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The Mass Spectra and Isotopic Purity of Compounds Proposed for Use in the "Master Analytical Scheme for the Analysis of Organic Compounds in Water"

In Partial Fulfillment of
EPA Interagency Agreement No. EPA-IAGD5-E684

E. White V, M. J. Welch*, and H. S. Hertz

Center for Analytical Chemistry
National Measurement Laboratory
National Bureau of Standards
U.S. Department of Commerce
Washington, DC 20234

*College of American Pathologists Research Associate

November 1980

Prepared for
U.S. Environmental Protection Agency
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U.S. DEPARTMENT OF COMMERCE, Philip M. Klutznick, *Secretary*
Jordan J. Baruch, *Assistant Secretary for Productivity, Technology, and Innovation*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

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This study was conducted as part of the
Federal Interagency Energy/Environment Research
and Development Program as part of Interagency Agreement
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Introduction

A "Master Analytical Scheme" for the analysis of organic compounds in water is being developed by the Environmental Protection Agency. It is the aim of this scheme to allow qualitative and quantitative analysis of organic chemicals in water by gas chromatography/mass spectrometry. A series of internal standards is required for the quantitative analyses associated with the scheme. The compounds of choice are stable isotope labeled materials. The National Bureau of Standards has analyzed a series of deuterium labeled compounds for potential use as the internal standards. The results of isotopic purity studies of these compounds as well as the mass spectra of these labeled materials are contained in this report.

Mass Spectra

Electron impact mass spectra of 70 eV were recorded on a Varian MAT 731 mass spectrometer at a source temperature of 150 °C; dodecyl phosphate-d_{25} trimethylsilyl derivative was recorded on a Varian MAT CH 7A at a source temperature of 250 °C. The sample inlet system was a small stainless steel resevoir at 100 °C except as noted on the spectra. The reported spectra are the average of six scans except for the trimethylsilyl derivatives of bisphenol A-d_{14} and mono-n-dodecyl phosphate-d_{25} which are single scans. Peaks at half-integer masses have been omitted from the acridine-d_9 and bromoethane-d_5 spectra.

Spectra for t-butanol-d_9, n-butyric acid-d_7, ethanol-d_5, and phenol-d_5, were obtained from the corresponding fully deuterated compounds by simultaneously introducing the fully deuterated compounds and a large excess of water from separate inlet resevoirs which share a common transfer line to the ion source.

The spectrum of bisphenol-A-d_{14} was obtained on a material prepared by six times dissolving a sample of bisphenol-A-d_{16} in methanol and evaporating to dryness. The trimethylsilyl ether derivative was used for the estimation of isotopic purity since further loss of deuterium was observed when bisphenol-A-d_{14} was exposed to water vapor in the ion source of the mass spectrometer.

Mono-n-dodecylphosphate-d_{23} did not give a mass spectrum representative of intact material when heated on a direct probe.

Isotopic Purity

Isotopic purities were calculated from an average of six scans of the molecular ion cluster of underivatized compounds obtained under the same conditions as the complete spectra except for: 1) bisphenol-A-d_{14} which was measured from the molecular ion of the trimethylsilyl derivative; 2)

n-butyric acid-d_7, ethanol-d_5, and phenol-d_5 which were measured on the molecular ions of the material formed by the simultaneous introduction of the corresponding fully deuterated compound and a large excess of water into the source of the mass spectrometer; 3] di-n-octyl ether which was measured at m/z 130 ($C_8D_{17}^+$); 4] t-butanol-d_9 which was measured at m/z 64 ($C_4D_8^{+\cdot}$) at a resolution of 5200. This resolution is sufficient to eliminate interference from oxygen containing fragments. The t-butanol-d_9 was formed from t-butanol-D_{10} by the simultaneous introduction of a large excess of water.

Identification of any commercial product does not imply recommendation or endorsement by the National Bureau of Standards, nor does it imply that the material or equipment indentified is necessarily the best available for the purpose.

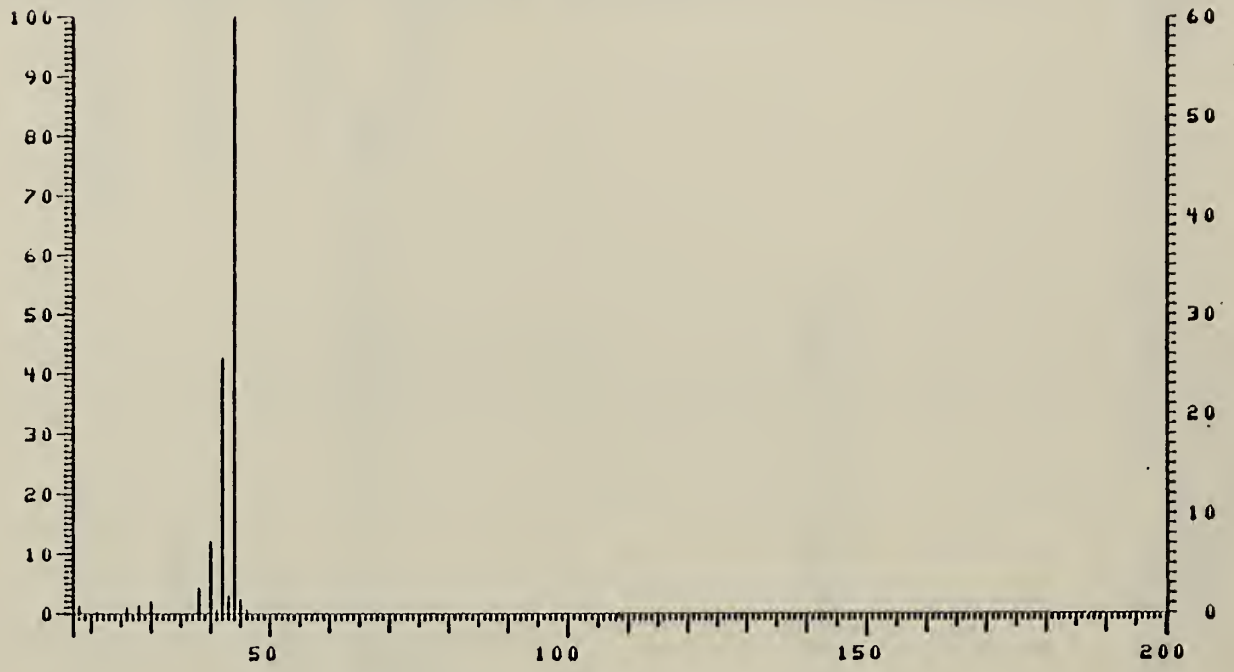
Isotopic Purity of Marker Compounds

Compound	No. of Deuterium Atoms Present In Compound		Atom % Deuterium[b]	Mole % Completely Labeled[b]
	As Supplied	After Exchange[a]		
Acetonitrile-d_3	3	3	99.3	98
Acridine-d_9	9	9	96.7	71
Anisole-2,4,6-d_3	3	3	96.1	88
Anthracene-d_{10}	10	10	99.4	94
Benzoic-d_5 acid	5	5	99.4	97
Bisphenol-A-d_{14}	16	14	98.6	81
Bromoethane-d_5	5	5	99.3	97
t-Butanol-d_9	10	9	99.5	94
n-Butylamine-d_9	9	9	99.3	94
n-Butyric-d_7 acid	7	7	99.3	95
Chlorobenzene-d_5	5	5	99.4	97
n-Decane-d_{22}	22	22	99.4	87
Diethyl ether-d_{10}	10	10	99.6	96
Di-n-octyl ether-d_{34}	34	34	99.7	94
Mono-n-dodecylphosphate-d_{25}	25	25	99.4	85
Ethanol-d_5	6	5	99.0	95
Hexamethylenetetramine-d_{12}	12	12	99.8	98
Naphthalene-d_8	8	8	98.6	89
2-Naphthalenesulfonic acid-d_7	7	7	98.6	87
Nitrobenzene-d_5	5	5	99.0	95
2-Phenylethyl-1,1,2,2-d_4-amine	4	4	99.2	97
Phenol-d_5	6	5	98.5	92
o-Xylene-d_{10}	10	10	99.4	94

[a] As used for spectra.

[b] For labeled positions after exchange.

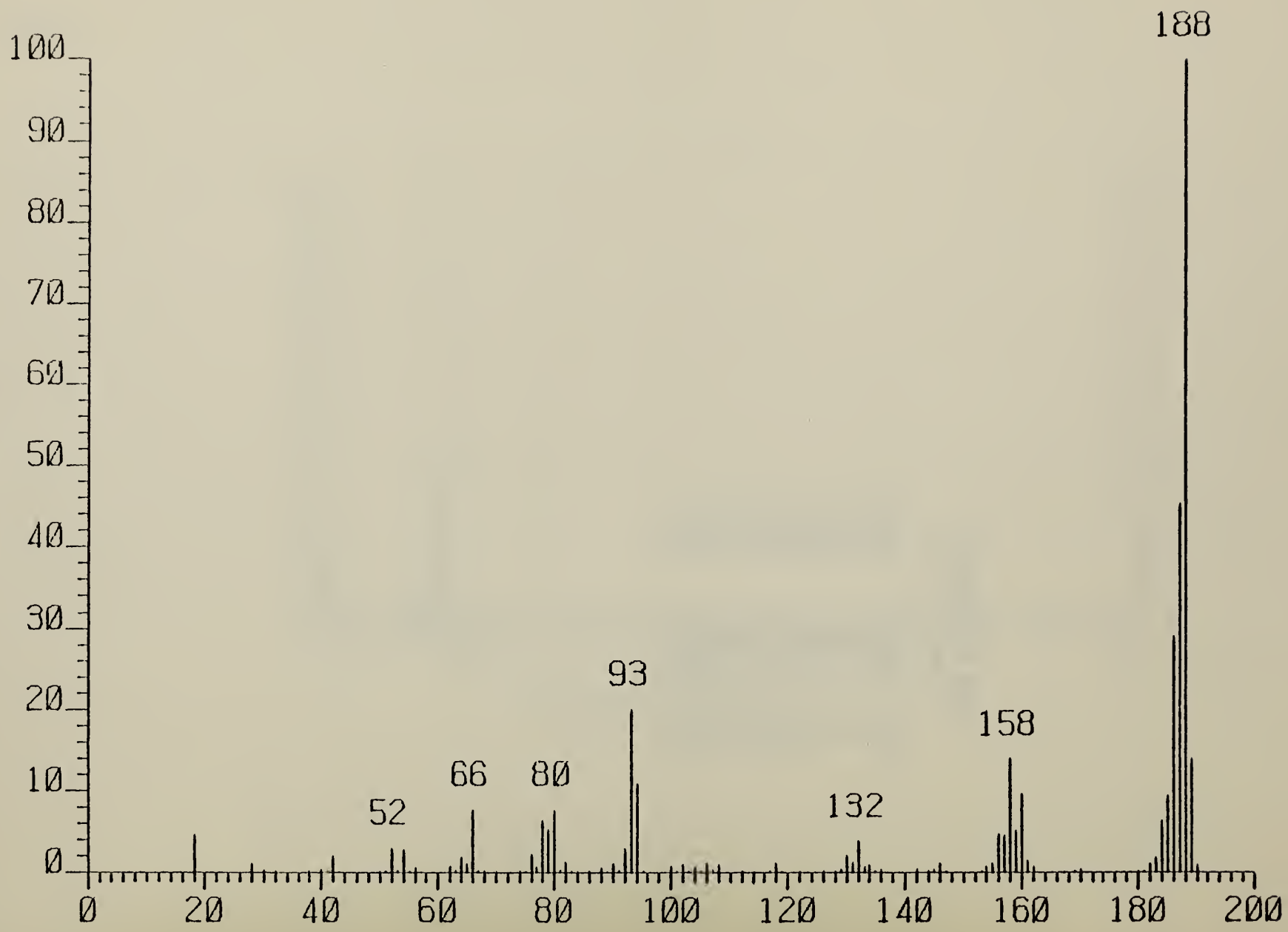
Mass Spectra



Mass Spectrum of Acetonitrile-d_3

Mass Spectrum of Acetonitrile-d_3

PEAK	I/BASE	MASS
5	1.57%	18.0
6	0.64%	21.0
7	0.26%	24.0
8	1.23%	26.0
9	1.38%	28.0
10	2.27%	30.0
12	4.57%	38.0
13	0.19%	39.0
14	12.00%	40.0
15	0.82%	41.0
16	42.96%	42.0
17	3.09%	43.0
18	100.00%	44.0
19	2.49%	45.0
20	0.83%	46.0



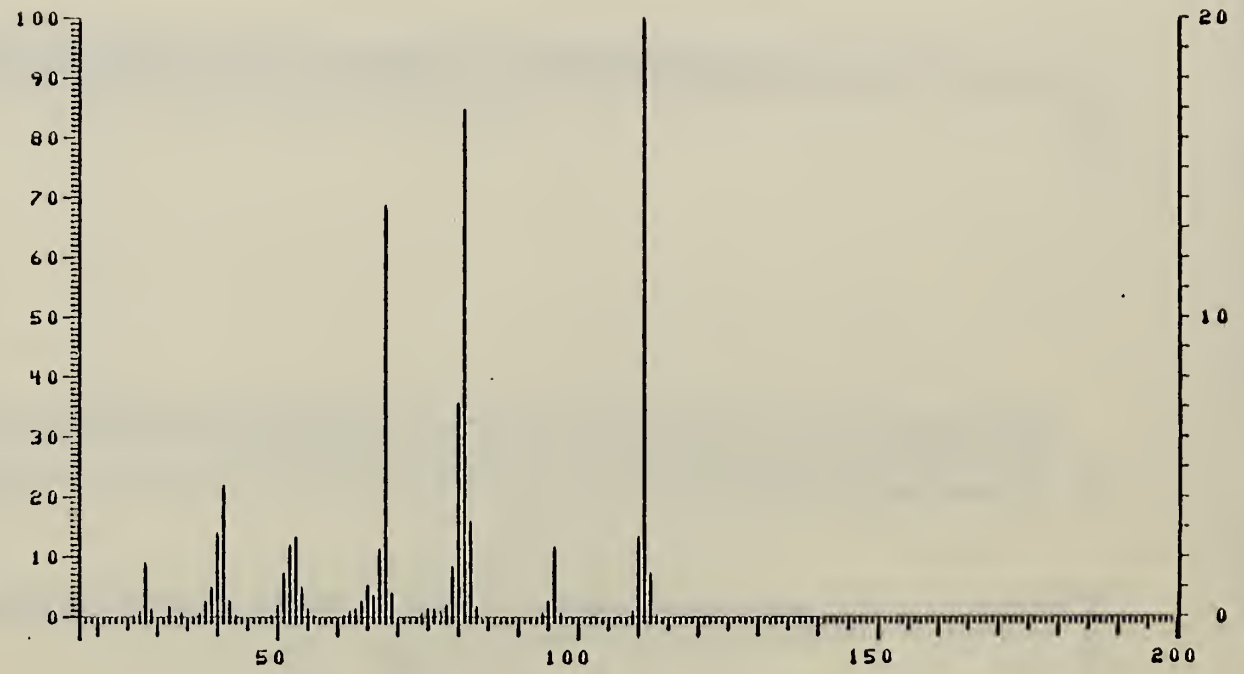
Mass Spectrum of Acridine-d_9 Inlet: Probe 32 °C, Ions at half-integer masses omitted.

