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# THE MASS SPECTRA OF VOLATILE CONSTITUENTS IN MILITARY EXPLOSIVES

## D.M. Anderson, F.B. Kistner and M.J. Schwarz

October 1969

CONDUCTED FOR

BARRIER AND INTRUSION DETECTION BRANCH U.S. ARMY ENGINEER RESEARCH AND DEVELOPMENT LABORATORIES

ΒY

CORPS OF ENGINEERS, U.S. ARMY COLD REGIONS RESEARCH AND ENGINEERING LABORATORY HANOVER, NEW HAMPSHIRE

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#### PREFACE

This report was prepared by Dr. Duwayne M. Anderson, Chief, Earth Sciences Branch, SP Frank B. Kistner, and CPT Maurice J. Schwarz, Research Division, U.S. Army Cold Regions Research and Engineering Laboratory. The report was prepared for the Barrier and Intrusion Detection Branch, U.S. Army Engineer Research and Development Laboratories, Fort Belvoir, Virginia.

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### THE MASS SPECTRA OF VOLATILE CONSTITUENTS IN MILITARY EXPLOSIVES

by

D.M. Anderson, F.B. Kistner and M.J. Schwarz

#### INTRODUCTION

This study was undertaken in order to determine the feasibility of detecting concealed explosive devices, such as anti-personnel or anti-tank mines, by means of a mass spectrometer detector. The principle of operation of the mass spectrometer is as follows:

A representative portion of the vapor of a substance is ionized and the resultant ions are separated into coherent ionic streams according to their mass to charge ratio (m/e) by passing them all through a magnetic field. The relative abundance of the various ions is then determined by measuring the electrical currents of the several ionic streams. All of these functions are necessarily accomplished in a high vacuum chamber. Generally, gases and liquids have vapor pressures large enough to be analyzed easily with conventional sampling techniques. Most solids have vapor pressures too low to be analyzed in a conventional manner. It was hoped that compounds used for military high explosives would have high enough vapor pressures to yield easily detectable, characteristic mass spectra. If several characteristic mass peaks were found to be common to all explosives, it would be possible to design a specially tuned mass spectrometer detector for use in locating hidden explosive devices by detecting the vapors emanating from them.

Five commonly used military high explosives were investigated: pressed trinitrotoluene (TNT), cast trinitrotoluene, composition B, composition A-3, and composition C-4 Table I summarizes the physical properties of these explosives. The most important data from the standpoint of this investigation, namely the vapor pressures of the various explosives, were unfortunately unknown. It was estimated, however, that the vapor pressures would be in the range  $10^{-3}$  to  $10^{-5}$  mm Hg. This estimate provided the incentive to proceed with the study, because if explosive vapors exist at those pressures in air, then, allowing for attenuation of the gas by a factor of  $10^7$  mm Hg. Partial pressures of this magnitude are not detectable with commercially available mass spectrometers. Hence the method was held to be promising.

#### **EXPERIMENTAL METHODS**

A Consolidated Electrodynamics Corp. 21-613 residual gas analyzer modified first to function as a mass spectrometer with capillary inlet and finally in its normal mode as a residual gas analyzer was used throughout the study. An ionization current of 25  $\mu$ a was used throughout. Samples of military explosives were obtained from the U.S. Army Engineer Research and Development Laboratories, Barrier and Intrusion Detection Branch, Fort Belvoir, Virginia. The five samples obtained were pressed TNT, cast TNT, composition B, composition A-3 and composition C-4. No special preparation of the samples was performed other than careful grinding to reduce them to a fine powder.

Explosives	Formula	Molecular Weight	Vapor Pressure ,	Melting Point <sup>O</sup> C	Explosion Temperature OC
T₩T	(NO2 <sup>')</sup> 3 C6H2 CH3	227.13	0.053 mm at 85 <sup>0</sup> C 0.106 mm at 100 <sup>0</sup> C	80.7 <sup>0</sup>	475 <sup>0</sup>
DNT .	(NO <sub>2</sub> ) <sub>2</sub> C6H <sub>3</sub> CH <sub>3</sub>	182.13		69.5 <sup>0</sup>	
RDX	$(NO_2)_3 N_3 (CH_2)_3$	222.15		202 <mark>0</mark>	260°
Composition B	55.2% RDX 40% TNT 1.2% Polyisoluctylene 0.6% WAX				278 <sup>0</sup>
Composition A-3	91% RDX 9% WAX				250 <sup>0</sup>
Composition C-4	91% RDX 2.1% Polyisobutylene 1.6% Motor Oil 5.3% Di(2-ethylehexyl) Sebacate				290°

#### Table I. Physical properties of military high explosives.

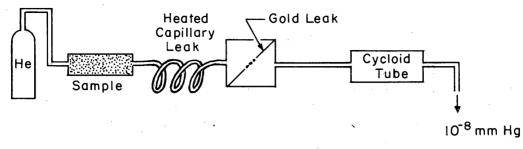
(From Military Explosives, DA Technical Manual TM 9-1910, 1955.)

