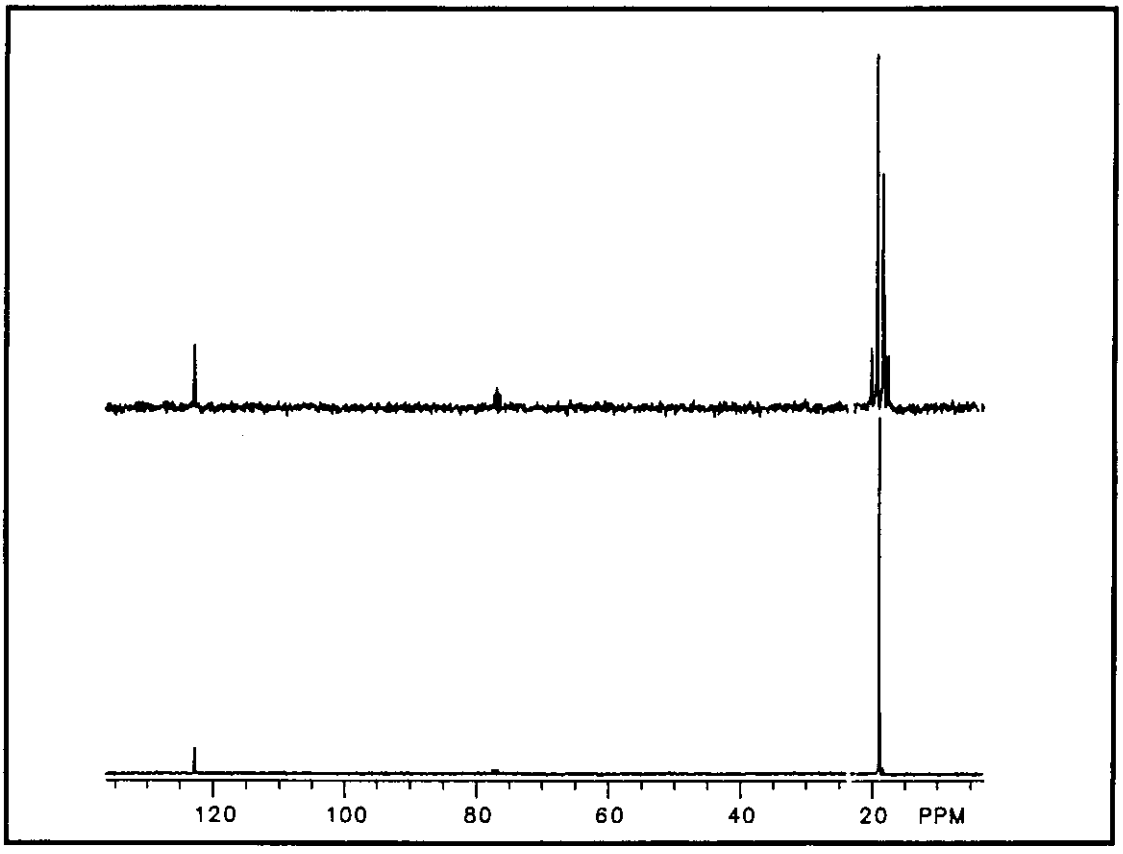
Problem 4

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





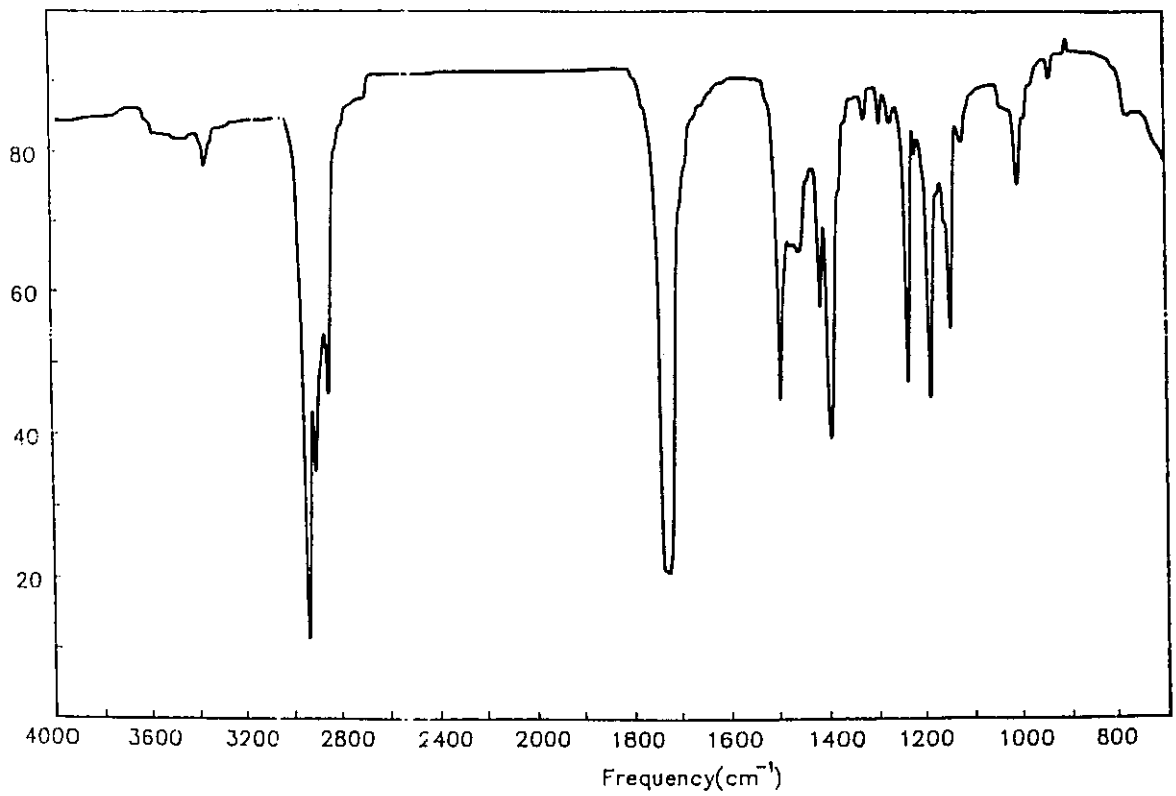

3.0
2.5
2.0
1.5
1.0
PPM

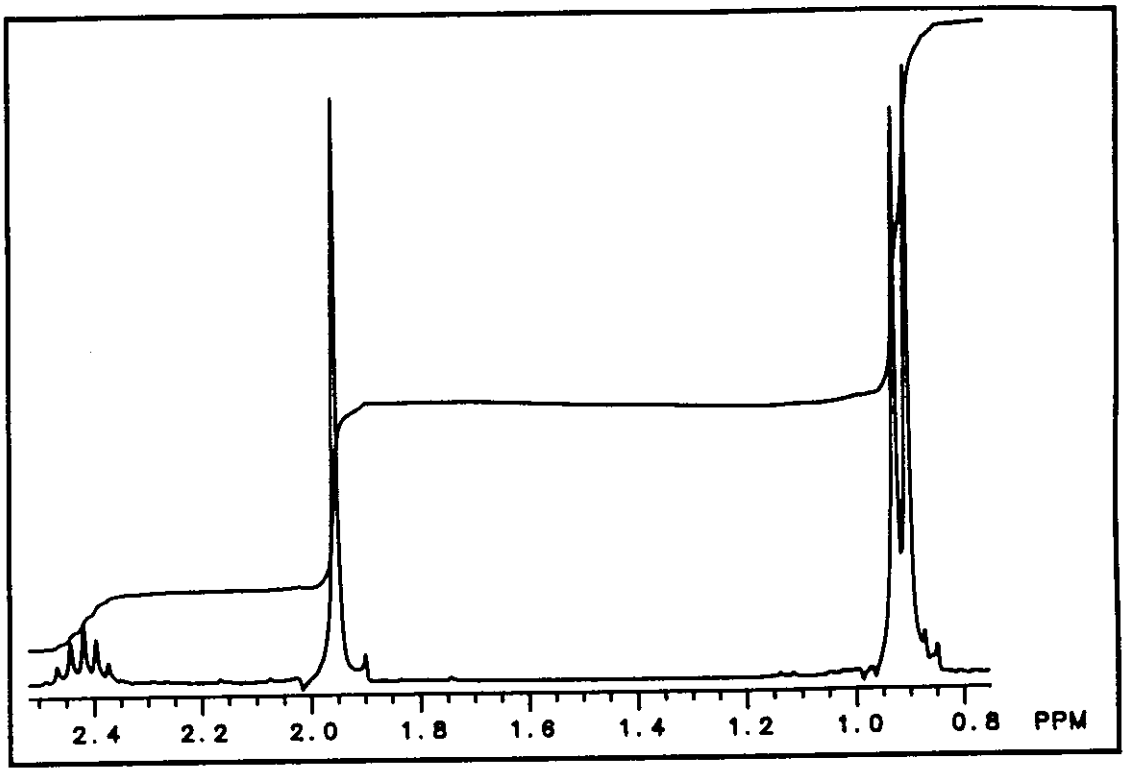

120
100
80
60
40
20
PPM

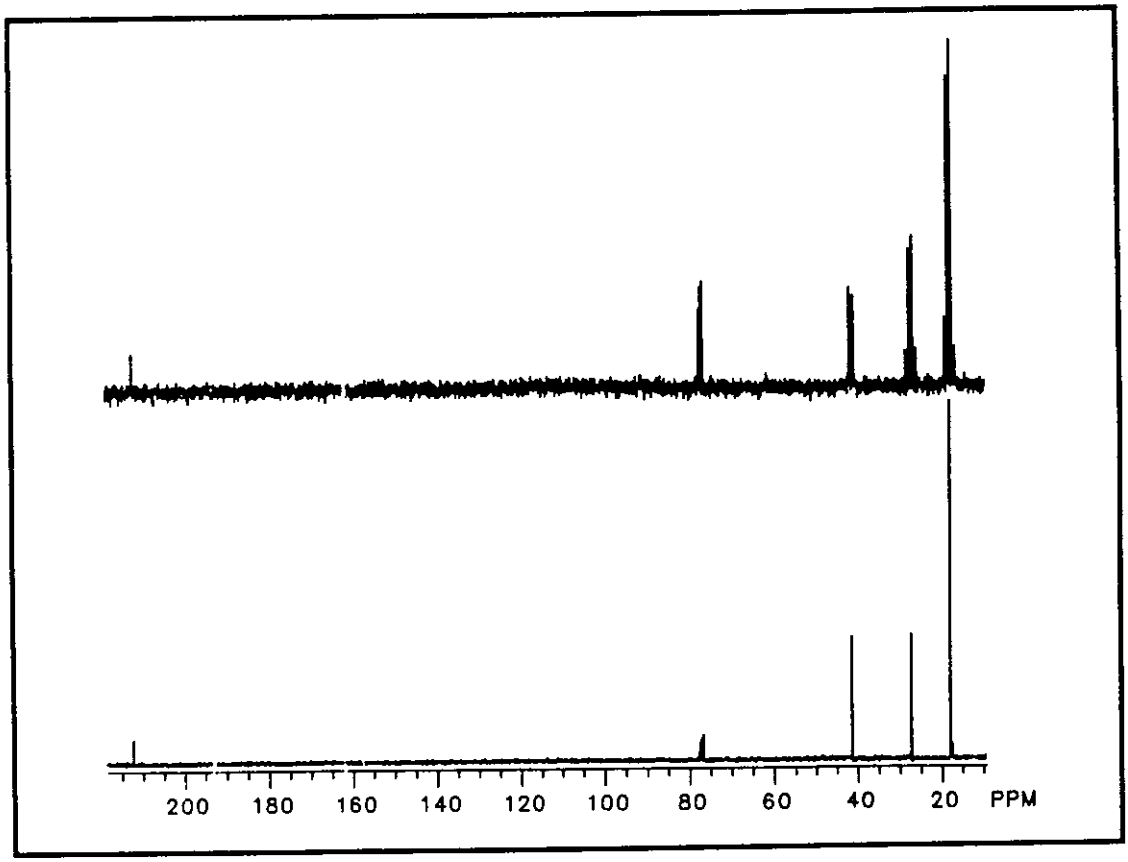
Problem 5

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass	R/A	Mass	R/A	Mass	R/A	Mass	R/A	Mass	R/A	Mass	R/A
25,	0.20	32,	0.10	42,	5.81	51,	0.30	58,	0.10	72,	0.20
26,	1.60	36,	0.10	43,	100.0	52,	0.10	59,	0.10	85,	0.10
27,	13.01	37,	0.60	44,	2.50	53,	0.40	63,	0.10	86,	9.81
28,	1.80	38,	1.10	45,	1.00	54,	0.10	67,	0.10	87,	0.60
29,	1.20	39,	6.71	46,	0.10	55,	0.60	69,	0.10	88,	0.10
30,	0.10	40,	0.90	49,	0.10	56,	0.20	70,	0.10		
31,	0.20	41,	13.01	50,	0.30	57,	0.20	71,	3.80		

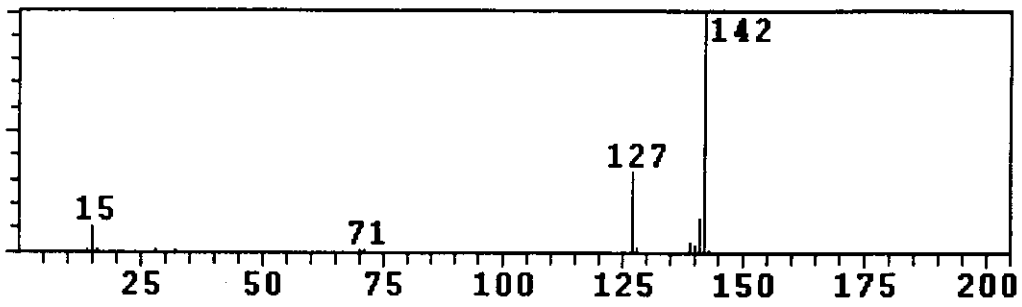


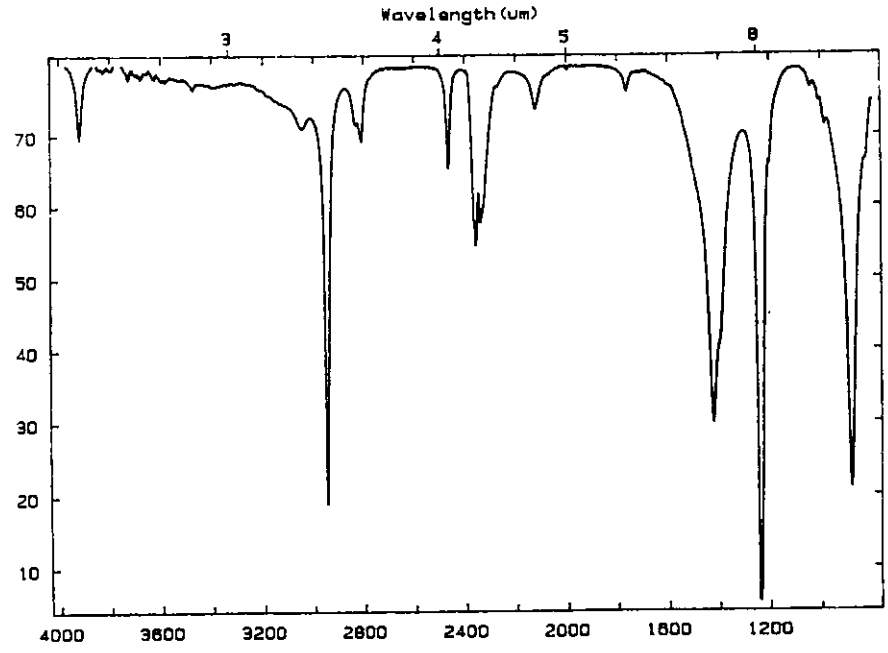

2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
PPM

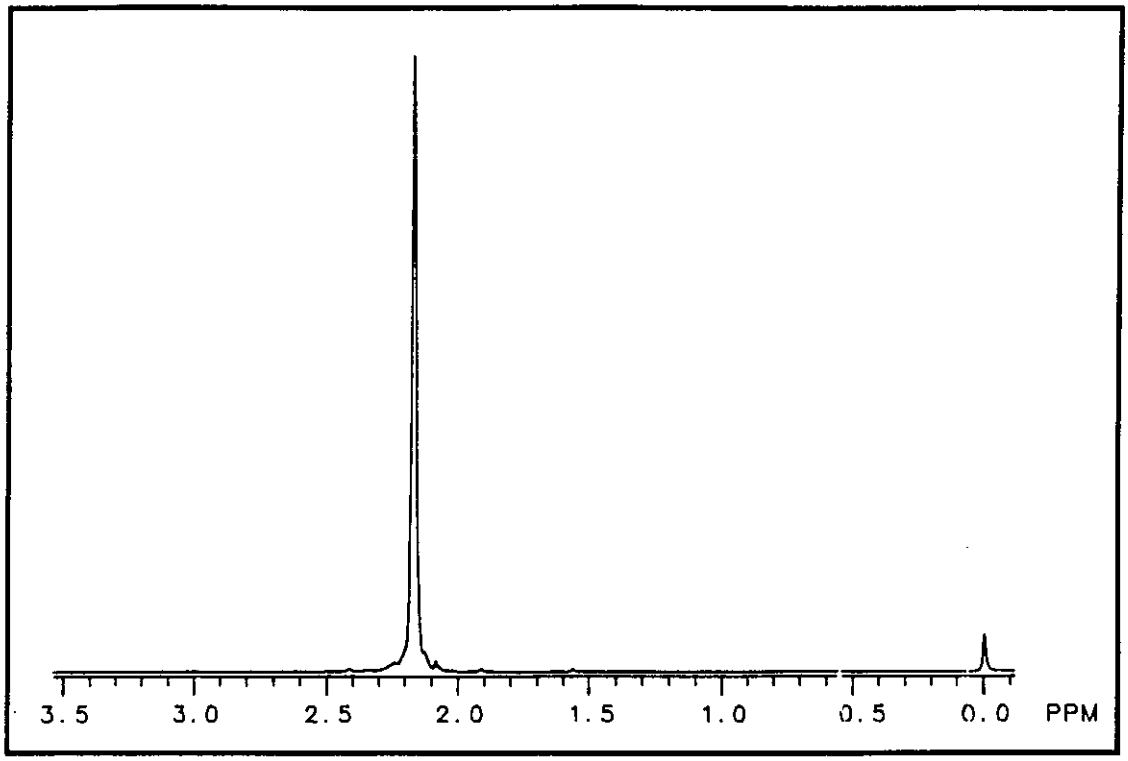

200
180
160
140
120
100
80
60
40
20
PPM

Problem 6

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na






3.5
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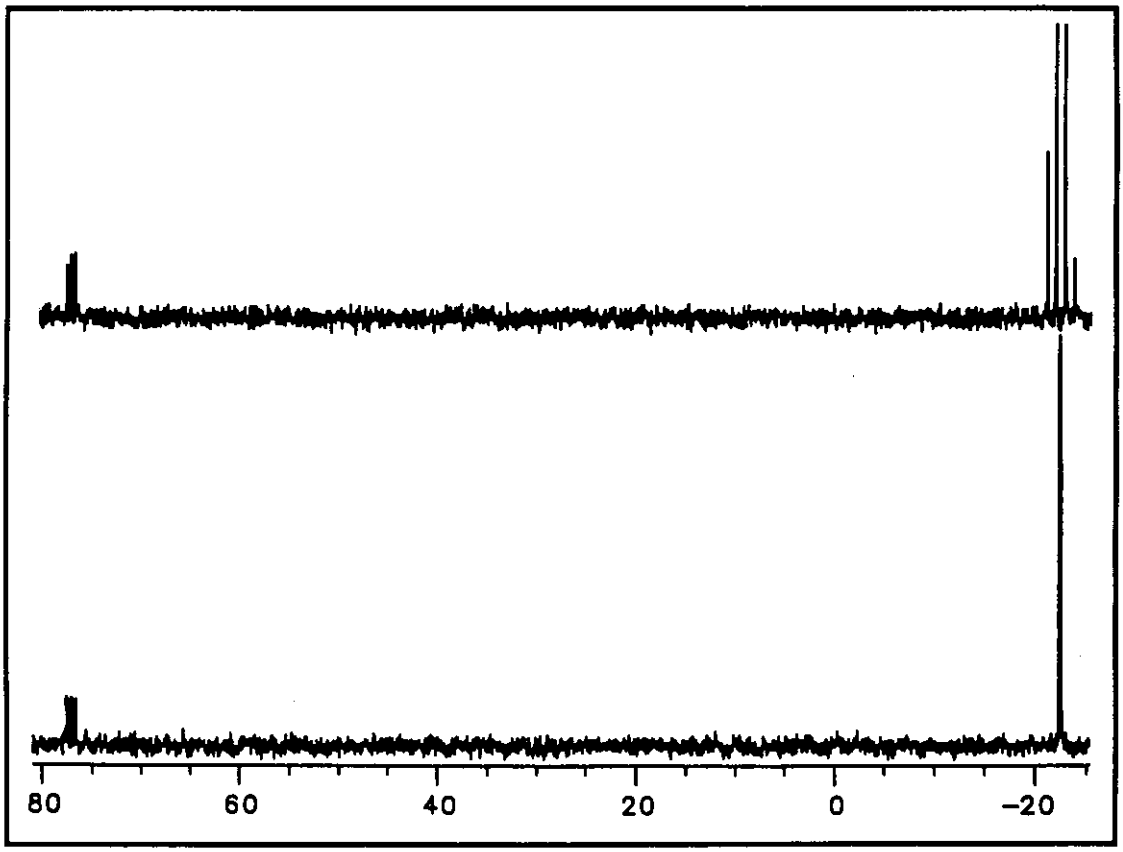
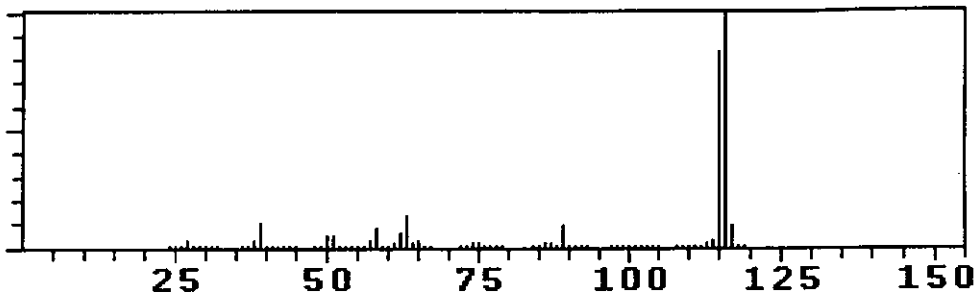
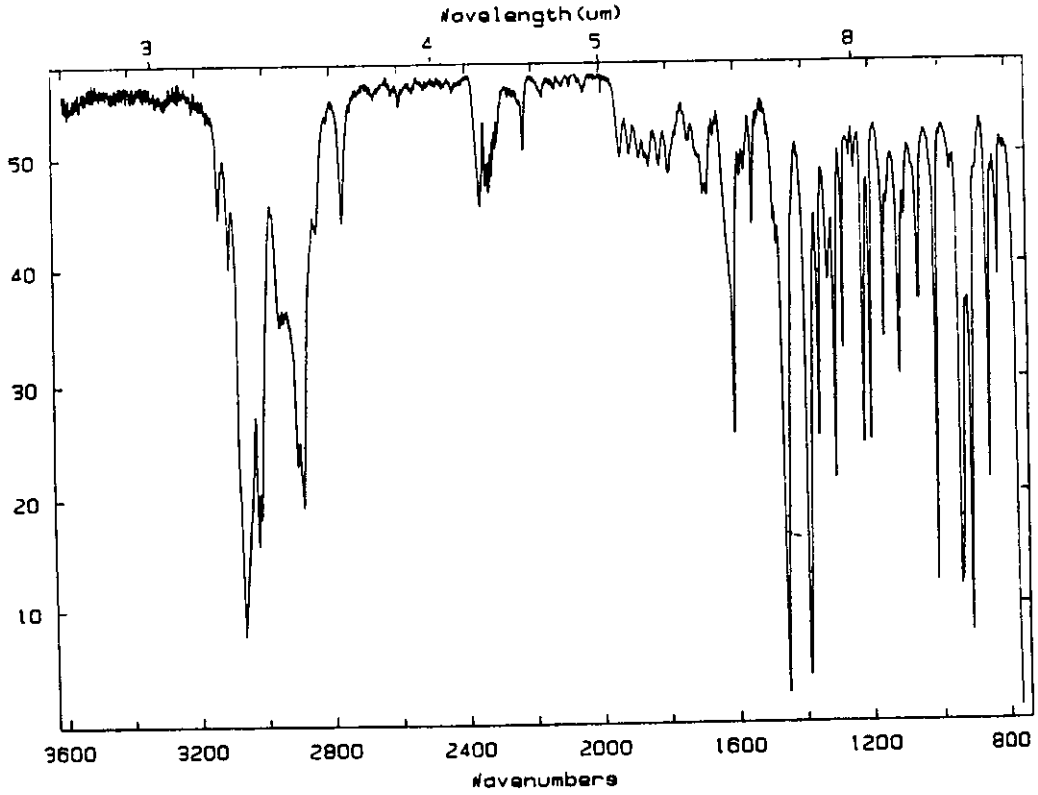
2.5
2.0
1.5
1.0
0.5
0.0
PPM

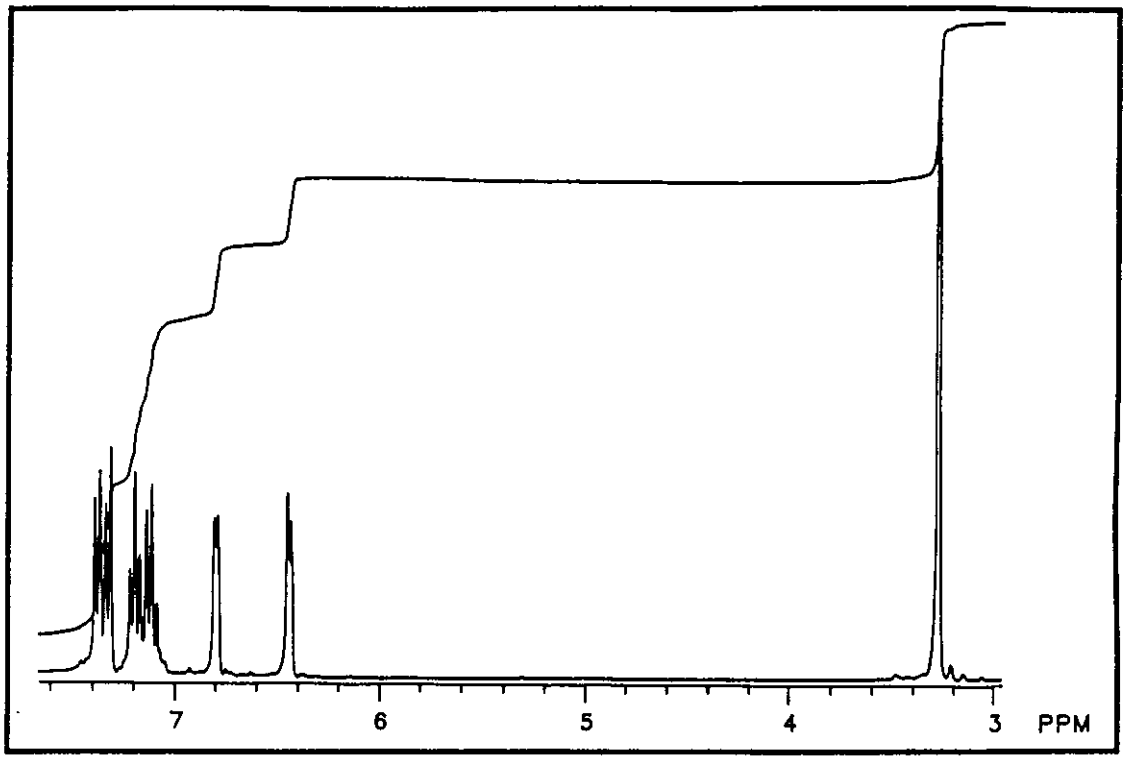

80
60
40
20
0
-20

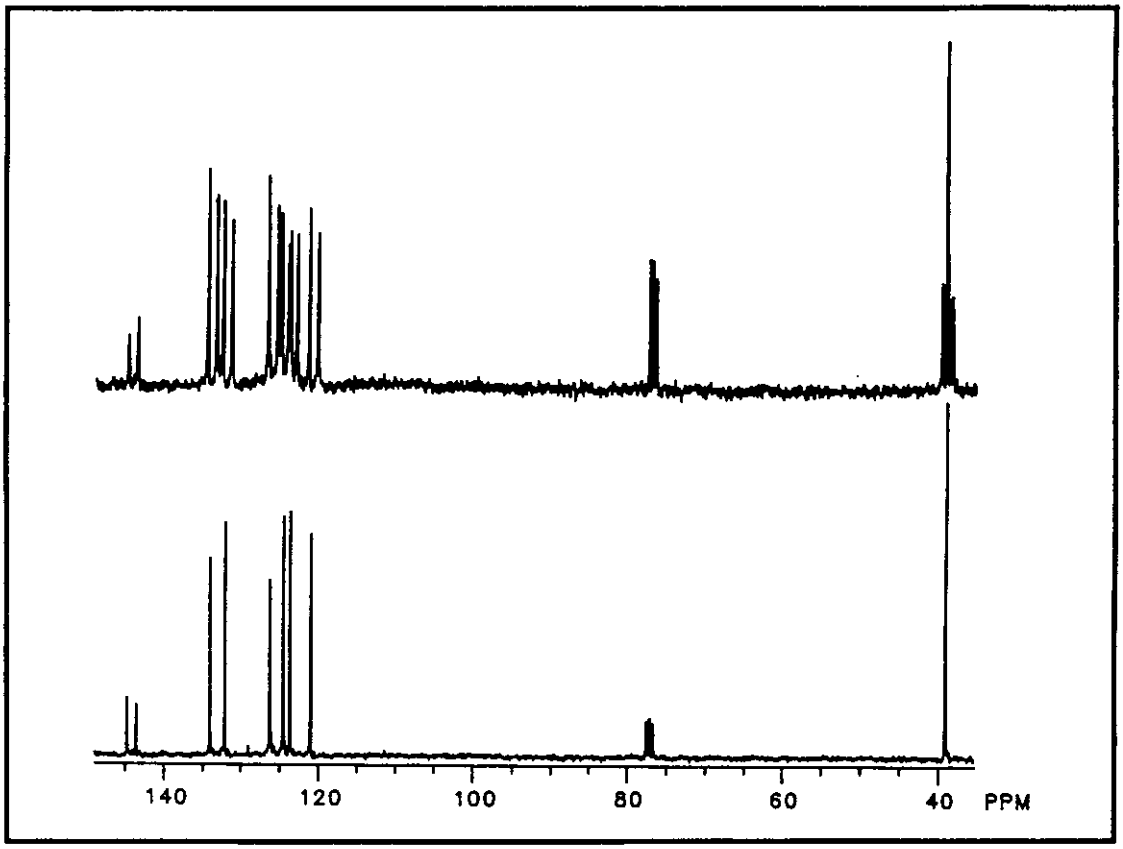
Problem 7

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



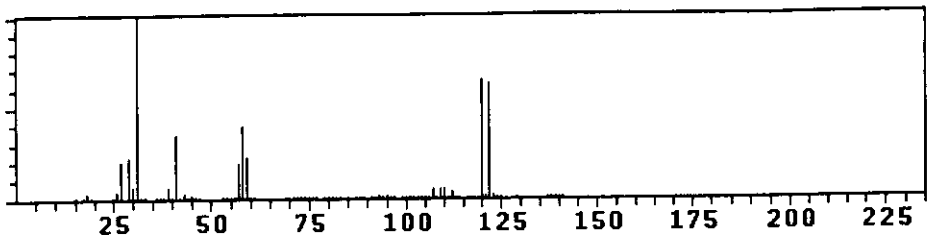


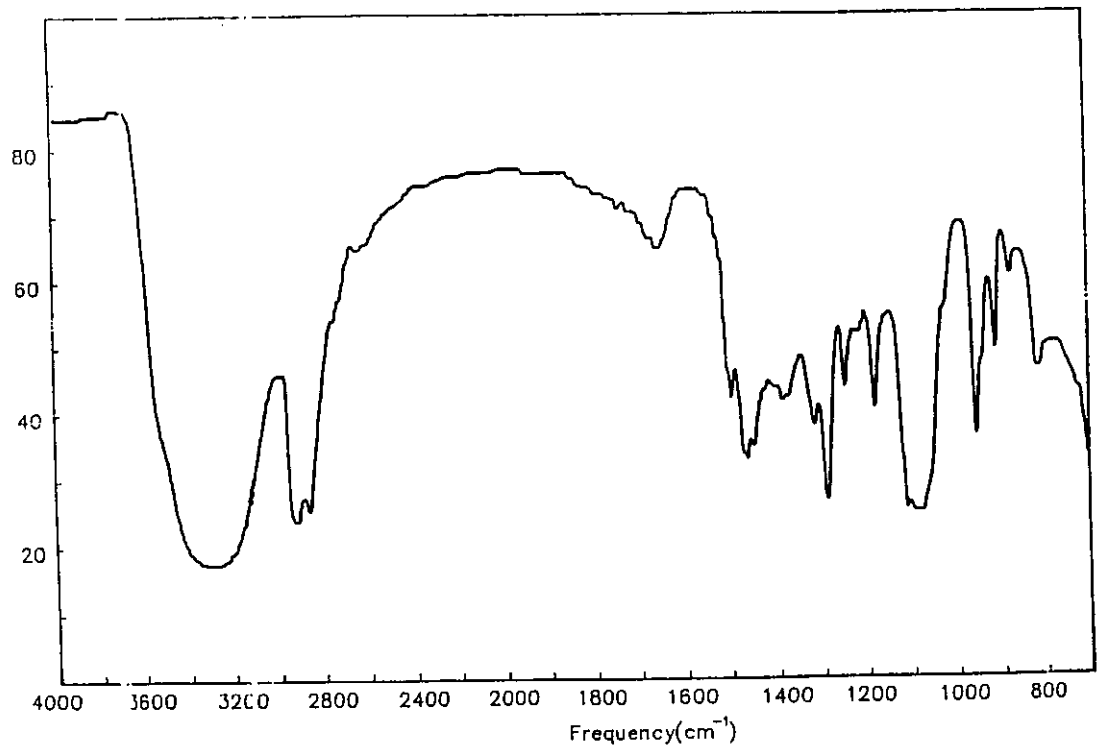

7
6
5
4
3
PPM

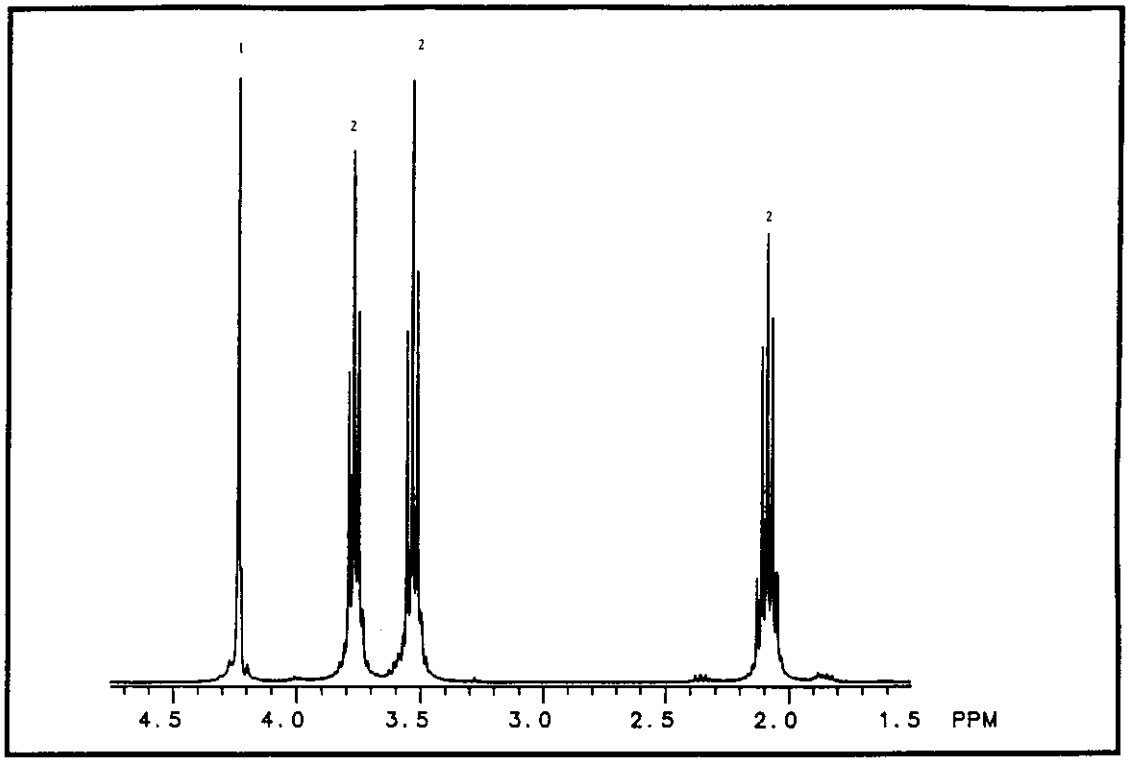

140
120
100
80
60
40
PPM

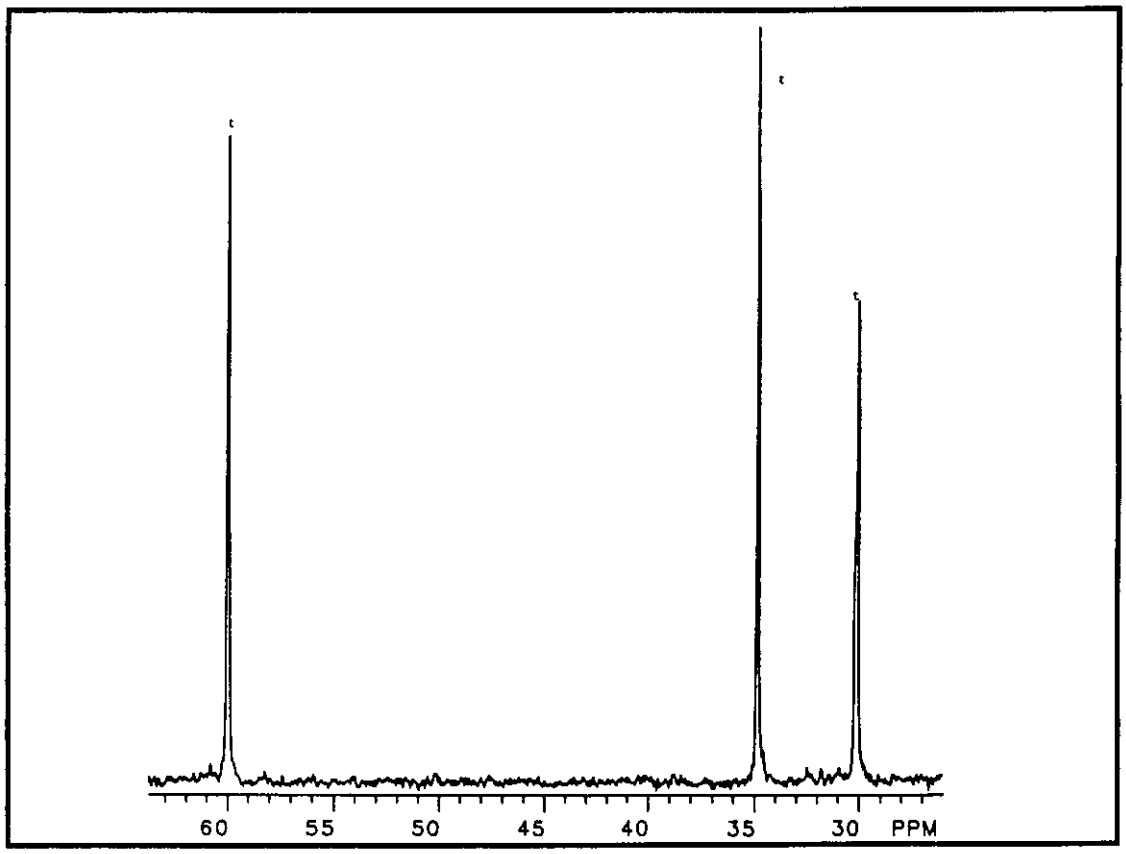
Problem 8

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





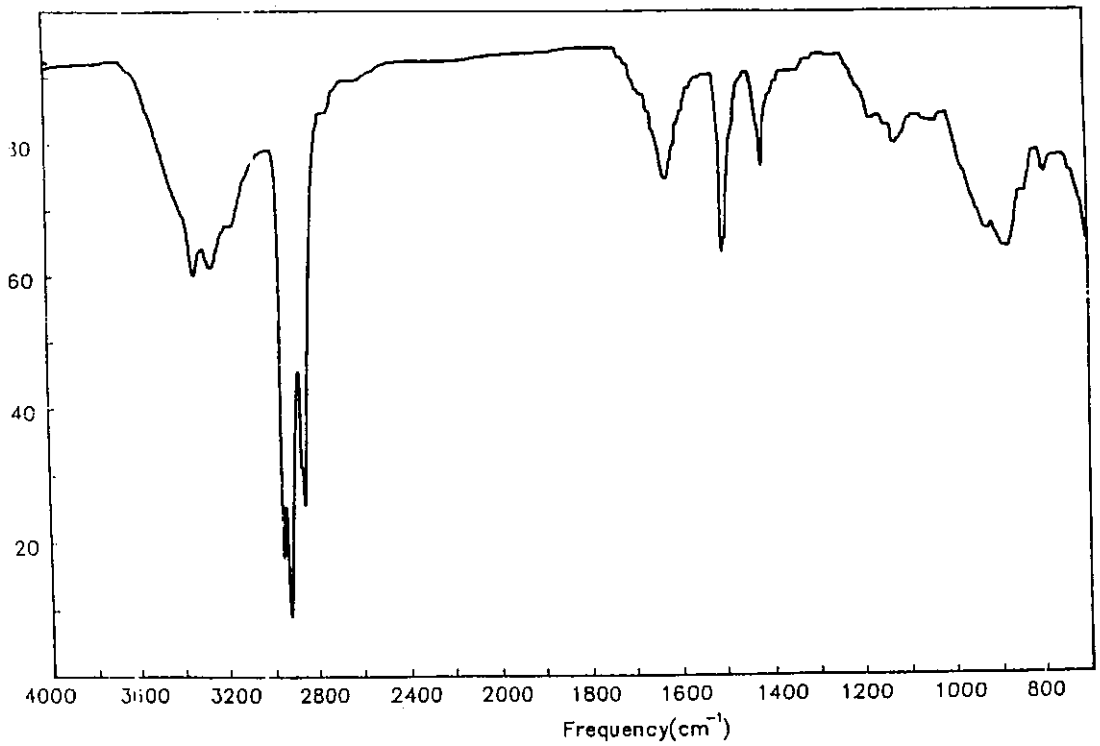

1
2
2
2
4.5
4.0
3.5
3.0
2.5
2.0
1.5
PPM

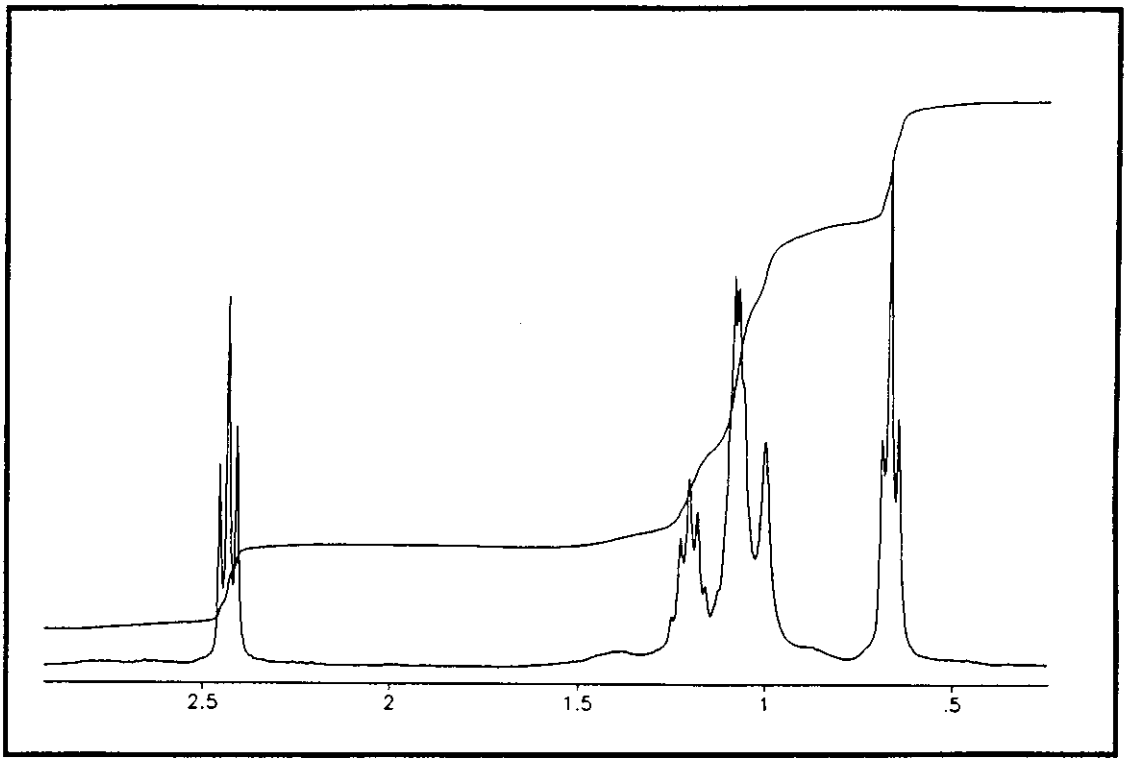

t
t
t
60
55
50
45
40
35
30
PPM

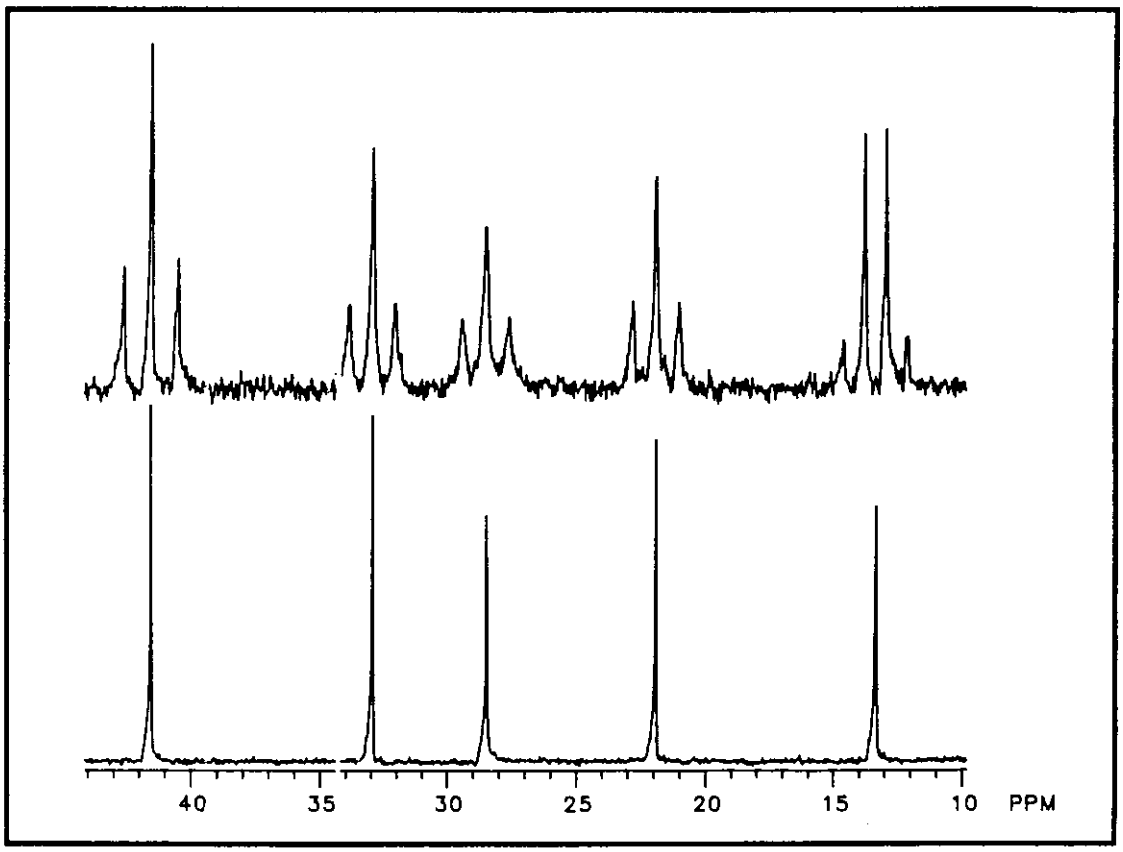
Problem 9

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
15, 0.50	29, 2.00	43, 2.00	56, 2.00	70, 0.70	86, 0.70
17, 0.20	30,100.0	44, 2.00	57, 0.30	71, 0.10	87, 8.00
18, 2.00	31, 2.00	45, 3.00	58, 1.00	72, 0.20	
27, 3.00	41, 4.00	46, 0.10	59, 0.20	84, 0.20	
28, 4.00	42, 3.00	55, 1.00	69, 0.50	85, 0.20	



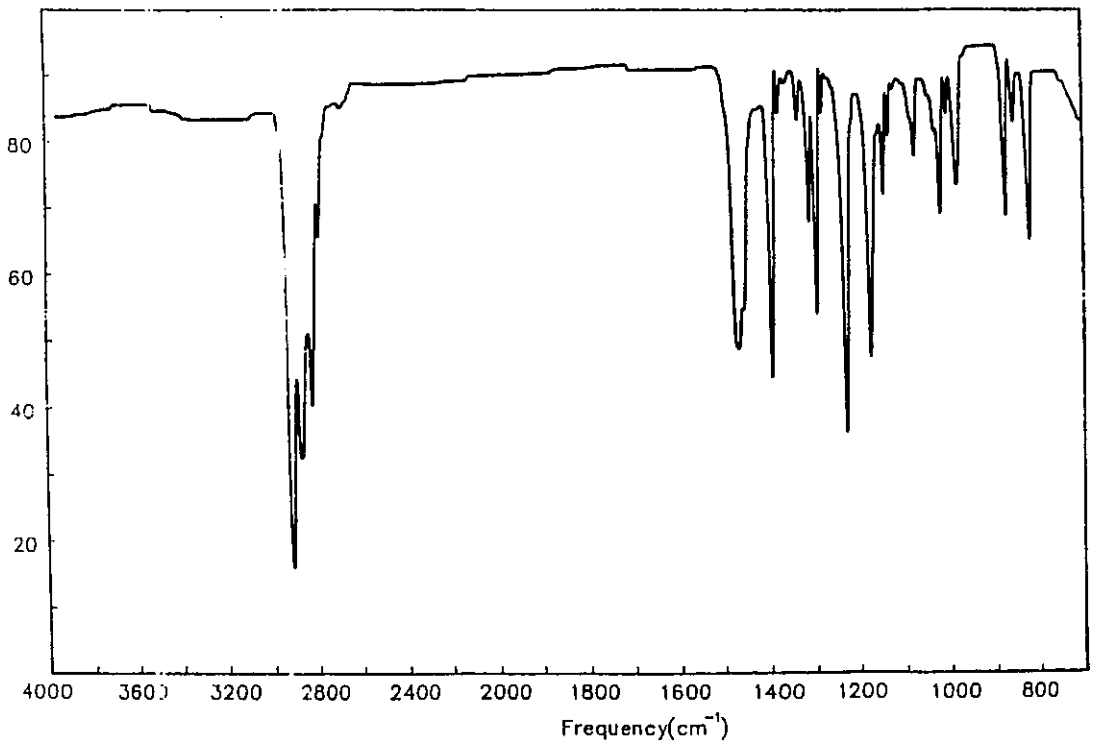

2.5
2
1.5
1
.5

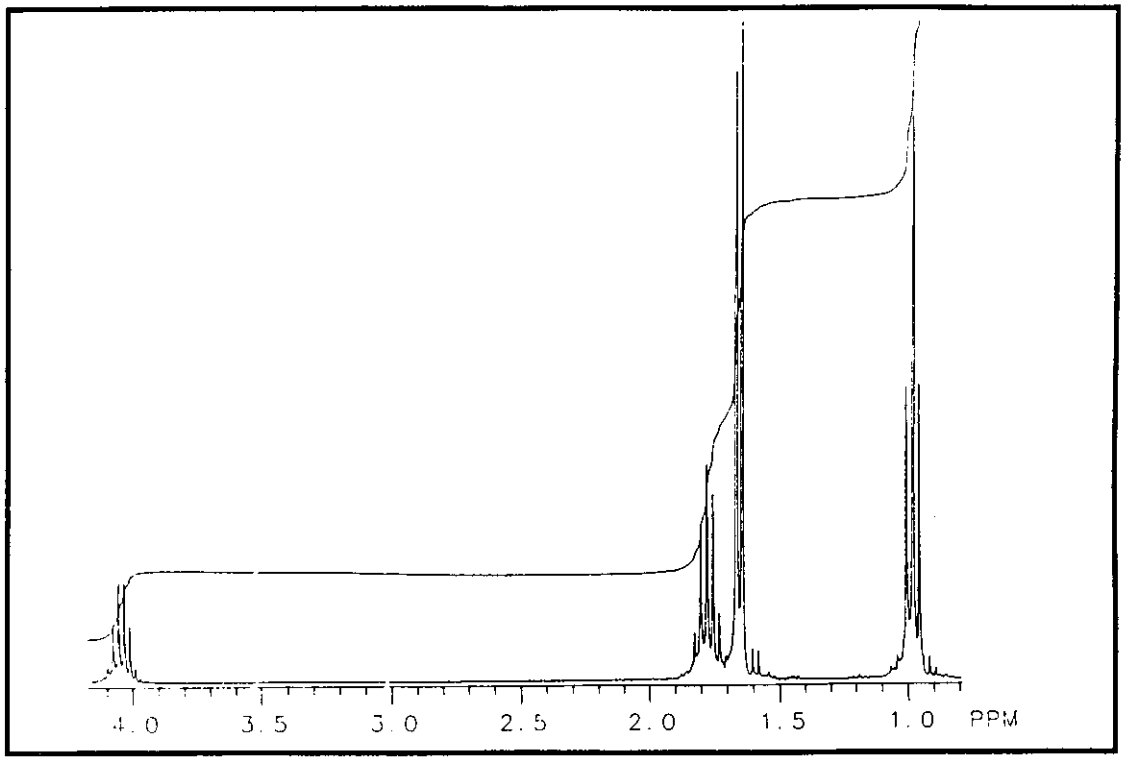

40
35
30
25
20
15
10
PPM

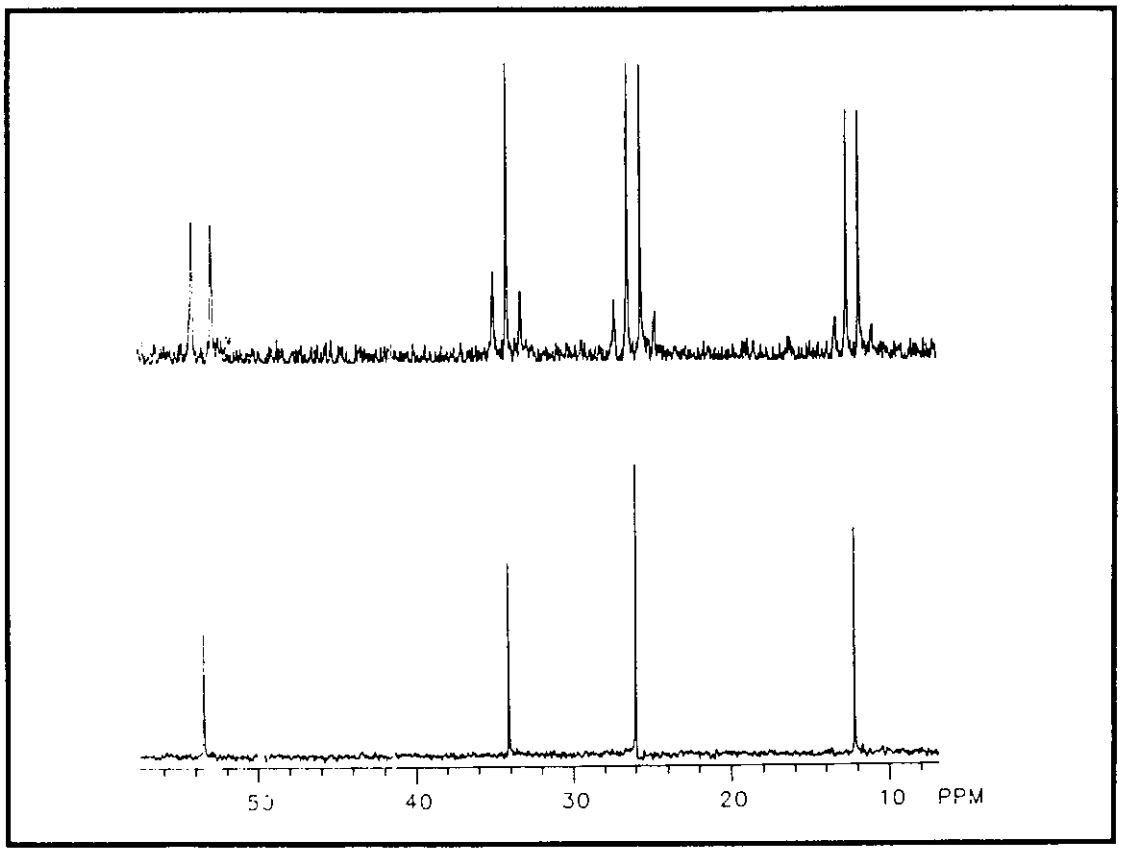
Problem 10

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
12, 0.50	26, 8.81	40, 2.60	54, 0.60	82, 0.60	106, 0.30
13, 0.70	27,33.83	41,60.37	55, 5.40	83, 0.10	107, 1.50
14, 1.70	28, 9.01	42, 3.50	56, 5.10	91, 0.10	108, 0.30
15, 7.51	29,56.97	43, 0.40	57,100.0	92, 0.10	109, 1.20
16, 0.20	29, 0.10	44, 0.10	58, 4.40	93, 0.50	117, 0.10
17, 0.10	30, 1.20	48, 0.10	59, 0.10	94, 0.10	119, 0.10
18, 0.10	32, 0.10	49, 0.70	71, 0.30	95, 0.40	121, 0.20
19, 0.10	36, 0.20	50, 2.30	72, 0.10	101, 0.10	125, 0.10
24, 0.10	37, 1.80	51, 2.00	79, 1.20	102, 0.10	136, 0.70
25, 0.90	38, 3.10	52, 0.70	80, 0.60	104, 0.10	138, 0.60
25, 0.20	39,20.32	53, 1.90	81, 1.10	105, 0.20	




4.0
3.5
3.0
2.5
2.0
1.5
1.0
PPM

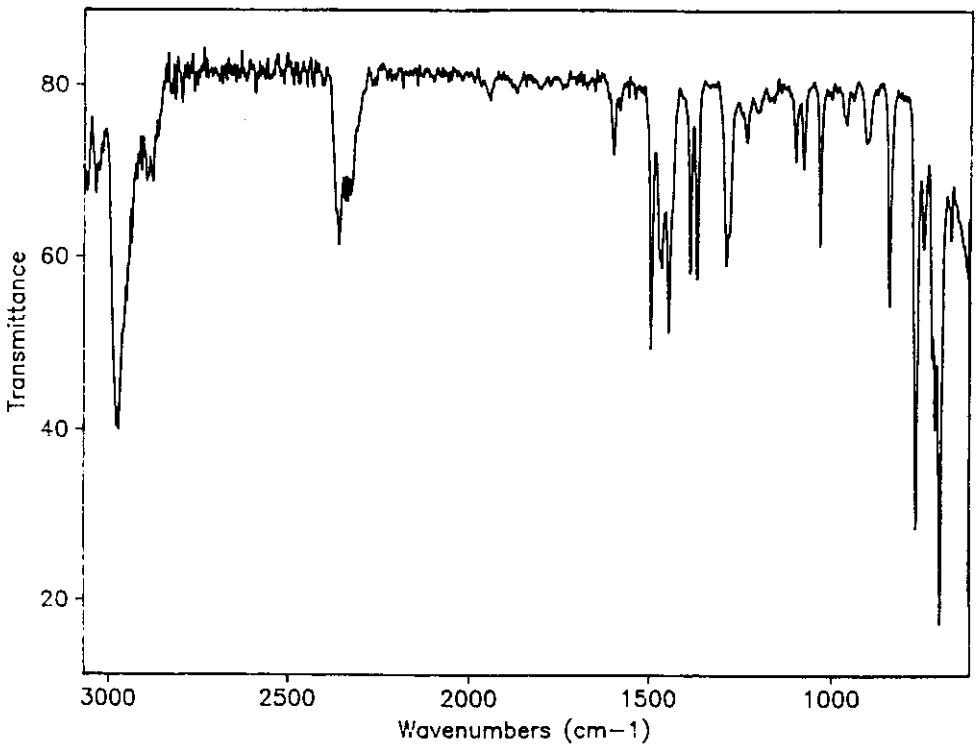

50
40
30
20
10
PPM

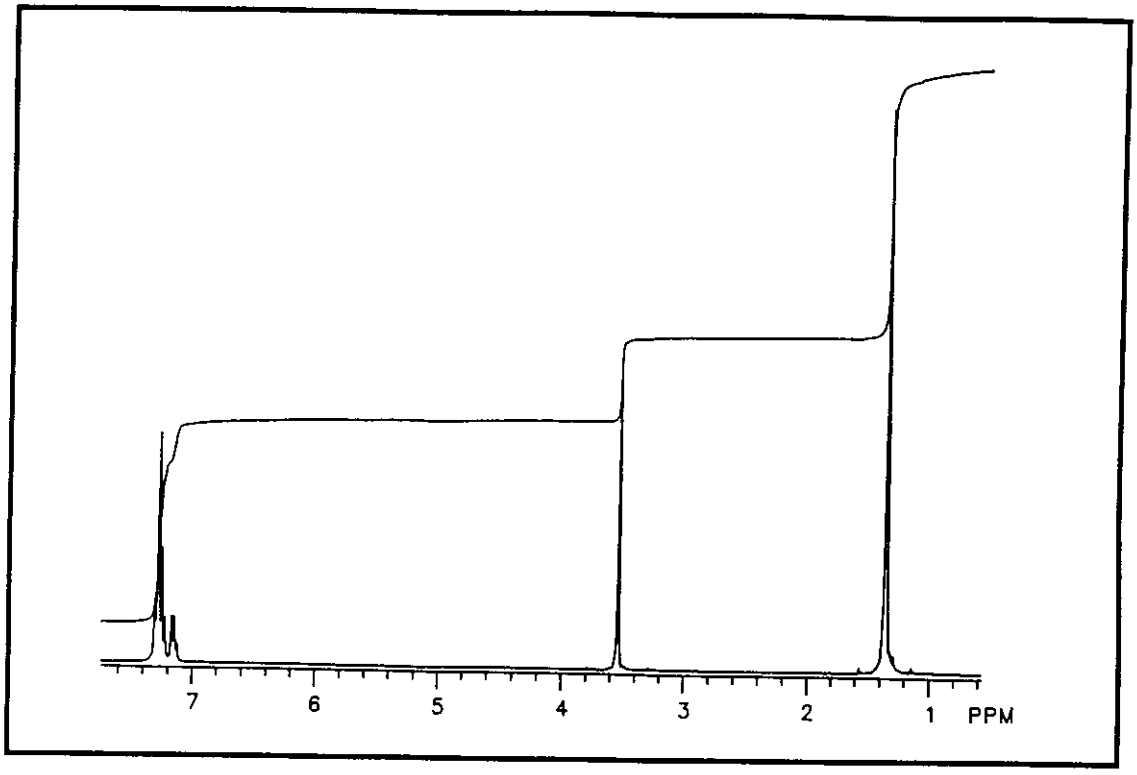
Problem 11

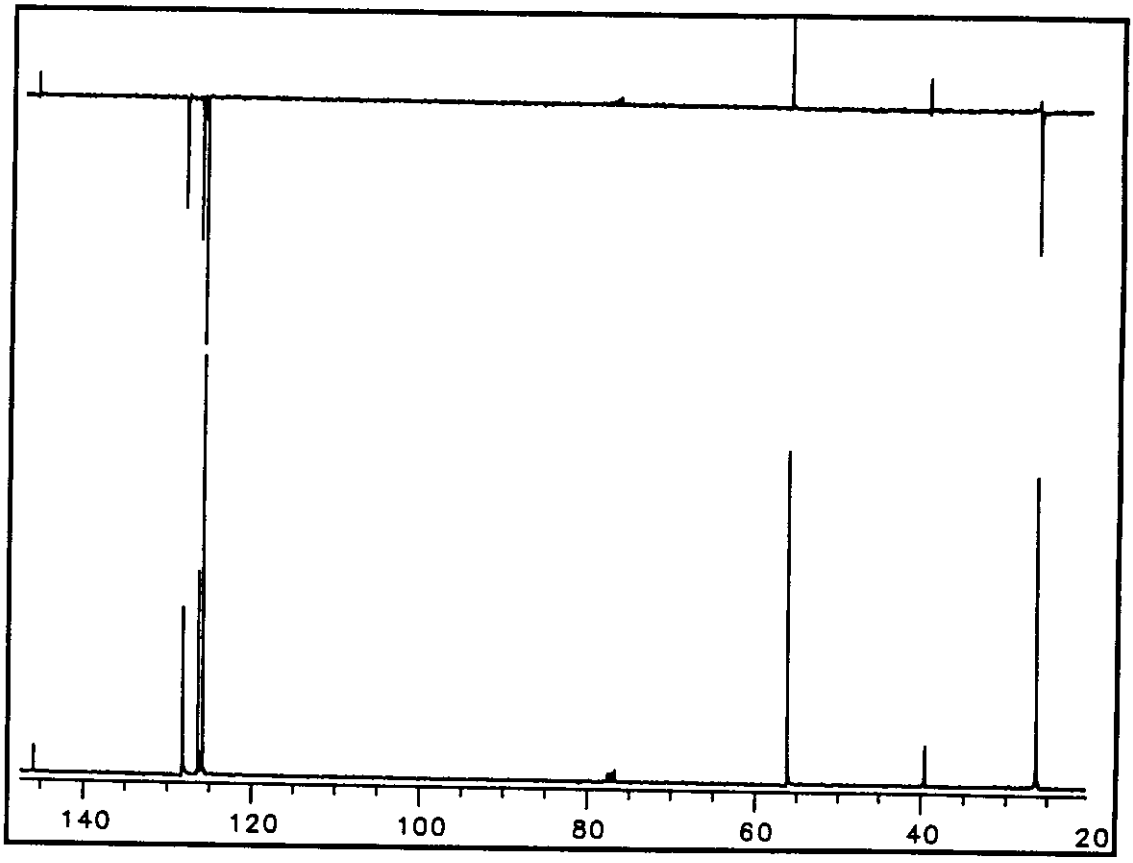
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
37	0.71	53	2.74	74	4.01	89	5.16	105	1.35	127	1.31
38	2.12	55	1.70	75	4.08	90	0.73	113	0.28	128	0.93
39	15.13	56	0.21	76	3.63	91	92.16	115	21.40	129	0.43
40	1.31	58	0.56	77	22.22	92	6.95	116	4.60	131	0.37
41	9.07	61	0.77	78	11.11	93	0.36	117	16.50	153	1.22
42	0.37	62	3.06	79	7.82	98	0.35	118	6.17	155	0.35
47	0.30	63	8.60	80	0.41	99	0.37	119	100.00	168	8.37
49	10.70	64	1.51	85	0.33	101	1.02	120	9.42	169	0.87
50	9.25	65	9.24	86	0.74	102	5.45	121	0.35	170	2.74
51	20.79	66	0.70	87	1.45	103	14.79	125	2.59	171	0.20
52	3.96	73	0.79	88	0.34	104	3.66	126	0.30		