Mass Spectrum of Acridine-d_9

Inlet: Probe 32 °C, Ions at half-integer masses omitted.

PEAK#	MASS	B
3	18.	4.58
8	28.	1.15
10	30.	0.36
11	32.	0.14
13	38.	0.23
15	40.	0.46
16	41.	0.27
17	42.	2.05
21	50.	0.14
22	51.	0.27
23	52.	2.97
24	53.	0.44
25	54.	2.75
26	55.	0.22
27	56.	0.49
32	62.	0.80
33	63.	0.30
34	64.	1.76
35	65.	1.01
36	66.	7.64
37	67.	0.24
38	68.	0.27
40	70.	0.19
44	74.	0.14
45	75.	0.19
46	76.	2.13
47	77.	0.78
48	78.	6.35
49	79.	5.25
50	80.	7.67
51	81.	0.43
52	82.	1.23
53	83.	0.13
54	84.	0.16
56	86.	0.18
58	88.	0.62
59	89.	0.17
60	90.	1.05
61	91.	0.40
62	92.	2.97
63	93.	20.01
64	94.	10.86
65	95.	0.15
69	100.	0.67
70	101.	0.15
71	102.	0.90

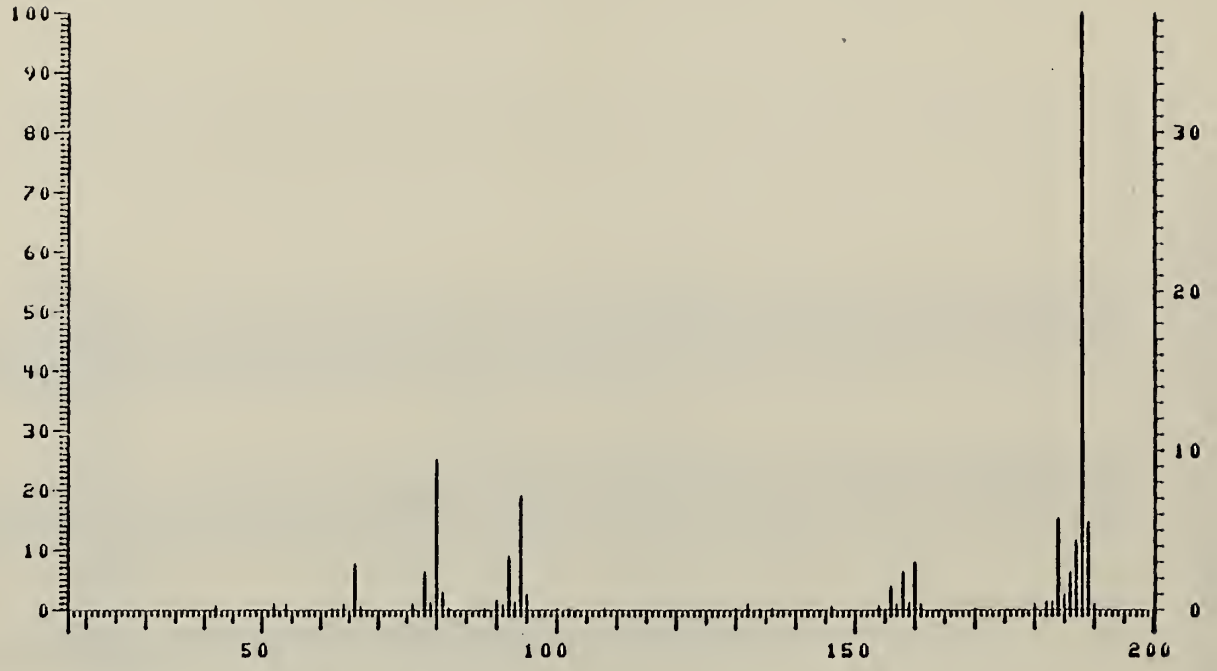
PEAK#	MASS	B
72	103.	0.21
73	104.	0.80
74	105.	0.28
75	106.	1.05
76	107.	0.30
77	108.	0.87
80	112.	0.11
82	114.	0.17
84	116.	0.10
85	117.	0.27
86	118.	1.17
87	119.	0.13
88	120.	0.10
90	122.	0.27
93	126.	0.12
95	128.	0.26
96	129.	0.41
97	130.	1.95
98	131.	1.21
99	132.	3.82
100	133.	0.66
101	134.	0.91
102	135.	0.24
103	136.	0.46
106	142.	0.30
108	144.	0.12
109	145.	0.36
110	146.	1.19
111	147.	0.13
113	153.	0.12
114	154.	0.75
115	155.	1.11
116	156.	4.73
117	157.	4.54
118	158.	13.89
119	159.	5.17
120	160.	9.64
121	161.	1.46
122	162.	0.73
124	169.	0.11
125	170.	0.44
128	180.	0.22
129	181.	0.26
130	182.	1.14
131	183.	1.80
132	184.	6.38
133	185.	9.46
134	186.	29.04
135	187.	45.35
136	188.	100.00
137	189.	13.94
138	190.	0.92



Mass Spectrum of Anisole-2,4,6-d_3

Mass Spectrum of Anisole-2,4,6-d_3

PEAK	I/BASE	MASS
3	0.10%	20.0
6	0.13%	25.0
7	0.53%	26.0
8	1.31%	27.0
9	9.26%	28.0
10	1.38%	29.0
11	0.23%	30.0
12	0.18%	31.0
13	1.97%	32.0
14	0.40%	33.0
15	0.63%	34.0
16	0.43%	36.0
17	0.99%	37.0
18	2.70%	38.0
19	5.08%	39.0
20	14.32%	40.0
21	22.22%	41.0
22	2.97%	42.0
23	0.36%	43.0
24	0.23%	48.0
25	0.57%	49.0
26	2.12%	50.0
27	7.39%	51.0
28	12.28%	52.0
29	13.64%	53.0
30	5.18%	54.0
31	1.36%	55.0
32	0.62%	56.0
33	0.26%	57.0
34	0.25%	60.0
35	0.41%	61.0
36	1.11%	62.0
37	1.35%	63.0
38	2.84%	64.0
39	5.35%	65.0
40	3.92%	66.0
41	11.62%	67.0
42	68.70%	68.0
43	4.17%	69.0
44	0.17%	70.0
45	0.21%	73.0
46	0.73%	74.0
47	1.63%	75.0
48	1.51%	76.0
49	1.00%	77.0
50	2.22%	78.0
51	8.35%	79.0
52	35.77%	80.0
53	84.69%	81.0
54	16.20%	82.0
55	1.73%	83.0
56	0.13%	84.0
58	0.13%	92.0
59	0.17%	93.0
60	0.69%	94.0
61	2.89%	95.0
62	11.95%	96.0
63	0.93%	97.0
65	0.22%	108.0
66	1.13%	109.0
67	13.45%	110.0
68	100.00%	111.0
69	7.41%	112.0
70	0.46%	113.0

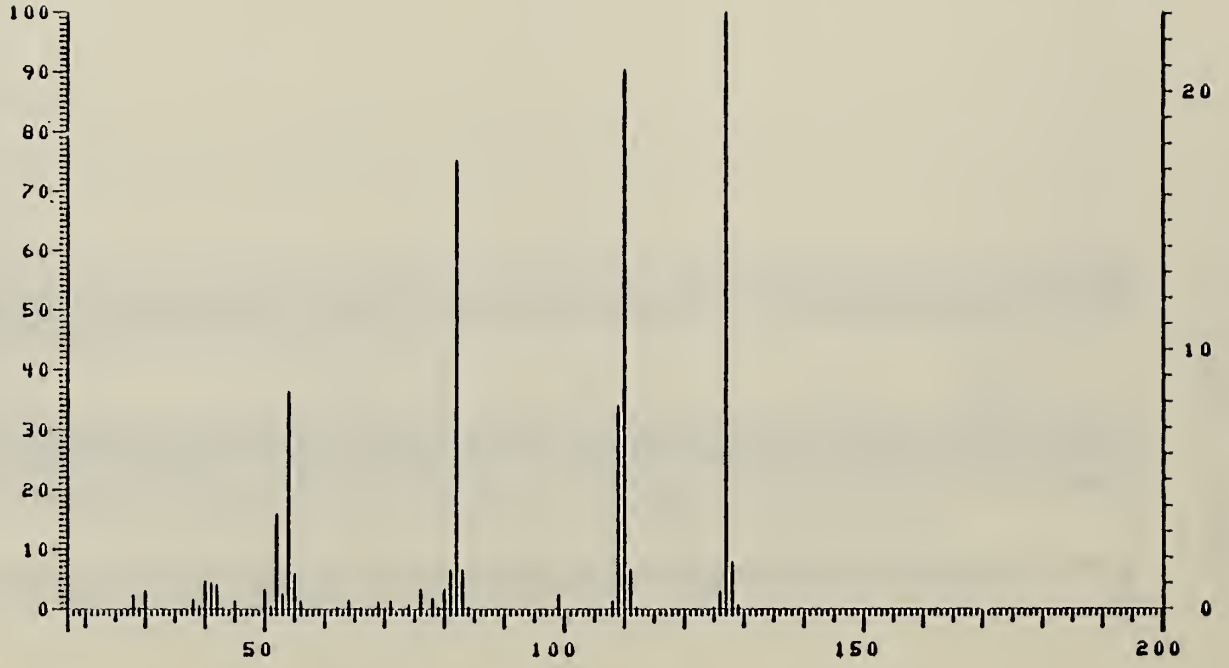


Mass Spectrum of Anthracene-d_{10} Inlet: Probe 40 °C

Mass Spectrum of Anthracene-d_{10}

Inlet: Probe 40 °C

PEAK	I/BASE	MASS
3	0.10%	30.0
5	0.71%	42.0
7	0.12%	50.0
8	0.11%	51.0
9	1.10%	52.0
10	0.11%	53.0
11	1.09%	54.0
13	0.19%	56.0
14	0.49%	62.0
15	0.54%	63.0
16	1.21%	64.0
17	0.26%	65.0
18	7.88%	66.0
19	0.86%	67.0
20	0.11%	68.0
21	0.17%	70.0
22	0.12%	74.0
23	1.27%	76.0
24	0.29%	77.0
25	6.54%	78.0
26	1.50%	79.0
27	25.30%	80.0
28	3.25%	81.0
29	0.59%	82.0
31	0.14%	84.0
33	0.17%	86.0
34	0.46%	88.0
36	1.91%	90.0
37	1.13%	91.0
38	9.02%	92.0
39	1.65%	93.0
40	19.10%	94.0
41	2.74%	95.0
42	0.58%	100.0
44	0.47%	102.0
45	0.26%	104.0
46	0.31%	106.0
47	0.37%	108.0
49	0.15%	112.0
50	0.17%	114.0
51	0.29%	118.0
52	0.32%	122.0
53	0.12%	124.0
54	0.14%	126.0
55	0.11%	128.0
56	0.43%	130.0
57	0.10%	131.0
58	1.01%	132.0
59	0.12%	133.0
60	0.35%	134.0
62	0.47%	136.0
63	0.13%	142.0
66	0.81%	146.0
67	0.10%	147.0
69	0.81%	154.0
70	0.16%	155.0
71	4.33%	156.0
72	1.06%	157.0
73	6.42%	158.0
74	1.52%	159.0
75	8.17%	160.0
76	1.05%	161.0
79	0.19%	168.0
80	0.40%	170.0
83	1.02%	180.0
84	0.26%	181.0
85	1.52%	182.0
86	1.47%	183.0
87	15.39%	184.0
88	2.87%	185.0
89	6.54%	186.0
90	11.87%	187.0
91	100.00%	188.0
92	14.73%	189.0
93	1.05%	190.0
95	0.19%	196.0

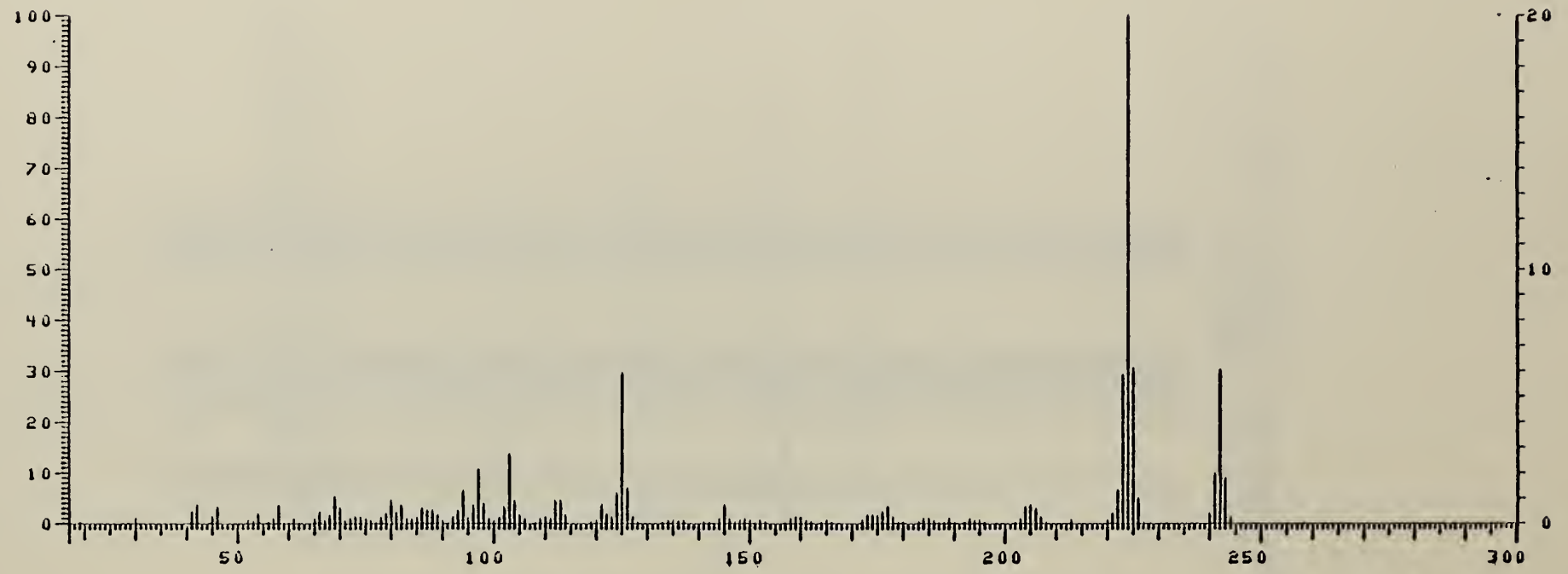


Mass Spectrum of Benzoic-d_5 acid Inlet: Probe 34 °C

Mass Spectrum of Benzoic-d_5 acid

Inlet: Probe 34 °C

PEAK	I/BASE	MASS
1	0.18%	26.0
2	2.52%	28.0
3	0.35%	29.0
4	3.04%	30.0
5	0.10%	31.0
6	0.15%	36.0
7	1.78%	38.0
8	0.82%	39.0
9	4.75%	40.0
10	4.39%	41.0
11	4.12%	42.0
12	0.42%	43.0
13	1.56%	45.0
14	0.13%	46.0
15	0.12%	48.0
16	3.35%	50.0
17	0.83%	51.0
18	16.14%	52.0
19	2.83%	53.0
20	36.49%	54.0
21	6.12%	55.0
22	1.60%	56.0
23	0.12%	57.0
24	0.23%	58.0
26	0.45%	62.0
27	0.10%	63.0
28	1.63%	64.0
29	0.34%	65.0
30	0.61%	66.0
31	0.13%	67.0
32	0.18%	68.0
33	1.22%	69.0
34	0.47%	70.0
35	1.41%	71.0
37	0.69%	74.0
38	0.15%	75.0
39	3.45%	76.0
40	0.32%	77.0
41	1.70%	78.0
42	0.47%	79.0
43	3.39%	80.0
44	6.96%	81.0
45	75.34%	82.0
46	6.92%	83.0
47	0.59%	84.0
48	0.25%	97.0
49	0.16%	98.0
50	2.49%	99.0
51	0.18%	100.0
53	1.46%	103.0
54	34.14%	109.0
55	90.37%	110.0
56	6.77%	111.0
57	0.40%	112.0
58	0.43%	125.0
59	3.21%	126.0
60	100.00%	127.0
61	8.07%	128.0
62	0.70%	129.0



