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MASS SPECTRA OF SOME ORGANIC AND INORGANIC COMPOUNDS

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UNIVERSITY OF
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*Radiation
Laboratory*

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AND INORGANIC COMPOUNDS

BERKELEY, CALIFORNIA

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UNIVERSITY OF CALIFORNIA

Lawrence Radiation Laboratory
Berkeley, California

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Amos S. Newton and Sylvia J. Waters

February 1959

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MASS SPECTRA OF SOME ORGANIC AND INORGANIC COMPOUNDS

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Lawrence Radiation Laboratory
University of California
Berkeley, California

February 1959

A compilation has been made of some mass spectra of various organic and inorganic compounds which we have run and which are not listed in previous compilations of mass spectral data.¹ These compounds were collected from various sources and many are the result of syntheses in the University of California Chemistry Department or the Lawrence Radiation Laboratory. All have appreciable vapor pressures at room temperatures and were run with a room temperature inlet system on a Consolidated Engineering Corporation Model 21-103 (a few were run on Model 21-102) analytical mass spectrometer.

1. Catalogue of Mass Spectral Data, American Petroleum Institute Research Project 44. F. D. Rossini, editor, Carnegie Institute of Technology, Petroleum Research Laboratory, Pittsburgh, Pennsylvania.

Name of compound: Allyl amine

Parent mass: 57

Structural formula: $\text{CH}_2=\text{CH}-\text{CH}_2\text{NH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	1.38	26	13.39	41	8.32
13	1.66	26.5	2.34	42	3.04
13.5	0.01	27	17.80	43	0.24
14	3.23	27.5	1.57	44	0.35
14.5	0.01	28	75.49	45	0.14
15	4.04	28.5	0.01	46	0.01
16	2.16	29	19.79	47	0.01
17	3.24	29.9	0.20	50	0.58
18	8.12	30	100.00	51	2.55
19	0.28	31	2.49	52	5.06
19.5	0.07	32	0.05	53	0.99
20	0.92	35	0.06	54	6.84
20.5	0.02	36	0.80	55	5.54
21	0.01	37	3.62	56	79.63
24	0.68	38	5.92	57	32.45
25	3.00	39	20.75	58	1.50
25.5	0.02	40	3.14	59	0.03

Relative sensitivity 0.52 at m/e 30 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 8.09.

Source: Eastman Kodak White Label

Name of compound: Allyl formate

Parent mass: 86

Structural formula: $\text{HCOOCH}_2\text{CH:CH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	2.55	32	0.61	53	0.79
13	3.48	33	0.09	54	0.15
14	4.51	36	1.10	55	3.48
15	7.13	37	7.86	56	3.46
16	1.33	38	13.79	57	100.00
17	0.89	39	75.40	58	27.94
18	1.26	40	22.75	59	1.13
19	1.00	41	35.01	60	0.15
20	0.09	42	2.96	68	0.09
21	0.09	43	4.74	69	0.06
22	0.04	44	3.25	70	0.03
24	0.70	45	2.90	71	0.04
25	3.15	46	2.45	73	0.06
26	17.48	47	3.34	74	0.09
27	33.78	48	0.06	77	0.06
28	23.10	51	0.03	85	0.04
29	84.04	52	0.12	86	0.59
30	14.41			87	0.06
31	35.80				

Relative sensitivity 0.51 at m/e 57 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.76.

Source: Eastman Kodak White Label.

Name of compound: Ammonium Carbamate

Parent mass: 78

Structural formula: $\text{NH}_2\text{COONH}_4$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	2.03	17	100.00	29	0.14
13	0.07	18	23.51	44	97.49
14	3.26	19	2.09	45	1.27
15	8.70	22	1.68	46	0.43
16	91.34	28	10.52		

Relative sensitivity 0.27 at m/e 17 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 8.01.

Source: Synthesis.

Name of compound: n-Amyl acetate

Parent mass: 130

Structural formula: $\text{CH}_3\text{CO}_2\text{C}_5\text{H}_{11}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.22	45	1.75	72	1.88
12	0.25	46	0.03	73	8.88
13	0.78	47	0.01	74	0.72
14	3.35	49	0.04	75	0.17
15	15.63	50	0.28	76	0.01
16	0.32	51	0.44	77	0.01
17	0.09	52	0.17	83	0.01
18	0.21	53	1.13	84	0.01
19	0.10	54	0.59	85	0.81
25	0.10	55	18.40	86	0.23
25.5	0.04	56	1.54	87	5.62
26	2.06	57	2.17	88	0.90
27	16.21	58	2.58	89	0.07
28	5.17	59	0.65	90	0.01
29	14.75	60	0.18	91	0.12
30	0.59	61	15.14	92	0.08
31	1.98	62	0.33	93	0.01
32	0.06	63	0.12	97	0.20
33	0.03	64	0.01	98	0.01
37	0.30	65	0.09	101	0.33
38	0.75	66	0.10	102	0.04
39	8.98	67	0.62	112	0.06
40	1.61	68	1.07	115	0.27
41	15.20	69	4.65	116	0.01
42	20.75	70	30.40	130	0.12
43	100.00	71	4.76	131	0.03
44	2.88				

Relative sensitivity 1.77 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.75.

Source: Eastman Kodak White Label.

Name of compound: Isoamyl acetate

Parent mass: 130

Structural formula: $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.22	45	1.88	75	0.24
12	0.25	46	0.07	76	0.01
13	0.80	49	0.04	82	0.01
14	3.53	50	0.34	83	0.04
15	16.60	51	0.51	84	0.05
16	0.34	52	0.18	85	0.75
17	0.05	53	1.14	86	0.50
18	0.12	54	0.74	87	2.16
19	0.09	55	26.86	88	0.30
25	0.09	56	2.38	89	0.05
25.5	0.03	57	2.92	90	0.01
26	1.61	58	1.33	91	0.05
27	14.56	59	0.20	92	0.04
28	4.41	60	0.17	94	0.02
29	11.98	61	7.93	97	0.26
30	0.47	62	0.20	98	0.02
31	1.50	63	0.08	101	0.69
32	0.04	64	0.01	102	0.10
33	0.01	65	0.05	103	0.02
36	0.01	66	0.04	111	0.01
37	0.32	67	0.20	112	0.19
38	0.80	68	0.17	113	0.04
39	9.54	69	3.33	115	0.42
40	1.45	70	35.76	116	0.04
41	14.60	71	2.73	128	0.05
42	12.22	72	1.43	129	0.14
43	100.00	73	8.29	130	0.02
44	2.75	74	1.52	131	0.01

Relative sensitivity 1.76 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.75.

Source: Eastman Kodak White Label.

Name of compound: Isoamyl amine

Parent mass: 87

Structural formula: $(\text{CH}_3)_2\text{CH}(\text{CH}_2)_2\text{NH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.24	35.5	0.02	59	1.05
12	0.09	36	0.04	60	0.03
13	0.18	37	0.39	61	0.01
14	0.72	38	0.83	62	0.02
15	3.86	38.5	0.02	63	0.04
16	0.33	39	5.62	64	0.01
17	0.71	40	0.94	65	0.04
18	5.35	41	6.01	66	0.03
19	0.02	42	3.56	67	0.07
25	0.10	43	3.31	68	0.10
26	1.13	44	4.25	69	0.20
26.5	0.01	45	1.38	70	3.04
27	7.66	46	0.03	71	0.26
28	8.00	49	0.06	72	0.35
29	4.00	50	0.33	73	0.60
30	100.00	51	0.38	74	0.04
31	2.33	52	0.22	77	0.02
32	0.36	53	0.43	78	0.05
32.5	0.02	54	0.39	83	0.04
33.5	0.08	55	2.42	84	0.06
34	0.01	56	1.23	86	0.23
34.5	0.04	57	0.58	87	2.59
35	0.03	58	1.40	88	0.17

Relative sensitivity 2.45 at m/e 30 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.80.

