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Mass Spectra and Analytical Correlations for 32 Alkyl Aryl Sulfides

UNITED STATES DEPARTMENT OF THE INTERIOR

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Mass Spectra and Analytical Correlations for 32 Alkyl Aryl Sulfides

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MASS SPECTRA AND ANALYTICAL CORRELATIONS FOR 32 ALKYL ARYL SULFIDES

by

J. E. Dooley[1] and R. F. Kendall[2]

ABSTRACT

A mass spectral scheme of analysis was devised which can be used to identify individually a single compound from a larger group of similar compounds. Mass spectra for 32 alkyl aryl sulfides are provided for future reference work, and analytical correlations used in producing the analytical scheme are discussed. Some of the correlations show that base peaks are either the same mass as the parent peaks or may be derived from cleavage alpha to the sulfur atom with migration of one hydrogen to the sulfur atom. Other spectral consistencies provide means of separating ortho-, meta-, and para-tolyl arrangements in an overall analytical scheme. Determinations of chain lengths and separation of isomeric species are also discussed.

INTRODUCTION

Recent developments (8)[3] in mass spectrometry have utilized computers to compare large volumes of reference data with an unknown mass spectrum and, hopefully, resolve the identity of the unknown compound. These computer techniques would be virtually nonexistent if appropriate catalogs[4] of reference spectral data were not available. Some of the excellent analyses and structural elucidations that are now being performed would likewise be tremendously hampered. Thus, the need and demand for standard spectral data are great, and the data reported here for 32 alkyl aryl sulfides represent another contribution in this area by the Bureau of Mines.

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[1] Chemist.

[2] Research physicist (optics).

[3] Underlined numbers in parentheses refer to items in the list of references preceding the appendix.

[4] American Petroleum Institute Research Project 44. Catalog of Mass Spectral Data. Chemical Thermodynamics Properties Center, Texas Agricultural and Mechanical University, College Station, Tex. 77840.

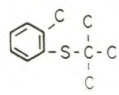
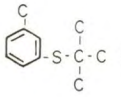
American Society for Testing and Materials. Index of Mass Spectral Data. Committee E-14 on Mass Spectrometry, 1916 Race Street, Philadelphia, Pa. 19103.

Sadtler Research Laboratories, Inc., 3316 Spring Garden Street, Philadelphia, Pa. 19104, keeps a spectral data file for many compounds and continually adds to the file. To obtain spectra for compounds, one must contact Sadtler.

Several authors (1-3, 5-6) have discussed mass spectral characteristics for a variety of organic sulfur compounds, but the availability of information for alkyl aryl sulfides has been limited. These compounds contain an aromatic ring and it was necessary in some instances to use the spectra of aromatic hydrocarbons (7, 10) in comparing structures of similar composition. Meyerson (10) observed that it is rather difficult to distinguish ortho-, meta-, and para-substituted tolyl rings and that no definitive rules can be established to resolve such isomers based strictly upon ring sites. Similar difficulties were encountered in attempting to distinguish the ortho-, meta-, and para-substituted alkyl aryl sulfides; however, some minute differentiations were observed that could be used in an isolation scheme to separate one isomer from another. Spectral consistencies used in the development of a characterization scheme are presented in addition to the mass spectral data for 32 alkyl aryl sulfides. Application of the analytical method is also discussed.

EXPERIMENTAL WORK

Data were obtained on a Consolidated Electrodynamics Corp. (CEC)[5] mass spectrometer, model 21-102, modified to the equivalent of model 21-103C. A CEC heated inlet system maintained sample vapor temperature at 140° C. Isatron temperature was controlled at 250° C. Magnetic field strength was 3,225 gauss with an ionizing current of 10 microamperes and an ionizing voltage of 70 volts. A 0.5-microliter constant-volume pipet was used to charge samples to the inlet through a gallium-covered glass frit. Pressures were measured with a CEC micromanometer. Sensitivities for parent and base peaks are given with each spectrum.

The phenyl and tolyl sulfides were synthesized by two different chemical procedures. Compounds that contained a t-butyl group were synthesized by the method of Fehnel and Carmack (4), and the other compounds were synthesized by the classical chemical process which incorporates the alkylation of the appropriate aromatic thiol with appropriate alkyl bromide. The synthesized compounds were purified by preparatory gas-liquid chromatography, and final purities were determined by standard gas-liquid chromatographic procedures. All compounds were purified to greater than 98.0 percent, except for 2-methyl-1-(2,2-dimethyl-1-thiapropyl) benzene  and 3-methyl-1-(2,2-dimethyl-1-thiapropyl) benzene  , which had purities of 95.9 and 97.4 percent, respectively.

[5]The mention of brand names is for identification only and does not imply endorsement by the Bureau of Mines.

DISCUSSION

Mass Spectral Data

Mass spectral data for the 32 alkyl aryl sulfides are presented in tables A-1 through A-4. A relative intensity (Rl), given for each ion in each spectrum, is based upon the percentage relationship of an ion to the most abundant ion species (base peak) in the spectrum. Base peaks and parent peaks are underlined, and the parent peaks are further denoted by the letter "P." Pertinent sensitivity data are provided at the top of each table. At the end of each table, the metastable and half peaks are listed. Since most of these peaks have insufficient resolution for accurate measurement of relative intensities, the suggested ion and location of each is noted. The approximate location was determined from spectral charts.

Analytical Correlations

Analytical correlations were observed which ultimately led to the development of a mass spectral method for identifying individual alkyl aryl sulfides. Regularities occurring in the spectra for base and parent peaks, alkyl chains, and ring sites provided the basis for a reasonable analytical scheme that was devised.

Base Peaks

Phenyl alkyl sulfides with a methyl or ethyl group attached to the sulfur produce a base and parent peak at the same m/e. Propyl or butyl substitutions result in cleavage alpha to the sulfur accompanied by hydrogen migration (from the chain to the sulfur) to form the base peak at m/e 110.

Tolyl alkyl sulfides show cleavages and rearrangements similar to those of the phenyl alkyl variety, except that in the case of a n-propyl substituent, the base peak appears one carbon number higher in mass number. The most intense ion in the spectra is either the parent ion (methyl, ethyl, n-propyl substitutions) or the m/e 124 ion (isopropyl and all butyl substitutions). In a manner similar to the processes occurring in the phenyl sulfides, cleavage alpha to the sulfur with accompanying hydrogen migration results in the m/e 124 ion in isopropyl- and butyl-substituted compounds.

Longer chains and branching at the carbon alpha to the sulfur enhance the intensity of the base peak with a corresponding loss in intensity of the parent ion.

Ring Differentiation

The m/e 91 ion intensity will resolve the phenyl and tolyl structures. An m/e 91 relative intensity of more than 24.19 percent verifies the tolyl structure. An intensity of less than 3.48 identifies the phenyl ring; the observation ignores the m/e 91 intensity of 22.74 shown for methyl phenyl sulfide since this compound would be eliminated by molecular weight considerations.

To make a reasonable separation of the three possible tolyl configurations (ortho-, meta-, para-), individual ion species from similar alkyl substitutions must be considered. For instance, in methyl-substituted tolyl sulfides, a compound showing an m/e 92 ion intensity equal to about 50 percent of the m/e 91 can only be a meta-tolyl type because the ortho and para arrangements show less than 20 percent m/e 92 to m/e 91. Confirmation of the methyl substitution in a meta-tolyl species may be found at m/e 105. In meta-tolyl, m/e 105 is about 18 percent relative to the base peak; ortho and para compounds with methyl substitution show less than 4.5-percent intensity relative to their respective base peaks.

Identification of Alkyl Chains

Compounds having methyl substitution can generally be determined from the parent ion and/or base peak. To resolve a tolyl methyl configuration from a phenyl ethyl sulfide, the m/e 110 intensity is useful. Tolyl methyl sulfides have m/e 110 ions less than 0.52 percent relative intensity, whereas phenyl ethyl sulfide has an m/e 110 intensity of 66.47 percent.

In addition to molecular weight considerations, an ethyl substitution in tolyl sulfides may be determined by the intensity of the m/e 119 ion. An m/e 119 ion intensity between 2.37 percent and 5.80 percent indicates the alkyl substituent is ethyl. For phenyl sulfides, however, the ethyl substitution is better defined by the m/e 110 to m/e 109 ratio of intensities. A ratio more than 1.0 and less than 3.0 identifies the alkyl chain as an ethyl group.

Propyl groups may be determined from the intensity of m/e 43 ions. An intensity greater than 14.28 percent shows the ion is derived mainly from the propyl grouping. To resolve isopropyl and n-propyl groups, the ratio of m/e 43 to m/e 29 may be used. An m/e 43 to m/e 29 ratio more than 3.0 but less than 5.0 verifies the group to be n-propyl. A ratio greater than 26.0 but less than 99.0 indicates the group is isopropyl. Metastable ions at m/e 39.1 and 42.6 also support the propyl substituent identification.

Butyl groups are easily defined by the presence of a metastable peak at m/e 29.5 (3) and by the intensity of the m/e 57 peak. An m/e 57 intensity greater than 5.68 percent determines the alkyl substituent to be a butyl group. In addition, the intensity of the m/e 57 ion indicates, to some extent, which particular butyl group may be present. An m/e 57 ion intensity of 5.68 to 8.05 percent indicates the n-butyl grouping; 10.03 to 14.76 percent identifies a s-butyl group; 19.23 to 40.75 percent indicates isobutyl or t-butyl. For tolyl sulfides, the overlap of ion intensities for isobutyl and t-butyl groups can be resolved by consideration of the intensity of the m/e 45 ion. After the group has been determined to be either isobutyl or t-butyl by the above procedure, then an m/e 45 ion intensity of approximately 10 to 24 percent verifies t-butyl, and about 35 to 50 percent identifies isobutyl.