Mass Spectrum of Bisphenol-A-d_{14} Inlet: Probe 79 °C

Mass Spectrum of Bisphenol-A-d_{14}

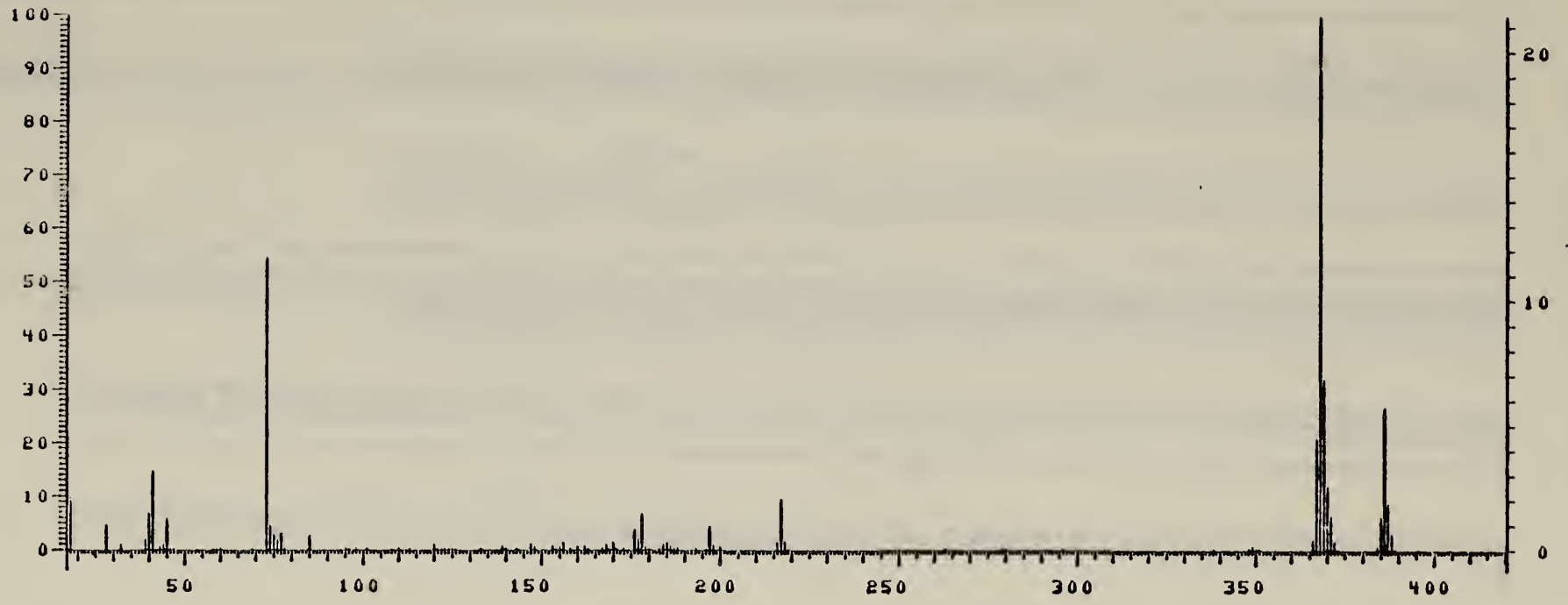
Inlet: Probe 79 °C

PEAK	I/BASE	MASS
1	0.54%	19.0
3	0.15%	29.0
4	1.19%	30.0
5	0.36%	31.0
6	0.13%	33.0
7	0.16%	34.0
8	0.10%	36.0
9	0.19%	38.0
10	0.11%	39.0
11	2.41%	41.0
12	3.78%	42.0
13	0.32%	43.0
14	1.42%	45.0
15	3.39%	46.0
16	0.14%	47.0
17	0.16%	48.0
18	0.26%	49.0
19	0.16%	50.0
20	0.21%	51.0
21	0.87%	52.0
22	0.93%	53.0
23	2.26%	54.0
24	0.26%	55.0
25	0.37%	56.0
26	1.22%	57.0
27	3.97%	58.0
28	0.43%	59.0
29	0.59%	60.0
30	1.19%	61.0
31	0.54%	62.0
32	0.27%	63.0
33	0.58%	64.0
34	1.15%	65.0
35	2.38%	66.0
36	0.98%	67.0
37	1.74%	68.0
38	5.62%	69.0
39	3.56%	70.0
40	0.73%	71.0
41	1.05%	72.0
42	1.48%	73.0
43	1.65%	74.0
44	1.31%	75.0
45	0.96%	76.0
46	0.37%	77.0
47	1.35%	78.0
48	2.06%	79.0
49	4.97%	80.0
50	2.47%	81.0
51	3.97%	82.0
52	1.00%	83.0
53	1.07%	84.0
54	1.44%	85.0
55	3.33%	86.0
56	2.71%	87.0
57	2.94%	88.0
58	1.67%	89.0
59	0.79%	90.0
60	0.62%	91.0
61	1.37%	92.0
62	2.86%	93.0
63	6.69%	94.0
64	1.89%	95.0
65	3.82%	96.0
66	10.72%	97.0
67	4.20%	98.0
68	1.13%	99.0
69	0.78%	100.0
70	1.57%	101.0
71	3.53%	102.0
72	13.69%	103.0
73	4.68%	104.0
74	1.85%	105.0
75	1.09%	106.0
76	0.32%	107.0
77	0.43%	108.0
78	1.09%	109.0
79	1.40%	110.0
80	1.27%	111.0
81	4.70%	112.0
82	4.95%	113.0
83	1.73%	114.0
84	0.22%	115.0
85	0.13%	116.0
86	0.13%	117.0
87	0.15%	118.0
88	0.61%	119.0
89	0.94%	120.0
90	3.97%	121.0
91	2.05%	122.0
92	1.36%	123.0
93	6.10%	124.0
94	29.84%	125.0
95	7.14%	126.0
96	1.44%	127.0
97	0.38%	128.0
98	0.21%	129.0
100	0.13%	131.0
101	0.26%	132.0
102	0.58%	133.0
103	0.68%	134.0
104	0.75%	135.0
105	0.79%	136.0
106	0.77%	137.0
107	0.30%	138.0
108	0.14%	139.0
109	0.16%	140.0
110	0.40%	141.0
111	0.34%	142.0
112	0.57%	143.0
113	1.11%	144.0
114	3.91%	145.0
115	1.11%	146.0
116	0.46%	147.0
117	0.74%	148.0
118	1.30%	149.0
119	0.70%	150.0
120	0.52%	151.0
121	0.69%	152.0
122	0.66%	153.0
123	0.20%	154.0
124	0.16%	155.0
125	0.32%	156.0
126	0.56%	157.0
127	1.08%	158.0
128	1.58%	159.0
129	1.43%	160.0
130	0.92%	161.0
131	0.54%	162.0
132	0.24%	163.0
133	0.48%	164.0
134	0.83%	165.0
135	0.38%	166.0
136	0.31%	167.0
137	0.20%	168.0
138	0.18%	169.0
139	0.22%	170.0
140	0.29%	171.0
141	0.85%	172.0
142	1.73%	173.0
143	1.97%	174.0
144	1.92%	175.0
145	2.40%	176.0
146	3.53%	177.0
147	1.59%	178.0
148	0.49%	179.0
149	0.51%	180.0
150	0.32%	181.0
151	0.28%	182.0
152	0.60%	183.0
153	1.10%	184.0
154	1.14%	185.0
155	0.71%	186.0
156	0.34%	187.0
157	0.57%	188.0
158	1.02%	189.0
159	0.47%	190.0
160	0.30%	191.0
161	0.55%	192.0
162	1.24%	193.0
163	0.68%	194.0
164	0.96%	195.0
165	0.66%	196.0
166	0.33%	197.0
168	0.14%	200.0
169	0.24%	201.0
170	0.37%	202.0
171	1.03%	203.0

Mass Spectrum of Bisphenol-A-d_{14}

Inlet: Probe 79 °C

172	3.44%	204.0
173	3.79%	205.0
174	3.28%	206.0
175	1.48%	207.0
176	0.49%	208.0
177	0.22%	209.0
179	0.22%	212.0
180	0.69%	213.0
181	0.17%	214.0
183	0.16%	219.0
184	0.74%	220.0
185	2.17%	221.0
186	6.69%	222.0
187	29.43%	223.0
188	100.00%	224.0
189	30.86%	225.0
190	5.12%	226.0
191	0.54%	227.0
192	0.18%	238.0
193	0.59%	239.0
194	2.32%	240.0
195	10.04%	241.0
196	30.40%	242.0
197	9.25%	243.0
198	1.55%	244.0
199	0.16%	245.0



Mass Spectrum of Bisphenol-A-d_{14}, bis(trimethylsilyl) ether Inlet: Probe 46 °C

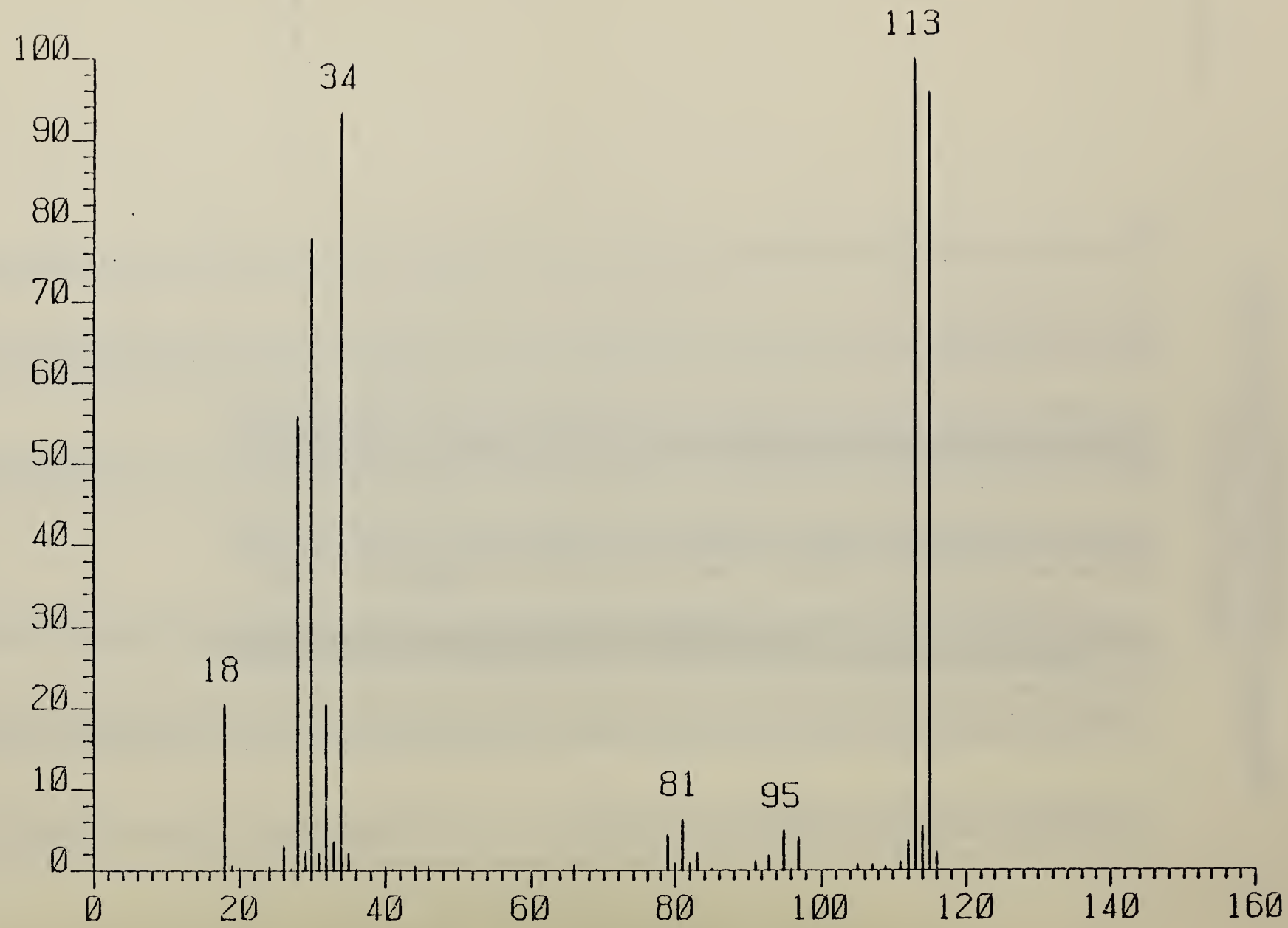
Mass Spectrum of
Bisphenol-A-d_{14}, bis(trimethylsilyl) ether