Source: Eastman Kodak White Label

Name of compound: IsoAmyl nitrite

Parent mass: 117

Structural formula $(\text{CH}_3)_2 \text{CH CH}_2 \text{CH}_2 \text{ONO}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.41	41	90.56	67	0.16
13	0.62	42	13.03	68	0.15
14	3.65	43	34.98	69	2.92
15	10.97	44	4.56	70	2.58
16	0.83	45	3.40	71	13.92
17	0.14	46	0.65	72	1.35
18	0.17	47	0.04	73	0.10
19	0.41	48	0.04	74	0.10
24	0.03	49	0.23	75	0.04
25	0.29	50	1.12	76	0.16
25.2	0.02	51	1.27	77	0.02
25.6	0.03	52	0.38	78	0.01
26	4.71	53	2.06	83	0.03
27	39.56	54	0.47	84	0.03
28	8.63	55	9.06	85	0.78
29	100.00	56	3.48	86	0.67
29.5	0.04	57	57.01	87	0.08
30	55.47	58	3.63	88	0.03
31	7.44	59	0.21	89	0.03
32	0.33	60	32.42	102	0.06
33	0.07	61	0.56	103	0.07
36	0.08	62	0.17	104	0.02
37	1.50	63	0.05	108	0.01
38	3.17	64	0.02	150	0.09
39	29.55	65	0.02		
40	4.27	66	0.03		

Relative sensitivity 0.75 at m/e 29 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.77.

Source: Eastman Kodak White Label.

Name of compound: Arsine (Arsenic hydride)

Parent mass: 78

Structural formula: AsH_3 UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	1.17	27	0.07	40	0.01
12	0.03	28	0.40	41	0.04
13	0.01	29	0.07	42	0.04
14	0.04	30	0.02	43	0.04
15	0.04	31	0.05	44	0.09
16	0.07	32	0.07	45	0.04
17	0.29	35	0.12	46	0.01
18	0.02	36	0.56	49	0.04
19	0.01	37	0.05	75	35.30
20	0.01	37.5	1.06	76	<u>100.00</u>
21	0.01	38	1.84	77	23.84
25	0.01	38.5	0.22	78	72.23
26	0.04	39	0.05		

Relative sensitivity 8.97 at m/e 76 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.74.

Source: Synthesis.

Name of compound: Azomethane

Parent mass: 58

Structural formula: $\text{CH}_3\text{N} = \text{NCH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.70	30	2.80	49	0.02
12	1.16	31	0.06	50	0.18
13	3.50	32	0.11	52	0.10
14	10.39	35	0.01	53	0.66
15	100.00	36	0.01	54	0.06
16	1.25	38	0.06	55	0.16
17	0.04	39	0.06	56	0.18
18	0.10	40	0.16	57	1.74
24	0.06	41	2.31	58	15.54
25	0.13	42	17.84	59	0.43
26	1.77	43	35.10	71	0.04
27	12.86	44	0.76	72	0.07
27.5	0.04	45	0.01	73	0.02
28	28.95	46	0.01	86	0.01
29	1.88	47	0.01	88	0.02

Relative sensitivity 1.09 at m/e 15 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.65.

Source: Synthesis.

Name of compound: Boron trifluoride

Parent mass: 68 (B^{11})

Structural formula: BF_3

UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
1	0.06	24.5	1.21	45	0.03
10	1.49	27	0.03	46	0.24
11	5.41	28	0.26	47	0.65
14	0.04	29	0.33	48	26.85
14.5	0.13	30	1.14	49	<u>100.00</u>
15	0.48	32	0.07	64	0.32
16	0.04	35	0.05	65	0.10
18	0.05	36	0.20	66	0.36
19	3.15	38	0.13	67	1.32
20	0.11	43	0.03	68	4.79
24	0.32	44	0.09		

Relative sensitivity ~0.50 at m/e 49 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: 98.5%

$\frac{43}{58}$ for n-butane ~7.99.

Source: Matheson.

Remarks - Run at low field.

Name of compound: Isobutyl acetate.

Parent mass: 116

Structural formula: $\text{CH}_3\text{CO}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.20	41	12.92	68	0.01
12	0.31	42	4.32	69	0.04
13	0.92	43	<u>100.00</u>	70	0.19
14	3.53	44	3.55	71	2.45
15	14.96	45	1.18	72	0.26
16	0.33	46	0.03	73	14.72
17	0.07	49	0.04	74	1.46
18	0.16	50	0.20	75	0.29
19	0.07	51	0.23	76	0.01
25	0.14	52	0.07	82	0.02
26	1.53	53	0.37	83	0.03
27	10.69	54	0.19	84	0.01
28	3.07	55	2.19	85	0.06
29	9.41	56	23.01	86	1.97
30	0.63	57	3.96	87	0.41
31	1.84	58	0.40	88	0.06
32	0.04	59	0.43	101	0.19
33	0.15	60	0.13	102	0.03
37	0.41	61	2.74	115	0.08
38	0.94	62	6.74	116	0.10
39	7.93	63	0.01	117	0.01
40	1.29	67	0.02		

Relative sensitivity 2.09 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.79.

Source: Eastman Kodak White Label.

Name of compound: Carbon Suboxide

Parent mass: 68

Structural formula: C_3O_2 UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	54.75	34	5.69	57	0.10
13	2.29	34.5	0.17	58	0.16
14	2.15	36	4.91	60	0.03
15	2.97	37	10.89	61	0.04
16	3.89	38	14.01	62	0.04
17	0.10	39	42.94	63	0.13
18	0.43	40	139.19	64	0.17
19	1.37	41	11.12	65	0.29
19.5	1.10	42	2.28	66	0.30
20	0.71	43	1.95	67	0.33
22	0.14	44	8.75	68	100.00
24	20.01	45	0.14	69	4.01
25	2.59	46	0.06	70	1.20
25.5	10.35	48	0.35	74	0.07
26	5.40	49	1.12	76	0.07
26.5	0.04	50	3.36	77	0.23
27	7.97	51	3.21	78	0.95
28	35.62	52	5.59	79	0.19
29	5.09	53	5.03	80	0.12
30	0.14	54	6.52	91	0.30
31	0.06	55	1.61	92	0.19
32	0.09	56	2.38		

Relative sensitivity 0.36 at m/e 68 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity :

 $\frac{43}{58}$ for n-butane 8.08.

Source: synthesis.

Name of compound: Threo-3-Chloro 2 acetoxabutane

Parent mass: 150 (Cl^{35})Structural formula: $\text{CH}_3(\text{CH}_2\text{COO})\text{CHCHClCH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.25	44	2.74	75	0.37
13	0.78	45	0.23	76	0.07
14	3.14	47	0.05	77	0.13
15	12.62	48	0.09	78	0.02
16	0.30	49	0.57	79	0.02
17	0.01	50	0.51	83	0.07
18	0.03	51	0.75	84	0.01
19	0.08	52	0.20	85	0.01
22	0.02	53	1.21	86	0.02
24	0.01	54	0.70	87	24.25
25	0.17	55	8.02	88	1.07
25.5	0.02	56	0.92	89	0.30
26	2.40	57	0.48	90	2.38
27	12.90	58	0.04	91	0.88
28	3.33	59	0.02	92	0.79
29	5.60	60	0.07	93	0.18
30	0.13	61	1.85	97	0.01
31	0.14	62	0.49	101	0.06
32	0.02	63	2.31	102	0.01
35	0.12	64	0.21	106	0.02
36	0.18	65	0.70	107	0.04
37	0.26	66	0.02	108	0.01
38	0.52	69	0.02	109	0.02
39	3.85	71	0.21	114	0.28
40	0.37	72	4.07	115	0.11
41	2.53	73	1.37	116	0.01
42	2.38	74	0.07	134	0.27
43	<u>100.00</u>			136	0.08

Relative sensitivity 2.54 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity: 3.3% 3-chloro-2-butanol removed from spectrum.

 $\frac{43}{58}$ for n-butane 7.74.

Source: Synthesis.