Mass Spectral Method for Identifying Individual Alkyl Aryl Sulfides

From the mass spectral data and correlations, an analytical scheme, shown in figure 1, was developed which utilizes intensity and m/e differences in parent, base, and other peaks to separate the various isomers in this group of alkyl aryl sulfides. To apply the scheme to an unknown spectrum, the parent mass peak must first be determined and located on the chart. Obviously, a parent peak at m/e 124 can only result from the methyl-substituted phenyl sulfide, thereby establishing the identity of the compound as indicated on the schematic.

The phenyl ethyl sulfide and three tolyl methyl sulfides require more deduction. All of these have the same base peaks and the same parent peaks at m/e 138. However, the intensity of m/e 110 in these compounds provides guidance in separating the phenyl structure from the tolyl configuration. An m/e 110 intensity greater than 65 percent of the base peak shows the compound is phenyl ethyl sulfide. An m/e 110 intensity less than 65 percent means the compound is one of the tolyl methyl sulfides. As shown in figure 1, the m/e 137 intensity will then serve to identify the individual tolyl methyl sulfide.

Phenyl propyl and tolyl ethyl sulfide identification require a similar approach. Parent peaks appear in the spectra at m/e 152. Phenyl propyl compounds show base peaks at m/e 110, whereas tolyl ethyl sulfides have base peaks at m/e 152. To further separate the n-propyl from the isopropyl group in the phenyl propyl sulfides, the parent peak intensity is considered. A parent peak intensity of about 40 percent relative to the base peak means the compound contains the n-propyl group. Otherwise, a relative intensity of about 75 percent indicates the isopropyl group. Tolyl ethyl sulfides are separated by the m/e 123 to m/e 124 ratio as illustrated in figure 1.

A parent peak at m/e 166 indicates either a phenyl butyl sulfide or a tolyl propyl sulfide. A base peak at m/e 110 establishes the phenyl structure with further characterization of the butyl chains accomplished by the intensity of the m/e 57 ion. A base peak at m/e 166 indicates the tolyl n-propyl structure with the relative intensities of the m/e 45 and m/e 124 ions used to further deduce the individual tolyl ring involved. A base peak at m/e 124 appears in tolyl isopropyl sulfide spectra, and identity of the tolyl ring is derived from the m/e 91 to m/e 89 ratio.

Tolyl butyl sulfides are indicated by the appearance of a parent peak at m/e 180 and a base peak at m/e 124. The relative intensity of the m/e 57 ion may be used to separate n-butyl and s-butyl chains from isobutyl and t-butyl groups. An m/e 57 relative intensity of 5 to 9 percent of the base peak shows the alkyl group is n-butyl, 10 to 15 percent verifies the s-butyl group, and 19 to 41 percent indicates the isobutyl and t-butyl groups. The m/e 45 and m/e 123 relative intensities are then useful in isolating the isobutyl from the t-butyl chain and in characterizing the three tolyl configurations involved.

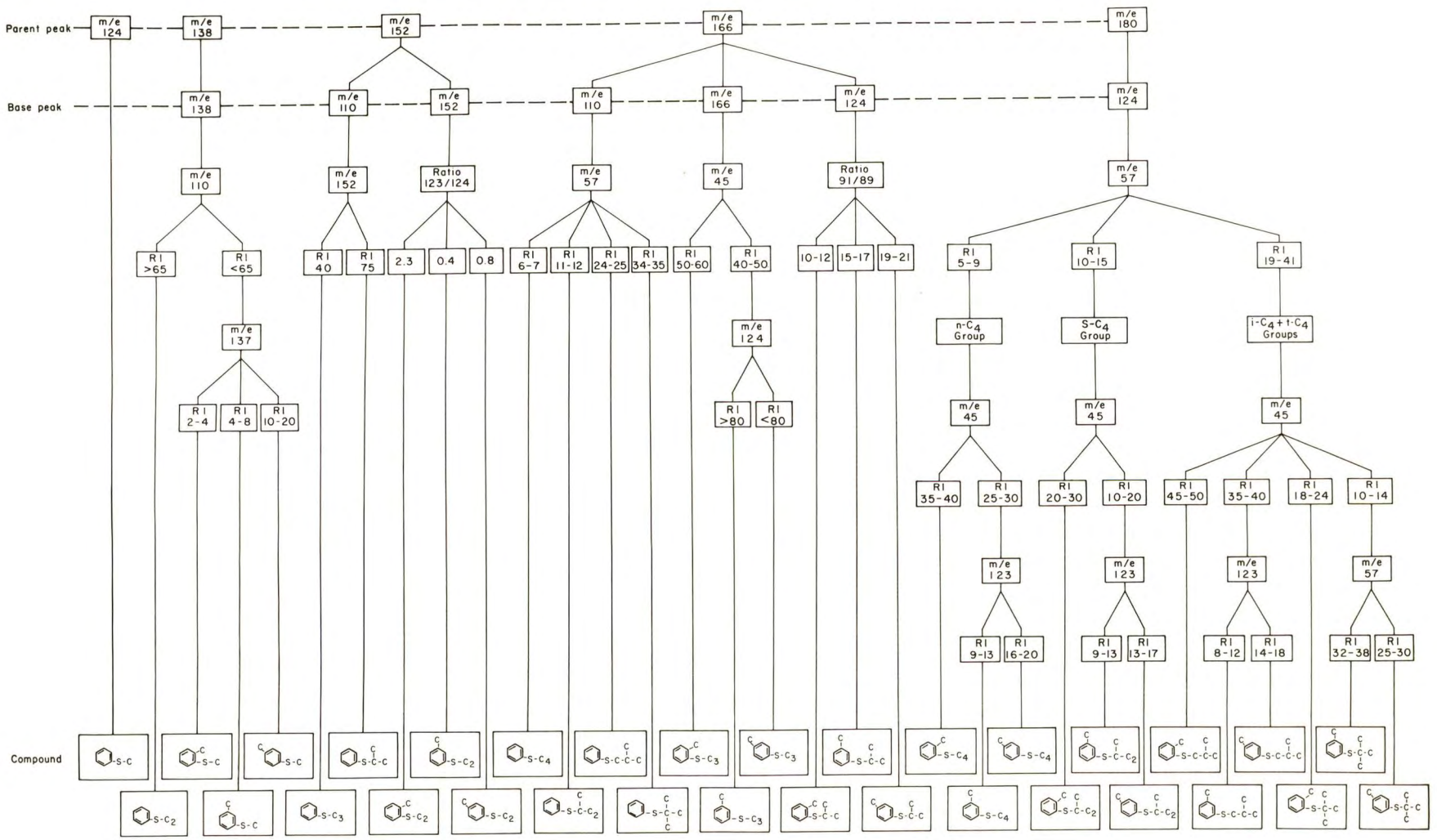


FIGURE 1. - Mass Spectral Scheme for Isolating Individual Alkyl Aryl Sulfides.

CONCLUSIONS

Mass spectral data were determined on 32 previously unavailable alkyl aryl sulfides. Some spectral consistencies observed in the data have made possible the development of an analytical scheme for detecting and identifying individual sulfide isomers from a larger group of sulfur compounds. The method utilizes spectral characteristics derived from parent and base peaks, alkyl chain lengths and structural configurations, and differences in ring structure to determine the identity of an individual compound. In block diagram form, the scheme provides a useful technique for the identification of alkyl aryl sulfides on an individual basis.