The samples were introduced into the analyzing portion of the instrument in several ways. One method involved placing a 5-g sample into a helium gas flow having a pressure of 1 atmosphere. The stream was then introduced to a heated capillary leak which led into a dynamic vacuum of about 1 mm Hg. This sample was then admitted to the cycloid tube analyzer through a gold leak (see Fig. 1). The spectra obtained in this manner were indistinguishable from background spectra obtained with no explosive present.

The second method was essentially the same as the first except that the samples were placed closer to the detector tube by putting them directly upon the gold leak (see Fig. 2). Again, the spectra obtained in this manner were essentially the same as those of the background spectra.

The third method employed a glass inlet system usually used for introduction of gaseous samples. A 0.2-g sample was placed in this system (see Fig. 3) and the pressure reduced to below  $1 \times 10^{-5}$  mm Hg. Helium gas was then added as ballast until a pressure of 1 mm Hg was attained. This mixture was analyzed and again the results were inconclusive in that no peaks other than those attributable to background were observed.

Finally, as a last resort, the instrument was operated as a residual gas analyzer. The gold leak was removed, leaving no obstacle between the analyzer and the sample (see Fig. 4). The sample was placed in the system and the pressure was reduced to  $1 \times 10^{-5}$  mm Hg. The system was then opened to the cycloid tube and the spectra of the bases remaining in the system were recorded. Backgrounds were recorded for identical conditions except that the explosive was not present.





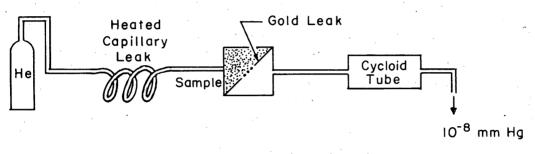


Figure 2.

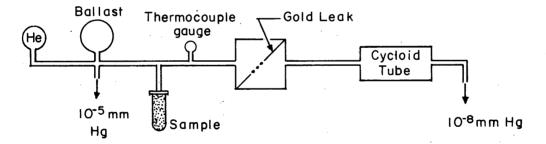
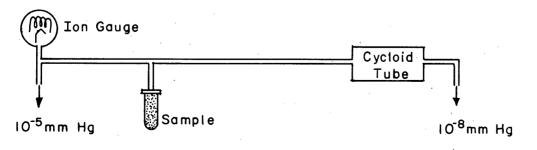


Figure 3.





#### RESULTS

All attempts to detect traces of the explosive vapors mixed with air or helium failed when the mixture was drawn into the capillary inlet and passed in front of the gold leak at the detector tube inlet. Failure to detect the explosive could be explained two ways:

1) Explosive vapors were present below threshold limits of detection.

2) Explosive vapors decomposed when heated and the resulting ionic species were unrecognizable or indistinguishable from normal background spectra.

The first explanation is obviously the most likely of the two but the second explanation could not be ruled out. If the explosive vapors were present below threshold limits this might be explained by the vapor pressure itself being too low or by failure of the explosive vapors to rise to their equilibrium partial pressures in the gas mixture. Attempts to detect the explosive vapors mixed and equilibrated with helium at 1 mm Hg pressure also failed, indicating that the vapor pressures of these explosives are too low to permit detection by the mass spectrometer with the inlet systems employed. The question was finally resolved by opening the cycloid tube to the explosive and pumping down the system to  $10^{-5}$  mm Hg. Vapors emanating from the explosives were then detected as residual gases by the instrument operating in its most sensitive mode. The data obtained are given in Appendix A but are summarized in Table II. The figures for each mass number represent

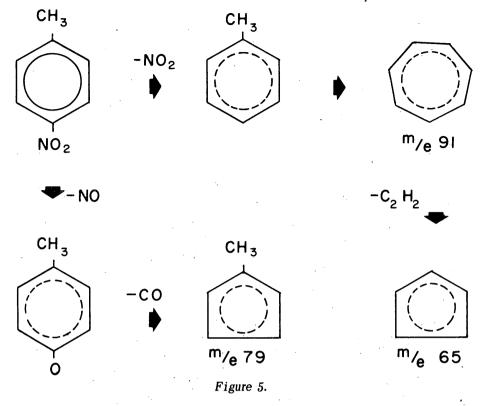
#### Table II. Mass spectral patterns.

Sample No. Compound Mass No.	l pr <b>esse</b> d TNT	2 cast TNT	3 composition B	4 composition A-3	5 composition C-4	p-nitro- toluene <sup>a</sup>	2,4-di- nitro-b toluene	toluene <sup>C</sup>
30	1.90	10.84	8.59	.19		4.17	14.80	
38	·29	1.86	1.64	~ ·		2.39		4.51
39	1.08	5.84	4.80	.29	3.82	20.4	14.4	18.31
4í	.21	.94	•98	1.34	8.04	5.83		2.44
42	.05	•5 <sup>2</sup>	.71	.50	3.73	.78		•38
43	•55	2.66	4.98	1.58	6.74	9.36		3.16
50	.61	2.54	2.32			5.14	5.9	5.49
51	•73	3.88	3.33			8.81	11.0	9.24
52	.49	2.48	2:02			2.39	9•5	2.31
52 555	.09	.83	.64	1.04	8.73			
56		•32		•55	3.18			
57	.21	.62	•75	1.54	11.75	•		
62	•53	2.43	1.94	•15		3.67	7.0	3.61
63	1.55	7.13	5.72			12.66	26.2	7.91
64	.68	2.74	2.26			3.62	12.8	1.93
65		1.08	.82			56.42	4.3	13.18
69				1.0	4.21			
70				•5	3.18			
71				1.0	3.18	0	0.5	
77	•53	2.06	1.75			8.07	8.2	1.1
78	•57	2.58	2.30			1.88	11.4	.13
79						7.89	5 <u>.</u> 6	
88	2.74	11.19	9.79		<i>c</i> ,	•32		•11
89	1.21	4.9	4.2		.64	9.36	50.7	3.74
90	.42	1.5	1.48			3.53	24.3	2.02
91						100.0	6.7	100.0

