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MASS SPECTROMETRY OF AEROSPACE MATERIALS

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16. Abstract

Mass spectrometry is used for chemical analysis of aerospace materials and contaminants. Years of analytical aerospace experience have resulted in the development of specialized techniques of sampling and analysis which are required in order to optimize results. This work has resulted in the evolution of a hybrid method of indexing mass spectra which includes both the largest peaks and the structurally significant peaks in a concise format. With this system, a library of mass spectra of aerospace materials has been assembled, including the materials responsible for 80 to 90 percent of the contamination problems at Goddard Space Flight Center during the past several years.

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MASS SPECTROMETRY OF AEROSPACE MATERIALS

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INTRODUCTION

The critical cleanliness requirements of advanced optical experiments (especially ultraviolet optics) and other types of detectors demand extreme vigilance during fabrication, handling, and testing to ensure proper responses and the production of reliable data during launch and flight operations. Mass spectrometry is a powerful tool for organic chemical analysis and is used frequently in aerospace technology to identify contamination on spacecraft hardware, to verify sources of this contamination, and to evaluate materials for use in space and test environments.

The results of several years of aerospace analytical work using mass spectrometry demonstrate that a number of specialized techniques for sampling and analysis are required to obtain good analytical results. Although 80 to 90 percent of contamination problems involve 100 or less chemical species, the majority of these are not listed in standard mass spectral reference sources. This document brings together a description of practical analytical procedures with an easy-to-use collection of mass spectral patterns commonly encountered in aerospace work.

ANALYTICAL APPARATUS

Instrumental requirements for a comprehensive analytical facility (figure 1) include a low-resolution mass spectrometer with a mass range at least up to 700 with unit resolution. The sample input facilities should include a direct-evaporation solids probe, a heated gas inlet with reservoir and calibrated leak, a liquid-evaporation inlet, and a coupled gas chromatograph (GC). The mass spectrometer should be capable of scanning the entire mass range in 5 or 6 seconds without loss of resolution in order to handle GC samples adequately and, ideally, should be equipped with a dedicated minicomputer for data accumulation, storage, and manipulation. This requirement is necessary for facilitating timely and complete interpretation of the enormous amount of information which can be generated. It is also desirable to have an integrator on the GC system to permit quantitative analysis and a high-speed printer/plotter for outputting data rapidly in meaningful form. Descriptions of the details of theory and operation of these instruments can be found in References 1, 2, and 3. Other desirable accessories are a computer library and an oscilloscopic data-display unit.