Inlet: Probe 46 °C

PEAK	I/BASE	MASS
4	0.33%	18.0
6	0.11%	20.0
8	0.17%	26.0
9	0.20%	27.0
12	0.10%	31.0
13	0.96%	38.0
14	2.13%	39.0
15	6.98%	40.0
16	14.55%	41.0
17	0.48%	42.0
18	0.76%	43.0
19	0.90%	44.0
20	5.78%	45.0
21	0.68%	46.0
22	0.43%	47.0
23	0.26%	48.0
24	0.17%	49.0
25	0.30%	50.0
26	0.16%	51.0
27	0.10%	52.0
28	0.10%	54.0
31	0.34%	58.0
32	0.35%	59.0
33	0.46%	60.0
34	0.14%	61.0
35	0.18%	62.0
36	0.25%	63.0
37	0.19%	66.0
38	0.36%	69.0
39	0.19%	70.0
40	0.31%	71.0
41	0.20%	72.0
42	54.44%	73.0
43	4.88%	74.0
44	3.14%	75.0
45	2.21%	76.0
46	3.16%	77.0
47	0.42%	78.0
48	0.21%	79.0
49	0.15%	80.0
50	0.16%	81.0
51	0.33%	82.0
52	0.10%	83.0
53	0.49%	84.0
54	3.20%	85.0
55	0.22%	86.0
56	0.15%	87.0
57	0.23%	91.0
58	0.10%	92.0
60	0.20%	94.0
61	0.49%	95.0
62	0.34%	96.0
63	0.33%	97.0
64	0.34%	98.0
65	0.18%	99.0
66	0.21%	100.0
67	0.48%	101.0
69	0.15%	104.0
71	0.22%	106.0
72	0.33%	107.0
73	0.39%	108.0
74	0.29%	109.0
75	0.35%	110.0
76	0.33%	111.0
77	0.22%	112.0
78	0.96%	113.0
79	0.22%	114.0
81	0.22%	116.0
84	0.15%	119.0
85	1.05%	120.0
86	0.42%	121.0
87	0.64%	122.0
88	0.56%	123.0
89	0.38%	124.0
90	0.46%	125.0
91	0.38%	126.0
92	0.10%	127.0
93	0.15%	128.0
94	0.18%	129.0
95	0.19%	130.0
96	0.30%	131.0
97	0.24%	132.0
98	0.35%	133.0
99	0.22%	134.0
100	0.11%	135.0
101	0.15%	136.0
102	0.24%	137.0
103	0.40%	138.0
104	0.95%	139.0
105	0.48%	140.0
106	0.14%	141.0
107	0.14%	142.0
108	0.44%	143.0
109	0.11%	144.0
110	0.23%	145.0
111	0.37%	146.0
112	1.40%	147.0
113	1.10%	148.0
114	0.21%	149.0
115	0.17%	150.0
116	0.12%	151.0
117	0.32%	152.0
118	1.26%	153.0
119	0.77%	154.0
120	0.77%	155.0
121	1.36%	156.0
122	0.31%	157.0
123	0.40%	158.0
124	0.44%	159.0
125	1.01%	160.0
126	0.52%	161.0
127	1.04%	162.0
128	0.73%	163.0
129	0.24%	164.0
130	0.11%	165.0
131	0.27%	166.0
132	0.68%	167.0
133	1.77%	168.0
134	0.71%	169.0
135	1.51%	170.0
136	0.50%	171.0
137	0.31%	172.0
138	0.34%	173.0
139	0.32%	174.0
140	0.23%	175.0
141	4.75%	176.0
142	3.54%	177.0
143	9.24%	178.0
144	0.98%	179.0
145	0.42%	180.0
146	0.22%	181.0
147	0.20%	182.0
148	0.35%	183.0
149	1.09%	184.0
150	2.65%	185.0
151	0.93%	186.0
152	0.40%	187.0
153	0.40%	188.0
154	0.15%	189.0
155	0.16%	190.0
156	0.10%	191.0
157	0.22%	192.0
158	0.66%	193.0
159	0.16%	194.0
160	0.13%	195.0
161	0.66%	196.0
162	4.45%	197.0
163	1.03%	198.0
164	0.48%	199.0
165	0.88%	200.0
166	0.27%	201.0
167	0.25%	202.0
168	0.18%	203.0
169	0.11%	204.0
170	0.10%	205.0
171	0.14%	206.0
172	0.12%	207.0
177	0.18%	213.0
178	0.15%	214.0
179	0.26%	215.0
180	1.58%	216.0
181	9.35%	217.0
182	1.72%	218.0
183	0.64%	219.0
184	0.15%	220.0
187	0.13%	227.0
188	0.12%	228.0
189	0.11%	229.0
190	0.14%	230.0

Mass Spectrum of
Bisphenol-A-d_{14}, bis(trimethylsilyl) ether
Inlet: Probe 46 °C

191	0.20%	231.0
192	0.11%	232.0
197	0.12%	242.0
198	0.23%	243.0
199	0.14%	244.0
200	0.11%	245.0
201	0.13%	246.0
202	0.18%	247.0
204	0.11%	249.0
206	0.10%	252.0
207	0.11%	257.0
208	0.14%	258.0
209	0.17%	259.0
210	0.29%	260.0
211	0.31%	261.0
212	0.20%	262.0
213	0.36%	263.0
214	0.12%	264.0
215	0.10%	265.0
217	0.11%	274.0
218	0.16%	275.0
219	0.22%	276.0
220	0.32%	277.0
221	0.16%	278.0
222	0.44%	279.0
223	0.60%	280.0
224	0.15%	281.0
228	0.13%	293.0
230	0.20%	295.0
231	0.35%	296.0
232	0.15%	297.0
233	0.10%	298.0
235	0.22%	313.0
238	0.10%	320.0
240	0.19%	335.0
241	0.12%	337.0
242	0.51%	338.0
243	0.14%	339.0
245	0.11%	347.0
246	0.36%	348.0
247	0.87%	349.0
248	0.56%	350.0
249	0.40%	351.0
250	0.16%	352.0
251	0.11%	354.0
253	0.32%	365.0
254	2.15%	366.0
255	21.18%	367.0
256	100.00%	368.0
257	32.27%	369.0
258	12.22%	370.0
259	6.36%	371.0
260	1.69%	372.0
261	0.51%	373.0
262	0.10%	374.0
263	0.11%	383.0
264	0.90%	384.0
265	6.44%	385.0
266	26.97%	386.0
267	8.33%	387.0
268	3.11%	388.0
269	0.64%	389.0
270	0.11%	390.0

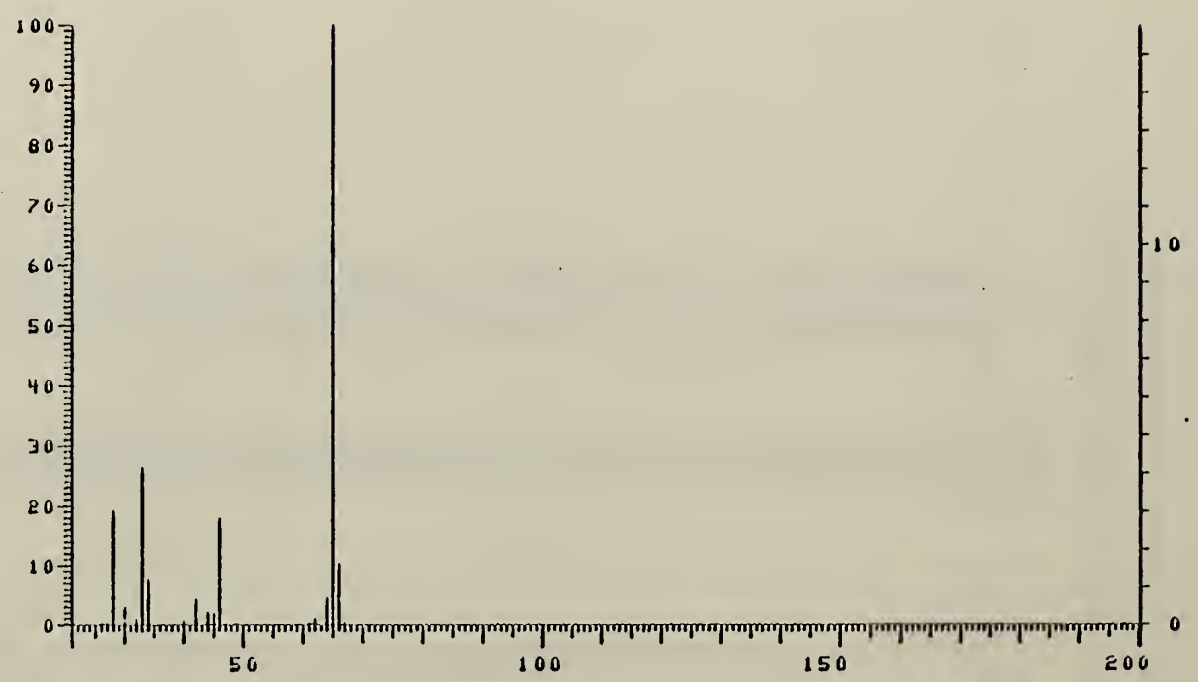


Mass Spectrum of Bromoethane-d_5 Ions at half-integer masses omitted.

Mass Spectrum of Bromoethane-d_5

Ions at half-integer mass omitted.

PEAK#	MASS	B
4	18.	20.48
5	19.	0.82
6	20.	0.46
7	24.	0.55
9	26.	3.04
10	27.	0.46
11	28.	55.89
12	29.	2.44
13	30.	77.75
14	31.	2.14
15	32.	20.41
16	33.	3.56
17	34.	93.42
18	35.	2.15
19	36.	0.11
21	40.	0.62
22	41.	0.25
23	42.	0.28
25	44.	0.64
26	46.	0.61
28	50.	0.34
33	66.	0.67
34	69.	0.11
35	79.	4.29
36	80.	0.92
37	81.	6.25
38	82.	0.88
39	83.	2.26
40	85.	0.17
41	91.	1.08
42	93.	1.85
43	95.	4.83
44	96.	0.16
45	97.	4.01
48	105.	0.63
49	107.	0.80
51	109.	0.55
52	111.	1.14
53	112.	3.60
54	113.	100.00
55	114.	5.46
56	115.	95.98
57	116.	2.22

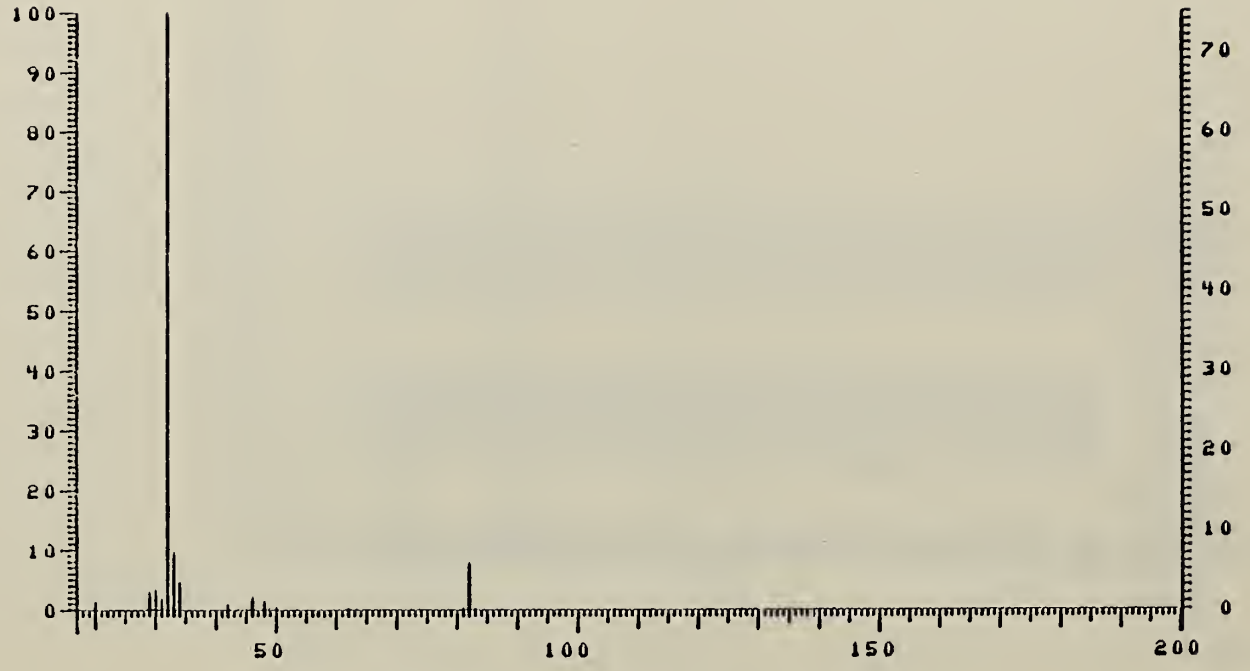


Mass Spectrum of t-Butanol-d_9 Observed $M^{+\cdot}$, m/z 83 (0.09%)

Mass Spectrum of t-Butanol-d_9

Observed $M^{+\cdot}$, m/z 83 (0.09%)

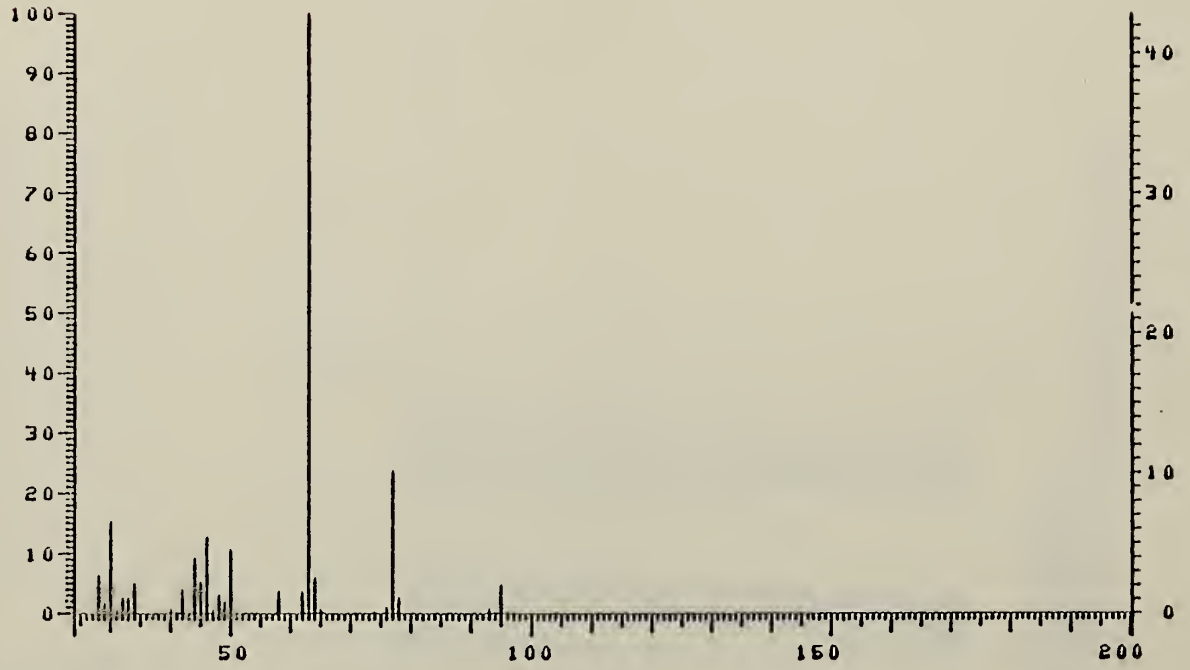
PEAK	I/BASE	MASS
8	0.32%	22.0
9	0.11%	25.0
10	0.54%	26.0
11	0.53%	27.0
12	19.35%	28.0
13	0.57%	29.0
14	3.08%	30.0
15	0.18%	31.0
16	1.07%	32.0
17	26.38%	33.0
18	7.86%	34.0
19	0.21%	35.0
20	0.29%	38.0
21	0.12%	39.0
22	0.69%	40.0
23	0.28%	41.0
24	4.37%	42.0
25	0.27%	43.0
26	2.22%	44.0
27	2.16%	45.0
28	18.00%	46.0
29	0.62%	47.0
30	0.26%	48.0
31	0.38%	49.0
32	0.12%	50.0
33	0.25%	52.0
34	0.20%	54.0
36	0.10%	56.0
37	0.24%	58.0
38	0.38%	61.0
39	1.23%	62.0
40	0.33%	63.0
41	4.78%	64.0
42	100.00%	65.0
43	10.37%	66.0
44	0.65%	67.0