7
6
5
4
3
2
1
PPM

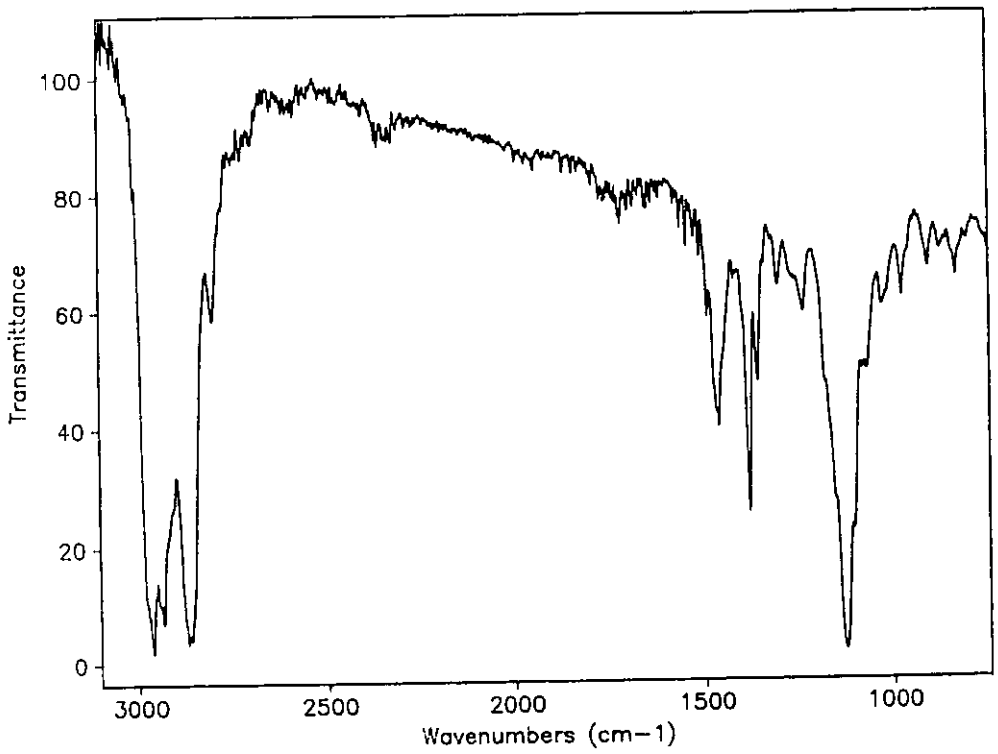

140
120
100
80
60
40
20

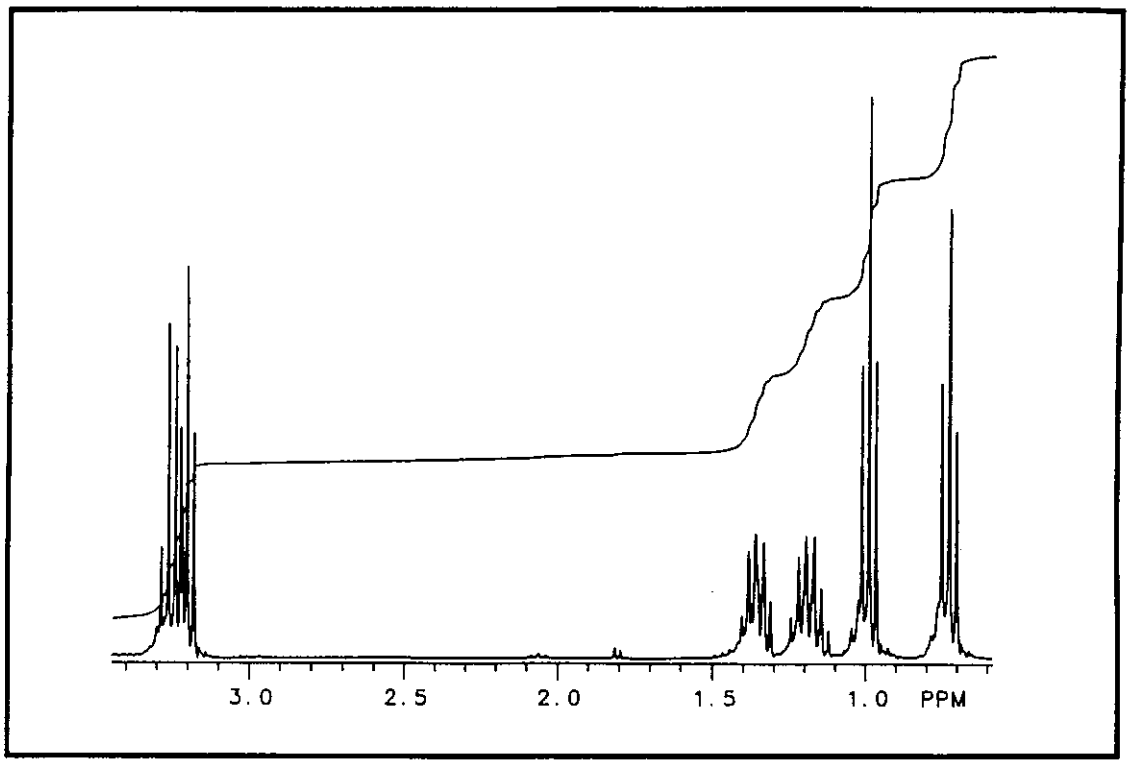
Problem 12

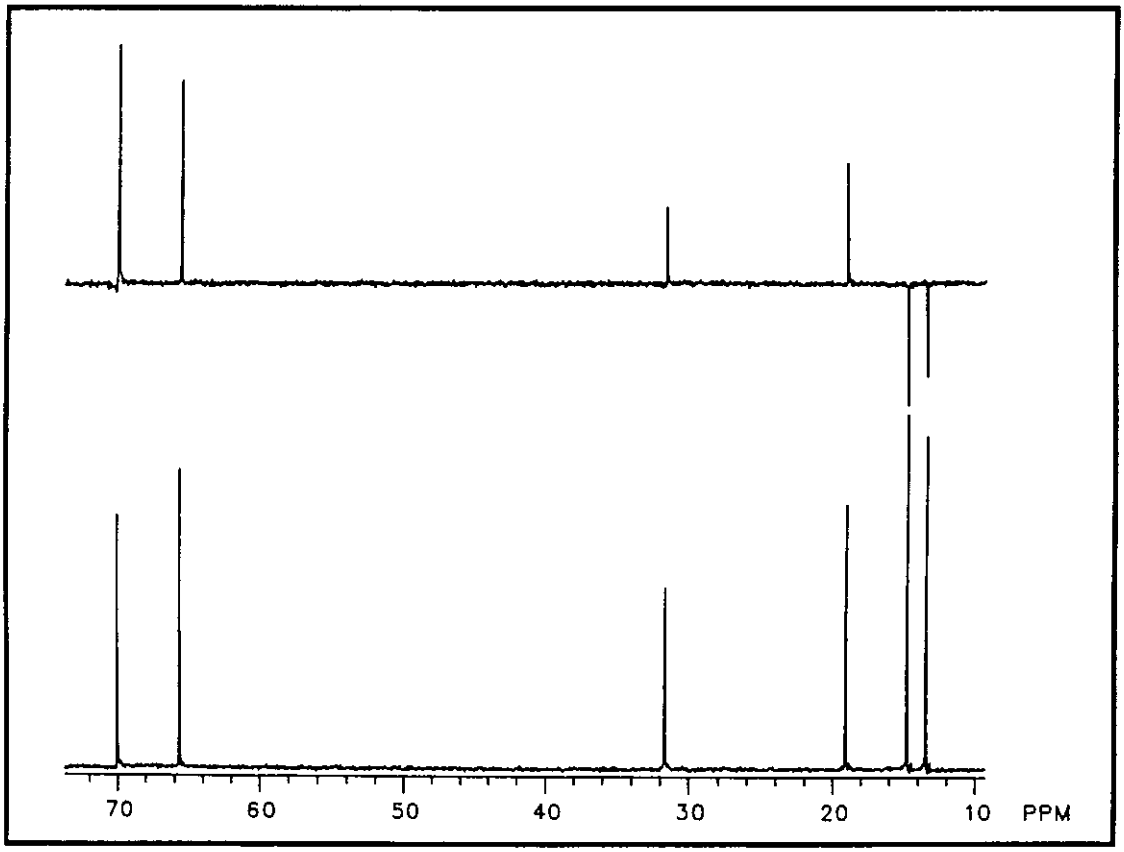
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z	
30	0.37	43	100.00	55	2.78	69	0.38
31	9.46	44	2.39	56	4.87	83	2.70
32	0.17	45	1.49	57	2.59	85	0.72
37	0.76	49	0.21	58	14.56	98	4.46
38	1.62	50	1.07	59	53.48	99	0.74
39	9.51	51	1.18	60	1.90	101	35.92
40	1.58	52	0.31	61	0.49	102	2.15
41	9.15	53	1.50	62	0.28		
42	9.01	54	0.23	63	0.21		



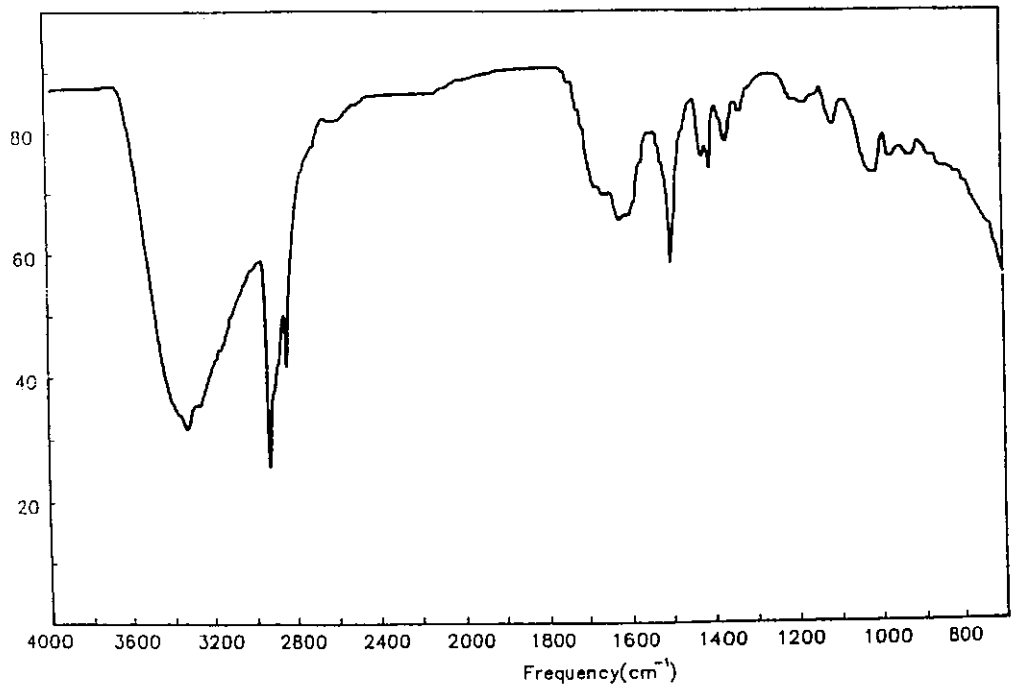

3.0
2.5
2.0
1.5
1.0
PPM

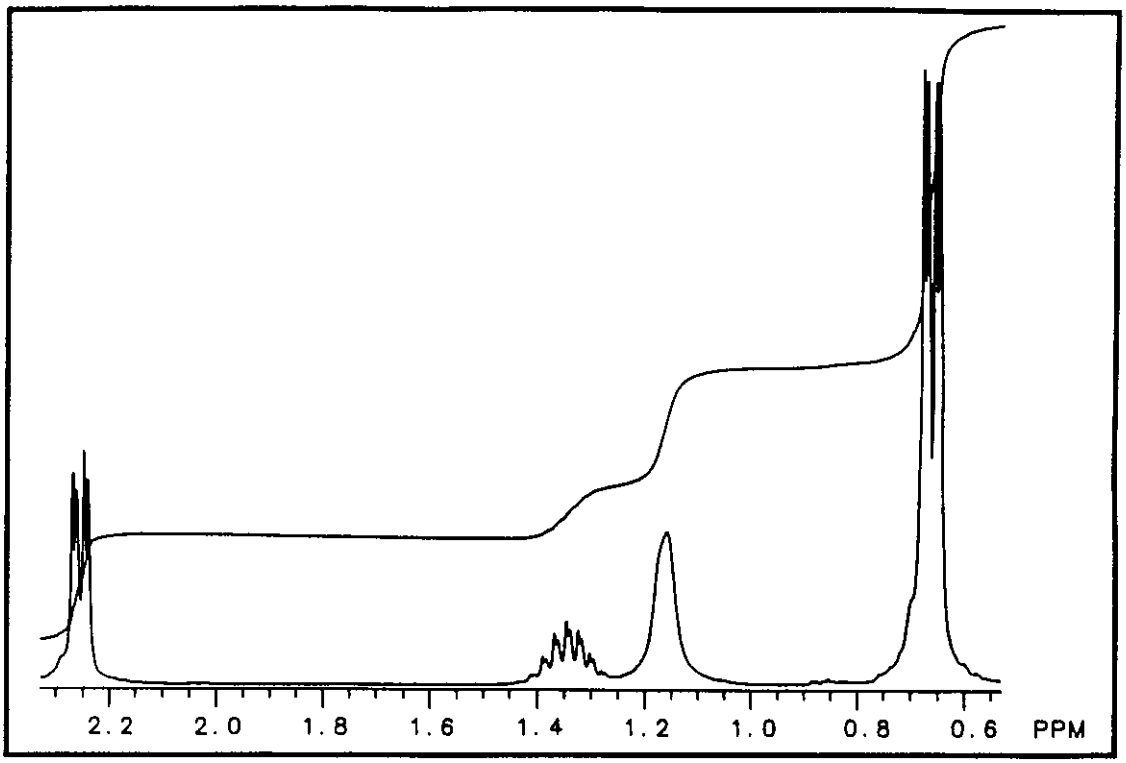

70
60
50
40
30
20
10
PPM

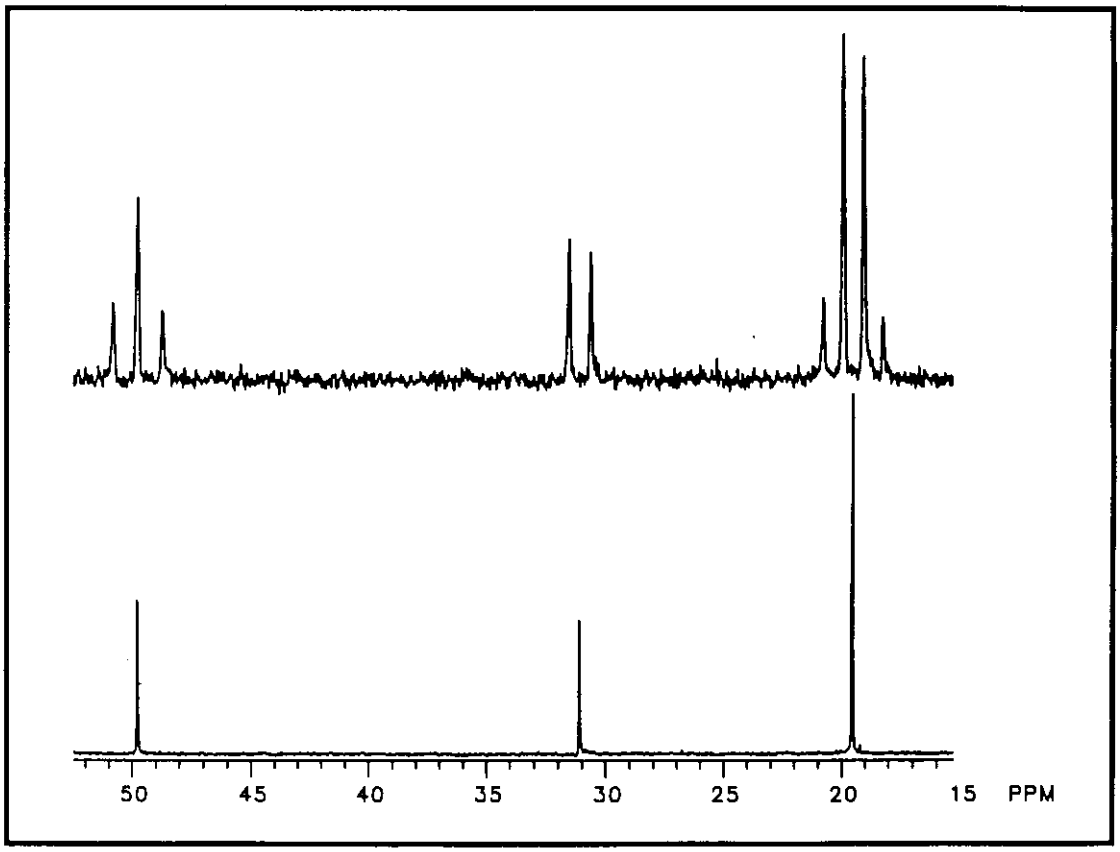
Problem 13

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
12, 0.10	26, 0.90	32, 0.10	40, 0.60	52, 0.30	68, 0.10
13, 0.10	26, 0.10	33, 0.10	41, 5.71	53, 0.30	69, 0.10
14, 0.40	27, 5.10	33, 0.10	42, 1.70	54, 0.50	70, 0.20
15, 2.70	27, 0.10	34, 0.10	43, 1.60	55, 1.80	71, 0.10
16, 0.30	28, 9.11	34, 0.10	44, 1.30	56, 1.90	72, 1.30
17, 0.30	29, 3.10	36, 0.10	45, 0.10	57, 0.80	73, 4.80
18, 2.00	30,100.0	37, 0.40	49, 0.10	58, 1.60	74, 0.30
19, 0.10	31, 2.30	38, 0.80	50, 0.10	59, 0.20	
25, 0.10	32, 0.30	39, 4.10	51, 0.20	60, 0.10	



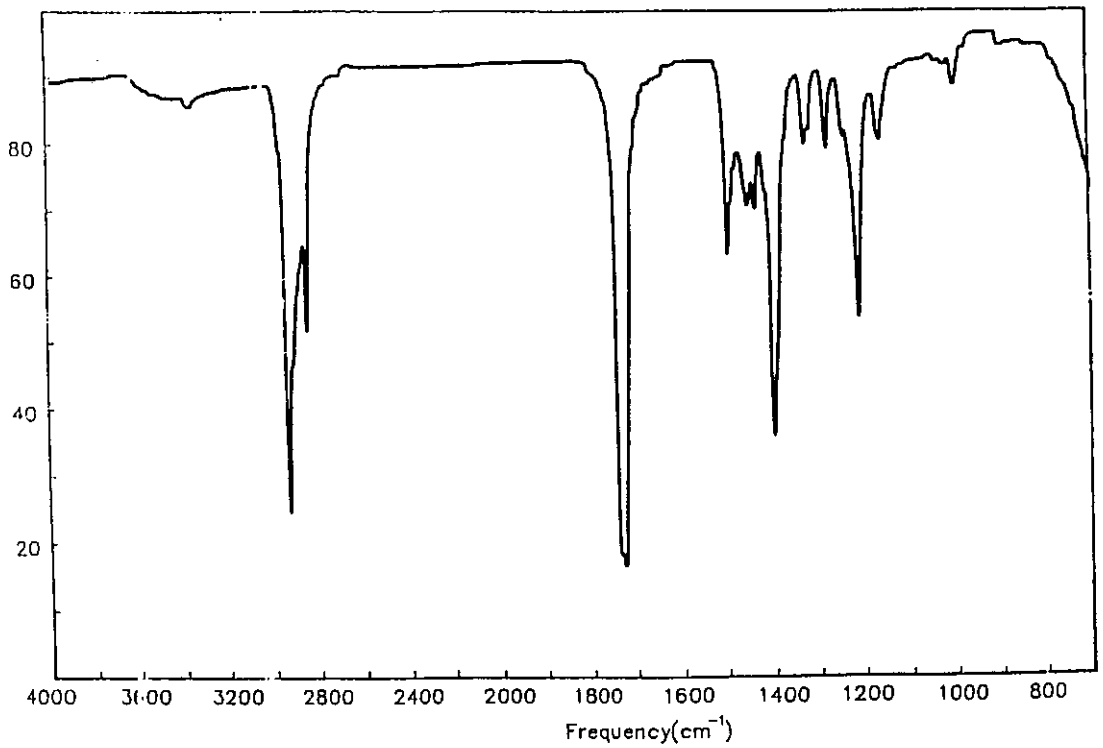

2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
PPM

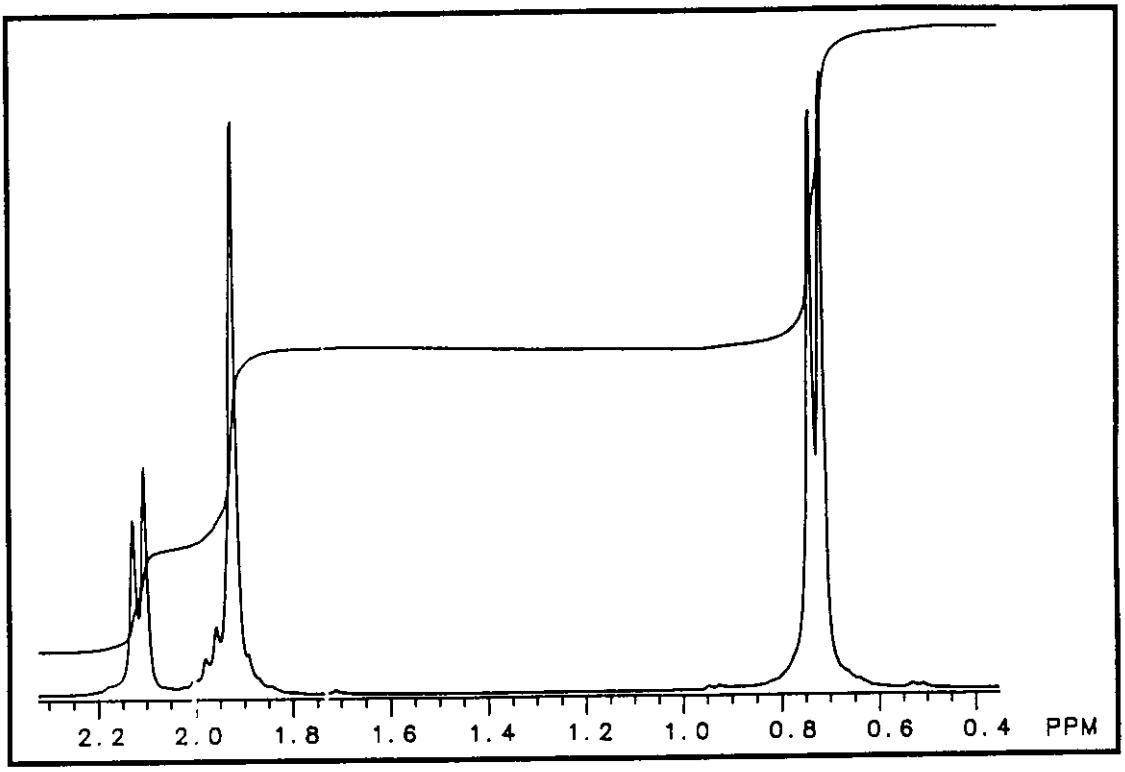

50
45
40
35
30
25
20
15
PPM

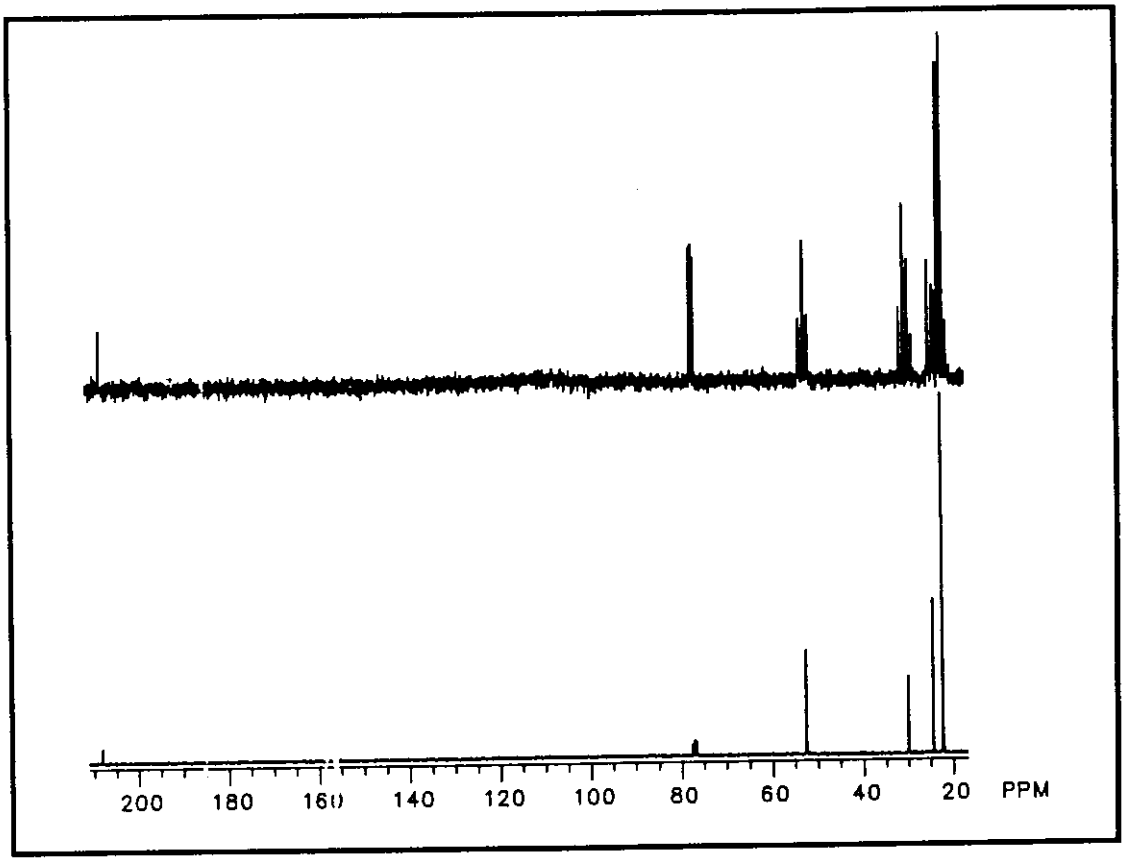
Problem 14

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
13, 0.90	29,23.92	45, 1.60	59, 3.80	72, 1.20	93, 0.10
14, 4.70	30, 0.80	46, 0.10	60, 0.20	77, 0.10	95, 0.10
15,27.12	31, 0.80	48, 0.10	61, 0.10	78, 0.10	96, 0.10
16, 0.70	32, 0.10	49, 0.30	62, 0.20	79, 0.10	97, 0.10
17, 0.10	36, 0.10	50, 1.40	63, 0.30	81, 0.20	98, 0.20
18, 0.60	37, 1.60	51, 1.50	64, 0.10	82, 0.20	99, 0.10
19, 0.10	38, 3.60	52, 0.40	65, 0.30	83, 0.80	100,15.71
19, 0.10	39,25.22	53, 1.70	66, 0.10	84, 0.30	101, 1.10
24, 0.10	40, 3.80	54, 0.40	67, 2.50	85,21.92	102, 0.10
25, 0.30	41,37.03	55, 2.90	68, 0.30	86, 1.20	
26, 3.50	42,12.41	56, 2.10	69, 1.20	87, 0.10	
27,24.22	43,100.0	57,37.53	70, 0.20	91, 0.10	
28, 3.60	44, 4.20	58,60.17	71, 0.40	92, 0.10	



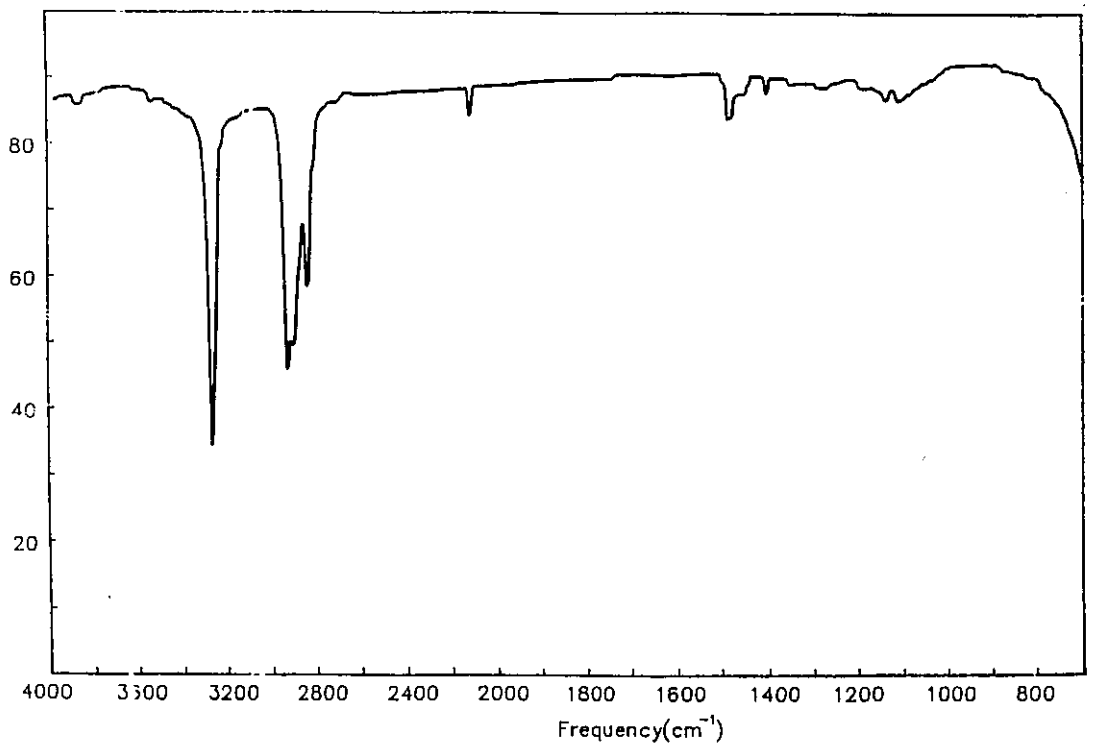

2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
PPM

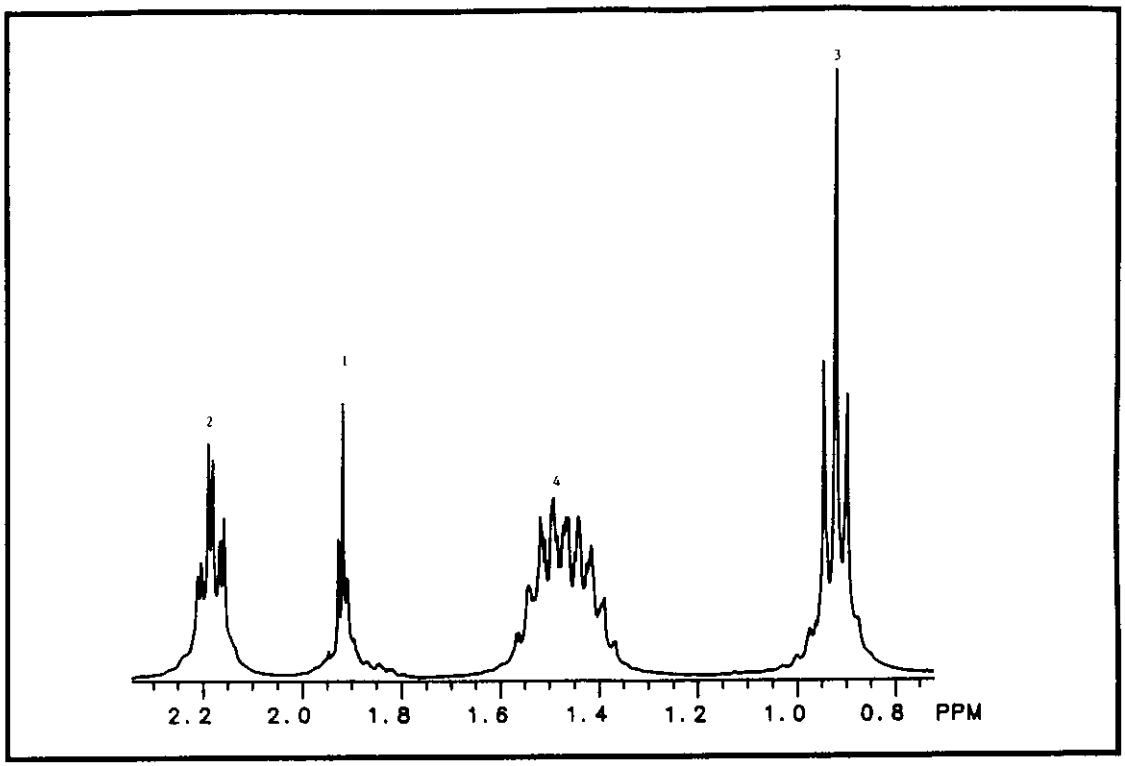

200
180
160
140
120
100
80
60
40
20
PPM

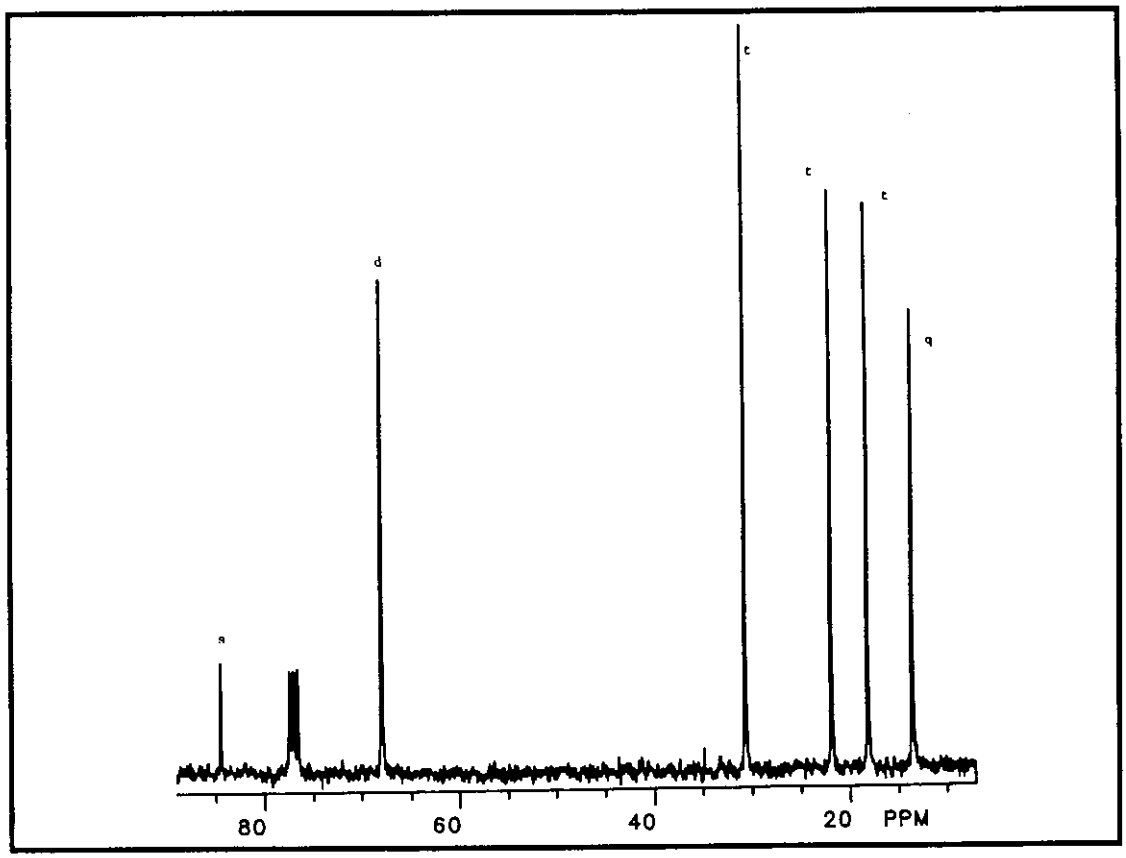
Problem 15

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
1, 1.10	28, 7.21	38, 8.81	49, 0.10	62, 1.00	75, 0.40
2, 0.10	28, 0.20	38, 0.10	50, 7.51	63, 2.00	75, 0.10
12, 0.30	29, 7.51	39,47.64	51, 9.51	63, 0.20	76, 0.10
13, 0.50	30, 0.20	39, 1.50	52, 5.00	64, 0.30	77, 2.00
14, 1.00	31, 0.20	40,27.72	53,16.61	65, 4.60	77, 0.20
15, 5.10	31, 0.10	41,67.48	54,28.73	66, 1.60	78, 0.40
16, 0.20	32, 0.30	42,17.12	55, 3.60	67,100.0	79, 2.00
24, 0.10	32, 0.10	43,51.37	55, 3.60	68, 5.61	80, 0.30
25, 0.60	35, 0.10	44, 1.80	56, 4.10	69, 0.10	81,11.31
25, 0.10	36, 0.30	45, 0.10	57, 0.20	72, 0.10	82, 0.80
26, 6.41	37, 4.20	48, 0.10	60, 0.10	73, 0.20	83, 0.10
27,64.78	37, 0.20	49, 1.30	61, 0.60	74, 0.70	

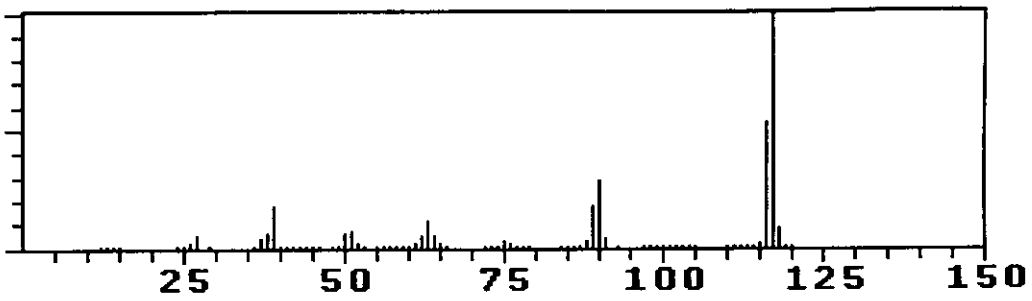


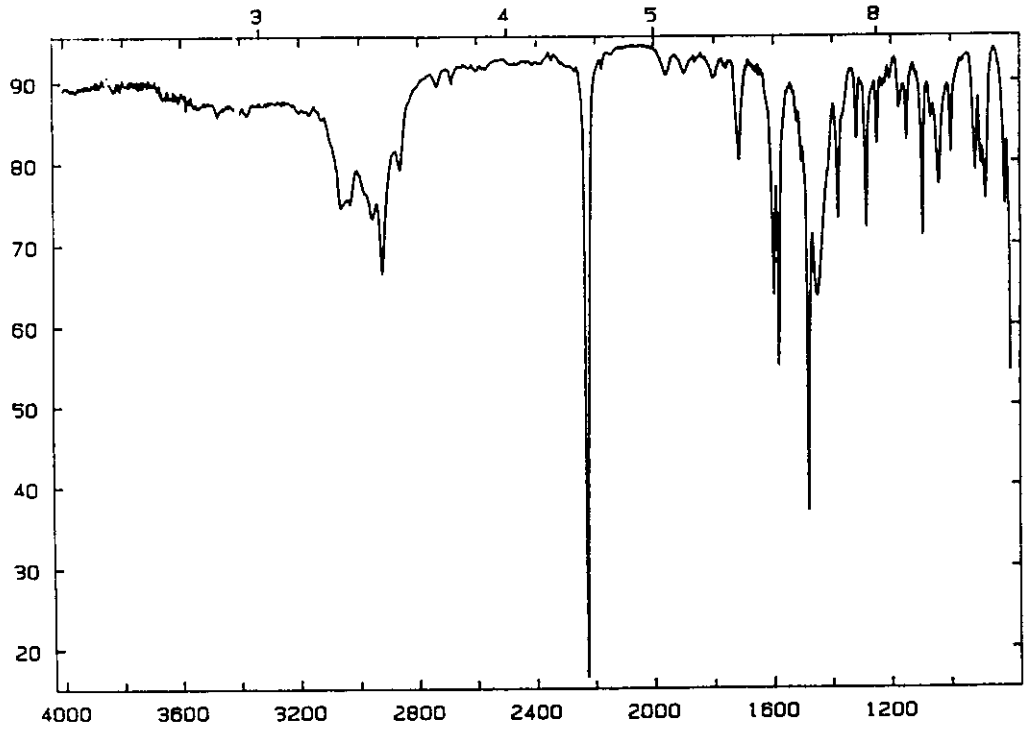

3
1
2
4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
PPM

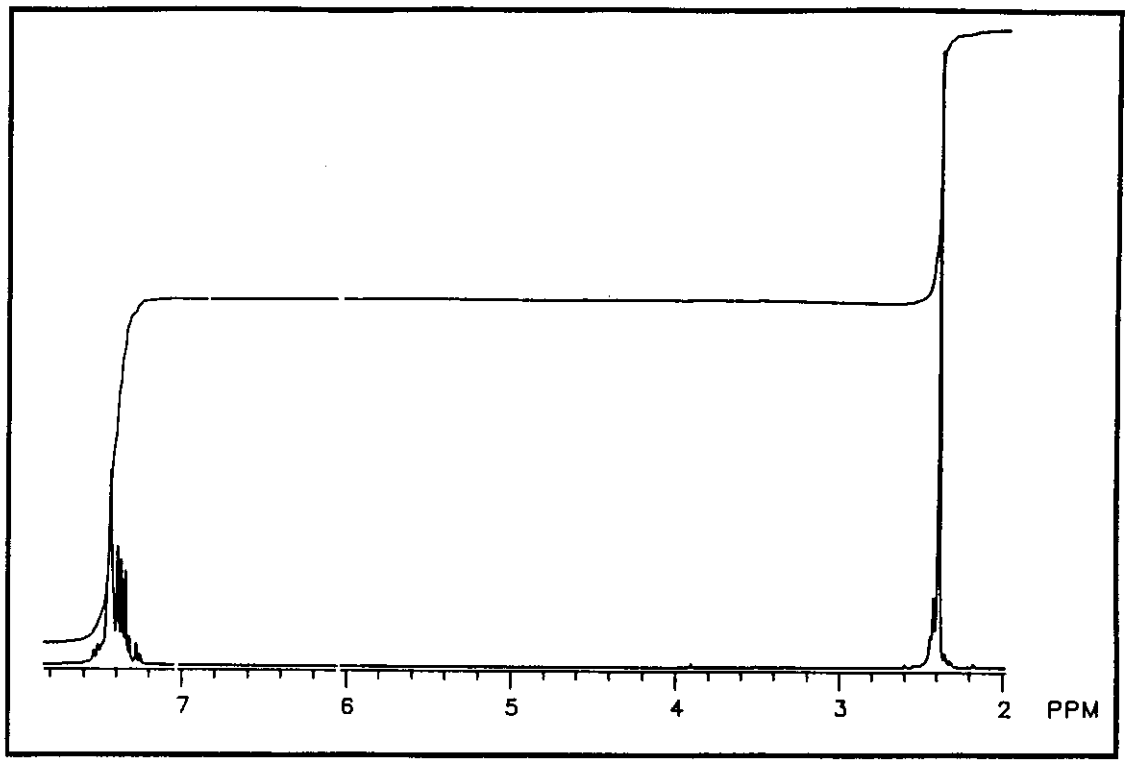

c
c
c
d
a
q
80
60
40
20
PPM

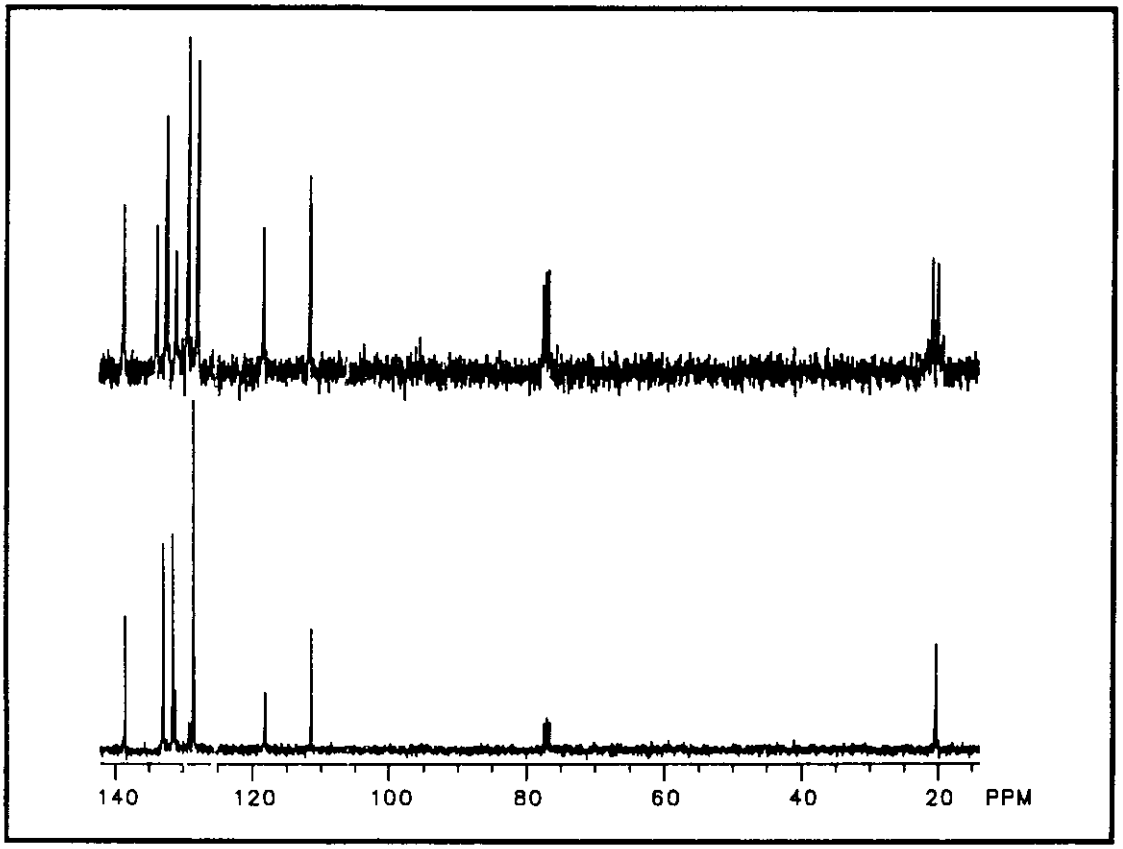
Problem 16

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 82.0% C; 6.0% H; 12.0% N



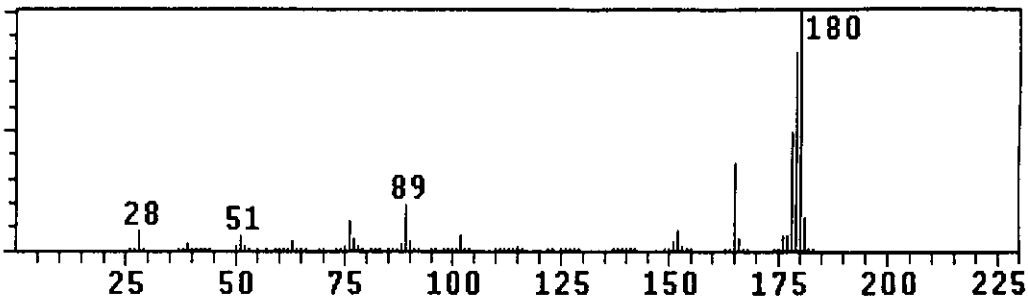


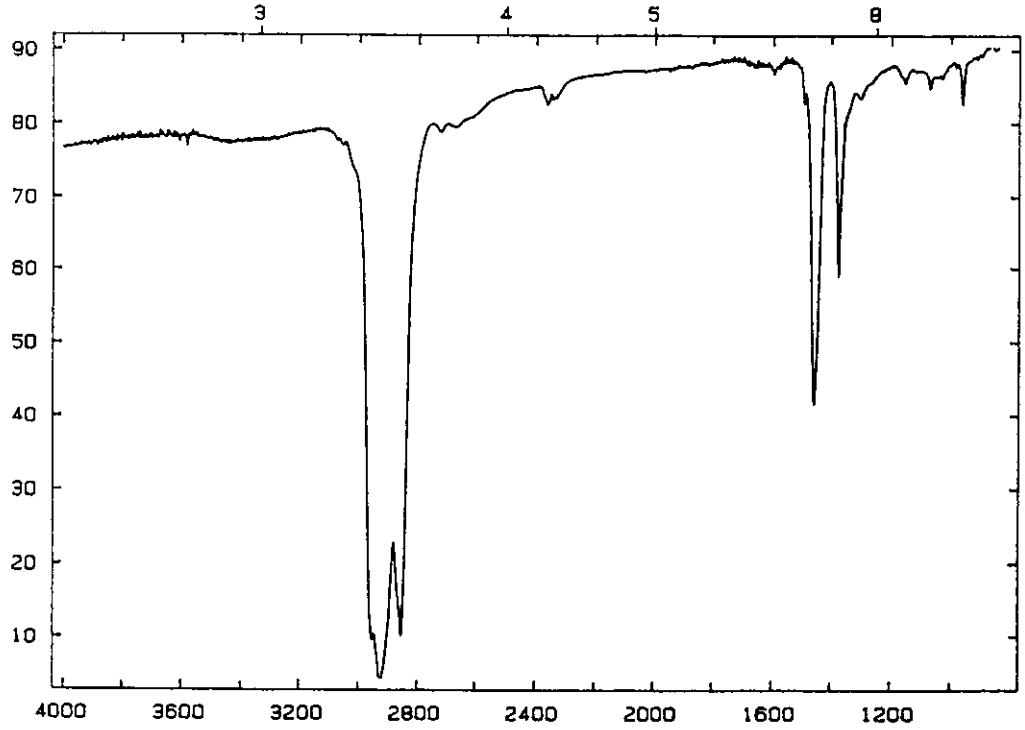

7
6
5
4
3
2
PPM

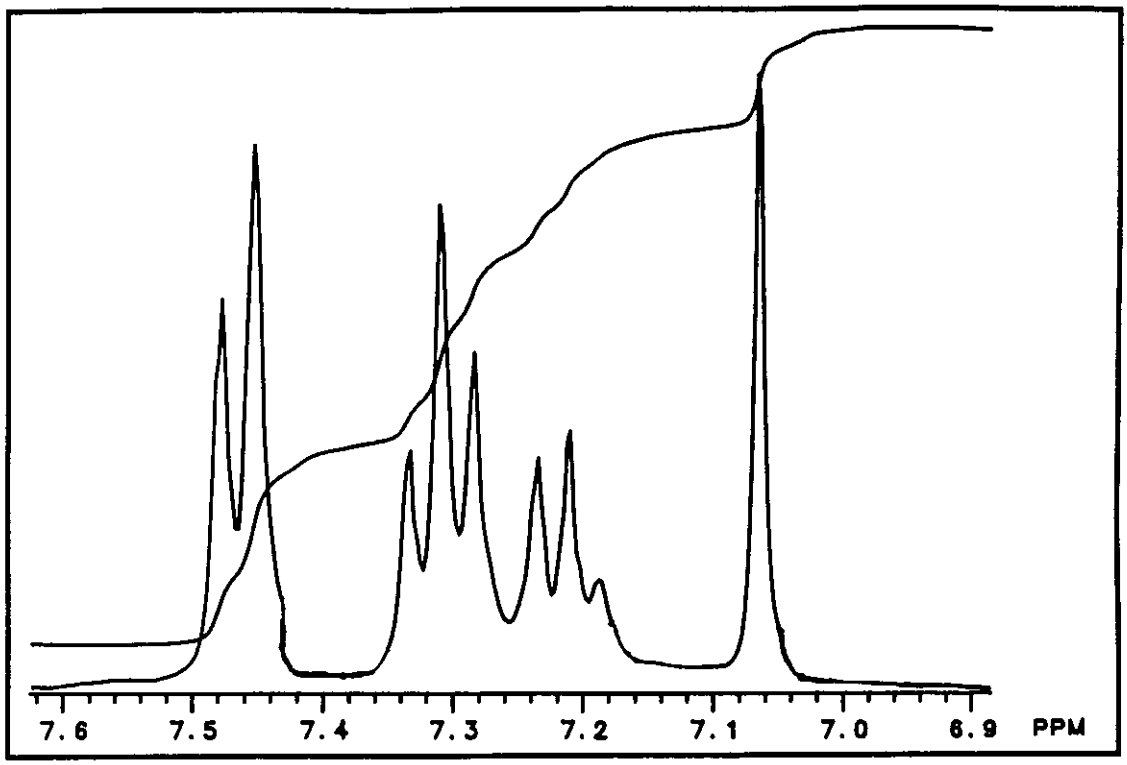

140
120
100
80
60
40
20
PPM

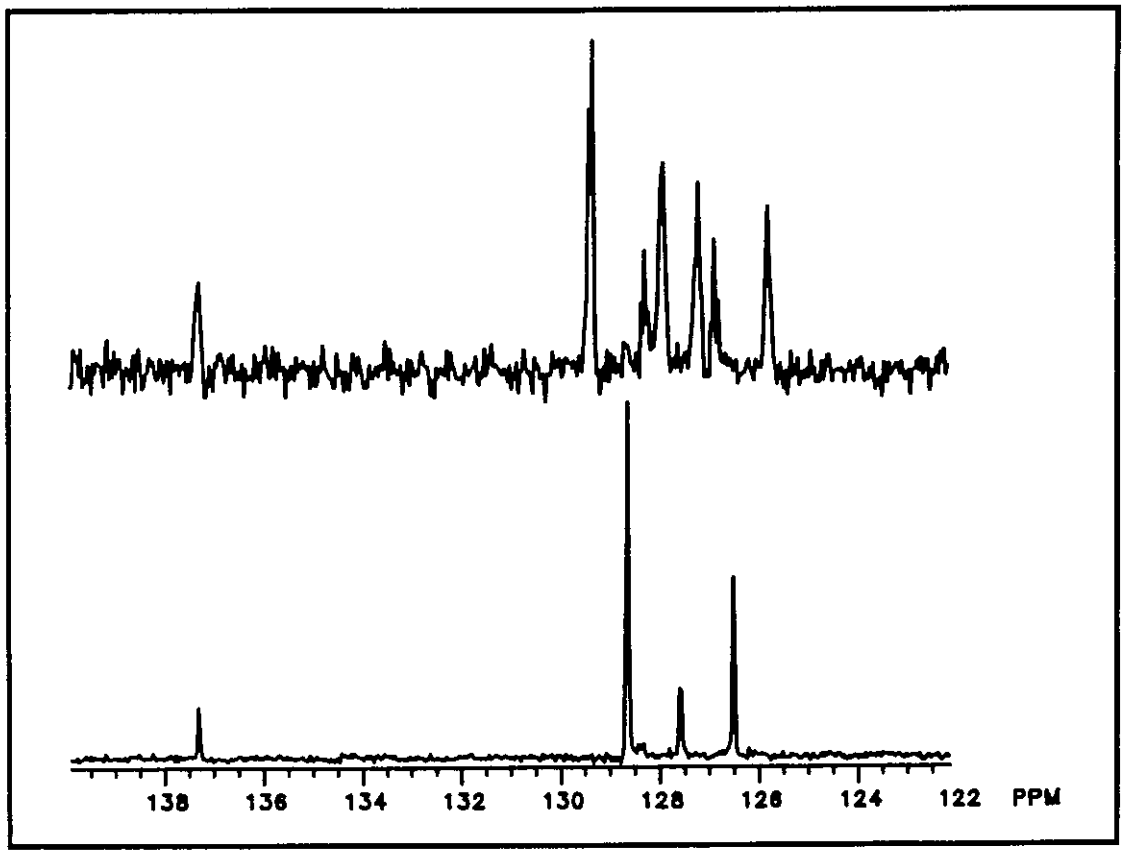
Problem 17

Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 93.3% C; 6.7% H






7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
PPM

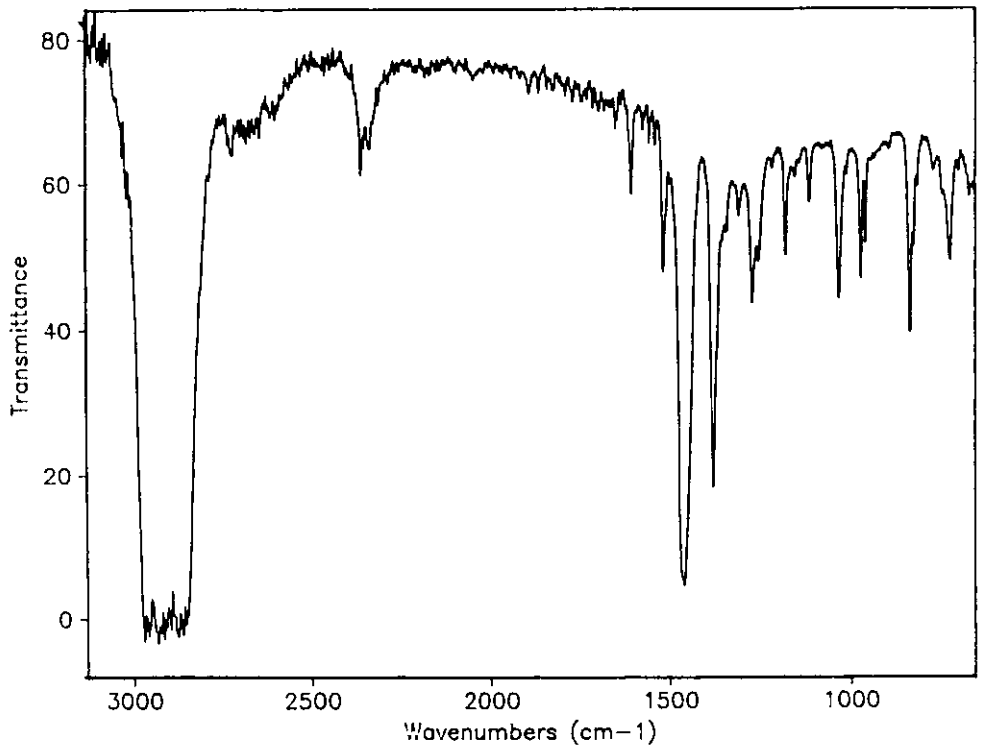

138
136
134
132
130
128
126
124
122
PPM

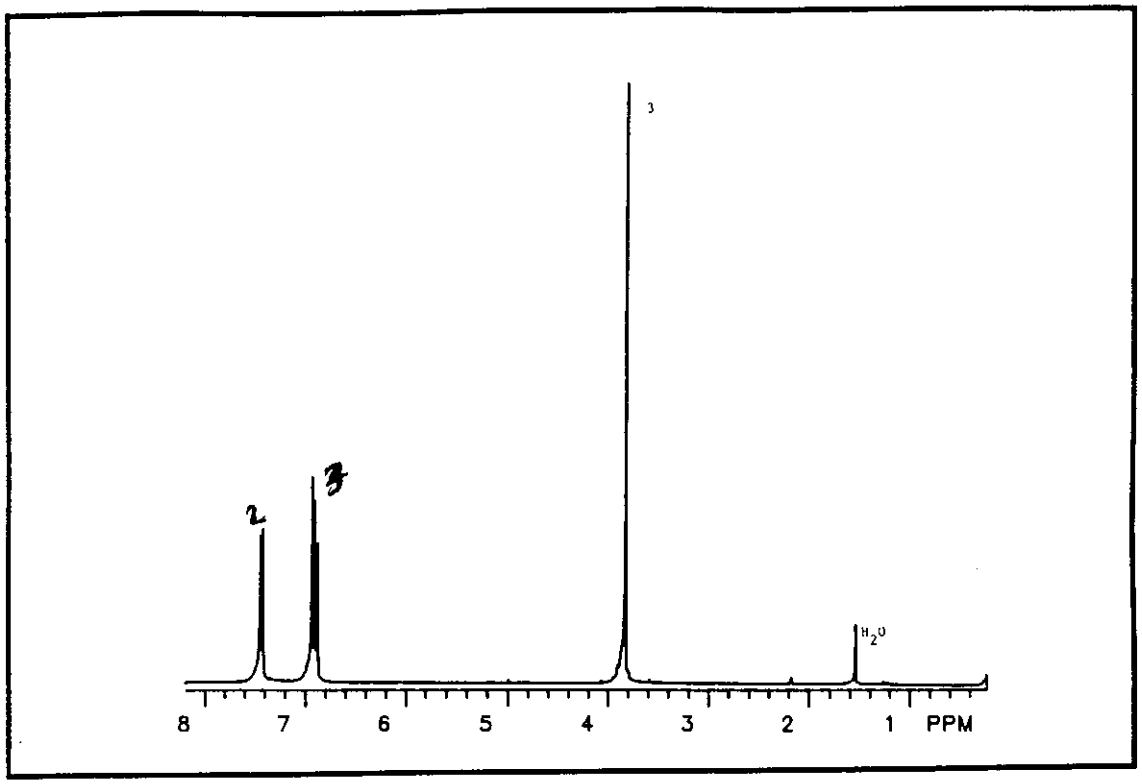
Problem 18

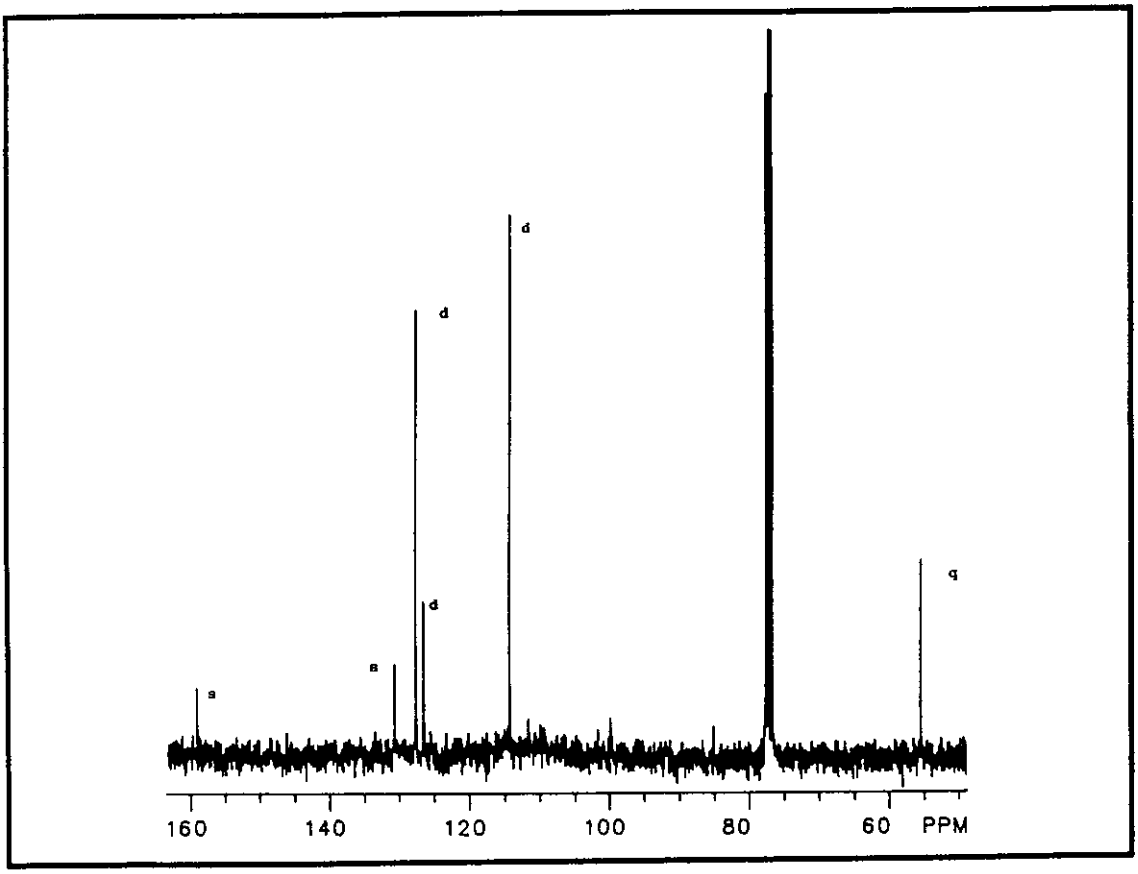
Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 80.0% C; 6.7% H

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z		m/z		m/z	
32	11.70	62	1.47	79	0.46	96	0.12	115	2.84	141	0.75	168	0.44	196	1.18
38	0.40	63	4.61	81	1.74	97	2.04	116	0.26	145	0.15	169	0.34	197	2.24
39	3.34	64	1.84	82	2.71	98	0.72	117	1.43	147	0.14	171	0.44	198	0.20
40	0.89	65	1.98	83	1.45	99	0.60	120	6.70	150	0.58	176	0.59	207	0.53
41	2.14	67	0.21	83	1.33	101	0.82	121	0.17	151	2.59	177	0.70	208	0.40
43	3.16	69	2.11	84	0.25	102	1.90	123	0.93	152	11.71	178	1.29	209	1.40
44	4.49	70	0.55	85	1.03	103	0.50	125	0.14	153	16.98	179	0.77	210	1.99
45	1.80	70	0.51	86	0.65	104	0.17	126	1.83	154	6.49	180	0.43	223	0.16
50	1.74	71	1.69	87	1.00	104	0.38	127	2.81	155	1.31	181	5.50	224	0.67
51	3.28	73	4.03	88	0.87	105	1.27	128	3.00	156	0.32	182	7.79	225	50.02
52	0.84	74	1.47	89	4.22	108	0.51	129	0.25	163	1.43	183	1.21	226	8.11
53	0.68	75	2.36	90	0.43	109	0.12	132	1.36	164	2.27	192	0.21	227	0.64
55	3.39	76	3.81	91	2.27	111	0.47	137	0.15	165	22.34	193	0.94	240	100.00
56	0.35	77	3.30	92	0.17	113	1.64	139	2.94	166	7.89	194	1.68	241	17.77
57	2.82	78	1.42	95	0.52	114	0.37	140	0.45	167	2.15	195	1.72	242	1.87