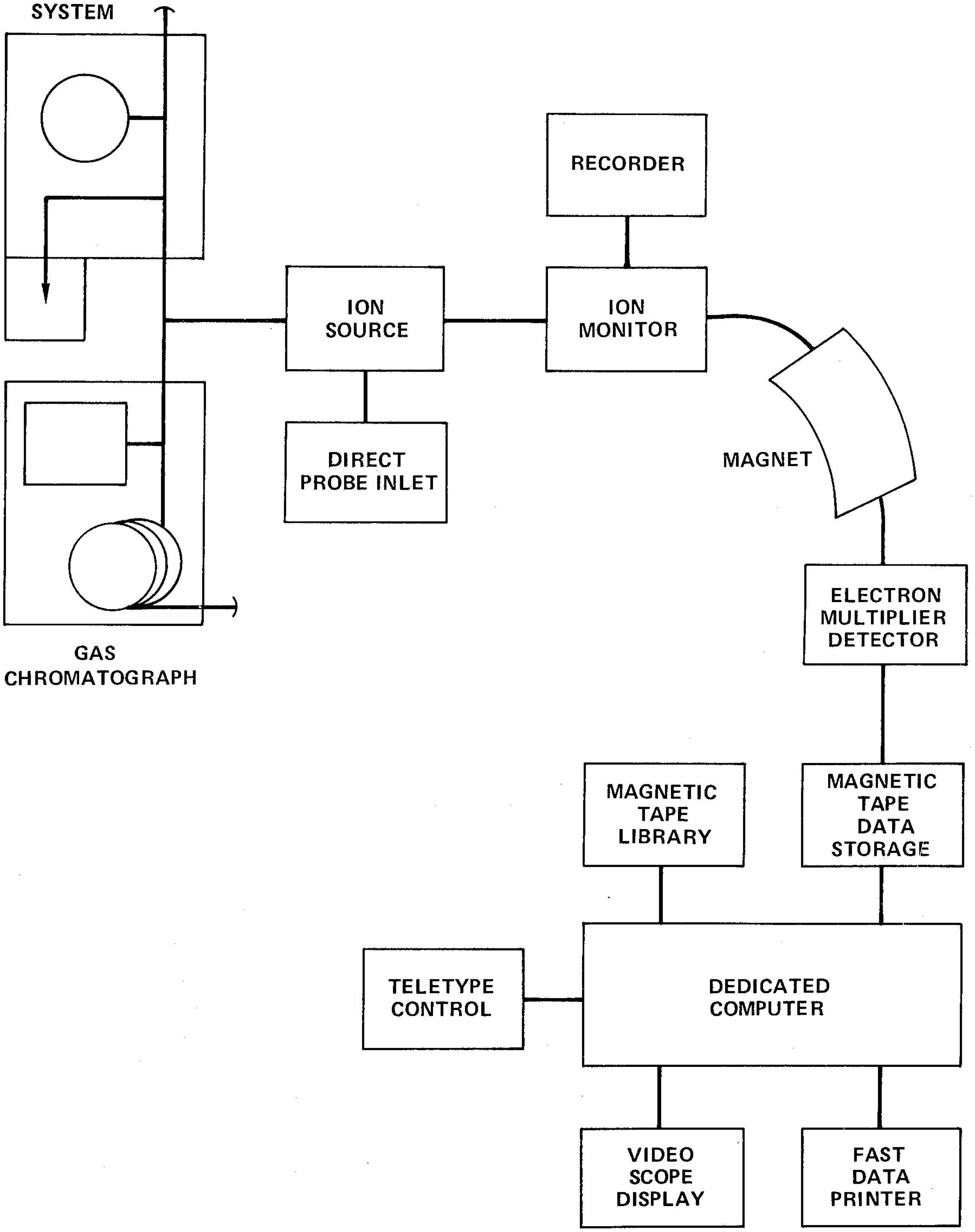

Figure 1. Analytical mass spectrometry system.

Besides the mass-spectral facility, an infrared spectroscopy capability is very important for providing sample screening and reinforcement of mass-spectral findings. As in any analytic effort, all possible sources of diagnostic information must be utilized.

SAMPLING TECHNIQUES

In analytical chemistry, it is important to obtain a representative sample that is not altered or comtaminated by the sampling technique because it is often necessary to determine the nature of a contaminant with only a few micrograms of material. Extreme care must be taken in such cases to ensure cleanliness of sampling devices (swabs, beakers, and syringes) and purity of the solvents used.

One of the most effective means of collecting small samples of contamination from spacecraft, experiment modules, or test facilities is by wiping with a dry or solvent-dampened cotton swab, followed by extraction of the swab in the laboratory. However, this procedure requires fastidious adherence to strict cleaning procedures and control of experimentally-induced background contaminant levels. All cotton, cotton swabs, and wiping cloths contain large amounts of organic impurities (such as cottonseed oil, adhesives, and sizing compounds) and other additives which must be completely removed before the item is suitable for sample-collection use. This task is most readily accomplished by extraction, using a Soxhlet Extractor. An effective extraction program for most uses includes 24-hour cycling with absolute ethanol, followed by 6 hours with spectrograde chloroform. If another solvent is to be used for sample collection, it should also be included in the extraction program. After extraction, the swabs should be dried and stored in a noncontaminating environment.

Small parts, such as solid-state devices, mirrors, and bearings, may be carried to the laboratory where the contaminant is removed by rinsing with an organic solvent. It is sometimes necessary to remove very small samples by dissolving them in a drop of solvent which is retrieved in a microsyringe for transport to the laboratory. Very often it is possible to remove solids by scraping them into a glass container or noncontaminating envelope. It is important that the container used to carry the sample does not contribute its own materials to the sample, and plastic cap liners, plasticized containers, and rubber seals or gaskets should be avoided.

Vaporization and condensation of marginally volatile materials are the most prevelant processes leading to spacecraft contamination in thermal-vacuum test chambers and in flight. The extent and nature of these outgassing and condensing processes is most readily determined by the use of liquid-nitrogen-cooled cold fingers installed in vacuum test chambers and operated during testing of flight hardware. These devices allow collection of the condensables emanating from the spacecraft or test equipment which might comprise contamination. Mass-spectral analysis of these residues, along with examination of hardware and test equipment, usually leads to identification of contamination sources.

An extensive program designed to reduce the incidence of outgassing problems in all Goddard projects is carried out by the Materials Engineering Branch (MEB). Through this program, thousands of materials have been subjected to a standard outgassing test, and from it, minimum standards have been designated that all materials must meet before being approved for spaceflight use (Reference 4). The MEB material engineers work with project scientists in attempting to eliminate all potential high-outgassing materials from spacecraft components.

ANALYTICAL TECHNIQUES

Standard operating techniques for mass spectrometry are well covered in various texts (References 1, 2, and 3) and in the instrument manuals and publications supplied with each mass spectrometer system. Therefore, only a few specialized procedures and concepts relating to aerospace analyses will be mentioned here.

Sample handling procedure is determined by a variety of considerations, including the amount, physical state, purity or complexity, vapor pressure, polarity, and thermal stability of the sample. Before beginning an analysis, it is desirable to determine how much information is required and what the aim of the analysis should be. For example, if a sample of lubricant is submitted for determining whether the proper type was used, it is unnecessary to run a complete gas-chromatograph/mass-spectrometer (GC/MS) analysis to identify the type of lubricant and the additives, impurities, and isomeric species. In fact, it probably would be sufficient to run only an infrared spectrum and a GC analysis with no mass spectrometry at all.