Name of compound: Ethyro-3-chloro 2-butanol

Parent mass: 108 (Cl³⁵)Structural formula: $\text{CH}_3\text{CHClCH}_2\text{CH}_2\text{OH}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.29	42	1.69	70	0.03
13	0.63	43	13.20	71	0.37
14	2.12	44	2.20	72	0.34
15	8.08	45	100.00	73	0.85
16	0.31	46	2.20	74	0.04
17	0.25	47	0.30	75	0.30
18	0.36	48	0.22	76	0.06
19	3.19	49	0.71	77	0.12
24	0.09	50	0.48	78	0.21
25+	0.60	51	0.81	79	0.03
25.5	0.09	52	0.19	80	0.07
26	4.80	53	0.93	83	0.03
27	21.11	54	0.24	87	0.15
28	3.50	55	5.43	88	0.01
29	18.07	56	0.52	89	0.04
30	0.74	57	4.07	90	0.10
31	2.99	58	0.31	91	0.16
32	0.05	59	0.03	92	0.10
33	0.01	60	0.14	93	2.28
34	0.01	61	0.45	94	0.09
35	0.51	62	0.50	95	0.70
36	0.78	63	1.53	96	0.03
37	0.88	64	0.22	105	0.01
38	1.09	65	0.74	106	0.01
39	3.59	66	0.03	107	0.16
40	0.37	67	0.10	108	0.03
41	2.01	69	0.04	109	0.05

Relative sensitivity 1.78 at m/e 45 referred to n-butane m/e 43.

Instrument model: CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.81.

Source: Synthesis.

Name of compound: Threo 3-Chloro 2-butanol

Parent mass: 108 (Cl³⁵)Structural formula: $\text{CH}_3\text{CH}(\text{Cl})\text{CHOHCH}_3$ UNCERTIFIED MASS SPECTRUM

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.31	44	2.28	73	0.76
13	0.64	45	100.00	74	0.04
14	2.12	46	2.19	75	0.27
15	8.05	47	0.31	76	0.06
16	0.32	48	0.21	77	0.12
17	0.27	49	0.69	78	0.22
18	0.33	50	0.81	79	0.04
19	3.24	51	0.79	80	0.08
24	0.08	52	0.19	81	0.03
25	0.59	53	0.91	83	0.04
25.5	0.09	54	0.23	84	0.01
26	4.87	55	5.45	85	0.01
27	21.24	56	0.49	86	0.02
28	3.55	57	4.20	87	0.14
29	18.66	58	0.33	89	0.03
30	0.76	59	0.03	90	0.09
31	3.09	60	0.14	91	0.16
32	0.04	61	0.44	92	0.10
33	0.01	62	0.44	93	2.75
34	0.02	63	1.47	94	0.11
35	0.52	64	0.19	95	0.88
36	0.81	65	0.73	96	0.02
37	0.89	66	0.03	97	0.02
38	1.08	67	0.11	105	0.02
39	3.58	69	0.05	106	0.15
40	0.38	70	0.04	107	0.03
41	2.07	71	0.36	108	0.06
42	1.68	72	0.27	109	0.06
43	12.60				

Relative sensitivity 1.80 at m/e 45 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.81.

Source: Synthesis.

Name of compound: Chloro methyl ether

Parent mass: 80 (Cl^{35})Structural formula: $\text{Cl CH}_2\text{OCH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.05	30	4.92	50	0.12
12	1.56	31	1.09	51	5.36
13	3.32	32	0.12	52	0.26
14	9.34	33	0.04	53	0.32
15	38.89	35	3.40	60	0.02
16	1.15	36	1.97	61	0.06
17	0.62	37	1.37	63	0.54
17.5	0.03	38	0.64	65	0.20
18	0.06	39	0.11	73	0.02
18.5	0.04	40	0.02	74	0.20
19	0.04	41	0.08	76	0.02
22	0.04	42	0.29	77	0.04
24	0.02	43	0.55	78	0.03
24.5	0.02	44	1.48	79	0.96
25	0.02	45	100.00	80	0.56
26	0.08	46	2.26	81	0.33
27	0.14	47	1.36	82	0.20
28	3.22	48	1.43	83	0.04
29	43.16	49	13.92		

Relative sensitivity 0.93 at m/e 45 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: 24.1% of Methylal removed from the spectrum.

 $\frac{43}{58}$ for n-butane 7.62.

Source: Eastman Kodak White Label.

Name of compound: Cyclohexyl amine (Amino hexa hydrobenzene)

Parent mass: 99

Structural formula: $\text{CH}_2\text{-CH}_2\text{-CH}_2\text{-CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.08	39.5	0.02	65	0.27
13	0.11	40	1.24	66	0.23
14	0.54	40.5	0.08	67	1.40
14.9	0.03	41	6.86	68	0.49
15	4.03	42	7.32	69	0.65
16	0.43	43	29.61	70	5.59
17	1.21	44	2.18	71	0.37
18	4.27	45	0.22	72	0.01
19	0.08	45.5	0.02	73	0.01
20	0.01	46	0.01	74	0.03
25	0.09	46.5	0.12	75	0.03
26	1.80	47	0.03	76	0.01
26.5	0.02	47.5	0.05	77	0.37
27	9.57	48	0.01	78	0.14
27.5	0.03	49	0.11	79	0.47
28	14.75	50	0.54	80	0.19
29	5.03	51	0.93	81	0.71
30	14.47	52	0.60	82	0.70
31	0.47	53	1.66	83	0.07
32	0.04	54	2.25	84	0.08
32.5	0.02	55	2.24	93	0.05
33.5	0.09	56	100.00	94	0.06
34	0.01	57	6.50	95	0.01
34.5	0.09	58	0.22	96	0.09
35	0.01	59	0.04	97	0.02
36	0.02	60	0.04	98	1.21
37	0.37	61	0.04	99	11.43
38	0.97	62	0.08	100	1.47
38.5	0.01	63	0.15	101	0.65
39	7.15	64	0.04	102	0.12

Relative sensitivity 1.48 at m/e 56 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature 250°.

Additional information:

Glass inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.92.

Source: Eastman Kodak White Label.

Name of compound: 1,2-Dibromo propane

Parent mass: 200 (Br⁷⁹)Structural formula: $\text{CH}_3\text{CHBrCH}_2\text{Br}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	1.15	46	0.01	83	0.13
13	1.54	47	0.01	84	0.01
14	2.84	48	0.01	85	0.01
15	5.82	49	0.07	91	0.49
16	0.11	50	0.03	92	0.35
17	0.02	51	0.05	93	5.29
18	0.07	52	0.01	94	0.39
19	0.07	53	0.05	95	4.79
19.5	0.03	54	0.02	96	0.07
20	0.03	55	0.30	97	0.17
24	0.45	56	0.03	102	0.04
25	2.14	57	0.09	103	0.04
26	10.23	58	0.03	104	0.30
27	27.88	59	0.10	105	2.39
28	2.09	60	0.06	106	0.93
29	0.29	60.5	0.12	107	10.91
30	0.02	61	0.05	108	0.84
31	0.39	61.8	0.10	109	9.11
32	0.04	62	0.02	110	0.09
35	0.07	63	0.32	115	0.03
36	0.94	64	0.02	116	0.03
37	6.24	65	0.10	117	0.10
38	10.40	75	0.01	118	0.01
39	48.39	76	0.08	119	0.50
40	5.02	77	0.25	120	0.14
41	100.00	78	0.04	121	66.36
42	8.53	79	3.35	122	2.71
43	0.36	80	1.11	123	64.52
44	0.03	81	3.19	124	2.50
45	0.18	82	1.09		

Relative sensitivity 0.79 at m/e 41 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane ~7.95 (average from Apr. 27 and May 20 butanes).

Source: Eastman Kodak White Label.

Remarks - Parent peaks outside range and not scanned.