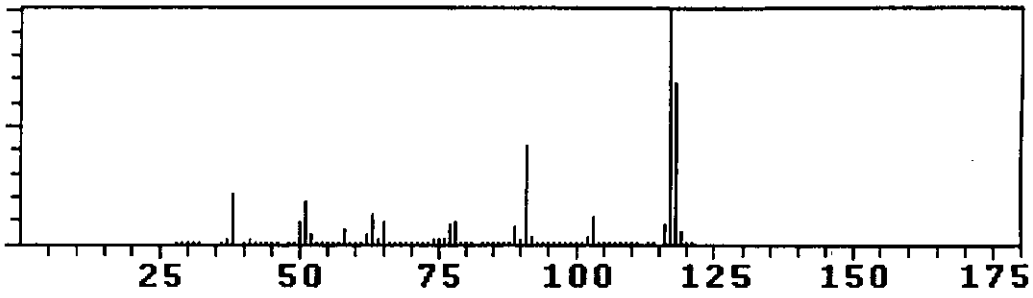


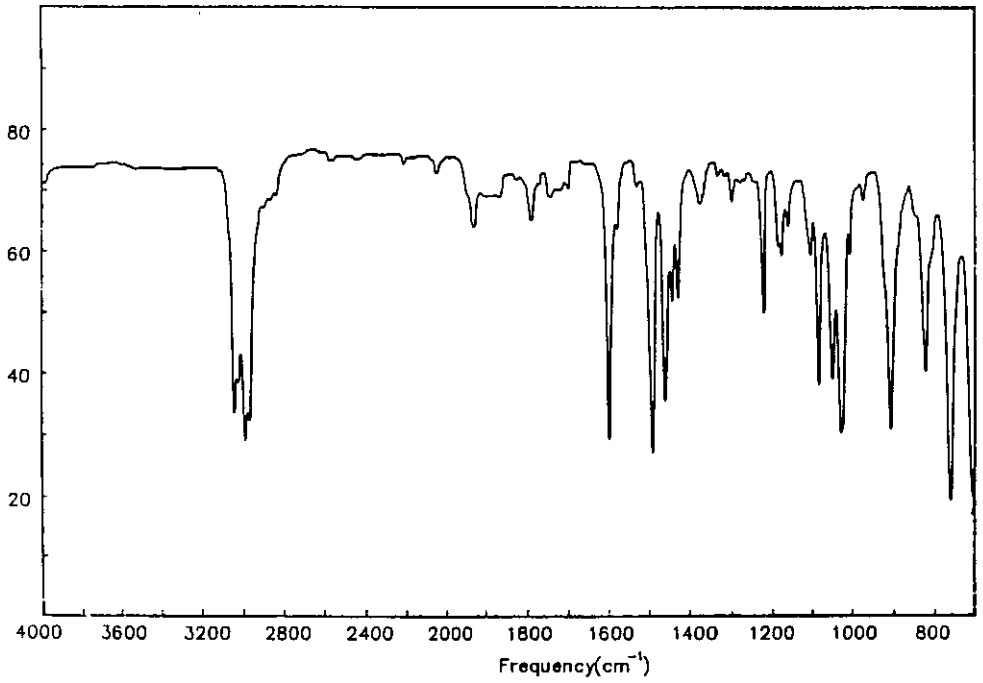

3
2
3
H_2O
8
7
6
5
4
3
2
1
PPM

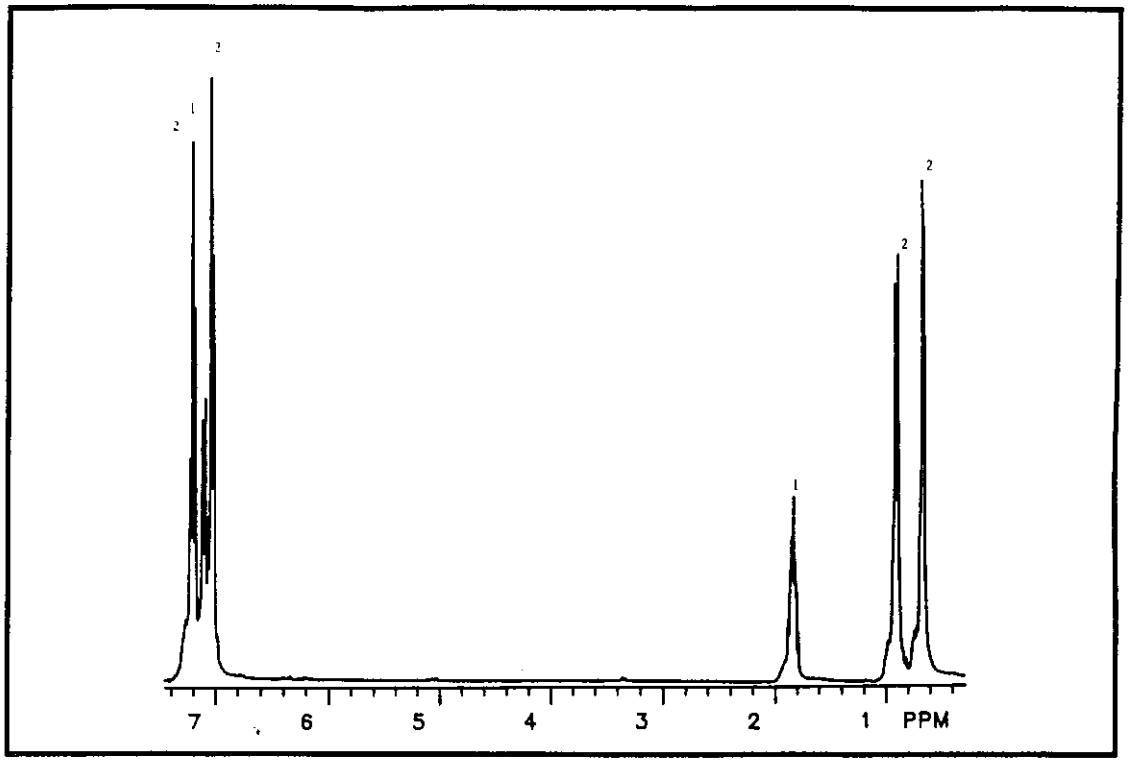

d
d
d
s
s
q
160
140
120
100
80
60
PPM

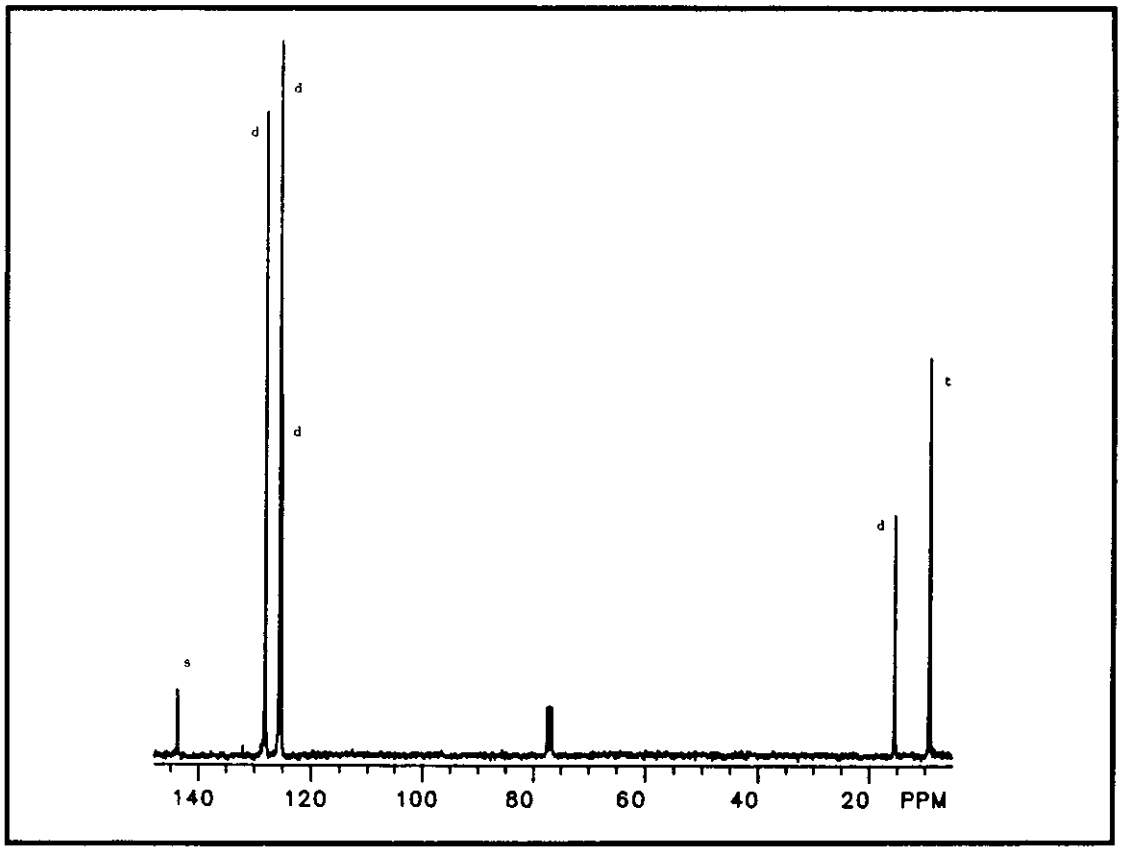
Problem 19

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 91.5% C; 8.5% H



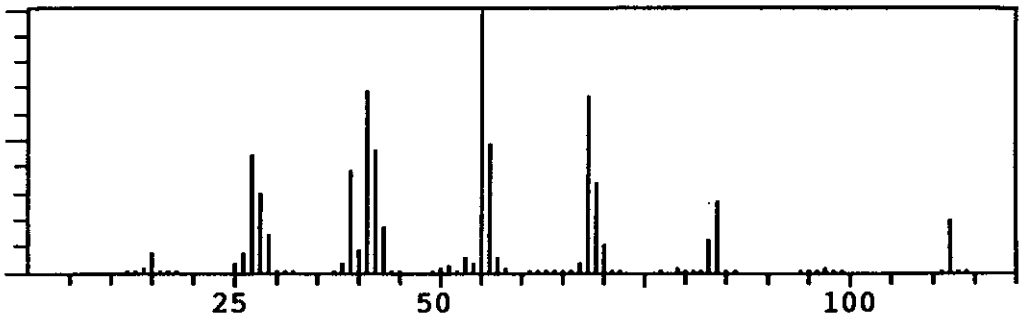


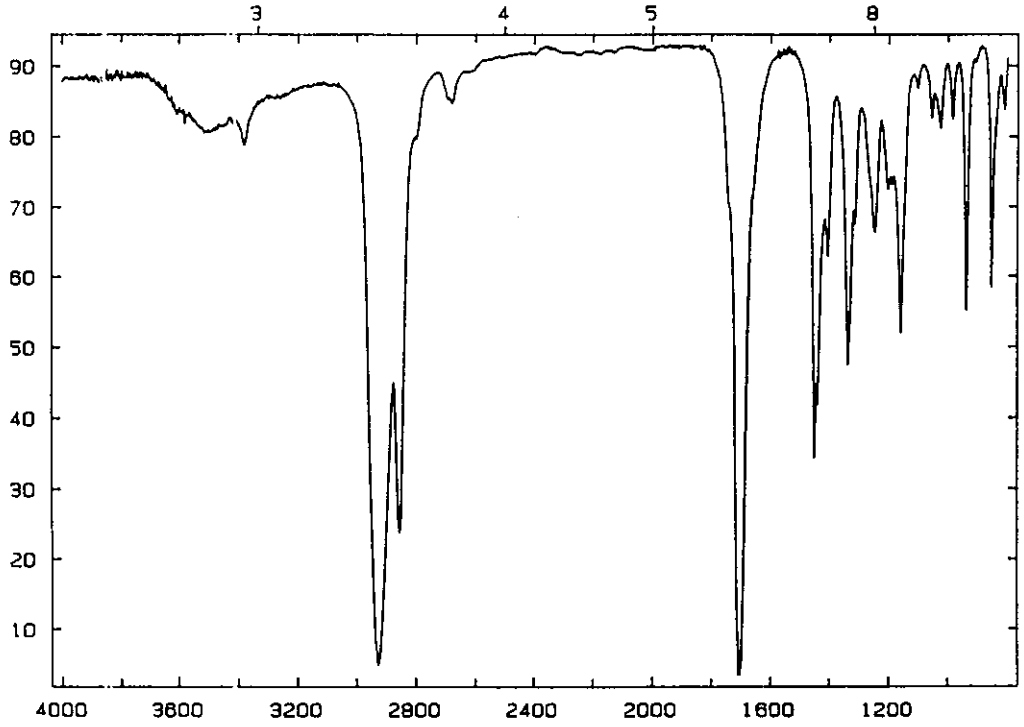

2
2
1
2
1
2
2
7
6
5
4
3
2
1
PPM

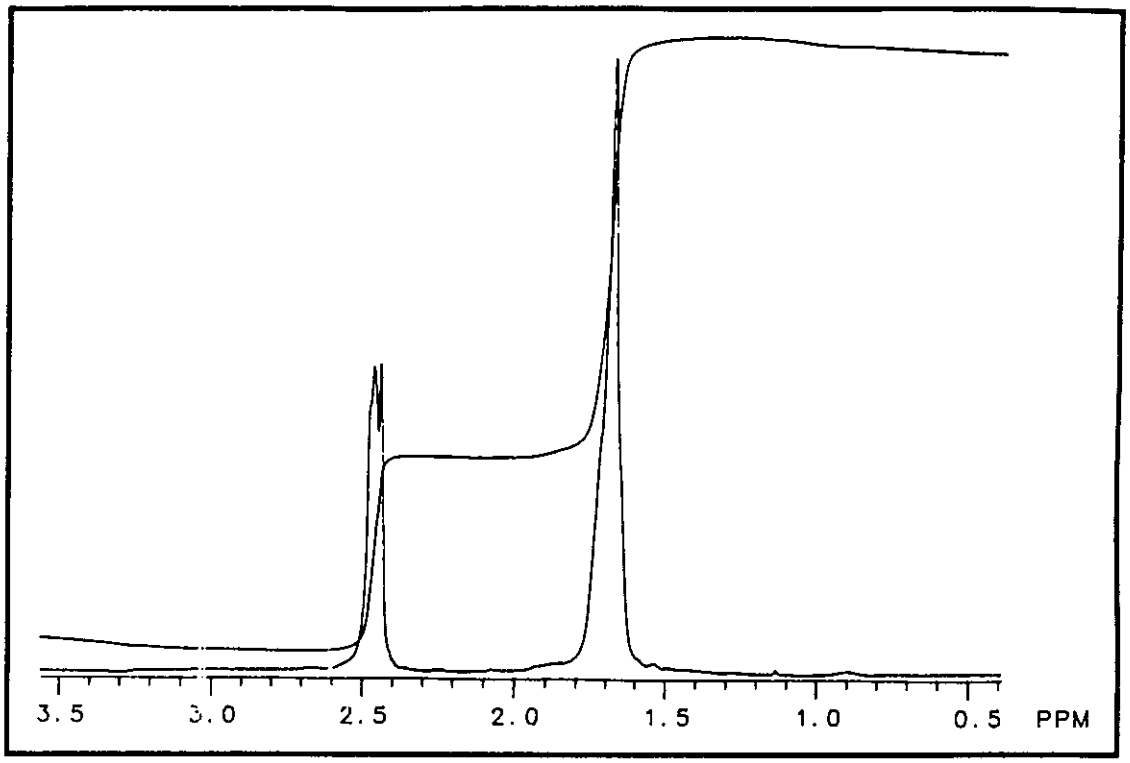

d
d
d
s
t
d
140
120
100
80
60
40
20
PPM

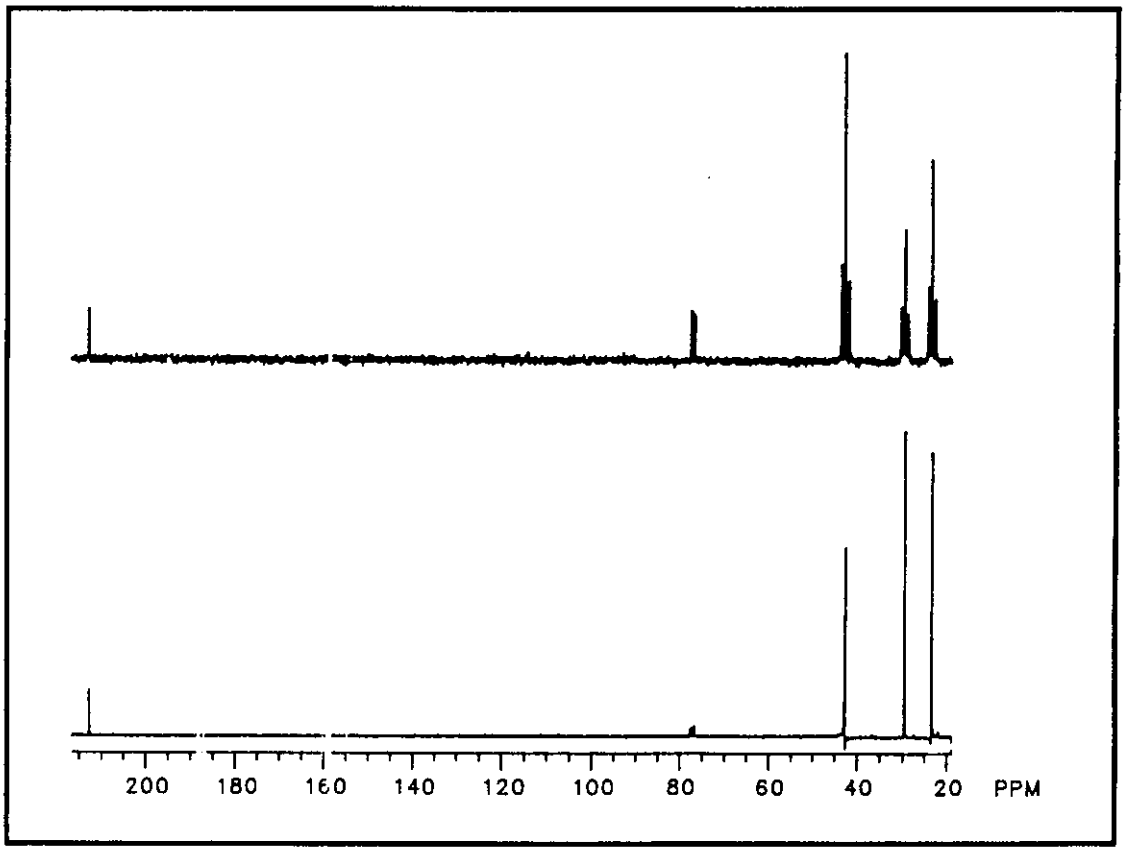
Problem 20

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



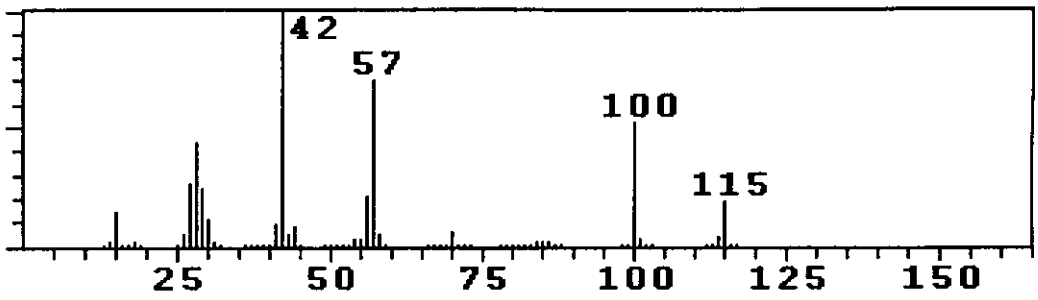


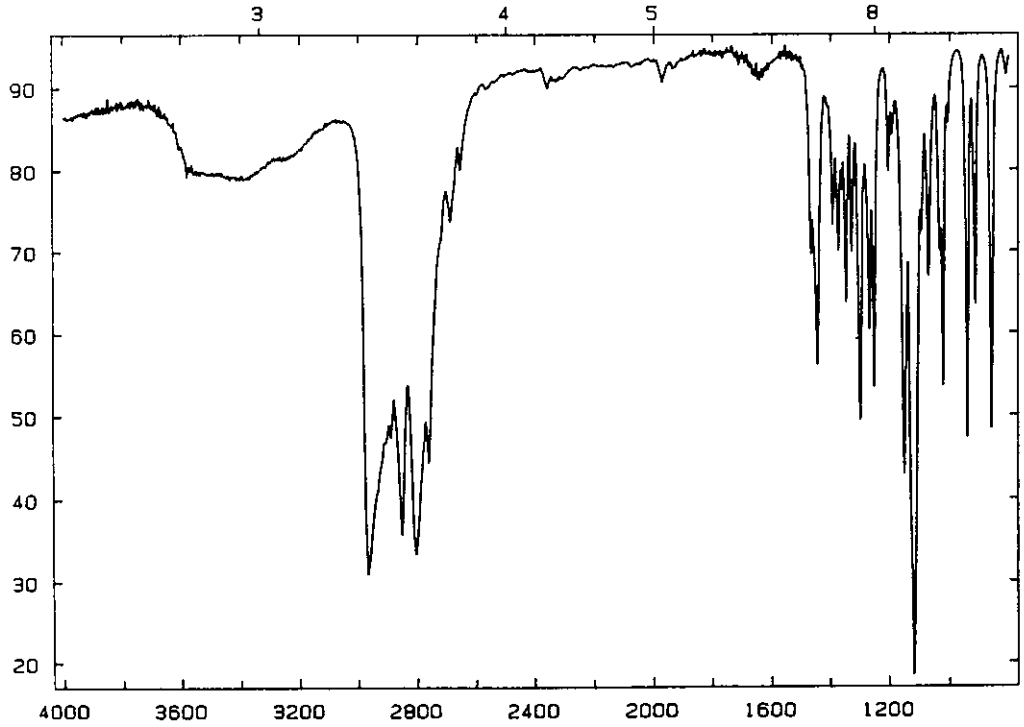

3.5
3.0
2.5
2.0
1.5
1.0
0.5
PPM

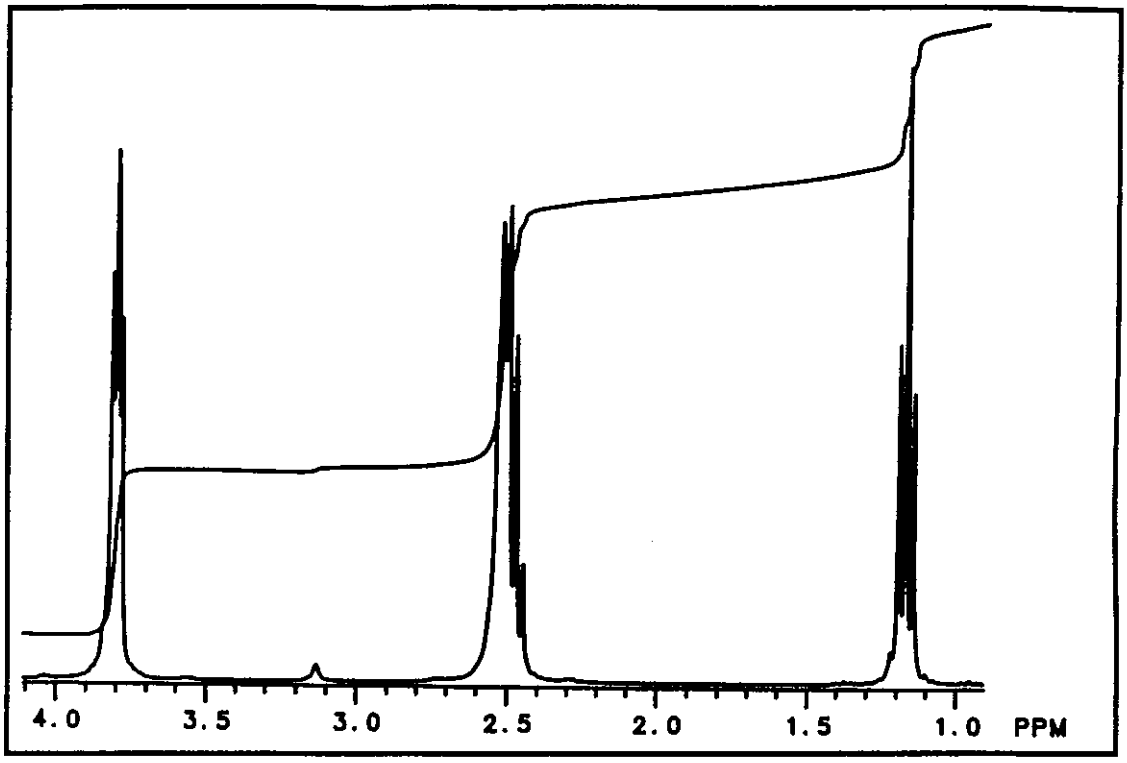

200
180
160
140
120
100
80
60
40
20
PPM

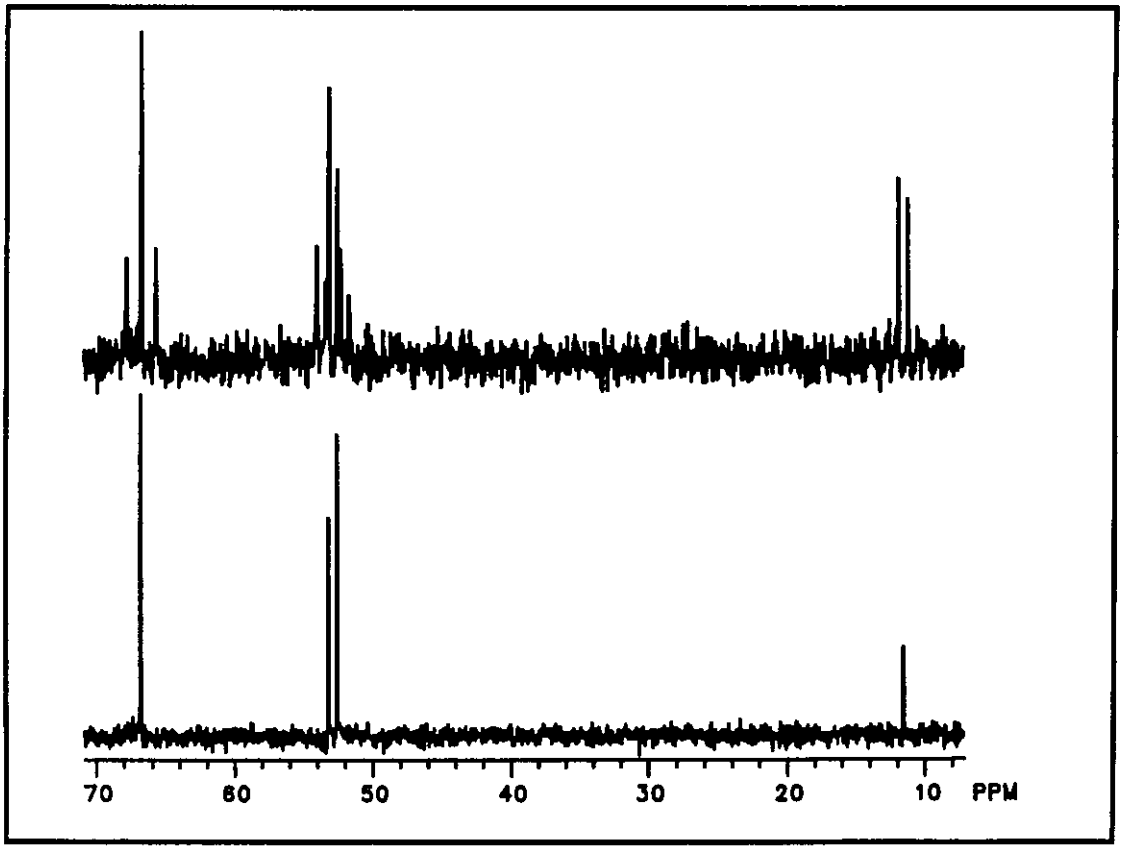
Problem 21

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 62.6% C; 11.4% H; 12.2% N



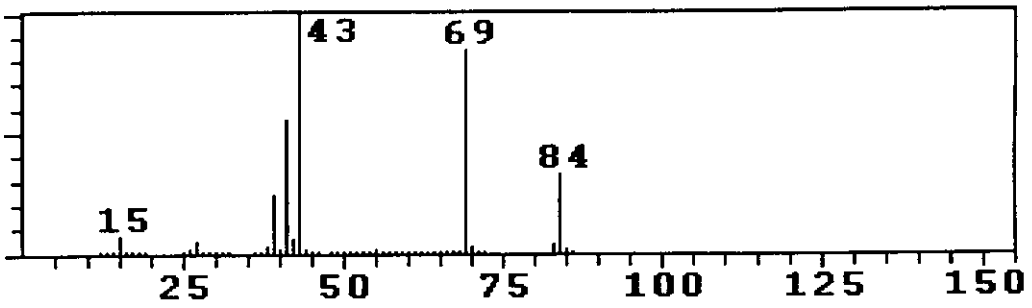


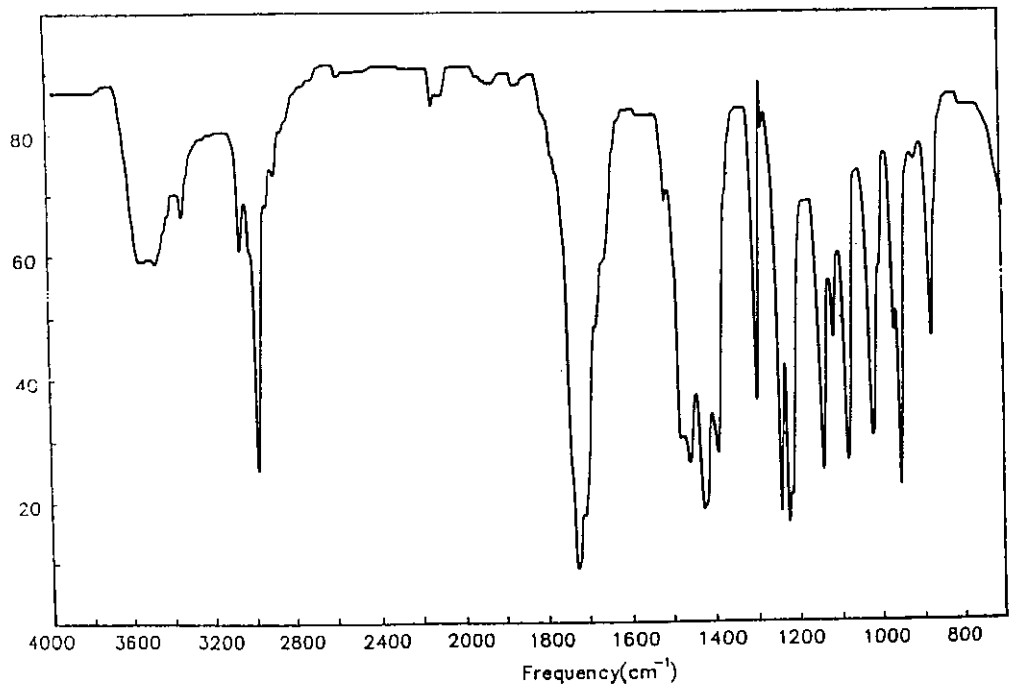

4.0
3.5
3.0
2.5
2.0
1.5
1.0
PPM

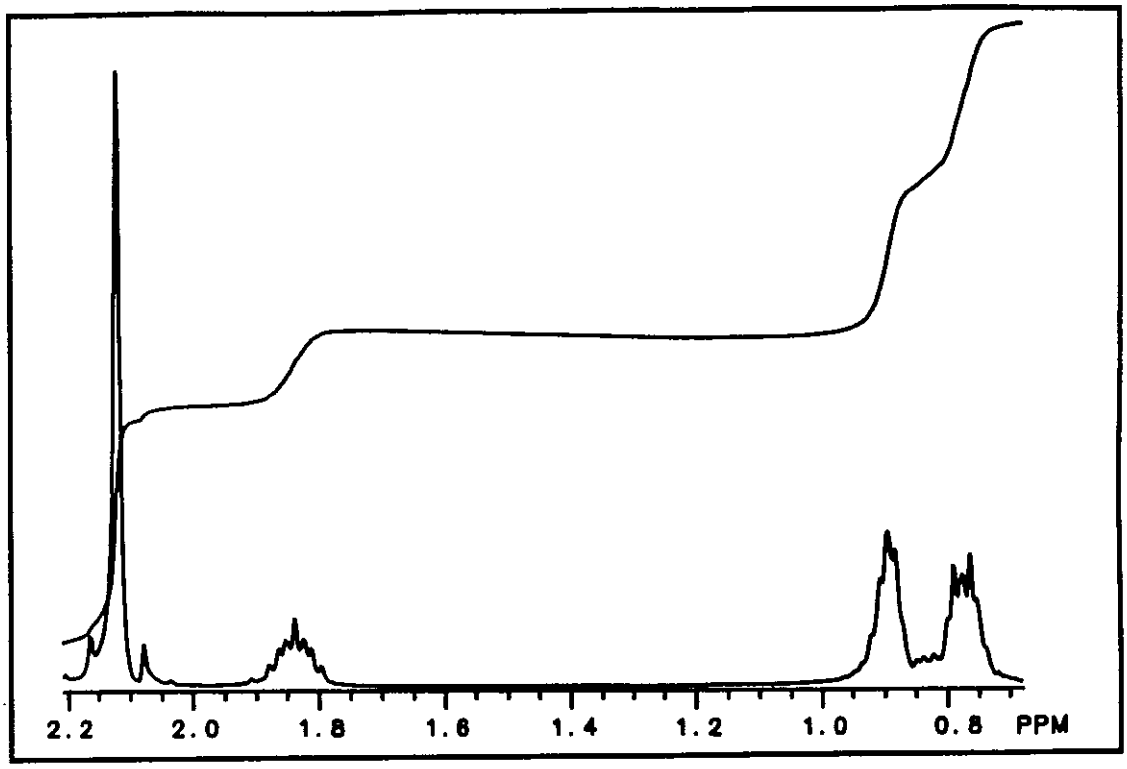

70
60
50
40
30
20
10
PPM

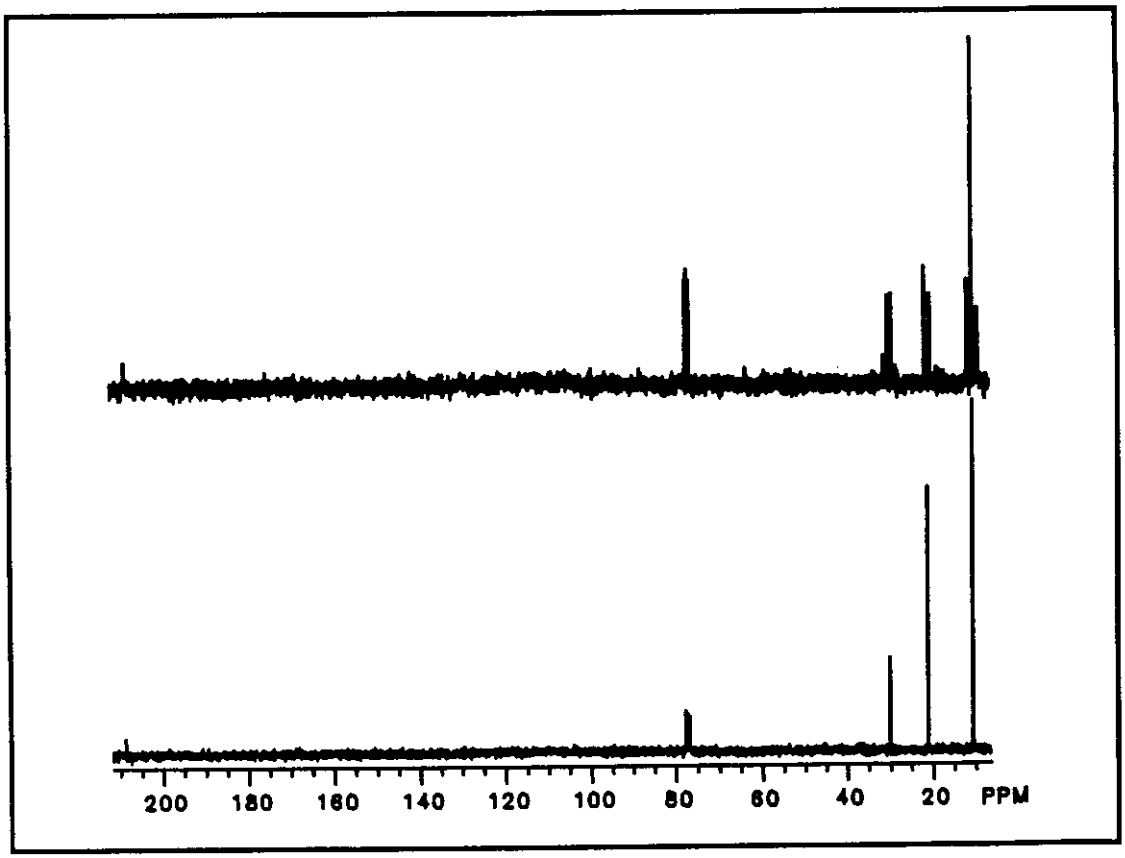
Problem 22

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 71.4% C; 9.6% H



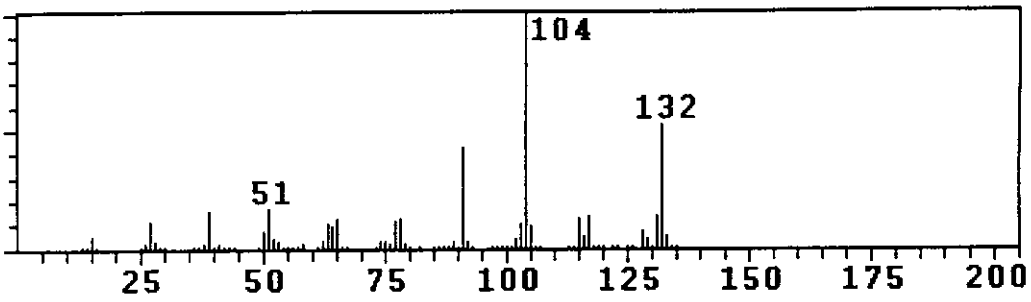


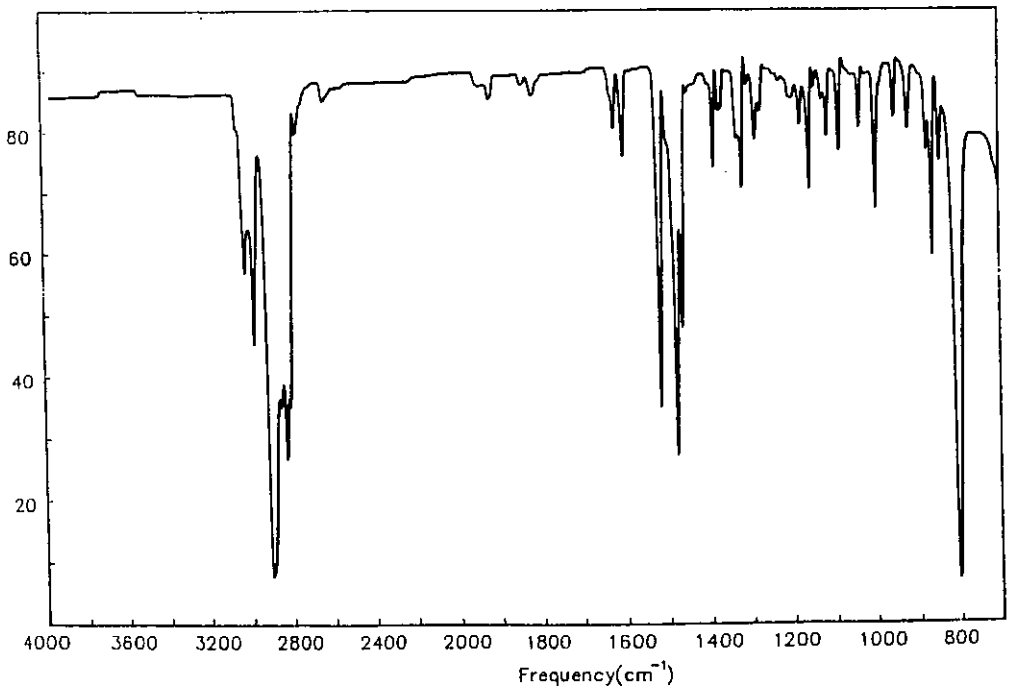

2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
PPM

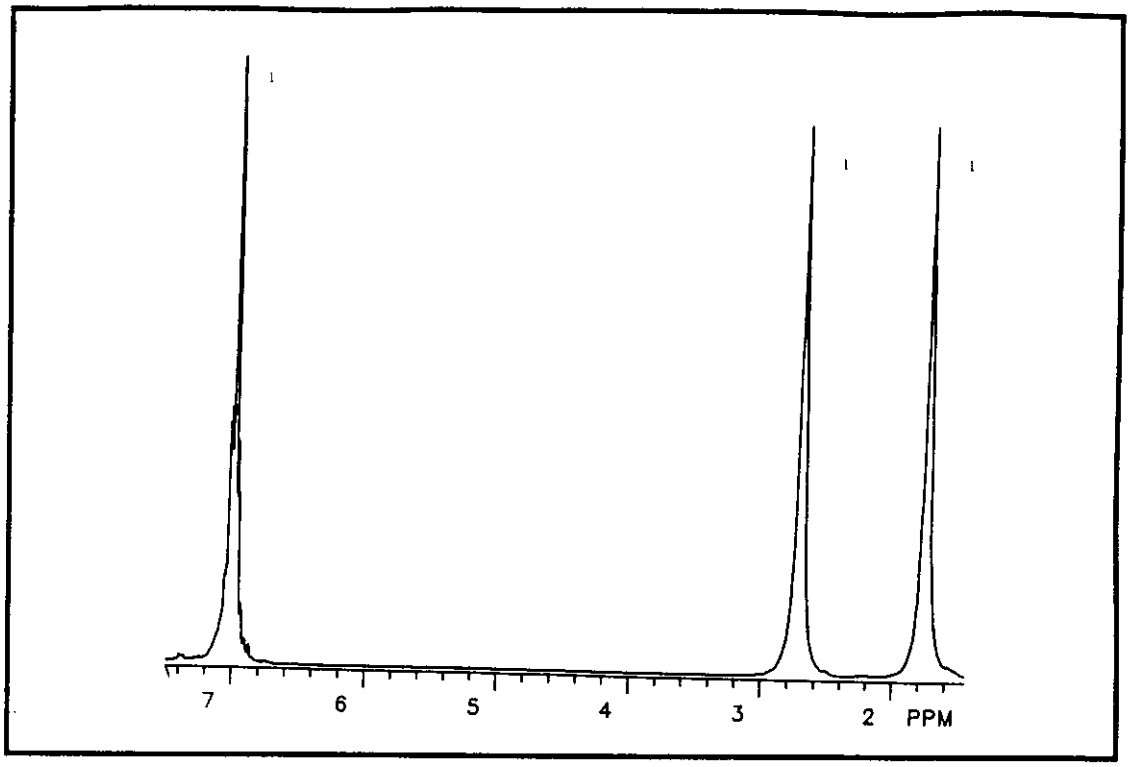

200
180
160
140
120
100
80
60
40
20
PPM

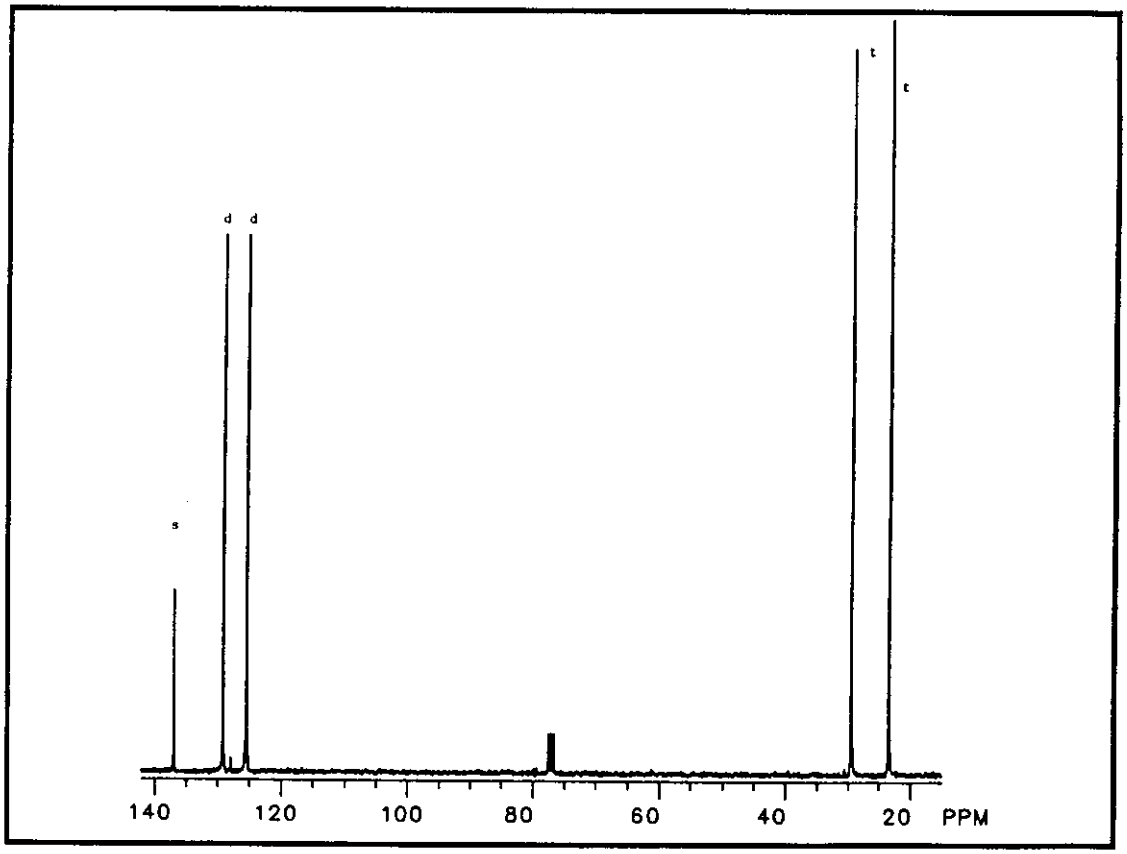
Problem 23

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 90.8% C; 9.2% H



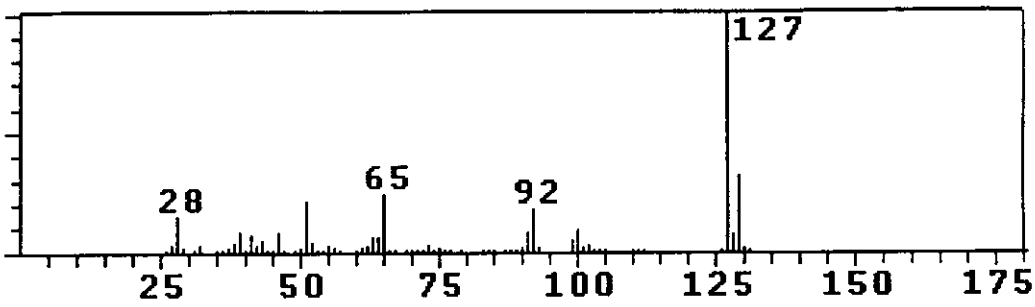


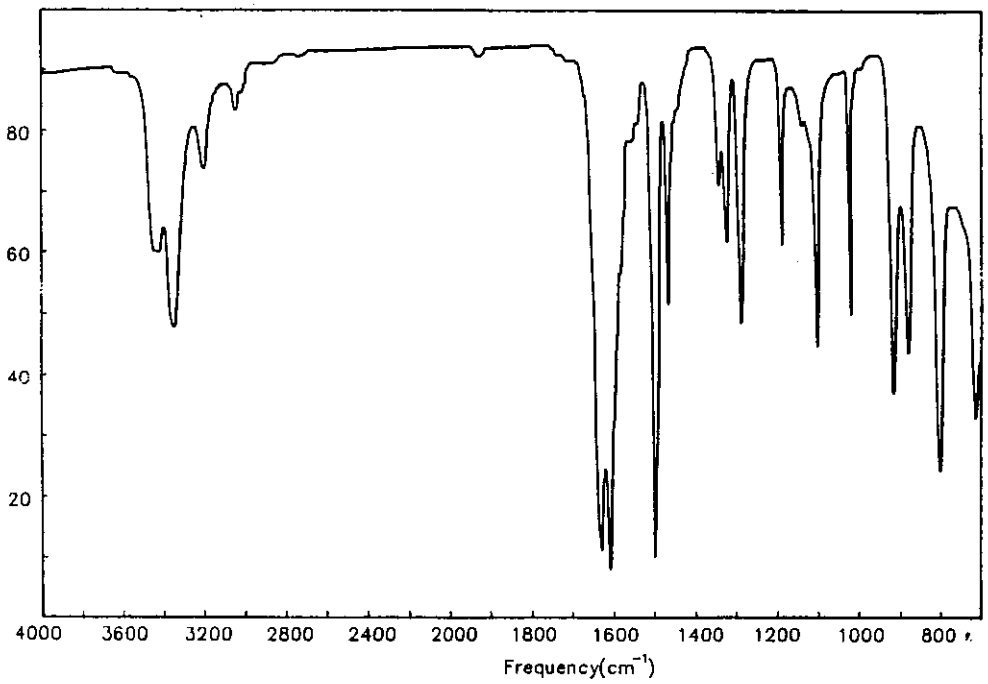

1
1
1
7
6
5
4
3
2
PPM

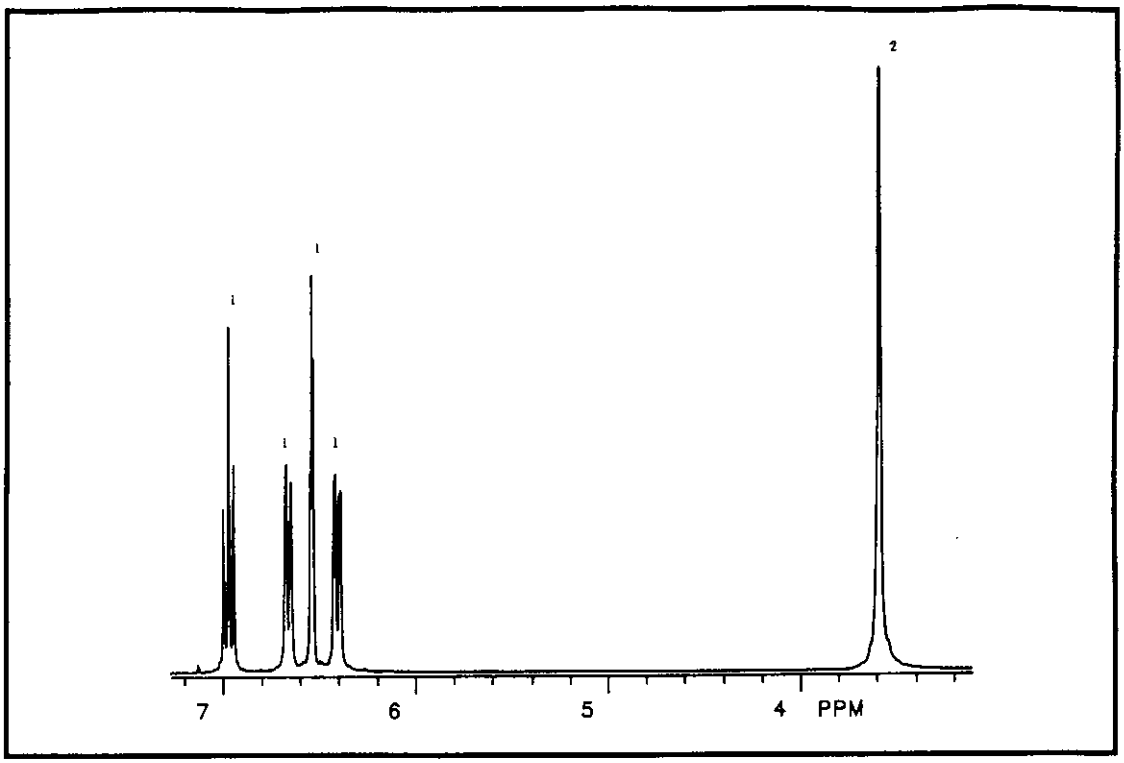

t
t
d
d
s
140
120
100
80
60
40
20
PPM

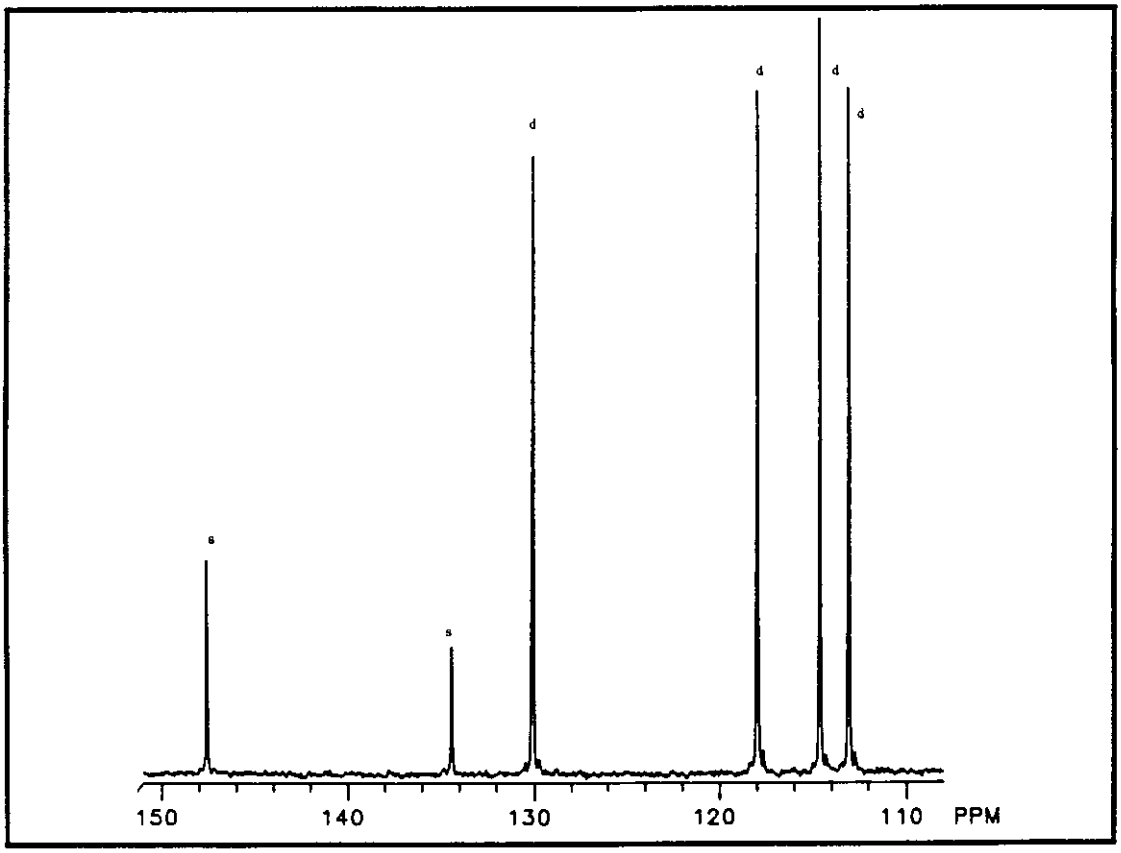
Problem 24a

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



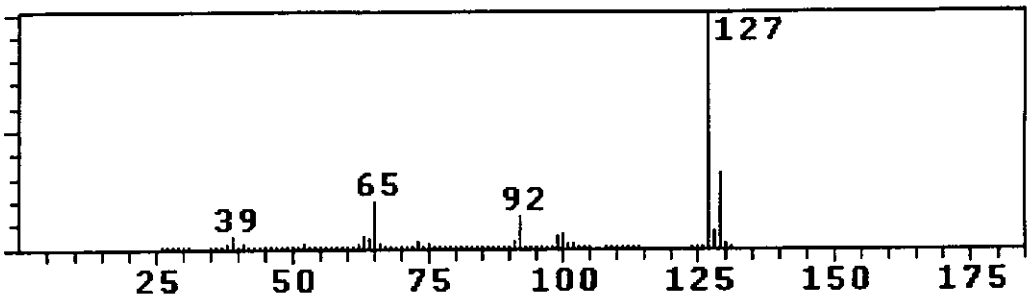


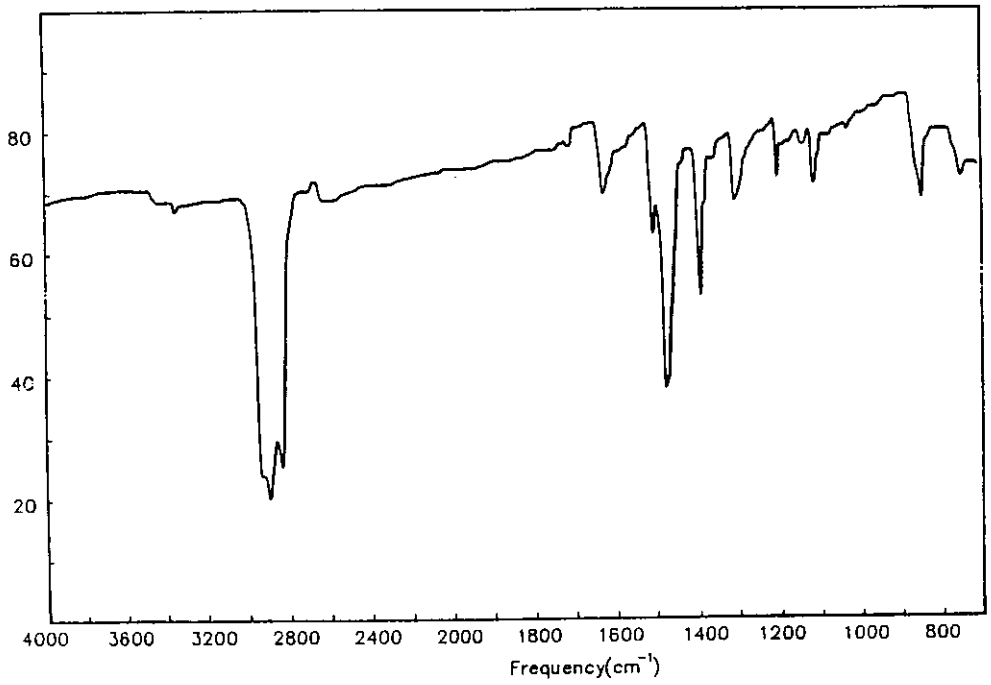

2
1
1
1
1
7
6
5
4
PPM

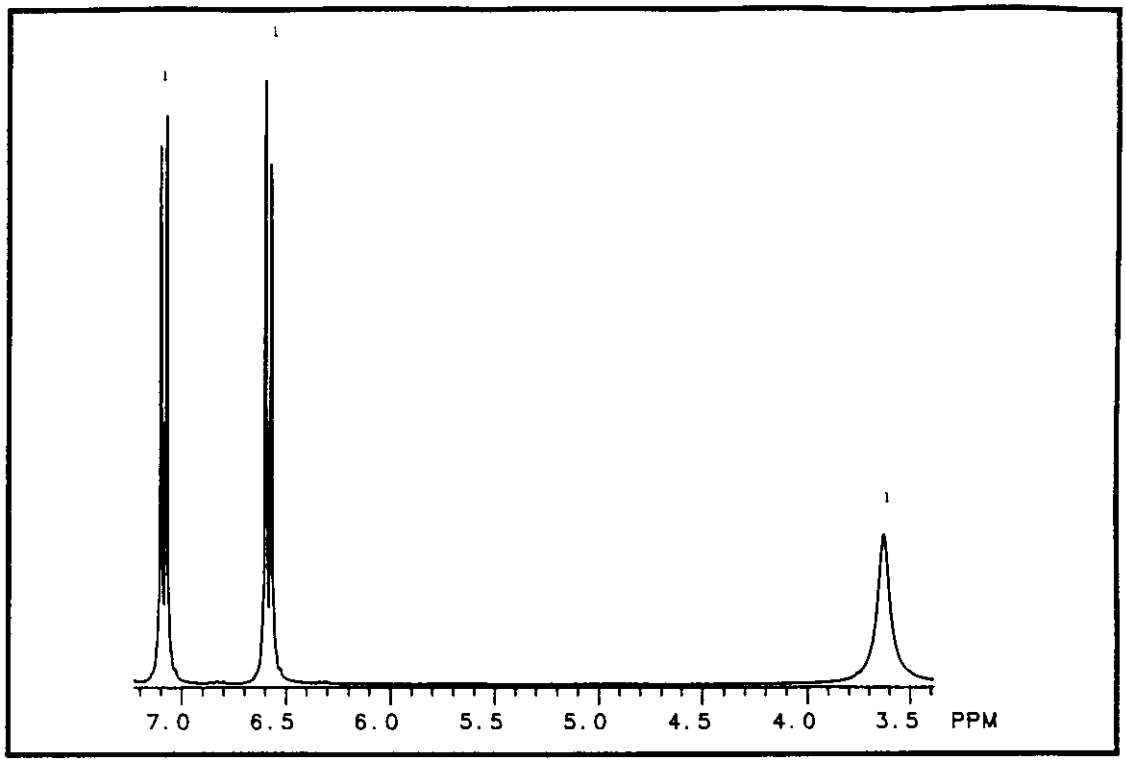

d
d
d
d
s
s
150
140
130
120
110
PPM

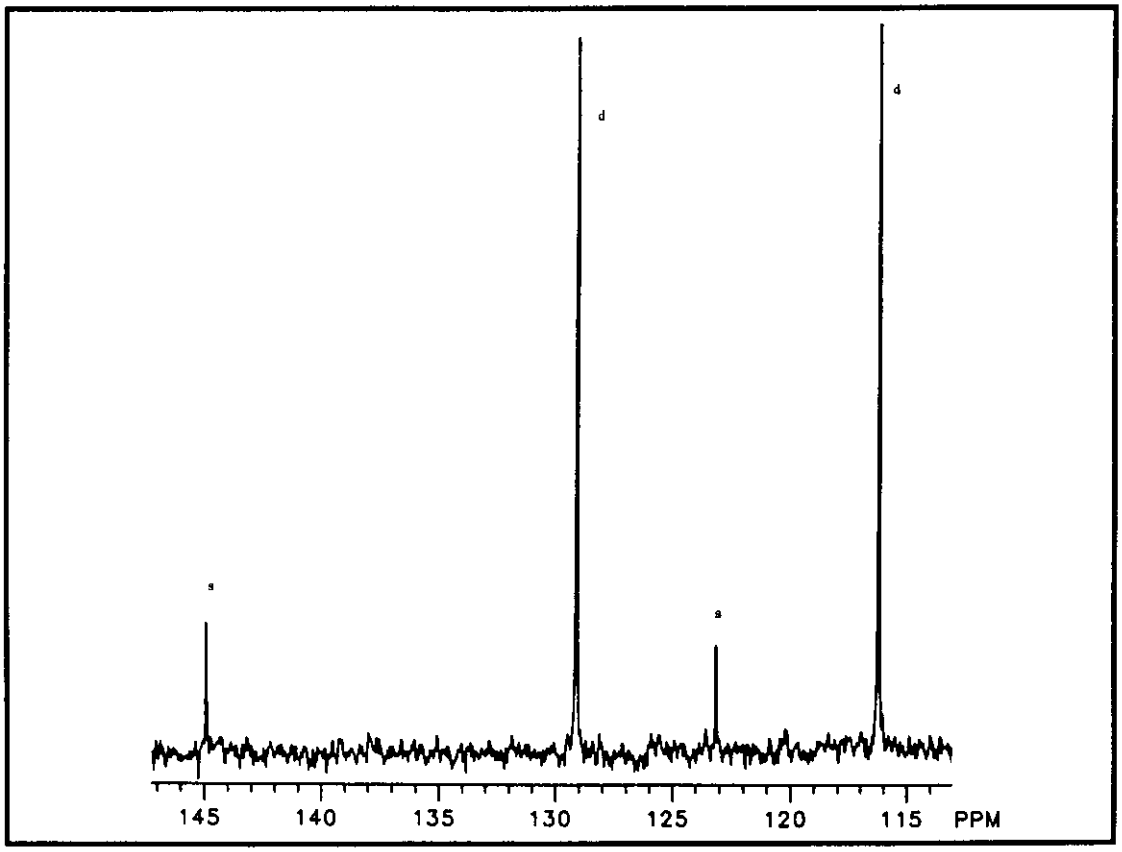
Problem 24b

Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



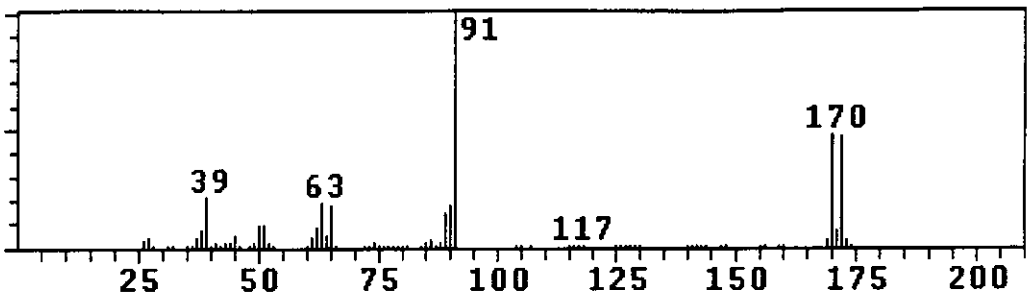


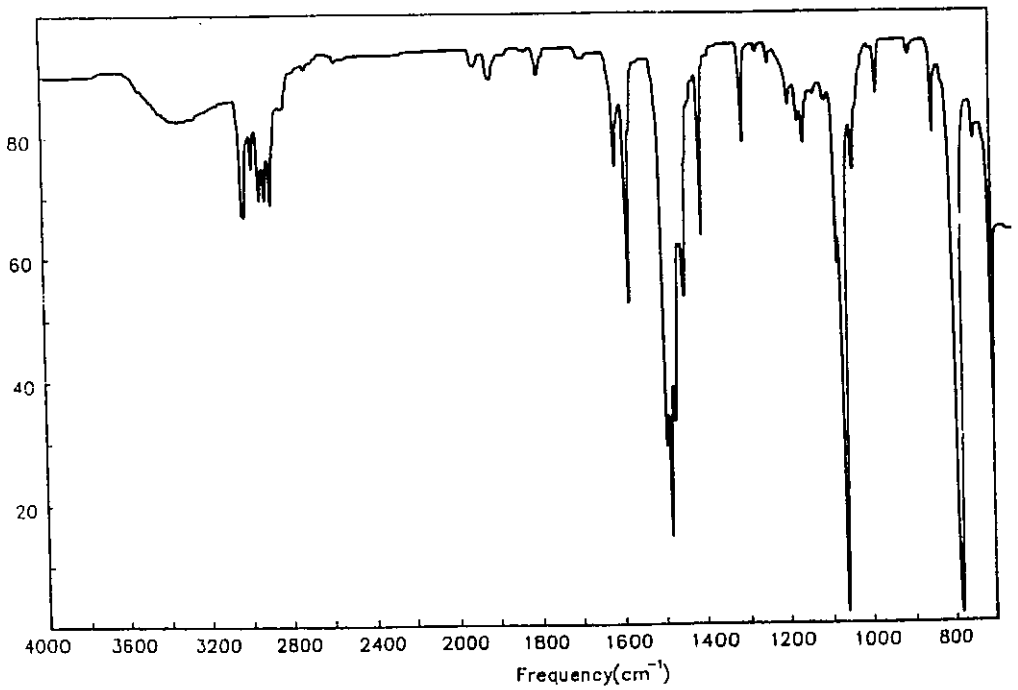

1
1
1
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
PPM

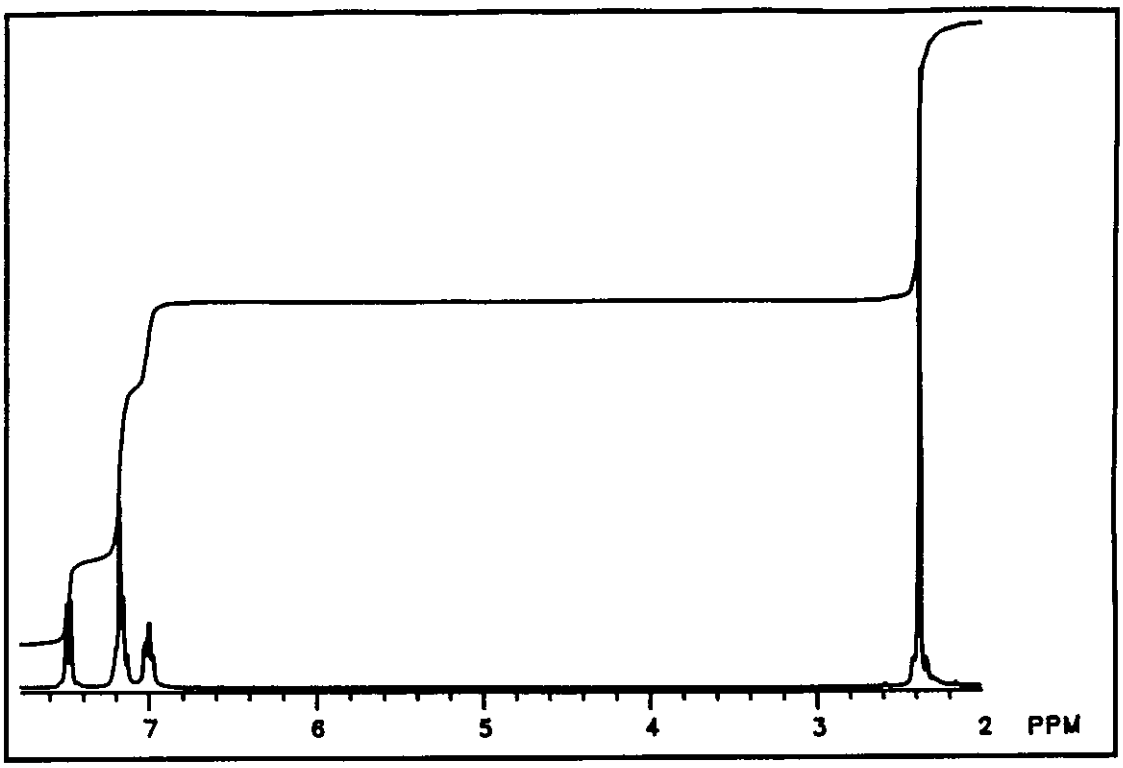

s
d
s
d
145
140
135
130
125
120
115
PPM

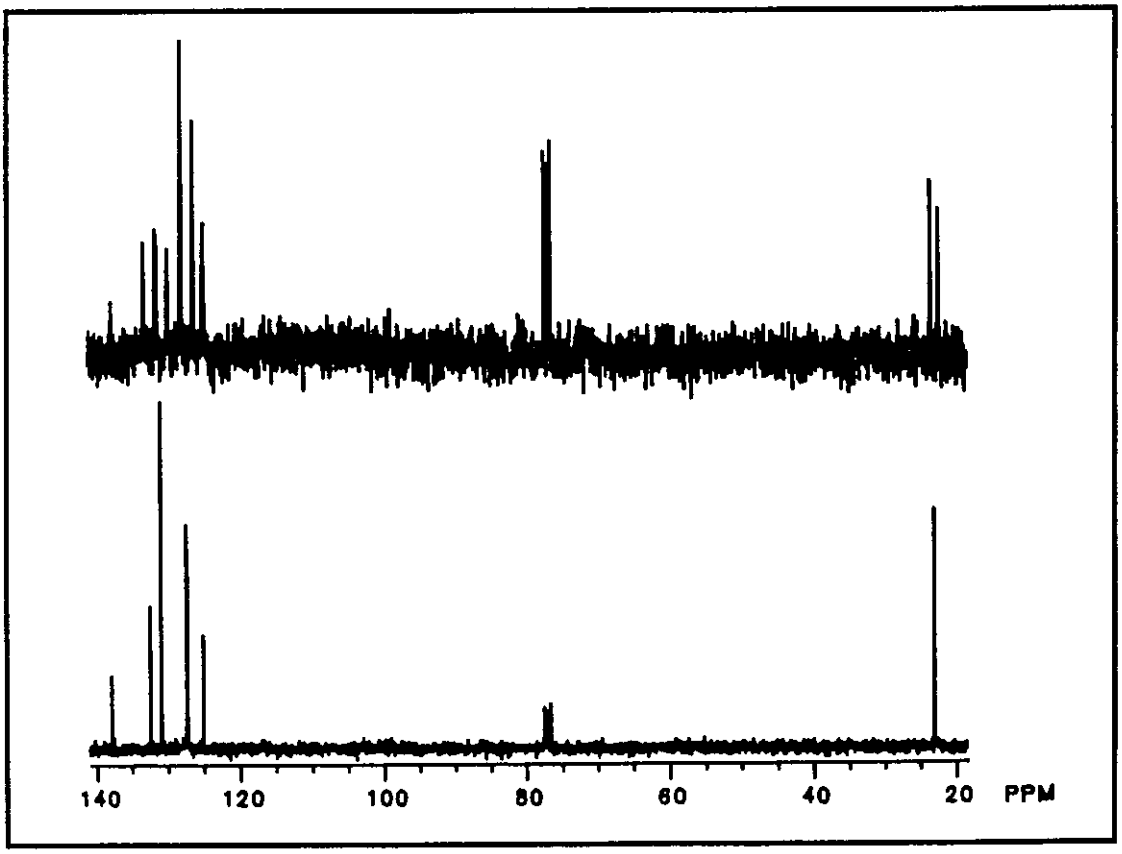
Problem 25a

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 49.2% C; 4.1% H



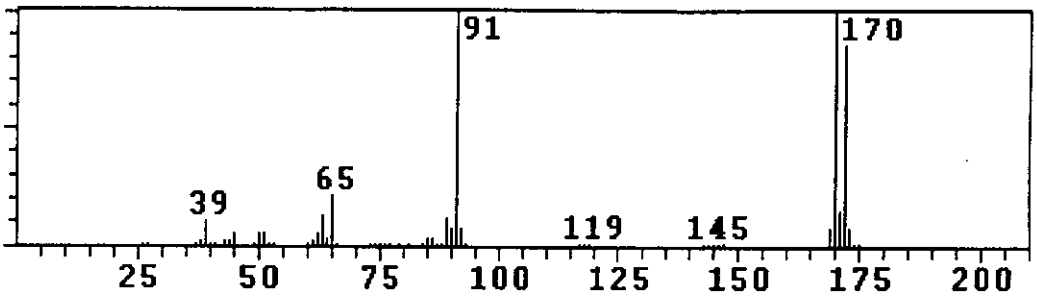


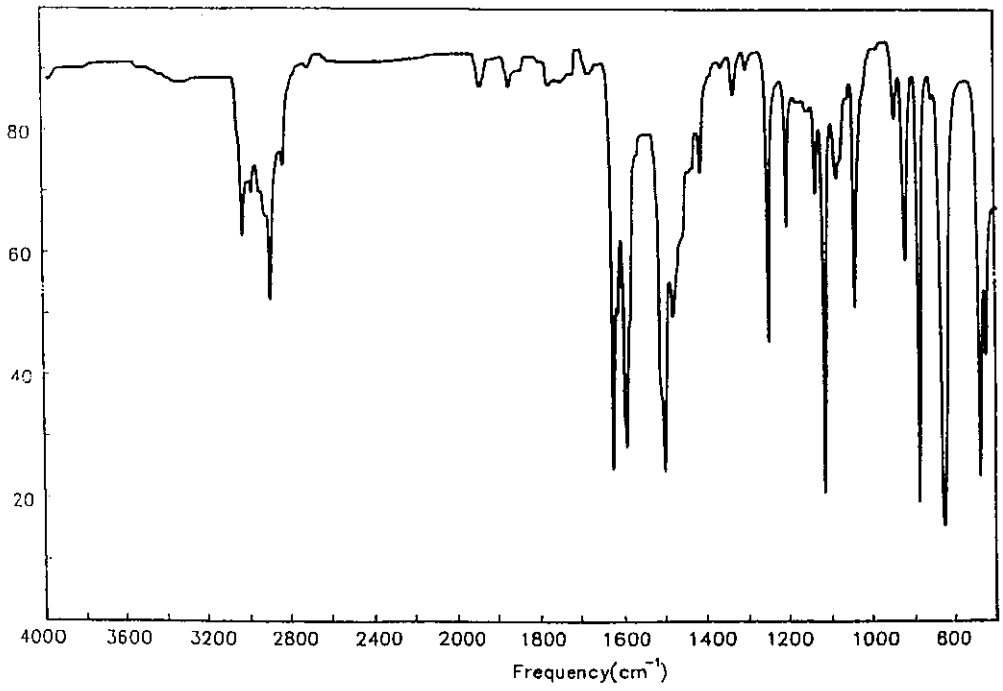

7
6
5
4
3
2
PPM

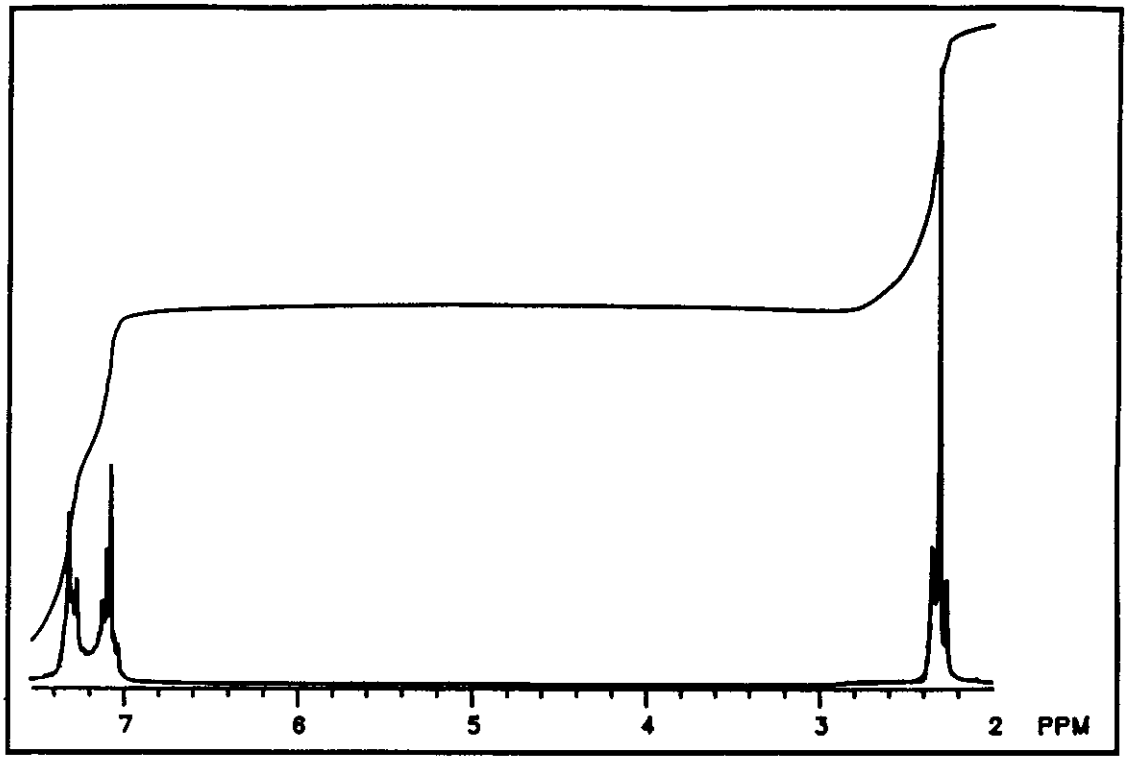

140
120
100
80
60
40
20
PPM

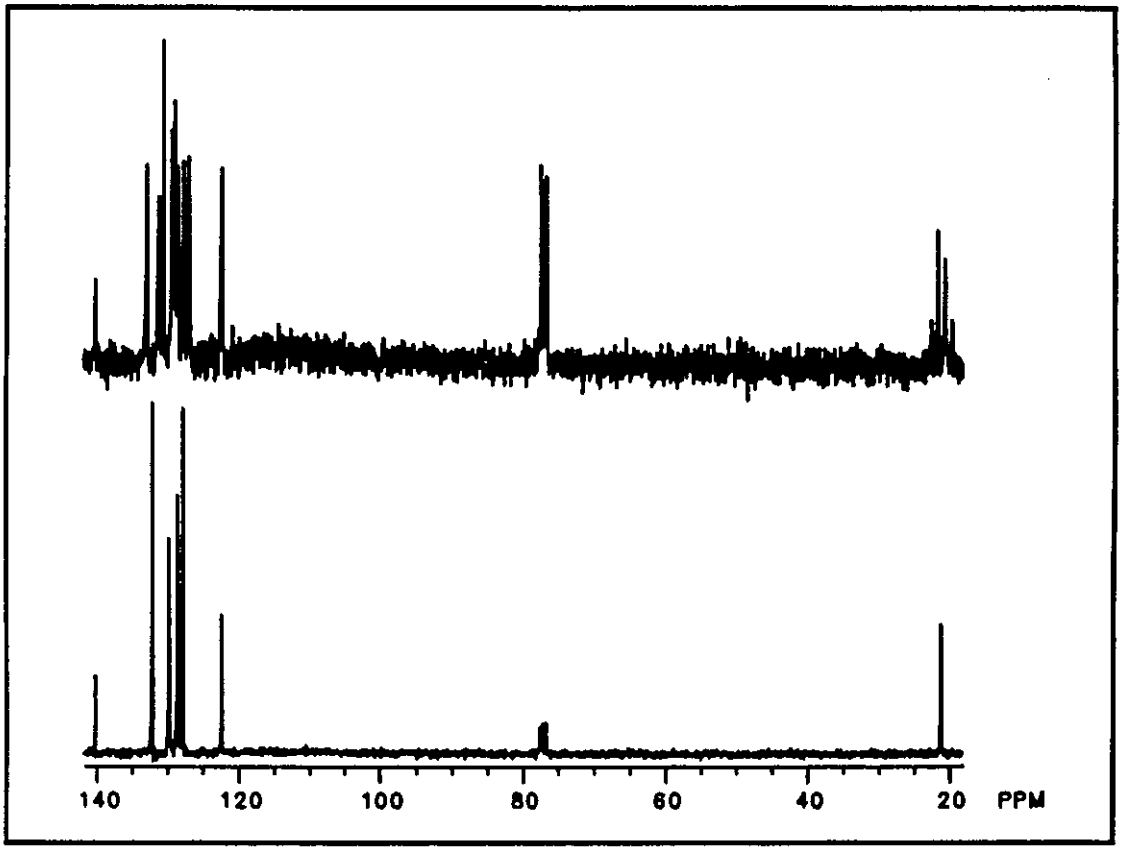
Problem 25b

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 49.2% C; 4.1% H






7
6
5
4
3
2
PPM

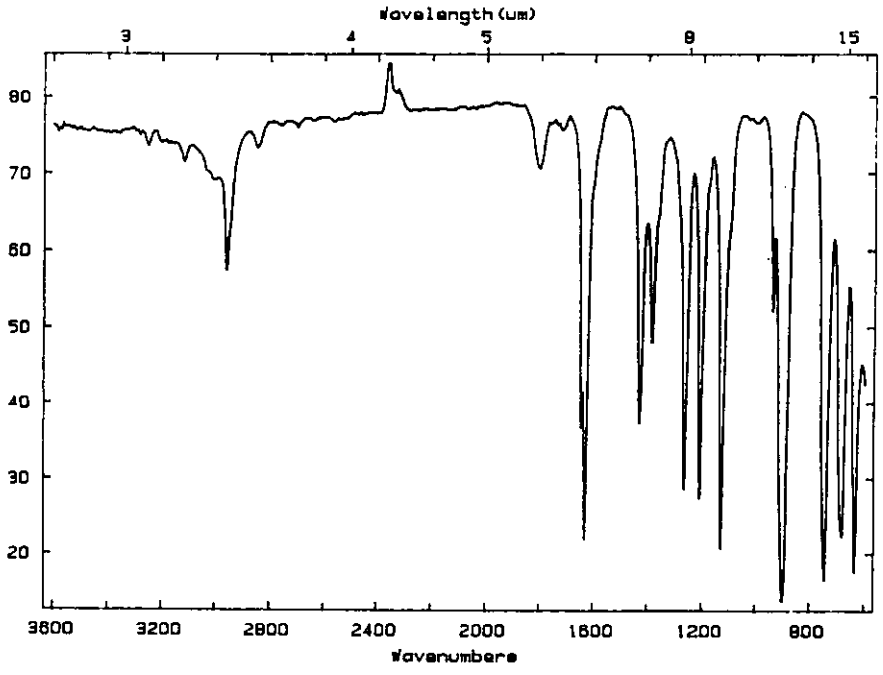

140
120
100
80
60
40
20
PPM

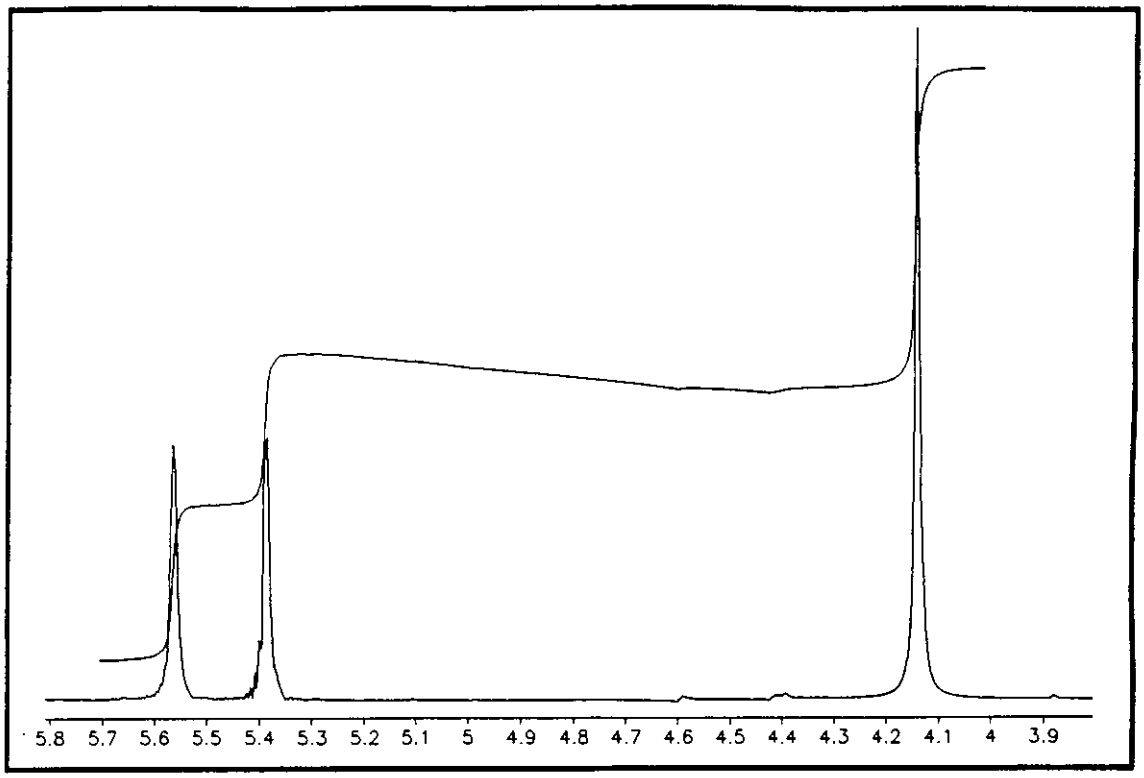
Problem 26

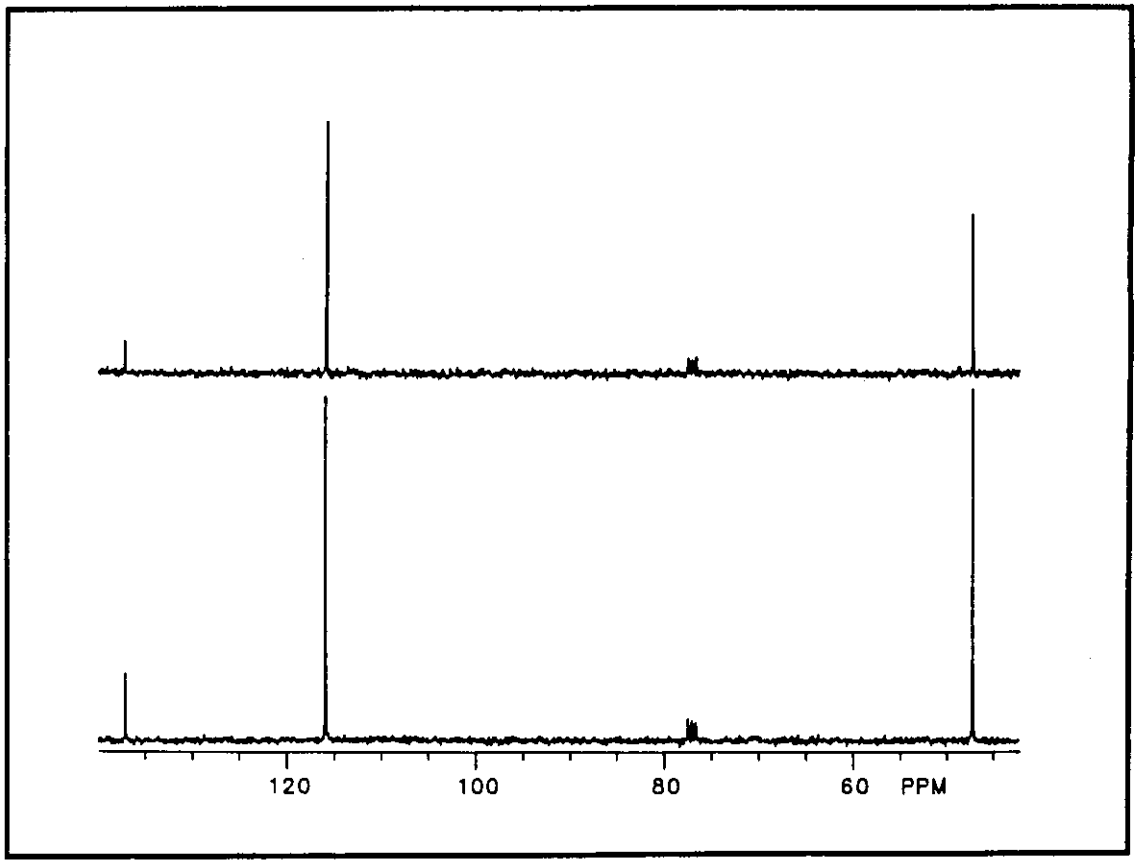
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