The greatest utility of the GC/MS combination in aerospace analysis is with samples of vacuum-condensed residue. The greatest proportion of these residues are susceptible to gas-chromatographic separation because they are readily volatile under GC conditions and are generally soluble in common organic solvents. In addition, these residues are usually complex mixtures of 50 or more separable entities and cannot be identified easily in any batch-type technique. The exact chromatographic conditions, such as column length, sample size, and flow rate, are determined by the requirements of the particular mass spectrometer and separator system. However, successful separation of vacuum-condensable mixtures requires the use of a stable high-temperature column packing with a low-bleed rate, such as OV-17 or Dexsil 300 GC. If the column can separate compounds such as decyl phthalates and tricresyl phosphates, it will be suitable for most vacuum-condensable mixtures.

When a GC/MS analysis has been completed, the results should be reconciled with the findings of the infrared spectrum of the mixture. If the infrared shows additional species, such as amines or acids (which might not pass through the chromatograph), the sample should be run again in the direct probe. Subtraction of mass-spectral peaks obtained in the GC/MS run from those of the mixture in the direct-probe run can often lead to identification of the additional materials.

Successful identification of many classes of aerospace materials depends on the skillful operation of the direct-probe inlet on the mass spectrometer. This inlet can be used to analyze low-volatility liquids, such as heavy oils, waxes, and greases, as well as solids. If the probe can be heated to 723 to 773 K, most polymeric materials can be volatilized sufficiently for identification. Optimum results are obtained by careful control of the heating rate—an art learned only by experience. The aim should be to heat fast enough to get sufficient partial pressures for identification and slow enough to get fractionation of multicomponent materials. It is mandatory to limit the size of the sample so that the operating pressure of the system is not exceeded and the length of time required to volatilize the sample is not excessive. The direct-inlet system is the most sensitive because all of the sample reaches the analyzer tube. Thus, it is often the only method available for obtaining information about very small samples, such as those visible only under the microscope.

Analyses of gases and gas mixtures are often required in connection with spark-chamber or detector atmospheres or propellants for rocket motors and thrusters. These can usually be studied by using the standard gas-inlet system which includes a filling manifold, a heated reservoir, and a controlled leak into the mass spectrometer. With appropriate references, a mixture can usually be identified both qualitatively and quantitatively. However, if small impurities must be identified, the gas chromatograph should be used.

Another use of the mass spectrometer is to obtain outgassing profiles of materials. This can be accomplished either by programmed heating of the material in the liquid inlet, followed by bleeding outgassed products through the controlled leak, or by calibrated use of the direct probe. In either case, the result is partial pressure output, indicating the rate of total outgassing (on the total-ion monitor), as well as identification of outgassed materials. Relating of results obtained by these procedures to standard outgassing test results is dependent on various parameters, such as pumping speed and throughput of the system, temperature control, and precision of sample size. At best, this relation can be established in a semi-quantitative fashion.

MASS-SPECTRAL INTERPRETATION

Before interpretation of the spectra from a sample begins, it is desirable to consider the quality of those spectra because the interpretation can be no better than the quality of the spectra permits. Spectra usually may be improved by using computer operations such as spectrum averaging and background subtraction. It is sometimes possible to eliminate peaks from impurities by raising thresholds; at other times, it is desirable to increase the abundance of high-mass peaks by weighted multiplication. When mixtures are run in the solids probe, it is often possible to subtract spectra obtained at one temperature from those at a higher or lower temperature to obtain a useful spectrum for identification. Also, if mixture spectra have been obtained and one or more components are known, spectra for these components may be subtracted peak for peak from the total spectrum. Other specialized data transformations can be made as the particular situation dictates.

If a good spectrum of a pure compound has been obtained, the material can be identified on theoretical grounds. The techniques for this operation are detailed explicitly by McLafferty (Reference 5). Spectral information, such as isotopic abundance, parent-peak identification, even and odd electron ions, neutral losses, and metastable ions, is combined to yield structural identification.

In the usual and more realistic cases of mass-spectral analysis, neither sufficiently good spectra nor available time exist for the theoretical approach. The "fingerprint comparison" method must then be used, which requires that the mass spectrum has been obtained previously and is on file. The most successful method for fingerprint comparison involves the memory and experience of the mass spectrometrist. However, when this method fails, a reference library must be consulted. This information is available in either published reference books (References 6, 7, and 8) or computer data banks (References 9 and 10). Data in reference books may be arranged either according to molecular weight or by the six or ten most-abundant mass peaks.