<sup>a</sup> Imperial Chemical Industries, Ltd., Uncertified Mass Spectrum, ASTM No. 1536

U. S. Army Natick Laboratory, Analytical Chemistry Division

<sup>C</sup> Consolidated Electrodynamics Corporation, Spectral Catalogue



the difference between the ion current at that mass due to the explosive less that observed under the same conditions when no explosive was present in the system (less background). The last three columns of Table II contain the mass spectral patterns of some similar compounds for which data are available.

The spectra of samples 1, 2 and 3, the ones containing TNT, are easily distinguished from the other samples. The prominent peaks are at m/e 30, 39, 43, 50, 51, 62, 63, 64, 77, 78, 88, 89, 90. There were other larger detectable peaks at much higher mass numbers but because the instrument available for this work is capable of good resolution only at m/e 12 to 150 it was not possible to resolve their m/e ratios.

Although the somewhat crude nature of these spectra makes detailed interpretations too tenuous to warrant lengthy consideration, a few observations at least can be made. In addition to samples 1, 2 and 3, nitrotoluene and dinitrotoluene yield large peaks at m/e 30. This peak is probably due to the NO<sup>+</sup> ion as has been observed for a variety of nitro-compounds.\*† The remaining prominent peaks are due no doubt to more complex fragmentation and to various rearrangements † which these aromatic nitro-compounds undergo when bombarded by electrons. Some possible processes are summarized in Figure 5.

Peaks attributable to the processes shown in Figure 1 can be seen in the residual spectra of samples 1, 2 and 3. In view of the similarity in the patterns of 1, 2 and 3 to those of the model compounds, nitrotoluene, dinitrotoluene and toluene, this is good evidence that the patterns are due at least in part to trinitrotoluene. The spectra of samples 4 and 5 indicate a quite different composition for these explosives although it is not possible from the spectra alone to deduce their

<sup>\*</sup> R. Boschan and S.R. Smith, Mass spectra of nitrate esters, nitro compounds, and several other nitrogen compounds. U.S. Naval Ordnance Test Station, Navord Report No. 5412, 1957.

<sup>&</sup>lt;sup>†</sup> J.H. Benyon, Mass spectrometry and its applications to organic chemistry. Elsevier Publishing Company, Amsterdam, 1960.

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formulations. Clearly, however, it is established that these explosives can be characterized in the sense that they each yield a distinctive chemical signature to the mass spectrometer detector. In the case of explosives containing TNT, it is evident that they all will have some peaks in common.

Without a more thorough investigation it is not precisely clear how an explosive detector based upon the mass spectrometer alone as a detector could be made to function as a universal explosives alarm. A decisive conclusion on the basis of the limited data now available is not possible but it is likely that detailed analysis of the complete mass spectra of various explosives would uncover possible schemes. It is even more likely that other detectors in combination with mass spectrometry can be built into an integrated explosives detection system.

During this investigation it was learned that a similar study was being carried on by Dravnieks and Weber for the Federal Aviation Agency.\* They utilized vapor phase chromatography to accomplish separations and several kinds of detectors in an attempt to devise a bomb detection system. Moderate success was achieved in detecting explosives in a closed space from which relatively large quantities of air were drawn out through a trap that extracted the explosive vapors. The vapors were periodically released from the trap and analyzed by one or several detectors. It appears from the data in Table II that the mass spectrometer detector could be made to function usefully in a similar arrangement; but it is also clear from the results of this study that the vapor pressures of the common explosives are so low that great difficulties are involved in using presently available mass spectrometer circuitry and tubes to detect the presence of their volatile components in air without some degree of concentration. A simple "bomb sniffer" using presently available detectors, including the cycloid tube of the mass spectrometer employed in this study, probably is not possible. The data in Table II show that, assuming reasonable advances in detector sensitivity, a successful "explosives sniffer" utilizing a mass spectrometer detector will soon be within our technological ability to develop.

#### RECOMMENDATIONS

It is recommended that the complete mass spectra of important military explosives be obtained. Not all mass spectrometers are suitable for this determination since only the newer models are capable of resolving ions of very high mass. This study, for example, revealed that ions of mass 200 and above result from ionizing vapors of the explosives examined but the mass spectrometer available was not capable of resolving peaks due to these ions. The new mass spectrometer facility at U.S. Army Natick Laboratories is capable of performing this analysis. It is therefore advisable to request their aid in obtaining and analyzing these spectra.