35	8.53	47	3.05	60	2.07	72	1.28	83	2.22	109	1.58
36	6.13	48	2.13	61	10.23	73	5.47	84	0.15	110	27.26
37	19.28	49	20.96	62	1.01	75	100.00	85	1.46	111	1.92
38	22.13	50	1.01	63	3.28	76	4.56	87	0.23	112	17.87
39	72.64	51	6.59	64	0.09	77	35.84	95	0.20	113	0.80
40	7.69	52	0.11	70	0.17	78	1.25	97	0.13	114	2.87
41	0.24	59	0.32	71	0.46	82	0.16	107	0.10	115	0.10

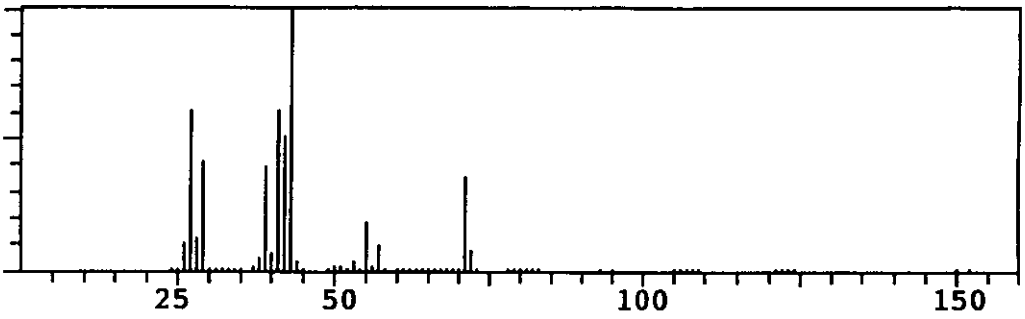


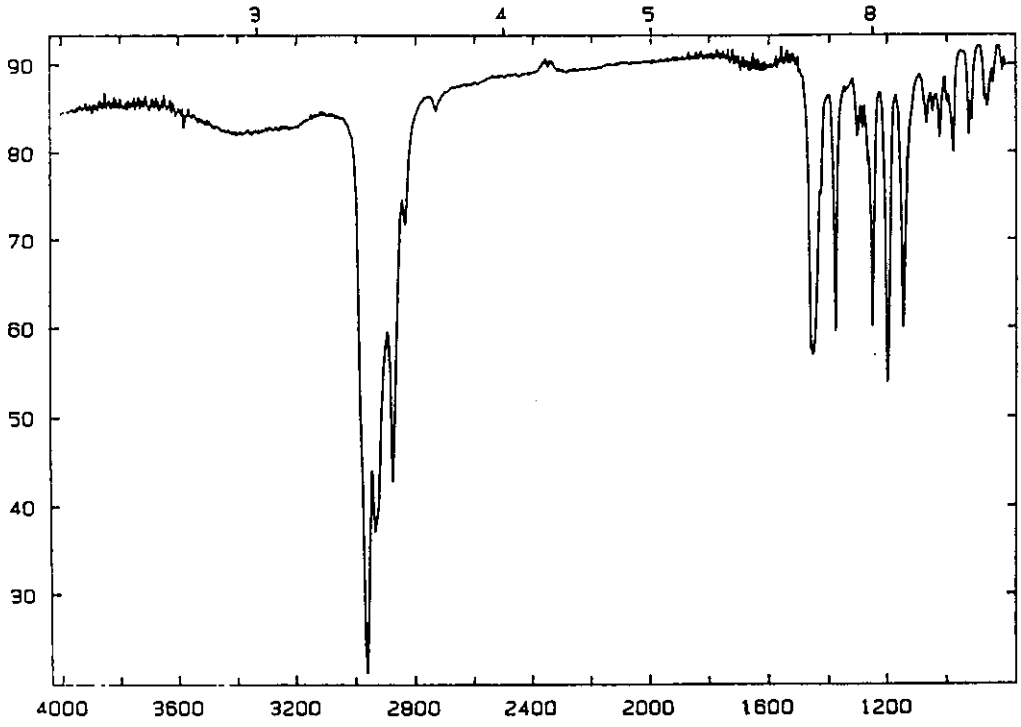

5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1 5 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4 3.9

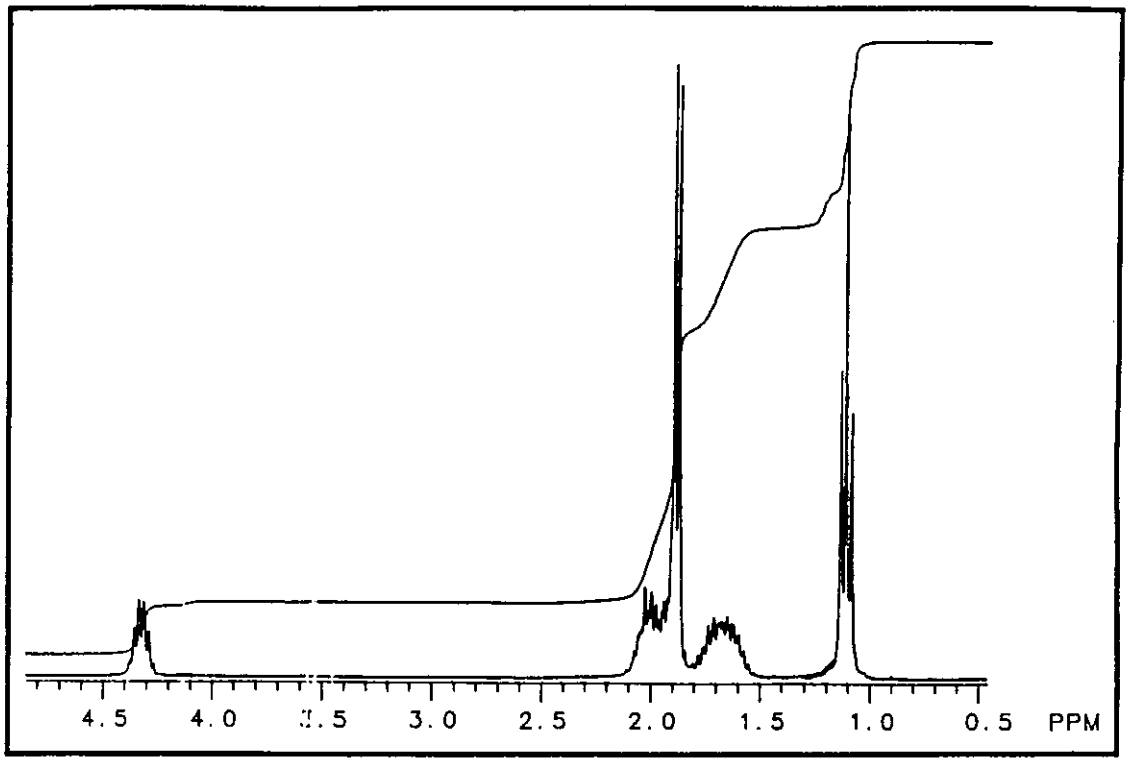

120 100 80 60 PPM

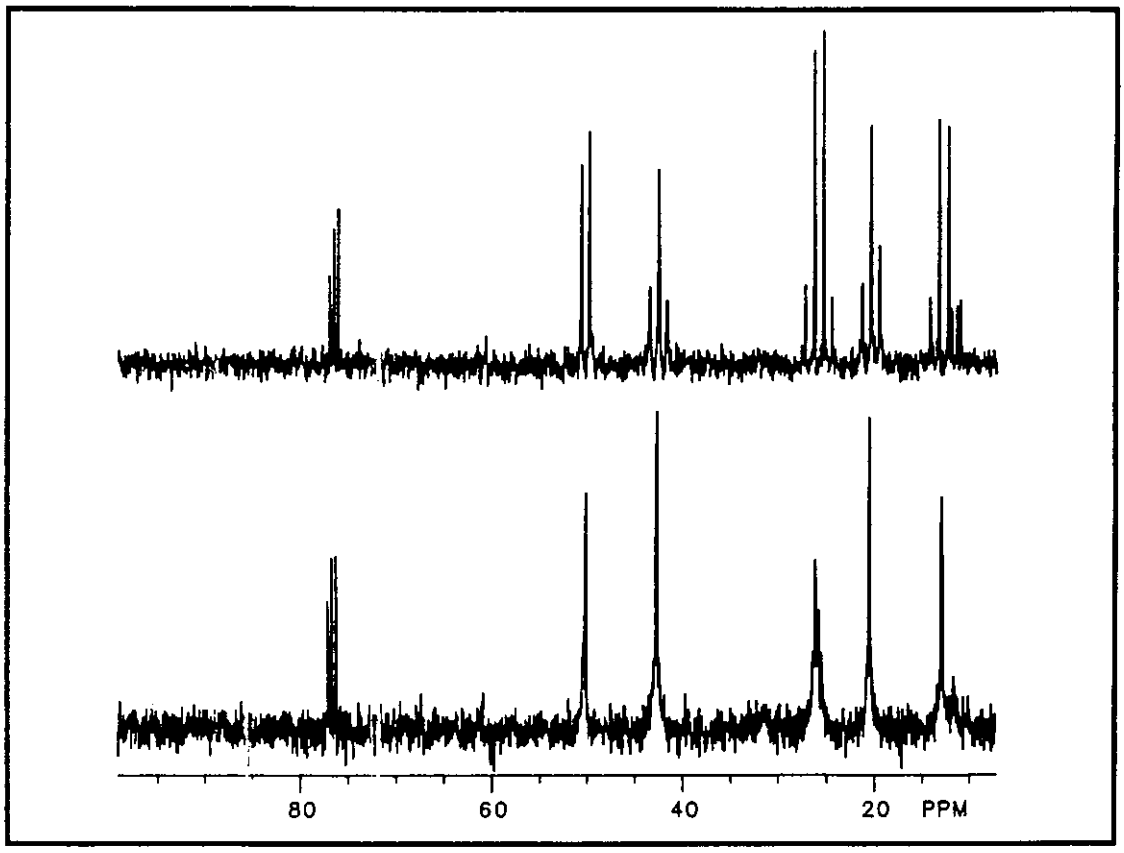
Problem 27

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



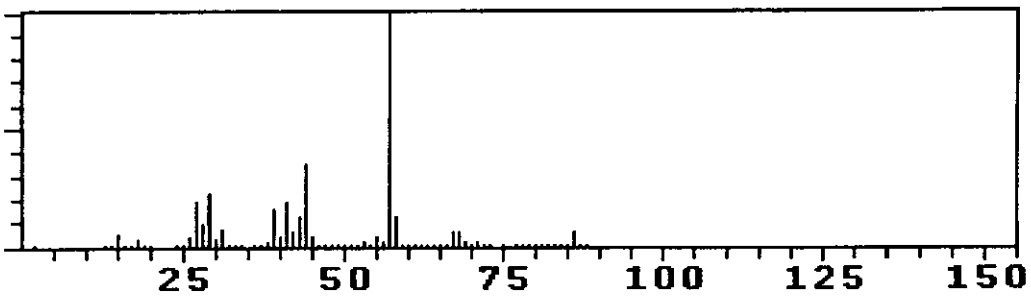


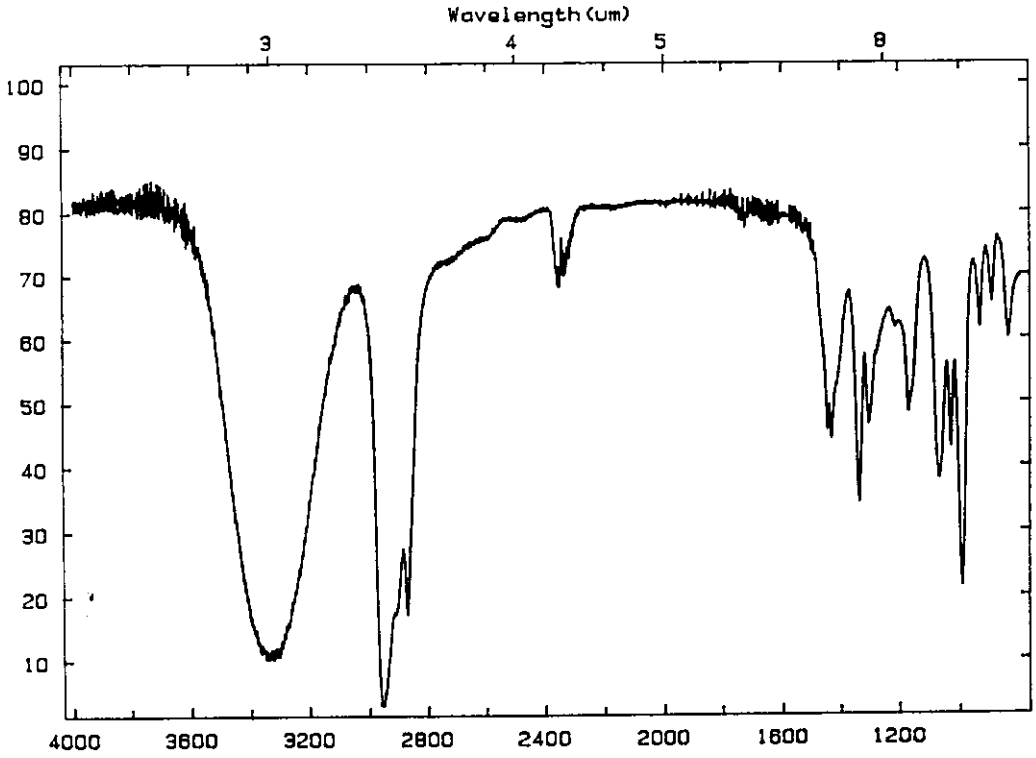

4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
PPM

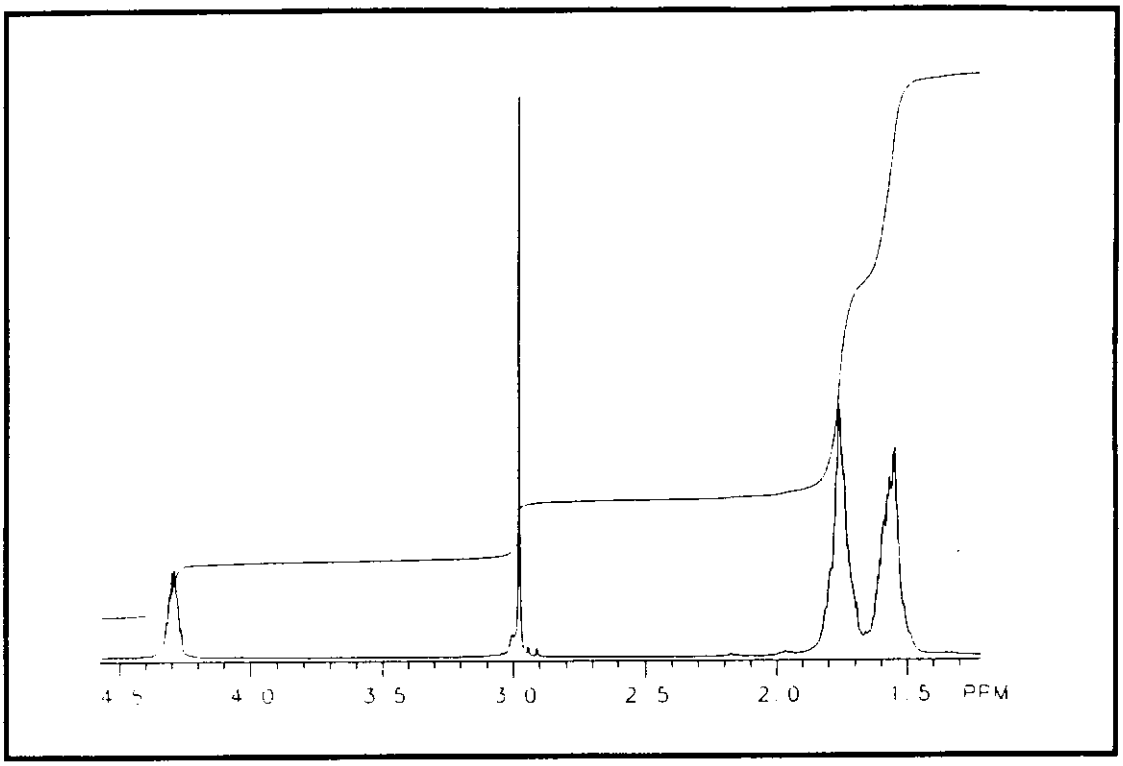

80
60
40
20
PPM

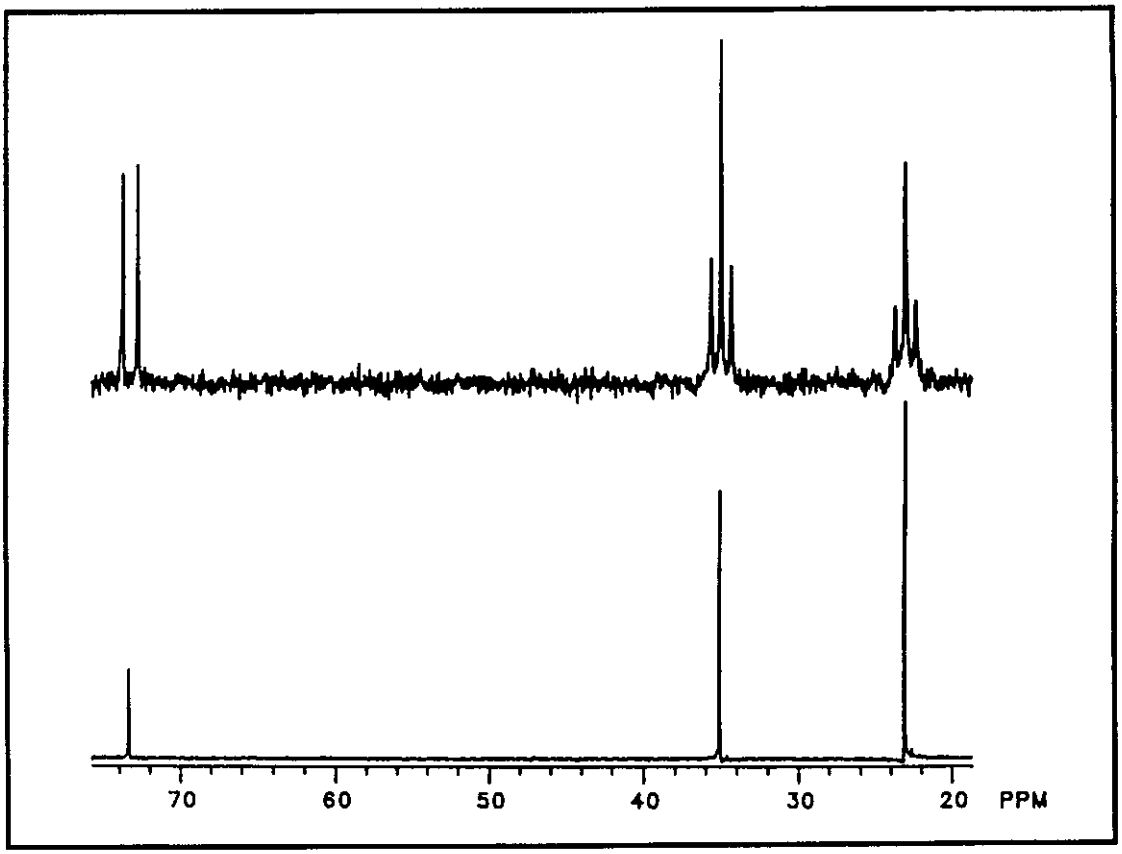
Problem 28

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





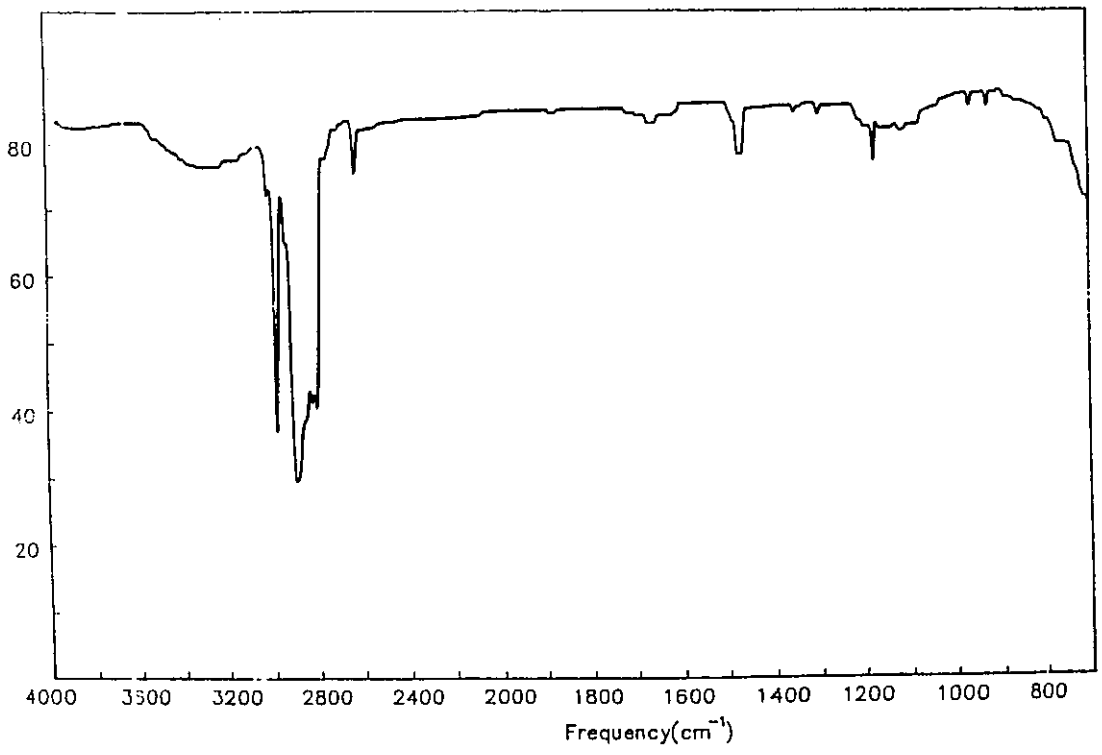

4.5
4.0
3.5
3.0
2.5
2.0
1.5
PPM

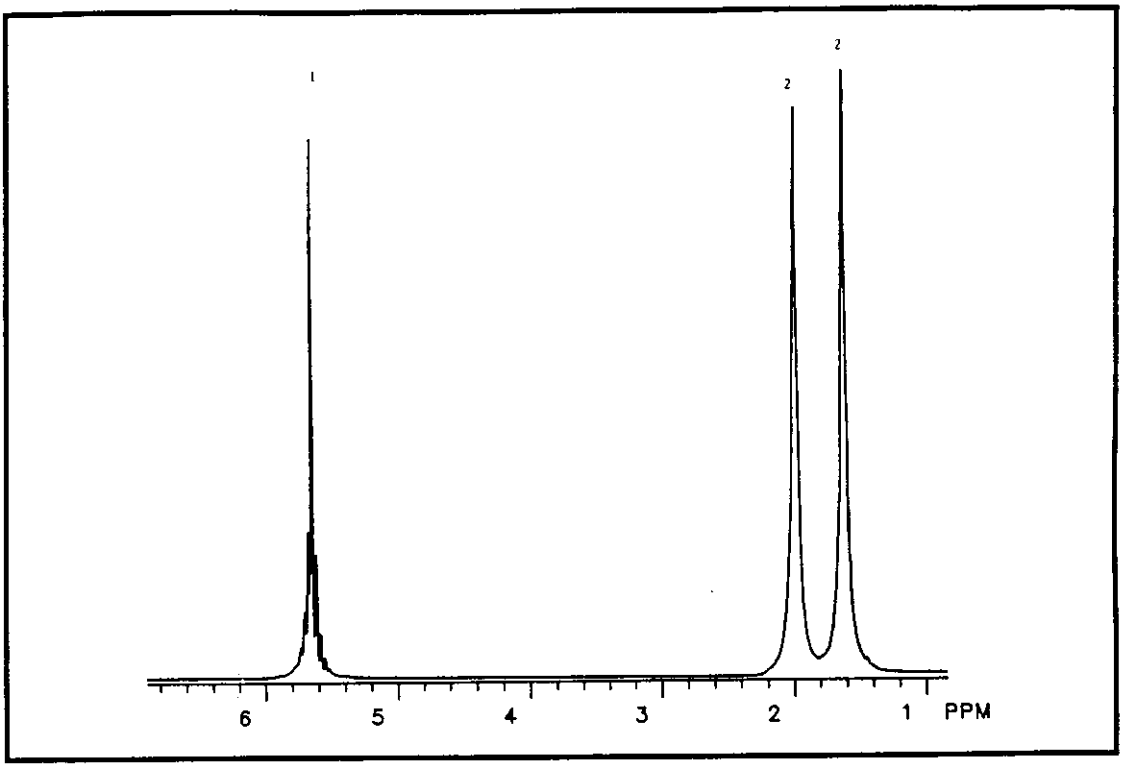

70
60
50
40
30
20
PPM

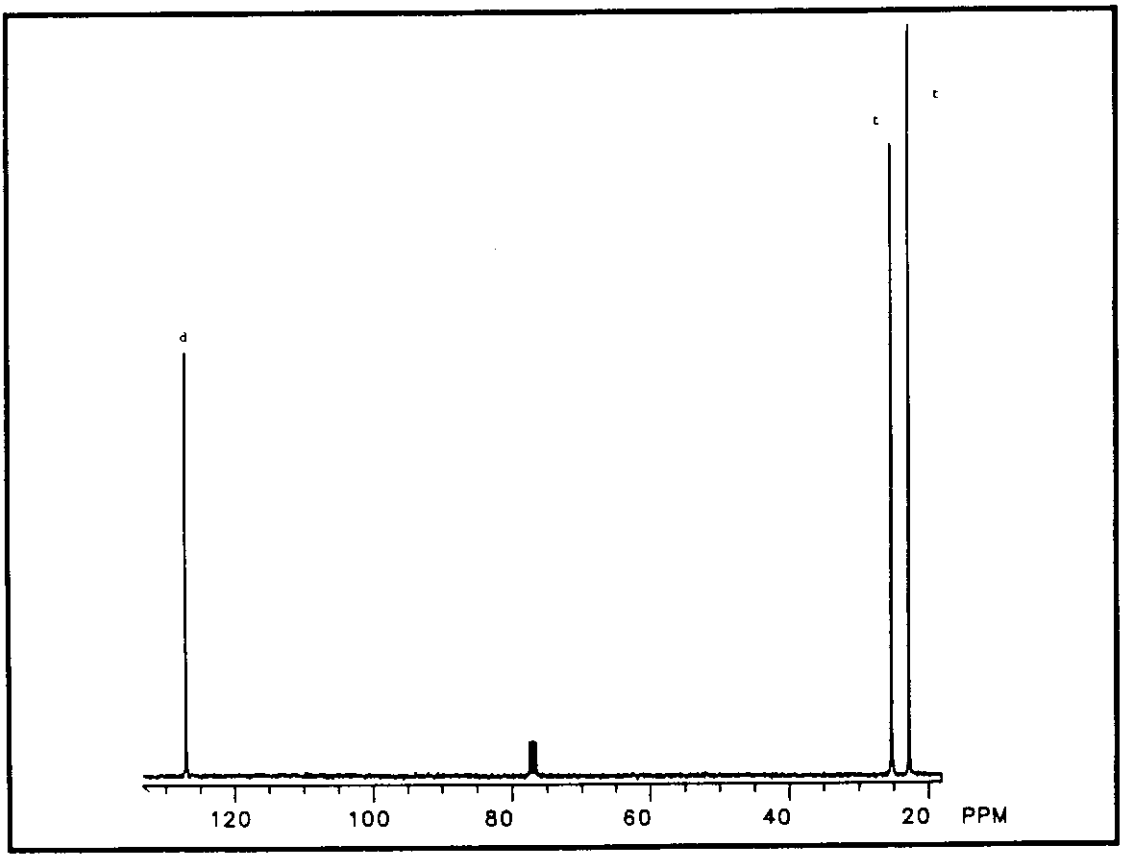
Problem 29

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
14, 0.50	37, 2.00	42, 3.00	54,80.01	66, 2.50	78, 1.40
15, 4.70	37, 0.30	43, 0.40	55, 6.30	67,100.0	79, 6.10
25, 0.30	38, 4.80	49, 1.00	56, 0.50	68, 5.40	80, 0.90
26, 5.70	39,41.30	50, 6.40	61, 0.30	73, 0.30	81,10.80
27,28.70	39, 0.50	51, 9.50	62, 0.60	74, 0.80	82,38.00
28, 8.00	40, 5.60	52, 4.80	63, 1.60	75, 0.60	83, 2.50
29, 3.30	41,40.30	53,13.20	65, 3.40	77, 5.00	

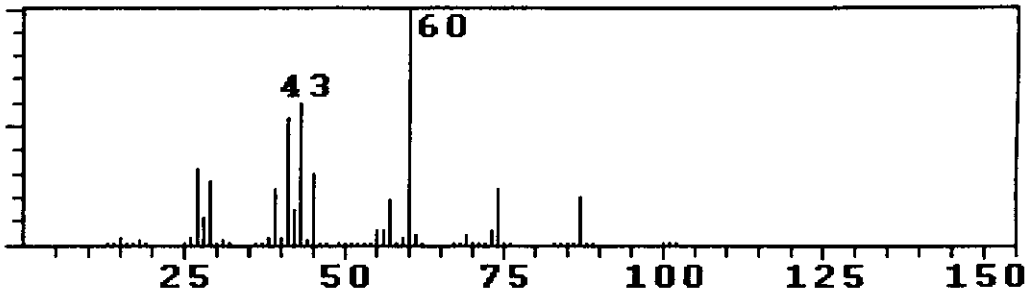


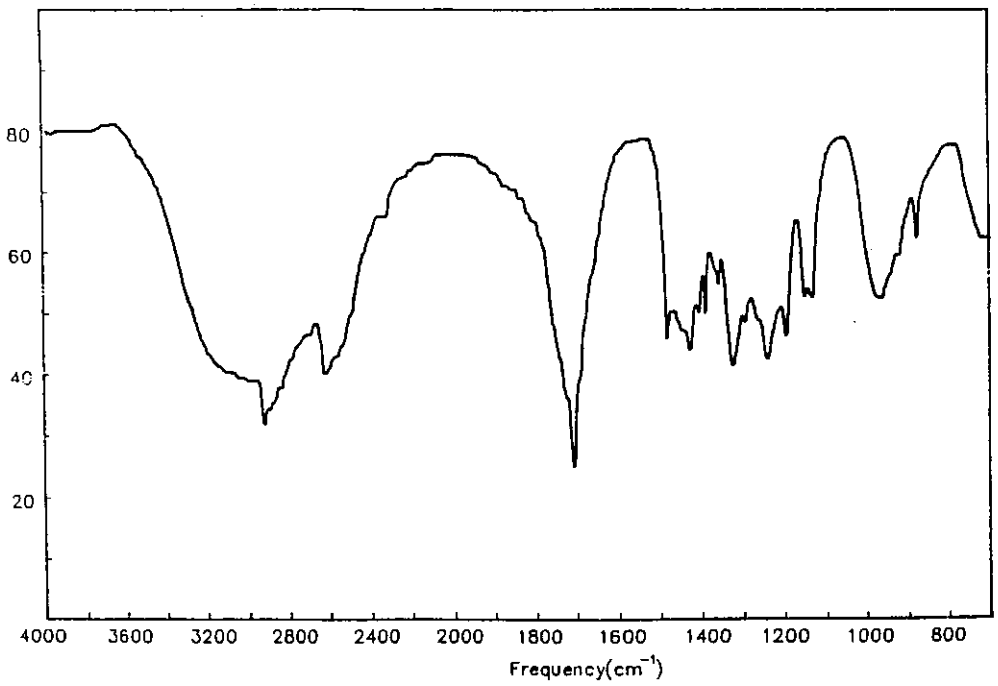

1
2
2
6
5
4
3
2
1
PPM

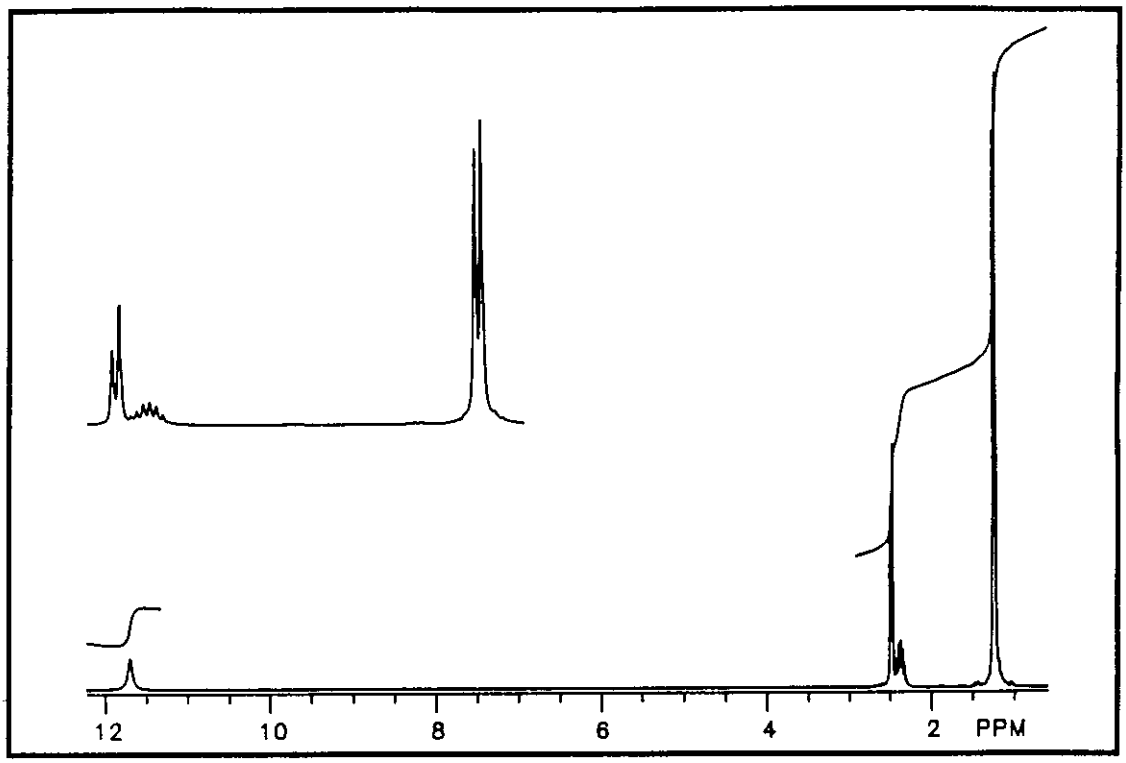

c
c
c
d
120
100
80
60
40
20
PPM

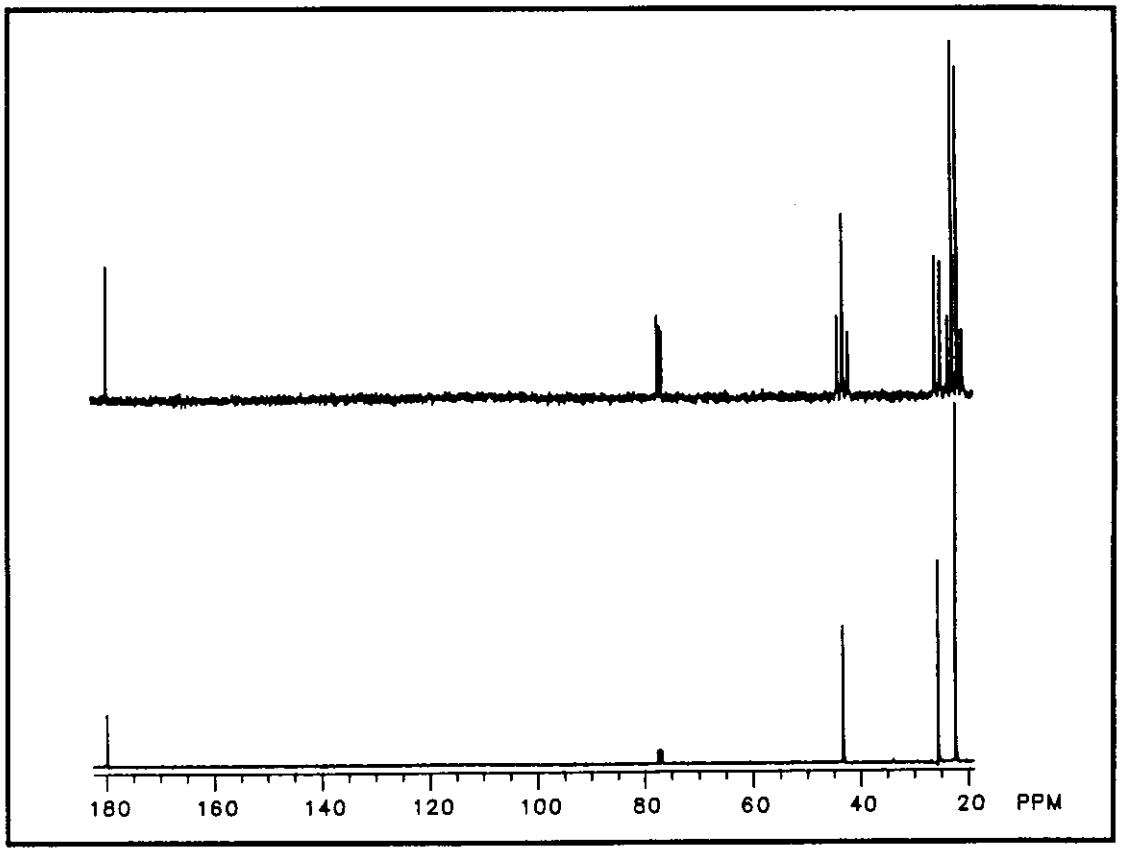
Problem 30

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





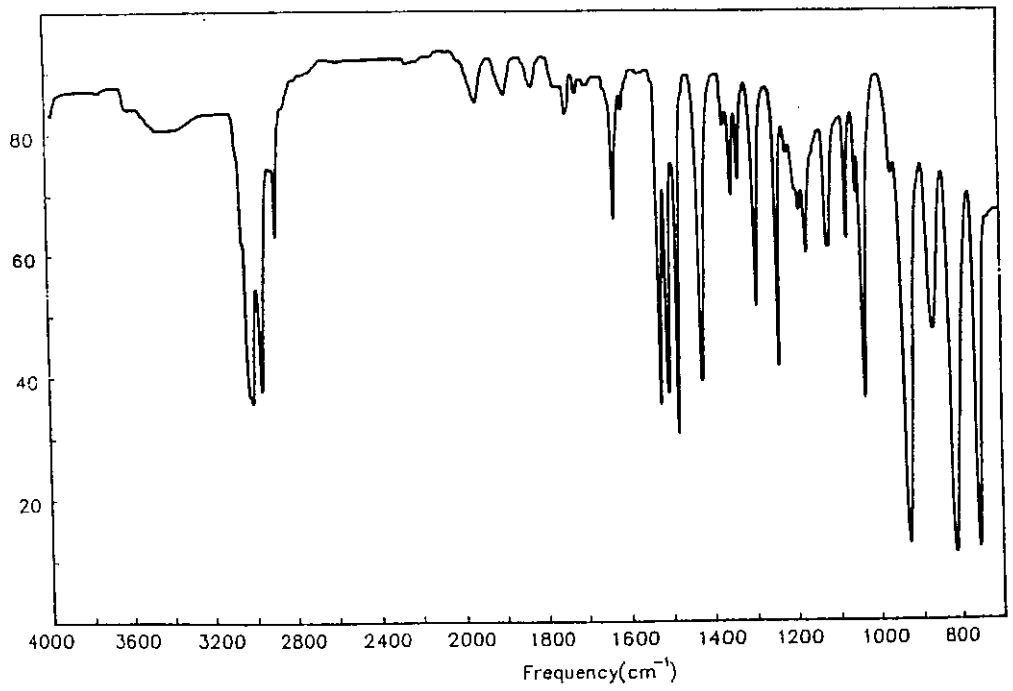

12
10
8
6
4
2
PPM

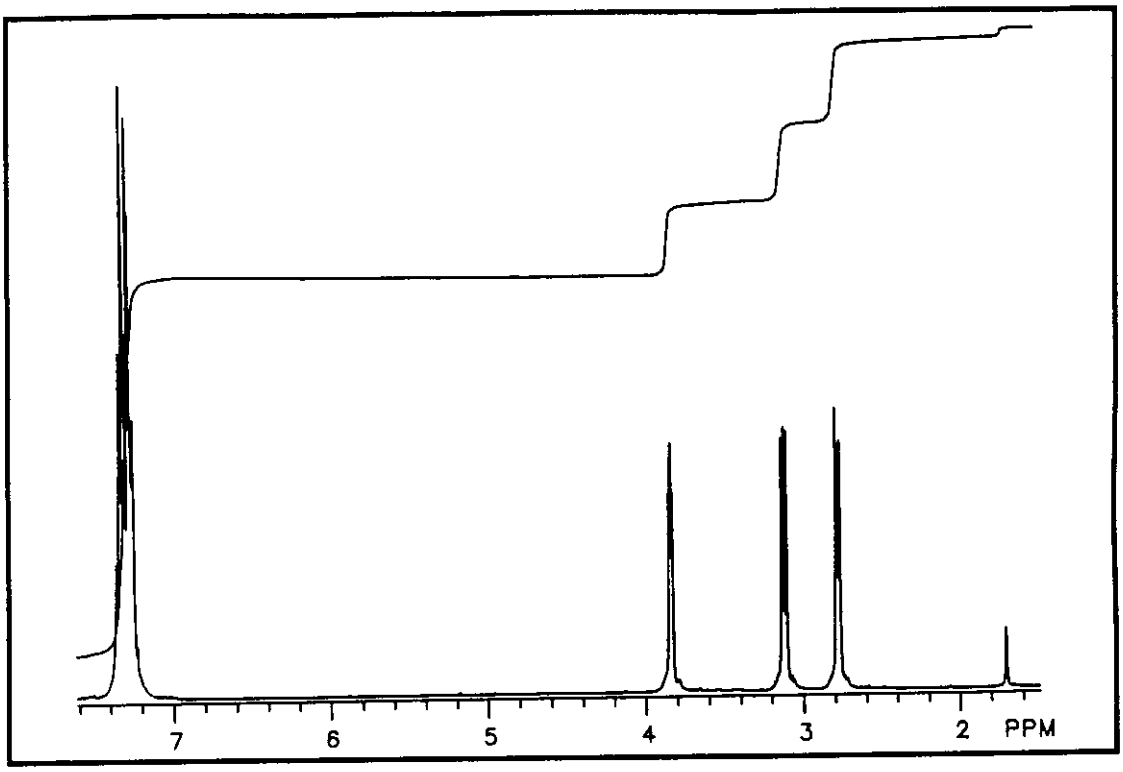

180
160
140
120
100
80
60
40
20
PPM

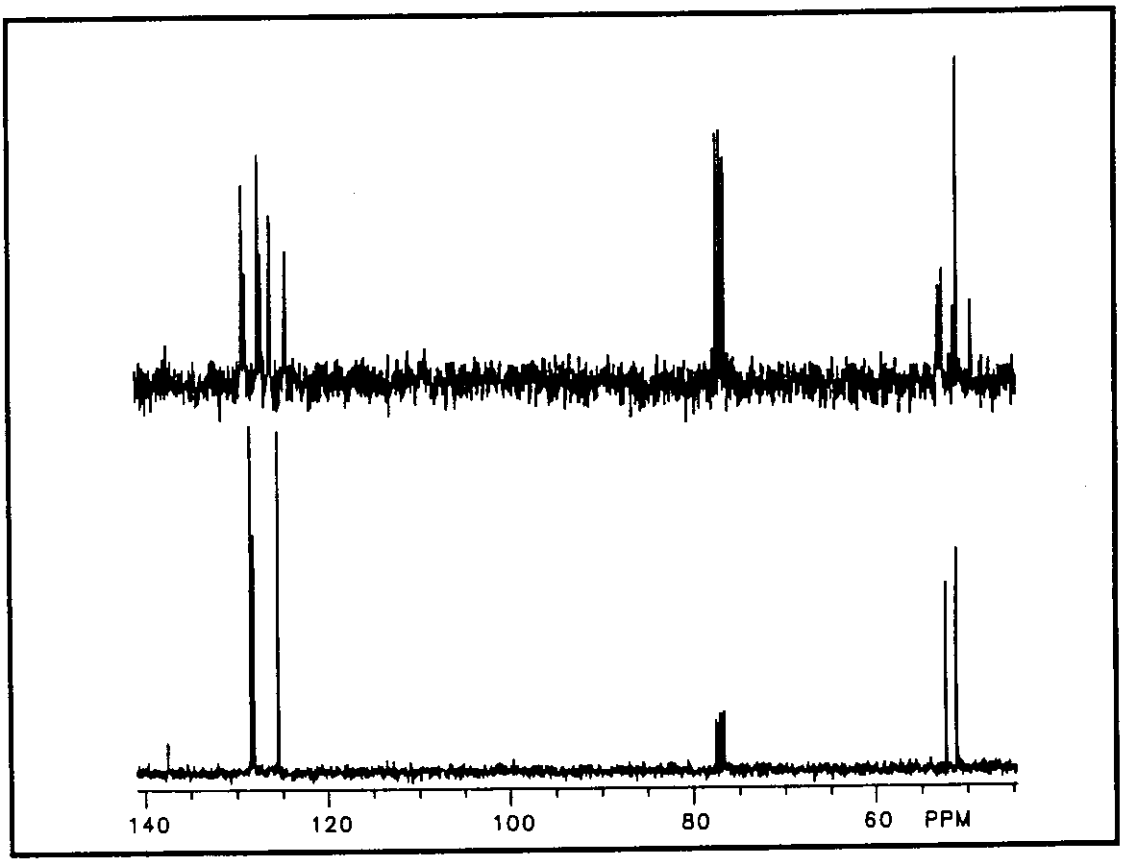
Problem 31

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
14, 0.20	38, 0.20	49, 0.10	64, 7.61	85, 0.60	104, 0.90
15, 0.30	39,14.11	50, 8.11	65,14.71	86, 1.20	105, 2.30
16, 0.10	40, 2.20	51,15.11	66, 1.10	87, 1.10	106, 0.30
17, 0.10	41, 1.60	51, 0.10	67, 0.10	88, 0.40	107, 2.60
18, 0.20	42, 0.30	52, 2.40	68, 0.10	89,73.39	108, 0.50
25, 0.10	42, 0.10	52, 0.20	72, 0.10	90,89.80	109, 0.20
26, 0.60	43, 1.10	53, 0.50	73, 0.60	91,100.0	118, 0.50
27, 2.10	43, 0.20	54, 0.10	74, 2.80	92,31.23	119,64.08
28, 0.50	44, 0.40	55, 0.20	75, 1.90	93, 2.20	120,62.58
29, 1.10	44, 0.20	56, 0.10	76, 1.20	94, 0.20	121, 5.71
30, 0.20	45, 1.10	57, 0.10	77, 8.11	95, 0.10	122, 0.40
31, 0.20	45, 0.30	59, 0.80	78, 2.00	97, 0.10	123, 0.10
32, 0.10	46, 0.50	59, 0.20	79, 0.90	98, 0.20	
36, 0.10	46, 0.10	60, 0.30	80, 0.10	99, 0.10	
37, 1.50	47, 0.10	61, 2.00	81, 0.10	101, 0.10	
37, 0.10	48, 0.10	62, 6.31	83, 0.10	102, 0.50	
38, 4.30	49, 0.90	63,18.02	84, 0.20	103, 1.10	