Cataloging by molecular weight is of limited value because it requires that the parent peak be known, which is very often not the case. Although serial arrangements by most-abundant species are the most efficient to use, they present another disadvantage. For many classes of compounds, the most-abundant species in the spectrum have little structural significance; therefore, positive identification cannot be made from these references alone. Computer data-bank searches usually use either of two approaches which tend to nullify the disadvantages of the printed references. In the first of these, the entire spectrum is divided into a number of smaller intervals (14 masses per interval or 20 masses per interval, etc.), and the two or three largest peaks in each interval are retained and compared to those of the unknown. This system has the advantage of retaining the most-abundant peaks in the spectrum, as well as the most structurally significant peaks. A similarity index is then given depending on the percentage of matches in the reduced spectra. The major disadvantage of this system is the fact that the intensity of the spectra becomes very important in determining the value of the similarity index. Thus, a weak spectrum and a strong spectrum of the same material may show very poor correlation.

The second computer approach involves interactive communications between the analyst and the data bank. The analyst enters the mass and intensity range of a peak, and the computer responds with the number of references on file that have that combination. Entering a large peak and three or four structurally significant peaks is usually enough to identify a compound if it is contained in the data bank.

Unfortunately, a large percentage of the materials which the aerospace analyst must identify are not included in any of the available mass-spectral data filing systems. To alleviate this problem, a listing of spectra obtained over a period of years at Goddard Space Flight Center has been included as an appendix to this report. The format for this data is intended to combine both the largest-peaks system and the structurally significant-peaks requirement. Although this format is admittedly quite subjective, it is designed to aid in efficient and rapid identifications.

MASS-SPECTRAL INDEXING OF AEROSPACE MATERIALS

Experience has shown the need for a ready-reference indexing method similar to the one presented here and that of the Appendix, Mass-Spectral Index of Aerospace Materials. The spectra are ordered according to the mass (M/E) of the most intense peak in the spectrum.

The next four most intense peaks are given, along with their relative abundances (RA), expressed in percent of the base peak (100-percent peak). Because the strongest peaks in the spectrum often contribute relatively little structural information (as in the case of aliphatic hydrocarbons), an additional listing has been included of up to four structurally significant peaks and their relative abundances. These peaks were chosen by an arbitrary and subjective consideration of each individual spectrum and the factors required for its identification. In some cases, the most intense peaks provide sufficient structural information, and no further masses are listed.

As an example of the use of this indexing method, consider the following entry for the common plasticizer, di- (2 ethyl hexyl) phthalate (DEHP).

M/E	M/E,RA	M/E,RA	M/E,RA	M/E,RA	M/E,RA	M/E,RA	M/E,RA	M/E,RA
149	167-88	57-72	70-66	55-58	112-32	113-34	279-40	

In this example, 149 is the base peak (most intense peak), with the next four peaks and their relative abundances directly following. These five peaks are sufficient for identifying the compound as an aliphatic ester of phthalic acid. However, the next three peaks are required for differentiating the octyl phthalate from hexyl, decyl, tridecyl, or mixed esters.

The names of materials included in this index and corresponding to the various spectra, range from pure chemical compounds to generic-name materials to brand-name products. Association of a spectrum with a material implies only that the analyzed product may have originated from that material. Because many products are complex mixtures, several different and distinct mass-spectral patterns are possible from the same material. For example, the outgassed part of a product (vacuum-condensable material (VCM)) may be different from the solvent-extractable part, and both may be different from the bulk of the material. However, each of these might be designated under the original product name. In actual practice, especially when a contaminant is being analyzed, it is often more important to identify possible sources rather than unique chemical structures. Thus, this index of spectra was prepared to provide some clue to contaminant origin in the maximum number of cases.

As a final note on analysis, it must be reemphasized that, for proper identification, all pertinent information about a sample must be considered. Its physical properties, history, source, and infrared spectra are all important aids to the analyst. Successful mass-spectral identification usually involves a hybrid combination of all this available information in order to respond with useful and timely answers to problems.

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National Aeronautics and Space Administration
Greenbelt, Maryland April 27, 1976

REFERENCES

1. McLafferty, F. W., *Mass Spectrometry of Organic Ions*, Academic Press, New York, 1963.
2. Biemann, Klaus, *Mass Spectrometry: Organic Chemical Applications*, McGraw-Hill, New York, 1962.
3. McFadden, William, *Techniques of Combined Gas Chromatography/Mass Spectrometry: Applications in Organic Analysis*, John Wiley & Sons, New York, 1973.
4. Campbell, William A., Richard S. Marriott, and John J. Park, *Outgassing Data for Spacecraft Materials*, NASA TN D-8008, July 1975.
5. McLafferty, F. W., *Interpretation of Mass Spectra*, W. A. Benjamin, Reading, Mass., 1973.
6. Stenhagen, E., S. Abrahamsson, and F. W. McLafferty, *Atlas of Mass Spectral Data*, John Wiley & Sons, New York, 1969.
7. Index of Mass Spectral Data, ASTM Committee E-14 on Mass Spectrometry, American Society for Testing and Materials, 1969.
8. Cornu, A. and R. Massot, *Compilation of Mass Spectral Data*, Heydon and Son, London, 1966.
9. Mass Spectral Search System, Data Base Services, Cyphernetics Corporation, Ann Arbor, Michigan, 1975.
10. Varian, MAT, Spectro System 100 MS, Library Search Program, Springfield, New Jersey, 1974.