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APPENDIX.--MASS SPECTRAL DATA FOR 32 ALKYL ARYL SULFIDES

TABLE A-1. - Mass spectral data for eight alkyl phenyl sulfides

	(1-Thiaethyl)-benzene	(1-Thiapropyl)-benzene	(1-Thiabutyl)-benzene	(2-Methyl-1-thiapropyl)-benzene	(1-Thiapentyl)-benzene	(2-Methyl-1-thiabutyl)-benzene	(3-Methyl-1-thiabutyl)-benzene	(2,2-Dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
Molecular weight	124	138	152	152	166	166	166	166
Magnetic field, gauss	3,225	3,225	3,225	3,225	3,225	3,225	3,225	3,225
Sensitivity, divisions/micron								
Base peak	54.86	42.26	52.25	87.12	77.37	90.64	56.91	100.91
Parent peak	54.86	42.26	39.24	34.75	37.07	29.44	35.65	11.38
n-Butane, m/e 43 peak	49.28	49.04	49.04	49.28	49.04	49.04	49.28	49.04
Ionizing current, microamperes	10	10	10	10	10	10	10	10
m/e	Relative intensities,[1] percent							
24	0.09	0.18	0.04	0.02	0.02	0.01	-	0.01
25	.40	1.47	.33	.18	.17	.14	0.13	.09
26	2.09	10.63	4.21	1.99	3.46	2.50	2.28	1.21
27	3.67	31.32	29.74	15.90	21.19	15.93	20.98	9.15
28	.10	2.69	1.93	.81	3.37	2.28	2.03	1.39
29	.03	18.23	3.40	.18	24.95	24.22	24.81	17.55
30	-	.39	.07	-	.55	.57	.57	.41
32	.91	.76	.56	.26	.21	.17	.23	.18
33	.37	.50	.24	.15	.12	.11	.14	.10
34	.25	.43	.25	.16	.17	.13	.20	.11
35	.05	.90	.06	.04	.10	.12	.07	.02
36	.35	.20	.13	.08	.03	.03	.06	.04
37	3.12	2.53	1.95	1.36	.75	.71	1.24	.84
38	4.73	4.80	4.50	3.24	2.10	1.95	3.49	2.31
39	14.77	20.69	26.85	19.54	16.83	16.31	28.30	18.85
40	.56	1.05	1.88	1.55	1.17	1.06	2.20	1.55
41	.24	.33	17.30	12.69	13.99	16.58	26.58	20.91
42	.02	.04	1.36	1.03	.86	.88	2.31	1.18
43	.05	.09	14.92	17.68	.55	.10	4.47	.10
44	.91	.41	.64	.63	.13	.09	.26	.10
45	21.81	31.82	31.10	6.74	17.85	6.08	31.03	4.68
46	5.80	1.75	2.29	.27	1.30	.25	2.33	.17
47	4.26	1.68	2.66	.64	1.78	.58	2.54	.45
48	.65	.18	.17	.04	.10	.04	.18	.03
49	1.93	1.19	.67	.40	.35	.27	.46	.35
50	14.23	11.56	7.76	4.01	4.60	3.43	6.44	2.88
51	23.32	23.01	18.88	8.40	11.77	8.08	17.00	5.56
52	2.73	2.48	1.93	.90	1.31	.93	1.87	.67
53	.60	.79	.57	.28	1.21	1.35	1.85	.97
54	.27	.20	.09	.07	.22	.18	.25	.16
55	.05	.09	.05	.03	2.91	2.86	4.45	2.17
56	.16	.19	.06	.05	.77	.95	.99	1.02
57	2.56	3.54	1.97	1.46	6.53	11.71	24.52	34.48
58	2.24	5.17	3.05	2.22	1.88	1.92	2.56	2.40
59	1.07	5.56	2.14	4.07	2.15	4.33	1.76	2.11
60	.38	4.19	.35	.49	.44	.62	.27	.15
61	1.38	3.90	.71	.59	.47	.62	.48	.34
62	4.75	2.50	1.39	.62	.73	.65	.98	.60
63	4.35	5.09	3.42	2.22	2.03	1.63	2.73	1.61
64	.73	.97	.67	.45	.41	.35	.55	.32
65	15.06	20.75	16.41	12.01	11.30	10.94	13.75	10.53
66	1.07	17.22	10.56	9.20	6.02	6.01	6.12	4.69
67	.19	1.03	.67	.56	.35	.35	.42	.27
68	.40	.31	.21	.14	.10	.08	.33	.12
69	11.68	15.56	10.29	6.97	6.15	5.50	7.90	5.36
70	1.11	1.30	.93	.61	.53	.47	.74	.45
71	1.31	2.16	1.97	1.08	1.10	.96	1.76	.71
72	.42	.19	.24	.09	.11	.11	.32	.07
73	1.14	.78	1.18	.64	.45	.68	1.18	1.19
74	4.58	3.36	2.59	1.28	1.10	.81	1.64	.76
75	2.53	2.24	1.87	1.08	.98	.69	1.38	.57
76	1.68	1.69	1.51	.75	.79	.57	1.24	.46
77	9.23	14.80	14.78	6.01	9.65	5.72	13.65	3.52
78	29.45	5.89	3.19	1.44	2.42	1.47	3.71	.76
79	4.29	4.80	3.74	.28	2.18	.32	3.89	.13
80	.48	.43	.41	.12	.17	.05	.30	.04
81	2.08	2.26	1.34	.92	.71	.63	.95	.62
82	3.88	4.33	2.53	1.83	1.58	1.38	2.03	1.31
83	1.54	2.09	1.47	1.06	.92	.87	1.17	.79
84	.54	6.99	4.50	3.96	2.34	2.31	2.48	1.92
85	.18	.50	.33	.27	.28	.21	.30	.16
86	.08	.35	.23	.19	.13	.12	.15	.09
87	.05	.10	.05	.02	.11	.14	.29	.09
88	.05	.16	-	-	.06	.06	.08	-
89	.55	.42	.44	.08	.37	.15	.51	.06
90	.62	.17	.20	.04	.14	.05	.23	.02
91	22.74	2.00	3.10	.76	2.66	.96	3.48	.36
92	1.81	.23	.34	.09	.25	.09	.33	.04
93	.70	.64	.38	.28	.22	.20	.28	.14
94	.11	.11	.07	.04	.04	.04	.06	.03
95	.21	.49	.35	.21	.19	.16	.27	.12
96	.14	.10	.08	.02	.04	.01	.08	-
97	.73	.65	.57	.10	.39	.12	.61	.04
98	.10	.07	.06	-	.03	-	.05	-
99	.04	.04	.06	-	.02	-	.04	-
100	-	-	-	-	-	-	-	-
101	-	.06	.06	.02	.02	.03	-	-
102	-	.20	.11	.08	.08	.10	.09	.03
103	-	1.27	.38	.86	.45	1.08	.25	.06
104	.03	1.08	.26	.81	.38	.99	.16	.03

See footnote at end of table.

TABLE A-1. - Mass spectral data for eight alkyl phenyl sulfides--Continued

	(1-Thiaethyl)-benzene	(1-Thiapropyl)-benzene	(1-Thiabutyl)-benzene	(2-Methyl-1-thiapropyl)-benzene	(1-Thiapentyl)-benzene	(2-Methyl-1-thiabutyl)-benzene	(3-Methyl-1-thiabutyl)-benzene	(2,2-Dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
105	0.24	4.13	0.25	0.21	0.52	0.24	0.33	0.09
106	.25	.54	.16	.10	.19	.08	.13	.06
107	.40	.41	.28	.18	.19	.15	.23	.13
108	4.46	4.88	3.32	2.09	2.19	1.74	2.77	1.63
109	45.48	23.97	18.79	15.27	16.48	14.81	15.85	11.09
110	3.61	66.47	100.00	100.00	100.00	100.00	100.00	100.00
111	2.09	6.15	8.41	8.31	8.22	8.41	8.49	8.53
112	.14	3.16	4.56	4.59	4.66	4.78	4.61	4.70
113	-	.26	.30	.31	.32	.31	.33	.33
114	-	-	.04	.03	.03	.04	.05	.03
115	-	-	.39	.14	.18	.16	.51	.14
116	-	-	.16	.06	.11	.09	.26	.06
117	.02	-	.34	.12	.29	.13	.34	.17
118	-	-	.20	.05	.05	.05	.09	.07
119	.02	-	.07	.05	.03	-	.05	-
120	.02	-	.03	-	-	-	.03	-
121	.98	1.34	1.27	.25	.77	.30	1.32	.08
122	.43	.50	.39	.06	.22	.06	.38	.01
123	8.48	65.26	61.40	1.09	28.36	1.58	61.21	.62
124	100.00P	5.53	5.31	.13	3.23	.17	8.74	.06
125	8.77	3.07	2.86	.05	1.41	.07	3.16	.03
126	4.68	.23	.23	-	.14	-	.38	-
127	.34	.03	-	-	.02	-	.05	-
128	.03	-	-	-	.03	.01	.07	-
129	-	-	-	-	.02	-	.05	-
130	-	-	-	-	-	-	.03	-
131	-	-	-	-	.04	.01	.05	-
132	-	-	-	-	.04	-	.03	-
133	-	.08	.04	.07	.05	.10	.05	-
134	-	.34	.38	.26	.30	.36	.43	.14
135	-	1.05	.90	.95	1.05	1.31	.70	.15
136	-	.24	.15	.19	.21	.28	.15	.03
137	-	1.84	1.41	4.81	2.78	10.62	1.70	.03
138	-	100.00P	.21	.63	.29	1.08	.17	-
139	-	9.55	.07	.24	.14	.25	.09	-
140	-	4.76	-	.03	-	.04	-	-
141	-	.40	-	-	-	-	-	-
142	-	.04	-	-	-	-	-	-
145	-	-	-	-	-	-	.04	-
147	-	-	.10	.02	.07	.06	.19	.03
148	-	-	.02	-	-	.03	.07	-
149	-	-	.25	.08	.07	.24	.49	.11
150	-	-	.07	.03	-	.04	.09	.02
151	-	-	.40	.22	.11	.57	.71	1.64
152	-	.10(imp)	75.10P	39.89P	.04	.08	.23	.17
153	-	-	7.96	4.21	-	.03	.05	.08
154	-	-	3.65	1.95	-	-	-	-
155	-	-	.34	.18	-	-	-	-
156	-	-	-	.01	-	-	-	-
161	-	-	-	-	-	-	.03	-
163	-	-	-	-	-	.02	.04	-
164	-	-	-	-	.03	.02	.04	-
165	-	-	-	-	.25	.16	.49	.05
166	-	-	-	-	47.92P	32.48P	62.64P	11.28P
167	-	-	-	-	5.63	3.86	7.33	1.31
168	-	-	-	-	2.30	1.64	3.14	.56
169	-	-	-	-	.24	.16	.32	.06
170	-	-	-	-	-	-	.02	-
180	-	-	-	-	.04	-	-	-
m/e	Metastable peaks (X = present, O = undetected)							
25.2	O	X	O	O	O	X	O	X
26.8	O	X	O	O	O	O	O	O
28.8	O	X	O	O	O	O	O	O
29.5	O	O	O	O	X	X	X	X
37.2	O	O	X	X	X	X	X	X
38.8	O	X	O	O	X	X	X	X
39.1	O	O	X	X	O	O	O	O
40.8	O	O	O	O	O	X	X	X
41.0	O	O	O	X	O	O	O	O
41.8	O	O	O	O	X	O	O	O
42.6	O	O	X	X	O	O	O	O
44.0	O	X	O	O	O	O	O	O
44.8	X	X	X	X	X	O	X	O
45.8	X	O	O	O	O	O	O	O
49.5	X	X	O	O	O	O	O	O
50.6	X	X	X	O	X	O	X	O
56.7	O	O	O	O	X	X	X	X
58.8	O	O	O	O	O	X	O	O
64.7	X	X	X	X	X	X	X	X
65.7	O	X	O	O	X	X	O	O
67.0	X	O	O	O	O	O	O	O
73.0	O	O	O	O	X	X	X	X
76.5	X	X	O	O	O	O	O	O
77.5	X	O	O	O	O	O	O	O
80.0	O	O	X	X	O	O	O	O
83.5	O	X	O	X	O	O	O	O
88.0	X	X	O	O	O	O	O	O
107.0	X	O	X	X	X	X	X	X
122.0	X	X	X	O	O	O	X	O

See footnote at end of table.