Name of compound: Diethyl selenide (mono)

Parent mass: 138 (Se⁸⁰)Structural formula: $\text{CH}_3\text{CH}_2\text{SeCH}_2\text{CH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.77	43	0.13	80	26.97	109	22.93
12	0.51	44	0.05	81	11.48	110	69.14
13	1.00	45	0.14	82	43.01	111	5.63
14	2.49	46	0.09	83	10.83	112	12.32
15	4.30	47	0.19	84	7.36	113	0.41
16	0.11	48	0.01	85	1.68	114	0.17
17	0.02	50	0.07	86	0.04	117	0.26
18	0.09	51	0.07	87	0.16	119	2.27
24	0.35	53	0.12	88	0.27	120	1.74
25	2.46	55	1.49	89	1.63	121	5.52
26	24.24	56	0.13	90	1.99	122	0.44
27	<u>100.00</u>	57	0.56	91	6.72	123	11.48
28	11.66	58	0.09	92	4.25	124	0.27
29	99.03	59	0.10	93	14.51	125	1.98
30	2.19	60	0.07	94	3.89	126	0.04
31	0.02	61	0.23	95	16.18	132	0.81
32	0.11	62	0.13	96	0.85	133	0.18
33	0.07	63	0.04	97	2.64	134	8.49
34	0.12	64	0.02	101	0.62	135	7.52
35	0.09	66	0.24	102	0.77	136	21.91
36	0.02	74	0.08	103	2.59	137	1.69
37	0.10	75	0.32	104	4.39	138	45.08
38	0.11	76	1.81	105	9.48	139	2.64
39	0.83	77	2.36	106	20.81	140	8.15
40	0.12	78	11.59	107	27.85	141	0.53
41	9.99	79	11.66	108	39.13	142	0.13
42	0.36						

Relative sensitivity 0.54 at m/e 27 referred to n-butane m/e 43.

Instrument model: CEC 21-103

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.79.

Source: Eastman Kodak White Label.

Name of compound: 2,5-Dimethyl 2,4-hexadiene

Parent mass: 110

Structural formula: $(CH_3)_2C=CHCH=C(CH_3)_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.81	41.5	0.09	60	0.14	87	0.25
12	0.12	42	3.73	61	0.56	89	0.51
13	0.23	43	8.03	62	1.42	90	0.75
14	1.02	43.5	0.07	63	3.45	91	6.88
15	12.46	44	0.44	63.5	0.33	92	1.89
16	0.39	44.5	0.10	64	0.94	93	9.16
17	0.05	45	0.83	65	7.16	94	3.33
18	0.04	45.5	0.43	66	3.69	95	100.00
24	0.07	46	0.54	67	50.98	96	77.78
24.7	0.10	46.5	0.45	68	14.91	97	0.35
25	0.07	47	0.56	69	6.16	98	0.07
26	2.45	47.5	0.65	70	1.33	99	0.10
27	27.79	48	0.53	71	0.12	100	0.16
28	4.44	49	0.50	72	0.04	101	0.40
29	11.39	50	4.64	73	0.24	102	0.12
30	0.28	51	11.04	74	0.65	103	0.14
31	0.13	51.5	0.20	75	0.75	104	0.10
32	0.10	52	4.93	77	12.58	105	0.34
35	0.04	52.5	0.29	78	3.33	106	0.18
36	0.16	53	22.19	79	11.04	107	0.58
37	1.34	53.5	0.35	80	4.26	108	0.31
37.2	0.25	54	5.23	81	13.34	109	2.25
38	3.94	55	35.13	82	3.11	110	56.26
38.5	0.19	55.5	0.22	83	1.84	111	5.00
39	39.57	56	4.82	84	0.81	112	0.25
39.5	0.21	57	0.73	85	0.45	113	0.54
40	6.81	58	0.10	86	0.36	114	0.10
41	44.11	59	0.33			125	0.04

Relative sensitivity 0.82 at m/e 95 referred to n-butane m/e 43.

Instrument model: CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.93

Source: Monomer Polymer Corp.

Name of compound: 2,2 Dimethoxy propane (acetone dimethyl acetal)

Parent mass: 104

Structural formula: $\text{CH}_3\text{C}(\text{OCH}_3)_2\text{CH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.93	32	10.32	52	0.05
12	1.17	33	1.98	53	0.48
13	2.39	34	0.07	54	0.16
14	7.56	35	0.04	55	3.00
15	37.16	36	0.26	56	0.56
15.5	0.08	37	2.20	57	4.23
16	0.76	37.2	0.19	58	0.58
17	0.42	38	4.27	59	0.59
18	0.16	39	21.76	60	0.03
19	0.26	39.5	0.16	69	0.04
19.5	0.05	40	8.07	70	0.03
20	0.05	41	33.81	71	0.28
20.7	0.08	42	46.60	72	18.74
23	0.04	43	63.37	73	100.00
24	0.10	44	1.66	74	4.45
25	0.69	45	8.07	75	0.36
25.2	0.19	46	0.21	76	0.02
26	4.66	47	3.81	88	0.07
27	22.18	48	0.10	89	23.14
28	6.47	49	0.03	90	1.03
29	38.72	50	0.04	91	0.13
30	3.33	51	0.05	104	0.00
31	21.26				

Relative sensitivity 0.70 at m/e 73 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature. Purity: > 98%

 $\frac{43}{58}$ for n-butane 7.96.

Source: Synthesis.

Name of compound: Di-iso-propyl amine

Parent mass: 101

Structural formula: $[(CH_3)_2CH]_2NH$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.27	38	0.86	64	0.02
12	0.11	39	7.67	65	0.02
13	0.29	39.3	0.05	66	0.04
14	1.45	40	1.53	67	0.11
15	15.61	40.5	0.07	68	0.48
16	0.55	41	12.78	69	0.16
17	0.26	41.5	0.01	70	2.25
18	4.06	42	14.48	71	0.77
19	0.02	42.5	0.01	72	0.79
22	0.21	43	12.19	73	0.12
25	0.07	43.9	0.15	73.5	0.11
26	1.51	44	100.00	80	0.04
27	13.24	45	2.57	81	0.02
28	11.73	46	0.01	82	0.10
29	1.45	50	0.04	83	0.04
30	3.86	51	0.11	84	0.67
31	0.08	52	0.28	85	0.39
32	0.07	53	0.14	86	39.73
33.5	0.12	54	0.52	87	2.22
34	0.09	55	0.21	88	0.05
34.5	0.52	56	1.96	98	0.06
35	0.11	57	0.58	99	0.06
35.5	0.02	58	8.69	100	1.42
36	0.01	59	0.31	101	4.39
37	0.37	60	0.01	102	0.30

Relative sensitivity 1.78 at m/e 44 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.63.

Source: Eastman Kodak White Label

Name of compound: Di-n-propyl amine

Parent mass: 101

Structural formula: $(\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{NH}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.43	38	1.16	67	0.13
12	0.13	39	11.29	68	0.75
12.6	0.09	39.2	0.27	69	0.20
13	0.27	40	1.73	70	4.69
14	1.37	41	23.63	71	0.56
15	9.19	42	8.73	72	100.00
16	0.23	43	32.56	73	4.70
17	0.32	44	10.79	74	0.06
18	2.50	45	0.29	78	0.02
25	0.20	46	0.02	79	0.01
26	3.50	50	0.05	80	0.06
26.5	0.02	51	0.16	81	0.02
27.5	28.79	51.5	0.02	82	0.08
28	21.25	52	0.42	83	0.03
29	10.18	53	0.21	84	0.52
30	92.15	54	1.10	85	0.05
31	1.45	55	0.62	86	2.90
32	0.05	56	4.39	87	0.18
32.5	0.03	57	1.16	88	0.01
33.5	0.12	58	6.73	98	0.24
34	0.03	59	0.29	99	0.35
34.5	0.05	60	0.02	100	2.39
35	0.02	64	0.02	101	10.12
36	0.02	65	0.02	102	0.68
37	0.51	66	0.02		

Relative sensitivity 1.19 at m/e 72 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.63.

Source: Eastman Kodak White Label

Name of compound: Di-n-propyl ether

Parent mass: 102

Structural formula: $(C_2H_5CH_2)_2O$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.15	32	0.09	55	2.74
12	0.09	33	0.03	56	0.21
13	0.15	35	0.01	57	1.01
14	0.80	36	0.04	58	0.53
15	4.08	37	0.31	59	3.16
16	0.39	38	0.76	60	0.14
17	1.36	39	8.04	61	0.09
18	4.54	40	1.31	69	0.04
19	0.09	41	18.23	70	0.01
20	0.08	42	4.33	71	0.19
24	0.01	43	100.00	72	0.07
25	0.13	44	4.86	73	16.39
25.3	0.01	45	1.67	74	0.71
26	2.51	46	0.04	75	0.04
27	22.02	50	0.01	87	0.13
28	3.99	51	0.01	100	0.08
29	8.33	52	0.01	101	0.15
30	0.83	53	0.05	102	7.12
31	6.21	54	0.05	103	0.37

Relative sensitivity 1.76 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.88.