Mass Spectrum of n-Butylamine-d_9

Mass Spectrum of
n-Butylamine-d_9

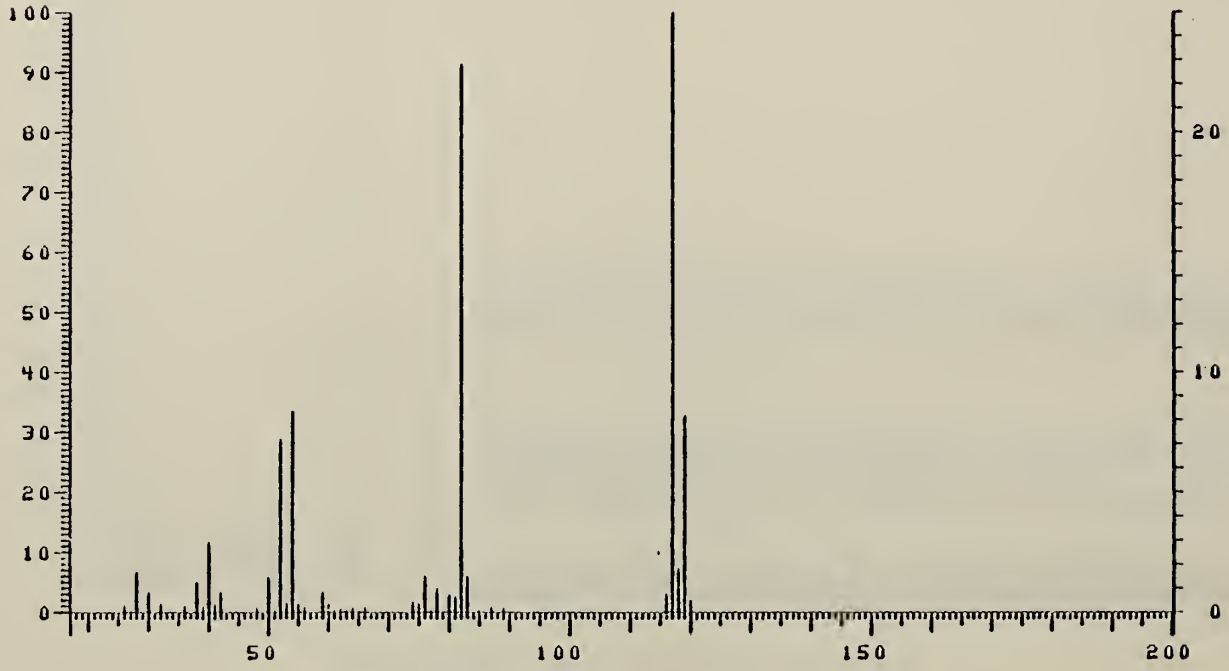
PEAK	I/BASE	MASS
2	1.55%	20.0
3	0.30%	21.0
5	0.13%	27.0
6	3.23%	29.0
7	3.54%	30.0
8	2.09%	31.0
9	100.00%	32.0
10	9.84%	33.0
11	4.82%	34.0
12	0.10%	35.0
16	1.29%	42.0
17	0.18%	43.0
18	0.62%	45.0
19	2.28%	46.0
20	0.30%	47.0
21	1.38%	48.0
22	0.34%	49.0
23	0.37%	50.0
24	0.13%	51.0
29	0.21%	60.0
30	0.10%	61.0
31	0.36%	62.0
32	0.33%	64.0
33	0.33%	80.0
34	0.55%	81.0
35	7.86%	82.0
36	0.62%	83.0



Mass Spectrum of n-Butyric-d_7 acid

Mass Spectrum of n-Butyric-d_7 acid

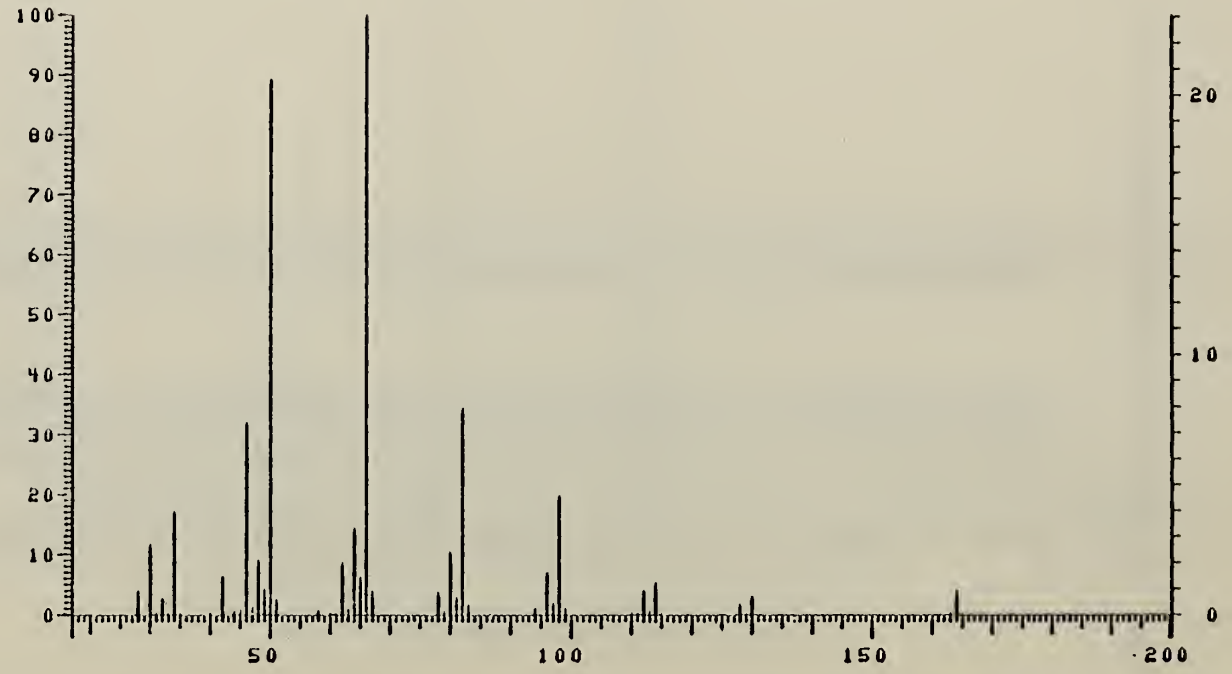
PEAK	I/BASE	MASS
10	0.14%	26.0
11	0.18%	27.0
12	6.42%	28.0
13	1.73%	29.0
14	15.48%	30.0
15	0.77%	31.0
16	2.81%	32.0
17	2.99%	33.0
18	5.12%	34.0
19	0.12%	35.0
20	0.10%	36.0
21	0.31%	38.0
22	0.68%	40.0
23	0.37%	41.0
24	4.32%	42.0
25	0.39%	43.0
26	9.64%	44.0
27	5.41%	45.0
28	12.74%	46.0
29	0.88%	47.0
30	3.19%	48.0
31	2.07%	49.0
32	10.73%	50.0
33	0.36%	51.0
35	0.19%	57.0
36	3.94%	58.0
37	0.14%	59.0
38	0.16%	61.0
39	3.69%	62.0
40	100.00%	63.0
41	6.10%	64.0
42	0.73%	65.0
44	0.49%	74.0
46	1.27%	76.0
47	23.76%	77.0
48	2.86%	78.0
49	0.23%	79.0
50	0.92%	93.0
51	0.35%	94.0
52	4.74%	95.0
53	0.40%	96.0



Mass Spectrum of Chlorobenzene-d_5

Mass Spectrum of Chlorobenzene-d_5

PEAK	I/BASE	MASS
2	0.13%	19.0
4	0.26%	24.0
5	0.12%	25.0
6	1.08%	26.0
7	0.62%	27.0
8	6.98%	28.0
10	3.36%	30.0
12	1.54%	32.0
13	0.29%	35.0
14	1.08%	36.0
15	0.20%	37.0
16	5.12%	38.0
17	1.31%	39.0
18	11.95%	40.0
19	1.34%	41.0
20	3.44%	42.0
21	0.13%	43.0
22	0.20%	44.0
23	0.30%	47.0
24	0.99%	48.0
25	0.15%	49.0
26	5.79%	50.0
27	0.53%	51.0
28	28.69%	52.0
29	1.78%	53.0
30	33.52%	54.0
31	1.47%	55.0
32	0.89%	56.0
33	0.22%	57.0
34	0.13%	58.0
35	3.41%	59.0
36	1.36%	60.0
37	0.66%	61.0
38	0.30%	62.0
39	0.60%	63.0
40	0.85%	64.0
41	0.37%	65.0
42	0.74%	66.0
43	0.10%	67.0
44	0.15%	72.0
45	0.29%	73.0
46	1.74%	74.0
47	1.54%	75.0
48	6.15%	76.0
49	0.66%	77.0
50	4.14%	78.0
51	0.37%	79.0
52	3.20%	80.0
53	2.99%	81.0
54	91.44%	82.0
55	6.05%	83.0
56	0.17%	84.0
57	0.63%	85.0
58	0.96%	87.0
60	0.30%	89.0
61	0.20%	91.0
62	0.17%	99.0
64	0.33%	115.0
65	3.07%	116.0
66	100.00%	117.0
67	7.62%	118.0
68	32.32%	119.0
69	2.09%	120.0



Mass Spectrum of n-Decane-d_{22}

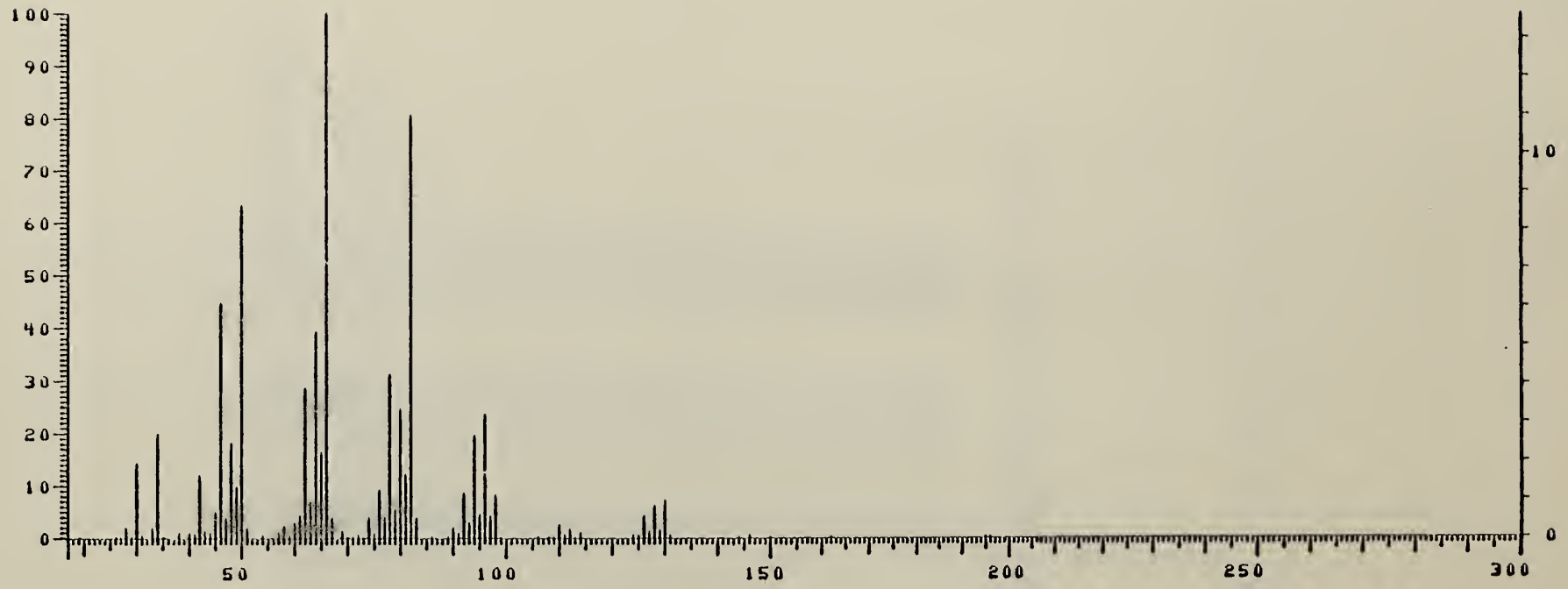
Mass Spectrum of n-Decane-d_{22}

PEAK	I/BASE	MASS
5	4.16%	28.0
6	0.24%	29.0
7	11.67%	30.0
8	0.34%	31.0
9	2.68%	32.0
10	0.61%	33.0
11	17.14%	34.0
12	0.37%	35.0
13	0.25%	38.0
14	0.55%	40.0
15	0.14%	41.0
16	6.39%	42.0
17	0.22%	43.0
18	0.89%	44.0
19	1.02%	45.0
20	32.00%	46.0
21	1.38%	47.0
22	9.30%	48.0
23	4.54%	49.0
24	89.63%	50.0
25	2.81%	51.0
26	0.13%	52.0
27	0.19%	54.0
29	0.79%	58.0
31	0.54%	60.0
32	0.43%	61.0
33	8.94%	62.0
34	1.18%	63.0
35	14.34%	64.0
36	6.61%	65.0
37	100.00%	66.0
38	4.22%	67.0
41	0.26%	74.0
42	0.27%	76.0
43	0.26%	77.0
44	3.83%	78.0
45	0.90%	79.0
46	10.48%	80.0
47	3.05%	81.0
48	34.43%	82.0
49	1.77%	83.0
50	0.32%	92.0
51	0.11%	93.0
52	1.05%	94.0
53	0.60%	95.0
54	7.24%	96.0
55	2.19%	97.0
56	19.69%	98.0
57	1.31%	99.0
58	0.36%	110.0
59	0.41%	111.0
60	4.33%	112.0
61	0.87%	113.0
62	5.59%	114.0
63	0.42%	115.0
65	0.19%	127.0
66	1.76%	128.0
67	0.51%	129.0
68	3.31%	130.0
69	0.27%	131.0
71	0.58%	163.0
72	4.04%	164.0
73	0.42%	165.0

Mass Spectrum of Diethyl ether-d_{10}

Mass Spectrum of Diethyl ether-d_{10}

PEAK	I/BASE	MASS
3	0.95%	19.0
4	0.38%	20.0
5	1.69%	22.0
6	0.12%	24.0
7	0.62%	26.0
8	0.12%	27.0
9	88.17%	28.0
10	0.75%	29.0
11	11.94%	30.0
12	0.31%	31.0
13	18.38%	32.0
14	1.54%	33.0
15	100.00%	34.0
16	1.07%	35.0
17	0.28%	36.0
18	0.27%	38.0
20	1.23%	40.0
21	0.10%	41.0
22	0.79%	42.0
23	0.10%	43.0
24	0.43%	44.0
25	0.19%	45.0
26	9.70%	46.0
27	0.36%	47.0
28	0.46%	48.0
29	0.52%	49.0
30	16.14%	50.0
31	0.45%	51.0
32	0.17%	54.0
33	0.16%	62.0
34	0.79%	65.0
35	28.87%	66.0
36	0.90%	67.0
38	0.17%	69.0
39	1.00%	82.0
40	0.70%	83.0
41	15.78%	84.0
42	0.75%	85.0
43	0.26%	86.0