TABLE A-1. - Mass spectral data for eight alkyl phenyl sulfides--Continued

	(1-Thiaethyl)-benzene	(1-Thiapropyl)-benzene	(1-Thiabutyl)-benzene	(2-Methyl-1-thiapropyl)-benzene	(1-Thiapentyl)-benzene	(2-Methyl-1-thiabutyl)-benzene	(3-Methyl-1-thiabutyl)-benzene	(2,2-Dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Half peaks (X = present, O = undetected)							
25.5	O	O	O	O	O	X	O	O
37.5	X	X	O	O	O	O	O	O
38.5	X	X	O	O	O	O	O	O
40.5	X	O	O	O	O	O	O	O
46.5	X	O	O	O	O	O	O	O
52.5	X	X	O	X	O	O	O	O
53.5	X	X	O	O	O	O	O	O
54.5	X	X	X	X	X	X	X	X
55.5	X	X	O	O	O	O	O	O
58.5	X	O	O	O	O	O	O	O
60.5	X	X	X	O	X	O	X	O
61.5	X	X	X	O	X	O	X	O
62.5	X	O	O	O	O	X	O	O
67.5	O	X	X	X	X	X	X	X
68.5	O	X	X	X	X	O	X	X
73.5	O	O	O	O	O	O	X	X
74.5	O	O	O	O	O	O	X	X
75.5	O	O	O	O	O	O	X	X

[1]Underlined values indicate parent and base peaks. Parent peaks are further noted with a "P" after the appropriate relative intensity. Ion contributions due to impurities are indicated by "imp" after the appropriate relative intensities.

TABLE A-2. - Mass spectral data for eight alkyl-o-tolyl sulfides

	2-Methyl-1-(1-thiaethyl)-benzene	2-Methyl-1-(1-thiapropyl)-benzene	2-Methyl-1-(1-thiabutyl)-benzene	2-Methyl-1-(2-methyl-1-thiapropyl)-benzene	2-Methyl-1-(1-thiapentyl)-benzene	2-Methyl-1-(2-methyl-1-thiabutyl)-benzene	2-Methyl-1-(3-methyl-1-thiabutyl)-benzene	2-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
Molecular weight	138	152	166	166	180	180	180	180
Magnetic field, gauss	3,225	3,225	3,225	3,225	3,225	3,225	3,225	3,225
Sensitivity, divisions/micron								
Base peak	52.56	47.64	42.90	60.95	59.69	73.40	48.31	89.35
Parent peak	52.56	47.64	42.90	36.17	39.46	32.50	37.38	11.93
n-Butane, m/e 43 peak	49.43	49.43	49.43	49.43	48.08	49.43	48.08	48.08
Ionizing current, microamperes	10	10	10	10	10	10	10	10
m/e	Relative intensities,[1] percent							
24	0.03	0.07	0.03	-	-	0.03	-	-
25	.19	.67	.21	0.14	0.13	.09	0.08	0.06
26	1.98	8.50	4.38	2.35	3.67	2.53	2.21	1.19
27	5.29	28.64	37.18	22.42	25.50	18.33	23.28	10.20
28	.29	2.73	2.50	1.10	4.18	2.57	2.22	1.42
29	.46	17.93	4.20	.93	32.10	29.97	29.62	18.47
30	-	.38	.09	-	.71	.66	.64	.42
32	.63	.53	.42	.24	.17	.15	.20	.15
33	.42	.45	.28	.19	.14	.14	.15	.13
34	.37	.50	.37	.25	.22	.21	.24	.17
35	.20	.72	.05	.06	.13	.13	.07	.03
36	.12	.07	.08	.06	.03	.03	.03	.03
37	1.93	1.22	1.48	1.12	.57	.50	.92	.57
38	4.52	3.40	4.43	3.24	2.08	1.74	3.20	1.81
39	19.81	19.19	31.57	23.13	19.66	17.22	30.88	17.30
40	1.45	1.37	2.75	2.15	1.59	1.37	2.79	1.68
41	2.26	2.44	21.34	17.00	18.23	19.35	31.24	21.56
42	.09	.11	1.74	1.35	1.09	1.11	2.75	1.22
43	.21	.12	19.26	24.24	.75	.15	5.21	.50
44	.64	.34	.83	.89	.19	.13	.31	.10
45	46.26	50.76	55.43	30.07	37.37	25.67	48.29	21.82
46	3.51	1.83	2.47	.82	1.56	.69	2.06	.56
47	4.06	3.02	4.31	2.12	3.03	1.75	3.51	1.46
48	.63	.12	.16	.06	.11	.05	.14	.05
49	.82	.45	.34	.26	.20	.16	.24	.23
50	5.72	4.61	3.28	2.64	2.32	1.96	2.94	1.75
51	10.35	10.71	10.83	7.03	6.60	5.47	8.35	4.66
52	2.54	2.80	2.80	1.92	1.79	1.55	2.30	1.33
53	2.38	3.37	3.58	2.45	3.16	2.87	4.09	2.41
54	.16	.18	.20	.13	.32	.24	.33	.21
55	.05	.06	.16	.04	3.47	2.75	4.09	1.93
56	.08	.07	.05	.02	.57	.64	.74	.85
57	.97	1.14	.82	.62	8.05	14.76	29.62	40.75
58	1.58	2.57	2.10	1.65	1.44	1.46	2.18	2.32
59	1.30	3.87	2.61	3.66	2.15	3.18	2.42	1.73
60	.77	1.33	.39	.48	.47	.48	.29	.16
61	2.44	2.97	1.02	.75	.61	.65	.68	.38
62	4.99	3.66	3.06	1.91	1.62	1.21	2.06	1.01
63	12.68	10.74	10.38	6.46	5.37	4.56	7.81	3.65
64	3.22	2.79	2.87	1.78	1.76	1.31	2.24	1.01
65	11.88	12.62	15.59	8.15	10.31	6.75	13.55	4.28
66	.94	1.13	1.29	.79	.85	.63	1.07	.43
67	.45	.37	.53	.40	.34	.23	.42	.25
68	.44	.32	.32	.27	.17	.16	.21	.13
69	9.50	8.06	7.12	5.30	4.01	3.48	4.91	3.25
70	1.83	1.73	1.63	1.18	.94	.81	1.15	.77
71	2.28	3.02	3.26	2.22	1.95	1.69	2.54	1.47
72	.33	.27	.33	.19	.18	.17	.30	.13
73	.47	.41	1.24	.90	.37	.59	.92	1.07
74	1.54	1.20	1.60	.94	.56	.45	.90	.49
75	1.26	1.19	1.53	1.07	.71	.55	1.11	.51
76	.81	.95	.86	.59	.55	.39	.72	.31
77	12.44	17.83	18.62	12.89	12.53	9.96	14.61	8.76

See footnote at end of table.