APPENDIX
MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS

BASE PEAK	MOST INTENSE PEAKS				STRUCTURALLY SIGNIFICANT PEAKS				MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
28	42- 73	56-73	41-58	27-43	84-39	85-32	123-11	125-10	Hysol EA934 Structural Adhesive
28	43- 38	36-33	44-28	41-26	104-22	148-10	203-20	263-10	3M Nextel Black Velvet 401
28	61- 75	42-53	102-40	73-34	60-26	115-24	268-13	326-21	DC 93-046 Adhesive
29	28- 88	54-72	43-60	40-50	82-16	84-28	152-11		White Nylon
29	57- 98	41-87	56-78	27-53	88-21	86-20	101-13		Butyl Oleate
36	38- 90	78-70	52-20	98-5					Polyvinyl Chloride
36	38- 96	180-70	182-66	232-20	266-20				Polyvinylidine Chloride
41	55- 87	43-68	69-59	39-48	141-16	268-13	296-14		Apiezon "H" Grease
41	55- 78	56-68	70-46	69-42	84-27	112-15	142-4	193-4	Tris (2 Ethyl hexyl) Trimellitate
41	69- 88	100-56	39-44	99-19					Methyl Methacrylate
41	137- 97	119-58	57-56	121-54	217-27	219-30	417-13	419-11	Stur-D-Lace P18DP Lacing Tape VCM
41	137- 97	119-83	121-79	39-67	217-53	219-48	417-22	419-24	Tris 2,3 DiBromopropyl Phosphate "Fyrol HB-32"
43	59-100	41-57	72-48	69-31	122-9	136-7			Oleoamide
43	67- 71	81-70	69-63	98-58	166-34	262-15	280-11		Spraylat Black Strip Coating
43	73- 94	57-91	60-88	55-77	129-48	141-51	256-37	284-26	Apiezon "T" Grease
44	30- 99	46-99	28-96	55-91	60-27	61-17	71-20		Nitrocellulose - Decomposition
44	45- 95	28-94	29-49	69-45	113-40	134-17	253-24	293-16	Loctite Refrigerant Sealant
44	58- 87	59-56	161-26	103-24	100-23	205-15	219-15		Armstrong A-31 Epoxy Catalyst
44	73-100	30-65	56-28	42-23	86-20				Diethylene Triamine (DTA Curing Agent)
44	73- 81	94-25	56-13	43-11					Epon Curing Agent "U"
44	73- 93	99-74	116-68	56-59	142-16				Triethylene Tetramine (TETA Curing Agent)
44	117-100	74-99	73-95	56-89					Epon Curing Agent "T"
45	57-100	41-89	28-89	29-85	75-70	88-47	101-36	102-30	Dibutoxy Ethoxy Ethyl Adipate
45	89- 63	133-43	57-43	161-36	205-21	487-21	531-19		Triton X-100 (Alkyl Phen oxy Poly Ethoxy Ethanol)
45	355- 70	89-58	311-57	57-51	135-45	161-46	399-23		Triton X-100 (Alkyl Phen oxy Poly Ethoxy Ethanol)
55	41- 97	27-76	57-70	69-68	98-63	264-18	399-26	515-18	Dibutyl Tin Di Oleate
55	41- 80	67-74	81-63	79-63	95-62	149-12	173-8	261-9	Linseed Oil

*M/E is mass to charge ratio and RA is relative abundance of that peak in percent of base peak (strongest peak).

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS (Continued)