The work of Dr. Dravnieks at the Illinois Institute of Technology, Chicago, Illinois, consisting of the gathering, cataloging and comparison of chemical signatures of vapors found in the air, merits continued support. His work is particularly valuable from the standpoint of explosives detection because of his long and rich experience with the signatures obtainable from a variety of detectors and detector systems.

Rapid advances are being made in mass spectrometer instrumentation. As soon as a significant increase in detector sensitivity is reached, the complete spectra of the important explosives should be analyzed to determine those peaks or peak combinations and sequences that are sufficiently distinct from common vapors found in air to be exploited; then, attempts to devise means of detecting them under various circumstances of interest can reasonably be expected to be successful.

\* A. Dravnieks and H. Weber, Bomb detection system study, IIT Research Institute, Final Report No. IITRI-C6026-13, 1965.

#### APPENDIX A

The mass spectra up to about m/e = 100 are shown as relative outputs. The relative output is the oscillograph recorder response, at constant sensitivity, to ion currents obtained at various mass/charge ratios. The arbitrary units, therefore, are recorder chart divisions. The relative outputs are then expressed in percent, based upon the nitrogen peak (m/e 28) as unity. The residual spectra were then obtained by subtracting the corresponding background from sample outputs.

The chart comparing the mass spectra of cast TNT to that of the background is also given for purposes of illustration and comparison. It and all the other charts can be reconstructed from the tabular data if desired.

	Sam	ole	Backg	round	Resid	lual
	Relative	Percentage	Relative	Percentage	Relative	Percentage
m/e	Output	Output	Output	Output	Output	Output
12	5.2	2.6	4.0	2.03	1.2	•57
14	19.8	9.93	19.5	9•9	•3	.03
15	1.2	.6	1.0	.51	.2	•09
16	10.0	5.0	6.3	3.2	3.7	2.8
17	32.5	16.3	9.5	4.82	23.0	11.48
18	107.7	53.9	30.5	15.5	77.2	38.4
20	•5	.25	1.0	•51	5	26
26	•6	•3	0	. 0	.6	•3
27	2.7	1.35	1.2	.61	1.5	.74
28	199.5	100.0	196.8	100.0	2.7	0
29	4.9	2.46	2.8	1.42	2.1	1.04
30	2.3	1.15	1.9	•96	.4	•19
32.	6.0	3.0	4.5	7.28	1.5	.72
39	2.1	1.05	1.5	.76	.6	•29 •06
40	6.2	3.1	6.0	3.04 .66	.2 2.7	1.34
41 42	4.0	2.0	1.3 0	•00	1.0	•5
42 43	1.0 6.2	.50 3.1	3.0	1.52	3.2	1.58
43 44	47.5	23.8	47.5	24.1	0	3
55	3.0	1.5	•9	.46	2.1	1.04
56	1.5	•75	• •	.2	1.1	•55
57	3.5	1.75	1.0	•51	2.5	1.54
60	1.2	.6	0	0	1.2	.6
62	.8	.4	•5	· .25	•3	.15
63	1.2	.6	1.2	.61	0	01
69	7.0	1.0	0	0	2.0	1.0
70	1.0	•5	0	0	1.0	•5
71	2.0	1.0	0	· 0	2.0	1.0
88	1.0	•5	1.0	.51	0	0.01
94	2.5	1.25	•7	•35	1.8	•9
96	2.3	1.15	•9	.46	1.4	.69