7
6
5
4
3
2
PPM

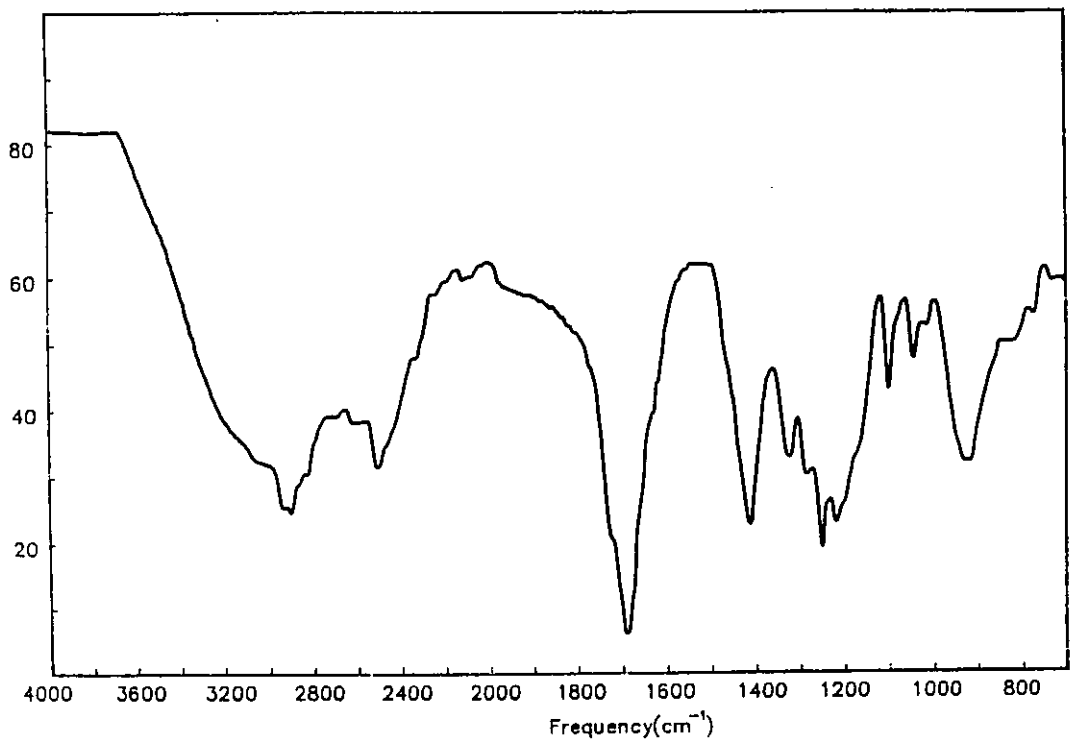

140
120
100
80
60
PPM

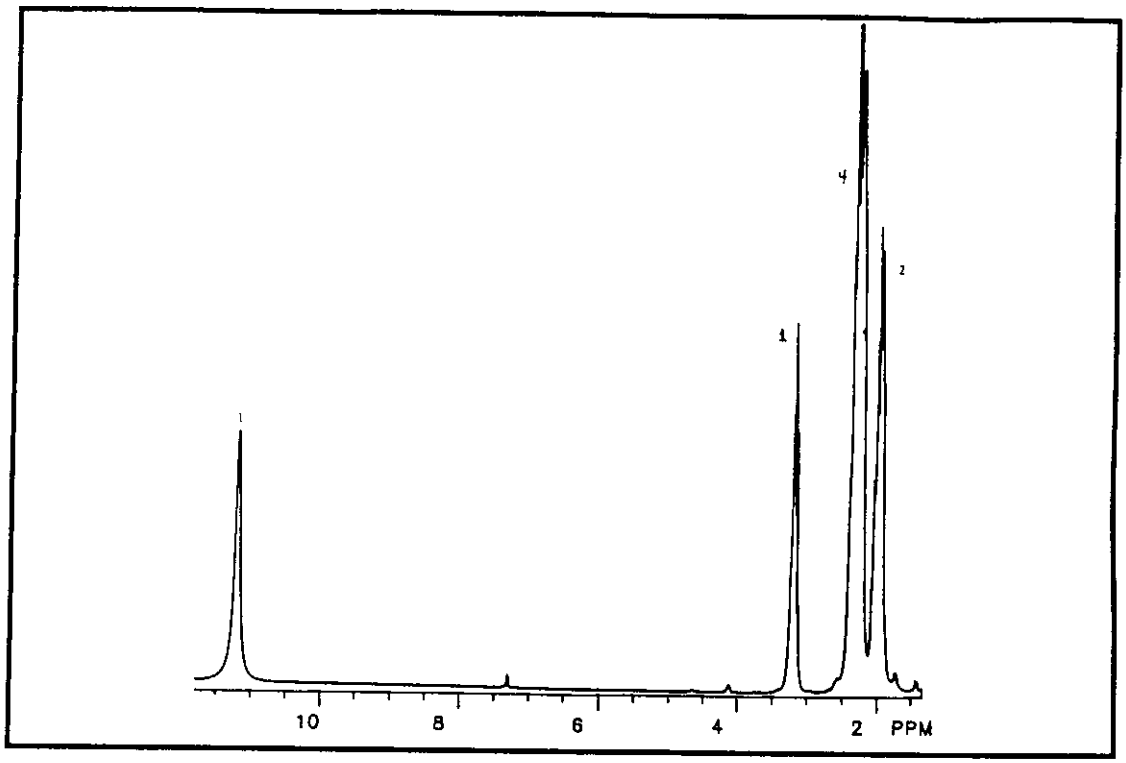
Problem 32

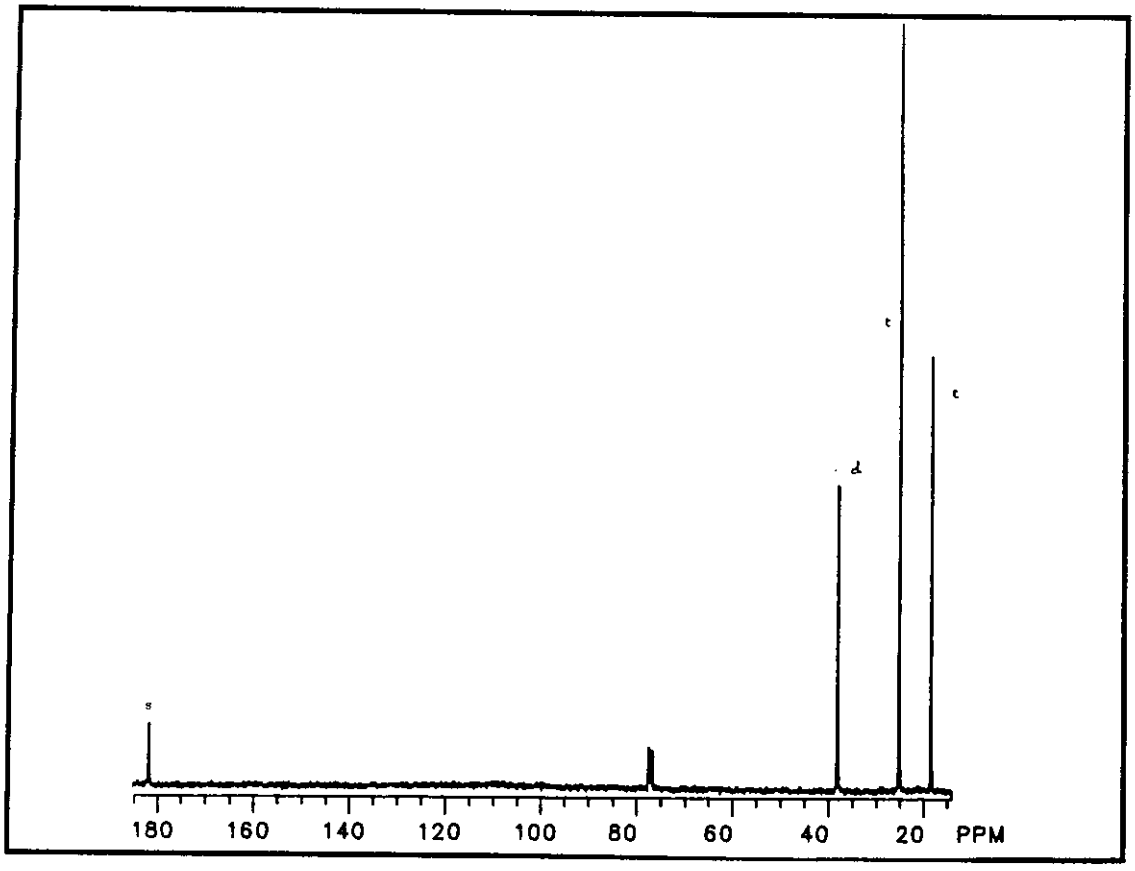
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z	
30	0.74	43	14.05	55	100.00	67	0.20	81	2.55
31	1.39	44	14.59	56	24.33	68	0.23	82	15.01
32	0.28	45	28.80	57	6.07	69	0.41	83	3.18
34	0.02	46	1.19	58	10.63	70	0.07	84	0.25
35	0.02	47	0.28	59	0.46	71	3.98	85	4.57
36	0.30	48	0.21	60	1.73	72	14.89	86	0.21
37	2.36	49	1.58	61	0.14	73	34.16	87	0.08
38	3.87	50	6.03	62	0.06	74	1.30	97	0.08
39	22.49	51	5.65	63	0.04	75	0.19	99	8.13
40	2.73	52	1.94	64	0.04	77	0.10	100	6.61
41	12.49	53	12.47	65	0.05	78	0.03	101	1.23
42	2.99	54	18.23	66	0.16	79	0.08	102	0.08

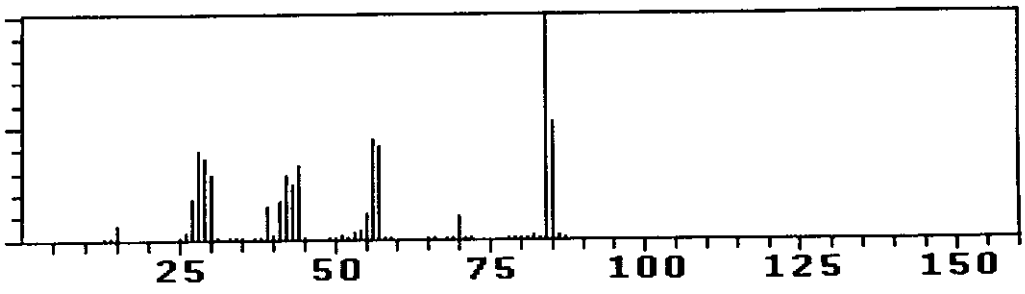


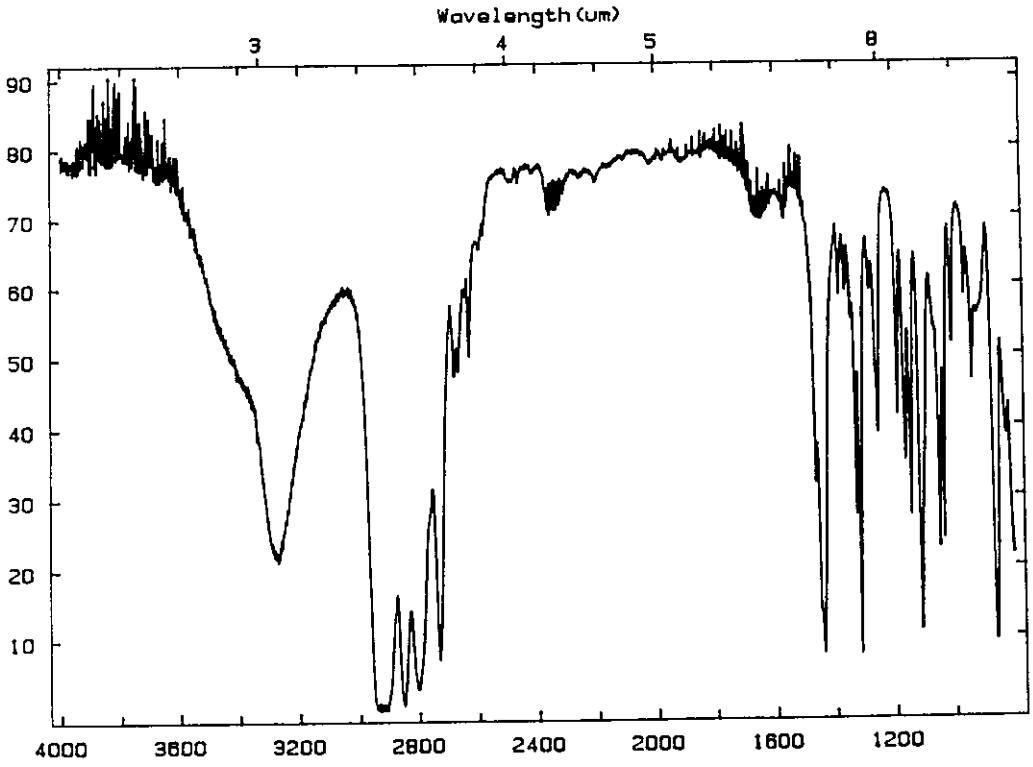

10
8
6
4
2
PPM

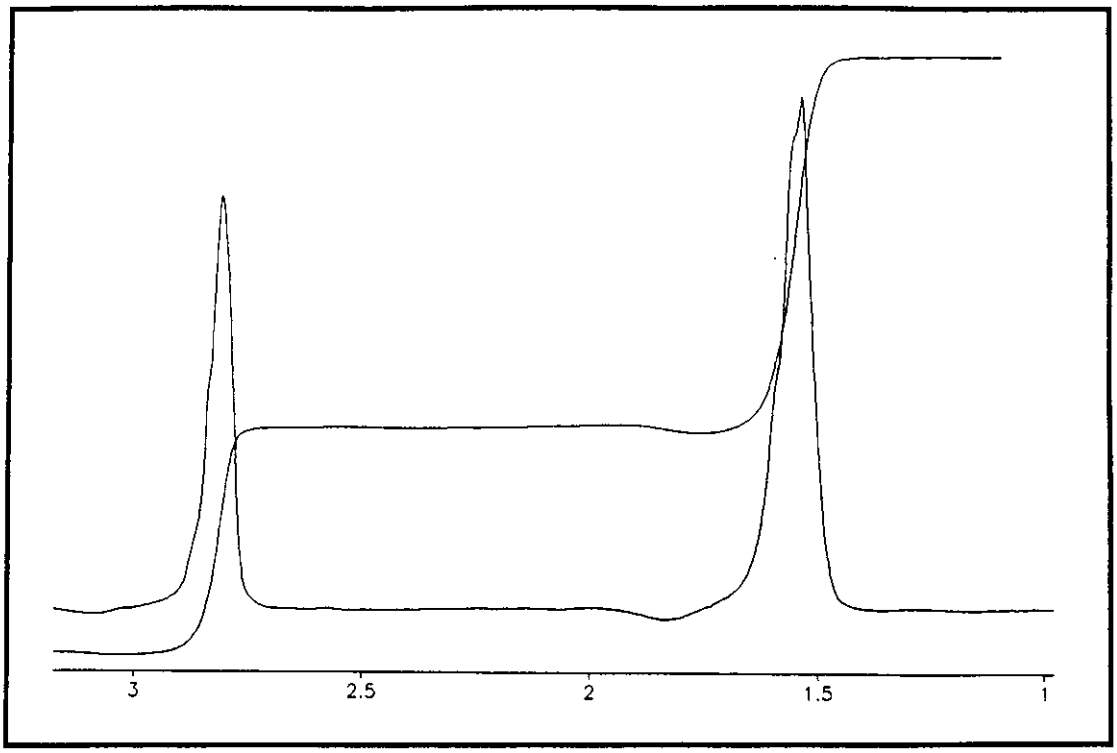

180
160
140
120
100
80
60
40
20
PPM

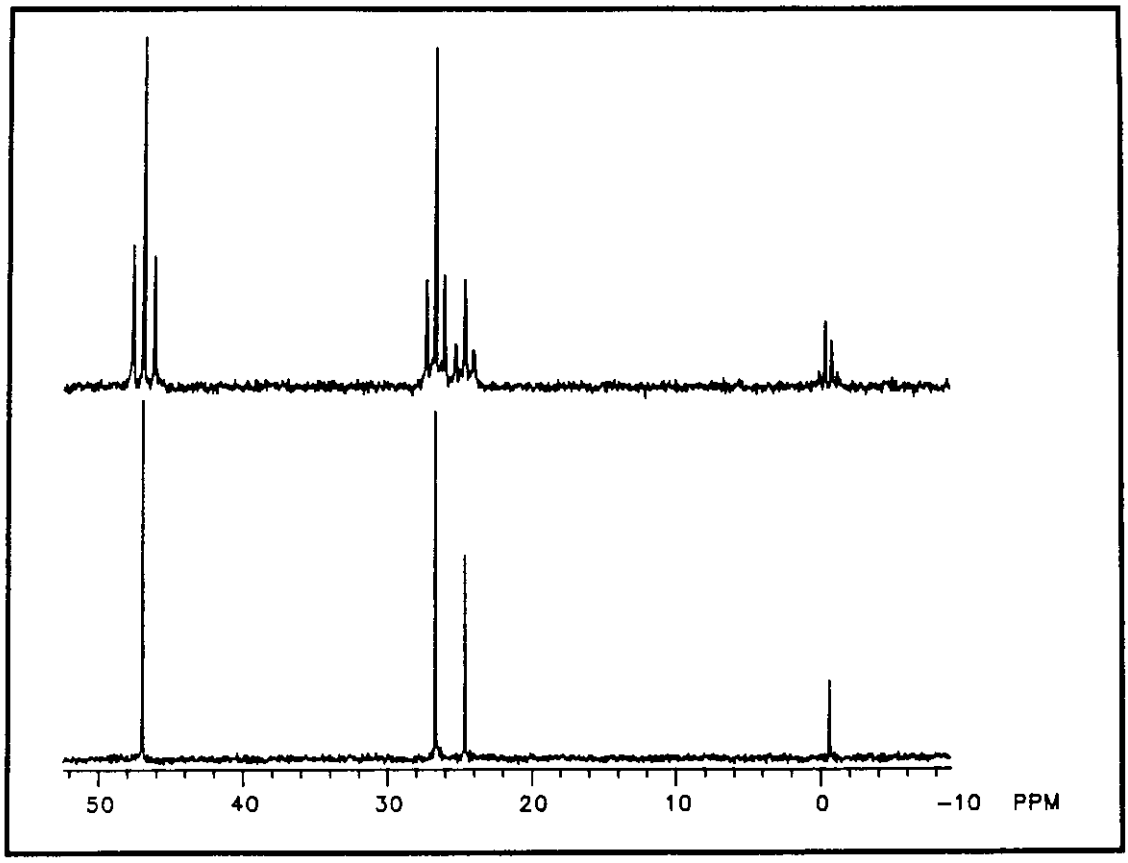
Problem 33

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





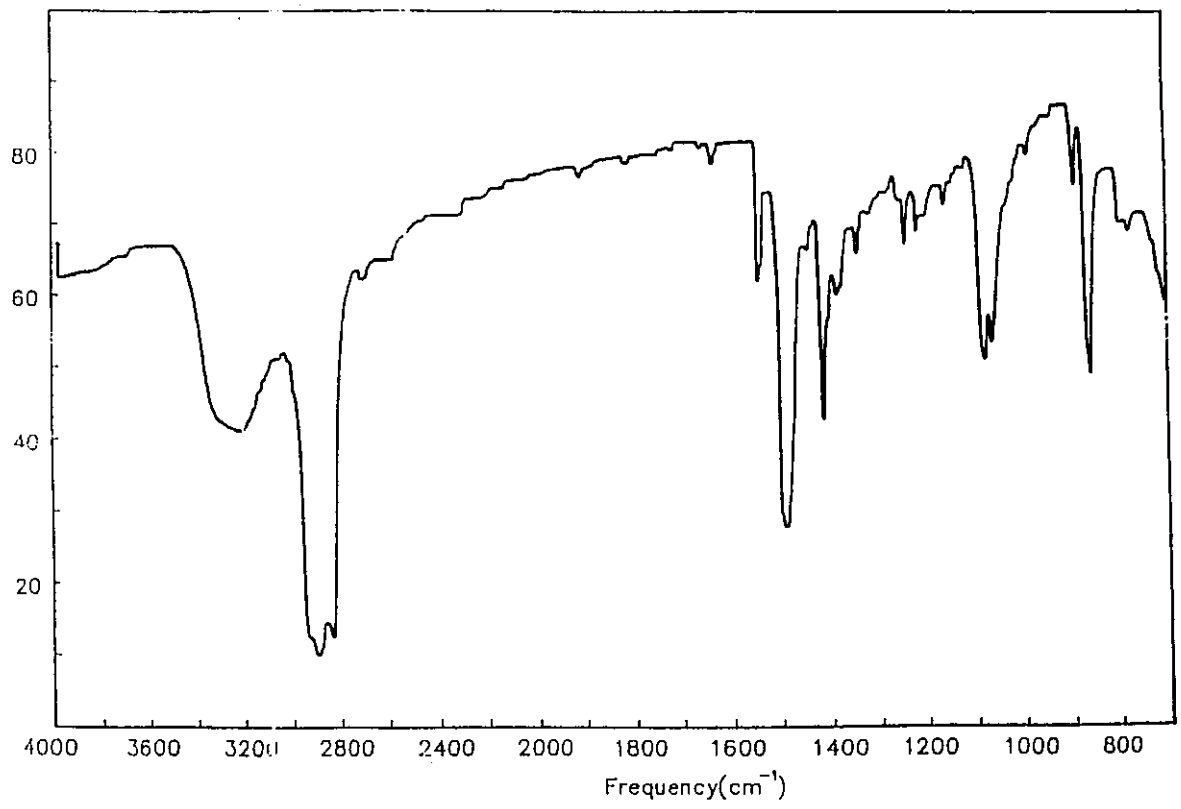

3
2.5
2
1.5
1

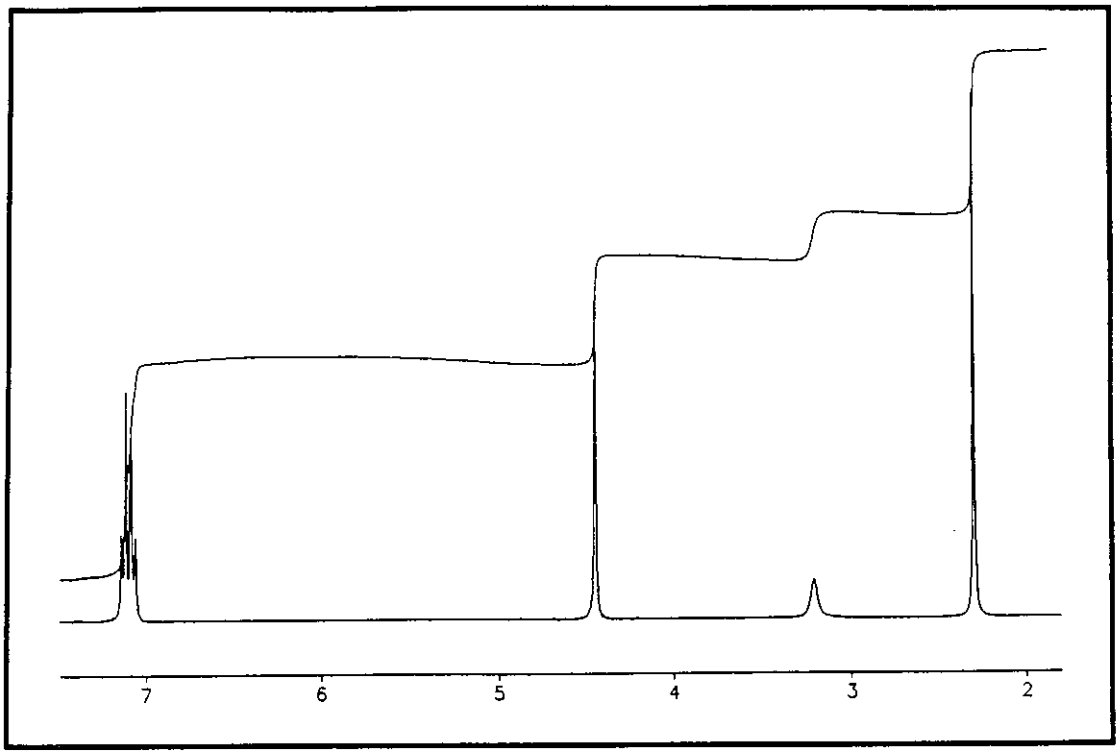

50
40
30
20
10
0
−10
PPM

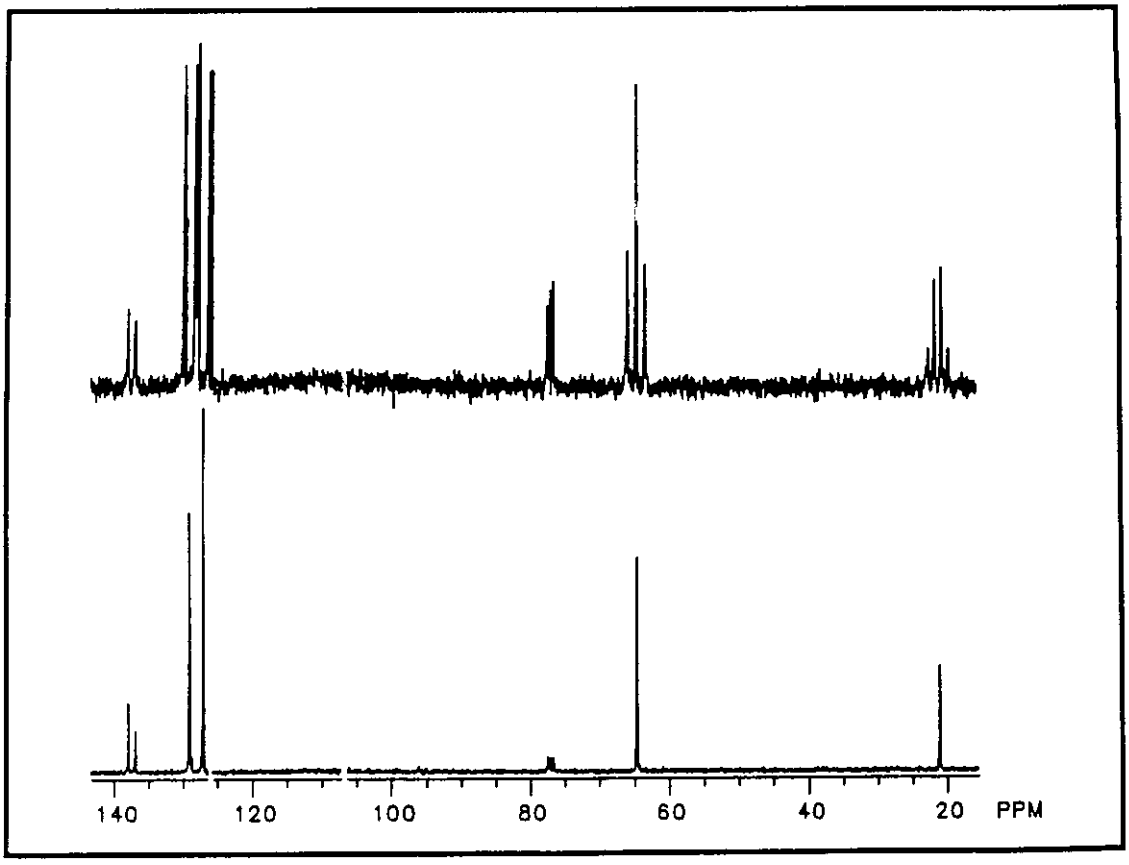
Problem 34

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
15, 4.80	40, 4.90	57, 0.70	74, 4.50	91,61.18	108, 7.81
16, 0.30	41,10.01	58, 0.20	75, 3.60	92, 6.91	109, 0.50
17, 1.90	42, 1.10	59, 1.20	76, 2.60	93,47.34	110, 0.10
18, 5.91	43, 2.60	60, 8.51	77,61.68	94, 4.40	112, 0.10
19, 0.50	44, 0.80	61, 4.50	78,14.61	95, 0.40	115, 0.10
20, 0.10	45, 1.20	62,10.01	79,65.58	96, 0.10	117, 0.10
24, 0.10	46, 0.40	63,21.82	80, 4.40	97, 0.10	118, 0.20
25, 0.20	47, 0.40	64, 5.30	81, 0.60	98, 0.40	119, 7.11
26, 2.70	48, 0.30	65,27.83	82, 0.10	99, 0.10	120, 3.60
27,12.81	49, 2.60	66, 3.70	83, 0.10	100, 0.10	121,19.62
29, 7.91	50,18.82	67, 1.10	84, 0.30	101, 0.30	122,81.49
30, 1.00	51,30.13	68, 0.40	85, 1.10	102, 1.70	123, 7.21
31, 4.80	52, 8.31	69, 0.20	86, 1.90	103, 7.41	124, 0.50
36, 0.10	53, 9.11	70, 0.20	87, 1.60	104,12.71	125, 0.10
37, 2.30	54, 0.70	71, 0.20	88, 0.50	105,21.42	
38, 5.71	55, 2.10	72, 0.30	89, 8.41	106, 3.50	
39,28.73	56, 0.30	73, 1.00	90, 3.90	107,100.0	



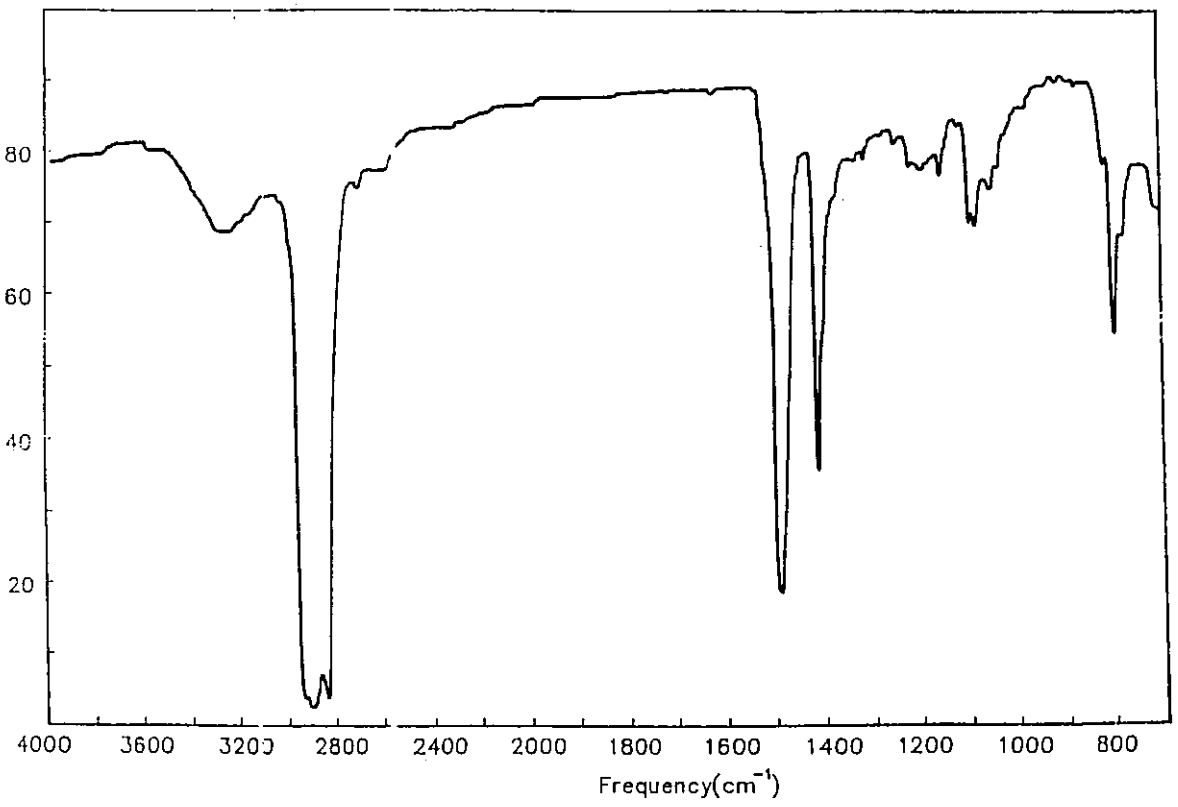

7
6
5
4
3
2

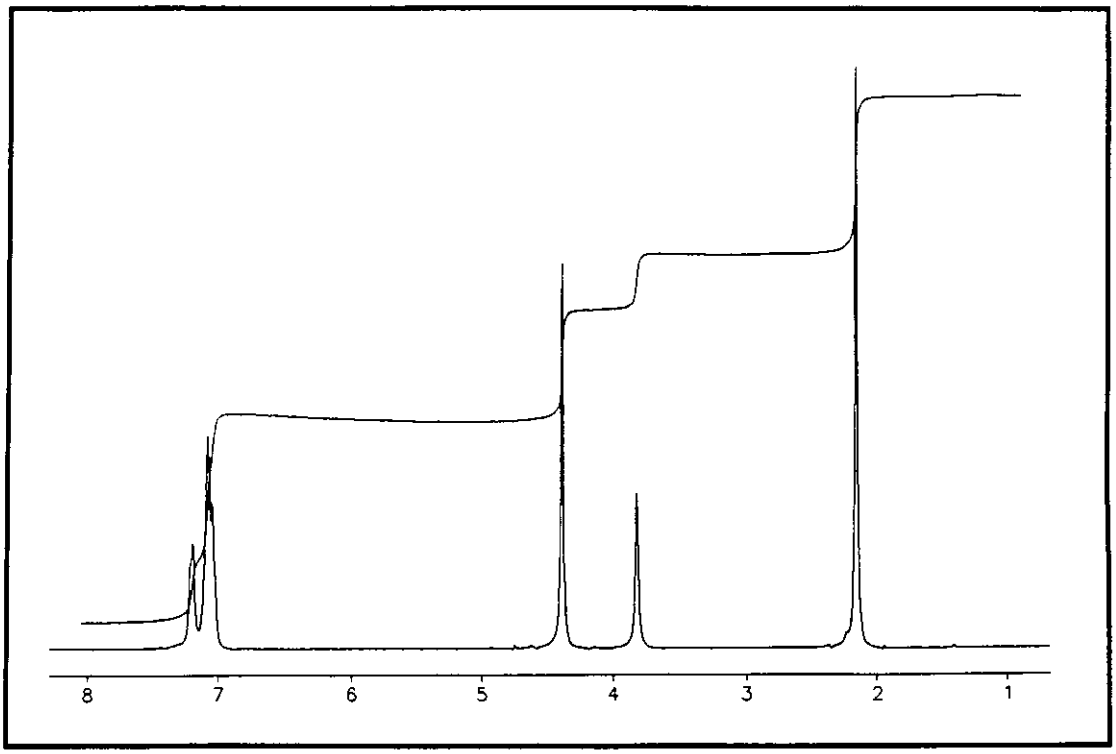

140
120
100
80
60
40
20
PPM

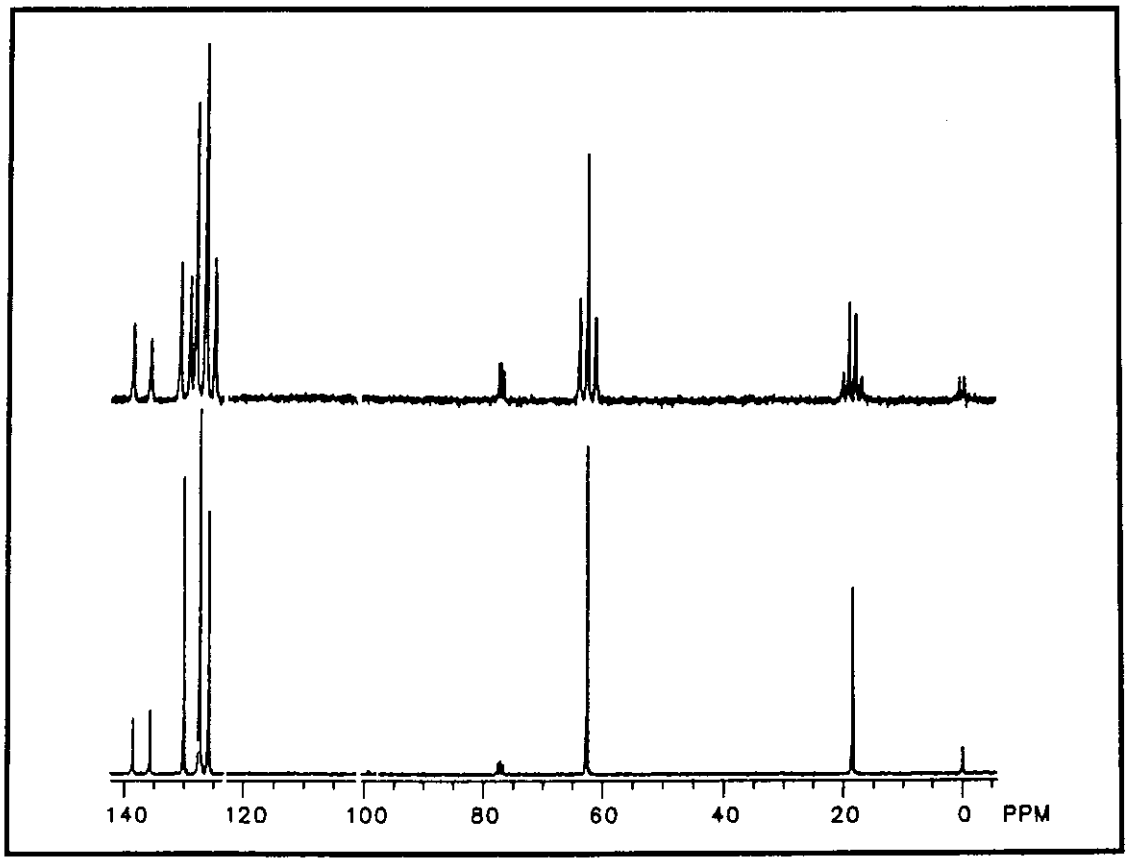
Problem 35

Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
15, 0.20	42, 0.30	52, 0.20	66, 1.60	86, 0.70	104,100.0
18, 0.20	43, 1.50	53, 3.20	67, 0.40	87, 0.60	105,16.92
26, 0.50	44, 0.30	53, 0.30	69, 0.20	88, 0.20	106, 1.00
27, 4.00	44, 0.10	54, 0.30	73, 0.30	89, 4.00	107,33.33
28, 2.70	45, 1.00	55, 0.70	74, 1.60	90, 1.30	108, 2.60
29, 1.90	45, 0.50	59, 0.80	75, 1.30	91,36.43	109, 0.20
31, 1.60	46, 0.50	60, 5.61	76, 1.10	92, 3.70	119, 3.60
32, 0.60	47, 0.20	60, 1.20	77,37.13	93,20.22	120, 1.00
37, 0.80	49, 0.50	61, 1.20	78,16.72	94, 1.70	121, 5.61
38, 2.20	50, 5.00	62, 3.10	79,38.63	95, 0.20	122,29.53
39,13.21	51,14.71	63, 8.11	80, 2.60	98, 0.20	123, 2.60
40, 1.40	51, 0.50	64, 1.80	81, 0.30	101, 0.20	124, 0.20
41, 3.30	52, 4.40	65,15.21	85, 0.40	103,14.21	

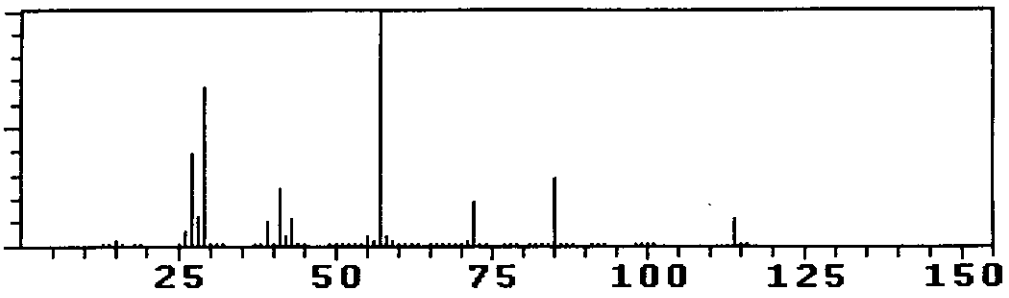


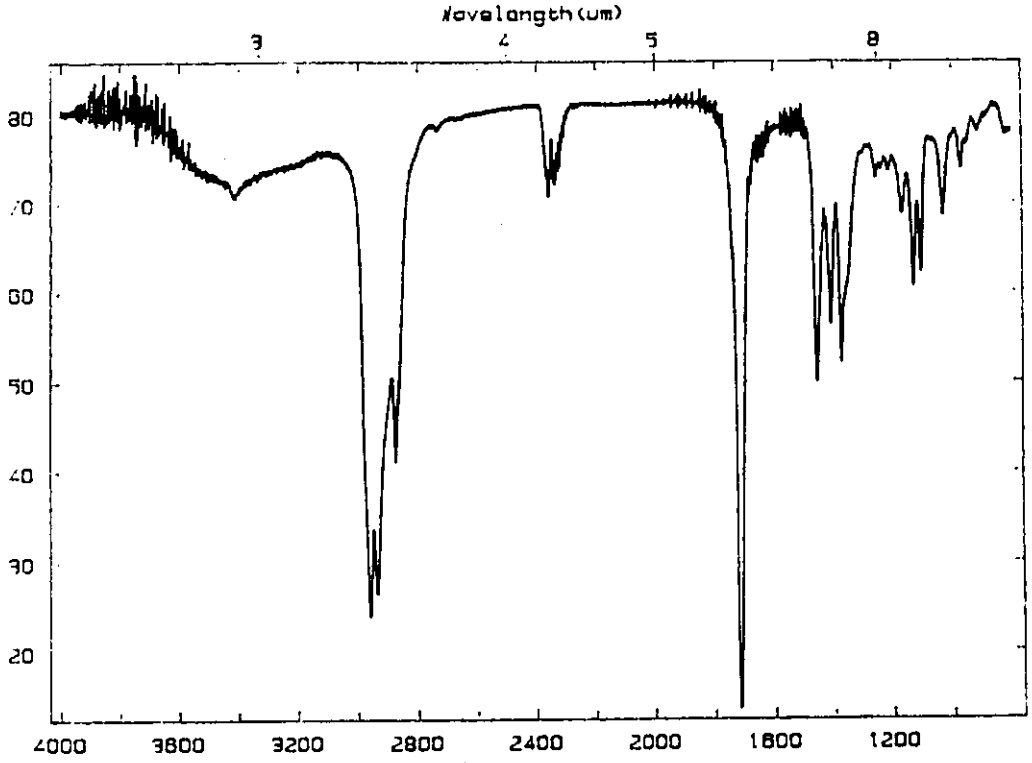

8
7
6
5
4
3
2
1

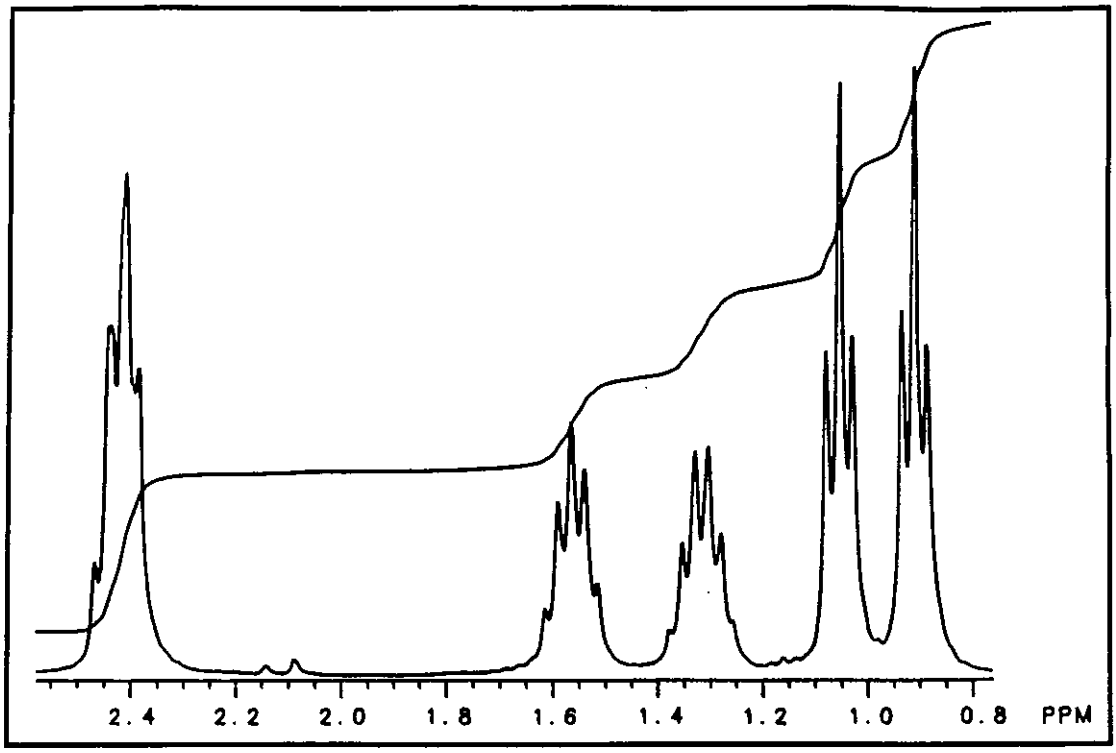

140
120
100
80
60
40
20
0
PPM

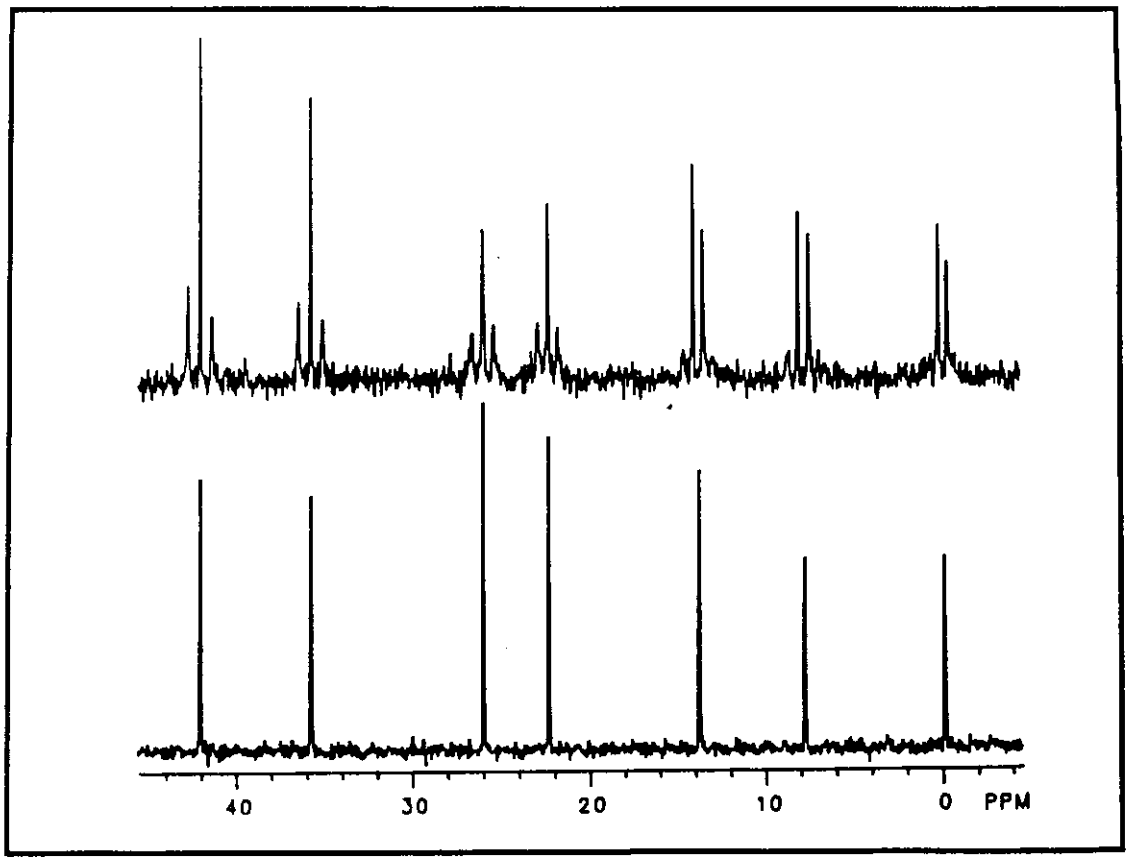
Problem 36

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na





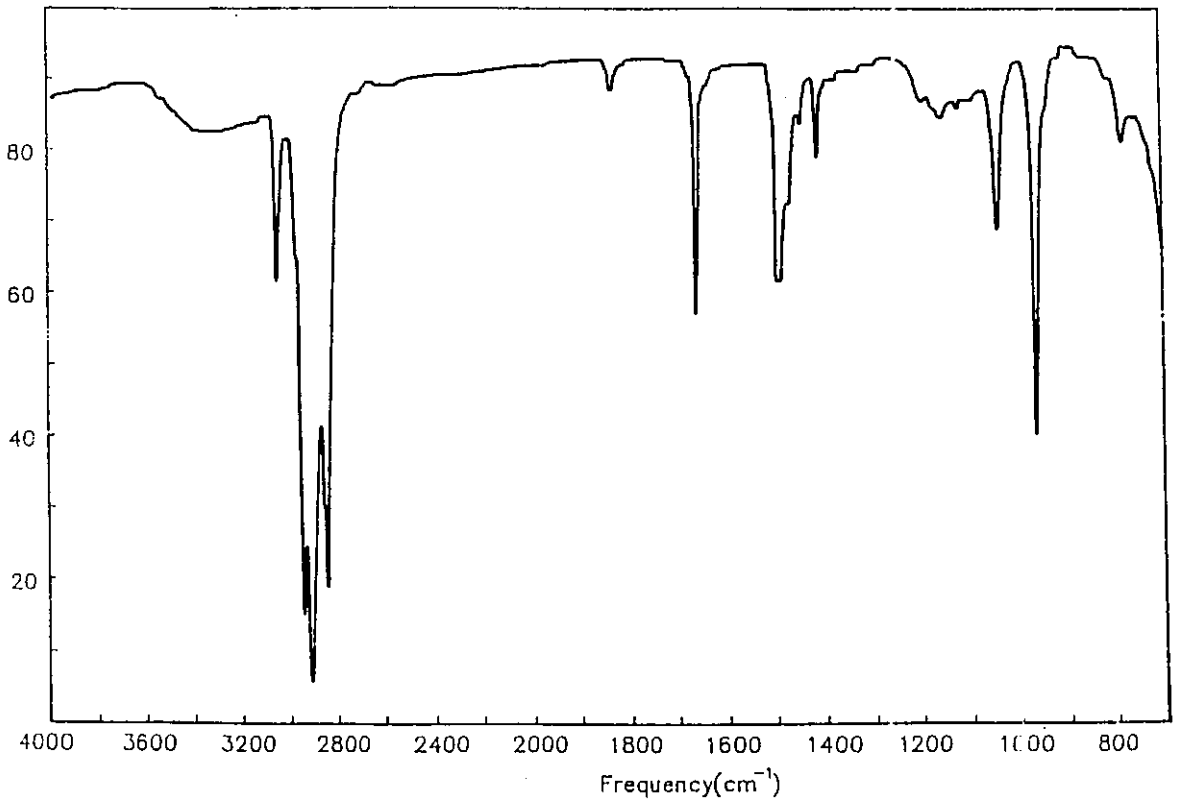

2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
PPM

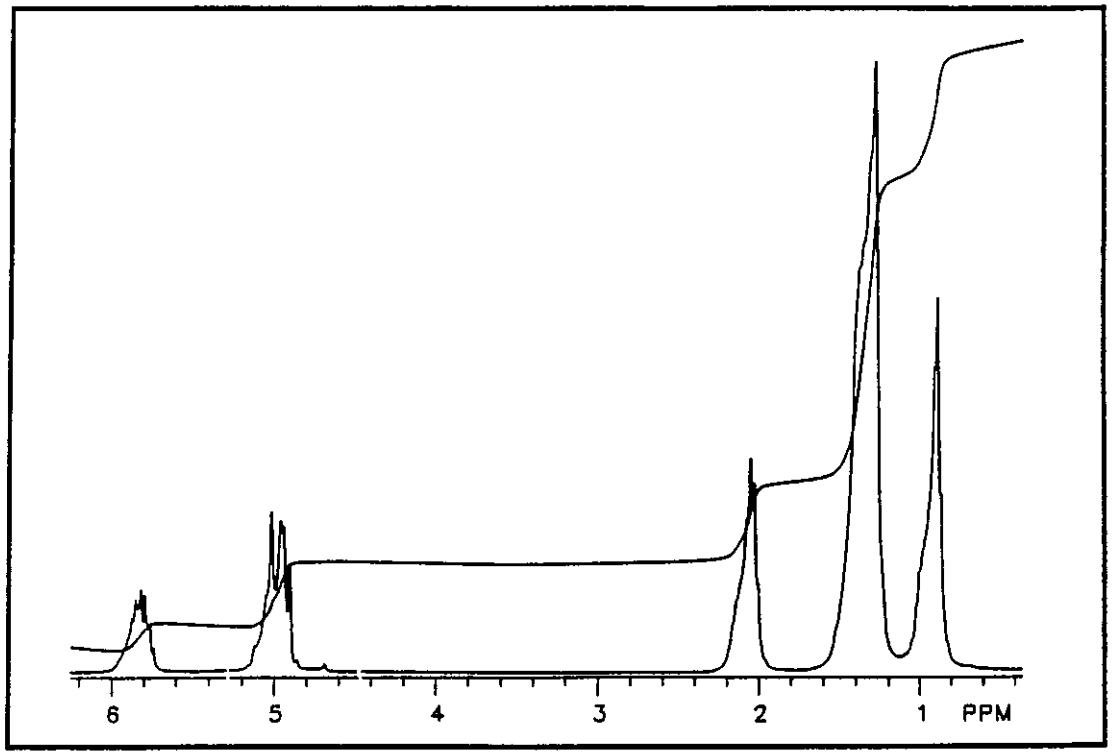

40
30
20
10
0
PPM

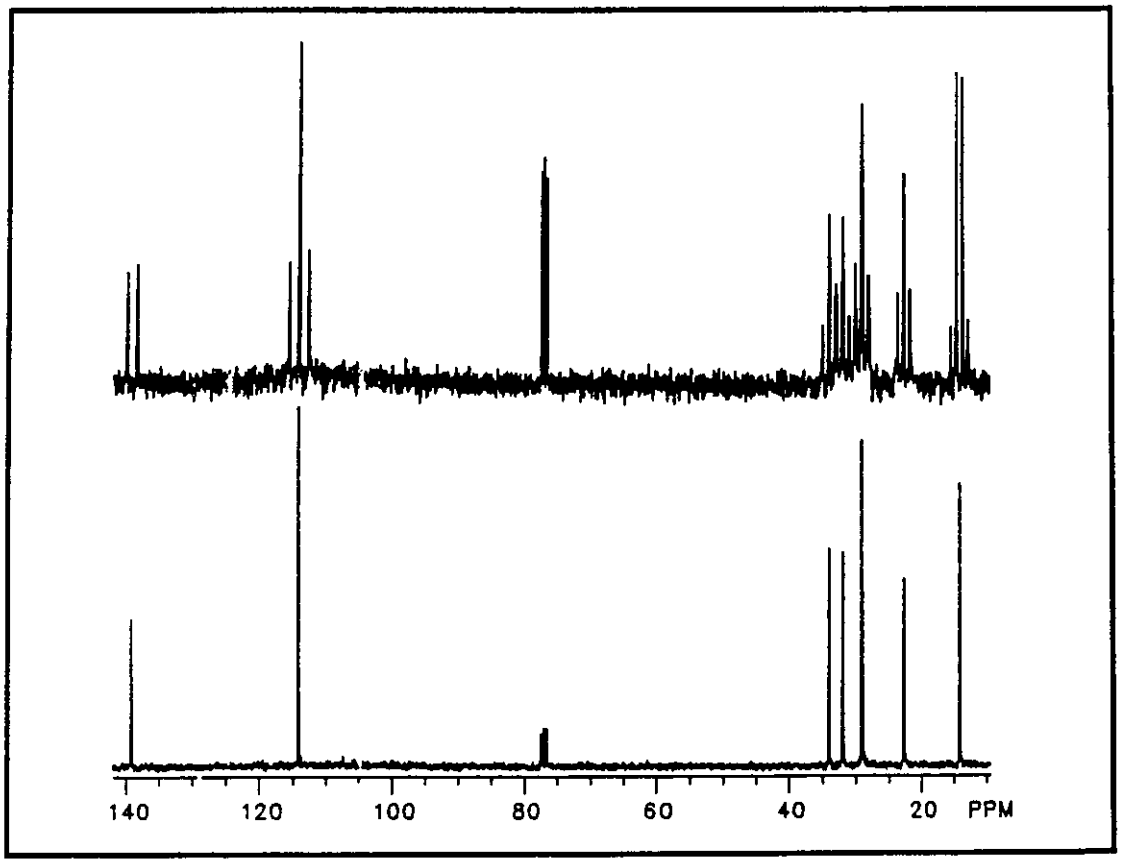
Problem 37

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
21, 0.03	36, 0.03	49, 0.21	61, 0.16	72, 0.31	84,13.38
24, 0.04	37, 0.70	50, 1.32	62, 0.30	73, 0.11	85, 0.87
25, 0.12	38, 2.05	51, 2.64	63, 0.53	74, 0.12	91, 0.11
26, 2.72	39,38.78	52, 1.07	64, 0.07	75, 0.07	95, 0.04
27,36.06	40, 5.55	53, 8.03	65, 1.25	77, 0.65	96, 0.02
28, 0.56	41,95.06	54, 7.15	66, 0.46	78, 0.14	97, 2.13
29,43.64	42,61.82	55,94.33	67, 4.95	79, 0.53	98, 0.13
30, 0.93	43,100.0	56,69.81	68, 4.63	80, 0.06	110, 0.02
31, 0.86	44, 2.83	57,11.25	69,31.95	81, 0.35	112, 2.59
33, 0.02	45, 0.09	58, 0.44	70,55.80	82, 3.88	113, 0.25
35, 0.03	47, 0.11	60, 0.08	71, 7.90	83,20.37	




6
5
4
3
2
1
PPM

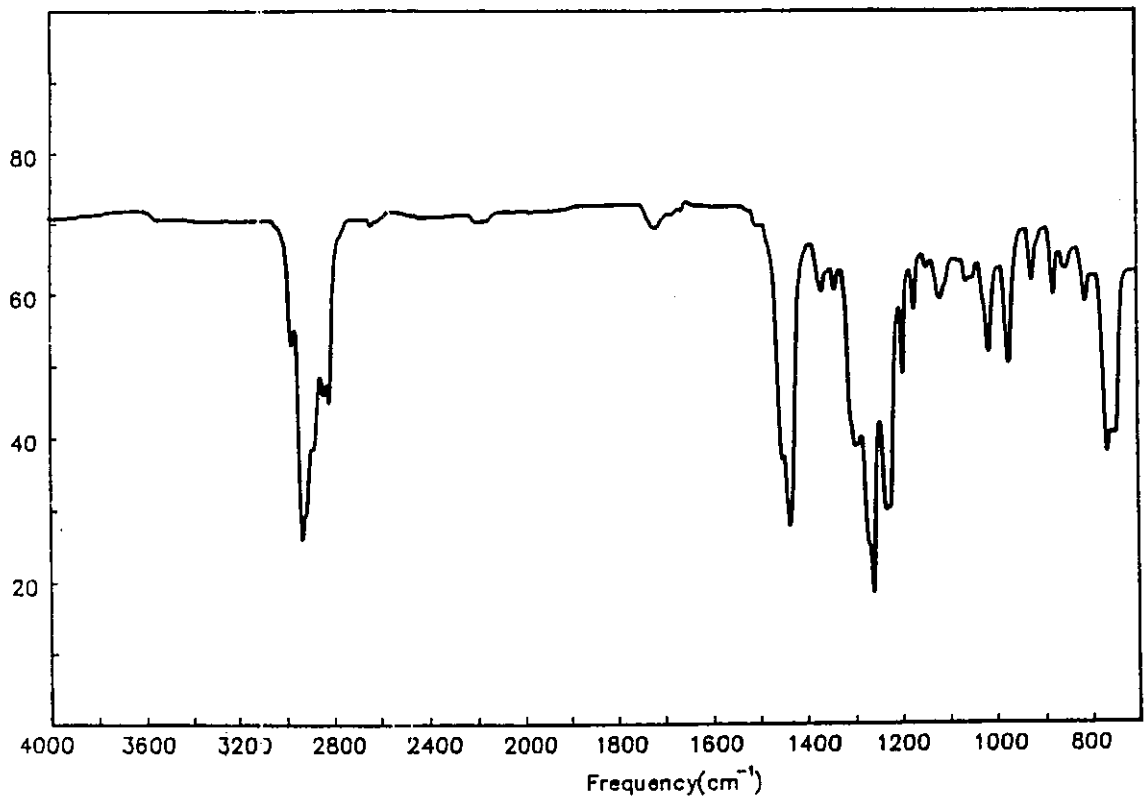

140
120
100
80
60
40
20
PPM

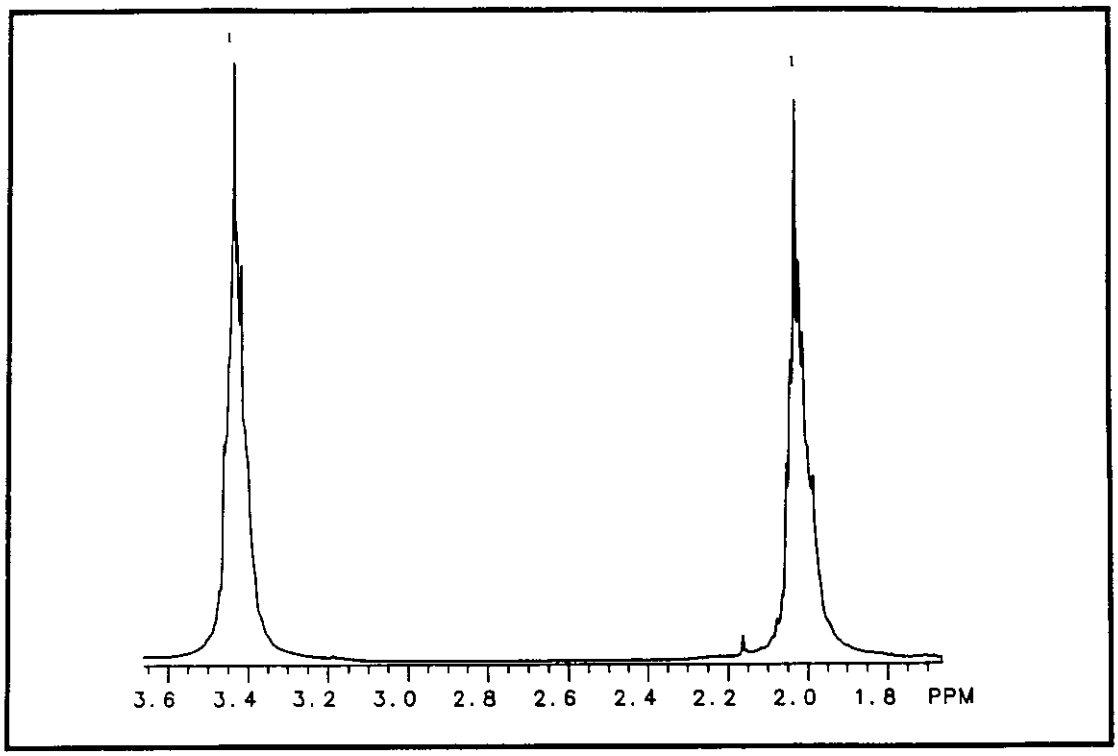
Problem 38

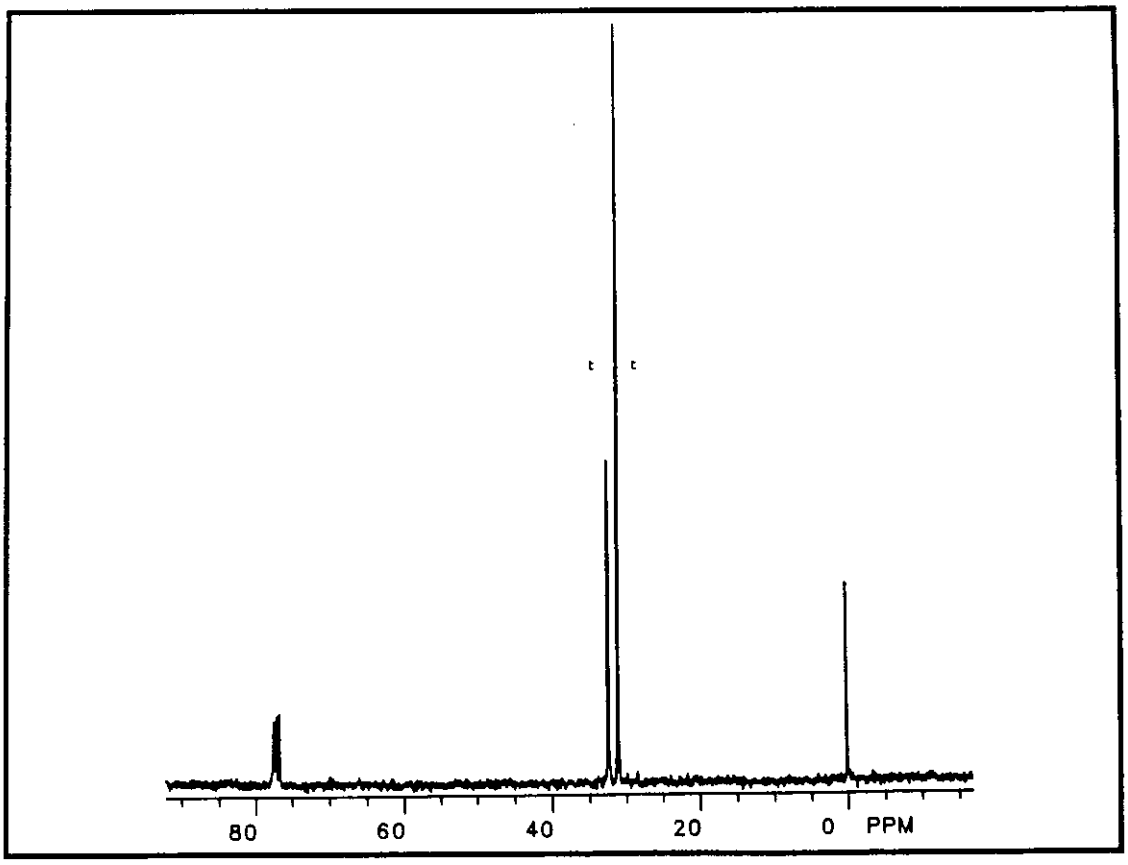
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/e		m/e		m/e		m/e		m/e	
37	1.90	50	4.50	79	6.54	106	5.18	137	71.28
38	3.67	51	4.51	80	4.00	107	12.30	138	3.12
39	27.90	52	1.51	81	6.97	108	5.00	214	0.48
40	2.55	53	10.60	82	3.95	109	10.81	215	0.03
41	17.39	54	4.76	93	8.08	134	6.13	216	0.91
42	1.52	55	100.00	95	7.39	135	72.40	217	0.03
49	1.15	56	4.70	105	1.25	136	9.20	218	0.46



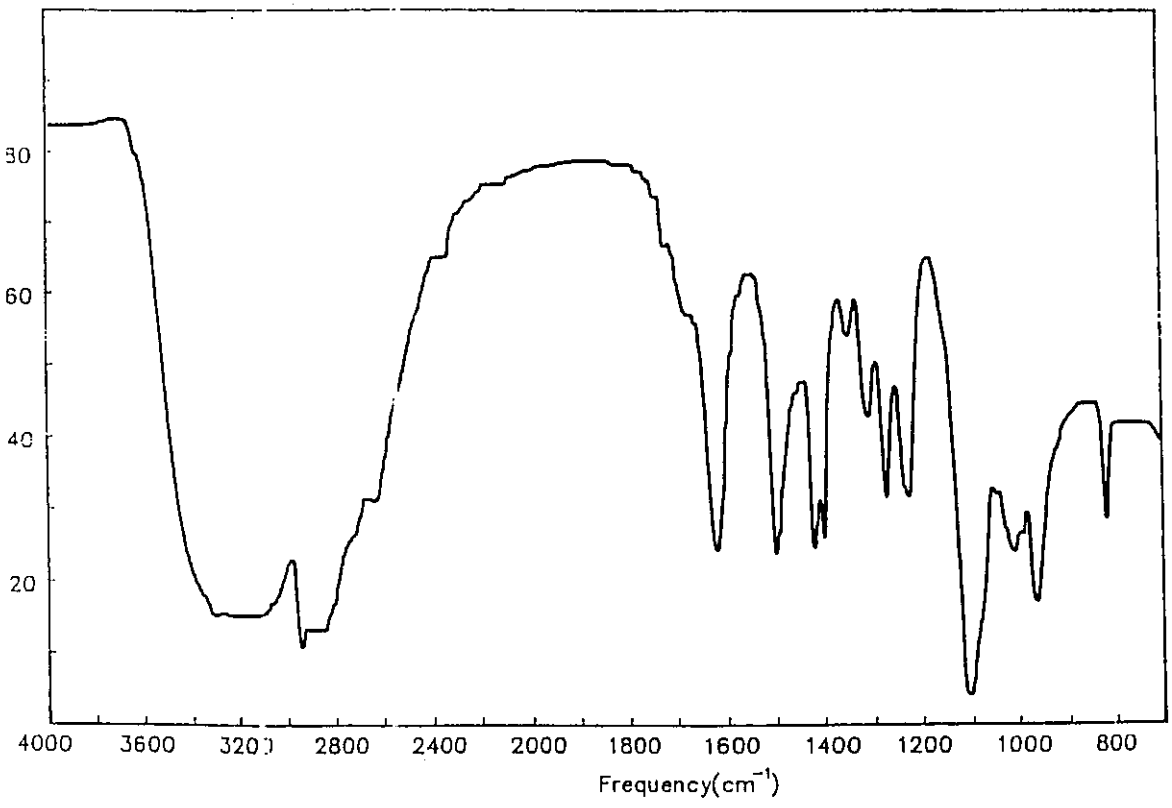

1
1
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
PPM

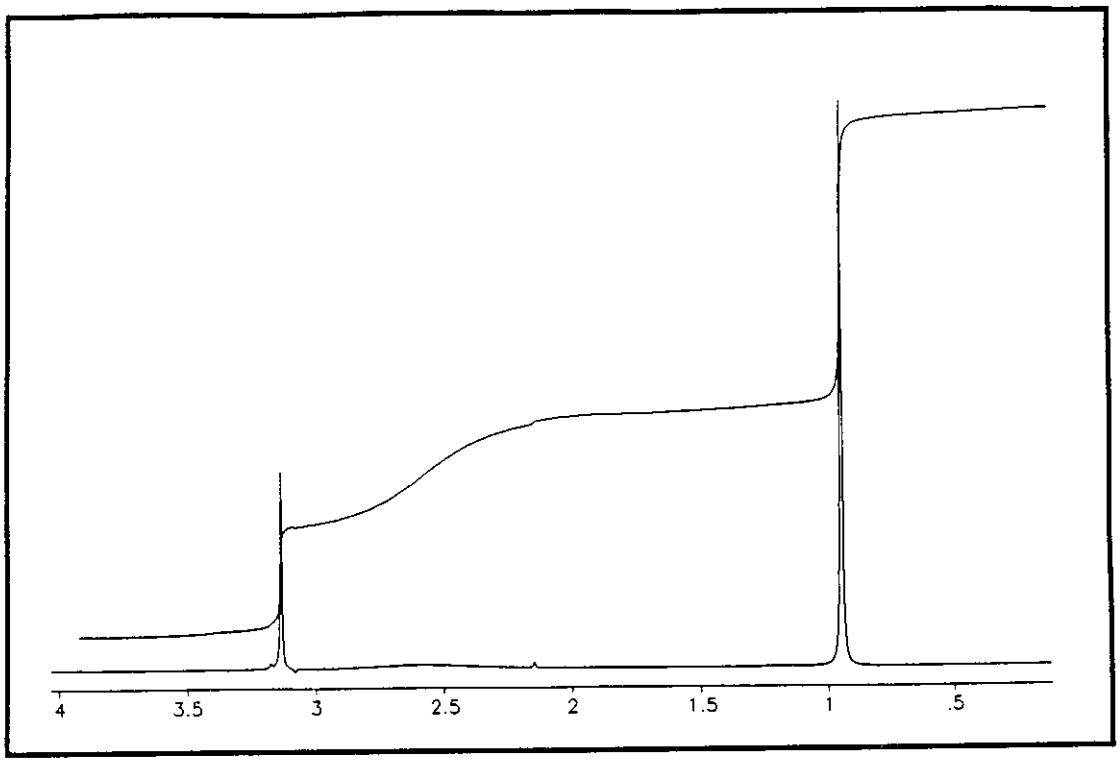

t
t
80
60
40
20
0
PPM

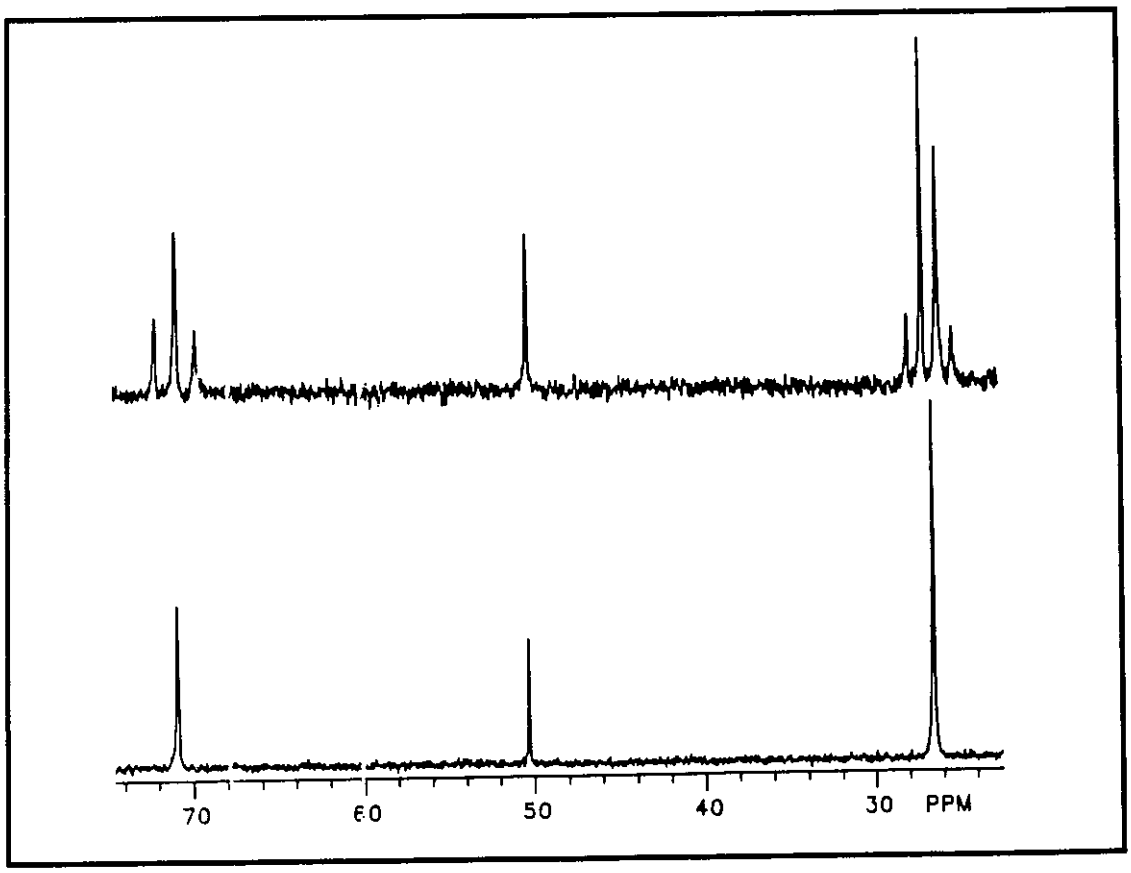
Problem 39

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A	Mass R/A
14, 0.50	29, 7.51	42,13.41	55, 2.00	65, 0.10	75, 0.20
15, 4.90	30, 9.91	43, 6.21	56, 9.81	66, 0.10	82, 0.10
16, 0.20	31, 4.40	44, 1.90	57, 4.90	67, 0.10	84, 0.20
17, 0.70	32, 0.80	45, 1.00	58,100.0	68, 0.10	85, 0.10
18,17.22	36, 0.30	46, 0.20	59, 4.70	69, 0.70	86, 0.20
19, 0.30	37, 0.30	49, 0.10	60, 0.30	70, 0.80	87, 0.10
25, 0.10	38, 0.80	50, 0.20	61, 0.50	71, 0.40	88, 0.10
26, 0.90	39, 4.80	51, 0.30	62, 0.10	72, 2.90	
27, 4.50	40, 1.60	52, 0.50	63, 0.10	73, 0.70	
28,11.31	41,18.02	54, 0.70	64, 0.10	74, 3.40	