TABLE A-2. - Mass spectral data for eight alkyl-o-tolyl sulfides--Continued

	2-Methyl-1-(1-thiaethyl)-benzene	2-Methyl-1-(1-thiapropyl)-benzene	2-Methyl-1-(1-thiabutyl)-benzene	2-Methyl-1-(2-methyl-1-thiapropyl)-benzene	2-Methyl-1-(1-thiapentyl)-benzene	2-Methyl-1-(2-methyl-1-thiabutyl)-benzene	2-Methyl-1-(3-methyl-1-thiabutyl)-benzene	2-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
78	5.41	6.17	6.53	3.94	4.23	3.04	5.35	2.44
79	7.63	8.20	8.26	5.67	5.64	4.77	6.09	3.90
80	.59	1.11	1.28	1.07	.79	.75	.86	.57
81	1.01	.94	.78	.60	.43	.38	.55	.36
82	1.94	2.01	1.79	1.32	1.04	.89	1.26	.81
83	.66	.82	.90	.59	.51	.43	.59	.54
84	.68	1.11	1.18	.95	.74	.67	.80	.68
85	.65	.47	.45	.27	.43	.23	.45	.37
86	.93	.62	.52	.32	.40	.23	.43	.21
87	.79	.58	.54	.32	.63	.51	1.08	.35
88	.45	.36	.40	.28	.37	.29	.44	.17
89	8.54	7.88	8.45	5.68	5.38	4.29	6.50	3.21
90	6.23	5.53	6.19	5.38	3.84	3.58	4.18	2.55
91	37.76	51.82	71.97	61.32	43.73	40.22	48.89	27.69
92	6.81	8.06	6.95	5.25	4.31	3.69	4.54	2.36
93	2.64	3.87	5.17	1.00	2.69	.63	4.66	.46
94	.53	.57	.60	.21	.29	.12	.45	.10
95	1.32	1.21	1.11	.77	.61	.52	.74	.47
96	.66	.67	.66	.45	.41	.32	.45	.26
97	2.14	3.06	3.57	2.06	2.22	1.54	2.82	1.36
98	.21	.41	.47	.35	.28	.23	.32	.19
99	.11	.22	.19	.11	.13	.09	.14	.08
100	-	.16	-	-	-	-	-	-
101	.04	.19	.06	-	.05	-	.05	-
102	.19	.31	.27	.08	.18	.09	.25	.03
103	.77	.85	1.10	.15	.70	.16	1.14	.06
104	.71	.82	1.17	.09	.79	.10	1.30	.04
105	3.14	.80	1.86	.53	1.38	.56	1.45	.14
106	.39	.19	.33	.12	.19	.11	.23	.06
107	.15	.16	.15	.11	.09	.09	.08	.05
108	1.57	2.14	2.17	1.54	1.36	1.16	1.52	1.02
109	.55	1.00	1.19	.73	.70	.50	.84	.38
110	.52	.27	.31	.23	.23	.17	.24	.13
111	.41	.17	.17	.10	.11	.07	.14	.07
112	.20	-	.04	-	-	-	-	.03
113	-	-	-	-	-	-	-	.02
115	-	.69	.68	.51	.52	.56	.45	.16
116	.05	.28	.34	.26	.23	.24	.23	.09
117	.19	.96	.59	.70	.34	.75	.25	.09
118	.06	.72	.27	.81	.28	.93	.13	.03
119	.17	2.72	.31	.19	.70	.21	.20	.07
120	.27	.51	.27	.12	.30	.11	.21	.07
121	10.22	10.03	9.41	5.21	6.13	3.90	7.61	2.84
122	3.56	4.27	3.62	1.50	2.32	1.05	3.01	.73
123	56.52	55.15	21.21	11.89	13.26	8.76	10.48	4.67
124	5.21	24.34	82.20	100.00	100.00	100.00	100.00	100.00
125	2.65	4.33	7.88	8.89	9.17	9.00	.14	9.48
126	.21	1.19	3.90	4.57	4.71	4.67	4.69	4.68
127	.03	.15	.34	.37	.39	.40	.42	.38
128	-	-	.15	.07	.13	.11	.23	.08
129	-	-	.11	.05	.09	.07	.19	.06
130	-	-	.06	-	.07	.06	.11	.03
131	-	-	.21	.07	.17	.09	.18	.09
132	-	-	.15	.06	.04	.05	.07	.07
133	.08	.10	.49	.19	.09	.04	.10	.02
134	.60	.89	1.22	.55	.85	.56	1.06	.21
135	.72	1.40	2.00	.60	1.67	.77	1.97	.13
136	.21	.87	.61	.70	.47	.83	.48	.04
137	2.52	32.78	60.48	.99	29.15	1.22	59.25	.45
138	100.00P	3.29	6.02	.26	3.32	.18	7.59	.16
139	9.60	1.58	2.95	.06	1.44	.07	2.99	.04
140	4.77	.15	.27	-	.14	-	.31	.02
141	.39	-	-	-	.03	-	.03	.02
142	.04	-	-	-	-	-	-	-
145	-	-	-	-	.03	.03	.04	.02
146	-	-	-	-	.03	.05	.04	.02
147	-	.14	.28	.19	.25	.25	.34	.10
148	-	.07	.17	.11	.09	.16	.19	.06
149	-	.34	.37	.59	.35	.71	.47	.16
150	-	.16	.15	.15	.10	.20	.13	.04
151	.04(imp)	1.18	1.46	4.44	2.21	9.66	1.43	.04
152	.32(imp)	100.00P	.23	.82	.28	1.18	.17	.42
153	.06(imp)	10.67	.09	.25	.09	.49	.07	.06
154	.03(imp)	4.88	-	.04	-	.05	-	.03
155	.03(imp)	.46	-	-	-	-	-	-
156	.02(imp)	.05	-	-	-	-	-	-
161	-	-	-	-	.04	.04	.07	.02
162	-	-	-	-	-	-	.04	.02
163	-	-	.23	.06	.05	.16	.28	.07
164	-	-	.14	.04	-	.05	.07	.02
165	-	-	.59	.30	.24	.52	.93	1.44
166	-	-	100.00P	59.34P	.04	.12	.48	.18
167	-	-	11.80	6.85	-	.03	.07	.08
168	-	-	5.06	2.96	-	-	-	.03
169	-	-	.51	.29	-	-	-	-
170	-	-	-	.02	-	-	-	-
177	-	-	-	-	-	.03	.07	.02
178	-	-	-	-	.06	.03	.07	-

See footnote at end of table.

TABLE A-2. - Mass spectral data for eight alkyl-o-tolyl sulfides--Continued

	2-Methyl-1-(1-thiaethyl)-benzene	2-Methyl-1-(1-thiapropyl)-benzene	2-Methyl-1-(1-thiabutyl)-benzene	2-Methyl-1-(2-methyl-1-thiapropyl)-benzene	2-Methyl-1-(1-thiapentyl)-benzene	2-Methyl-1-(2-methyl-1-thiabutyl)-benzene	2-Methyl-1-(3-methyl-1-thiabutyl)-benzene	2-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
179	-	-	-	-	0.29	0.21	0.56	0.06
180	-	-	0.14(imp)	-	66.10P	44.28P	77.38P	13.36P
181	-	-	-	-	8.50	5.71	9.93	1.72
182	-	-	-	-	3.40	2.28	3.96	.68
183	-	-	-	-	.37	.25	.42	.08
184	-	-	-	-	.04	.02	.03	-
m/e	Metastable peaks (X = present, O = undetected)							
25.2	O	X	O	O	X	X	X	X
29.5	O	O	O	O	X	X	X	X
37.2	O	O	X	X	X	X	X	X
38.8	X	O	O	O	X	X	X	X
39.1	O	O	X	X	O	O	O	O
40.8	O	O	X	X	X	X	X	X
42.6	O	O	X	X	O	O	O	O
44.8	X	X	X	X	X	X	X	X
56.7	O	O	O	O	O	O	O	X
57.2	X	O	O	O	O	O	O	O
67.0	O	X	X	X	X	X	X	X
68.0	O	X	O	O	O	O	O	O
75.2	O	O	X	X	X	X	X	X
76.5	X	X	X	X	X	X	X	X
77.5	O	O	O	O	X	X	O	O
78.5	O	O	O	X	O	O	O	X
85.5	O	O	O	O	X	X	X	X
88.2	X	X	X	X	O	O	O	O
88.5	O	O	O	O	X	X	X	X
90.5	X	X	X	X	X	X	X	X
93.0	O	O	X	X	O	O	O	O
120.0	X	X	X	X	X	X	X	X
m/e	Half peaks (X = present, O = undetected)							
25.5	O	O	O	O	O	O	O	X
42.5	X	O	O	O	O	O	O	O
43.5	X	O	O	O	O	O	O	O
44.5	X	O	O	O	O	O	O	O
45.5	X	X	O	O	O	O	O	O
46.5	X	X	O	O	O	O	O	O
47.5	X	X	O	O	O	O	O	O
52.5	X	O	O	O	O	O	O	O
58.5	X	X	X	O	O	O	O	O
59.5	X	X	O	O	O	O	O	O
60.5	X	X	X	X	X	X	X	X
61.5	X	X	X	X	X	X	X	X
66.5	X	O	O	O	O	O	O	O
67.5	X	X	X	X	X	X	X	X
68.5	X	X	X	X	X	O	X	X
69.5	X	O	O	O	O	O	O	O
73.5	O	O	X	X	X	X	X	X
74.5	O	O	X	X	X	X	X	X
75.5	O	O	O	X	O	O	O	O
80.5	O	O	O	O	O	O	X	O
81.5	O	O	O	O	O	O	X	X
82.5	O	O	O	O	O	O	X	X

[1]Underlined values indicate parent and base peaks. Parent peaks are further noted with a "P" after the appropriate relative intensity. Ion contributions due to impurities are indicated by "imp" after the appropriate relative intensities.

TABLE A-3. - Mass spectral data for eight alkyl-m-tolyl sulfides

	3-Methyl-1-(1-thiaethyl)-benzene	3-Methyl-1-(1-thiapropyl)-benzene	3-Methyl-1-(1-thiabutyl)-benzene	3-Methyl-1-(2-methyl-1-thiapropyl)-benzene	3-Methyl-1-(1-thiapentyl)-benzene	3-Methyl-1-(2-methyl-1-thiabutyl)-benzene	3-Methyl-1-(3-methyl-1-thiabutyl)-benzene	3-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
Molecular weight	138	152	166	166	180	180	180	180
Magnetic field, gauss	3,225	3,225	3,225	3,225	3,225	3,225	3,225	3,225
Sensitivity, divisions/micron								
Base peak	59.99	48.37	40.96	64.76	60.42	77.47	48.16	94.79
Parent peak	59.99	48.37	40.96	37.54	39.37	34.43	36.01	13.30
n-Butane, m/e 43 peak	49.28	49.28	49.28	49.36	49.36	49.43	49.36	48.08
Ionizing current, microamperes	10	10	10	10	10	10	10	10
m/e	Relative intensities,[1] percent							
24	0.03	0.07	0.04	-	-	-	-	-
25	.15	.63	.22	0.13	0.11	0.09	0.08	0.05
26	1.53	7.99	4.38	2.13	3.49	2.31	2.02	1.02
27	4.45	28.63	36.73	21.08	25.57	17.48	22.84	9.46
28	.22	2.60	2.27	1.09	4.18	2.46	2.23	1.35
29	.21	18.34	5.12	.31	29.53	27.12	25.64	16.92
30	-	.40	.12	-	.64	.61	.57	.39
32	.57	.48	.47	.22	.20	.14	.22	.13
33	.27	.37	.26	.15	.13	.11	.14	.09
34	.21	.39	.33	.19	.26	.15	.23	.11
35	.08	.71	.06	.04	.11	.12	.07	.02
36	.11	.07	.07	.05	.02	.03	.04	.02
37	1.75	1.26	1.54	1.08	.59	.50	.91	.55
38	4.24	3.67	4.79	3.27	2.20	1.81	3.26	1.79
39	18.48	20.38	34.00	23.30	20.55	17.63	31.07	17.02
40	1.33	1.45	2.97	2.13	1.65	1.39	2.81	1.65
41	2.34	2.80	21.67	16.35	17.03	17.98	28.38	20.29
42	.11	.13	1.76	1.28	1.07	1.04	2.44	1.14

See footnote at end of table.