Source: Eastman Kodak White Label.

Name of compound: Ethyl benzyl ether

Parent mass: 136

Structural formula: $C_2H_5OCH_2C_6H_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.54	41	2.82	62	1.95	92	78.72
12	0.21	42	0.44	63	5.83	93	5.74
13	0.42	43	1.41	64	1.78	94	0.21
14	1.77	43.5	0.03	65	15.81	99	0.24
15	1.55	44	0.34	66	0.96	100	0.33
16	0.31	44.5	0.06	67	0.08	101	0.38
17	0.06	45	0.60	67.5	0.24	102	0.10
18	0.08	45.5	0.21	68	0.06	103	0.08
19	0.08	46	0.26	73	0.21	104	0.10
24	0.05	46.5	0.15	74	1.01	105	3.27
25	0.24	48	0.06	75	1.41	106	1.57
26	2.60	49	0.41	76	1.06	107	17.14
27	10.92	50	5.37	77	17.23	108	2.58
28	2.57	51	13.19	78	4.12	109	0.20
29	13.83	52	3.37	79	33.24	120	0.05
30	2.06	53	1.60	80	2.54	121	0.05
31	4.70	54	0.08	81	0.13	122	0.08
32	0.08	55	0.13	85	0.34	125	0.06
36	0.06	57	0.36	86	0.36	126	0.16
37	0.75	58	0.47	87	0.24	128	0.06
37.5	0.06	59	0.69	88	0.31	135	9.95
38	2.37	60	0.13	89	4.63	136	8.48
38.5	0.08	60.5	1.23	90	3.81	137	0.80
39	13.21	61	0.62	91	<u>100.00</u>	138	0.06
40	1.01						

Relative sensitivity 1.01 at m/e 91 referred to n-butane m/e 43.

Instrument model: CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.63.

Source: Eastman Kodak White Label

Name of compound: Ethyl n-caproate

Parent mass: 144

Structural formula: $\text{CH}_3(\text{CH}_2)_4\text{CO}_2\text{C}_2\text{H}_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.45	40	4.64	66	0.28	91	0.11
12	0.23	41	42.95	67	0.88	92	0.14
13	0.45	42	35.00	68	0.89	95	0.06
14	2.42	43	85.91	69	8.48	96	0.14
15	11.95	44	4.08	70	22.20	97	1.90
16	0.54	45	22.95	71	26.82	98	1.36
17	0.10	46	0.63	72	1.81	99	53.86
18	0.14	47	0.56	73	27.42	100	3.85
19	0.77	48	0.25	74	4.76	101	26.21
24	0.05	49	0.10	75	1.02	102	3.46
25	0.27	50	0.52	76	0.08	103	0.31
25.2	0.34	51	1.39	77	0.12	104	0.04
26	7.84	52	0.54	78	0.15	105	0.11
26.2	0.32	53	2.95	79	0.11	113	0.08
27	68.71	54	1.29	80	0.41	114	0.33
28	18.68	55	23.41	81	0.56	115	8.44
29	98.41	56	5.73	82	0.23	116	0.92
30	3.53	57	5.21	83	1.47	117	4.75
31	3.78	58	0.51	84	0.23	118	0.34
32	0.19	59	1.61	85	0.46	119	0.04
33	0.11	60	45.00	86	0.25	127	0.31
34	0.14	61	24.70	87	7.30	129	0.36
37	0.58	62	0.86	88	100.00	143	0.16
38	0.23	63	0.32	89	5.80	144	1.49
39	23.18	65	0.33	90	0.61	145	0.25
39.5	0.43						

Relative sensitivity 0.67 at m/e 88 referred to n-butane m/e 43

Instrument model: CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.94.

Source: Synthesis

Name of compound: Ethyl n-valerate

Parent mass: 130

Structural formula: $\text{CH}_3(\text{CH}_2)_3\text{CO}_2\text{C}_2\text{H}_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.32	46	0.47	74	1.76
13	0.61	47	0.41	75	0.64
14	3.33	48	0.01	76	0.04
15	11.12	49	0.09	77	0.05
16	0.52	50	0.71	78	0.29
17	0.13	51	0.95	79	0.03
18	0.24	52	0.42	80	0.01
19	0.66	53	1.78	81	0.03
24	0.05	54	0.78	82	0.06
25	0.39	55	13.36	83	1.30
25.2	0.09	56	9.64	84	0.79
25.5	0.03	57	51.15	85	56.87
26	8.75	58	2.52	86	3.42
27	55.34	59	1.87	87	1.98
28	23.17	60	32.14	88	58.40
29	<u>100.00</u>	61	15.23	89	2.87
30	3.52	62	0.48	90	0.24
31	3.47	63	0.09	91	0.22
32	0.08	64	0.01	92	0.04
36	0.03	65	0.03	100	0.67
37	1.15	66	0.03	101	15.08
38	1.35	67	0.10	102	2.00
39	15.15	68	0.11	103	5.66
40	1.96	69	0.56	104	0.34
41	34.20	70	9.15	105	0.05
42	11.34	71	0.49	115	1.16
43	12.67	72	0.10	130	0.88
44	1.69	73	16.79	131	0.11
45	16.49				

Relative sensitivity 0.83 at m/e 29 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 7.87.

Source: Eastman Kodak White Label.

Name of compound: Ethyl Isovalerate

Parent mass: 130

Structural formula: $(\text{CH}_3)_2\text{CHCH}_2\text{CO}_2\text{C}_2\text{H}_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.40	38	0.39	59	10.61	85	54.40
12	0.29	38.2	25.17	60	33.21	86	3.32
13	0.67	39	0.33	60.5	0.11	87	12.09
14	3.83	39.2	0.34	61	16.39	88	59.71
15	15.98	40	4.27	61.5	0.03	89	2.98
16	0.73	41	50.85	62	0.54	90	0.32
17	0.11	42	18.47	63	0.11	91	0.06
18	0.14	43	34.41	66	0.11	92	0.04
19	0.71	44	2.04	67	0.18	99	0.16
24	0.04	45	18.78	68	0.29	100	0.63
25	0.32	46	0.48	69	3.53	101	1.43
25.2	0.20	47	0.54	70	9.60	102	13.51
26	6.94	49	0.11	71	2.36	103	4.15
27	53.32	50	0.68	72	0.45	104	0.31
28	12.43	51	0.89	73	6.85	105	0.05
29	100.00	52	0.37	74	5.43	115	7.91
29.5	0.35	53	1.83	75	0.62	116	0.73
30	3.73	54	0.62	76	0.07	117	0.08
31	3.31	55	7.65	77	0.06	128	0.09
32	0.10	56	11.63	78	0.22	129	0.17
36	0.08	57	76.09	82	0.18	130	1.78
37	0.87	58	3.69	83	0.91	131	0.22
37.2	2.37	58.5	0.04	84	0.52		

Relative sensitivity 0.72 at m/e 29 referred to n-butane m/e 43

Instrument model: CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.94.

Source: Synthesis.

Name of compound: Fluorobenzene

Parent mass: 96

Structural formula: C_6H_5F UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.11	41	0.04	68	3.23
12	1.00	43	0.09	69	4.22
13	0.55	44	0.77	70	20.80
14	0.20	44.5	0.01	71	0.86
15	0.32	45	0.72	72	0.20
16	0.01	46	0.59	73	1.45
18	0.03	46.5	0.04	74	4.64
19	0.13	47	0.36	75	7.44
20	0.02	47.5	0.11	76	2.39
21	0.01	48	3.39	77	1.58
24	0.28	48.5	0.15	78	0.11
25	0.81	49	2.69	79	0.04
26	2.65	50	14.86	80	0.07
27	1.45	51	7.26	81	1.22
28	0.20	52	1.50	82	0.07
29	0.01	53	0.07	84	0.01
31	3.93	55	0.15	85	0.03
32	0.33	56	0.73	86	0.03
33	0.68	57	4.48	87	0.03
34	0.01	58	0.14	89	0.17
35	0.03	60	0.40	90	0.13
36	0.96	61	1.74	91	1.67
36.5	0.04	62	1.62	92	0.76
37	5.16	63	4.16	93	0.57
37.5	0.61	64	0.28	94	2.58
38	5.34	65	0.24	95	7.22
38.5	0.11	66	0.01	96	100.00
39	6.59	67	0.04	97	7.08
40	0.22			98	0.13

Relative sensitivity 1.39 at m/e 96 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.64.