#### MASS SPECTRUM OF COMPOSITION A-3

Relative m/ePercentage OutputRelative OutputPercentage OutputRelative OutputPercentage Output124.02.194.02.030.161418.510.119.59.9-1.0.2153.51.911.0.512.5.411611.56.296.33.25.23.091738.020.89.54.8228.515.9618123.067.230.515.592.551.7274.02.191.2.612.81.5628183.0100.0196.8100.0-13.80295.02.732.81.422.21.313017.59.551.9.9615.66.59333.01.64003.01.643910.22.561.5.764.644.80407.54.16.03.041.51.06413.01.641.3.661.7.96421.3.71001.3.714311.96.53.55.4.26.13.33523.72.02003.72.02531.6.87001.6.87541.3.721.3.75.5.55451.3.55001.		Sam	ple	Backg	round	Resid	lual
12 4.0 2.19 4.0 2.03 0 .16   14 18.5 10.1 19.5 9.9 -1.0 .2   15 3.5 1.91 1.0 .51 2.5 .41   16 11.5 6.29 6.3 3.2 5.2 3.09   17 36.0 20.8 9.5 4.82 28.5 15.96   18 123.0 67.2 30.5 15.5 92.5 51.7   27 4.0 2.19 1.2 .61 2.8 1.58   28 183.0 100.0 196.8 100.0 -13.8 0   29 5.0 2.73 2.8 1.42 2.2 1.31   30 17.5 9.55 1.9 .96 15.6 8.59   32 5.5 3.0 4.5 2.28 1.0 .72   38 3.0 1.64 1.3 .66 1.7 .96   41 3.0 1.64 1.3 .66 1.7 .96   42	. ,						
1418.510.119.59.9-1.0.2153.51.911.0.512.5.411611.5 $6.29$ $6.3$ $3.22$ $5.2$ $3.09$ 1738.020.89.5 $4.82$ 28.5 $15.96$ 18123.0 $67.2$ $30.5$ $15.5$ $92.5$ $51.7$ 27 $4.0$ $2.19$ $1.2$ $61$ $2.8$ $1.56$ 28183.0100.0196.8100.0 $-13.8$ 029 $5.0$ $2.73$ $2.8$ $1.42$ $2.2$ $1.31$ 30 $17.5$ $9.55$ $1.9$ $.966$ $15.6$ $8.59$ 32 $5.5$ $3.0$ $4.5$ $2.28$ $1.0$ $.72$ 38 $3.0$ $1.64$ $0$ $0$ $3.0$ $1.64$ 40 $7.5$ $4.1$ $6.0$ $3.04$ $1.5$ $1.06$ 41 $3.0$ $1.64$ $1.3$ $.666$ $1.7$ $.98$ 42 $1.3$ $.71$ $0$ $0$ $1.3$ $.71$ $43$ $11.9$ $6.5$ $3.0$ $1.52$ $8.9$ $4.96$ $44$ $45.0$ $24.6$ $47.5$ $24.1$ $-2.5$ $.5$ $45$ $1.3$ $.71$ $0.8$ $.41$ $.5$ $.3$ $46$ $1.8$ $.98$ $.2$ $.1$ $1.6$ $.88$ $50$ $4.6$ $2.52$ $.4$ $2$ $4.2$ $2.22$ $51$ $6.5$ $3.55$ $.4$ <th>m/e</th> <th>Output</th> <th>Output</th> <th>Output</th> <th>Output</th> <th>Output</th> <th>Output</th>	m/e	Output	Output	Output	Output	Output	Output
1418.510.119.59.9-1.0.2153.51.911.0.512.5.411611.5 $6.29$ $6.3$ $3.22$ $5.2$ $3.09$ 1738.020.89.5 $4.82$ 28.5 $15.96$ 18123.0 $67.2$ $30.5$ $15.5$ $92.5$ $51.7$ 27 $4.0$ $2.19$ $1.2$ $61$ $2.8$ $1.56$ 28183.0100.0196.8100.0 $-13.8$ 029 $5.0$ $2.73$ $2.8$ $1.42$ $2.2$ $1.31$ 30 $17.5$ $9.55$ $1.9$ $.966$ $15.6$ $8.59$ 32 $5.5$ $3.0$ $4.5$ $2.28$ $1.0$ $.72$ 38 $3.0$ $1.64$ $0$ $0$ $3.0$ $1.64$ 40 $7.5$ $4.1$ $6.0$ $3.04$ $1.5$ $1.06$ 41 $3.0$ $1.64$ $1.3$ $.666$ $1.7$ $.98$ 42 $1.3$ $.71$ $0$ $0$ $1.3$ $.71$ $43$ $11.9$ $6.5$ $3.0$ $1.52$ $8.9$ $4.96$ $44$ $45.0$ $24.6$ $47.5$ $24.1$ $-2.5$ $.5$ $45$ $1.3$ $.71$ $0.8$ $.41$ $.5$ $.3$ $46$ $1.8$ $.98$ $.2$ $.1$ $1.6$ $.88$ $50$ $4.6$ $2.52$ $.4$ $2$ $4.2$ $2.22$ $51$ $6.5$ $3.55$ $.4$ <td>12</td> <td>4.0</td> <td>2.19</td> <td>4.0</td> <td>2.03</td> <td>0</td> <td>.16</td>	12	4.0	2.19	4.0	2.03	0	.16
15 $3.5$ $1.91$ $1.0$ $.51$ $2.5$ $.41$ 16 $11.5$ $6.29$ $6.3$ $3.2$ $5.2$ $3.09$ 17 $38.0$ $20.8$ $9.5$ $4.82$ $28.5$ $15.96$ 18 $123.0$ $67.2$ $30.5$ $15.5$ $92.5$ $51.7$ 27 $4.0$ $2.19$ $1.2$ $.61$ $2.8$ $1.58$ 28 $183.0$ $100.0$ $196.8$ $100.0$ $-13.8$ $0$ 29 $5.0$ $2.73$ $2.8$ $1.42$ $2.2$ $1.31$ 30 $17.5$ $9.55$ $1.9$ $.96$ $15.6$ $8.59$ $38$ $3.0$ $1.64$ $0$ $0$ $3.0$ $1.64$ $40$ $7.5$ $4.1$ $6.0$ $3.04$ $1.5$ $1.06$ $41$ $3.0$ $1.64$ $1.3$ $.66$ $1.7$ $.98$ $42$ $1.3$ $.71$ $0$ $0$ $1.3$ $.71$ $44$ $45.0$ $24.6$ $47.5$ $24.1$ $-2.5$ $.5$ $45$ $1.3$ $.71$ $0.8$ $.41$ $.5$ $.3$ $44$ $45.0$ $24.6$ $47.5$ $24.1$ $-2.5$ $.5$ $45$ $1.3$ $.71$ $0.8$ $.41$ $.5$ $.3$ $5$ $1.3$ $.71$ $0.8$ $.41$ $.5$ $.3$ $44$ $45.0$ $24.6$ $47.5$ $24.1$ $-2.5$ $.5$ $5$ $1.3$ $.75$ $.66$ $1.3$ $.75$ $5$ <t< td=""><td>14</td><td>18.5</td><td></td><td></td><td>-</td><td>-</td><td></td></t<>	14	18.5			-	-	
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94 2.5 1.37 .7 .35 1.8 1.02							
	96	2.0	1.1	.9	• .46	1.0	.64