BASE PEAK	MOST INTENSE PEAKS				STRUCTURALLY SIGNIFICANT PEAKS				MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
55	41- 90	69-81	57-77	83-75	98-40	264-42	265-30		Neoprene Sleeving Extract
55	43- 58	41-55	29-42	141-41	342-5				NPT-4 Oil Bray Oil Co.
55	57- 84	43-74	98-47	112-45	127-33	141-32	183-41	226-29	Gude Nylace Style 18 B Lacing Tape VCM
55	57- 61	141-55	41-55	98-44	257-6	383-7			NPT-4 Oil Bray Oil Co.
55	67- 67	81-62	43-57	41-57	123-16	165-10	166-17	280-11	Castor Oil
55	129- 98	56-86	43-84	70-64	241-27	269-18			N-Octyl N-Decyl A dipate
56	31- 70	41-61	104-56	43-56	76-45	148-25			Mono-m-butyl Phthalate
56	57- 86	257-68	43-57	73-51	129-37	239-37	312-24		Butyl Palmitate
56	57- 96	285-78	43-77	73-60	129-56	267-41	340-44		Butyl Stearate
56	83- 91	43-91	69-85	97-80	153-70	209-70			Poly isobutylene
57	28- 94	55-84	69-80	95-74	112-54	123-44	208-68		Andok C Hydrocarbon Oil
57	43- 99	55-78	71-67	141-67	185-19	213-14	256-19	284-15	Cottonseed Oil
57	55- 86	43-74	69-70	83-64	125-21	137-12	141-12	153-11	Apiezon "T" Grease
57	55- 83	43-73	69-72	97-62	149-12	151-15	191-11		Vac Torr Oil
57	55- 93	43-87	69-85	129-84	141-19	269-36	287-19		Isodecyl A dipate
57	71- 65	55-63	43-60	69-60	97-51	123-22	125-27	141-20	Apiezon C, Hydro Carbon Oil
57	71- 69	43-63	55-62	69-62	125-24	155-15	165-11	181-8	DuoSeal Pump Oil
57	71- 59	43-64	55-54	69-52	139-25	141-22	155-12	169-9	Apiezon "B" Oil
57	71- 63	97-62	83-58	43-55	151-11	153-11			Sunvis 931 Oil
57	117- 64	41-39	43-37	29-37	120-14	155-20			Dibutyl Maleate
57	129- 96	70-72	55-64	41-63	112-43	147-22	241-10	259-6	Di (2 Ethyl hexyl) A dipate
57	183- 83	55-76	43-67	71-50	311-39	383-22	439-24		Gude "Q" Lacing Tape Extract
59	72- 83	55-55	43-36	69-32	126-18	128-10	337-27		Residue From Polyethylene Sheeting (erucamide)
59	117- 65	99-53	115-34	175-25					Polyproylene Glycol
63	125- 83	213-74	151-50	249-41					Chlorinated Organophosphorus Compound "Fyrol 99" Plasticizer
67	149- 82	54-68	82-60	41-49	84-22	167-34	249-6		Di-Cyclohexyl Phthalate
69	100-100	114-82	119-55	164-27	192-15	280-9			FC-78 Fluorinert Electronic Fluid - 3M
69	100-100	169-100	131-98	119-89	150-42	197-31	231-22		FC-77 Fluorinert Electronic Fluid - 3M

*M/E is mass to charge ratio and RA is relative abundance of that peak in percent of base peak (strongest peak).

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS (Continued)

BASE PEAK	MOST INTENSE PEAKS				STRUCTURALLY SIGNIFICANT PEAKS				MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
69	131- 97	119- 85	181- 76	100- 52	293- 18	393- 26	544-9		FC-48 Fluorinert Electronic Fluid- 3M
69	219-100	131- 98	100- 35	264- 35	414- 11	502- 15			FC-43 Fluorinert Electronic Fluid-3M
73	147- 56	44- 58	75- 55	221- 51	77- 39				3M Tape #433 VCM
73	147- 42	281- 34	207- 26	415- 24	461- 18	475- 13			RTV-11 VCM Methyl Silicone
73	207- 44	281- 43	147- 40	503- 21					RTV-11 VCM Methyl Silicone
73	207- 64	355- 40	147- 37	281- 34	429- 33	563- 11			RTV-11 VCM Methyl Silicone
73	207- 45	355- 45	147- 36	281- 30	489- 19				RTV-11 VCM Methyl Silicone
73	429- 44	207- 37	147- 34	355- 27	475- 8				RTV-11 VCM Methyl Silicone
75	77- 81	109- 62	125- 61	38- 60	149- 32	151- 20	345-24		Chemlok 234 B
75	99- 99	191- 95	381- 67	209- 66	321- 49	383- 42			Tris Dichloropropyl Phosphate
77	73- 92	137- 90	207- 73	59- 57	215- 34	237- 28	281- 31	355- 14	DC FS 1281 Fluorinated Silicone
77	147- 54	75- 53	44- 46	73- 43	149- 12	207- 15	221- 11		3M Tape #433 VCM Methyl Silicone
78	197- 67	135- 53	315- 47	393- 25					DC 710 Methyl Phenyl Silicone
78	315- 62	197- 50	135- 46	393- 38	408- 14	451- 12	529- 12		DC F-6-1105 Methyl Phenyl Silicone
79	67- 82	41- 74	95- 71	81- 86	108- 51	261- 26	306- 20		Ethyl Linolenate
80	52- 94	59- 85	66- 67	83- 61	51- 32	111- 39			Eastman 910 Cyano Acrylic Adhesive
81	100- 75	28- 56	31- 49	50- 21					Chemfluor Lab-Tape (TFE-TEFLON)
85	135- 40	101- 35	151- 35	131- 29	153- 18	201- 15	203- 14		Kel-F #90
86	118- 69	224- 31	56- 27	42- 27					"Fyrol 6" - Diethyl bis (2 hydroxy ethyl) amino-methyl Phosphate
88	263- 96	73- 87	261- 71	57- 52					Tin Oleate
91	92- 63	104- 41	39- 39	77- 31	215- 15	230- 28			Di Methyl Cresyl Phosphate
91	92- 74	182- 59	56- 55	149- 38					Butyl Benzyl Phthalate
94	86- 21	65- 20	66- 18	44- 16	105- 14				Diphenyl Phthalate
98	41- 89	43- 84	55- 79	29- 47	129- 21	284- 33	401- 15		Dibutyl Tin Distearate
99	113- 92	70- 90	55- 90	41- 71	211- 36	323- 14			Tris - (2 ethyl hexyl) Phosphate
100	57- 13	43- 13	55- 10	71- 7	101- 6				Outgassed Product from Polyurethane Foam
101	57- 76	56- 19	119- 17	158- 16					Di-isobutyl Succinate
104	91- 48	103- 46	78- 35	77- 28	128- 11	129- 15	141- 12		Gude 21 H Lacing Tape Extract
104	103- 63	78- 46	91- 29	77- 28					Loctite Sealant "D"