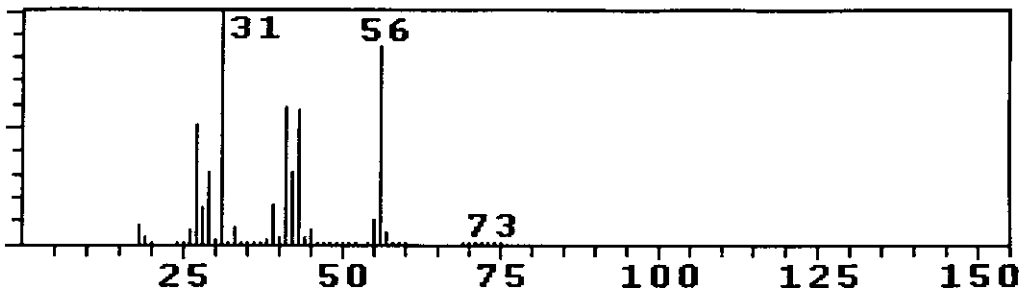


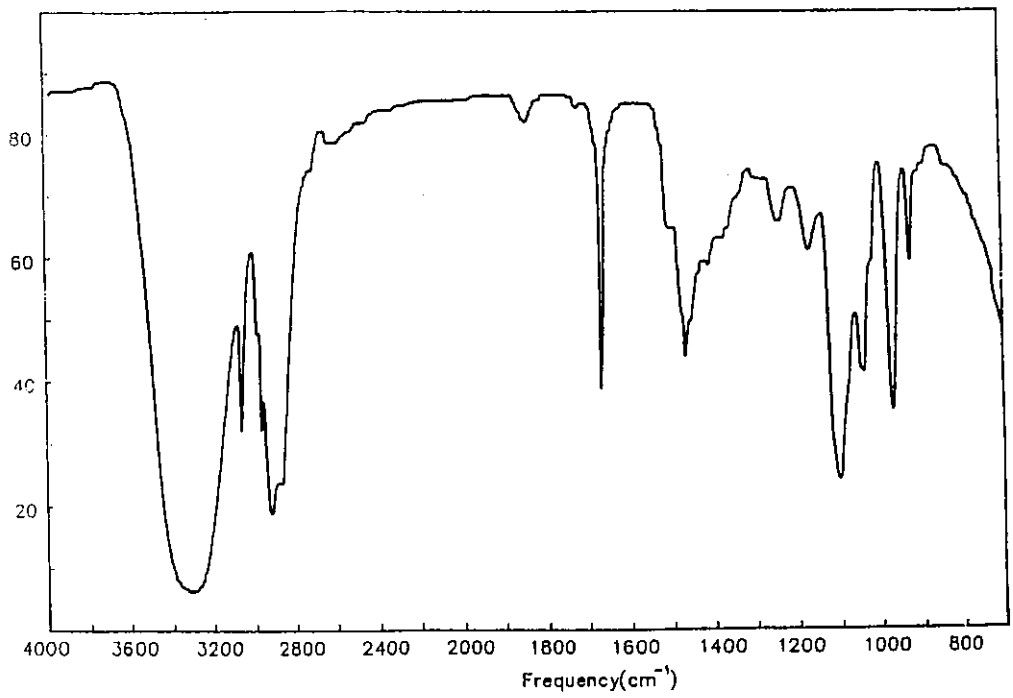

4
3.5
3
2.5
2
1.5
1
.5

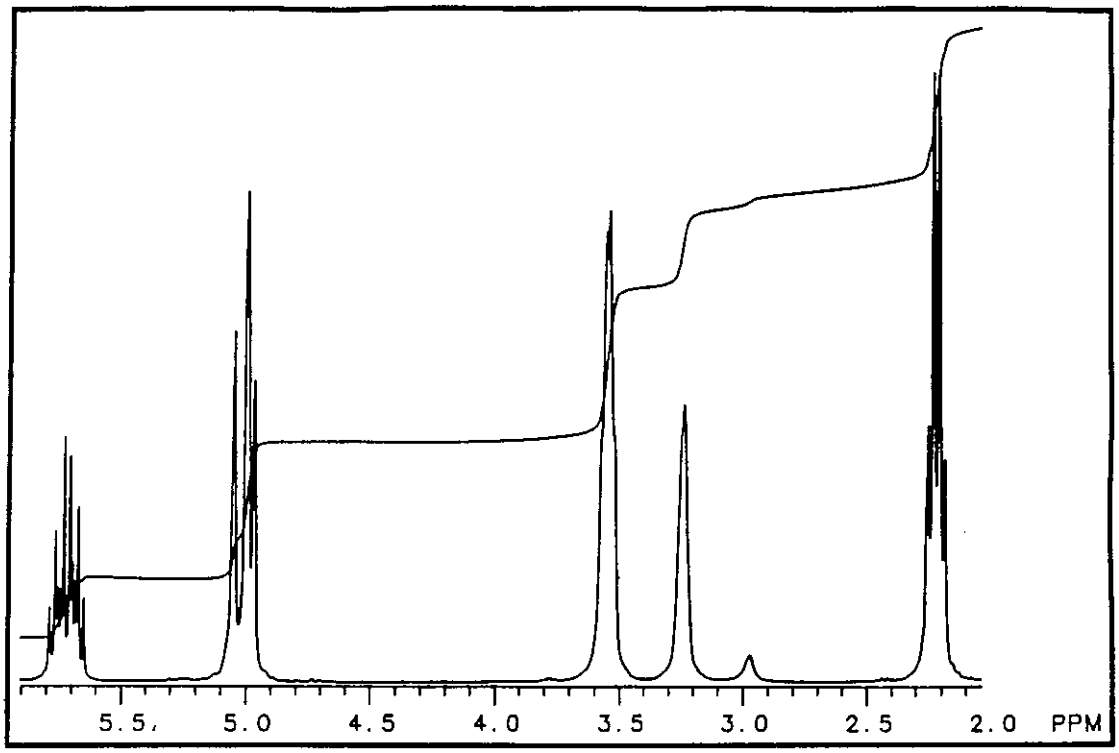

70
60
50
40
30
PPM

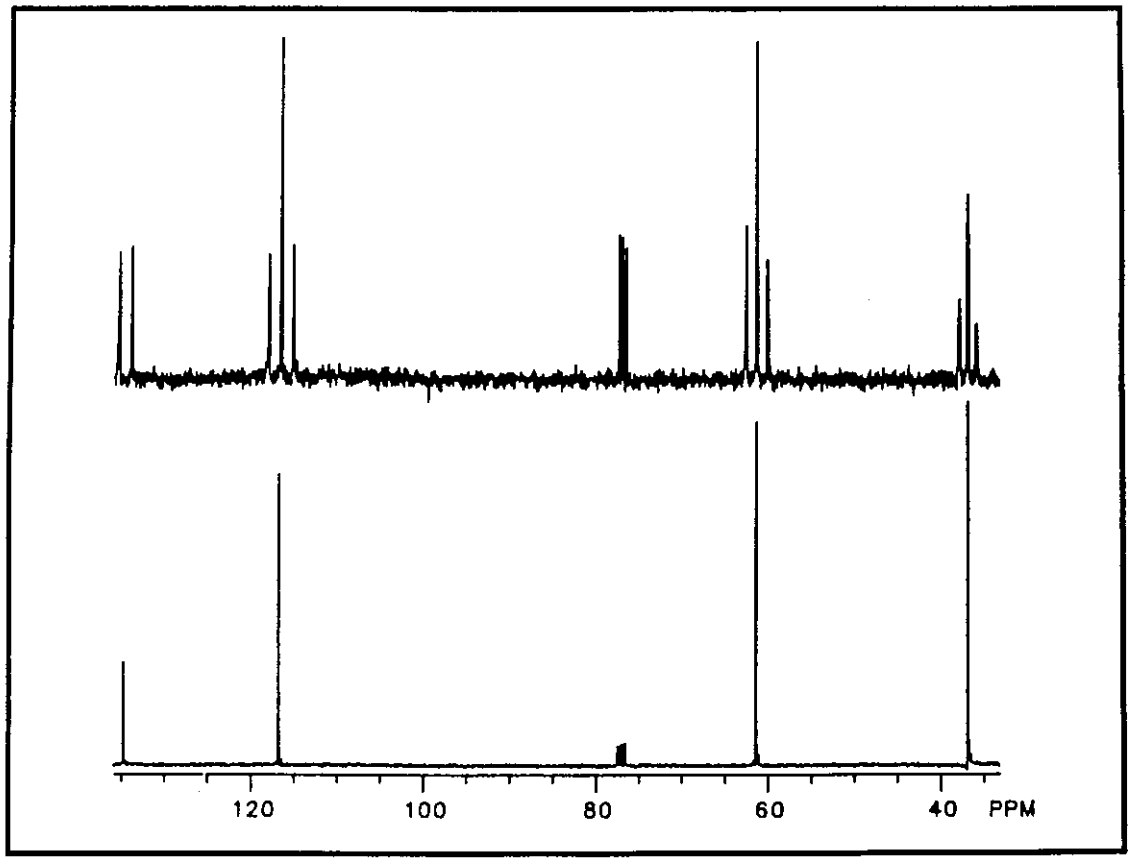
Problem 40

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



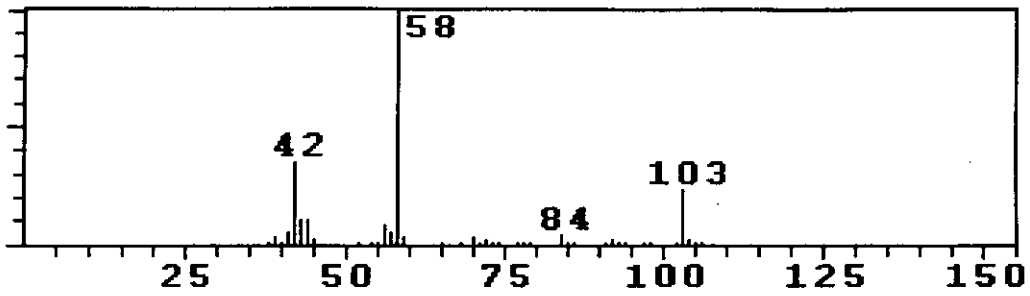


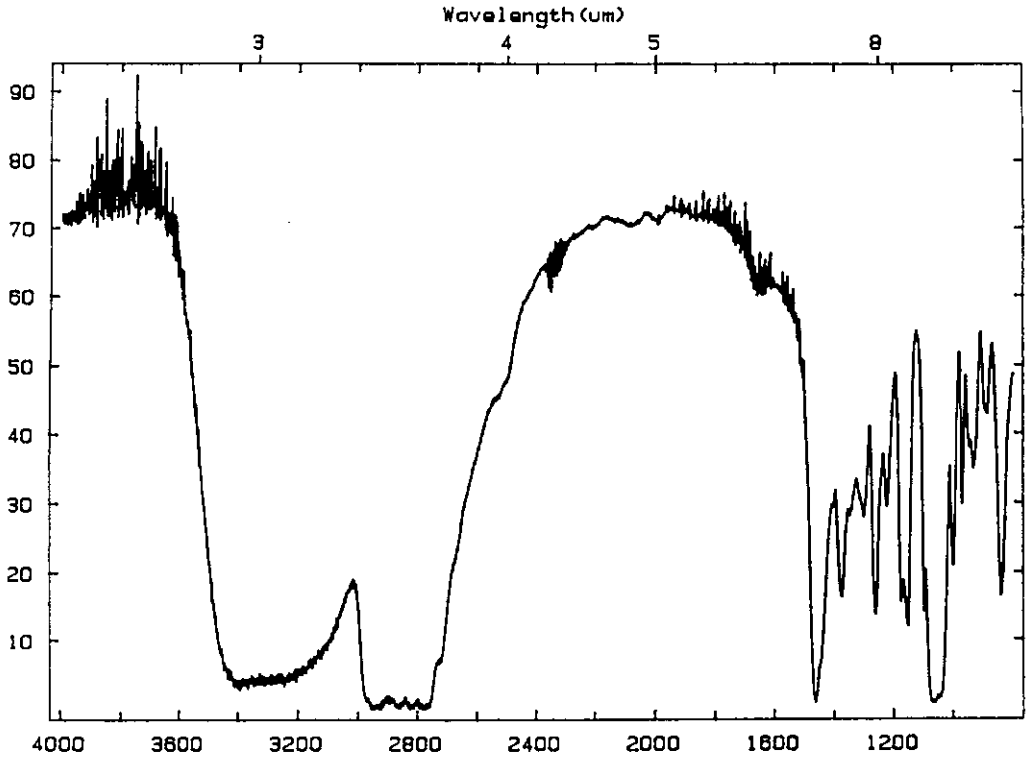

5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
PPM

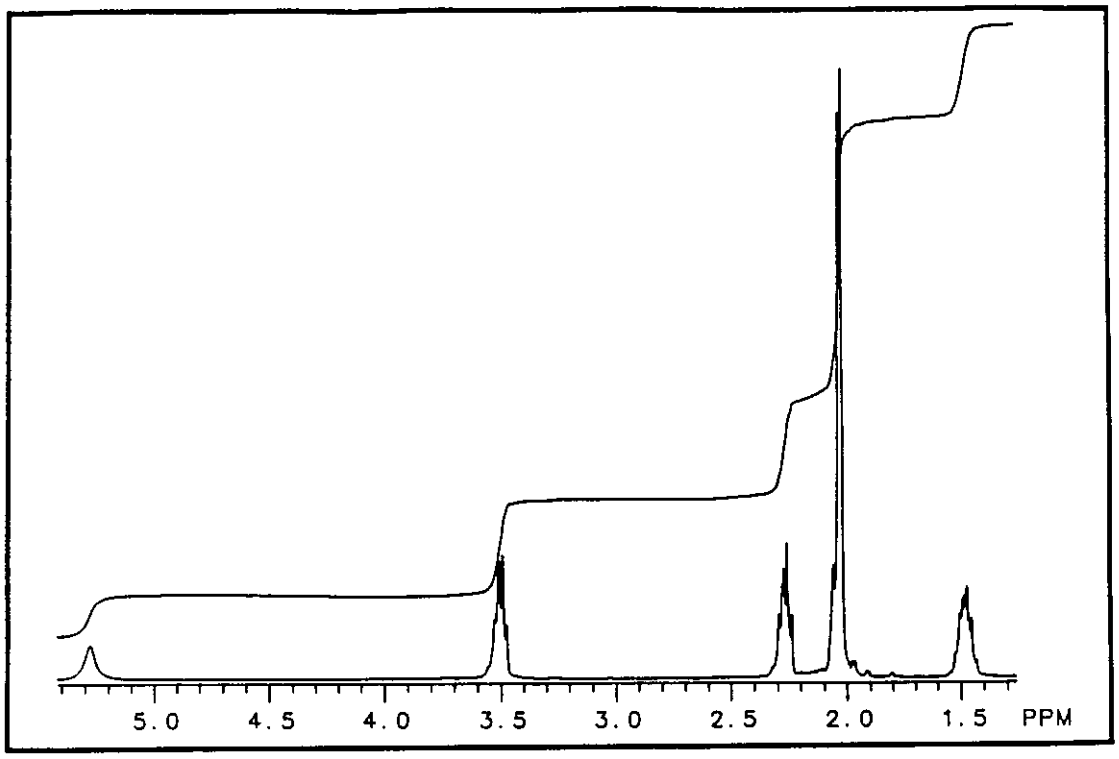

120
100
80
60
40
PPM

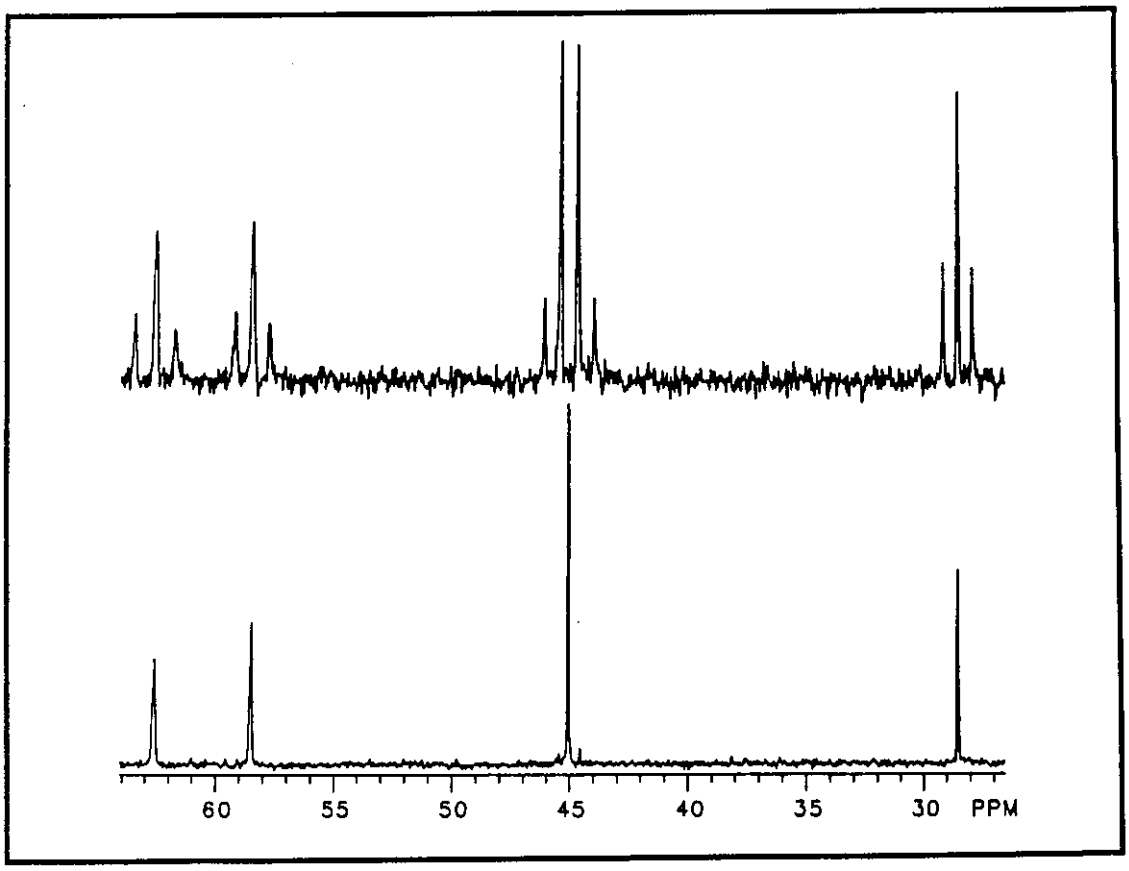
Problem 41

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na






5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
PPM

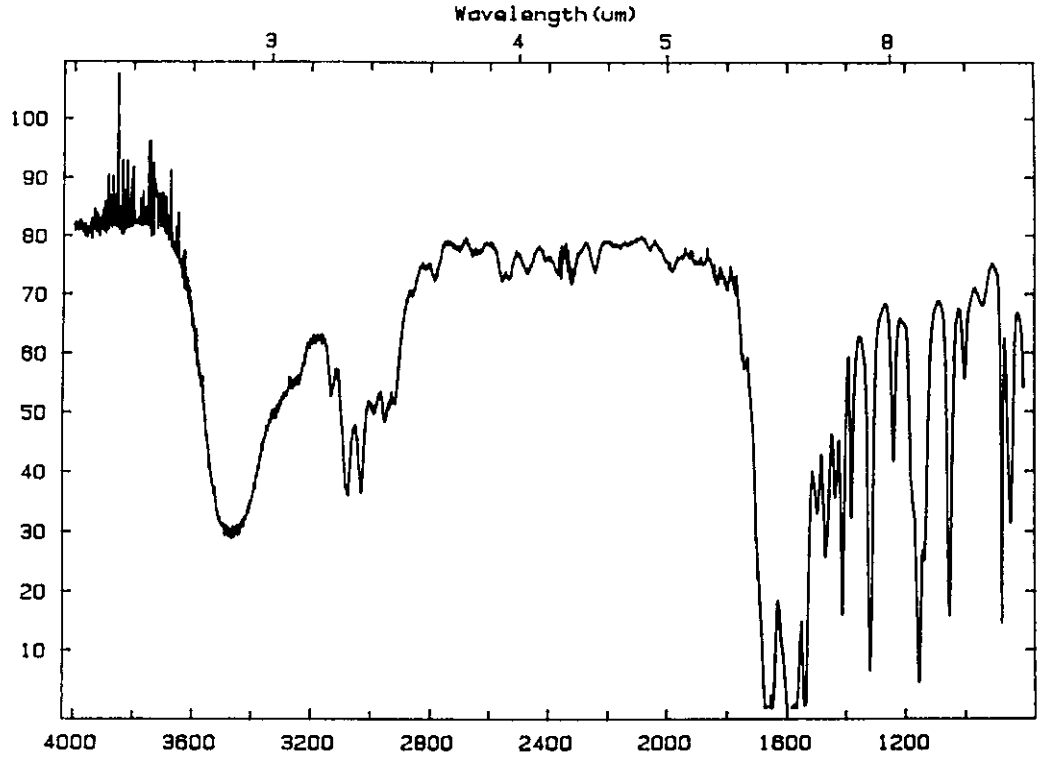

60
55
50
45
40
35
30
PPM

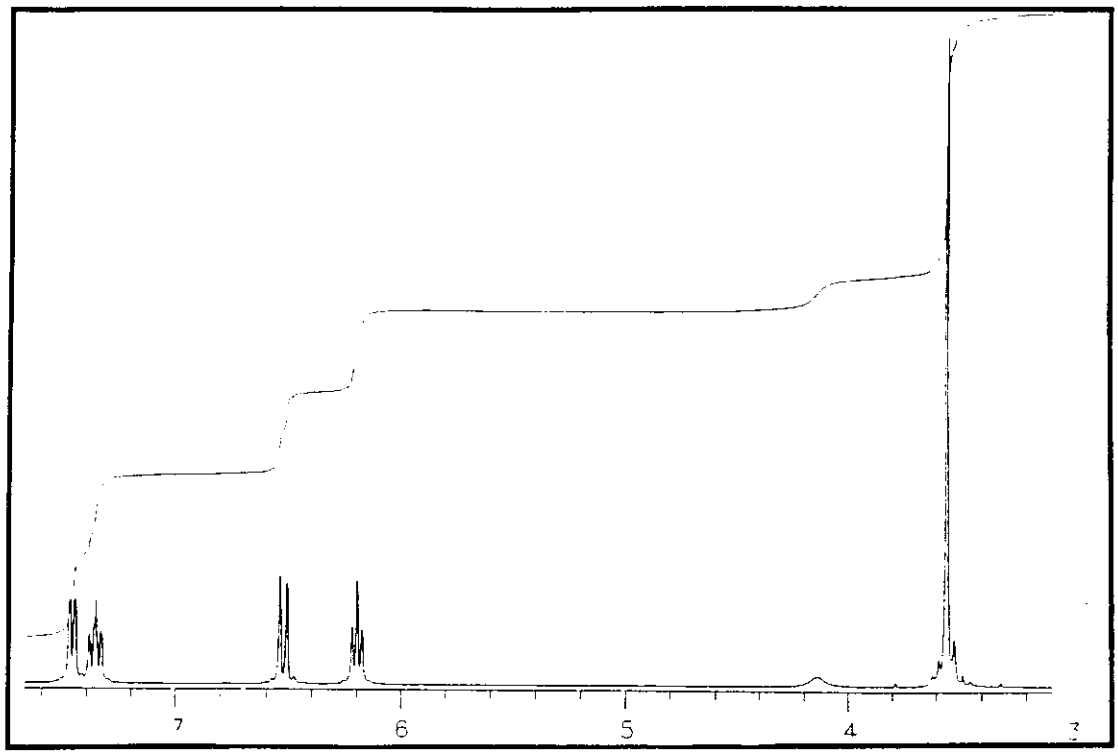
Problem 42

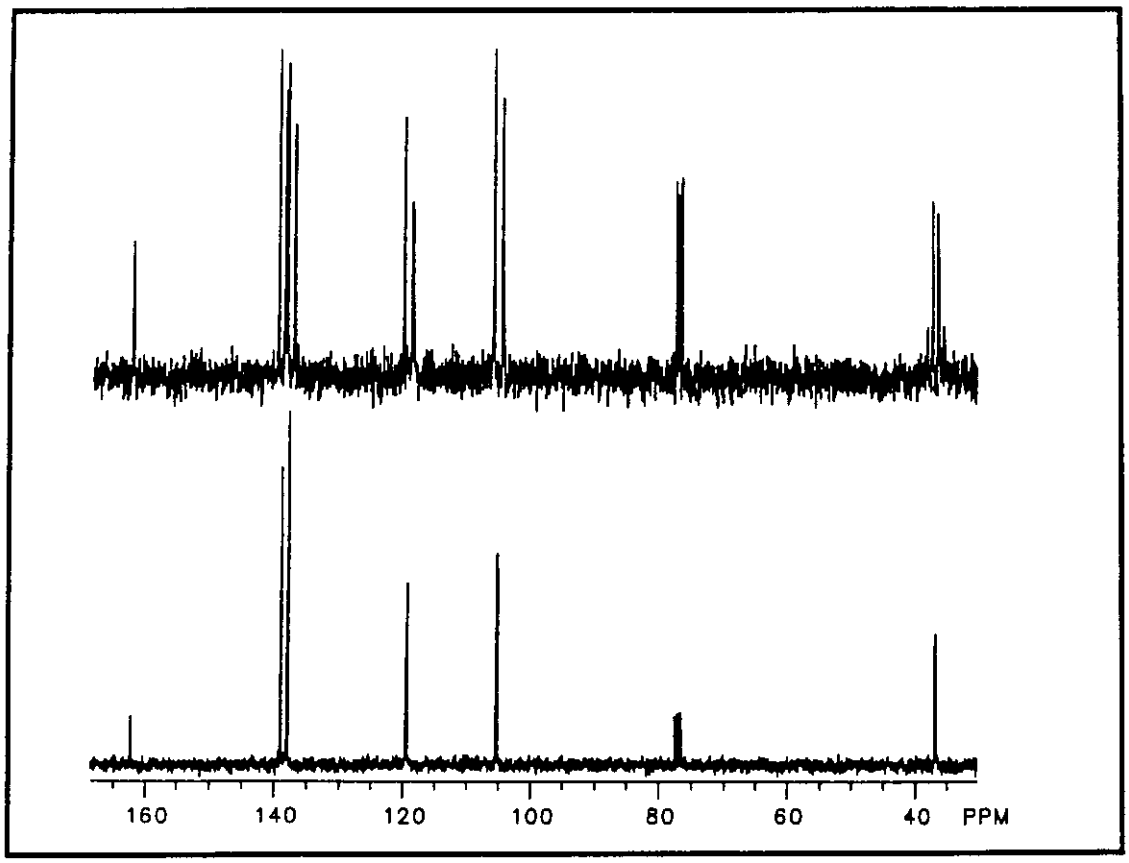
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z	
51	11.73	64	2.75	93	0.94
52	6.66	65	1.44	94	1.39
53	11.89	66	5.46	101	1.47
54	8.44	68	2.77	108	3.73
55	13.00	78	3.40	109	100.00
56	1.37	79	2.53	110	6.28
57	0.49	80	69.19		
58	1.26	81	88.63		
59	10.13	82	4.99		
60	0.46	83	5.24		
63	0.99	85	1.41		