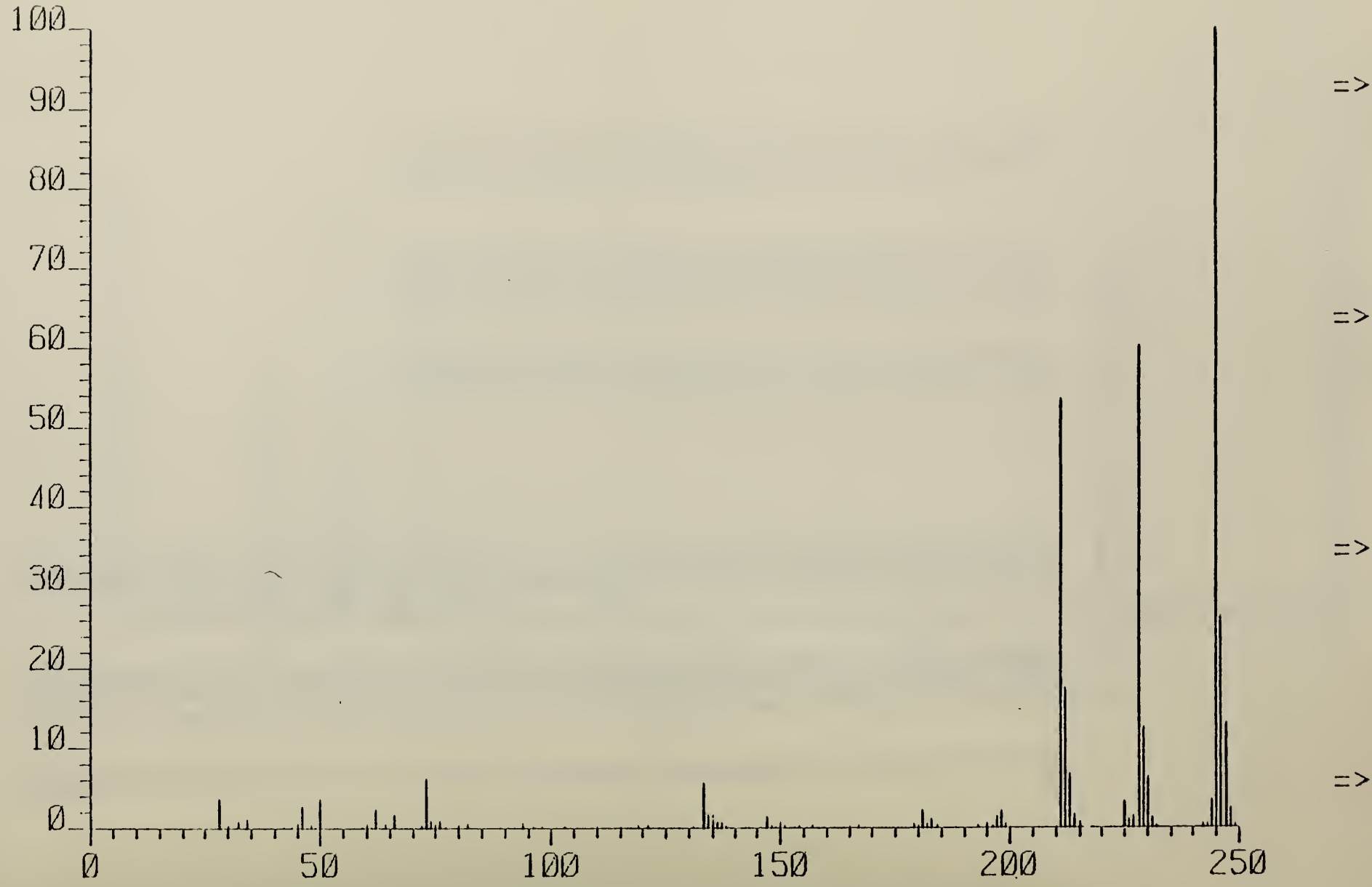


Mass Spectrum of Di-n-octyl ether-d_{34} Observed $M^{+\cdot}$, m/z 278 (0.08%)

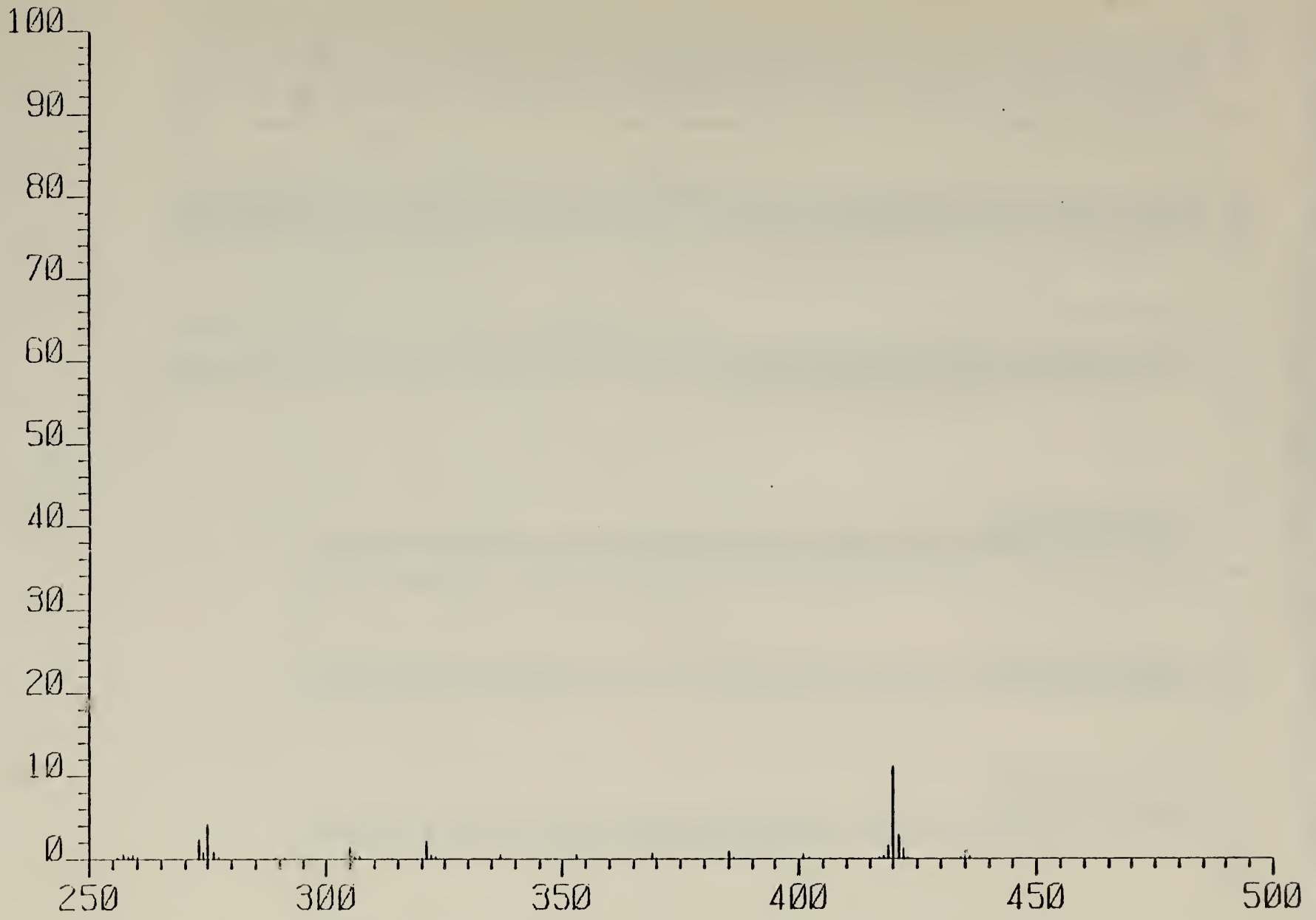
Mass Spectrum of Di-n-octylether-d_{34}

Observed $M^{+\cdot}$, m/z 278 (0.08%)

PEAK	I/BASE	MASS
2	0.60%	19.0
3	0.19%	21.0
4	0.11%	22.0
5	0.15%	23.0
7	0.35%	26.0
8	0.36%	27.0
9	2.23%	28.0
10	0.65%	29.0
11	14.38%	30.0
12	0.72%	31.0
13	2.17%	33.0
14	20.24%	34.0
15	0.46%	35.0
16	0.26%	36.0
17	0.10%	37.0
18	1.06%	38.0
19	0.25%	39.0
20	1.08%	40.0
21	1.25%	41.0
22	12.33%	42.0
23	1.45%	43.0
24	1.32%	44.0
25	5.01%	45.0
26	44.75%	46.0
27	4.00%	47.0
28	18.56%	48.0
29	10.24%	49.0
30	63.35%	50.0
31	2.08%	51.0
32	0.64%	52.0
33	0.12%	53.0
34	0.73%	54.0
35	0.22%	55.0
36	0.47%	56.0
37	1.02%	57.0
38	2.49%	58.0
39	0.91%	59.0
40	3.27%	60.0
41	4.55%	61.0
42	28.72%	62.0
43	7.17%	63.0
44	39.62%	64.0
45	16.68%	65.0
46	100.00%	66.0
47	4.27%	67.0
49	1.34%	69.0
50	0.48%	70.0
51	0.47%	71.0
52	0.67%	72.0
53	0.64%	73.0
54	4.32%	74.0
55	1.33%	75.0
56	9.50%	76.0
57	4.42%	77.0
58	31.35%	78.0
59	5.76%	79.0
60	24.70%	80.0
61	12.57%	81.0
62	80.85%	82.0
63	4.16%	83.0
64	0.14%	84.0
65	0.27%	85.0
66	0.47%	86.0
67	0.15%	87.0
68	0.33%	88.0
69	0.43%	89.0
70	2.12%	90.0
71	1.17%	91.0
72	8.71%	92.0
73	3.12%	93.0
74	19.77%	94.0
75	4.68%	95.0
76	23.91%	96.0
77	4.43%	97.0
78	8.54%	98.0
79	0.56%	99.0
84	0.17%	105.0
85	0.63%	106.0
86	0.18%	107.0
87	0.37%	108.0
88	0.55%	109.0
89	2.68%	110.0
90	0.75%	111.0
91	1.71%	112.0
92	0.65%	113.0
93	1.27%	114.0
94	0.11%	115.0
96	0.23%	119.0
98	0.16%	122.0
99	0.19%	123.0
100	0.77%	124.0
101	0.83%	125.0
102	4.61%	126.0
103	1.64%	127.0
104	6.38%	128.0
105	1.67%	129.0
106	7.38%	130.0
107	0.86%	131.0
109	0.16%	142.0
110	0.23%	143.0
111	0.49%	144.0
112	0.32%	145.0
113	0.68%	146.0
115	0.10%	148.0
116	0.66%	150.0
119	0.11%	159.0
120	0.21%	160.0
121	0.18%	161.0
122	0.48%	162.0
123	0.16%	169.0
124	0.16%	181.0
127	0.19%	194.0
128	0.37%	195.0
129	0.58%	196.0
131	0.12%	210.0



Mass Spectrum of Mono-n-dodecylphosphate-d_{25}, bis(trimethylsilyl)ether



Mass Spectrum of Mono-n-dodecylphosphate-d_{25}, bis(trimethylsilyl)ether

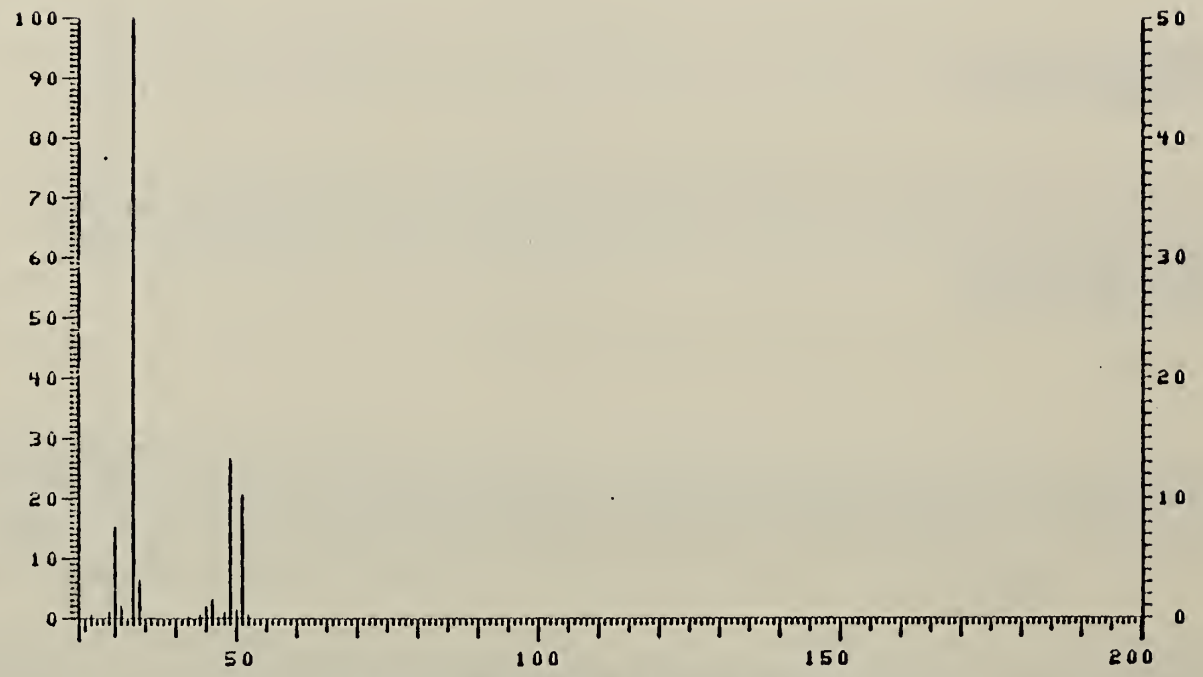
Inlet: Gas chromatograph

Mass Spectrum of Mono-n-dodecylphosphate-d_{25}, bis(trimethylsilyl) ether
Inlet: Gas chromatograph

PEAK#	MASS	B
1	28.	3.70
2	30.	0.30
3	32.	1.00
4	34.	1.10
5	40.	0.10
6	42.	0.20
7	43.	0.10
8	44.	0.20
9	45.	0.80
10	46.	2.70
11	47.	0.20
12	48.	0.60
13	49.	0.20
14	50.	3.60
15	51.	0.10
16	58.	0.10
17	59.	0.20
18	60.	0.50
19	61.	0.20
20	62.	2.40
21	63.	0.10
22	64.	0.60
23	65.	0.10
24	66.	1.60
25	72.	0.30
26	73.	6.10
27	74.	0.90
28	75.	0.60
29	76.	0.90
30	77.	0.20
31	78.	0.10
32	79.	0.10
33	80.	0.40
34	82.	0.50
35	90.	0.10
36	92.	0.10
37	93.	0.10
38	94.	0.50
39	96.	0.20
40	98.	0.20
41	103.	0.20
42	105.	0.10
43	110.	0.20
44	115.	0.20
45	117.	0.10
46	119.	0.40
47	120.	0.10
48	121.	0.30
49	124.	0.10
50	131.	0.20
51	133.	5.70
52	134.	1.60
53	135.	1.70
54	136.	0.70
55	137.	0.70
56	138.	0.40
57	139.	0.10
58	147.	1.40
59	148.	0.30
60	149.	0.20
61	150.	0.70
62	151.	0.30
63	152.	0.10
64	153.	0.20
65	154.	0.30
66	156.	0.10
67	157.	0.30
68	165.	0.20
69	167.	0.30
70	168.	0.10
71	179.	0.50
72	180.	0.30
73	181.	2.20
74	182.	0.60
75	183.	1.10
76	184.	0.30
77	185.	0.10
78	193.	0.30
79	195.	0.60
80	196.	0.30
81	197.	1.50
82	198.	2.20
83	199.	0.50
84	200.	0.20
85	207.	0.10
86	209.	0.10
87	210.	0.20
88	211.	53.50
89	212.	17.50
90	213.	6.80
91	214.	1.70
92	215.	0.30
93	216.	0.10
94	223.	0.10
95	225.	3.30
96	226.	1.10
97	227.	1.50
98	228.	60.20
99	229.	12.50