*M/E is mass to charge ratio and RA is relative abundance of that peak in percent of base peak (strongest peak).

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS (Continued)

BASE PEAK	MOST INTENSE PEAKS				STRUCTURALLY SIGNIFICANT PEAKS			MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
105	77- 72	106- 34	318-20	51-19				Resorcinol Mono Benzoate
108	122- 86	107- 77	209-57	224-57				Phenol Formaldehyde
113	69- 91	41- 56	112-33	86-23	114-16	200-15		Loctite Sealant "D"
113	69- 70	41- 35	112-21	86-17	200-10			Loctite "AA"
113	69- 82	41- 44	112-26	200-13				Loctite Refigerant Sealant
113	69- 60	41- 34	45-26	44-17	114-10	200-7		Loctite, Sealant A, Red
125	107-71	151- 70	137-47	81-36				Chlorinated Organo-phosphorus "Fyrol 99" plasticizer
135	377- 78	315- 73	197-66	73-59	451-28	470-38		Sperex SP-101 Hi temp White Paint (Methyl-Phenyl Silicone)
135	403- 65	73- 50	197-50	553-48				RTV-560 VCM Methyl Phenyl Silicone
137	59- 69	77- 59	215-48	237-44	159-36	219-14		FS-1281 Fluorinated Silicone
137	77- 57	59- 40	215-36	78-30				DC FS 1265 Fluorinated Silicone
137	215-100	59- 92	138-84	237-72	159-63	307-20		Dow Corning FS-1265 Fluorinated Silicone
141	55- 71	57- 52	41-45	71-35	257-14	397-13		NPT-4 Oil, Bray Oil Co.
141	57- 66	71- 39	43-38	55-33	212-12	243-22	383-18	Gude brod 18D96 Lacing Tape VCM
141	57- 66	71- 51	43-42	243-38	212-20	284-14	383-33	Stur-D-Lace 18 DU Lacing Tape - VCM
141	57- 65	71- 50	43-34	399-31	212-21	539-17		Lacing Twine SL-VCM
141	57- 60	71- 47	243-37	384-33				Stur-D-Lace B Style 18DB VCM
141	352- 94	142- 79	155-37	43-26				"Lion Oil" Hydrocarbon Diffusion Pump Oil
146	148- 64	111- 37	75-20	150-12				Dichloro benzene
148	174- 96	147- 91	121-52	122-47				Eccofoam FPH/12-10H Polyurethane
149	31- 26	57- 27	45-24	41-20	100-12	167-17		Cyclo hexyl o-Phthalate
149	57- 55	43- 51	71-45	85-37	141-25	167-17	307-34	Di-isodecyl Phthalate
149	57- 73	71- 55	43-50	349-50	167-39	183-12	335-20	Di- (Tridecyl) Phthalate
149	121- 80	164- 80	163-73	135-29	322-14			2,2' Methylene bis (6-tButyl 4 Methyl Phenol)
149	150- 48	223- 30	29-30	41-27	104-15	205-26		Dibutyl Phthalate
149	167- 88	57- 72	70-66	55-58	112-32	113-34	279-49	Di (2 ethylhexyl) Phthalate
149	177- 71	150- 33	176-25	65-18	222-14			Di ethyl Phthalate
149	279- 60	43- 58	150-56	57-53	167-12	261-14	390-3	Di-n-octyl Phthalate
149	533-100	103- 97	162-73	444-63	193-30	283-32		Mylar Polyester

*M/E is mass to charge ratio and RA is relative abundance of that peak in percent of base peak (strongest peak).

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS (Continued)