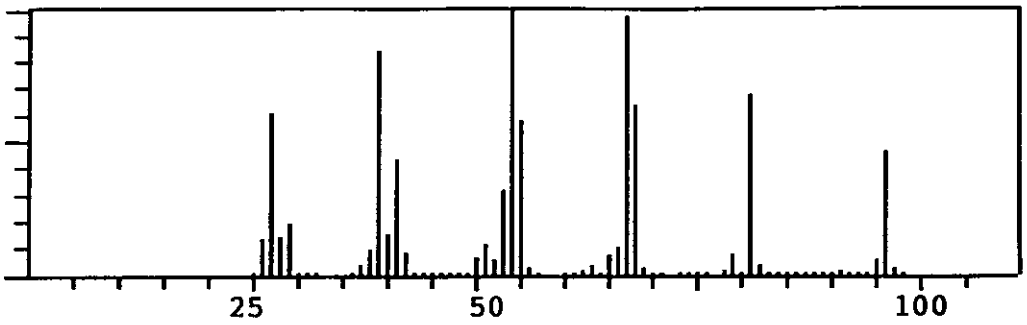


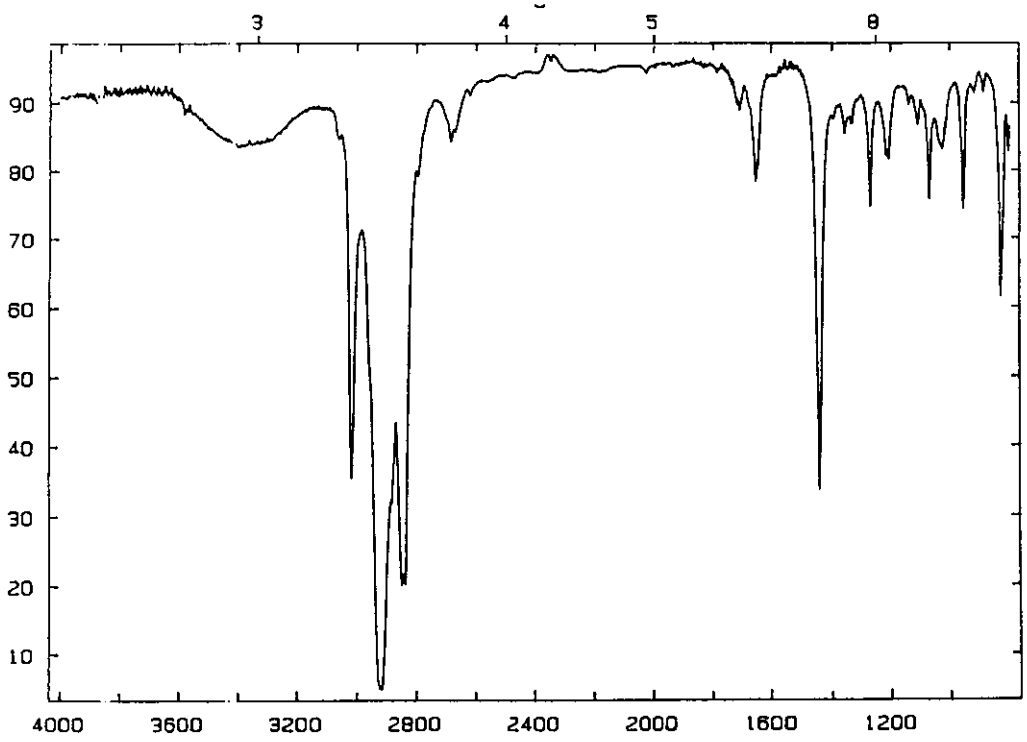

7
6
5
4
3

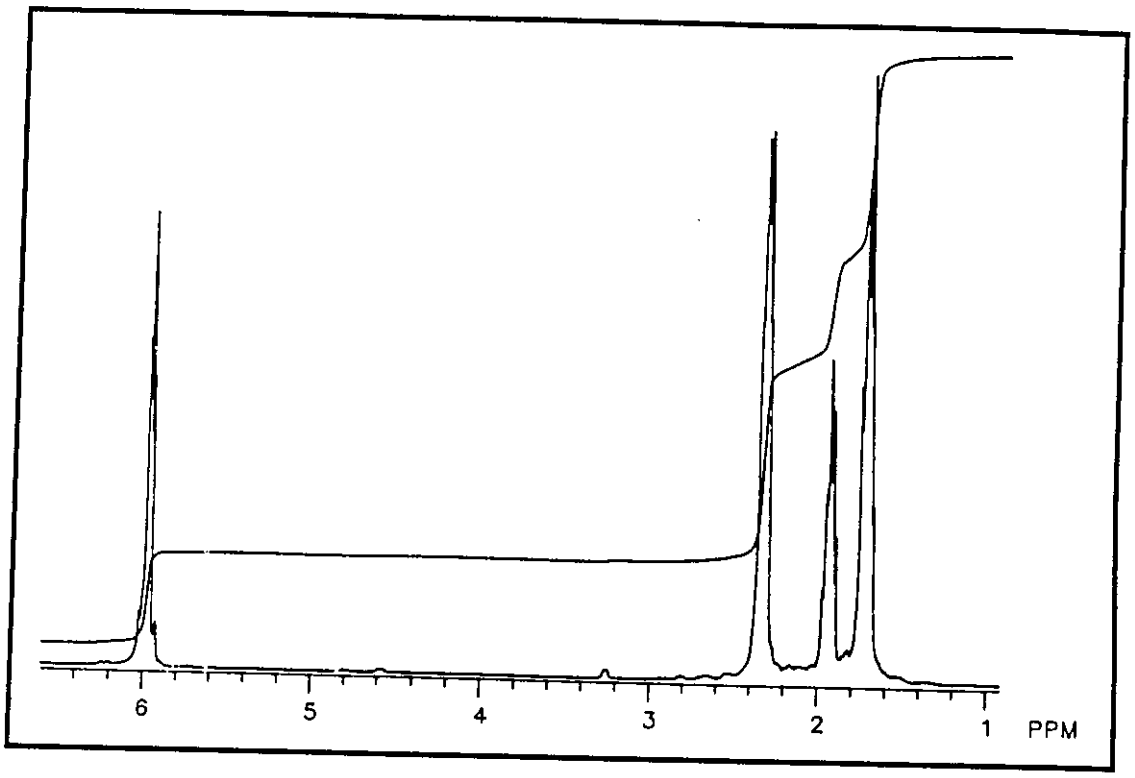

160
140
120
100
80
60
40
PPM

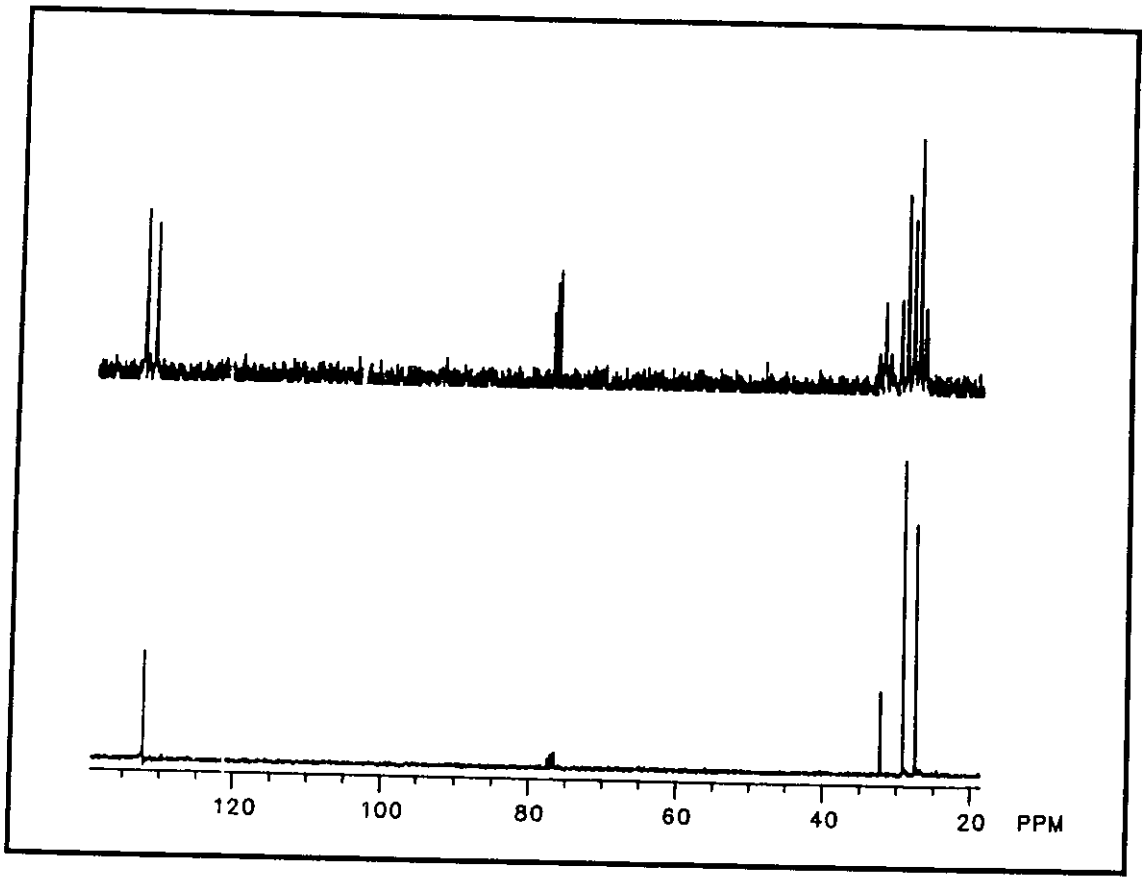
Problem 43

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



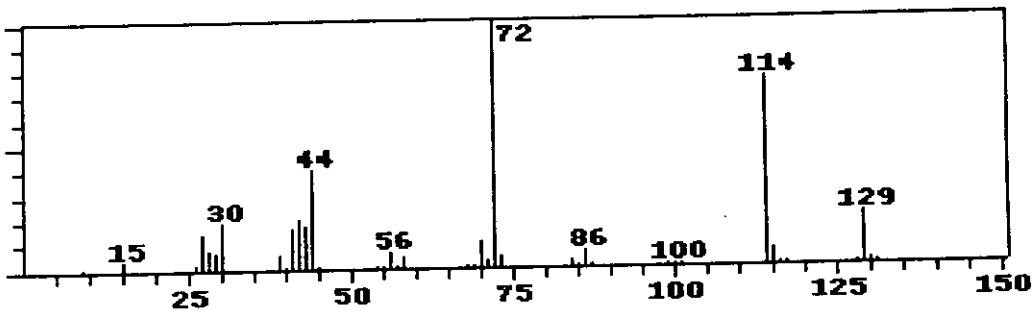


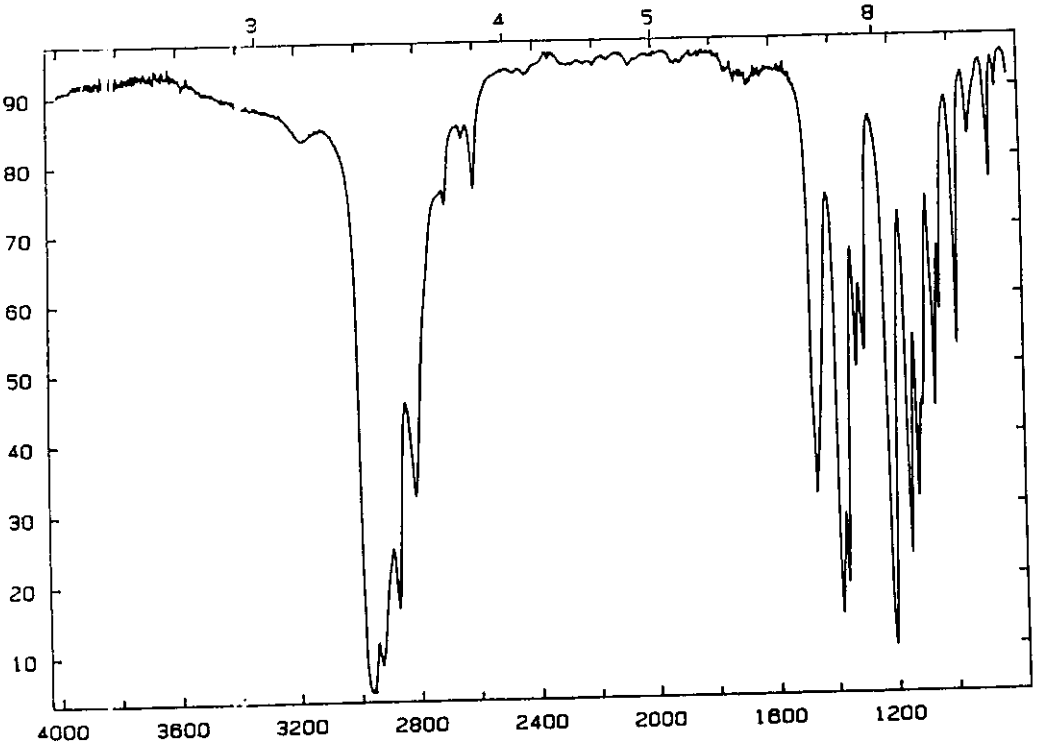

6
5
4
3
2
1
PPM

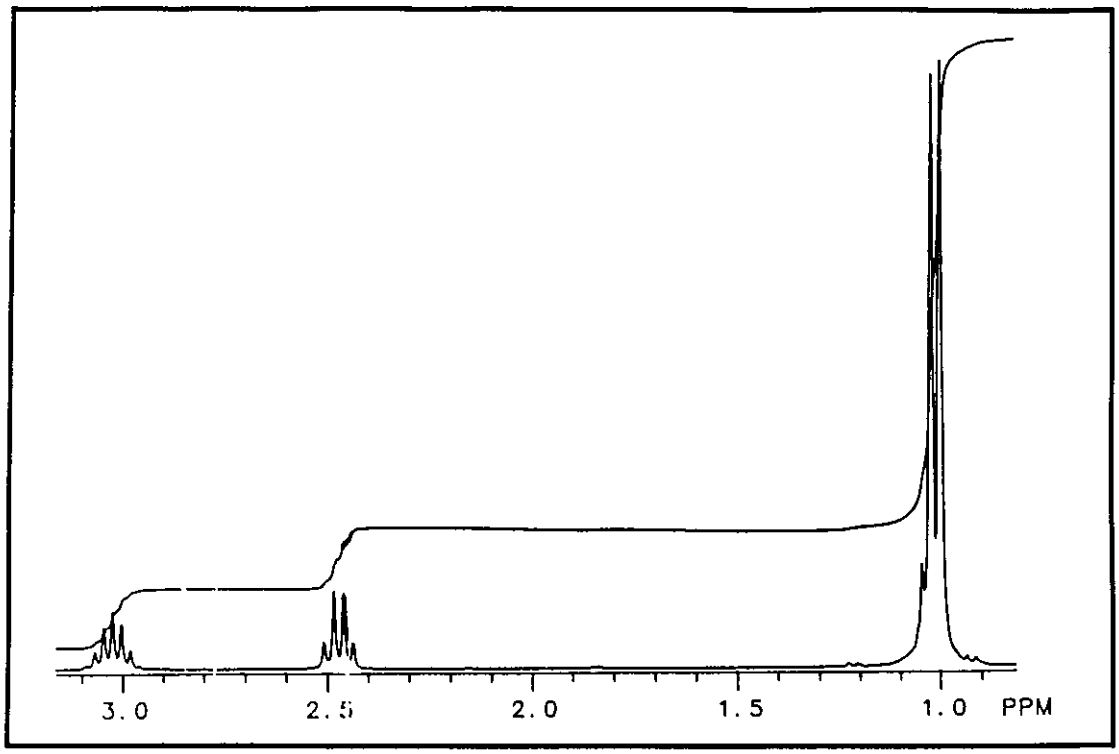

120
100
80
60
40
20
PPM

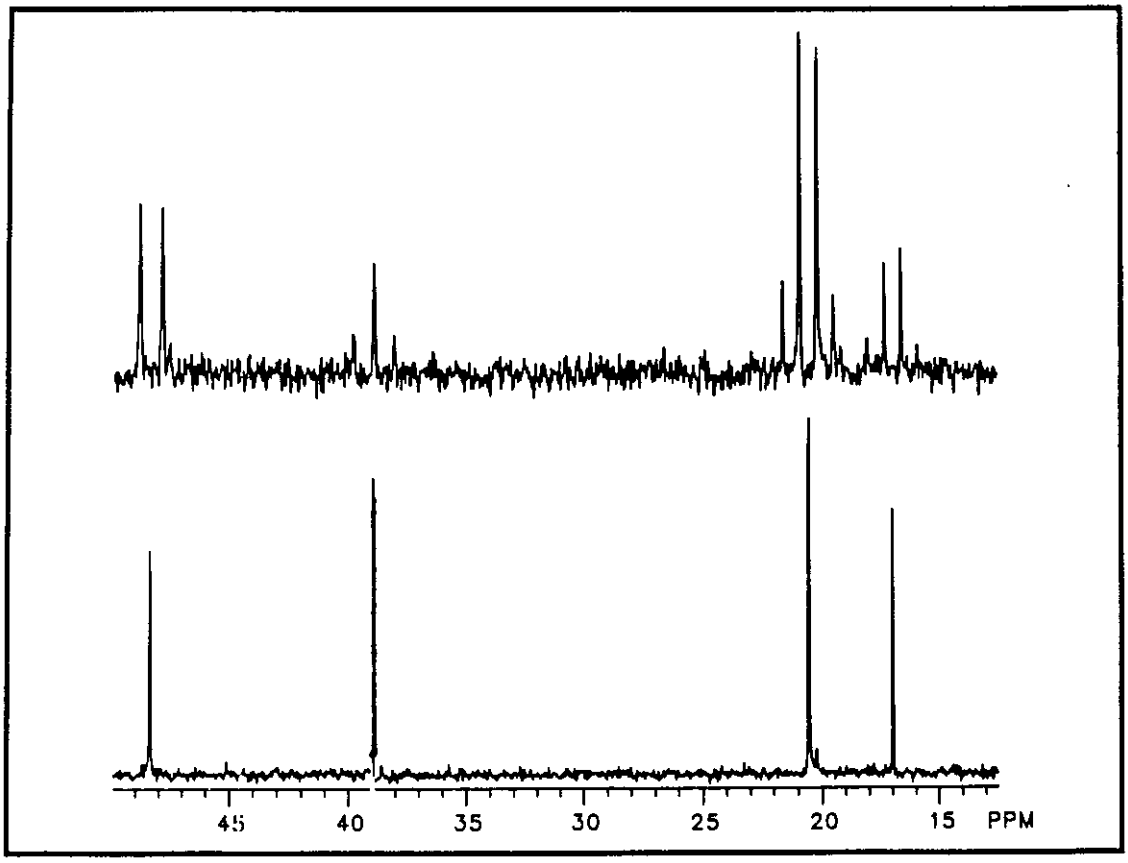
Problem 44

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



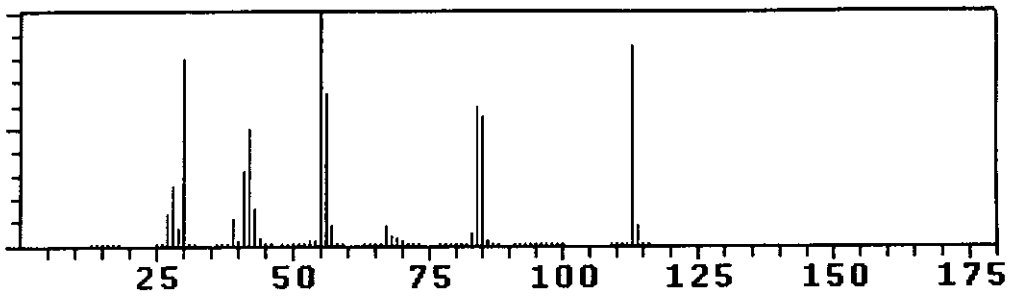


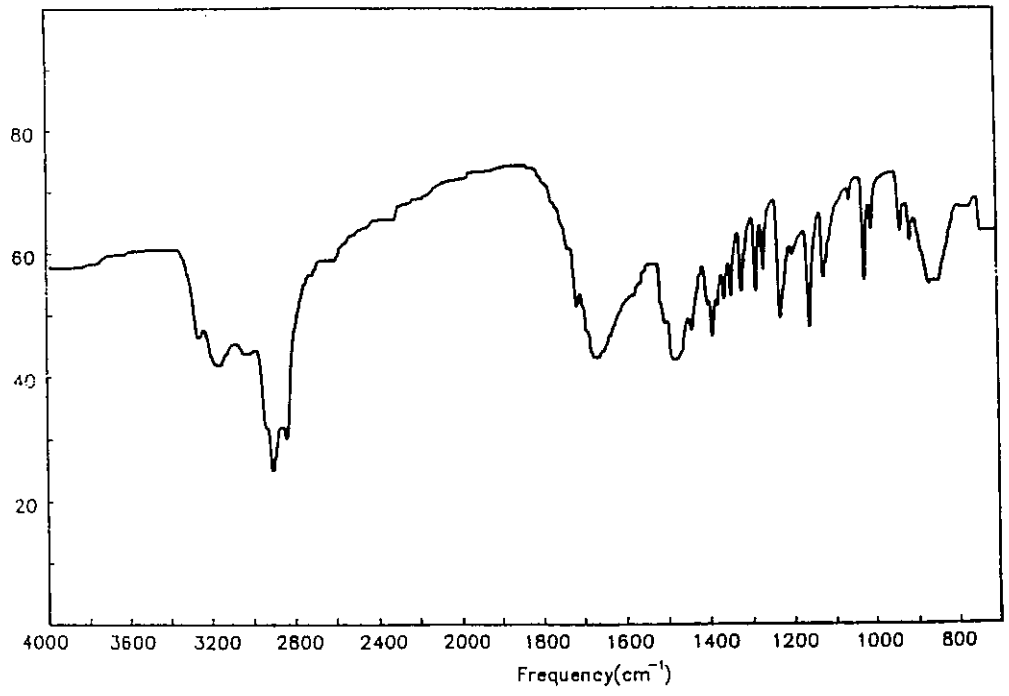

3.0
2.5
2.0
1.5
1.0
PPM

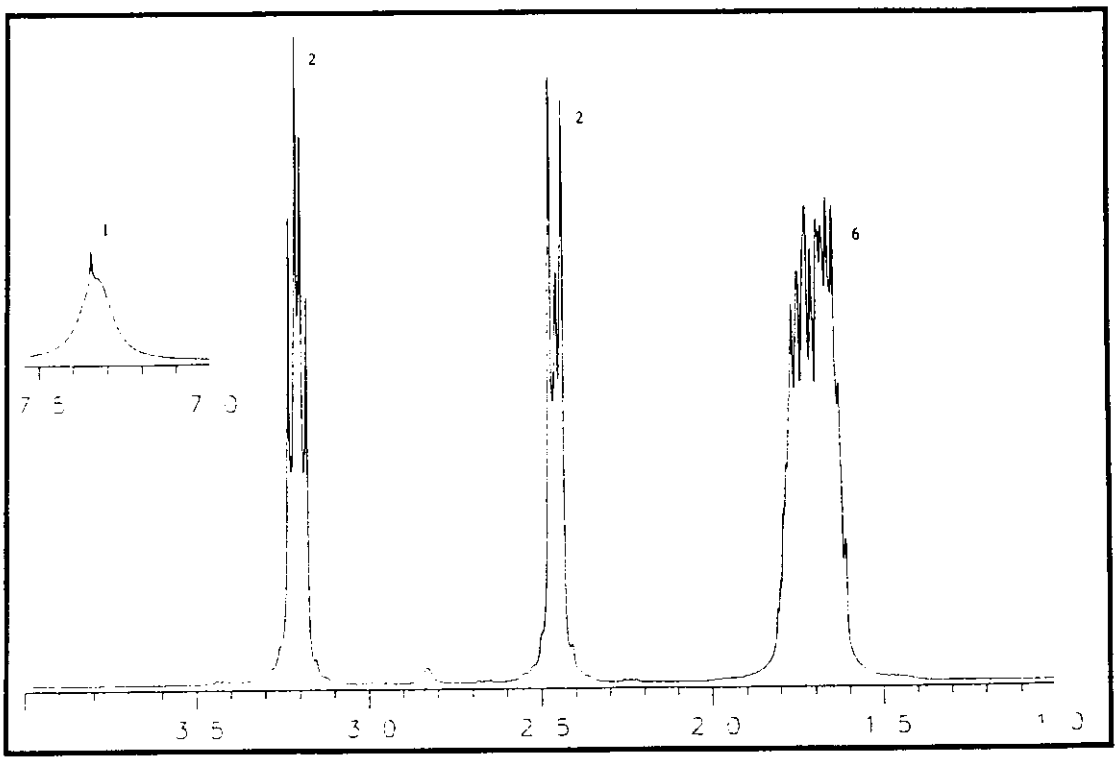

45
40
35
30
25
20
15
PPM

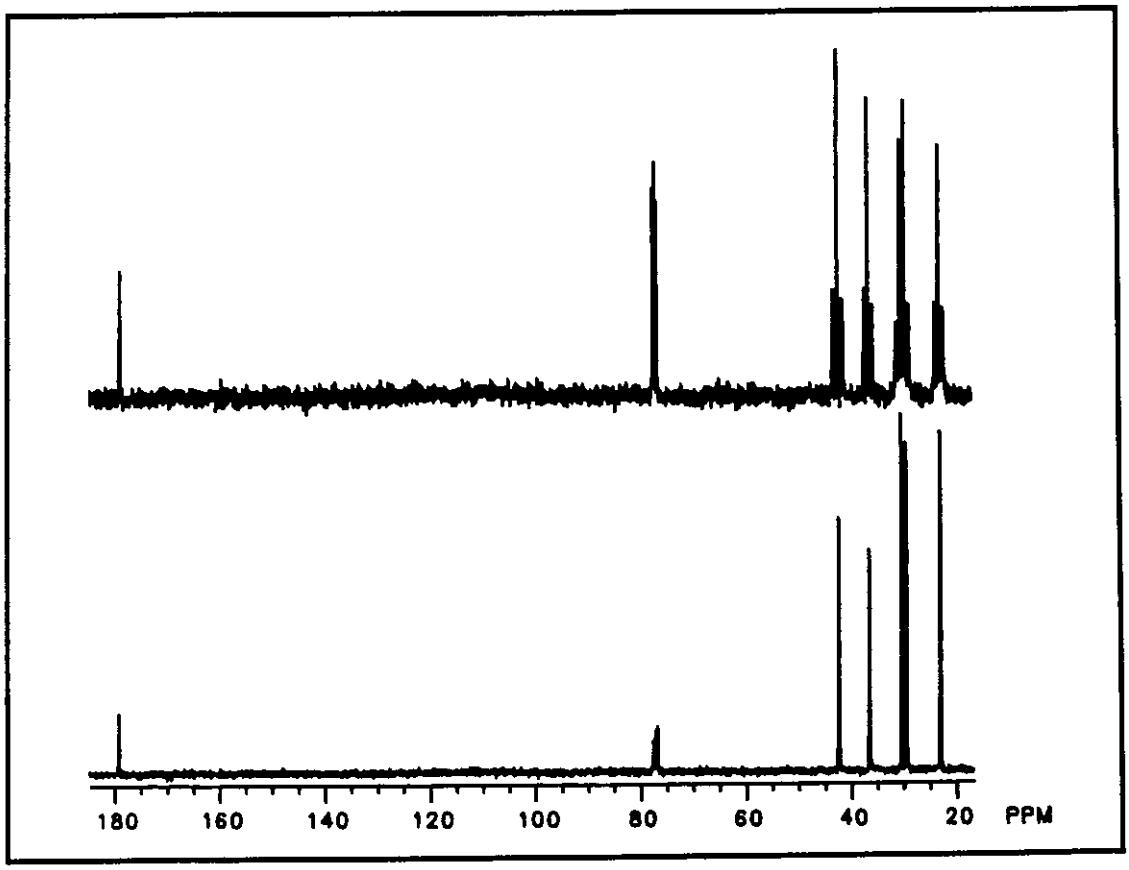
Problem 45

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 63.7% C; 9.8% H; 12.4% N



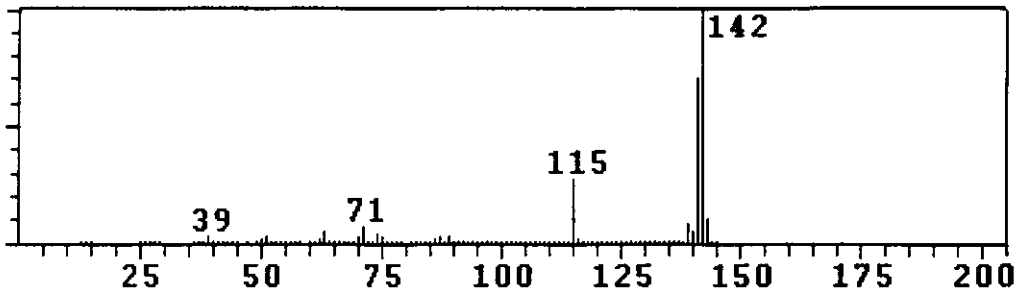


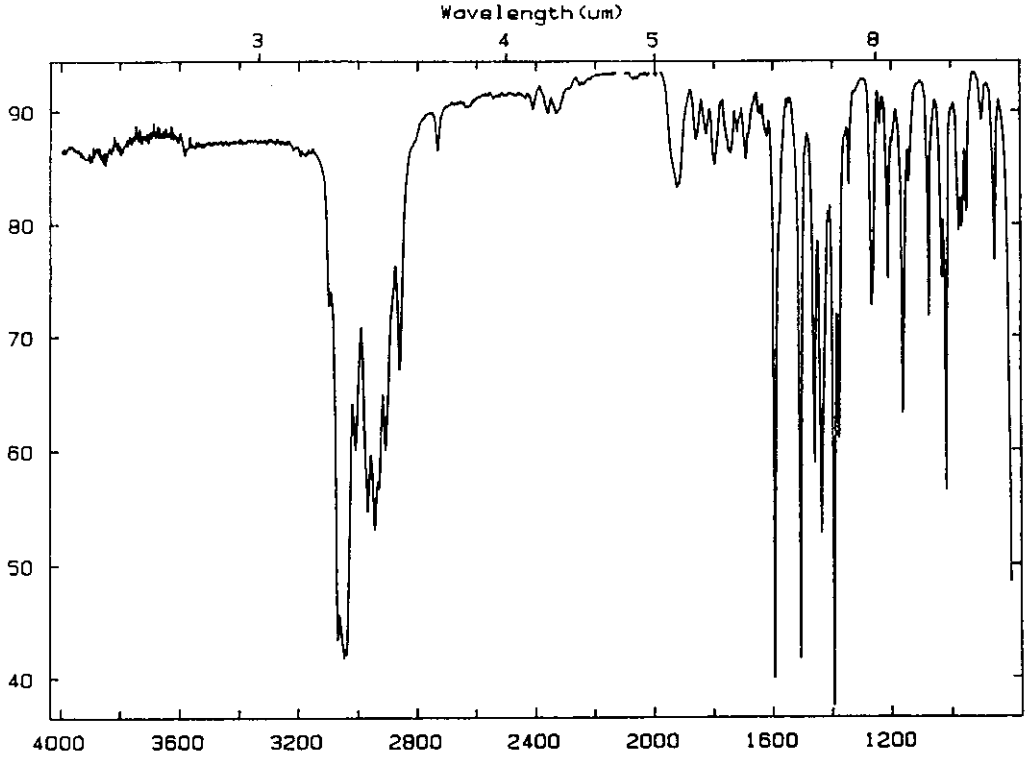

2
2
1
6
7 5
7 0
3 5
3 0
2 5
2 0
1 5

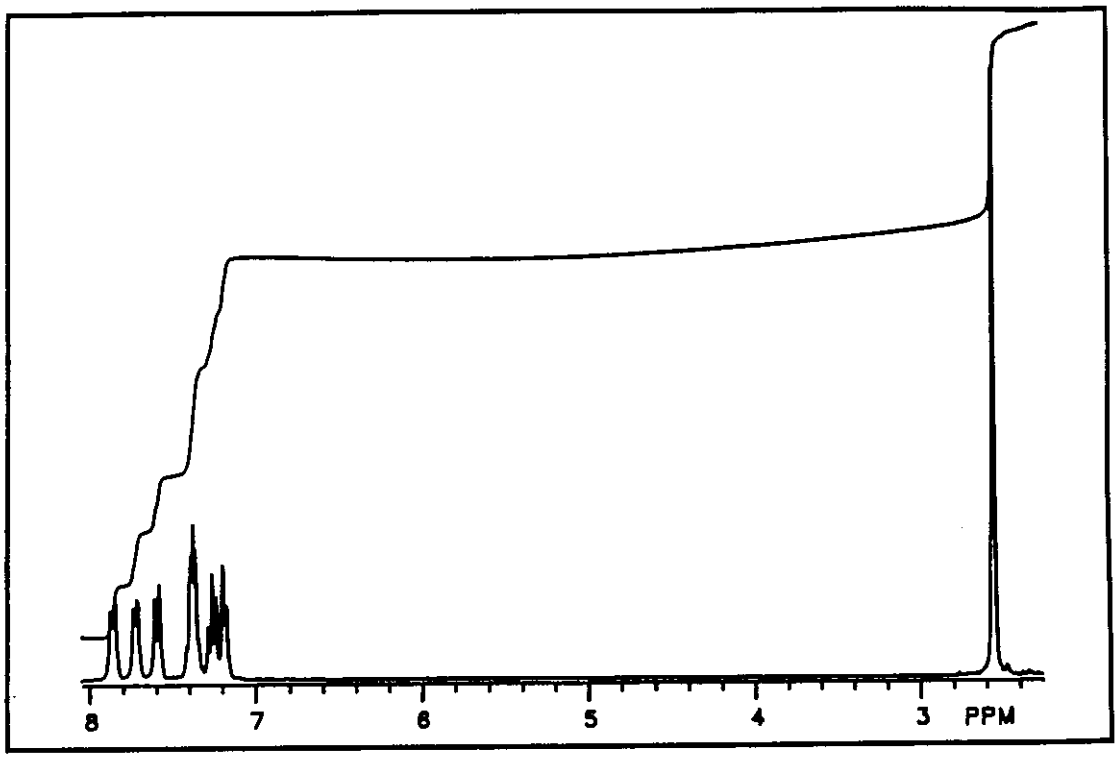

180
160
140
120
100
80
60
40
20
PPM

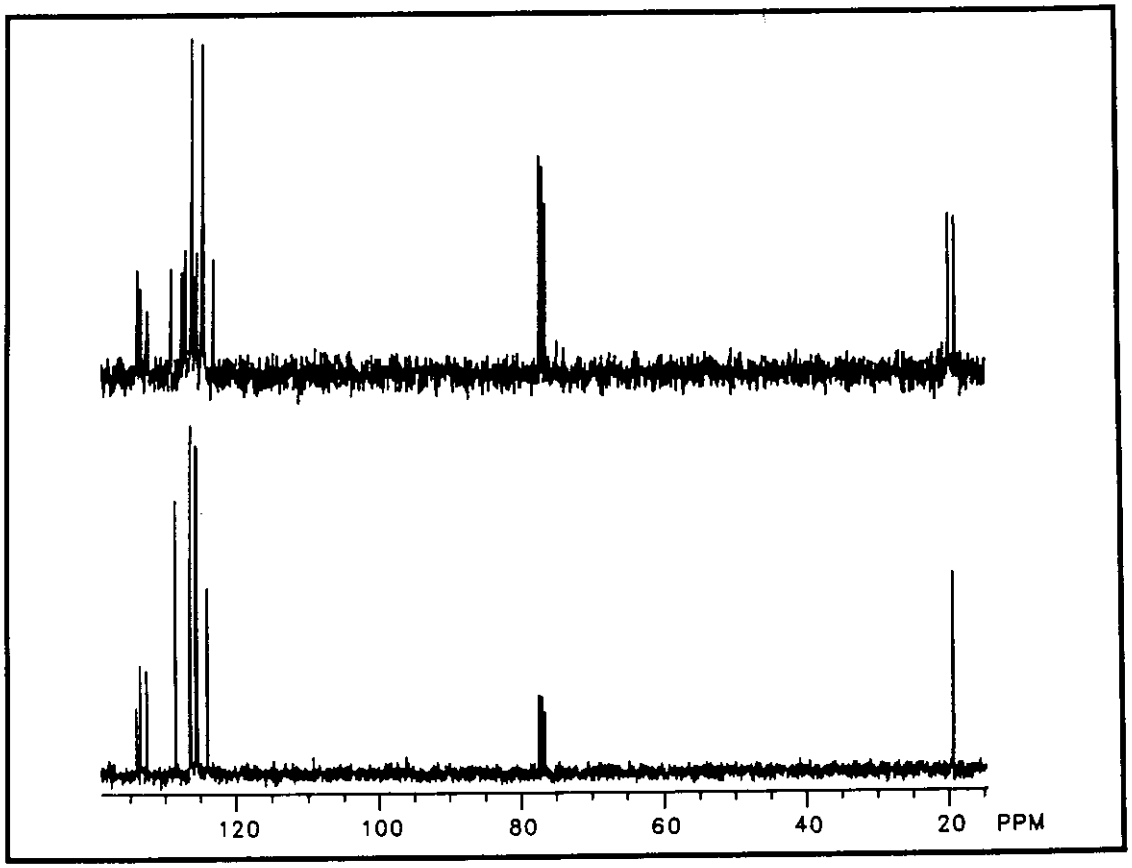
Problem 46

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 92.9% C; 7.1% H



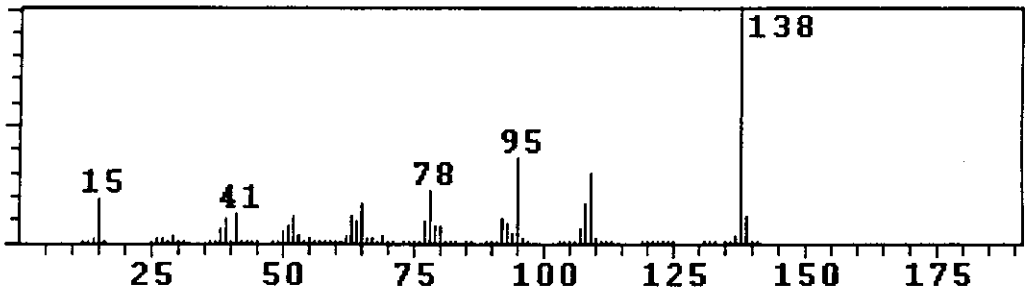


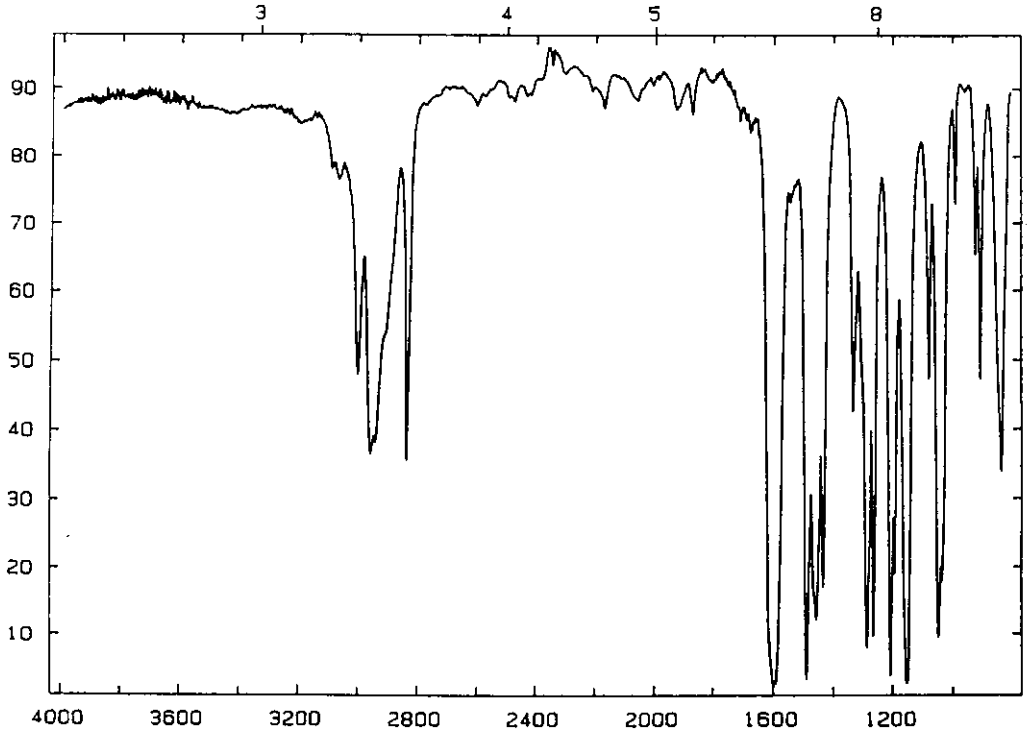

8
7
6
5
4
3
PPM

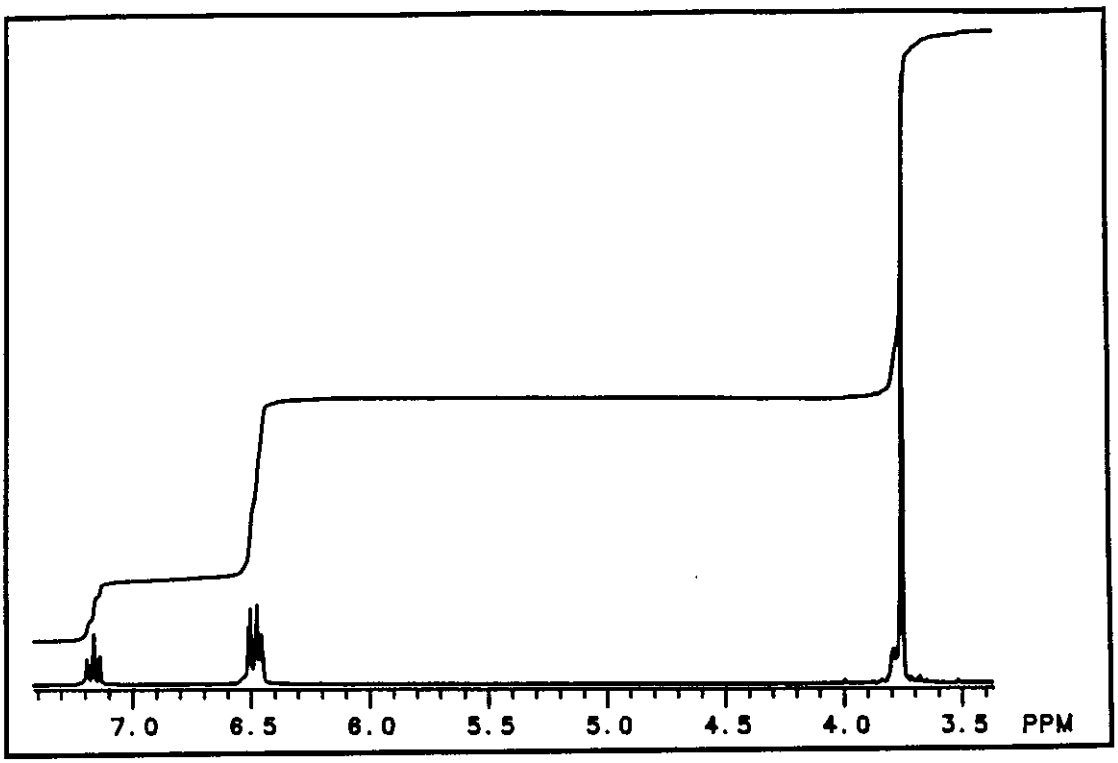

120
100
80
60
40
20
PPM

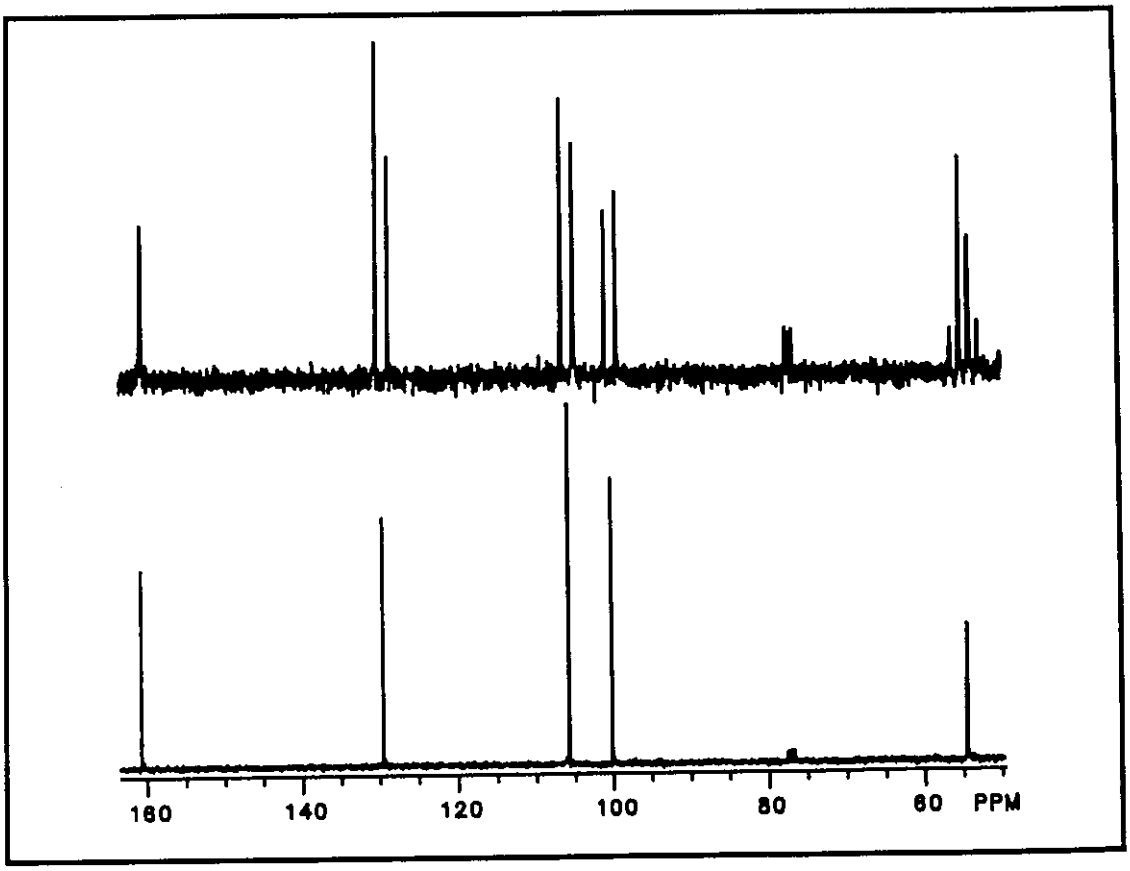
Problem 47

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na






7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
PPM

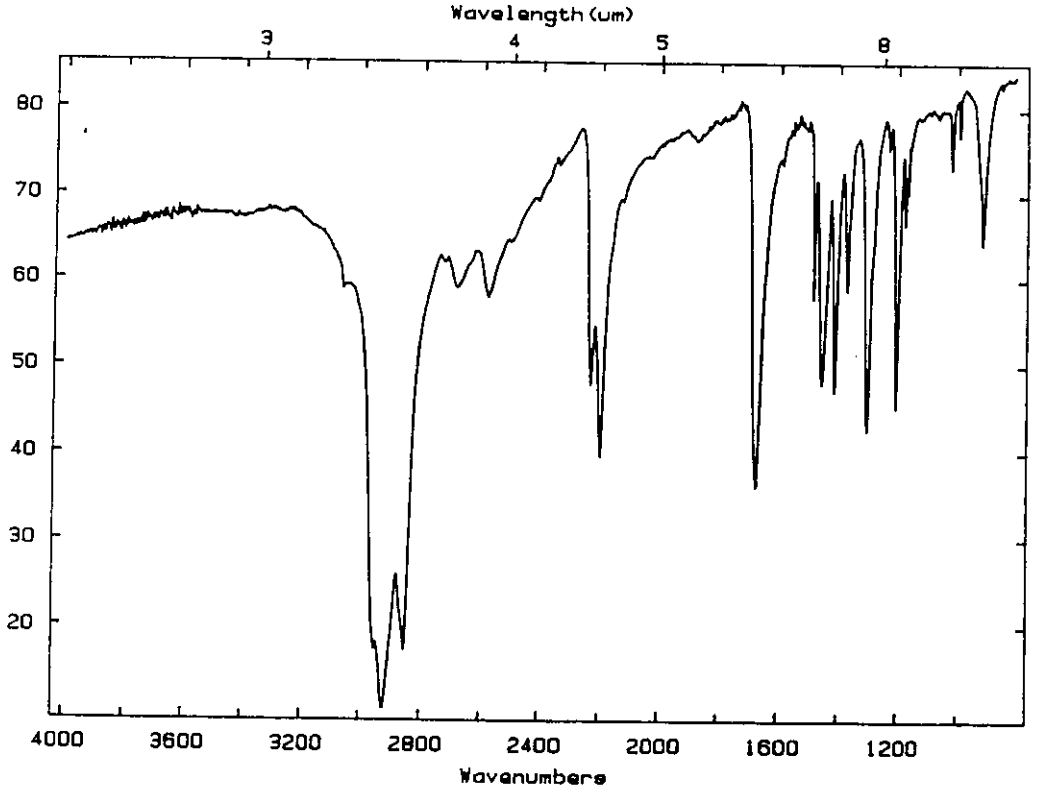

160
140
120
100
80
60
PPM

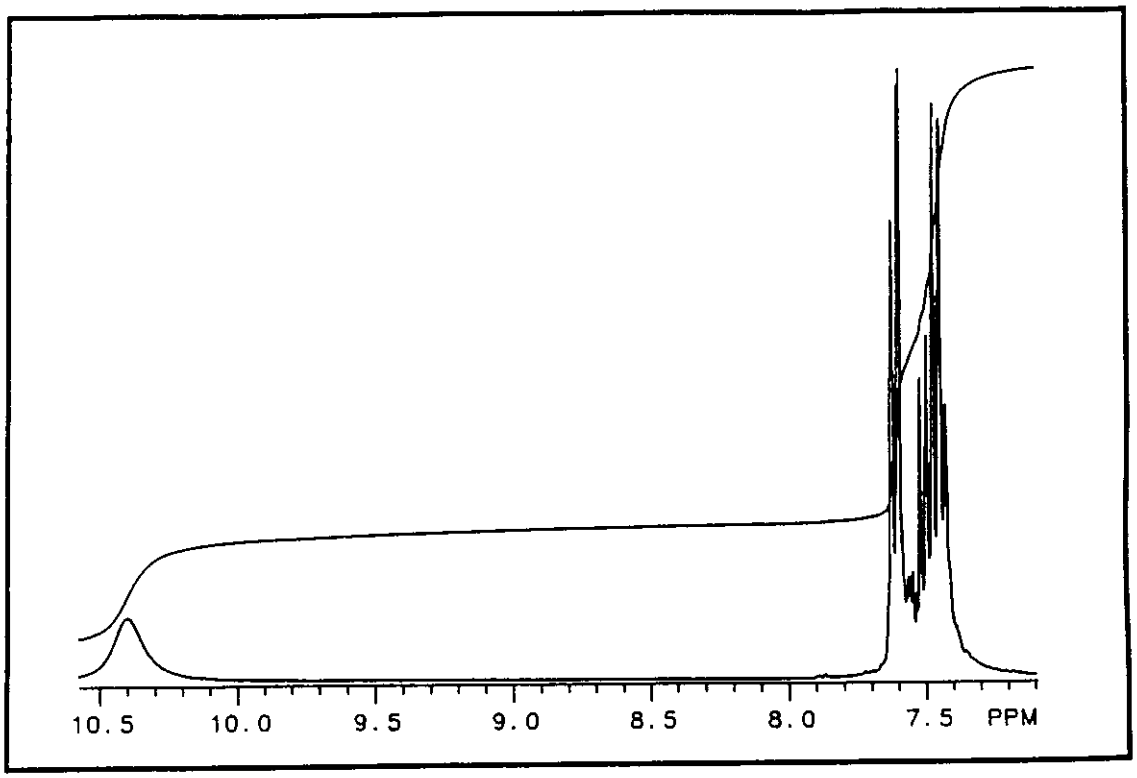
Problem 48

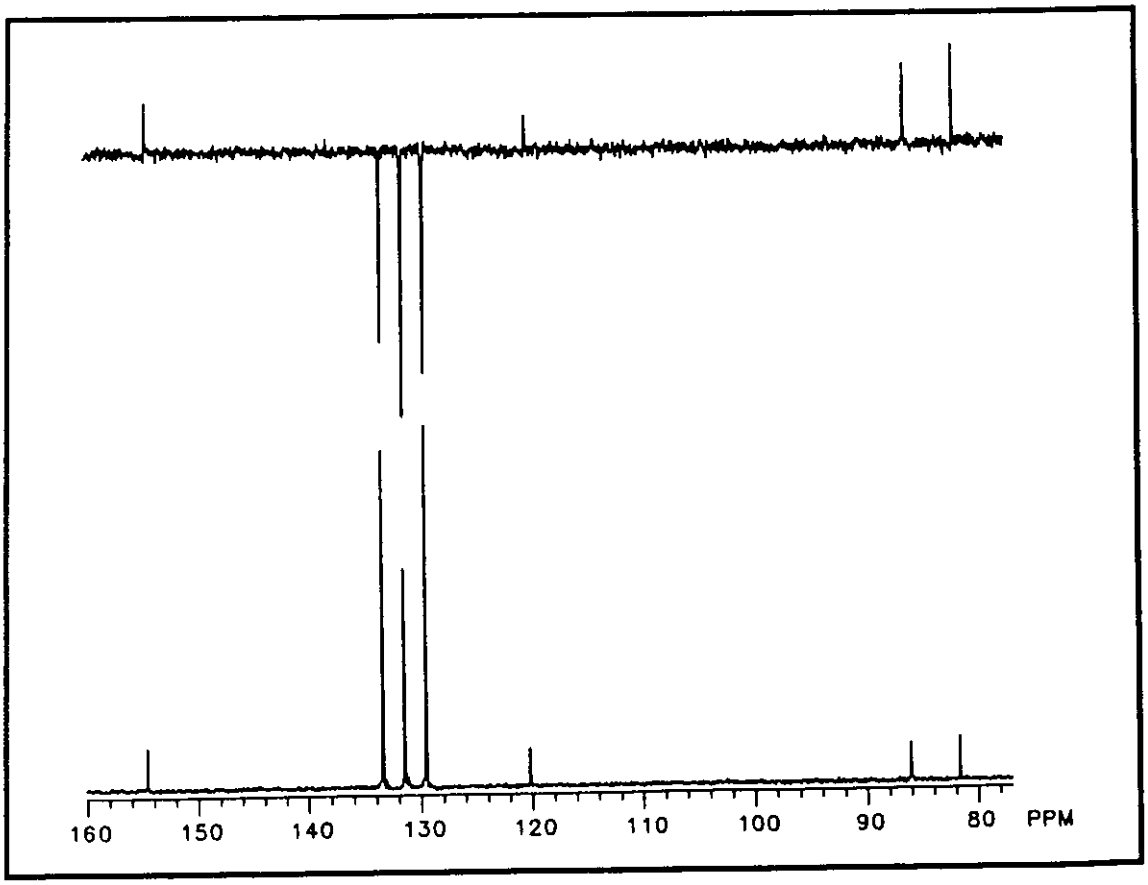
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 74.0% C; 4.1% H

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
32	0.11	51	11.54	64	1.92	85	0.19	98	3.78	119	1.54
37	1.83	52	5.36	73	3.39	86	0.34	99	0.76	129	30.67
38	2.09	53	0.20	74	16.78	87	1.45	100	0.25	130	3.07
39	3.61	59	0.98	75	15.81	88	0.06	101	6.02	131	0.14
44	20.09	60	0.22	76	26.91	89	5.93	102	100.00	146	37.36
45	1.32	61	3.80	77	3.88	90	1.76	103	8.75	147	3.94
49	2.81	62	5.43	78	0.05	91	0.08	117	0.27	148	0.23
50	13.46	63	8.56	84	1.30	97	0.59	118	17.19		




10.5
10.0
9.5
9.0
8.5
8.0
7.5
PPM

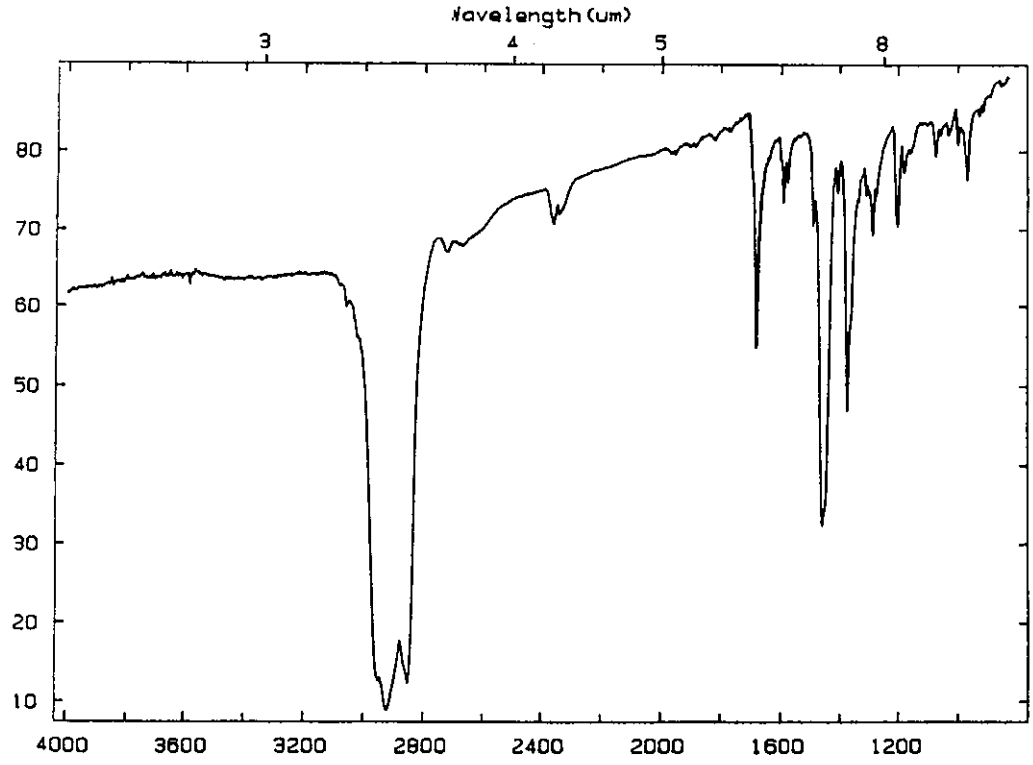

160
150
140
130
120
110
100
90
80
PPM

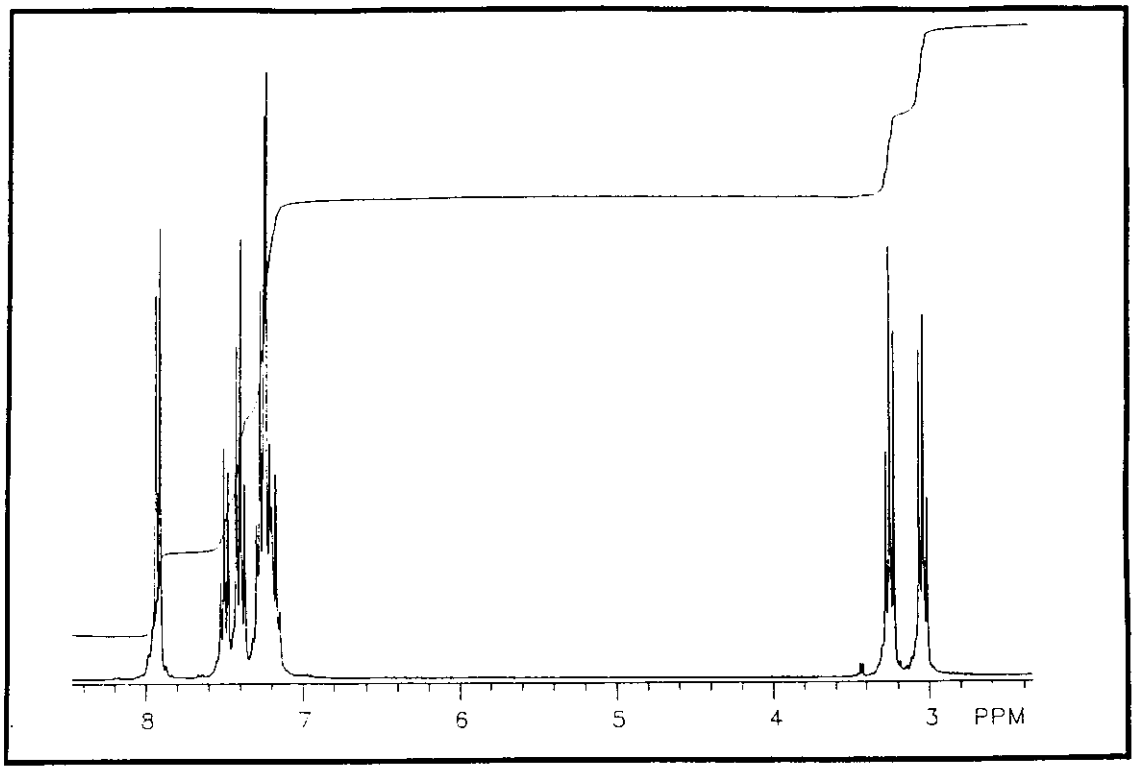
Problem 49

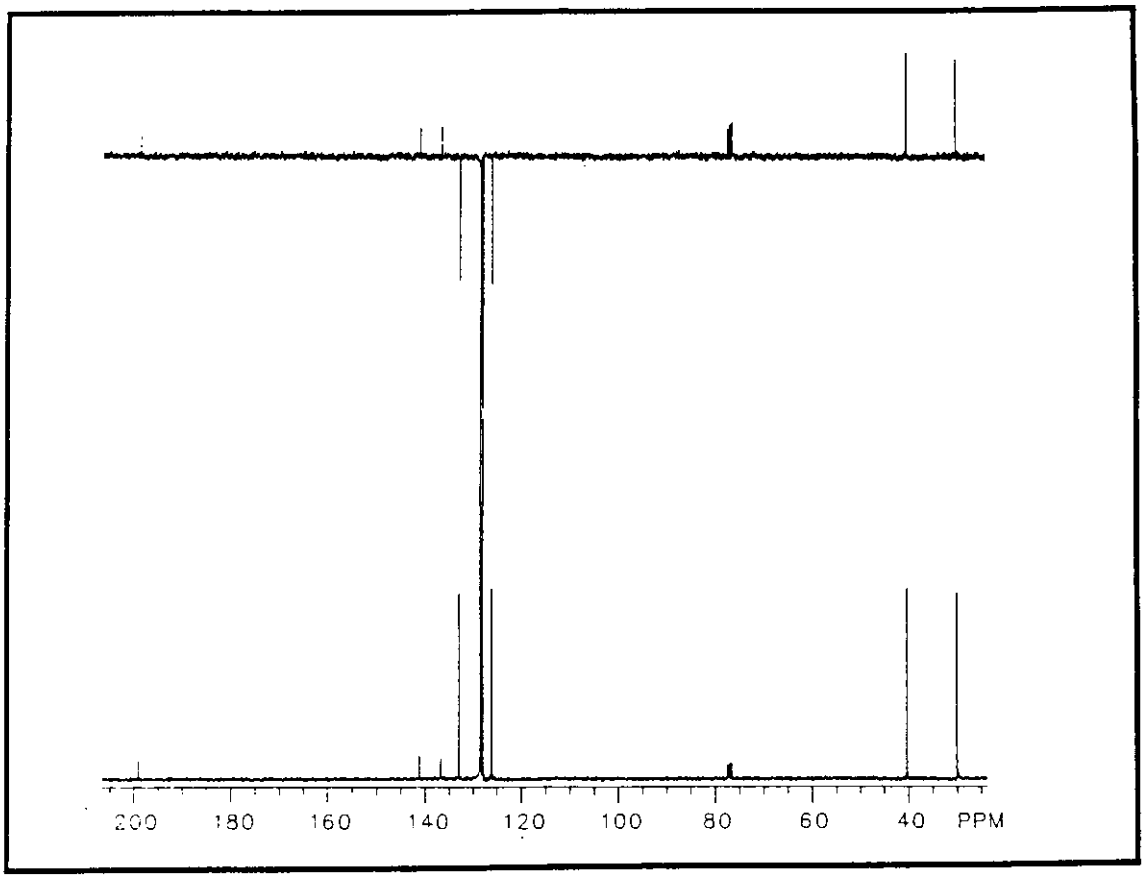
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis:

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
37	0.04	61	0.04	79	4.48	105	100.00	151	0.20	189	0.42
38	0.50	62	0.83	80	0.23	106	8.23	152	0.83	190	0.16
39	2.85	63	2.61	86	0.14	107	0.76	153	0.29	191	1.69
40	0.05	64	0.63	87	0.17	115	1.19	164	0.04	192	2.27
41	0.27	65	4.67	89	1.69	116	0.13	165	1.59	193	0.52
42	0.10	66	0.34	90	0.55	118	0.27	166	0.64	194	0.39
49	0.10	73	0.11	91	10.58	119	0.20	167	0.75	195	0.60
50	4.88	74	1.78	92	1.03	126	0.04	176	0.08	209	3.26
51	13.97	75	1.65	101	0.09	128	0.08	177	0.05	210	54.28
52	1.81	76	2.72	102	1.23	131	2.39	178	0.71	211	9.01
53	0.71	77	47.85	103	5.84	132	0.96	179	0.37	212	0.81
55	0.76	78	7.52	104	6.71	133	0.71	181	1.22		

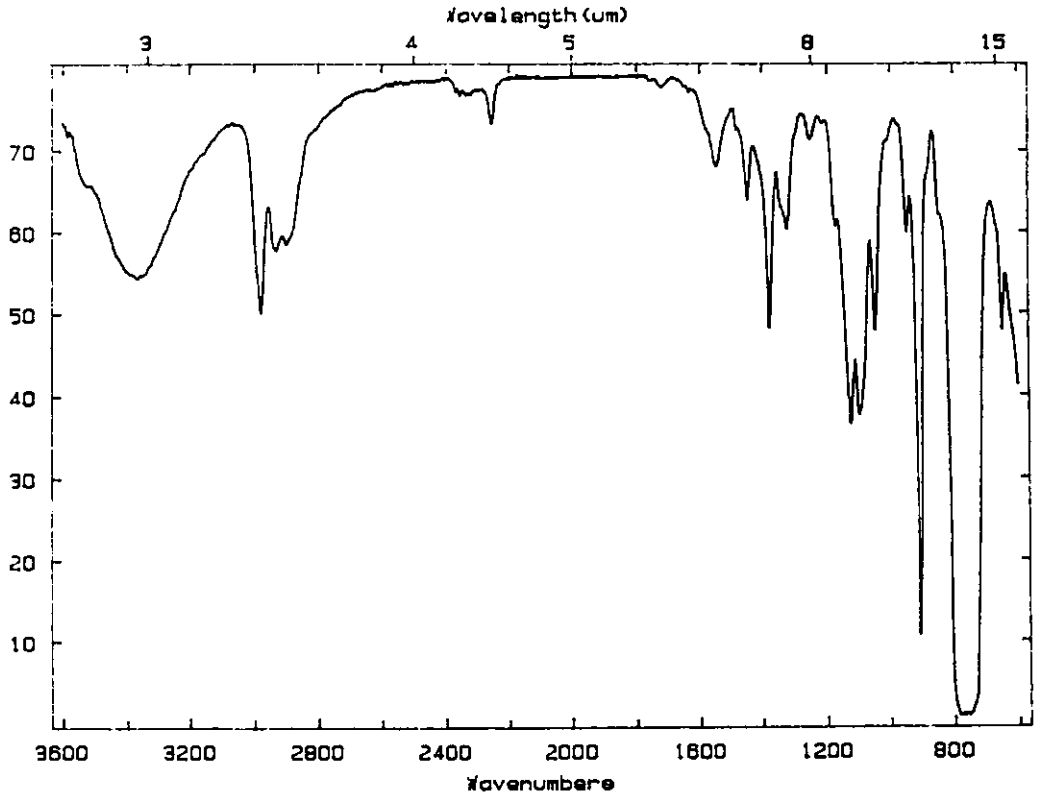


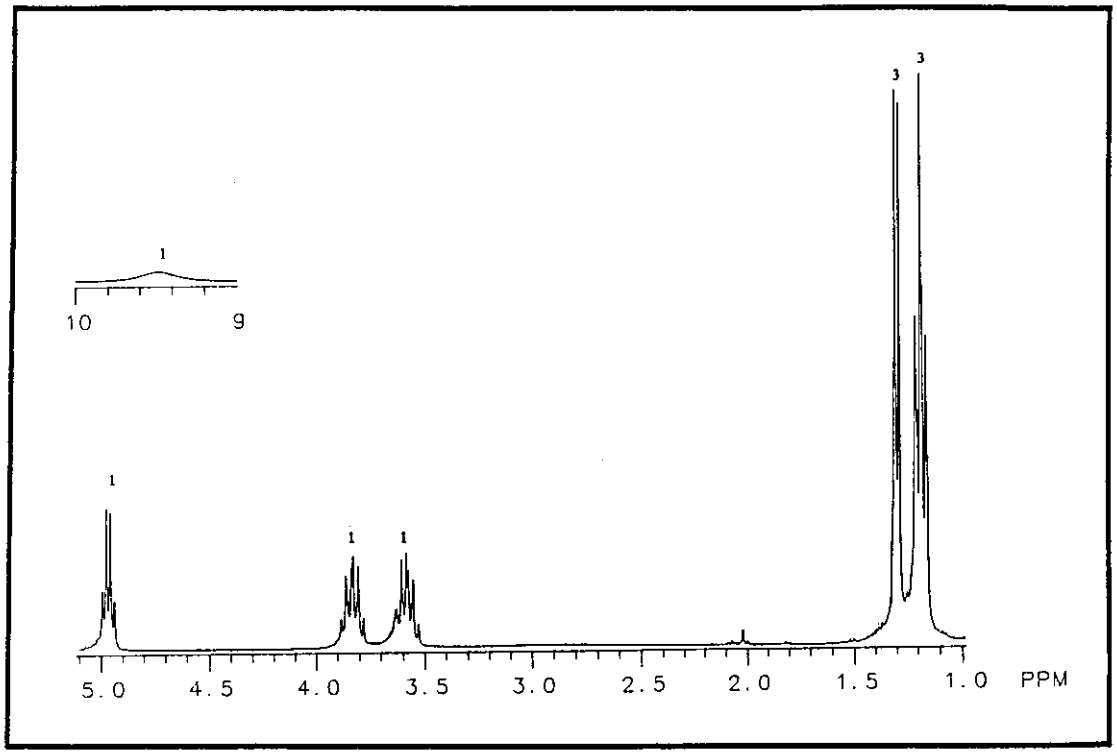

8
7
6
5
4
3
PPM

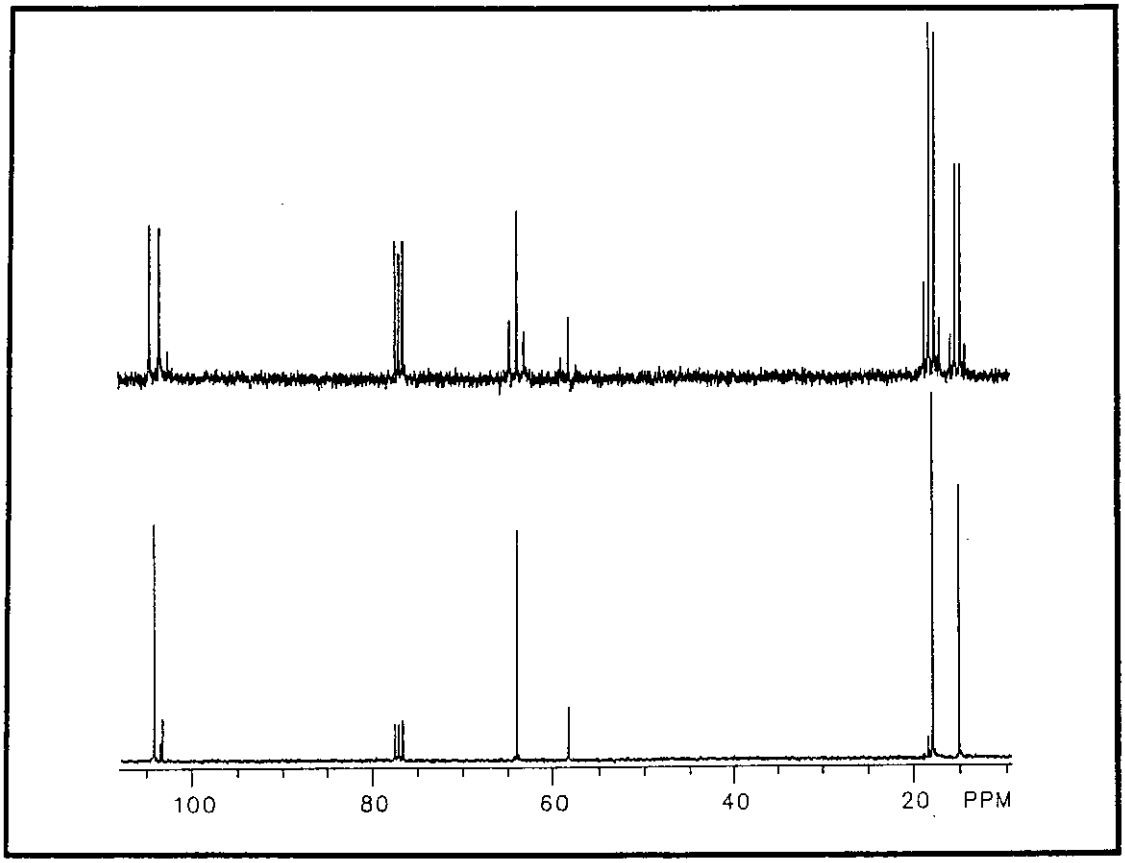

200
180
160
140
120
100
80
60
40
PPM

Problem 50

Exact Mass: 106.06
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: 45.2% C; 9.5% H
Comments: no mass spectra obtained; product decomposes violently upon heating




1
10
9
1
1
1
3
3
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
PPM

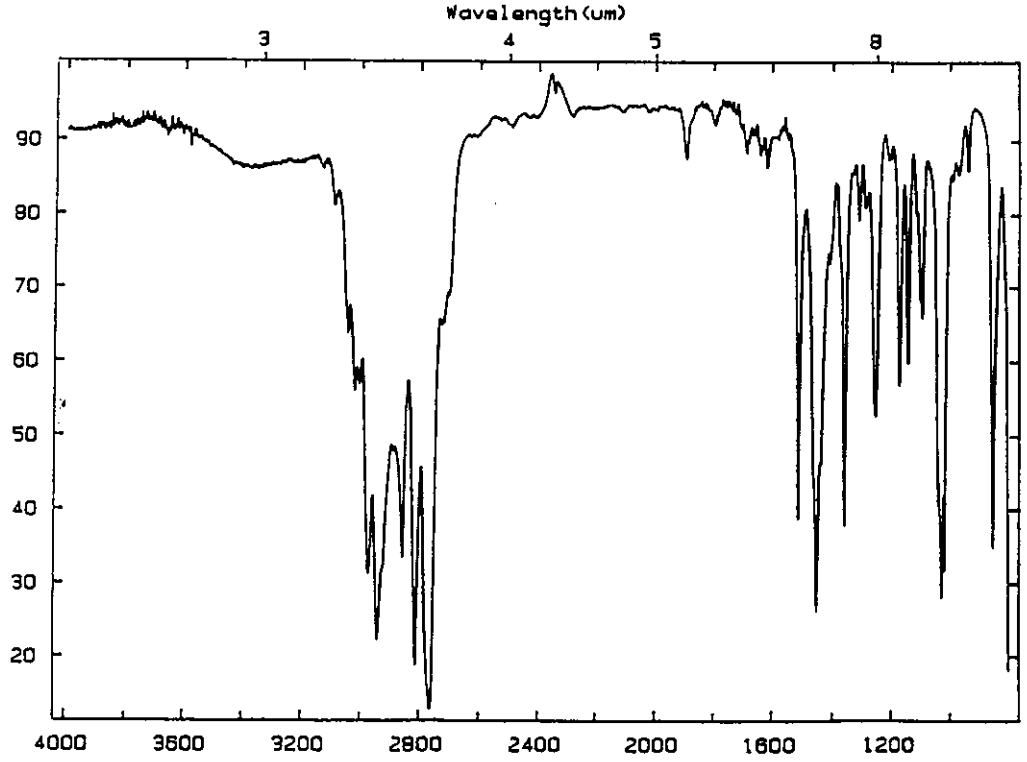

100
80
60
40
20
PPM

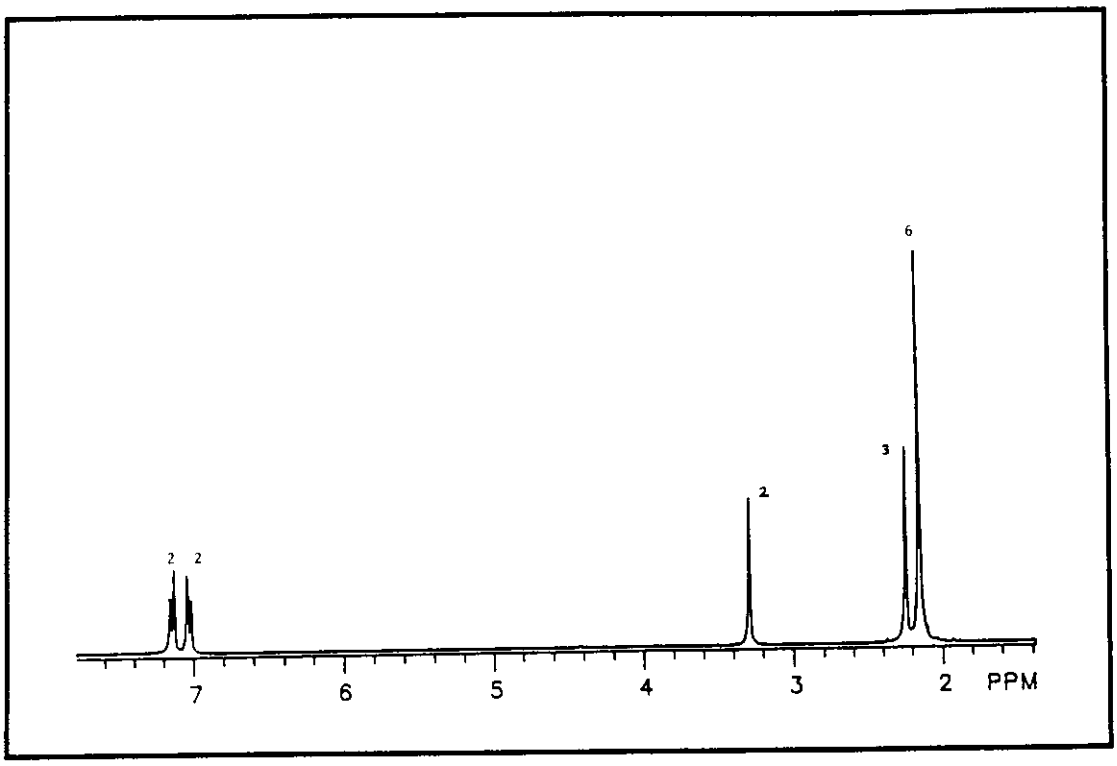
Problem 51

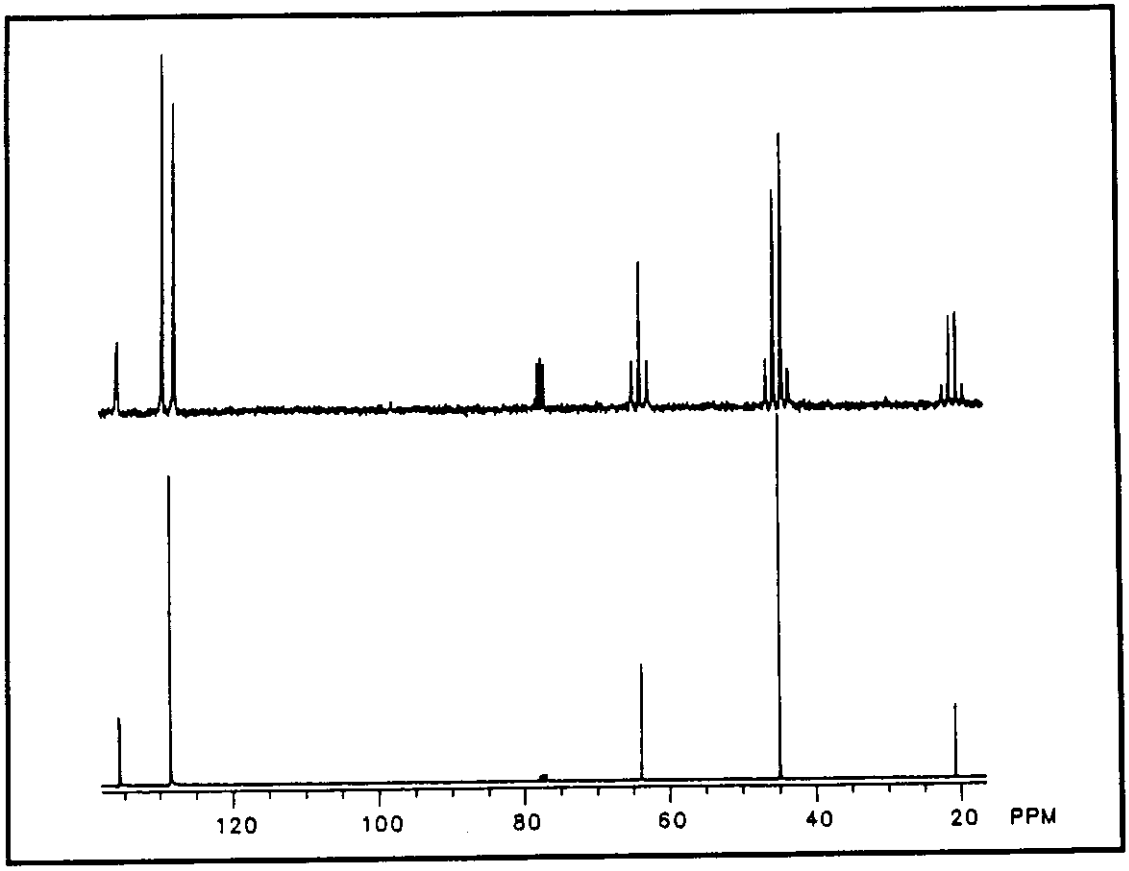
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
30	4.55	53	6.56	66	2.27	86	1.01	110	1.55	146	1.87
38	2.21	54	0.61	74	4.03	87	0.75	116	2.90	147	0.77
39	18.91	55	5.43	75	2.22	89	10.58	117	2.16	148	72.14
40	4.43	56	2.06	76	3.71	90	4.45	118	3.96	149	82.95
41	8.71	57	5.96	77	42.40	91	26.97	130	1.96	150	8.64
42	48.46	58	68.09	78	18.68	92	1.81	131	1.68		
43	13.45	59	5.07	79	26.16	98	1.09	132	9.39		
44	10.17	62	5.19	80	1.28	102	4.48	133	1.34		
50	9.85	63	15.78	82	3.32	103	22.56	134	10.43		
52	7.25	65	20.38	84	1.44	105	100.00	135	0.63		




6
3
2
2 2
7
6
5
4
3
2
PPM

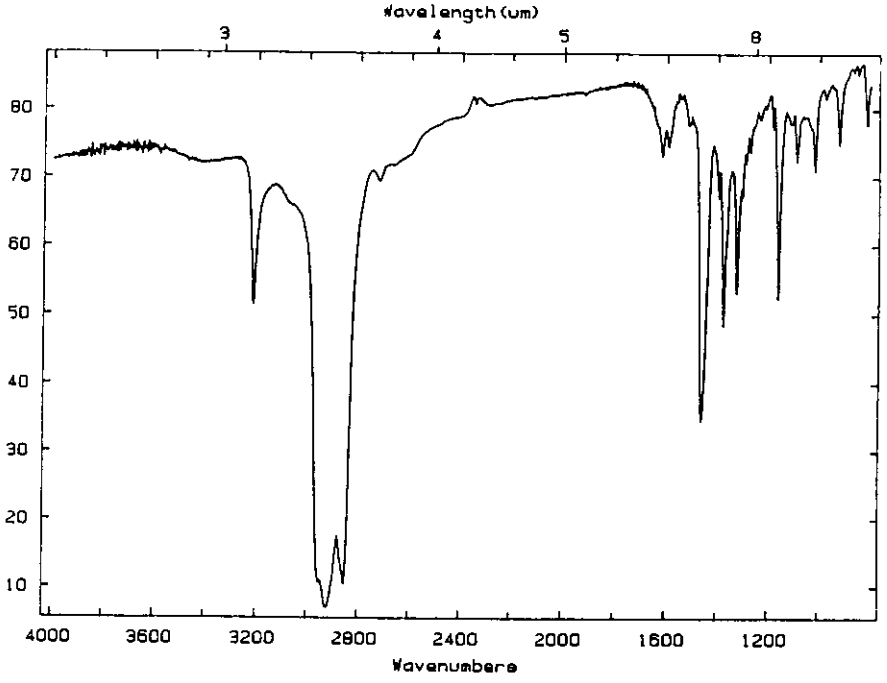

120
100
80
60
40
20
PPM

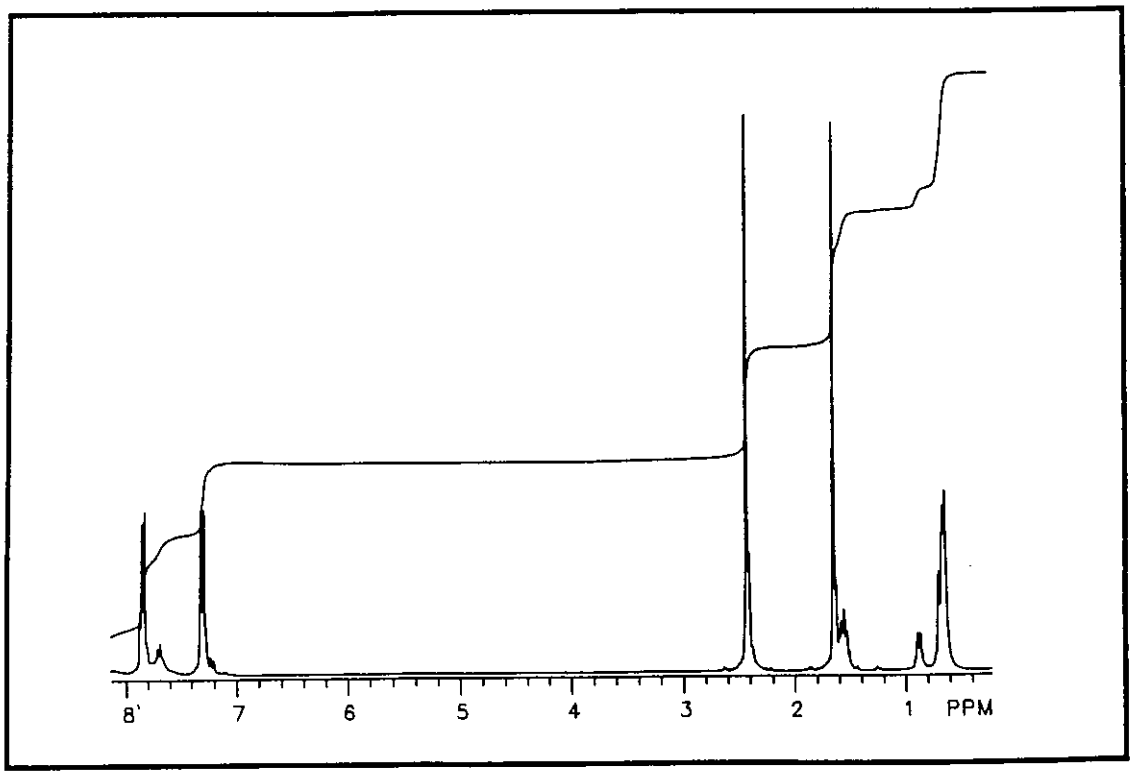
Problem 52

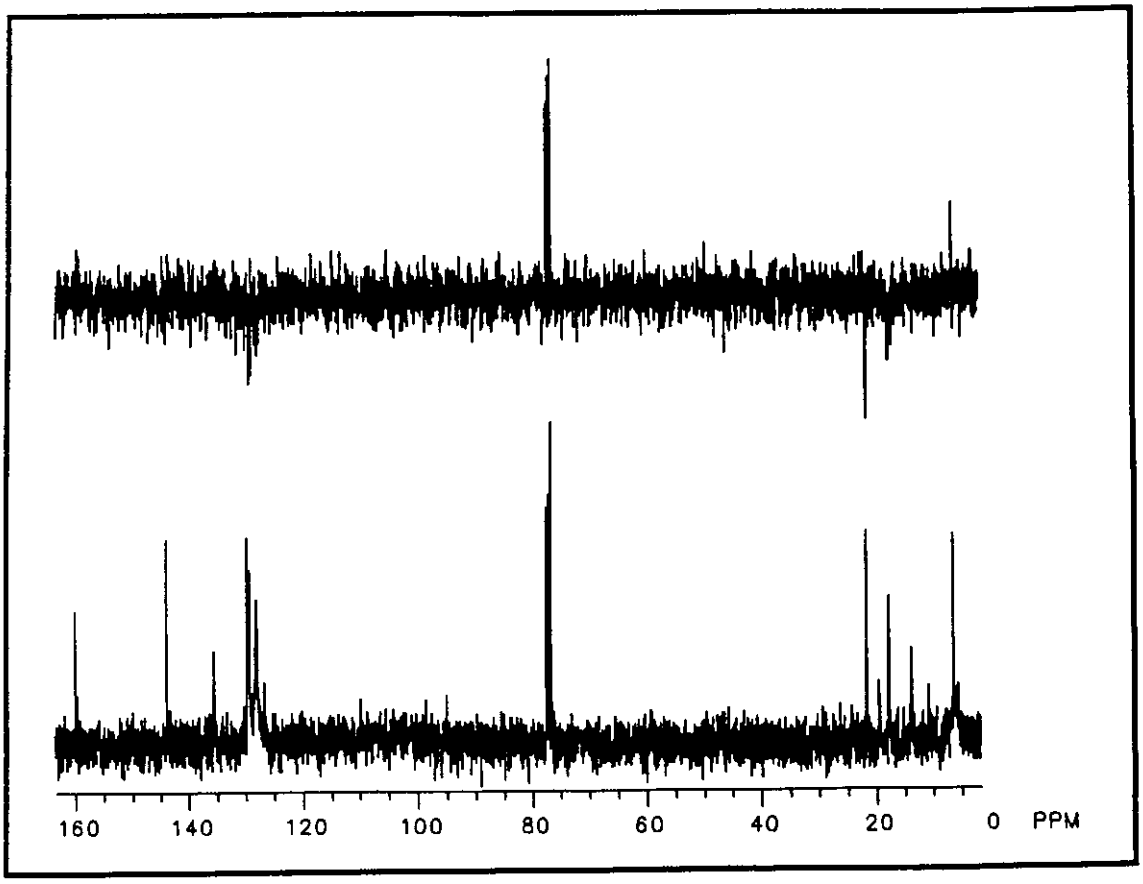
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z	
30	5.38	57	4.96	82	21.68	141	0.68
39	23.91	63	7.43	89	9.30	155	4.19
40	5.74	64	2.19	90	3.60	157	71.55
41	23.47	65	32.10	91	54.62	158	7.00
42	15.55	66	2.73	92	16.29	159	1.65
43	1.76	67	48.57	93	5.19	252	23.33
50	0.78	68	36.15	95	3.26	253	1.56
51	4.96	69	5.89	96	13.46		
52	1.30	70	10.42	97	100.00		
53	18.56	77	4.66	98	5.22		
54	1.90	80	15.45	139	20.61		
56	30.01	81	5.44	140	14.45		




8
7
6
5
4
3
2
1
PPM

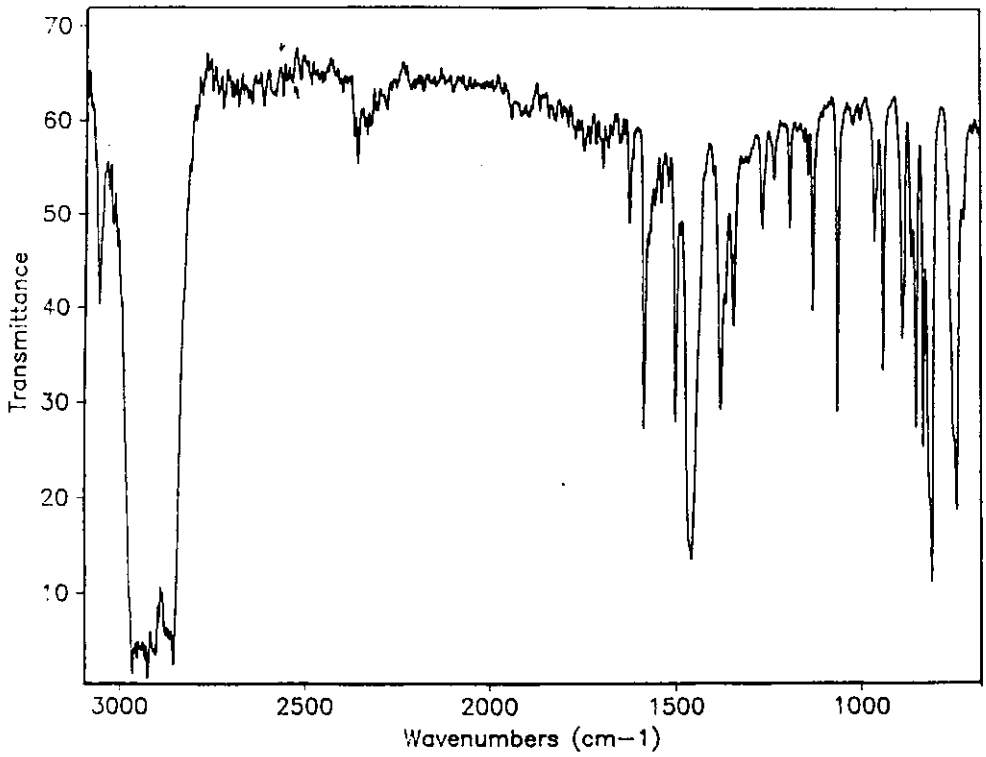

160
140
120
100
80
60
40
20
0
PPM

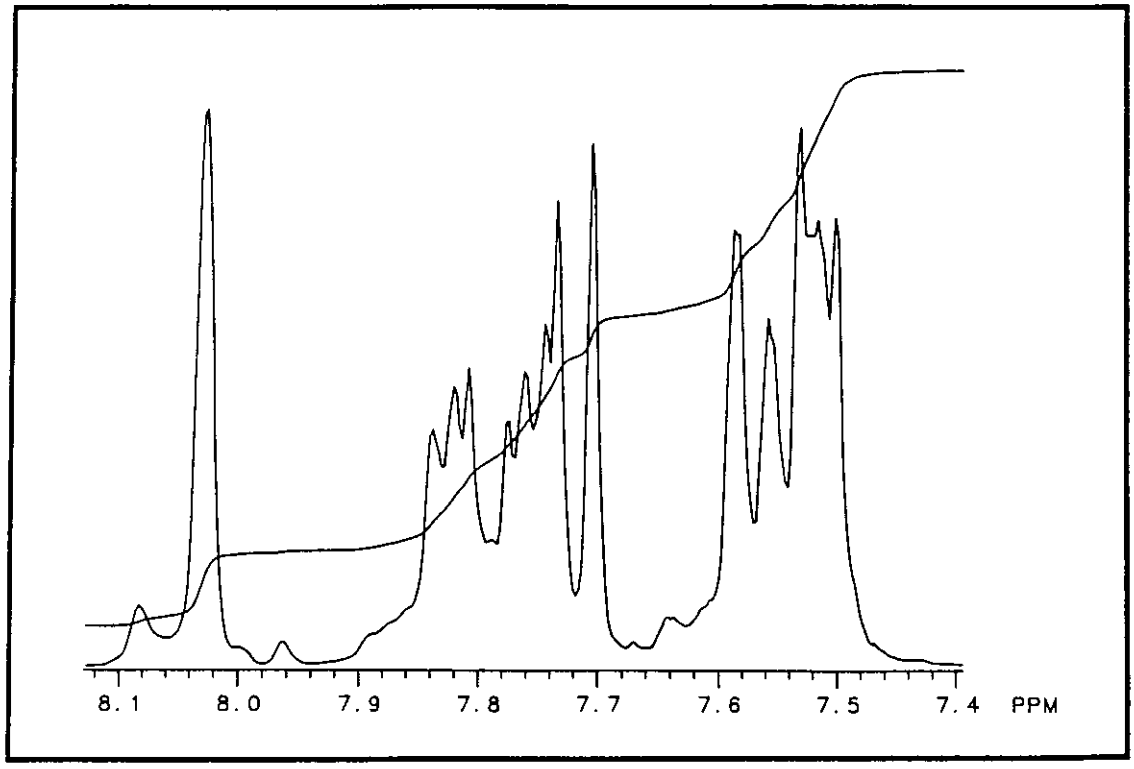
Problem 53

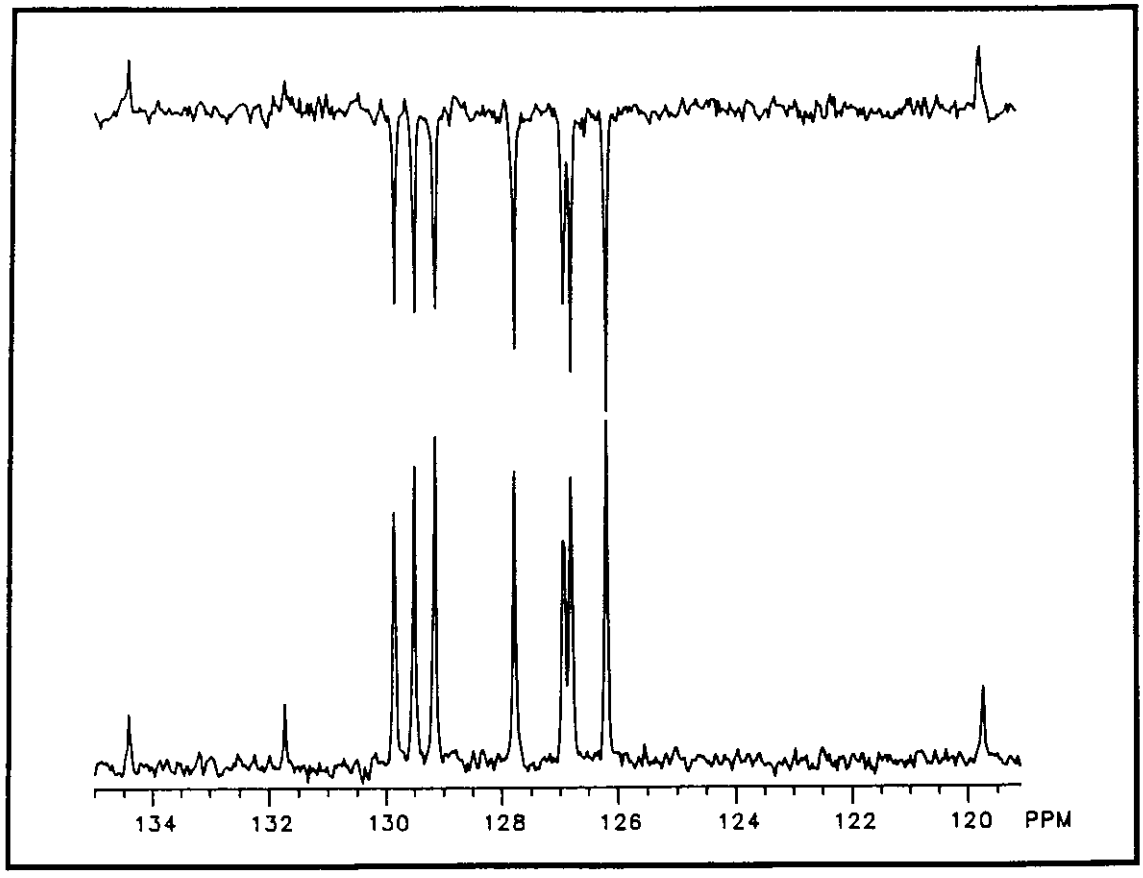
Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z	
38	0.60	76	3.03	99	2.08	127	64.92
50	2.82	77	6.00	100	1.90	128	7.01
51	2.43	79	0.83	101	5.32	206	100.00
61	1.66	85	1.20	103	4.37	207	11.30
62	2.75	86	1.82	104	3.63	208	96.52
63	6.92	87	2.60	122	0.49	209	10.70
74	6.42	91	0.43	125	1.62		
75	6.03	98	2.92	126	18.39		




8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
PPM

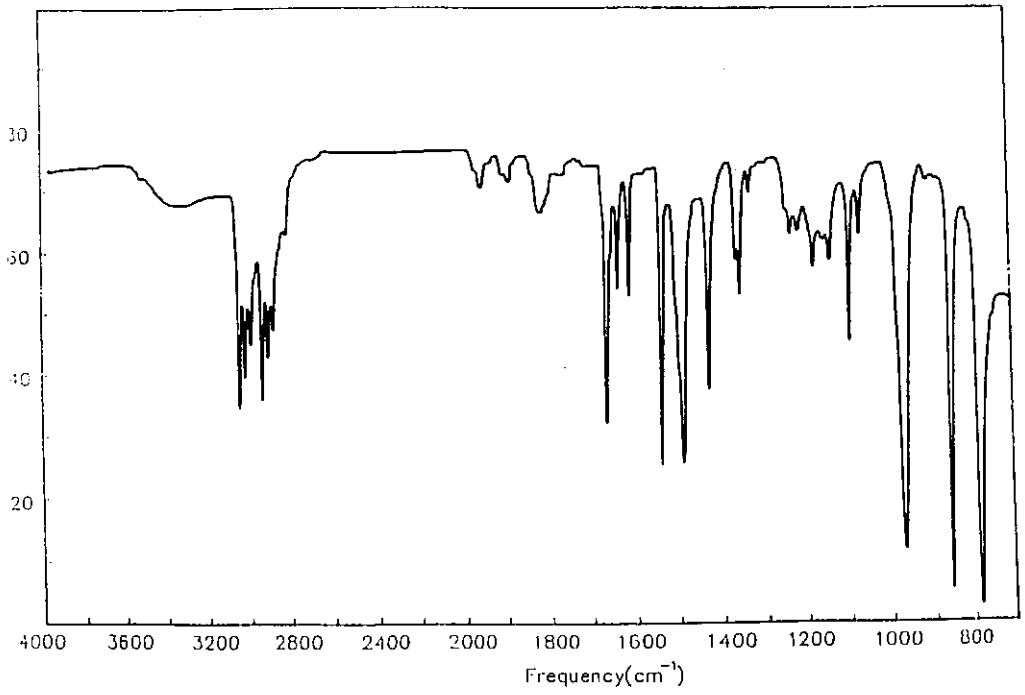

134
132
130
128
126
124
122
120
PPM

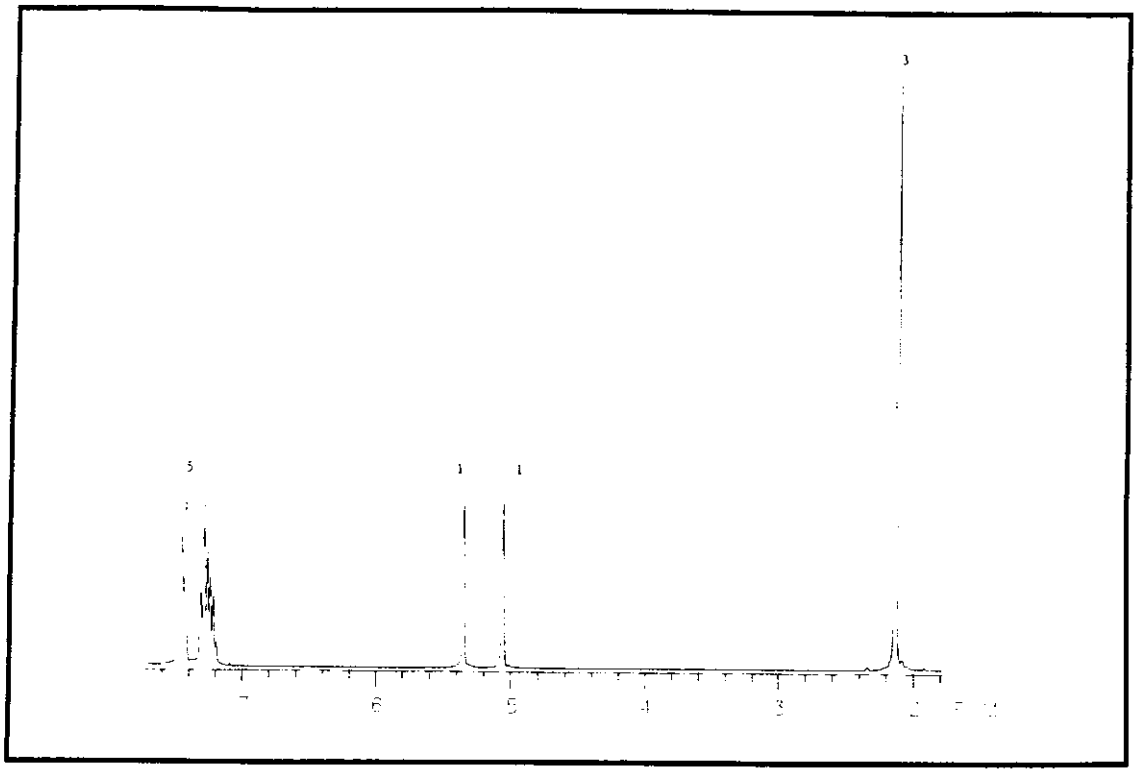
Problem 54

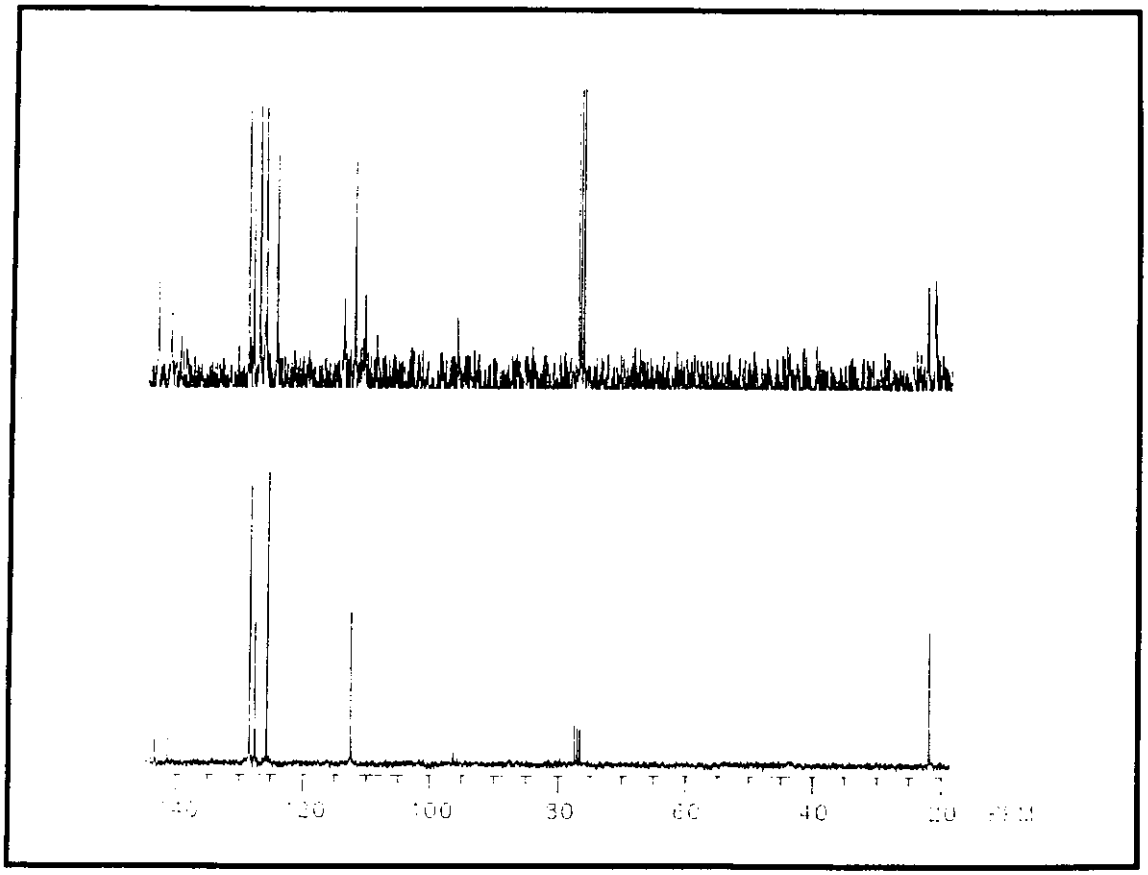
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z		m/z		m/z		m/z		m/z	
31	0.03	43	0.31	53	1.74	65	8.46	92	2.15	104	4.76
32	0.04	44	0.12	54	0.12	66	0.86	93	0.10	105	0.25
36	0.15	45	0.12	55	0.26	67	0.07	97	0.13	113	0.54
37	2.30	46	0.03	58	7.78	72	0.07	98	0.56	115	29.57
38	5.07	48	0.10	60	0.20	73	1.08	99	0.19	116	6.40
39	22.86	49	1.18	61	1.97	88	0.67	100	0.11	117	85.00
40	2.69	50	14.19	62	5.37	89	6.00	101	1.00	118	100.00
41	2.80	51	26.46	63	12.40	90	1.94	102	7.35	119	9.85
42	0.13	52	6.05	64	1.98	91	21.31	103	53.93	120	0.50