### MASS SPECTRUM OF COMPOSITION B

	Sam	n]e	Backg	round	Resid	lual
	Relative	Percentage	Relative	Percentage	Relative	Percentage
m/e	Output	Output	Output	Output	Output	Output
12	3.1	1.62	2.9	2.3	.2	68
14	12.8	10.2	12.3	9.74	•5	.46
15	2.5	1.98	•9	.71	1.6 6.2	1.27 4.95
16	12.2 58.0	9.7 46.0	6.0 11.5	4.75 9.1	46.5	36.9
17 18	192.0	152.0	37.0	29.3	155.0	121.3
20	1.0	•79	•7	•55	•3	.24
22	.8	.64	•7	•55	.1	•09
25	1.0	•79	0	0	1.0	•79
.26	1.1	.87	•5	.4	.6	- 47
27	8.7	· 6.9	1.4	1.1	7.3	5.8
28 0 <b>0</b>	126	100.0 7.54	126.6 2.6	100.0 2.06	6 6.9	0 7.48
2 <b>9</b> 30	9.5 4.0	3.18	4.1	3.24	1	06
31	1.0	•79	0	0	1.0	•79
32	5.3	4.21	5.2	4.11	.1	•1 ·
39	7.2	5.72	2.4	1.90	4.48	3.82
40	5.3	4.21	4.6	3.64	•7	•57
41	11.9	9.44	1.8	1.4 .4	10.1 4.7	8.04
42 43	5.2 11.9	4.13 9.44	•5 3.4	.4 2.7	4•7 8•5	3•73 6•74
43 44	32.8	25.9	34.0	27.9	-1.2	-2.0
55	11.0	8.73	0	0	11.0	8.73
56	4.0	3.18	0	Ο.	4.0	3.18
57	14.8	11.75	0	0	14.8	11.75
67	3.4	2.7	0	0	3.4	2.7
68	1.2	•95	0	0	1.2	•95
69 70	5.3 4.0	4.21 3.18	0 0	0	5.3 4.0	4.21 3.18
70 71	4.0	3.18	0	Ú Ő	4.0	3.18
81	3.6	2.86	0	0	3.6	2.86
82	1.3	1.03	Ò	0	1.3	1.03
83	3.7	2.94	0	0	3.7	2.94
84	1.2	•95	0	0	1.2	•95
85	2.1	1.67	0	0 2.4	2.1	1.67 42
88 89	2.5 1.8	1.98 1.43	3.0 1.0	•79	5 .8	.64
94	4.0	3.18	1.0	•79	3.0	2.39
95 .	1.0	•79	0	0	1.0	•79
96	4.9	3.89	•7	•55	4.2	3.34
97	3.9	3.1	0	0	3.9	3.1
98	1.2	•95	0	Ο.	1.2	•95