Source: Eastman Kodak White Label.

Name of compound: Formaldehyde Dimethyl Hydrazone

Parent mass: 72

Structural formula: $(\text{CH}_3)_2\text{NN}=\text{CH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	1.62	27	18.69	52	0.05
13	3.64	28	43.88	53	0.33
14	14.83	29	3.93	54	0.10
15	14.18	30	32.23	55	21.00
15.8	0.15	31	1.45	56	0.33
16	0.74	32	0.64	57	23.55
17	0.36	34	0.03	58	0.76
18	7.14	38	1.04	59	0.03
19	0.03	39	1.47	69	0.30
20	0.05	40	4.98	70	3.12
20.5	0.30	41	6.58	71	37.83
21	0.03	42	100.00	72	73.88
24	0.07	43	20.03	73	3.01
25	0.20	44	5.09	74	0.08
26	1.59	45	0.55	75	0.08
26.3	0.11				

Relative sensitivity 0.65 at m/e 42 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.74.

Source: Synthesis.

Name of compound: n-Heptyl alcohol (Heptanol-1)

Parent mass: 116

Structural formula: $\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OH}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.20	43	92.02	69	52.97
13	0.25	44	7.21	70	97.01
14	1.55	45	6.71	71	5.84
15	9.43	46	0.30	72	0.22
16	0.35	49	0.15	73	2.29
17	0.27	50	1.37	74	0.15
18	0.72	51	1.97	77	0.25
19	2.07	52	0.75	78	0.10
24	0.07	53	5.23	79	0.27
25	0.15	54	7.13	80	0.02
26	5.86	55	79.30	81	0.77
27	64.94	56	100.00	82	0.45
28	18.93	57	27.76	83	7.18
29	66.51	58	1.55	84	1.15
30	2.72	59	0.70	85	0.55
31	63.66	60	0.02	86	0.17
32	1.22	61	0.02	87	0.09
33	0.65	62	0.12	91	0.07
37	0.80	63	0.27	96	0.10
38	2.14	65	0.52	97	0.85
39	34.26	66	0.42	98	5.46
40	6.38	67	2.44	102	0.10
41	99.26	68	14.21	116	0.02
42	60.97				

Relative sensitivity 0.47 at m/e 56 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.90.

Source: Humphrey-Wilkinson Co.

Name of compound: Hexatriene (1,3,5 Hexatriene)

Parent mass: 80

Structural formula: $\text{CH}_2(\text{CH})_4\text{CH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.47	32.5	0.01	57	0.03
12	0.84	34	0.03	58	0.02
13	0.96	35	0.04	59	0.01
13.7	0.02	36	0.63	60	0.29
14	1.56	36.5	0.07	61	1.21
15	3.52	37	5.26	62	1.68
16	0.07	37.5	0.86	63	3.74
17	0.08	38	8.30	64	0.69
18	0.26	38.5	0.40	65	10.67
19	0.05	39	36.92	66	0.62
19.5	0.02	39.5	0.55	67	0.04
20	0.04	40	6.94	69	0.03
20.5	0.02	40.5	0.23	72	0.13
23.5	0.03	41	8.01	73	0.98
24	0.18	42.5	0.32	74	2.81
25	0.92	43	0.06	75	3.96
25.5	0.09	44	0.03	76	1.84
26	8.20	48	0.40	77	38.68
27	30.82	49	2.69	78	11.45
28	4.01	50	15.72	79	100.00
28.2	0.06	51	21.57	80	53.90
29	0.45	52	17.57	81	3.35
30	0.02	53	11.95	82	0.10
30.5	0.02	54	4.40	83	0.02
31	0.29	55	0.22	91	0.01
31.5	0.05	56	0.04	97	0.01
32	0.04				

Relative sensitivity 0.92 at m/e 79 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: Purified by
gas
chromatography. $\frac{43}{58}$ for n-butane 7.95.

Source: Synthesis.

Name of compound: Hydrazoic Acid (Azoimide)

Parent mass: 43

Structural formula: HN_3 UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.22	26	0.02	37	0.01
12	0.02	27	0.10	38	0.06
14	25.30	28	28.24	39	0.01
15	47.68	29	16.98	40	0.01
16	1.46	30	0.40	42	8.18
17	0.68	32	0.02	43	100.00
18	0.84	35	0.04	44	3.09
19	0.02	36	0.17	45	0.04
21	59.33				

Relative sensitivity 0.51 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.56.

Source: Synthesis.

Name of compound: Ketene

Parent mass: 42

Structural formula: $\text{H}_2\text{C} = \text{C} = \text{O}$ UNCERTIFIED MASS SPECTRUM

Submitted by: Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	12.49	24	4.36	40	5.10
13	13.08	25	5.81	41	26.52
14	100.00	26	1.61	42	93.93
15	1.15	27	0.05	43	2.14
16	1.02	28	11.32	44	0.01
17	0.05	29	6.83	45	0.02
20	0.04	30	0.07	53	0.01
20.5	0.49	31	0.01	55	0.04
21	1.84	32	0.01	58	0.03
21.5	0.04	36	0.01		

Relative sensitivity 0.54 at m/e 14 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature. Purity: 0.52% Propene,
0.68% Water, and
0.15% Ethane subtracted
from spectrum.

$\frac{43}{58}$ for n-butane 7.87.

Source: Synthesis.

Name of compound: Methyl isopropenyl ether

Parent mass: 72

Structural formula: $\text{CH}_3\text{OC}(\text{CH}_2)\text{CH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	1.08	31	5.76	49	0.02
13	2.38	32	0.13	50	0.04
14	7.99	33	1.60	51	0.04
15	22.87	34	0.02	52	0.08
16	0.37	35	0.04	53	0.70
17	0.04	35.5	0.04	54	0.20
18	0.04	36	0.56	55	1.15
19	0.15	37	4.66	56	0.72
19.5	0.07	37.2	0.33	57	5.98
20	0.06	38	8.61	58	0.26
24	0.23	39	38.00	59	0.03
24.5	0.04	39.2	0.12	69	0.05
25	1.27	40	16.52	70	0.03
25.2	0.21	41	61.21	71	0.16
26	7.78	42	100.00	72	45.60
27	36.32	43	18.80	73	1.93
28	6.65	44	0.68	74	0.14
29	32.48	45	1.02	78	0.02
30	1.52	46	0.03	86	0.02

Relative sensitivity 0.72 at m/e 42 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: 0.51%

 $\frac{43}{54}$ for n-butane 7.96.acetone dimethyl
acetal subtracted.

Source: Synthesis.

Name of compound: Methylisopropenyl ketone

Parent mass: 84

Structural formula: $\text{CH}_3\text{COC}(\text{CH}_2)\text{CH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.64	36	0.65	58	0.19
12	0.95	37	5.77	59	0.03
13	2.18	37.2	0.48	60	0.16
14	7.39	38	10.00	61	0.49
15	27.83	38.5	0.23	62	0.48
16	0.51	39	48.35	63	0.40
17	0.38	40	5.89	64	0.08
18	0.49	41	97.84	65	0.35
19	0.13	42	14.83	66	0.21
19.5	0.04	43	100.00	67	0.32
20	0.06	44	3.48	68	0.35
24	0.16	45	1.20	69	33.67
24.5	0.10	46	0.04	70	1.52
25	0.94	48	0.18	71	0.14
25.5	0.06	49	1.04	72	0.17
26	4.49	50	2.73	77	0.06
27	9.61	51	1.93	79	0.09
28	2.50	52	0.54	81	0.21
29	3.74	53	2.02	82	0.08
30	0.12	54	0.42	83	0.30
31	0.74	55	5.60	84	34.72
31.5	0.08	56	0.81	85	2.08
32	0.12	57	0.96	86	0.13
35	0.04				

Relative intensity 0.79 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: Some dimer present.

 $\frac{43}{58}$ for n-butane 8.00.

Source: Monomer Polymer Corp.