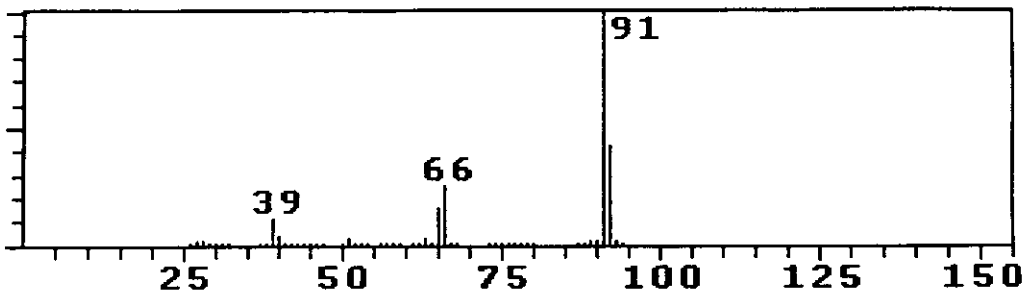


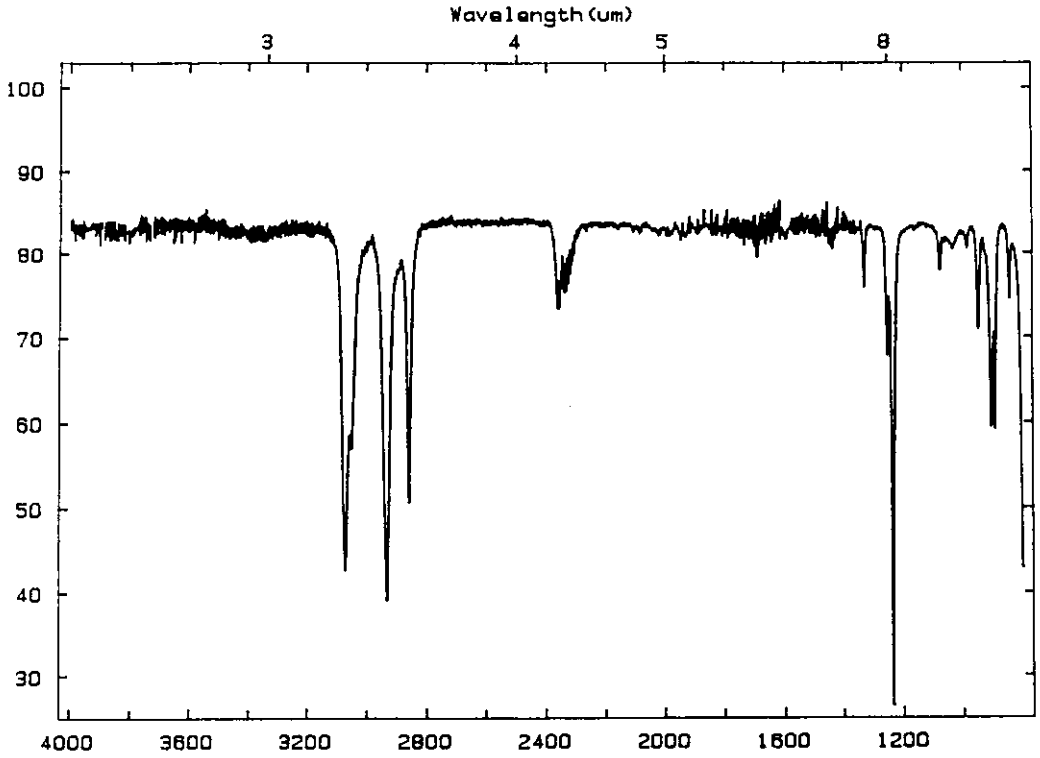

3
5
1
1
7
6
5
4
3

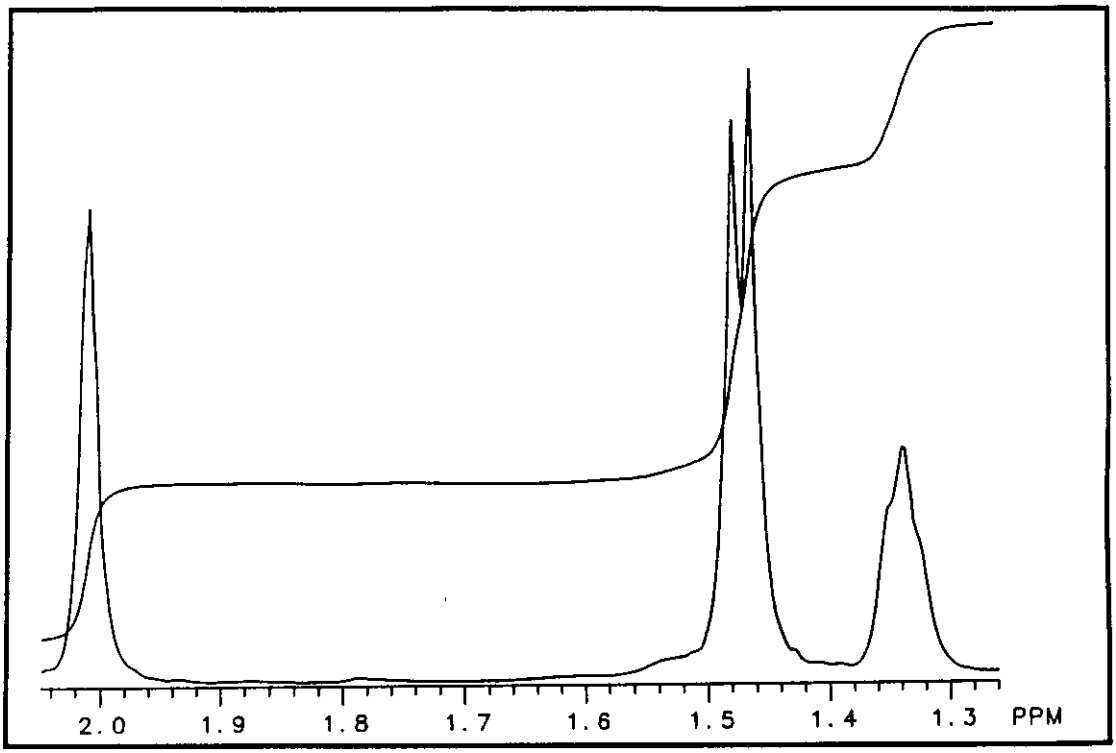

140
120
100
80
60
40
20

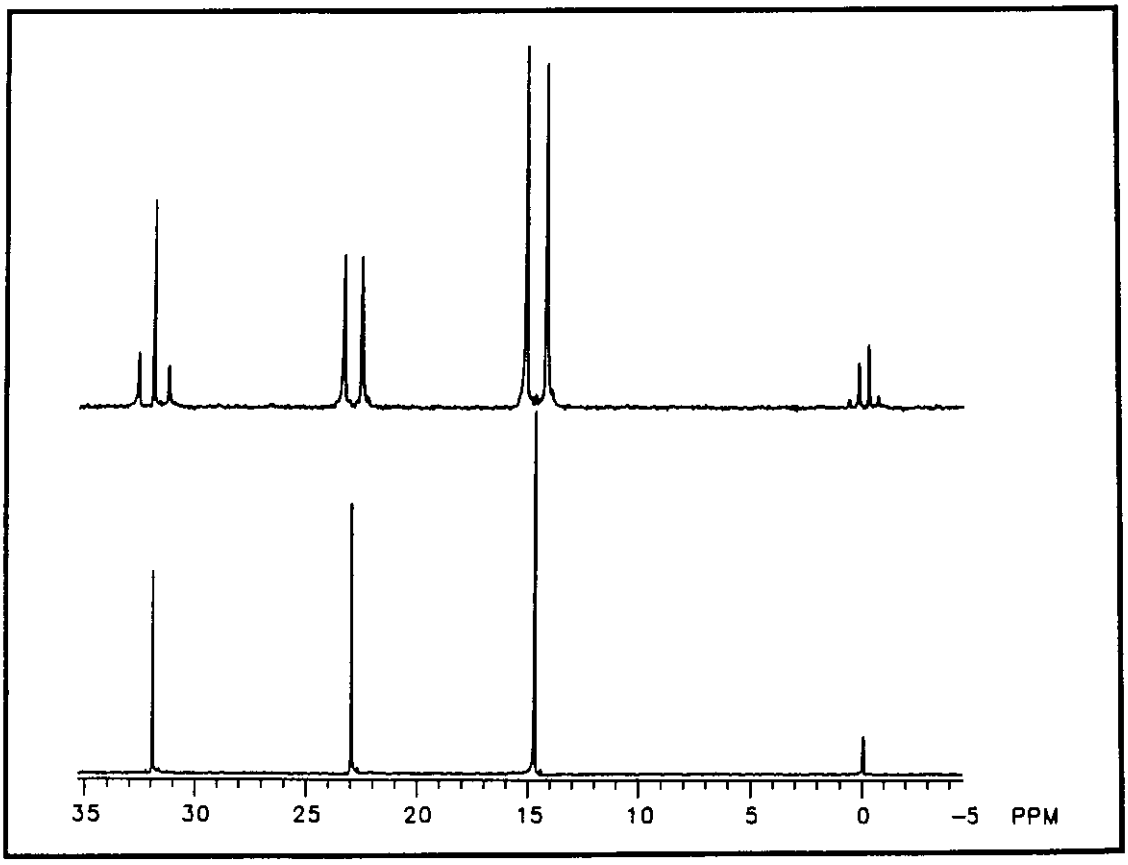
Problem 55

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



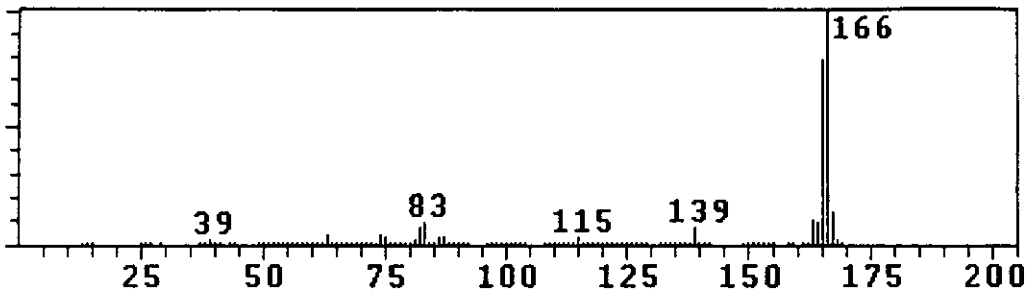


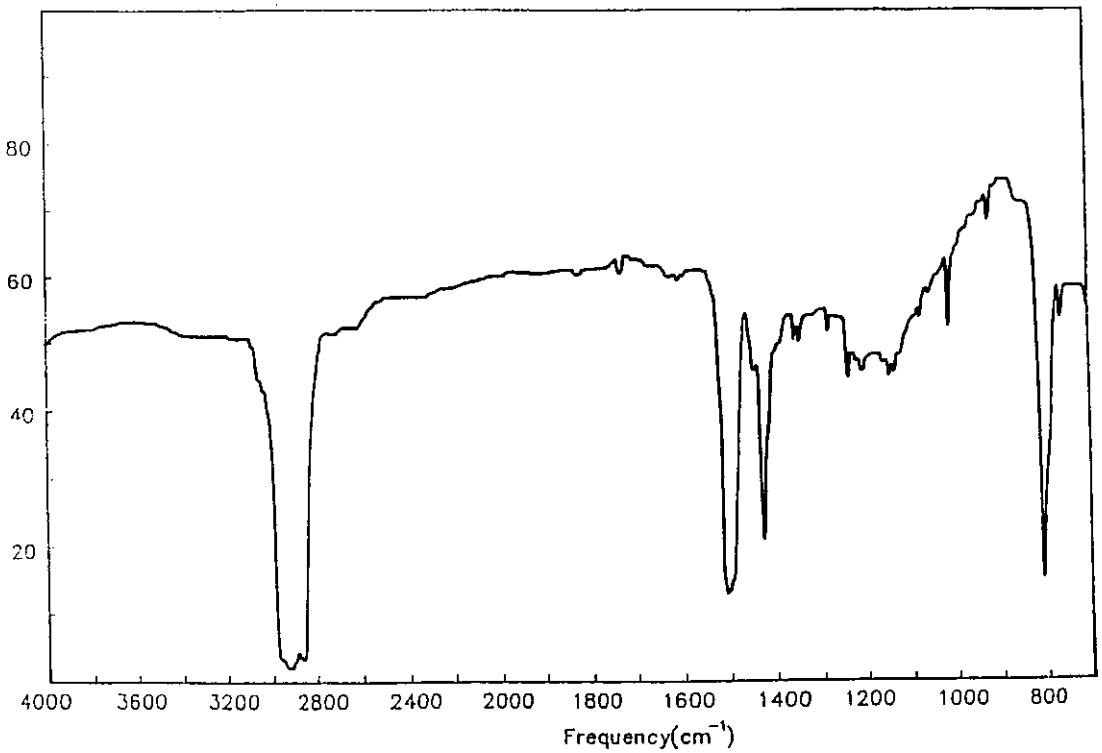

2.0
1.9
1.8
1.7
1.6
1.5
1.4
1.3
PPM

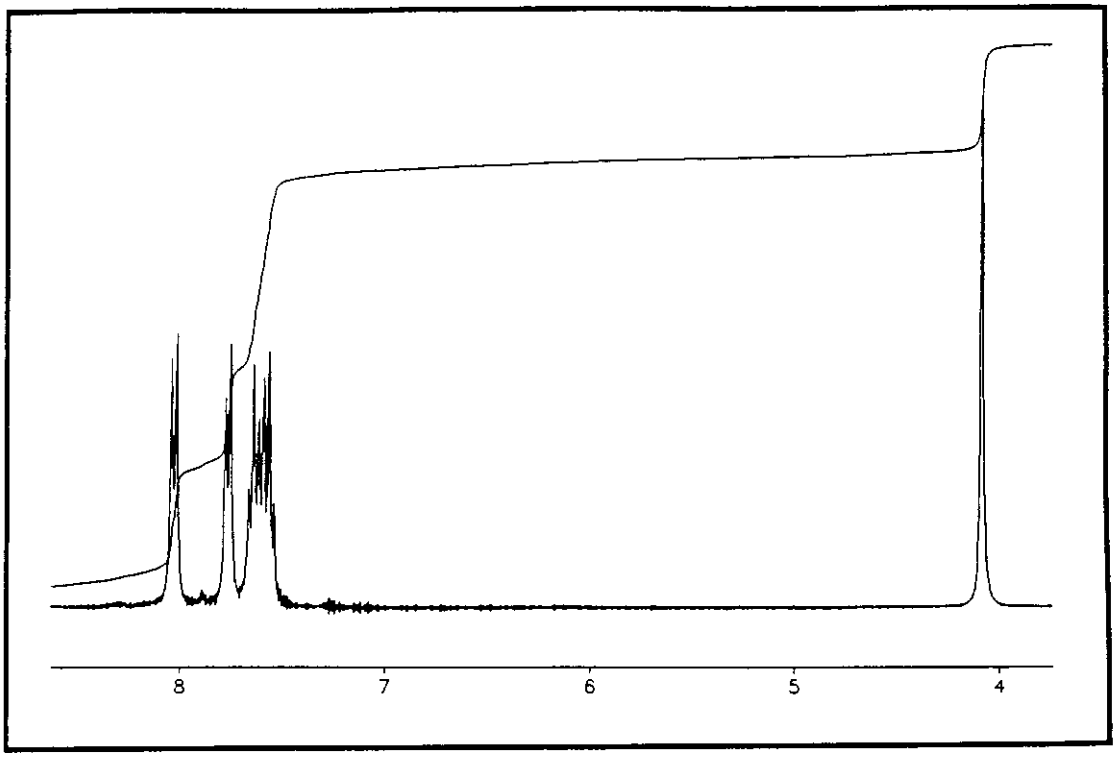

35
30
25
20
15
10
5
0
−5
PPM

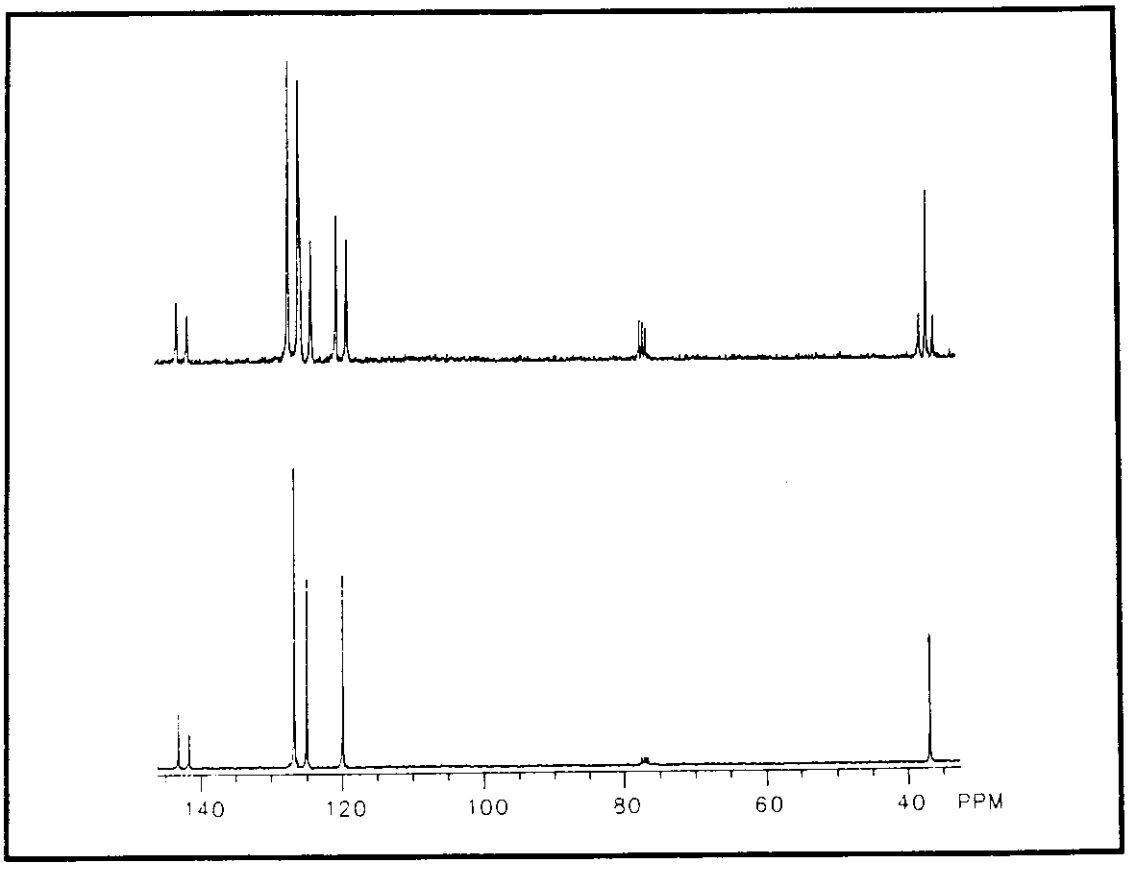
Problem 56

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



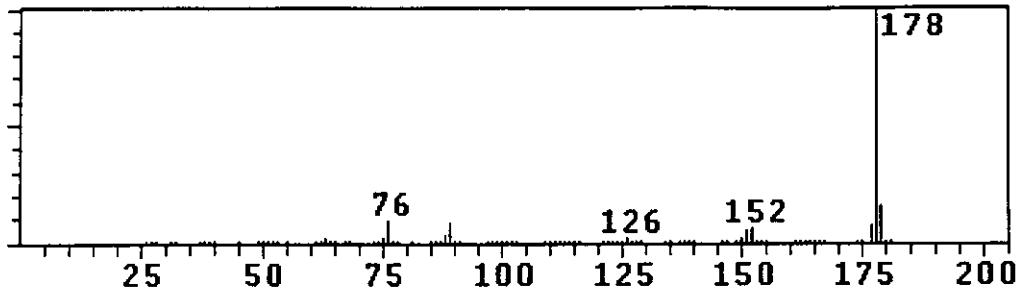


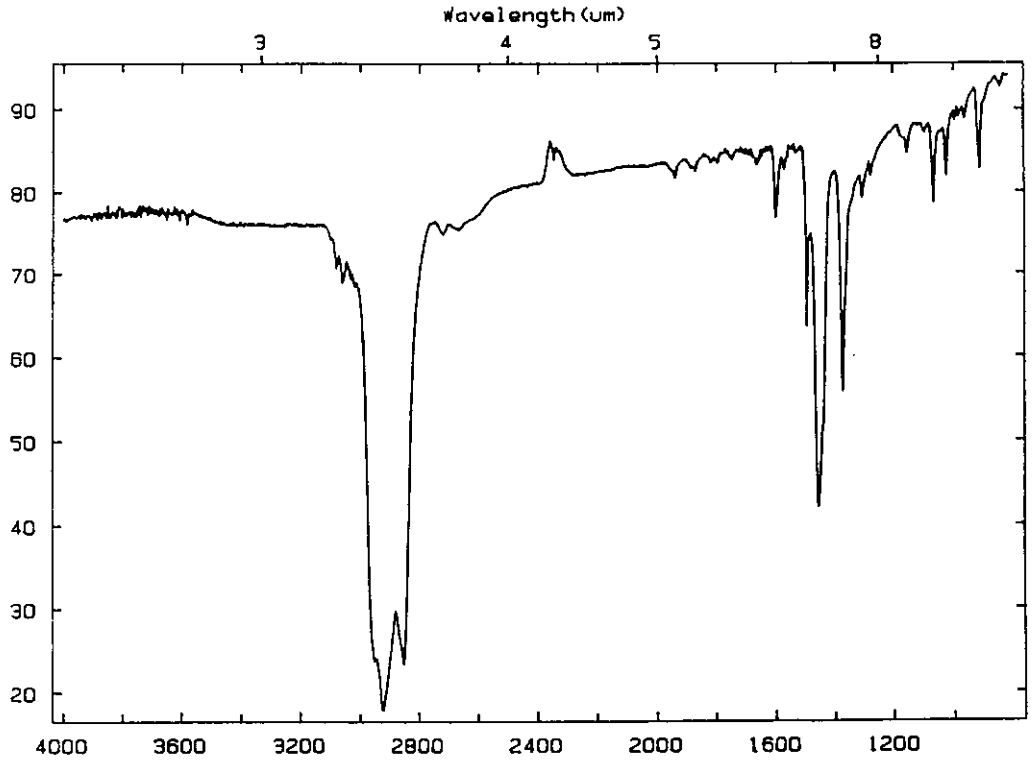

8
7
6
5
4

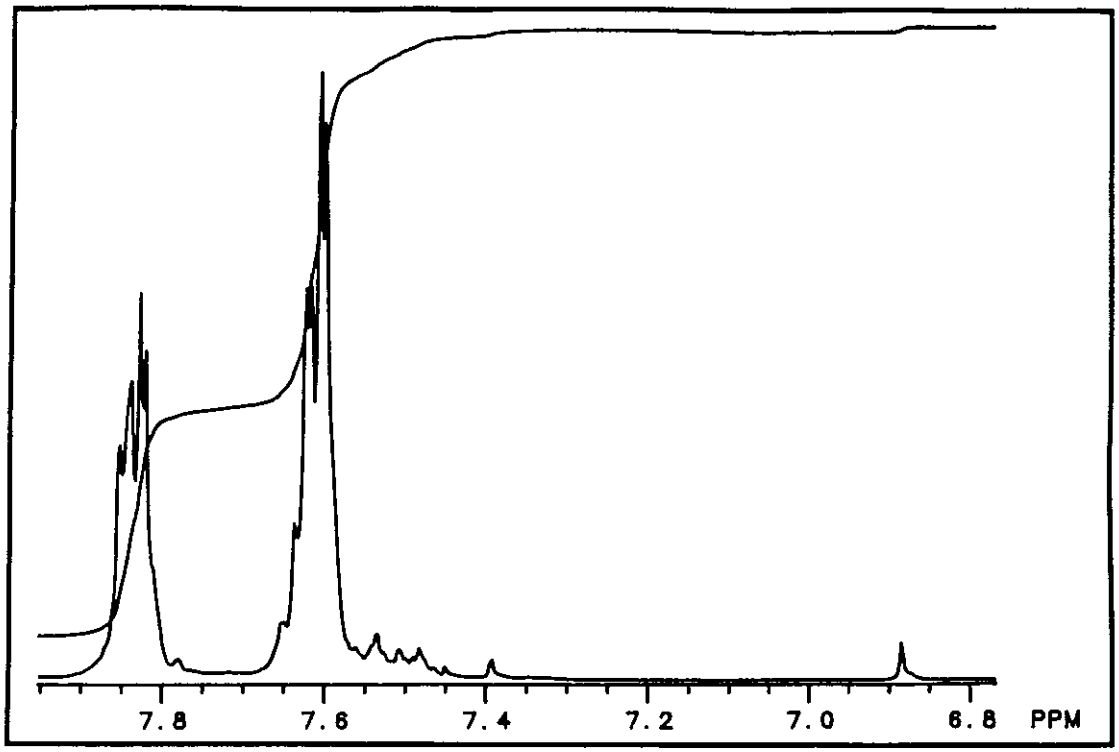

140
120
100
80
60
40
PPM

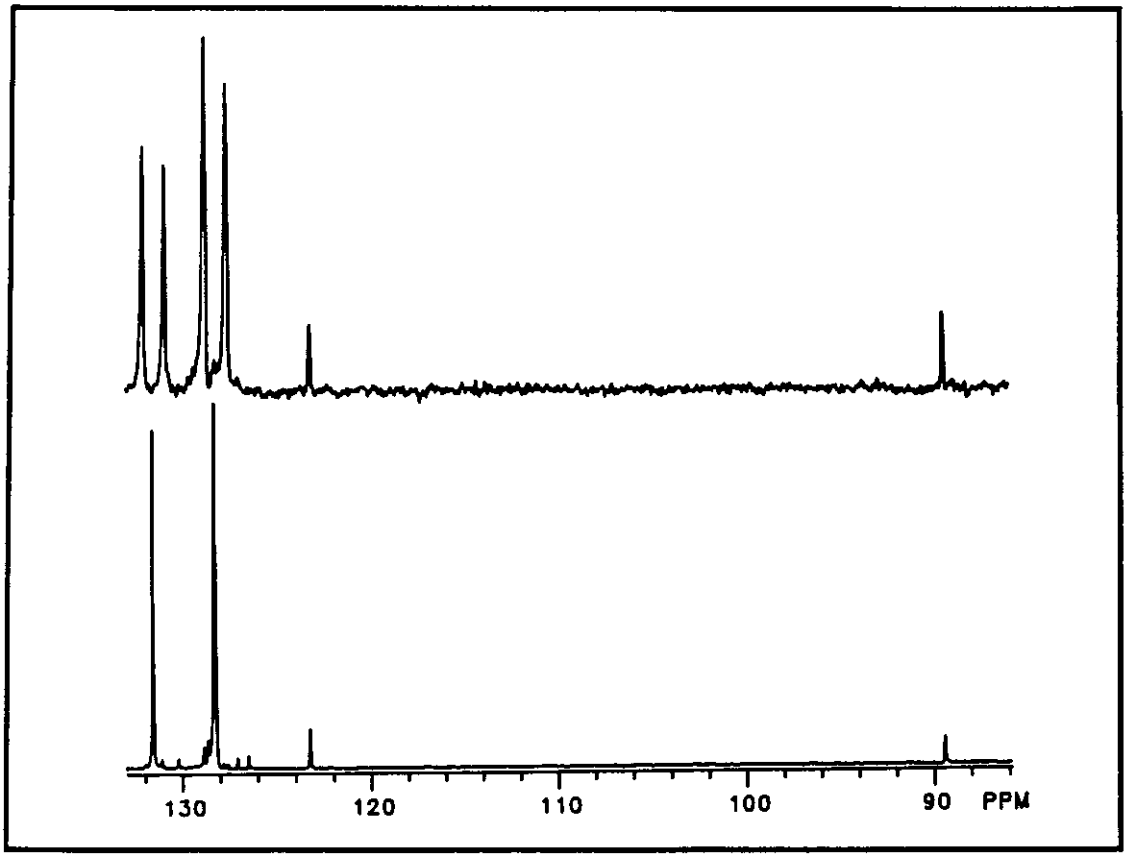
Problem 57

Exact Mass: na
IR: nujol
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



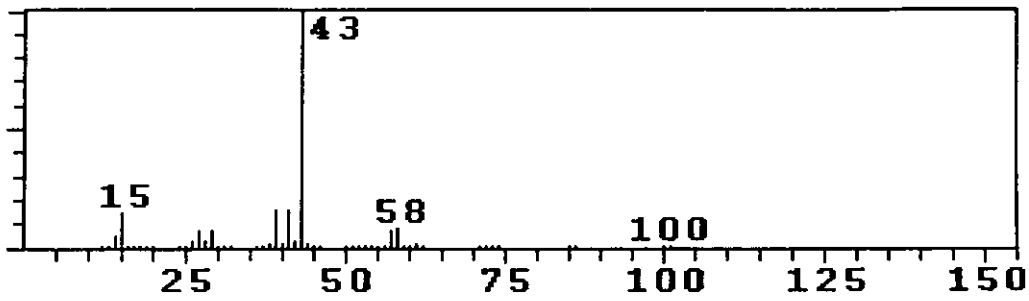


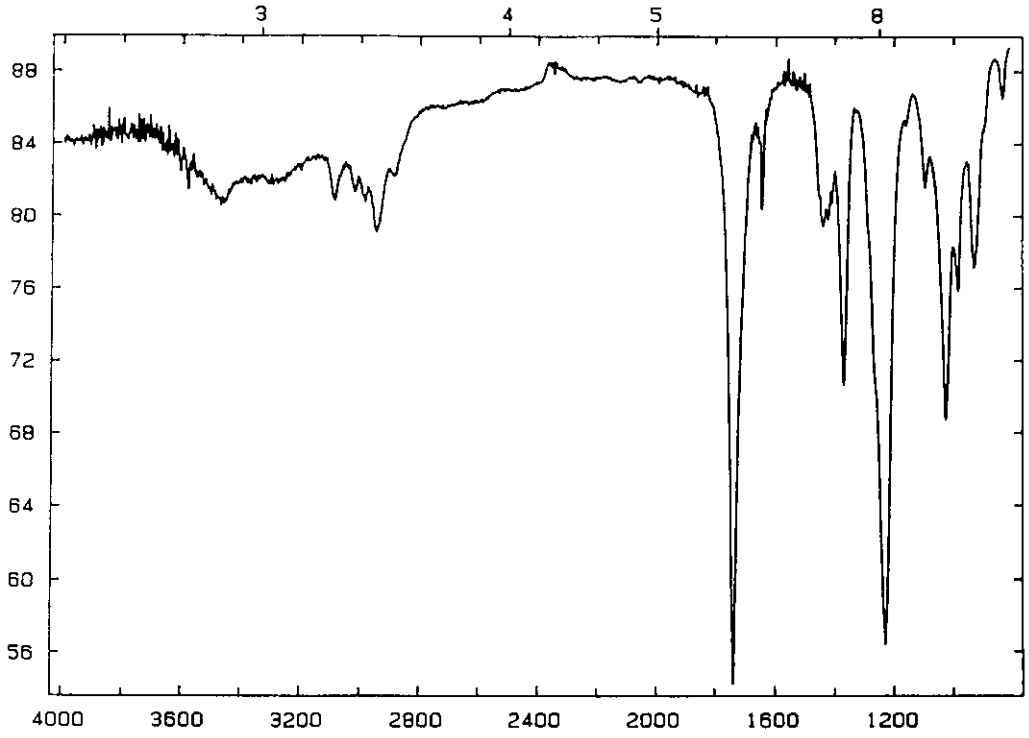

7.8
7.6
7.4
7.2
7.0
6.8
PPM

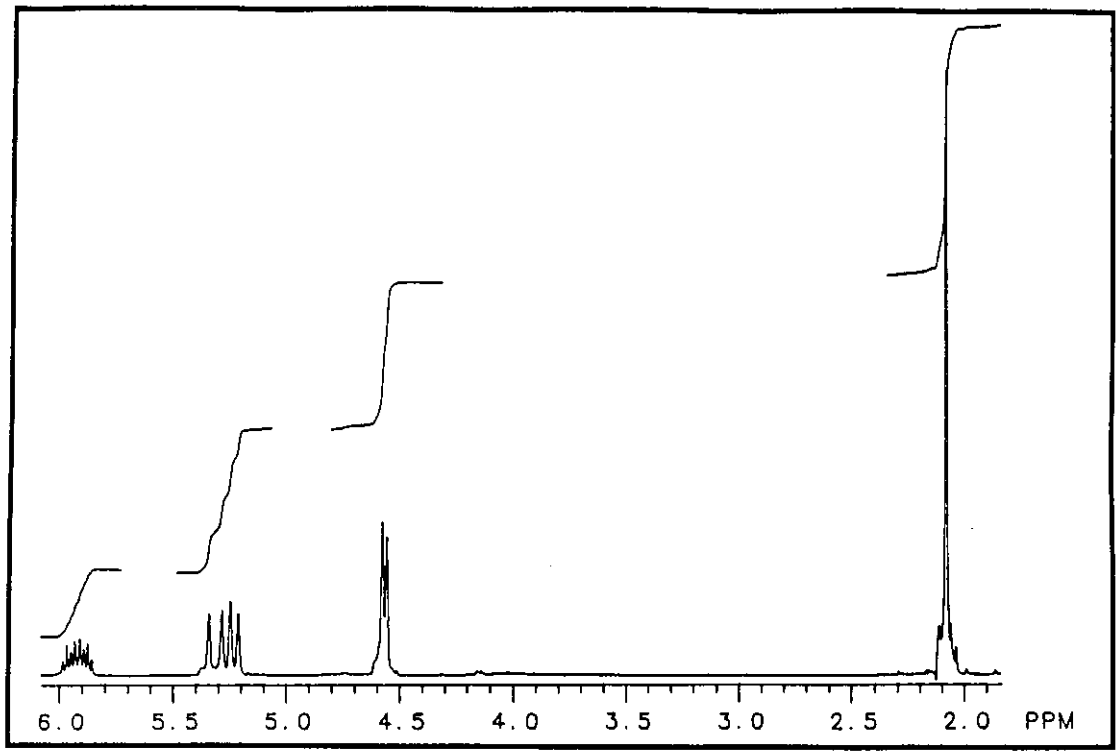

130
120
110
100
90
PPM

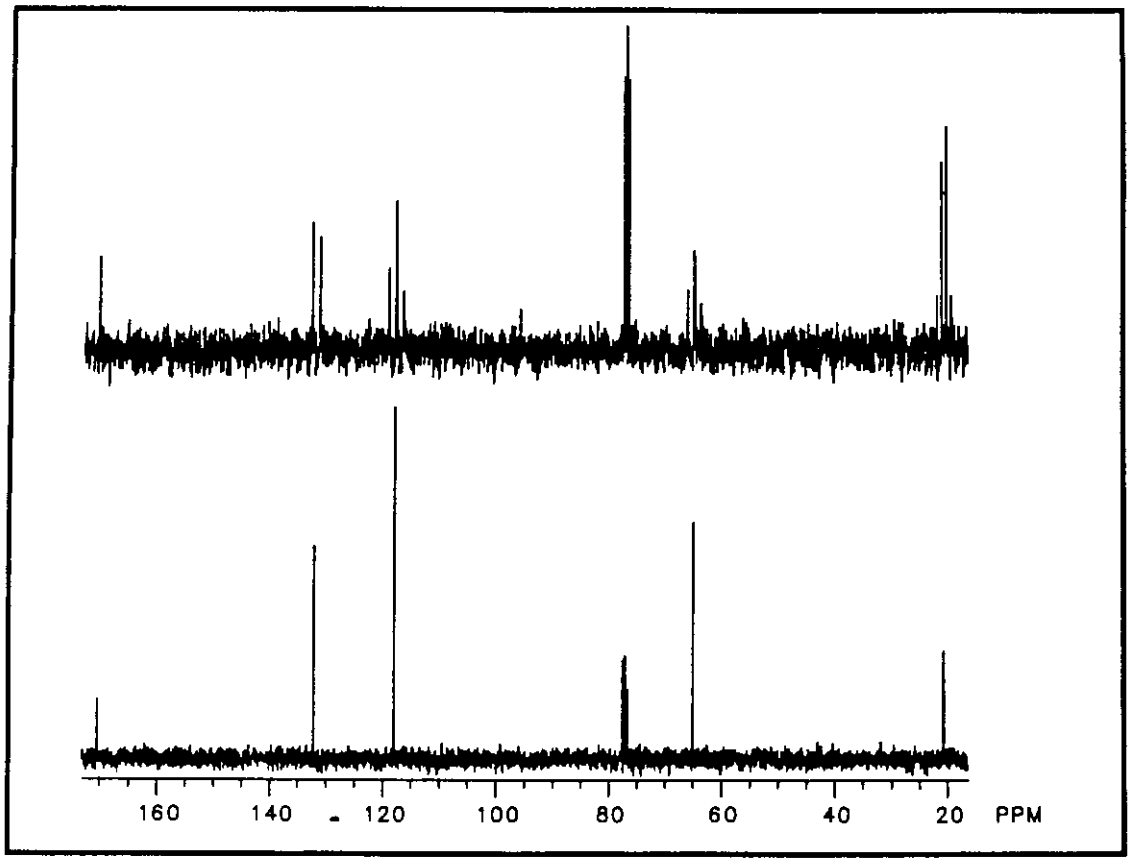
Problem 58

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na






6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
PPM

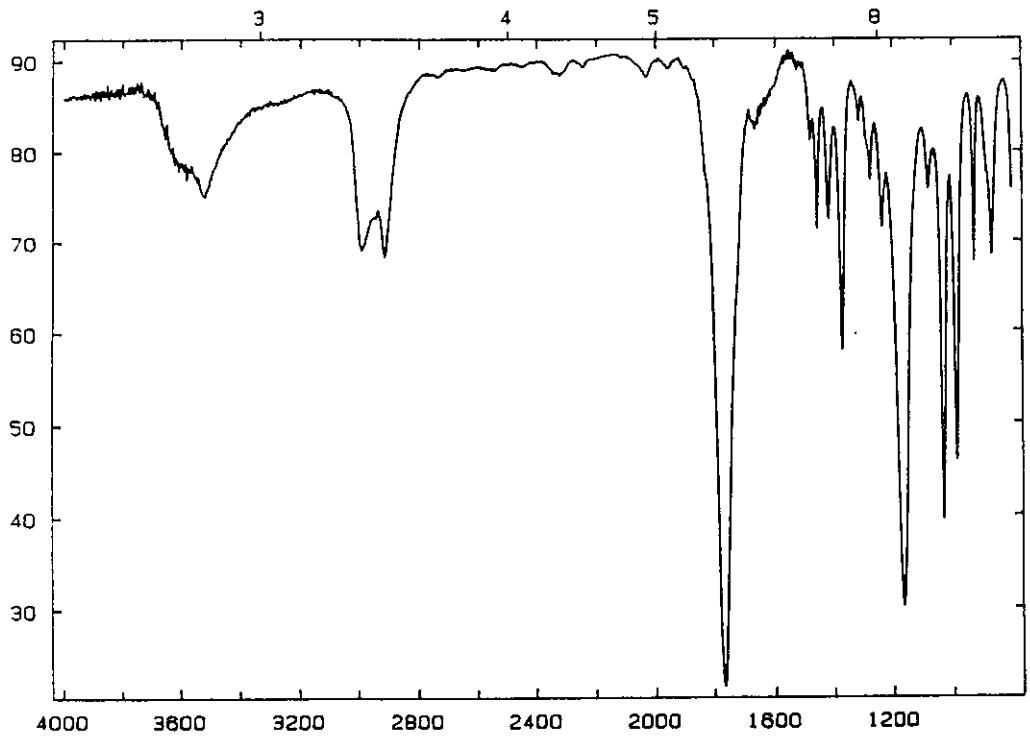

160
140
120
100
80
60
40
20
PPM

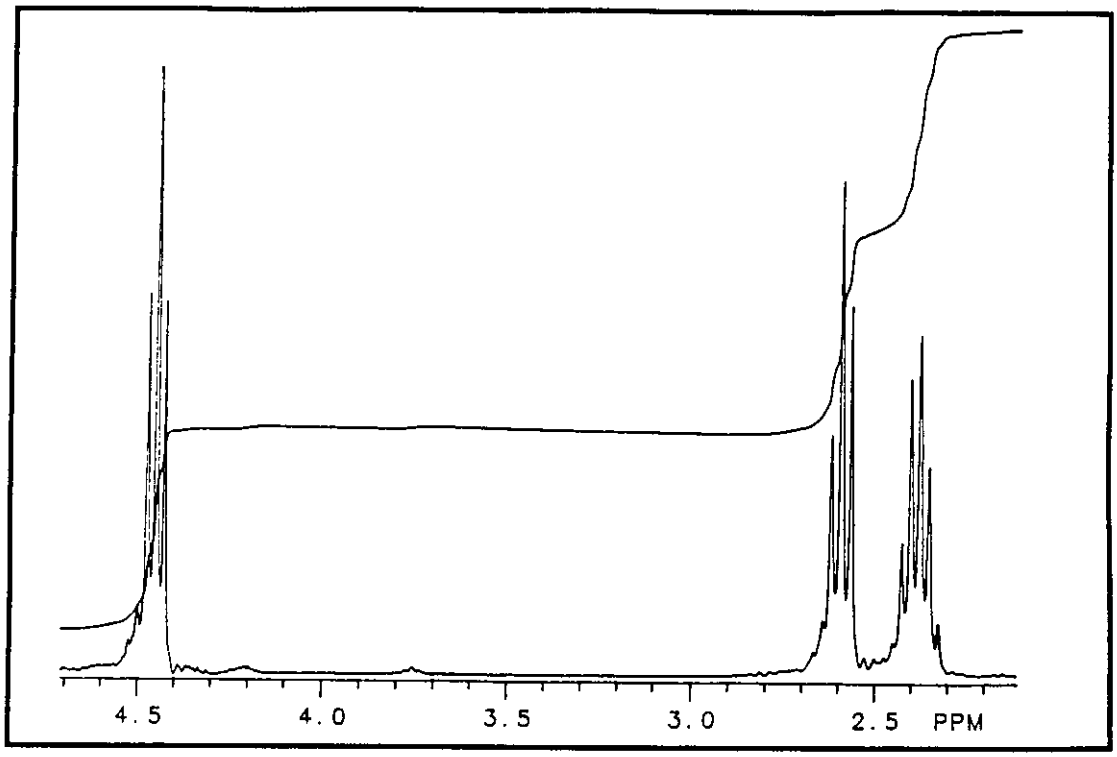
Problem 59

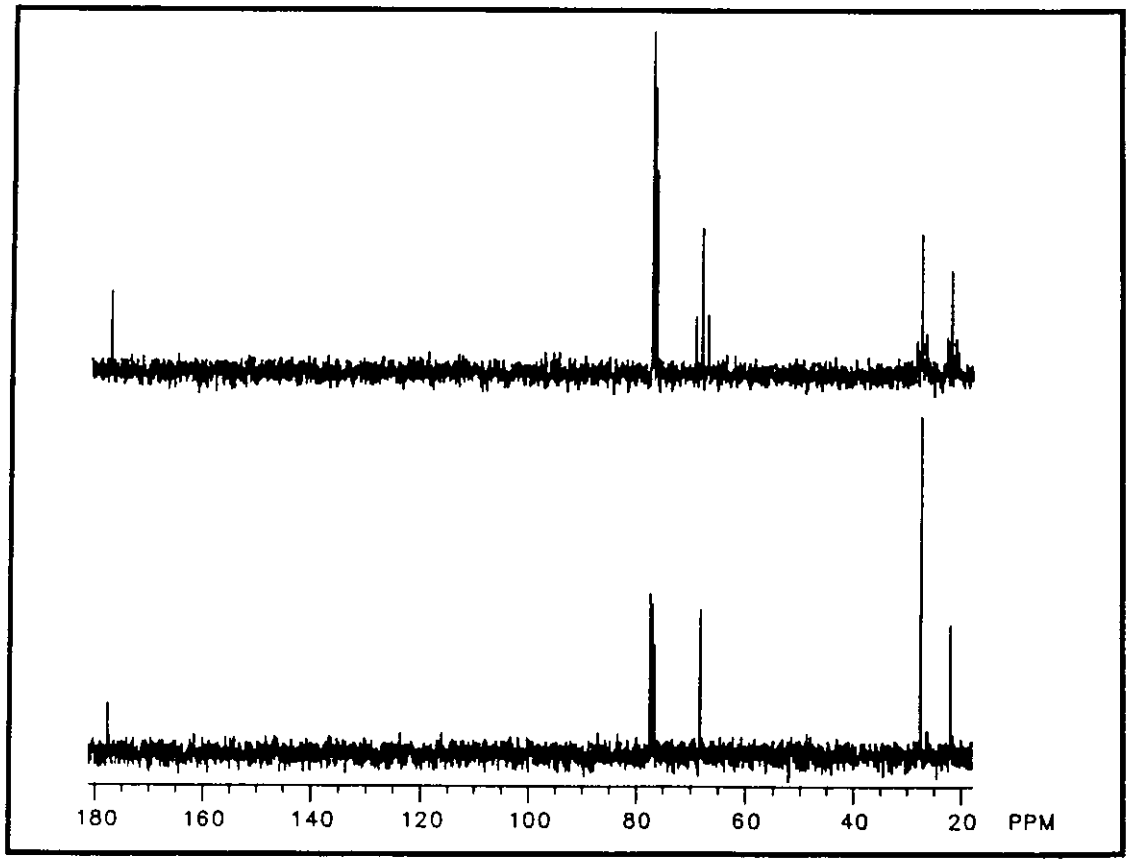
Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na

Mass Spectral Data

m/z		m/z	
30	9.14	55	8.85
37	5.84	56	22.91
38	9.84	57	3.98
39	36.51	85	7.68
40	17.64	86	27.74
41	69.56		
42	100.00		
43	7.59		
44	8.77		
45	1.27		
53	0.69		

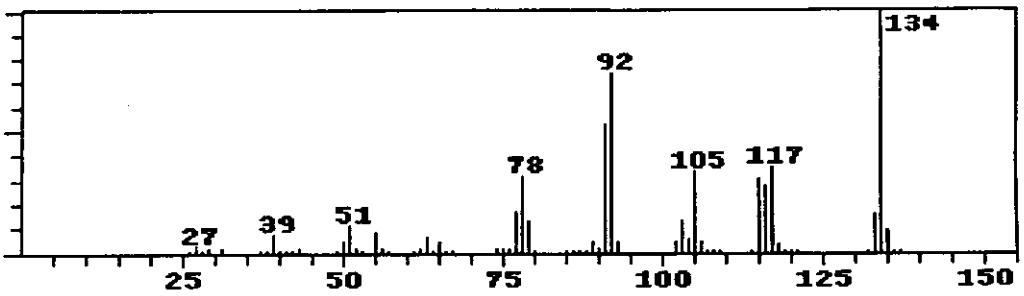


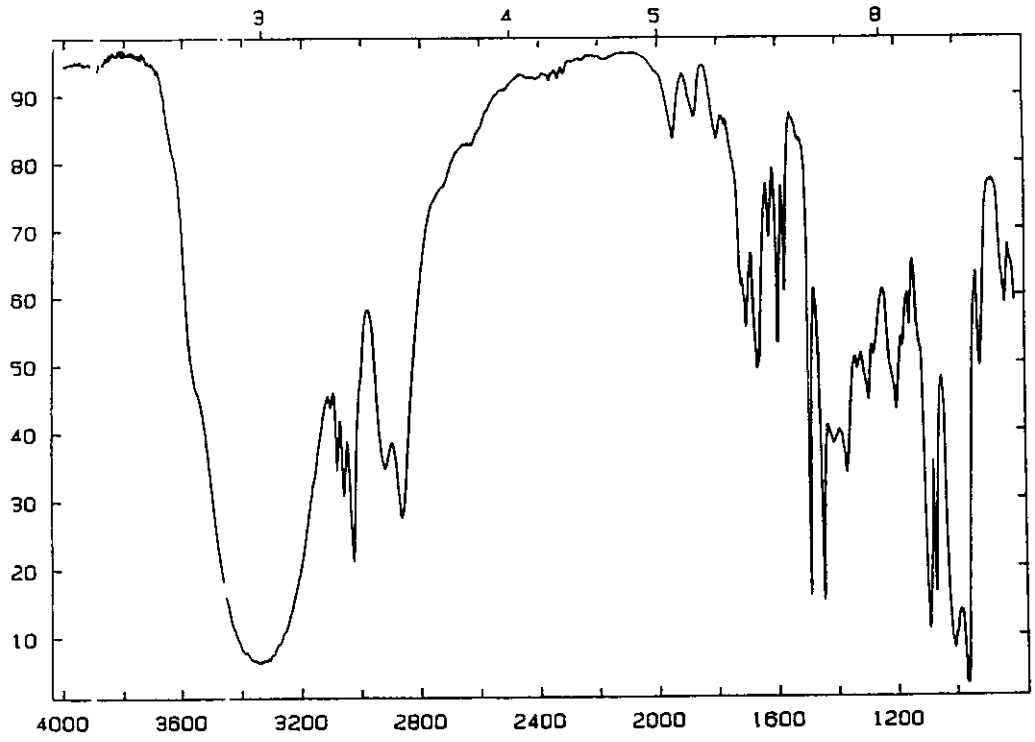

4.5
4.0
3.5
3.0
2.5
PPM

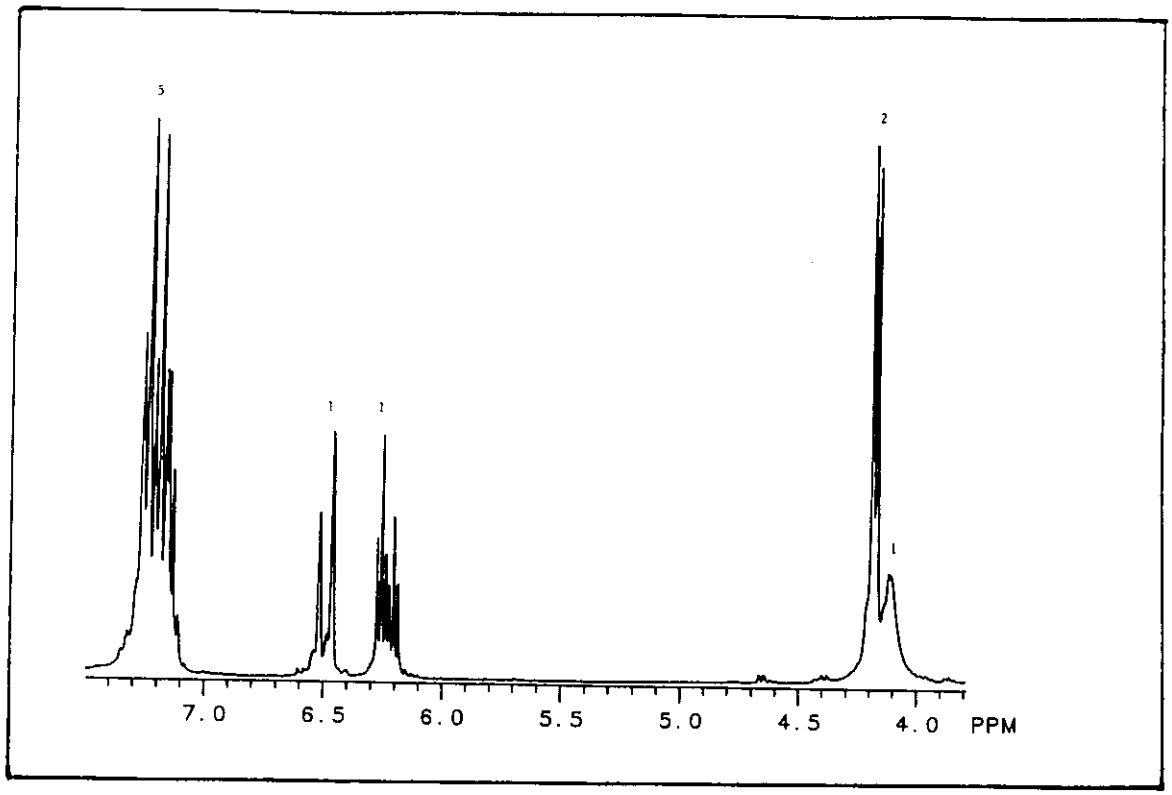

180
160
140
120
100
80
60
40
20
PPM

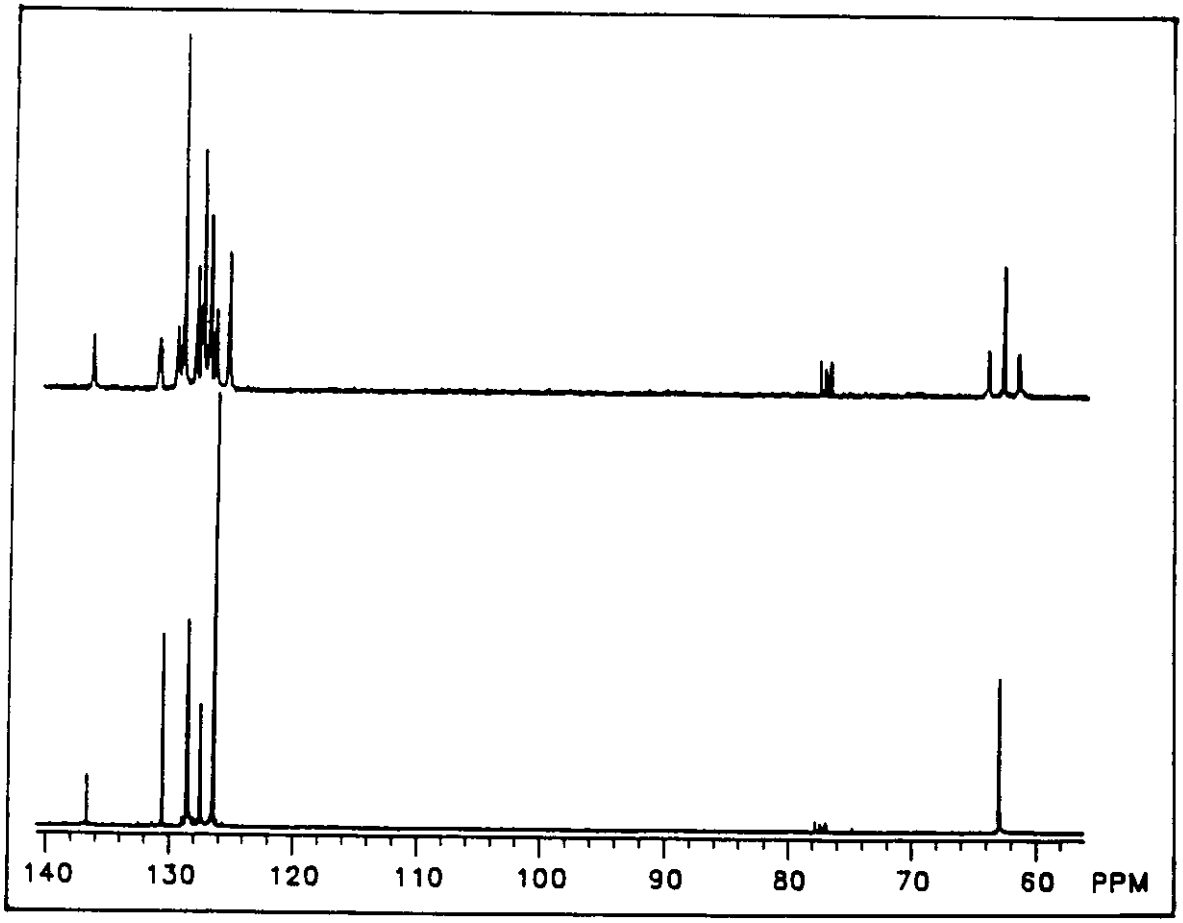
Problem 60

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na



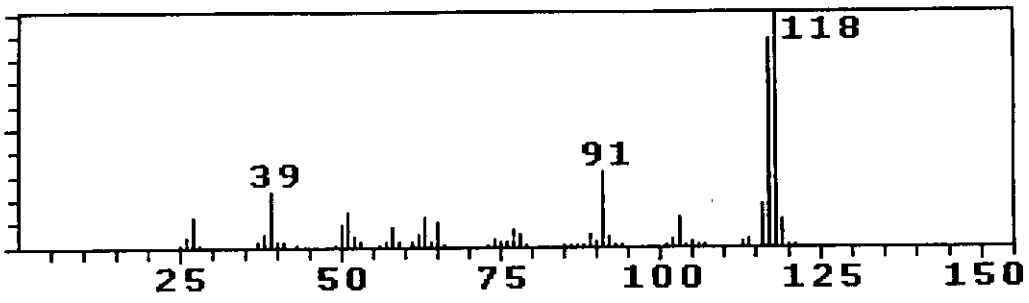


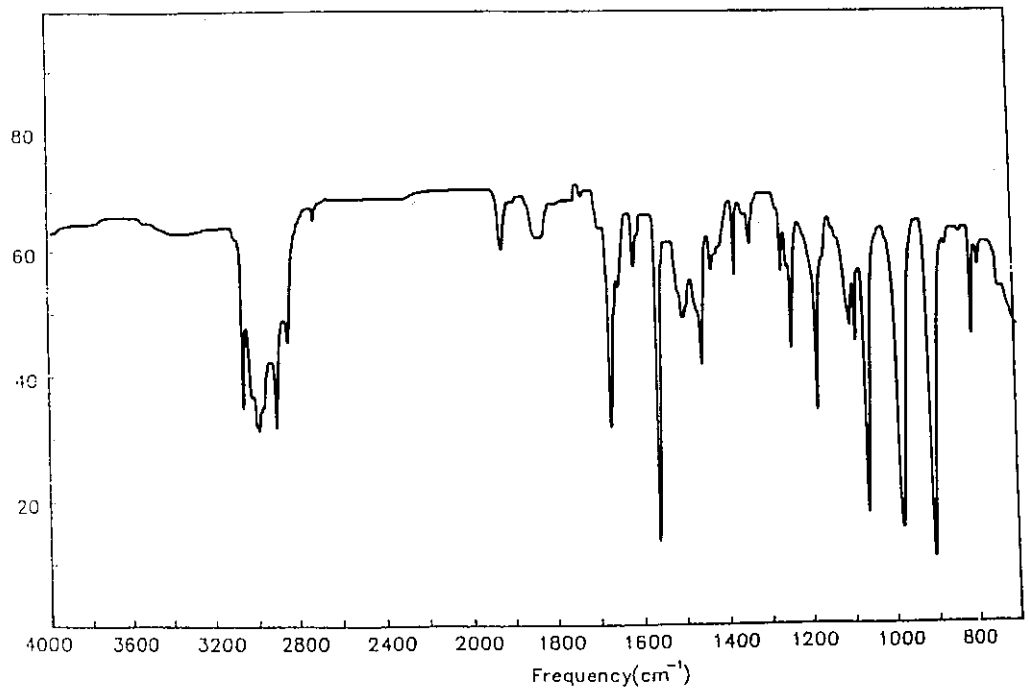

5
2
1
2
1
7.0
6.5
6.0
5.5
5.0
4.5
4.0
PPM

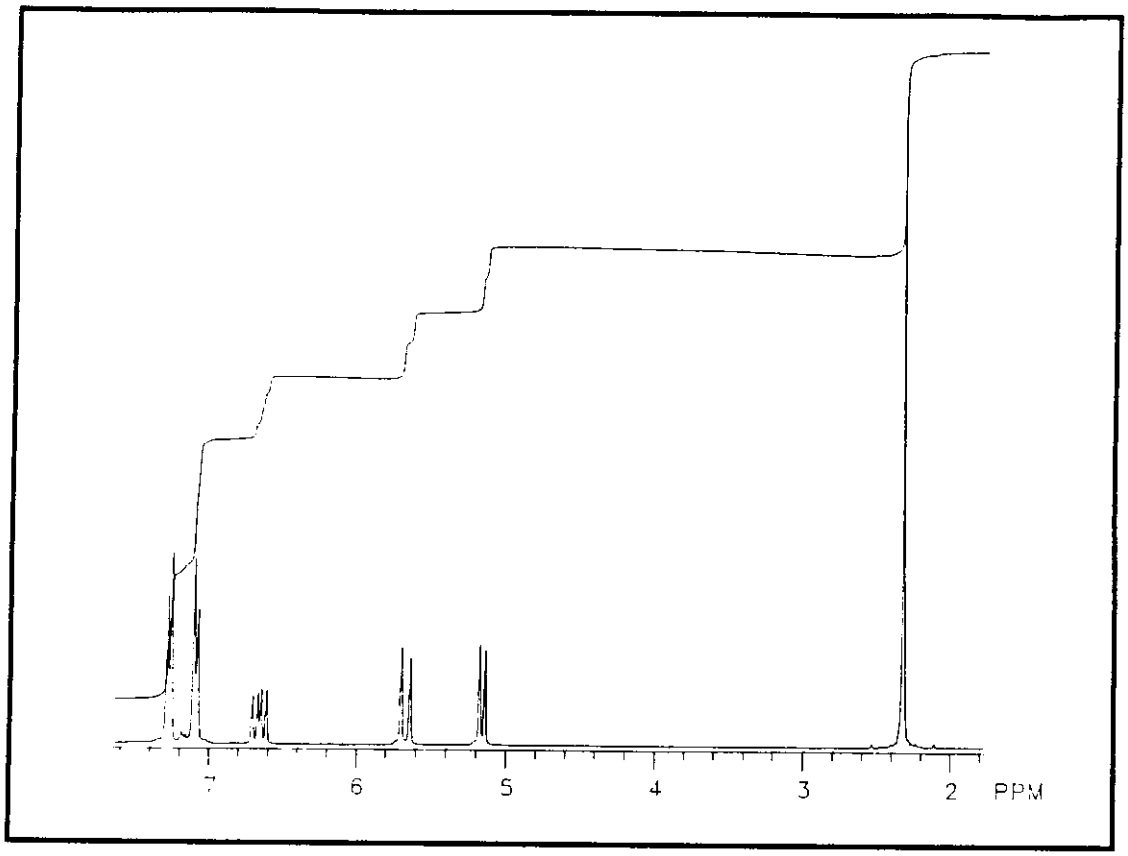

140
130
120
110
100
90
80
70
60
PPM

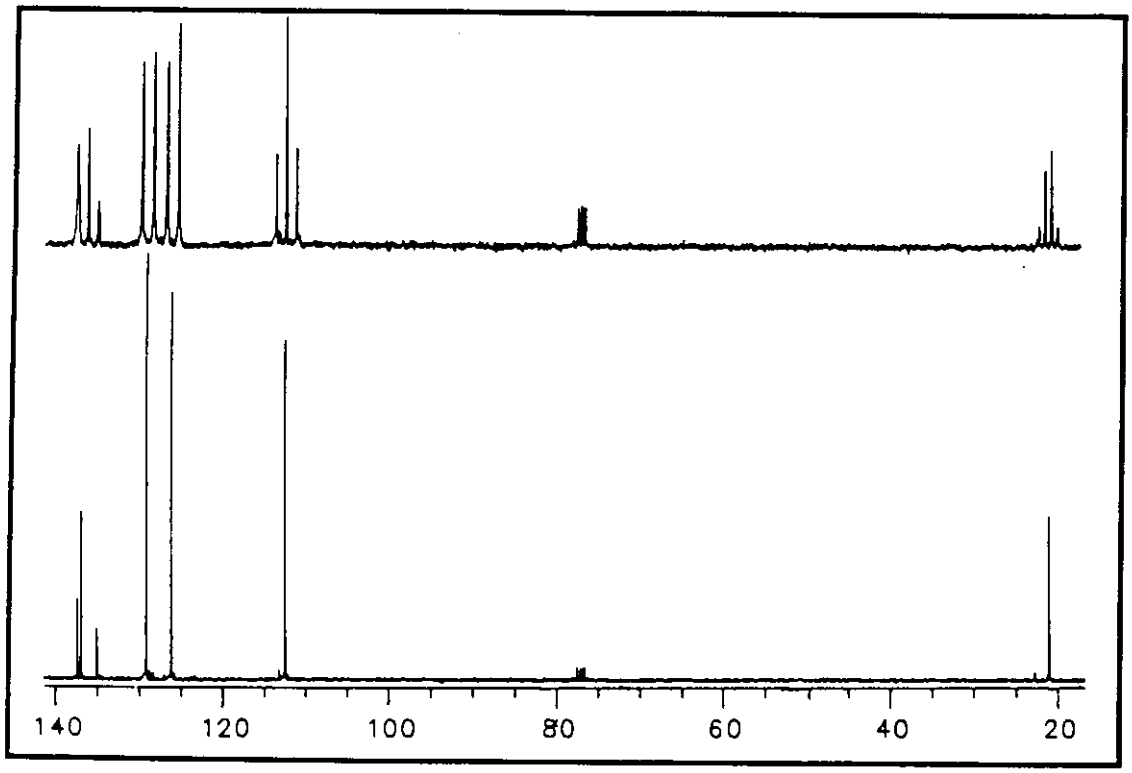
Problem 61

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na






7
6
5
4
3
2
PPM


140
120
100
80
60
40
20

Problem 62

Exact Mass: na
IR: neat
^{1}H NMR: $CDCl_3$
^{13}C NMR: $CDCl_3$
Analysis: na