## MASS SPECTRUM OF COMPOSITION C-4

MASS SPECTRUM OF PRESSED TRINITROTOLUENE	MASS	SPECTRUM	OF	PRESSED	TRINITROTOLUENE	
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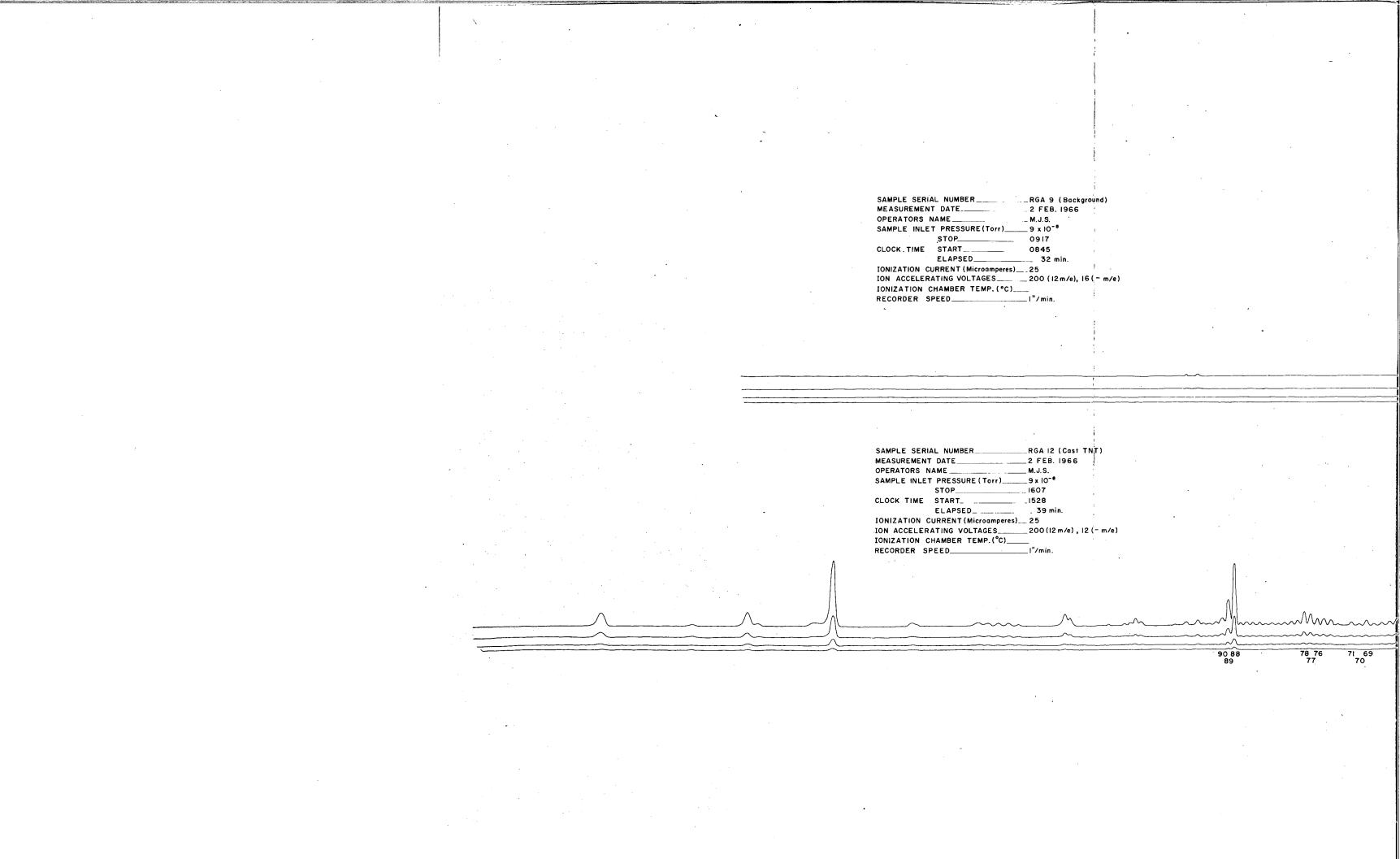
			· .	_ ·		
		nple	Backg		Resid	
	Relative	Percentage	Relative	Percentage	Relative	Percentage
m/e	Output	Output	Output	Output	Output	Output
12	1.4	.27	1.2	•17	.2	.10
14	46.8	8.86	31.8	4.6	15.0	4.26
15	4.6	.87	5.5	•79	9	•08
16	22.0	4.2	15.4	2.2	6.6	2.0
17	50 <b>.</b> 8 <sup>.</sup>	9.63	31.6	4.5	19.2	5.13
18	174.6	33.0	103.8	14.8	70.8	18.2
20	2.2	.42	1.6	.23	.6	,19
26	1.2	.23	1.4	.20	2	•03
27	40.0	7.57	3.4	•49	36.6	7.08
28	528.0	100.0	698.0	100.0	-170.0	0
29	8.2	1.55	9.0	1.3	8	.25
30	10.6	2.01	0.8	.11	9.8	1.90
32	118.2	22.4	169.8	24.4	-51.6	-2.0
36	1.0	•19	•8	•11	2	.08
37	1.2	.23	•5 .	•07	•7	.16
38	2.2	.42	•9	.13	1.3	.29
39	7.6	1.44	2.5	•36	5.1	1.08
40	13.4	2.54	18.0	2,56.	-4.6	02
41	4.0		3.8	•55	.2	.21
42	1.8	•34	2.0	.29	2	•05
43	16.0	3.04	17.4	2.49	-1.4	•55
44	7.0	1.33	6.8	•97	.2	•36
50	3.2	.61	0	0	3.2	.61
51	4.6	.87	1.0	.14	0 (	•73
52 52	2.6 .8	.49	0	0	2.6	.49
53	.0 2.6	.15 .49	0 2.8	0.40	.8 2	.15
55 56	.8	.49 .15	1.2		2 4	•09
57	<b>3.</b> 2 ·	.61	2.8	.17 .40	4	02 .21
58.	2.8	•53	4.0	•57	.4 -1.2	04
60	1.0	.19	•5	.07	•5	.12
61 61	.6	.11	0	0	.6	•11
62	2.8	•53	Õ	0	2.8	•53
63	8.2	1.55	0	0	8.2	1.55
64	3.6	.68	0	0	3.6	.68
69	1.4	.27	1.8	.26	4	.01
70	1.0	•19	1.0	.14	0	.05
71	1.2	.23	2.0	•29	8	06
74	.6	.11	0	0	.6	.11
75	1.2	.23	0	0	1.2	.23
76	1.0	.19	· 0	0.	· 1.0	.19
77	2.8	•53	Ó	0	2.8	•53
78	3.0	•57	0	0	3.0	•57
88	14.5	2.74	0	0	14.5	2.74
89	6.4	1.21	0	· 0	6.4	1.21
90	2.2	.42	0	0	2.2	.42
94	3.0	•57	1.5	.22	1.5	•35
96	2.2	.42	1.2	.17	1.0	.25