TABLE A-3. - Mass spectral data for eight alkyl-m-tolyl sulfides--Continued

	3-Methyl-1-(1-thiaethyl)-benzene	3-Methyl-1-(1-thiapropyl)-benzene	3-Methyl-1-(1-thiabutyl)-benzene	3-Methyl-1-(2-methyl-1-thiapropyl)-benzene	3-Methyl-1-(1-thiapentyl)-benzene	3-Methyl-1-(2-methyl-1-thiabutyl)-benzene	3-Methyl-1-(3-methyl-1-thiabutyl)-benzene	3-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
43	0.28	0.20	15.87	20.95	0.98	0.18	5.69	0.66
44	.55	.31	.73	.76	.20	.12	.32	.10
45	25.91	30.04	44.84	18.24	27.77	15.35	38.76	12.03
46	3.48	1.72	2.60	.55	1.52	.48	2.13	.34
47	3.46	2.09	3.52	1.42	2.47	1.19	2.97	.91
48	.43	.11	.19	.05	.10	.05	.16	.03
49	.71	.41	.33	.24	.20	.15	.23	.21
50	5.08	4.41	4.00	2.42	2.34	1.88	2.92	1.52
51	8.01	9.00	9.20	5.66	5.74	4.29	6.74	3.58
52	2.26	2.85	3.00	1.93	1.89	1.57	2.32	1.29
53	2.56	4.05	4.26	2.82	3.61	3.19	4.56	2.35
54	.17	.22	.23	.15	.32	.26	.35	.24
55	.14	.15	.11	.05	3.43	2.82	4.05	1.98
56	.12	.08	.04	.02	.64	.69	.73	.88
57	1.16	1.47	1.10	.84	5.68	11.50	20.21	35.33
58	1.49	2.97	2.52	1.92	1.61	1.54	2.00	2.15
59	1.07	4.33	2.90	3.98	2.44	3.66	2.52	1.74
60	.57	1.59	.45	.55	.47	.54	.29	.15
61	2.12	3.02	1.06	.75	.64	.66	.70	.36
62	4.42	3.60	3.25	1.81	1.66	1.19	2.09	.90
63	10.51	9.91	10.20	5.72	5.84	4.17	7.33	3.02
64	2.35	2.29	2.52	1.33	1.49	1.03	1.93	.70
65	10.30	12.71	16.91	8.06	10.70	6.74	13.90	4.10
66	.84	1.15	1.52	.82	.92	.66	1.13	.45
67	.38	.44	.55	.39	.36	.31	.43	.32
68	.77	.38	.41	.26	.24	.18	.37	.19
69	8.45	7.85	6.85	5.22	4.10	3.59	4.88	3.29
70	1.55	1.56	1.48	1.05	.85	.75	1.03	.66
71	2.02	2.97	4.01	2.12	1.98	1.69	2.55	1.41
72	.37	.26	.35	.19	.19	.18	.35	.12
73	.43	.41	1.34	.92	.47	.76	1.07	1.37
74	1.36	1.14	1.50	.88	.59	.46	.95	.46
75	1.14	1.17	1.51	1.05	.77	.58	1.13	.49
76	.82	1.09	.99	.59	.62	.42	1.00	.33
77	10.37	15.62	17.33	10.82	10.82	8.45	12.63	7.10
78	5.23	6.30	6.57	4.05	4.29	3.19	4.95	2.53
79	8.89	9.04	10.60	7.34	7.29	6.32	7.69	4.98
80	.81	2.08	2.26	1.84	1.36	1.26	1.38	.94
81	1.08	1.11	.94	.70	.52	.46	.65	.51
82	2.19	2.37	2.29	1.64	1.31	1.11	1.53	1.00
83	1.02	1.49	1.72	1.46	.90	.76	1.01	1.12
84	.69	1.38	1.39	1.55	.86	.78	.89	.81
85	.70	.61	.59	.34	.52	.30	.55	.49
86	.91	.67	.59	.33	.44	.25	.48	.21
87	.74	.56	.59	.32	.58	.48	.95	.33
88	.29	.30	.35	.20	.29	.22	.35	.11
89	4.94	5.17	6.21	3.39	3.90	2.74	4.75	1.79
90	2.83	3.54	4.05	2.80	2.46	1.99	2.81	1.34
91	32.08	61.44	70.46	54.20	41.68	35.88	44.72	24.19
92	16.18	8.84	7.15	5.01	4.58	3.60	4.83	2.15
93	3.46	5.71	6.43	1.05	3.22	.68	5.24	.46
94	.45	.62	.71	.20	.33	.12	.49	.09
95	1.19	1.29	1.17	.80	.64	.54	.76	.50
96	.66	.65	.61	.42	.38	.30	.42	.29
97	2.56	3.81	4.32	2.38	2.73	1.88	3.27	2.41
98	.29	.57	.62	.45	.38	.30	.42	.31
99	.14	.21	.25	.14	.15	.11	.18	.09
100	-	.07	.04	.03	.03	.03	-	-
101	.08	.22	.07	.03	.06	.04	.07	-
102	.22	.41	.27	.09	.20	.11	.25	.02
103	1.25	1.23	1.32	.17	.83	.19	1.25	.05
104	.95	1.14	1.39	.10	.88	.12	1.35	.03
105	17.90	1.19	2.96	.72	2.92	.84	2.78	.22
106	1.68	.25	.55	.15	.39	.14	.41	.07
107	.21	.22	.18	.16	.12	.13	.13	.08
108	2.58	3.55	3.58	2.68	2.40	2.08	2.57	1.83
109	.49	1.63	1.76	1.09	1.03	.79	1.16	.61
110	.32	.39	.40	.28	.28	.23	.29	.18
111	.27	.26	.21	.12	.14	.10	.17	.21
112	.07	.04	-	-	-	-	-	.18
113	-	-	-	-	-	-	-	.09
115	-	.67	.67	.54	.51	.61	.52	.16
116	-	.30	.39	.27	.24	.28	.29	.09
117	.12	1.19	.75	.95	.48	1.03	.31	.11
118	-	.83	.33	1.09	.42	1.23	.19	.02
119	.11	5.80	.30	.22	1.09	.27	.25	.05
120	.21	.73	.22	.10	.53	.10	.18	.05
121	7.05	6.74	6.51	3.50	4.14	2.73	4.87	2.03
122	2.44	2.58	3.05	1.10	1.96	.92	2.55	.69
123	23.54	12.62	13.39	11.18	11.04	11.00	9.96	6.52
124	2.06	32.50	86.83	100.00	100.00	100.00	100.00	100.00
125	1.05	3.23	8.18	9.15	9.34	9.21	9.35	9.30
126	.09	1.52	4.02	4.76	4.79	4.76	4.77	4.77
127	-	.20	.37	.38	.41	.42	.47	.39
128	-	-	.16	.08	.15	.12	.25	.08
129	-	-	.13	.05	.13	.10	.23	.05
130	-	-	.07	.03	.11	.07	.17	.03
131	-	-	.22	.13	.52	.14	.29	.12

See footnote at end of table.