BASE PEAK		MOST INTENSE PEAKS			STRUCTURALLY SIGNIFICANT PEAKS			MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
149	533- 51	104- 34	43-24	57-21	445-17	534-20		Dacron Polyester Extract
161	203- 75	218- 63	218-63	205-49	175-49			2,6 di (t-butyl) 3 (dimethyl amino) P-cresol
163	77- 48	164- 33	194-31	735-23				Dimethyl Phthalate
163	135- 40	178- 31	177-14	41-11	350-10			2,2' Methylene bis (6 t-Butyl 4 Ethyl Phenol)
166	165- 96	167- 21	82-21	83-15				Fluorene
169	69- 57	119- 56	147-37	335-28	285-24			Krytox 240-AB Fluorinated Hydrocarbon
169	119- 74	69- 74	147-52	335-48	97-32	285-42		Krytox Oil 143 AB
171	57- 56	70- 45	71-45	112-41	129-10	149-13	283-10	Di 2 Ethyl hexyl Azelate
174	55- 94	41- 80	28-72	81-62	145-51	148-46		Solithane 113 Polyurethane
174	69- 91	123- 83	41-78	148-61				Loctite "35"
174	148- 92	67- 89	123-89	41-77				Loctite Impact Resistant Adhesive 308
180	182-100	184- 96	145-92	109-90				Trichlorobenzene
183	105- 77	77- 40	184-14	165-11				Benzilic Acid
191	57- 66	206- 60	192-49	131-40				2,6 di (t-butyl) 3 (dimethyl amino) P-Cresol
191	205- 23	57- 20	206-19	192-15				2,4,di (t-butyl) Anisole
197	135- 88	315- 65	393-33	78-30	259-21	393-33	529-21	DC F-6-1105 Methyl Phenyl Silicone
205	220- 92	177- 57	163-56	207-54				2,5 di (t-butyl) Quinone
207	73- 75	44- 66	281-38	341-32	355-20	429-25		3M tape #433 VCM
207	73- 36	281- 25	208-25	96-18				Dow Corning "High Vacuum Grease"
207	73- 61	281- 24	208-21	221-21	341-8	355- 9		D.C. 510 Silicone Fluid
207	73- 55	281- 31	208-29	341-21	96-14	267-15	355-15	RTV-11 VCM Methyl Silicone
207	221- 74	73- 60	295-40	147-37	281-28	355-14	369-26	F-50 Methyl Silicone Oil
207	222- 44	57- 29	41-24	205-22				2,5 di (t-butyl) Hydro Quinone
207	281- 27	208- 24	73-21	96-16				Dow Corning 11 Compound Methyl Silicone
211	226- 26	212- 16	92-10	183-7				4-t-butyl 2 Phenyl Phenol
216	214- 72	218- 48	179-18	181-18				Tetrachlorobenzene
219	234- 25	220- 17	57-13	88-6				2, 6 di-t-butyl 4 ethyl phenol
221	73- 74	207- 63	295-52	147-47	281-34	369-36		GE Silicone Grease G-300
221	177- 74	248- 53	191-45	163-42	250-23			2,5 di (t-amyl) hydroquinone
227	151- 97	228- 93	77-31	105-24				2-Hydroxy 4-Methoxy Benzo Phenone

*M/E is mass to charge ratio and RA is relative abundance of that peak in percent of base peak (strongest peak).

MASS-SPECTRAL INDEX OF AEROSPACE MATERIALS (Continued)

BASE PEAK	MOST INTENSE PEAKS				STRUCTURALLY SIGNIFICANT PEAKS				MATERIAL
M/E	M/E RA*	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	M/E RA	
228	102- 96	60- 93	43-92	57-91	129-49	185-31	211-73	229-80	Isopropyl Myristate
247	57- 30	248- 19	262-14	41-12					2,4,6 Tri t-butyl Phenol
250	174- 89	208- 56	221-36	148-34					Chemglaze Z 306 Polyurethane Coating
253	331- 96	254- 61	346-58	332-43					RTV-560 VCM Methyl Phenyl Silicone
308	323- 69	342- 46	309-46	57-33					2-(3,5 di t-butyl 2 Hydroxy Phenyl) 5-Chloro Benzo Triazole
319	317- 86	57- 73	433-65	73-60	573-24	575-30			Dibutyl Tin Dilaurate
325	340- 40	29- 25	327-37	57-22	119-11	269-17			Armstrong A-31 Epoxy Resin
326	77- 79	170- 43	233-38	65-38					Triphenyl Phosphate
326	328- 67	324- 63	254-52	256-49					Penta Chlorobiphenyl
340	77- 70	65- 58	165-45	91-41					Di phenyl Cresyl Phosphate
354	115- 34	77- 33	355-33	141-32					Santovac 5 Poly Phenyl Ether
354	165- 30	355- 25	77-25	91-20					Phenyl Dicresyl Phosphate
360	362- 82	290- 55	358-55	288-40					Hexachloro bi phenyl
368	91- 27	369- 26	165-19	107-18					Tricresyl Phosphate
394	396- 96	398- 53	324-48	392-48					Heptachlorobiphenyl
405	327- 99	156- 83	343-54	328-54					RTV-560 VCM (566) Methyl Phenyl Silicone
447	77- 72	141- 54	168-53	115-46	223-42	233-21			Convalex 10 DP Oil
469	470- 43	197- 40	313-30	149-27	188-24	259-15	391-24		DC 704 Pump Fluid
479	135- 98	197- 90	73-50	481-43					RTV-560 VCM (or 566) Methyl Phenyl Silicone
529	451- 84	218- 68	43-54	73-46	319-36	373-40			D. C. 93-046 Adhesive Methyl Phenyl Silicone

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