Name of compound: Methyl n-propyl ether

Parent mass: 74

Structural formula: $\text{CH}_3\text{OCH}_2\text{C}_2\text{H}_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.24	31	2.77	46	2.21
13	0.53	32	0.08	47	0.22
14	1.90	33	0.80	53	0.08
15	14.27	35	0.04	55	0.16
16	0.37	35.5	0.06	56	0.09
17	0.31	36	0.14	57	0.28
18	0.06	37	0.61	58	0.18
19	0.08	38	1.18	59	0.74
20	0.06	39	5.66	60	0.01
24	0.03	40	0.95	71	0.17
25	0.25	41	8.56	72	0.10
26	0.78	42	2.55	73	1.54
27	12.89	43	4.46	74	12.89
28	3.68	44	0.58	75	0.56
29	17.82	45	<u>100.00</u>	76	0.03
30	1.14				

Relative sensitivity 1.36 at m/e 45 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 8.06.

Source: Synthesis.

Name of compound: Phenetole (Ethyl Phenyl Ether)

Parent mass: 122

Structural formula: $C_2H_5OC_6H_5$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.34	36	0.10	54	0.20	81	0.04
12	0.20	37	1.50	55	2.87	89	0.03
13	0.35	37.5	0.03	56	0.10	90	0.02
14	1.02	38	4.62	60	0.07	91	0.60
15	2.17	39	19.14	60.5	0.06	92	0.39
16	0.12	39.5	0.08	61	0.56	93	1.58
17	0.02	40	4.37	62	1.44	94	100.00
18	0.03	41	0.61	63	3.91	95	6.54
19	0.02	42	0.36	64	2.06	96	0.39
23.5	0.03	43	0.24	65	11.73	97	0.02
24	0.05	44	0.08	66	16.92	102	0.02
24.2	0.03	45	0.14	67	1.06	103	0.16
25	0.35	45.5	0.16	68	0.44	104	0.02
26	3.35	46	0.17	69	0.03	105	0.07
27	12.21	46.5	0.16	72.8	0.20	106	0.01
28	1.84	47	0.18	73	0.35	107	0.68
29	8.90	48	0.10	74	1.02	108	0.06
30	0.35	49	0.36	75	0.62	119	0.02
31	0.25	50	4.04	76	0.69	120	0.03
31.5	0.08	51	9.47	77	9.17	121	0.31
32	0.08	52	1.00	78	1.35	122	35.04
32.5	0.06	53	1.06	79	1.38	123	3.06
33.7	0.03	53.5	0.20	80	0.11	124	0.19

Relative sensitivity 1.45 at m/e 94 referred to n-butane m/e 43.

Instrument model: CEC-21-103.

Ionization chamber temperature: 250°

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.50.

Source: Eastman Kodak White Label (Purified).

Name of compound: Phenol

Parent mass: 94

Structural formula: C_6H_5OH UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.26	37	5.90	62	3.52
12	0.62	37.5	0.24	63	6.03
13	0.60	38	10.18	64	3.10
14	1.03	38.5	0.11	65	22.30
15	0.90	39	27.52	66	27.58
16	0.12	40	13.24	67	2.19
17	0.38	41	1.10	68	1.26
18	0.74	42	1.16	69	0.08
19	0.15	43	0.74	70	0.02
23.5	0.02	44	0.16	72	0.09
24	0.21	44.5	0.05	73	0.68
24.2	0.06	45	0.17	74	1.89
25	0.93	45.5	0.24	75	0.90
25.5	0.02	46	0.95	76	0.77
26	3.44	46.5	0.36	77	0.87
27	4.72	47	5.08	78	0.12
28	1.12	47.5	0.52	79	0.92
29	3.27	48	0.36	80	0.08
30	0.18	49	1.50	81	0.02
30.5	0.07	50	5.98	89	0.02
31	1.92	51	5.40	90	0.05
31.5	0.53	52	1.08	91	0.08
32	0.66	53	3.48	92	0.30
32.5	0.68	54	1.13	93	1.93
33	0.20	55	8.43	94	<u>100.00</u>
34	0.06	56	0.32	95	10.94
35	0.04	57	0.05	96	0.44
36	0.84	60	0.58	97	0.02
36.5	0.04	61	2.41		

Relative sensitivity 1.05 at m/e 94 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.60.

Source: Mallinckrodt

Name of compound: IsoPropenyl acetate

Parent mass: 100

Structural formula: $\text{CH}_3\text{CO}_2\text{C}(\text{CH}_3)(\text{CH}_2)$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.21	35	0.01	57	2.35
12	0.71	36	0.16	58	14.11
13	1.96	37	1.31	59	0.52
14	6.64	38	2.51	60	0.06
15	17.55	39	9.86	61	0.17
16	0.30	40	1.62	62	0.01
17	0.04	41	10.56	69	0.02
18	0.08	42	7.49	71	0.10
19	0.04	43	100.00	72	5.74
19.5	0.02	44	2.47	73	0.26
20	0.02	45	0.46	74	0.02
24	0.10	46	0.01	82	0.01
25	0.55	49	0.01	85	0.06
26	2.84	50	0.03	86	0.01
27	6.86	51	0.03	91	0.02
28	2.08	52	0.08	92	0.01
29	4.02	53	0.14	99	0.03
30	0.38	54	0.03	100	4.24
31	0.63	55	0.10	101	0.29
32	0.16	56	0.04	102	0.04
33	0.02				

Relative sensitivity 1.79 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.94.

Source: Eastman Kodak White Label, purified.

Name of compound: Iso-propyl amine

Parent mass: 59

Structural formula: $(\text{CH}_3)_2\text{CHNH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.43	26.5	0.30	43	6.83
12	0.50	27	8.40	43.4	0.03
13	0.94	27.5	0.11	44	<u>100.00</u>
14	3.10	28	11.09	45	2.60
15	13.58	29	1.73	46	0.02
16	1.26	30	5.86	50	0.07
17	1.15	30.1	0.01	51	0.30
18	21.51	31	0.15	52	0.54
19	0.15	32	0.04	53	0.05
19.5	0.01	36	0.13	54	0.34
20	0.01	37	0.92	55	0.06
20.5	0.02	38	1.92	56	0.54
21	0.01	39	6.29	57	0.37
24	0.08	40	3.53	58	6.06
25	0.43	41	10.48	59	2.17
26	2.38	42	15.41	60	0.08

Relative sensitivity 1.32 at m/e 44 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.80.

Source: Eastman Kodak White Label.

Name of compound: Isopropyl iodide

Parent mass: 170

Structural formula: $\text{CH}_3\text{CHICH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
18	0.01	51	0.03	99	0.06
19	0.12	52	0.02	100	0.06
19.5	0.04	53	0.07	101	0.07
20	0.06	54	0.02	102	0.04
20.5	0.04	55	0.23	111	0.04
24	0.20	56	0.13	112	0.09
25	0.77	57	1.03	113	0.02
26	5.04	58	0.11	125	0.04
27	48.63	59	0.14	127	16.73
28	4.15	63	0.05	128	2.76
29	0.71	64	0.02	129	0.11
30	0.03	67	0.04	136	0.20
31	0.08	69	0.20	138	0.19
35	0.04	70	0.05	139	0.20
36	0.58	71	0.04	140	0.13
37	3.28	77	0.03	141	0.30
38	5.74	79	0.02	142	0.07
39	27.52	81	0.04	151	0.03
39.2	0.82	83	0.17	152	0.11
40	3.96	84	0.03	153	0.10
41	52.26	85	0.03	154	0.06
42	4.99	87	0.23	155	1.23
43	100.00	91	0.02	156	0.06
44	3.34	95	0.01	168	0.07
45	1.82	96	0.02	170	41.76
46	0.06	97	0.26	171	1.34
50	0.02	98	0.04		

Relative sensitivity 1.06 at m/e 43 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: Impurities on
111,112,113 peaks. $\frac{43}{58}$ form n-butane 7.68.

Source: Eastman Kodak White Label.