TABLE A-3. - Mass spectral data for eight alkyl-m-tolyl sulfides--Continued

	3-Methyl-1-(1-thiaethyl)-benzene	3-Methyl-1-(1-thiapropyl)-benzene	3-Methyl-1-(1-thiabutyl)-benzene	3-Methyl-1-(2-methyl-1-thiapropyl)-benzene	3-Methyl-1-(1-thiapentyl)-benzene	3-Methyl-1-(2-methyl-1-thiabutyl)-benzene	3-Methyl-1-(3-methyl-1-thiabutyl)-benzene	3-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
132	-	-	0.19	0.09	0.10	0.07	0.11	0.10
133	0.05	0.11	.29	.21	.18	.05	.13	.02
134	.29	.78	1.02	.45	.78	.46	.78	.14
135	.76	1.77	2.25	.64	1.70	.74	1.84	.12
136	.30	1.03	.77	.92	.63	1.05	.54	.03
137	5.77	52.98	72.65	1.09	36.21	1.50	69.77	.39
138	100.00P	5.05	7.43	.16	4.31	.22	9.48	.05
139	9.71	2.57	3.70	.07	1.83	.09	3.61	.05
140	4.79	.22	.32	-	.20	-	.41	.02
141	.39	-	.03	-	.03	-	.05	.02
142	.03	-	-	-	-	-	-	-
145	-	-	-	-	.08	.05	.10	.02
146	-	-	-	-	.09	.07	.08	.02
147	-	.15	.33	.20	.29	.29	.44	.11
148	-	.09	.19	.16	.14	.22	.27	.08
149	-	.41	.51	.71	.52	.88	.61	.13
150	-	.22	.16	.21	.15	.28	.17	.04
151	-	1.83	1.38	6.39	2.83	13.85	1.66	.03
152	-	100.00P	.21	.77	.34	1.53	.18	-
153	-	9.87	.07	.33	.15	.69	.16	.17
154	-	4.81	-	.04	-	.07	-	.02
155	-	.43	-	-	-	-	-	-
156	-	.04	-	-	-	-	-	-
161	-	-	.06	-	.06	.06	.12	.02
162	-	-	-	-	-	.04	.07	-
163	-	-	.23	.10	.09	.23	.36	.08
164	-	.05(imp)	.19	.10	-	.07	.10	.02
165	-	-	.79	.46	.16	.77	.81	1.51
166	-	-	100.00P	57.97P	.16	.14	.14	.18
167	-	-	11.80	6.81	.03	.05	.05	.09
168	-	-	5.02	2.89	-	-	-	.09
169	-	-	.51	.30	-	-	-	.02
170	-	-	.04	.03	-	-	-	-
177	-	-	-	-	.03	.03	.06	.02
178	-	-	-	-	.16	.08	.07	.03
179	-	-	-	-	.56	.30	.62	.09
180	-	-	.07(imp)	-	65.15P	44.44P	74.78P	14.03P
181	-	-	-	-	8.46	5.69	9.57	1.83
182	-	-	-	-	3.37	2.31	3.85	.74
183	-	-	-	-	.37	.26	.42	.08
184	-	-	-	-	.04	.03	.05	-
m/e	Metastable peaks (X = present, O = undetected)							
25.2	O	X	O	O	X	X	X	X
29.5	O	O	O	O	X	X	X	X
37.2	O	O	X	X	X	X	X	X
38.8	O	O	O	O	X	X	X	X
39.1	O	O	X	X	O	O	O	O
40.8	O	O	O	X	X	X	X	X
42.6	O	O	X	X	O	O	O	O
44.8	X	X	X	X	X	X	X	X
56.7	O	O	O	O	O	O	O	X
62.5	X	O	O	O	O	O	O	O
67.0	O	X	X	X	X	X	X	X
75.2	X	X	X	X	X	X	X	X
76.5	X	X	X	X	X	X	X	X
78.5	X	X	X	X	X	X	X	X
80.0	X	O	O	O	O	O	O	O
85.5	O	O	O	O	X	X	X	X
88.2	X	X	X	X	X	X	X	X
90.5	X	X	X	X	X	X	X	X
93.0	O	O	X	X	O	O	O	O
120.0	X	O	X	X	O	X	X	O
m/e	Half peaks (X = present, O = undetected)							
42.5	X	O	O	O	O	O	O	O
43.5	X	O	O	O	O	O	O	O
45.5	X	O	O	O	O	O	O	O
46.5	X	X	O	O	O	O	O	O
47.5	X	O	O	O	O	O	O	O
48.5	X	O	O	O	O	O	O	O
52.5	X	O	O	O	O	O	O	O
58.5	X	X	X	X	O	O	O	O
59.5	X	X	O	O	O	O	O	O
60.5	X	X	X	X	X	X	X	X
61.5	X	X	X	X	O	X	X	X
67.5	X	X	O	X	X	X	X	X
68.5	X	X	O	X	X	X	X	X
69.5	X	O	O	O	O	O	O	O
73.5	O	O	X	X	X	X	X	X
74.5	O	O	X	X	X	X	X	O
75.5	O	O	O	X	O	X	O	O
76.5	O	X	O	O	O	O	O	O
80.5	O	O	O	O	O	O	X	O
81.5	O	O	O	O	O	O	X	O
82.5	O	O	O	O	O	O	X	X

[1]Underlined values indicate parent and base peaks. Parent peaks are further noted with a "P" after the appropriate relative intensity. Ion contributions due to impurities are indicated by "imp" after the appropriate relative intensities.

TABLE A-4. - Mass spectral data for eight alkyl-p-tolyl sulfides

	4-Methyl-1-(1-thiaethyl)-benzene	4-Methyl-1-(1-thiapropyl)-benzene	4-Methyl-1-(1-thiabutyl)-benzene	4-Methyl-1-(2-methyl-1-thiapropyl)-benzene	4-Methyl-1-(1-thiapentyl)-benzene	4-Methyl-1-(2-methyl-1-thiabutyl)-benzene	4-Methyl-1-(3-methyl-1-thiabutyl)-benzene	4-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
Molecular weight	138	152	166	166	180	180	180	180
Magnetic field, gauss	3,225	3,225	3,225	3,225	3,225	3,225	3,225	3,225
Sensitivity, divisions/micron								
Base peak	59.13	50.68	44.89	64.42	57.38	80.14	50.26	96.95
Parent peak	59.13	50.68	44.89	38.51	43.32	35.21	39.81	13.74
n-Butane, m/e 43 peak	48.08	48.08	48.37	48.37	48.37	48.37	48.37	48.37
Ionizing current, microamperes	10	10	10	10	10	10	10	10
m/e	Relative intensities,[1] percent							
24	0.03	0.07	-	0.02	-	-	-	-
25	.17	.60	0.20	.14	0.13	0.09	0.09	0.05
26	1.80	7.75	4.11	2.31	3.81	2.32	2.10	1.09
27	4.80	27.41	34.17	21.30	26.85	17.06	21.97	9.34
28	.29	2.81	2.50	1.27	4.48	2.69	1.84	1.47
29	.13	16.79	4.09	.32	32.01	25.76	24.77	15.92
30	-	.36	.09	-	.70	.57	.56	.37
32	.52	.50	.26	.24	.20	.15	.24	.17
33	.28	.32	.19	.16	.13	.10	.13	.09
34	.20	.34	.25	.22	.19	.14	.20	.12
35	.08	.58	.04	.03	.10	.10	.06	.02
36	.10	.06	.07	.05	.03	.03	.03	.03
37	1.60	1.03	1.29	1.00	.56	.44	.85	.48
38	3.64	2.78	3.80	2.87	2.02	1.50	2.86	1.50
39	15.96	15.76	27.22	20.89	19.24	15.37	27.80	15.02
40	1.16	1.14	2.46	2.02	1.60	1.26	2.66	1.51
41	2.03	2.37	18.71	15.83	17.61	16.70	27.39	18.61
42	.09	.10	1.71	1.37	1.21	1.06	2.93	1.09
43	.17	.11	14.28	18.80	.81	.16	5.19	.51
44	.22	.32	.64	.70	.20	.11	.29	.11
45	23.92	33.28	40.65	17.75	28.89	14.07	37.76	11.24
46	3.19	1.57	2.25	.54	1.52	.44	1.98	.32
47	3.09	2.00	3.09	1.37	2.40	1.08	2.76	.85
48	.42	.12	.15	.06	.10	.04	.13	.04
49	.75	.43	.33	.28	.19	.15	.23	.21
50	5.60	4.50	3.93	2.63	2.62	1.90	3.02	1.60
51	8.43	8.75	8.67	5.91	6.16	4.47	7.10	3.64
52	2.36	2.68	2.75	1.96	1.99	1.52	2.27	1.26
53	2.70	4.01	4.23	3.05	3.92	3.20	4.53	2.65
54	.18	.23	.23	.16	.35	.26	.35	.23
55	.06	.09	.09	.04	3.09	2.32	3.24	1.83
56	.14	.08	.03	.03	.55	.60	.64	.80
57	1.02	1.28	.93	.78	6.19	10.03	19.23	27.10
58	1.30	2.41	1.95	1.62	1.47	1.28	1.76	1.69
59	.89	3.48	2.32	3.58	2.12	3.27	2.10	1.50
60	.56	1.13	.35	.48	.46	.45	.29	.14
61	2.03	2.38	.93	.70	.59	.58	.62	.33
62	4.04	3.22	2.82	1.74	1.68	1.10	1.98	.85
63	9.93	8.59	8.67	5.28	5.64	3.70	6.66	2.73
64	2.14	1.94	2.06	1.18	1.40	.87	1.75	.60
65	9.04	10.38	13.45	7.02	9.66	5.61	11.89	3.50
66	.78	.97	1.19	.75	.86	.58	1.00	.40
67	.34	.35	.46	.39	.35	.30	.41	.29
68	.53	.34	.32	.24	.21	.17	.29	.17
69	9.85	8.97	7.95	6.22	5.15	4.06	5.61	3.66
70	2.16	2.16	2.01	1.57	1.35	1.07	1.49	.95
71	2.36	3.35	3.58	2.54	2.45	1.90	2.86	1.63
72	.44	.28	.36	.23	.23	.19	.34	.15
73	.50	.39	.91	.81	.38	.53	.80	1.06
74	1.34	1.07	1.26	.81	.54	.38	.72	.40
75	1.10	1.07	1.26	.93	.75	.53	.97	.44
76	.79	.95	.87	.53	.65	.40	.69	.34
77	10.31	14.98	15.99	11.15	11.98	8.44	13.04	7.01
78	5.57	5.71	5.85	4.01	4.37	3.01	4.75	2.38
79	10.21	10.66	11.19	8.65	9.19	6.88	9.00	5.70
80	.75	1.59	1.68	1.49	1.21	1.04	1.19	.79
81	.75	.77	.64	.53	.40	.32	.48	.33
82	1.74	1.90	1.70	1.35	1.12	.89	1.24	.80
83	.71	1.01	1.04	.78	.70	.56	.76	.75
84	.59	1.17	1.18	1.03	.84	.71	.82	.79
85	.67	.49	.45	.28	.48	.24	.47	.52
86	.94	.64	.53	.33	.48	.24	.48	.21
87	.78	.58	.55	.32	.59	.42	.86	.30
88	.30	.27	.31	.19	.30	.21	.38	.11
89	4.52	4.40	5.13	3.08	3.68	2.38	4.26	1.62
90	2.18	2.97	3.38	2.56	2.39	1.79	2.57	1.26
91	47.77	58.88	68.35	62.91	47.83	41.13	47.49	29.55
92	8.53	7.77	6.67	5.54	4.65	3.82	4.64	2.52
93	2.57	5.12	5.63	1.15	3.20	.67	4.87	.48
94	.43	.56	.64	.22	.34	.13	.47	.09
95	1.65	1.81	1.65	1.24	1.08	.82	1.15	.72
96	.80	.80	.76	.57	.59	.39	.55	.33
97	2.32	3.54	3.85	2.34	2.79	1.77	3.14	1.57
98	.25	.50	.55	.42	.38	.28	.40	.24
99	.13	.20	.21	.13	.15	.10	.16	.09
100	-	.08	-	.03	.03	-	-	-
101	.05	.19	.06	.03	.05	-	.06	-
102	.16	.33	.24	.08	.18	.09	.23	.03
103	.73	1.03	1.07	.15	.77	.17	1.10	.06
104	.52	.97	1.11	.09	.80	.10	1.17	.03
105	4.36	1.07	2.13	.63	2.12	.67	2.02	.18