Mass Spectrum of Mono-n-dodecylphosphate-d_{25}, bis(trimethylsilyl) ether
Inlet: Gas chromatograph

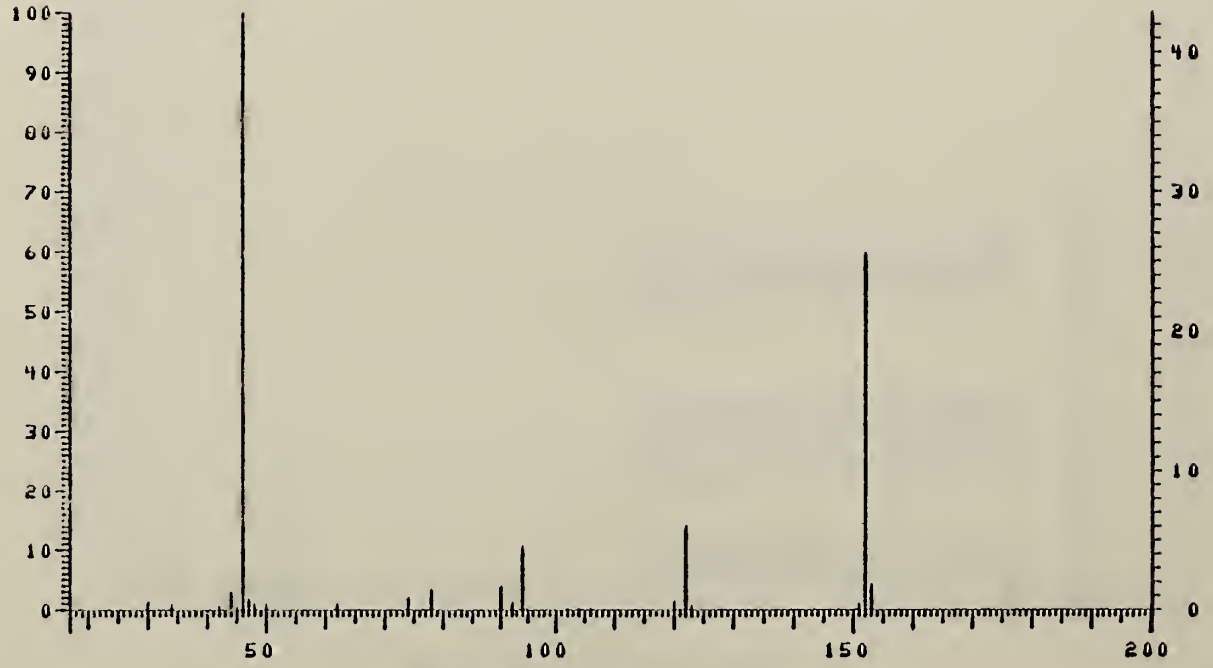
PEAK#	MASS	B
100	230.	6.40
101	231.	1.20
102	232.	0.30
103	239.	0.10
104	240.	0.10
105	242.	0.60
106	243.	0.50
107	244.	3.40
108	245.	100.00
109	246.	26.40
110	247.	13.10
111	248.	2.60
112	249.	0.60
113	256.	0.20
114	257.	0.50
115	258.	0.40
116	259.	0.60
117	260.	0.30
118	272.	0.10
119	273.	2.30
120	274.	1.00
121	275.	4.10
122	276.	0.90
123	277.	0.40
124	278.	0.10
125	289.	0.20
126	291.	0.20
127	299.	0.10
128	304.	0.10
129	305.	1.40
130	306.	0.30
131	307.	0.30
132	320.	0.20
133	321.	2.10
134	322.	0.50
135	323.	0.40
136	337.	0.50
137	338.	0.10
138	353.	0.50
139	354.	0.10
140	355.	0.10
141	368.	0.10
142	369.	0.70
143	370.	0.20
144	371.	0.10
145	384.	0.10
146	385.	0.90
147	386.	0.20
148	387.	0.10
149	400.	0.10
150	401.	0.60
151	402.	0.20
152	417.	0.20
153	418.	0.30
154	419.	1.60
155	420.	11.10
156	421.	3.00
157	422.	1.20
158	423.	0.20
159	433.	0.10
160	434.	0.20
161	435.	1.00
162	436.	0.30
163	437.	0.10



Mass Spectrum of Ethanol-d_5

Mass Spectrum of Ethanol-d_5

PEAK	I/BASE	MASS
13	0.77%	26.0
14	1.07%	29.0
15	15.43%	30.0
16	2.18%	31.0
17	100.00%	33.0
18	6.44%	34.0
19	0.22%	35.0
20	0.36%	42.0
21	0.24%	43.0
22	0.74%	44.0
23	2.19%	45.0
24	3.22%	46.0
25	0.37%	47.0
26	1.12%	48.0
27	26.95%	49.0
28	1.63%	50.0
29	20.75%	51.0
30	0.74%	52.0

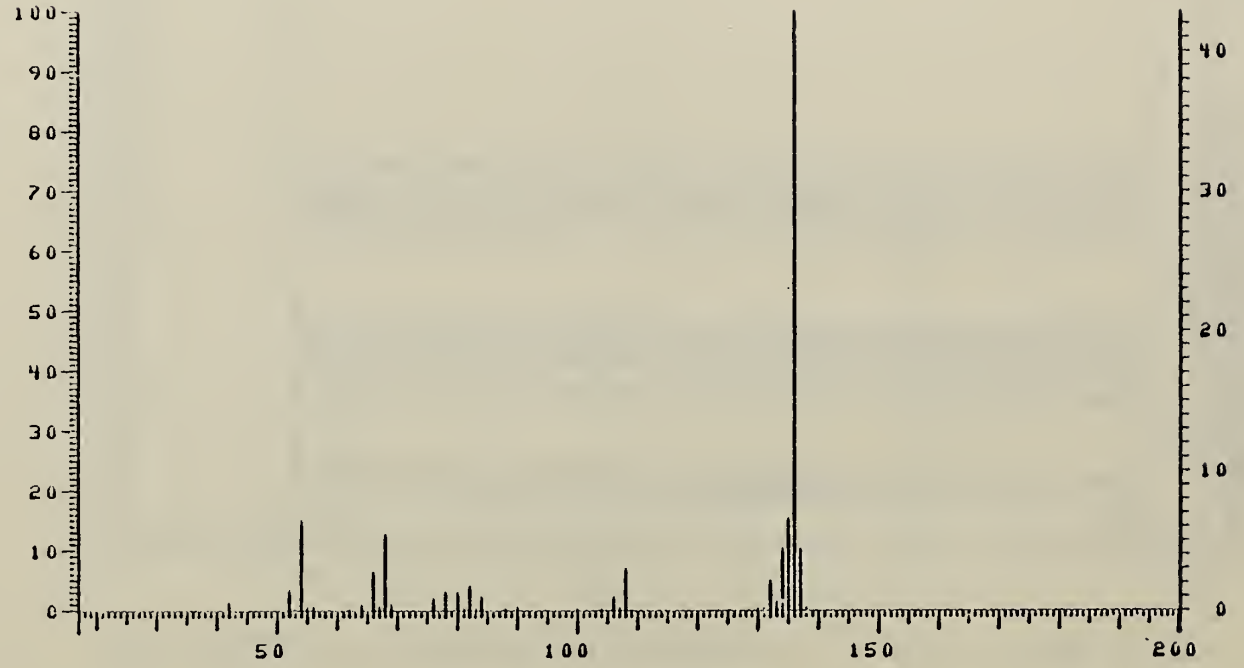


Mass Spectrum of Hexamethylenetetramine-d_{12} Inlet: Probe 26 °C

Mass Spectrum of
Hexamethylenetetramine-d_{12}

Inlet: Probe 26 °C

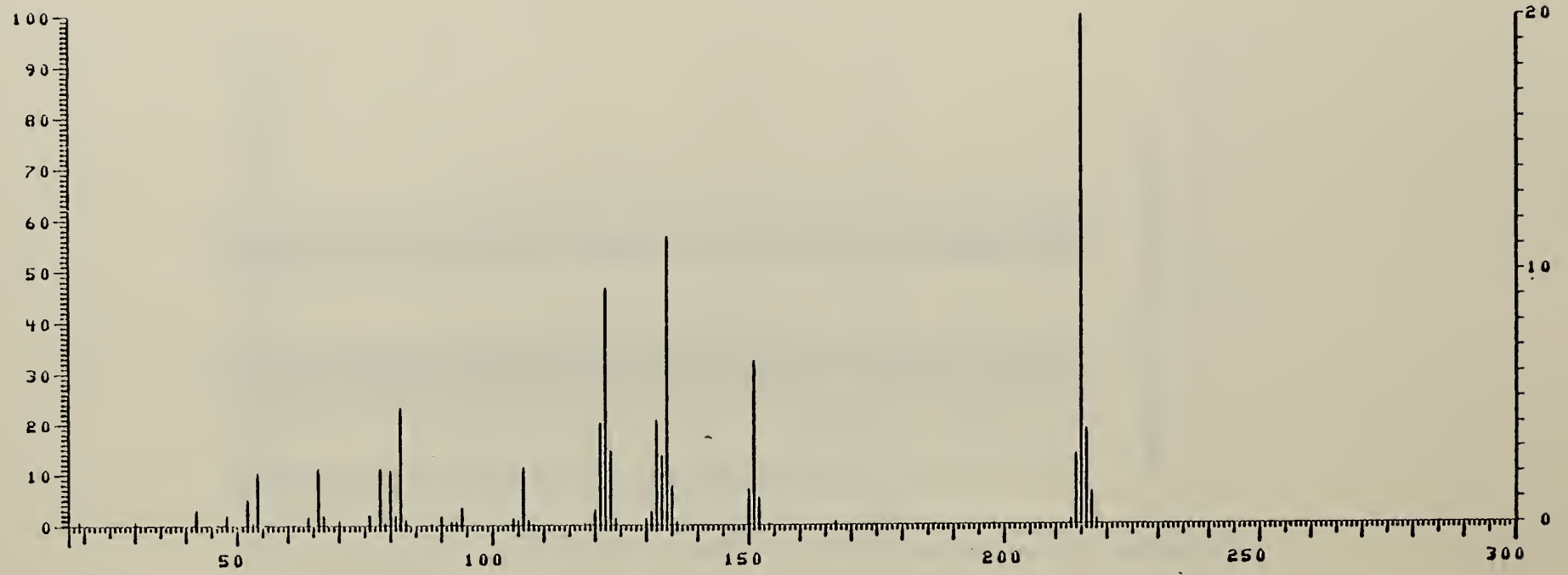
PEAK	I/BASE	MASS
2	0.11%	26.0
5	1.34%	30.0
7	1.03%	34.0
9	0.69%	42.0
11	3.06%	44.0
12	0.76%	45.0
13	100.00%	46.0
14	2.56%	47.0
15	1.02%	48.0
16	1.25%	50.0
17	0.22%	58.0
18	0.27%	60.0
19	0.18%	61.0
20	1.23%	62.0
21	0.17%	64.0
22	0.29%	66.0
23	2.29%	74.0
24	0.10%	75.0
25	0.25%	76.0
26	3.54%	78.0
27	0.13%	79.0
29	0.17%	88.0
30	4.03%	90.0
31	0.21%	91.0
32	1.55%	92.0
33	0.25%	93.0
34	10.86%	94.0
35	0.57%	95.0
36	0.49%	102.0
37	0.36%	104.0
38	0.61%	106.0
40	0.20%	118.0
41	1.59%	120.0
42	0.34%	121.0
43	14.19%	122.0
44	0.90%	123.0
45	0.11%	150.0
46	1.22%	151.0
47	59.69%	152.0
48	4.66%	153.0
49	0.18%	154.0



Mass Spectrum of Naphthalene-d_8

Mass Spectrum of Naphthalene-d_8

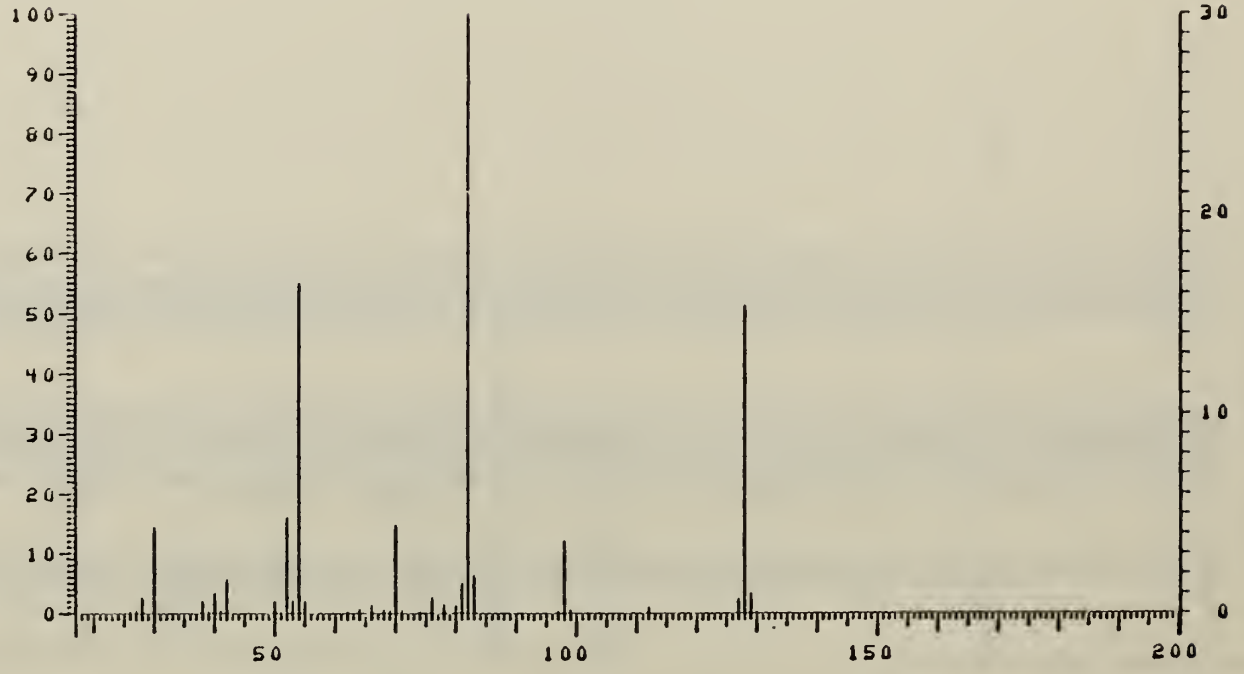
PEAK	I/BASE	MASS
1	0.31%	30.0
3	1.44%	42.0
4	0.18%	50.0
5	3.46%	52.0
6	0.36%	53.0
7	15.10%	54.0
8	0.86%	55.0
9	0.69%	56.0
11	0.40%	62.0
13	1.22%	64.0
14	0.25%	65.0
15	6.60%	66.0
16	0.79%	67.0
17	12.78%	68.0
18	1.18%	69.0
19	0.15%	70.0
20	0.21%	74.0
22	2.32%	76.0
23	0.30%	77.0
24	3.11%	78.0
25	0.27%	79.0
26	3.02%	80.0
27	0.47%	81.0
28	4.18%	82.0
29	0.56%	83.0
30	2.52%	84.0
31	0.17%	85.0
32	0.12%	86.0
33	0.40%	88.0
34	0.69%	90.0
36	0.24%	94.0
37	0.48%	100.0
38	0.22%	102.0
39	0.37%	104.0
40	0.23%	105.0
41	2.36%	106.0
42	0.97%	107.0
43	7.23%	108.0
44	0.65%	109.0
45	0.20%	118.0
48	0.38%	130.0
50	0.54%	131.0
51	5.04%	132.0
52	1.77%	133.0
53	10.54%	134.0
54	15.34%	135.0
55	100.00%	136.0
56	10.54%	137.0
57	0.84%	138.0
60	0.18%	150.0