Name of compound: Silicon Tetrachloride

Parent mass: 168 ($\text{Si}^{28}, \text{Cl}^{35}$)Structural formula: SiCl_4 UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	0.09	49.5	0.02	101	0.35
14	0.31	50	0.36	102	0.90
15	0.03	50.5	0.01	103	0.06
16	0.06	51	0.07	117	0.21
17.5	0.07	61	0.07	119	0.14
18	0.06	63	35.89	121	0.03
18.5	0.02	64	1.93	133	100.00
26	0.06	65	12.71	134	5.18
27	0.03	66	0.64	135	99.21
28	21.96	66.5	2.40	136	4.95
29	1.18	67	0.56	137	33.62
30	0.79	67.5	2.40	138	1.63
31.5	1.54	68	0.14	139	4.32
32	0.14	68.5	0.86	140	0.18
32.5	0.52	69	0.04	141	0.12
33	0.04	69.5	0.11	168	41.29
35	25.73	70	0.65	169	2.10
36	0.48	72	0.41	170	53.98
37	7.91	74	0.07	171	2.68
38	0.16	81	0.28	172	26.96
44	0.16	82	0.04	173	1.31
45	0.11	83	0.10	174	6.27
46	0.01	84	0.01	175	0.28
47	0.08	98	6.84	176	0.63
48	0.07	99	0.39	177	0.02
49	0.55	100	4.78	178	0.01

Relative sensitivity 0.63 at m/e 133 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 8.01.

Source: Fisher Technical.

Remarks: Masses 168 to 178 run at higher field. Ratios of lower peaks checked lower field ratios.

Name of compound: Trichloroethylene

Parent mass: 130 (Cl³⁵)Structural formula: CHClCCl₂UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
12	7.97	48.5	0.35	83	1.31
13	3.93	49	6.46	84	1.85
14	0.07	49.5	0.07	85	0.85
16	0.02	50	1.92	86	0.33
17.5	0.17	51	0.05	87	0.15
18	0.05	59	10.10	94	9.71
18.5	0.06	60	56.45	95	100.00
24	8.93	61	4.51	96	8.45
25	27.82	62	18.08	97	64.36
26	0.69	63	0.40	98	2.41
27	0.06	64.5	0.04	99	10.35
28	0.26	65	2.36	100	0.32
30	0.23	65.5	0.09	101	0.12
31	0.07	66	2.28	102	0.02
32	0.65	66.5	0.06	129	0.46
35	31.10	67	0.74	130	99.27
36	3.05	68	0.11	131	2.58
37	9.65	69	0.06	132	95.13
38	1.00	70	0.86	133	2.23
41	0.10	70.7	0.21	134	30.41
42	0.05	71	0.52	135	0.91
47	19.75	73	0.05	136	3.23
47.5	0.54	74	0.08	137	0.10
48	6.08	82	2.85		

Relative sensitivity 0.49 at m/e 95 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: Pure by gas chromatography.

 $\frac{43}{58}$ for n-butane 7.98.

Source: Eastman Kodak White Label, purified.

Name of compound: Trimethyl hydrazine

Parent mass: 74

Structural formula: $(\text{CH}_3)_2\text{NNHCH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	2.05	31	7.22	53	0.25
12	1.77	32	7.73	54	0.19
13	3.94	33	0.13	55	0.38
14	15.99	34	0.03	56	1.01
15	71.45	35	0.05	57	19.56
16	6.75	36	1.26	58	4.51
17	16.34	36.5	0.28	59	65.39
18	59.15	37	0.03	60	2.08
19	0.22	38	1.07	69	0.25
20	0.22	39	1.92	70	2.15
20.5	0.28	40	5.43	71	26.25
21	0.03	41	7.76	72	49.68
21.5	0.03	42	100.00	73	6.62
24	0.06	43	33.97	74	40.32
25	0.19	44	5.33	75	1.67
26	2.02	45	2.77	85	0.22
27	17.79	46	3.13	86	0.54
28	62.27	47	2.43	87	1.14
29	9.87	52	0.06	88	0.32
30	65.58				

Relative sensitivity 0.27 at m/e 42 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature.

Purity: Impurities on
85, 86, 87, 88
peaks. $\frac{43}{58}$ for n-butane 7.50.

Source: Synthesis.

Name of compound: Tri-n-Propyl Amine

Parent mass: 143

Structural formula: $(\text{CH}_3\text{CH}_2\text{CH}_2)_3\text{N}$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.28	40	1.09	70	2.56	99	0.17
12	0.06	41	23.83	71	0.69	100	1.15
12.7	0.04	42	17.54	72	18.25	101	0.20
13	0.11	43	26.28	73	0.82	102	0.03
14	0.59	44	5.44	74	0.01	103	0.03
15	6.44	45	0.17	77	0.07	104	0.02
16	0.14	45.5	0.16	78	0.04	105	0.35
17	0.05	47.5	0.02	79	0.04	106	0.08
18	0.39	49	0.01	80	0.08	110	0.08
25	0.04	50	0.05	81	0.07	111	0.04
25.2	0.01	51	0.12	82	0.30	112	1.08
26	1.44	52	0.19	83	0.17	113	0.10
27	24.53	53	0.24	84	3.42	114	100.00
28	7.55	54	1.35	85	0.57	115	8.87
29	8.11	55	1.01	86	8.49	116	0.89
29.8	0.21	56	33.35	87	0.46	119	0.01
30	25.30	57	2.57	88	0.01	120	0.10
31	0.37	58	3.89	91	0.38	124	0.03
32	0.04	59	0.15	92	0.02	126	0.06
37	0.21	65	0.07	94	0.02	128	0.45
37.3	0.04	66	0.06	95	0.03	129	0.03
38	0.43	67	0.19	96	0.07	142	1.16
39+	7.67	68	0.65	97	0.06	143	6.71
39.2	0.13	69	0.24	98	0.59	144	0.29

Relative sensitivity 1.76 at m/e 114 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°

Additional information:

Glass inlet - room temperature.

Purity:

 $\frac{43}{58}$ for n-butane 7.63.

Source: Eastman White Label

Name of compound: Vinyl methyl ether

Parent mass: 58

Structural formula: $\text{CH}_2\text{CHOCH}_3$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.98	30	5.58	45	0.39
12	3.98	31	40.26	46	0.10
13	9.65	32	2.56	52	0.05
14	24.60	33	0.18	53	0.14
15	100.00	35	0.05	54	0.04
16	0.77	36	0.19	55	0.54
17	0.14	37	0.11	56	0.16
18	0.17	38	0.18	57	4.73
24	1.26	39	0.61	58	77.49
25	5.57	40	0.79	59	2.66
26	28.86	41	2.73	60	0.19
27	60.24	42	19.94	72	0.05
28	65.87	43	68.54	75	0.04
29	62.77	44	1.80		

Relative sensitivity 0.43 at m/e 15 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature..

Purity: 95% pure.

 $\frac{43}{58}$ for n-butane 8.03.Methanol and acetylene
impurities not subtracted.

Source: Matheson.

Name of compound: Vinyl propionate

Parent mass: 100

Structural formula: $\text{CH}_3\text{CH}_2\text{CO}_2\text{CHCH}_2$ UNCERTIFIED MASS SPECTRUM

Submitted by Lawrence Radiation Laboratory, University of California, Berkeley.

<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>	<u>m/e</u>	<u>Relative intensity</u>
2	0.29	32.5	0.03	53	0.50
12	0.78	35.5	0.01	54	0.21
13	2.13	36	0.05	55	1.98
14	7.29	37	0.21	56	1.93
15	15.66	38	0.23	57	74.08
16	0.41	39	0.65	58	2.49
17	0.03	40	0.17	59	0.20
18	0.04	41	1.34	60	0.05
19	0.11	42	6.60	69	0.03
24	0.25	42.2	0.23	70	0.02
25	1.79	43	13.54	71	0.30
25.2	0.14	44	11.35	72	0.03
26	13.00	45	1.29	73	0.35
27	42.99	46	0.09	74	0.06
28	11.25	47	0.03	86	0.03
29	100.00	49	0.02	100	4.80
30	2.25	50	0.03	101	0.31
31	0.65	51	0.03	102	0.03
32	0.03	52	0.06		

Relative sensitivity 1.21 at m/e 29 referred to n-butane m/e 43.

Instrument model CEC 21-103.

Ionization chamber temperature: 250°.

Additional information:

Metal inlet - room temperature. Purity:

 $\frac{43}{58}$ for n-butane 8.00.

Source: Monomer-Polymer Corp.

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