See footnote at end of table.

TABLE A-4. - Mass spectral data for eight alkyl-p-tolyl sulfides--Continued

	4-Methyl-1-(1-thiaethyl)-benzene	4-Methyl-1-(1-thiapropyl)-benzene	4-Methyl-1-(1-thiabutyl)-benzene	4-Methyl-1-(2-methyl-1-thiapropyl)-benzene	4-Methyl-1-(1-thiapentyl)-benzene	4-Methyl-1-(2-methyl-1-thiabutyl)-benzene	4-Methyl-1-(3-methyl-1-thiabutyl)-benzene	4-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-Propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Relative intensities,[1] percent--Continued							
106	0.51	0.23	0.33	0.14	0.28	0.12	0.29	0.06
107	.16	.18	.15	.13	.11	.10	.11	.06
108	2.47	3.32	3.23	2.54	2.49	1.94	2.51	1.65
109	.49	1.32	1.36	.95	.93	.66	1.00	.51
110	.30	.31	.33	.25	.27	.19	.27	.15
111	.25	.18	.16	.09	.13	.08	.14	.10
112	.09	-	-	-	-	-	-	.05
113	-	-	-	-	-	-	-	.03
115	-	.50	.57	.45	.44	.49	.42	.12
116	-	.22	.28	.21	.18	.21	.21	.07
117	.13	.81	.51	.79	.41	.85	.26	.09
118	.03	.55	.27	.90	.32	.98	.17	.02
119	.13	2.37	.21	.20	.81	.24	.23	.05
120	.28	.39	.21	.11	.29	.10	.19	.06
121	8.93	7.33	6.69	4.46	5.18	3.27	5.59	2.41
122	4.79	3.10	3.32	1.66	2.55	1.29	2.84	.89
123	34.06	20.85	19.78	16.25	18.33	15.01	16.12	8.97
124	3.20	26.14	76.98	100.00	100.00	100.00	100.00	100.00
125	1.61	3.30	7.32	9.29	9.45	9.21	9.35	9.24
126	.13	1.41	3.63	4.74	4.73	4.69	4.73	4.72
127	-	.23	.32	.37	.39	.39	.43	.38
128	-	-	.13	.07	.13	.10	.22	.07
129	-	-	.09	.03	.10	.06	.19	.05
130	-	-	.07	.02	.08	.05	.13	.03
131	-	-	.14	.05	.23	.09	.20	.09
132	-	-	.11	.06	.05	.04	.07	.07
133	.05	.11	.17	.11	.08	.03	.09	.03
134	.52	.67	.80	.36	.67	.38	.66	.12
135	.74	1.56	1.76	.57	1.53	.61	1.54	.10
136	.47	.90	.68	.74	.55	.81	.64	.03
137	15.56	51.84	68.17	1.16	38.28	1.24	66.08	.32
138	100.00P	4.99	6.67	.15	4.37	.17	8.32	.05
139	10.03	2.48	3.30	.06	1.89	.06	3.34	.03
140	4.77	.23	.28	-	.18	-	.35	.02
141	.43	.04	.03	-	.03	-	.04	.03
142	.03	-	-	-	-	-	-	-
145	-	-	-	-	.03	.02	.05	.02
146	-	-	-	-	.04	.04	.05	.02
147	-	.14	.26	.15	.23	.21	.33	.08
148	-	.10	.13	.12	.11	.16	.20	.06
149	-	.38	.44	.57	.47	.70	.52	.11
150	-	.28	.11	.15	.14	.23	.13	.03
151	-	2.22	1.16	4.99	2.51	10.30	1.49	.03
152	.03(imp)	100.00P	.14	.65	.29	1.11	.17	-
153	-	10.68	.05	.25	.13	.52	.07	.03
154	-	4.88	-	.03	-	.04	-	-
155	-	.45	-	-	-	-	-	-
156	-	.04	-	-	-	-	-	-
161	-	-	.03	-	.05	.04	.10	.02
162	-	-	-	-	-	-	.05	-
163	-	-	.17	.07	.06	.15	.28	.07
164	-	-	.26	.13	-	.04	.09	.03
165	-	-	.81	.33	.13	.57	.76	1.36
166	-	-	100.00P	59.77P	.03	.13	.12	.17
167	-	-	11.82	6.99	-	.03	.05	.08
168	-	-	5.04	2.99	-	-	-	.02
169	-	-	.50	.31	-	-	-	-
170	-	-	.04	.03	-	-	-	-
177	-	-	-	-	-	.03	.06	.02
178	-	-	-	-	.18	.11	.19	.03
179	-	-	-	-	.59	.22	.69	.07
180	-	-	.07(imp)	-	75.50P	43.94P	79.20P	14.17P
181	-	-	-	-	9.79	5.66	10.30	1.85
182	-	-	-	-	3.89	2.26	4.10	.74
183	-	-	-	-	.43	.24	.45	.08
184	-	-	-	-	.03	.02	.04	-
m/e	Metastable peaks (X = present, O = undetected)							
25.2	O	X	O	O	X	X	X	X
29.5	O	O	O	O	X	X	X	X
37.2	O	O	X	X	X	X	X	X
38.8	X	O	O	O	O	O	X	X
39.1	O	O	X	X	O	O	O	O
40.8	O	O	X	X	O	X	X	X
42.6	O	O	X	X	O	O	O	O
44.8	X	X	X	O	X	X	X	X
46.8	O	O	X	O	O	O	O	O
50.8	X	O	O	O	O	O	O	O
56.7	O	O	O	O	O	O	X	X
60.2	X	O	O	O	O	O	O	O
62.5	X	O	O	O	O	O	O	O
67.0	O	X	X	X	X	X	X	X
75.2	O	O	X	X	X	X	X	X
76.5	X	X	X	X	X	X	X	X
78.5	X	X	X	X	X	X	X	X
85.5	O	O	O	O	X	X	X	X
88.5	X	X	X	X	X	X	X	X
90.5	X	X	X	X	X	X	X	X
93.0	O	O	X	X	O	O	O	O
120.0	X	X	X	X	X	X	X	X

See footnote at end of table.

TABLE A-4. - Mass spectral data for eight alkyl-p-tolyl sulfides--Continued

	4-Methyl-1-(1-thiaethyl)-benzene	4-Methyl-1-(1-thiapropyl)-benzene	4-Methyl-1-(1-thiabutyl)-benzene	4-Methyl-1-(2-methyl-1-thiapropyl)-benzene	4-Methyl-1-(1-thiapentyl)-benzene	4-Methyl-1-(2-methyl-1-thiabutyl)-benzene	4-Methyl-1-(3-methyl-1-thiabutyl)-benzene	4-Methyl-1-(2,2-dimethyl-1-thiapropyl)-benzene
Alkyl substituent.....	Methyl	Ethyl	n-propyl	Isopropyl	n-Butyl	s-Butyl	Isobutyl	t-Butyl
m/e	Half peaks (X = present, 0 = undetected)							
42.5	X	0	0	0	0	0	0	0
43.5	X	X	0	0	0	0	0	0
46.5	X	X	X	X	X	0	0	0
47.5	X	X	0	0	0	0	0	0
48.5	X	0	0	0	0	0	0	0
52.5	X	0	0	0	0	0	0	0
58.5	X	X	0	0	0	0	0	0
59.5	X	X	0	0	0	0	0	0
60.5	X	X	X	X	X	X	X	X
61.5	X	X	X	X	X	X	X	X
67.5	X	X	X	0	X	0	X	0
68.5	X	X	X	0	X	0	X	X
69.5	X	0	0	0	0	0	0	0
73.5	0	0	X	X	X	X	X	X
74.5	0	0	X	X	X	X	X	X
75.5	0	0	0	X	0	X	0	0
80.5	0	0	0	0	0	0	X	0
81.5	0	0	0	0	0	0	X	0
82.5	0	0	0	0	0	0	X	X

[1]Underlined values indicate parent and base peaks. Parent peaks are further noted with a "P" after the appropriate relative intensity. Ion contributions due to impurities are indicated by "imp" after the appropriate relative intensities.

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