Mass Spectrum of 2-Naphthalenesulfonic acid-d_7 Inlet: Probe 73 °C

Mass Spectrum of
2-Naphthalenesulfonic acid-d_7
Inlet: Probe 73 °C

PEAK	I/BASE	MASS
1	0.83%	19.0
2	0.71%	30.0
3	0.10%	34.0
5	3.05%	42.0
6	0.59%	46.0
7	2.28%	48.0
8	5.14%	52.0
9	0.84%	53.0
10	10.61%	54.0
11	0.34%	56.0
12	0.21%	59.0
13	0.54%	60.0
14	0.35%	61.0
15	1.68%	64.0
17	11.15%	66.0
18	2.22%	67.0
20	1.13%	70.0
21	2.29%	76.0
22	11.20%	78.0
23	0.87%	79.0
24	10.37%	80.0
25	2.12%	81.0
26	23.35%	82.0
27	1.25%	83.0
29	0.41%	88.0
30	1.87%	90.0
31	0.15%	91.0
32	0.91%	92.0
33	0.86%	93.0
34	3.52%	94.0
37	1.60%	104.0
38	1.25%	105.0
39	11.43%	106.0
40	1.10%	107.0
41	0.36%	108.0
42	0.19%	110.0
44	0.43%	113.0
45	0.34%	119.0
46	3.08%	120.0
47	20.62%	121.0
48	46.75%	122.0
49	14.70%	123.0
50	1.62%	124.0
51	1.42%	130.0
52	2.83%	131.0
53	20.68%	132.0
54	13.96%	133.0
55	56.92%	134.0
56	7.93%	135.0
57	0.78%	136.0
58	0.13%	137.0
59	0.12%	138.0
61	0.11%	148.0
62	0.90%	149.0
63	7.05%	150.0
64	32.42%	151.0
65	5.41%	152.0
66	0.45%	154.0
68	0.22%	164.0
70	0.30%	166.0
71	0.80%	167.0
72	0.19%	168.0
73	0.31%	182.0
74	0.11%	183.0
75	0.16%	197.0
76	0.59%	198.0
78	1.06%	213.0
79	14.23%	214.0
80	100.00%	215.0
81	19.13%	216.0
82	6.62%	217.0
83	1.00%	218.0
84	0.14%	219.0



Mass Spectrum of Nitrobenzene-d_5

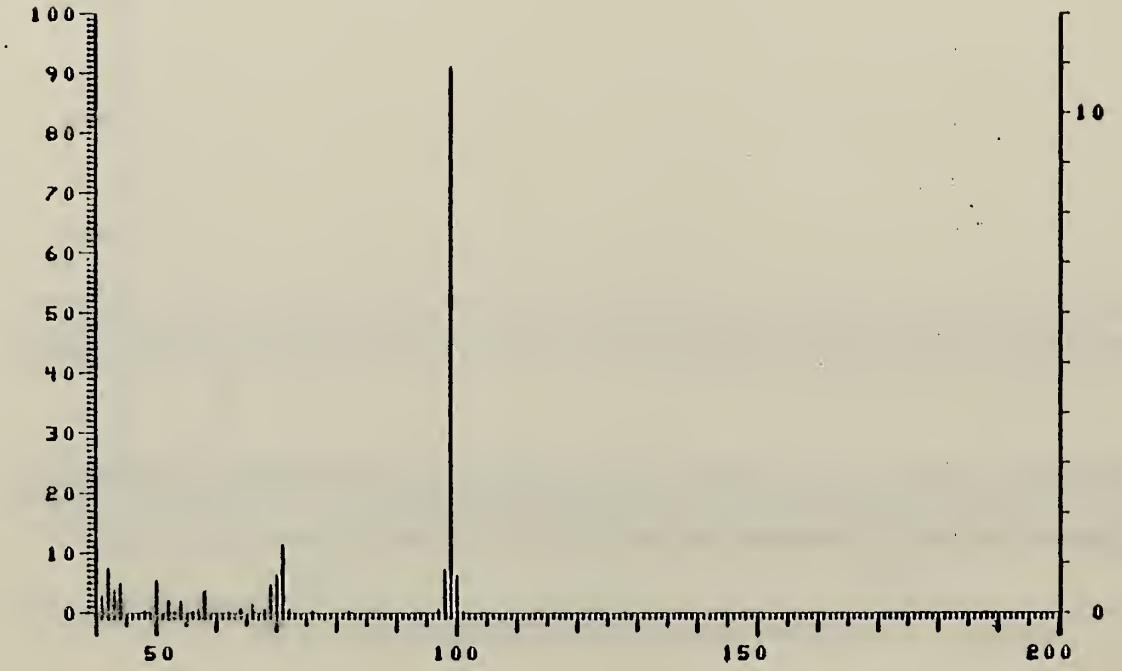
Mass Spectrum of Nitrobenzene-d_5

PEAK	I/BASE	MASS
3	0.51%	26.0
4	0.69%	27.0
5	2.98%	28.0
7	14.47%	30.0
8	0.10%	31.0
9	0.10%	32.0
10	0.10%	33.0
12	0.30%	35.0
13	0.25%	36.0
14	2.06%	38.0
15	0.35%	39.0
16	3.46%	40.0
17	0.99%	41.0
18	5.98%	42.0
19	0.22%	43.0
20	0.14%	44.0
21	0.17%	46.0
22	0.30%	48.0
23	2.20%	50.0
24	0.38%	51.0
25	16.27%	52.0
26	2.44%	53.0
27	55.19%	54.0
28	2.29%	55.0
29	0.13%	56.0
31	0.48%	62.0
32	0.80%	64.0
34	1.45%	66.0
35	0.11%	67.0
36	0.77%	68.0
37	0.81%	69.0
38	14.69%	70.0
39	0.99%	71.0
40	0.10%	72.0
41	0.52%	74.0
43	2.85%	76.0
44	0.22%	77.0
45	1.42%	78.0
46	0.16%	79.0
47	1.53%	80.0
48	5.02%	81.0
49	100.00%	82.0
50	6.45%	83.0
51	0.22%	84.0
52	0.19%	96.0
53	0.66%	97.0
54	12.17%	98.0
55	0.91%	99.0
56	0.10%	100.0
57	1.12%	112.0
59	2.60%	127.0
60	51.44%	128.0
61	3.59%	129.0
62	0.41%	130.0

Mass Spectrum of 2-Phenylethyl-1,1,2,2-d_4-amine

Mass Spectrum of
2-Phenylethyl-1,-,2,2-d_4-amine

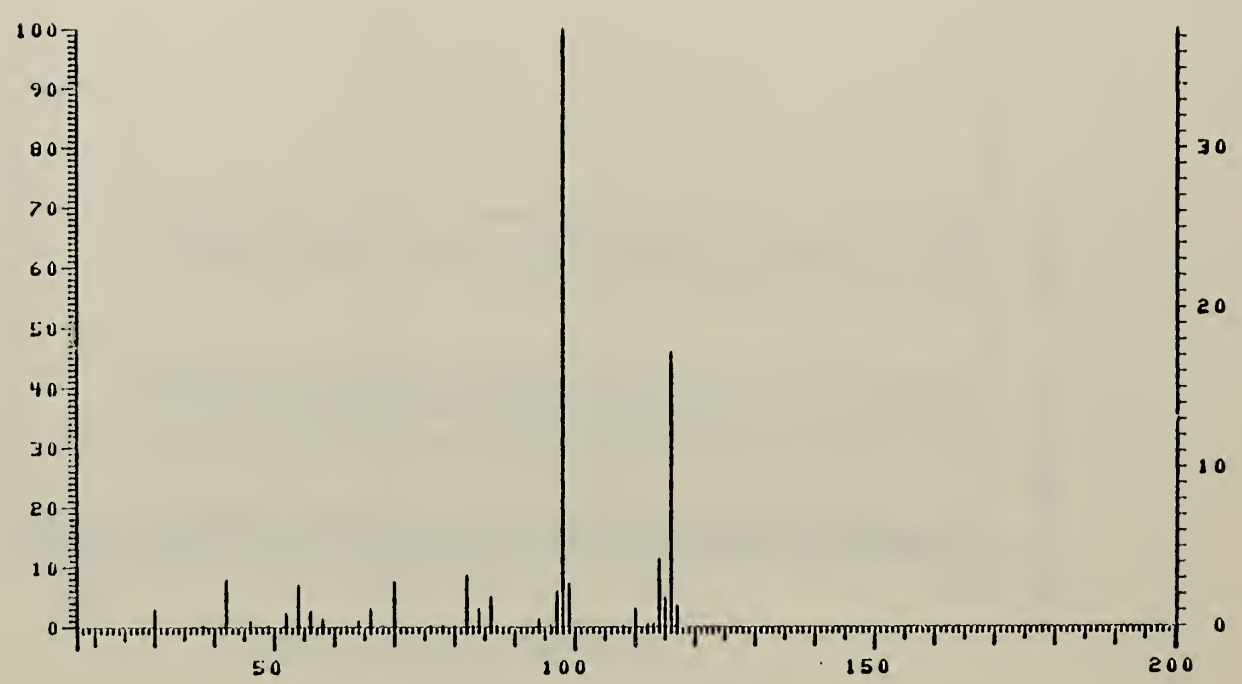
PEAK	I/BASE	MASS
1	0.11%	19.0
2	0.13%	27.0
3	1.54%	29.0
4	0.73%	30.0
5	1.48%	31.0
6	100.00%	32.0
7	29.09%	33.0
8	2.21%	34.0
9	0.14%	37.0
10	0.34%	38.0
11	1.09%	39.0
12	1.36%	40.0
13	0.74%	41.0
14	0.36%	42.0
15	0.45%	43.0
16	0.32%	45.0
17	0.28%	46.0
18	0.76%	50.0
19	1.54%	51.0
20	1.09%	52.0
21	0.78%	53.0
22	0.32%	54.0
23	0.16%	60.0
24	0.17%	61.0
25	0.33%	62.0
26	0.78%	63.0
27	0.94%	64.0
28	1.14%	65.0
29	2.79%	66.0
30	2.77%	67.0
31	0.30%	68.0
32	0.22%	74.0
33	0.20%	75.0
34	0.17%	76.0
35	0.40%	77.0
36	0.66%	78.0
37	0.88%	79.0
38	0.63%	80.0
39	0.31%	81.0
41	0.51%	90.0
42	0.77%	91.0
43	1.54%	92.0
44	8.91%	93.0
45	4.30%	94.0
46	0.70%	95.0
47	0.13%	96.0
48	0.15%	104.0
49	0.39%	105.0
50	0.51%	106.0
51	0.78%	107.0
52	0.11%	108.0
53	0.10%	109.0
55	0.20%	119.0
56	0.19%	120.0
57	0.30%	121.0
58	0.17%	122.0
59	0.40%	123.0
60	0.25%	124.0
61	4.86%	125.0
62	1.66%	126.0
63	0.25%	127.0



Mass Spectrum of Phenol-d_5

Mass Spectrum of Phenol-d_5

PEAK	I/BASE	MASS
24	3.10%	41.0
25	7.46%	42.0
26	4.19%	43.0
27	5.03%	44.0
28	0.18%	45.0
29	0.17%	46.0
31	0.42%	48.0
32	0.44%	49.0
33	5.44%	50.0
34	0.16%	51.0
35	2.21%	52.0
36	0.54%	53.0
37	2.28%	54.0
38	0.24%	55.0
39	0.35%	56.0
40	0.75%	57.0
41	3.70%	58.0
42	0.14%	59.0
43	0.14%	60.0
44	0.38%	62.0
46	0.75%	64.0
47	0.32%	65.0
48	1.62%	66.0
49	0.30%	67.0
50	0.97%	68.0
51	4.87%	69.0
52	6.62%	70.0
53	11.41%	71.0
54	0.72%	72.0
55	0.13%	74.0
56	0.53%	76.0
58	0.24%	78.0
59	0.30%	80.0
60	0.23%	81.0
61	0.62%	82.0
62	0.21%	96.0
63	0.68%	97.0
64	7.62%	98.0
65	91.10%	99.0
66	6.39%	100.0
67	0.37%	101.0



Mass Spectrum of o-Xylene-d_{10}

Mass Spectrum of o-Xylene-d_{10}

PEAK	I/BASE	MASS
1	3.15%	30.0
3	0.15%	34.0
4	0.37%	38.0
5	8.29%	42.0
7	1.23%	46.0
8	0.45%	49.0
9	0.21%	50.0
10	2.55%	52.0
11	0.22%	53.0
12	7.22%	54.0
13	0.30%	55.0
14	2.84%	56.0
15	1.58%	58.0
17	0.38%	62.0
18	1.11%	64.0
19	0.15%	65.0
20	3.29%	66.0
21	0.49%	68.0
22	0.15%	69.0
23	7.88%	70.0
24	0.15%	71.0
25	0.32%	72.0
27	0.54%	76.0
28	0.36%	78.0
29	0.40%	80.0
30	0.18%	81.0
31	8.99%	82.0
32	0.47%	83.0
33	3.30%	84.0
34	0.30%	85.0
35	5.21%	86.0
36	0.36%	87.0
37	0.13%	88.0
38	0.12%	90.0
39	1.39%	94.0
40	0.37%	96.0
41	6.14%	97.0
42	100.00%	98.0
43	7.37%	99.0
44	0.24%	100.0
45	0.49%	108.0
46	0.15%	109.0
47	3.27%	110.0
48	0.21%	111.0
49	0.78%	112.0
50	0.98%	113.0
51	11.52%	114.0
52	5.12%	115.0
53	46.30%	116.0
54	3.94%	117.0
55	0.15%	118.0

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Mass spectra for 24 deuterated organic compounds are given in tabular and graphical form. The mole percent deuterium at labelled positions as determined by mass spectrometry for 23 compounds is given.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)*

Deuterated compounds; isotopic purity; mass spectra; "Master Analytical Scheme"; organic compounds in water

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