APPENDIX A

TRINITROTOLUENE

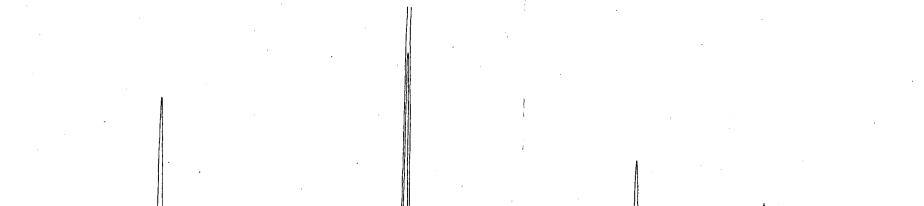
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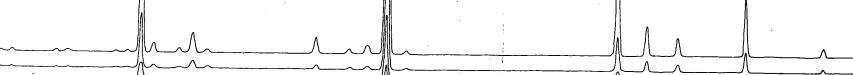
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	Sam		Backg			idu <b>al</b>
Ĩ.	Relative	Percentage	Relative	Percentage	Relative	Percentage
m/e	Output	Output	Output	Output	Output	Output
12	4.4	2.27	4.0	2.03	• 4	.24
14	18.7	9.65	19.5	9.9	8	25
15	2.2	1.13	1.0	•51	1.2	
16	10.7	5.5	6.3	3.2	4.4	2.3
17	31.7	16.4	9•5 ·	4.82	22.2	11.58
18		54.2				
	105.0		30.5	15.5	74.5	34.7
20	1.0	.52	1.0	.51	0	.01
26	1.5	•77	0	0	1.5	•77
27	4.2	2.16	1.2	.61	2.0	1.55
28	193.8	100.0	196.8	100.0	-3.0	0
29	5.0	2.58	2.8	1.42	2.2	1.16
30	22.9	11.8	1.9	•96	21.0	10.84
32	5.2	2.68	4.5	2.28	•7	•4
37	2.1	1.08	0	0	2.1	1.08
38	3.6	1.86	0	0	3.6	1.86
39	12.8	6.6	1.5	•76	11.3	5.84
40	7.9	4.08	6.0	3.04	1.9	1.04
41 .	3.1	1.6	1.3	.66	1.8	•94
42	1.0	.52	0	0	1.0	.52
43	8.1	4.18	3.0	1.52	5.1	2.66
44	48.8	25.2	47.5	24.1	1.3	1.1
45	1.3	.67	8	.41	•5	.26
46	1.9	•98	.2	.1	1.7	.88
49	1.0	.52	0	0	1.0	.52
50	5.3	2.74	•4	.2	4.9	2.54
51	7.9	4.08	•4	.2	7.5	3.88
52	4.8	2.48	0.	0	4.8	2.48
53	2.1	1.08	Õ	õ	2.1	1.08
55	2.5	1.29	•9	.46	1.6	.83
56	1.0	.52	.4	.2	.6	32
57	2.2	1.13	1.0	•51	1.2	.62
60	1.2	.62	0	0	1.2	.62
61	1.8	•93	õ	. 0	1.8	•93
62	5.2	2,68	•5	.25	4.7	2.43
63	15.0	7.74	1.2	.61	13.8	7.13
64	5.7	2.94	•4	.2	5.3	2.74
65	2.1	1.08	0	0	2.1	
76	2.5	1.29	0			1.08
	4.0			0	2.5	1.29
77 78		2.06	0	0	4.0	2.06
78	5.0	2.58	0	0	5.0	2.58
88	22.7	11.7	1.0	.51	21.7	11.19
89	9.5	4.9	0	0	9•5	4.9
90	2.9	1.5	0	0 .	°2 <b>.</b> 9	1.5

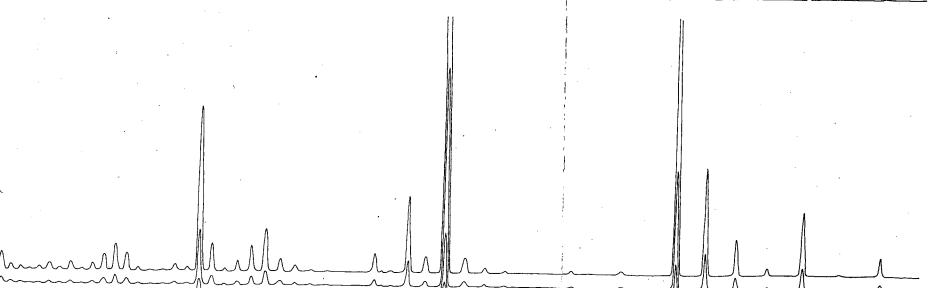


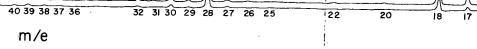












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13. ABSTRACT					
The mass spectra of the volat	ile constituents o	f the r	nilitarv e	cplosives: com	position
A-3, composition B, composi					
with a residual gas analyzer r					
plosives was too low for accu	rate measuremen	t with	the appar	atus at hand but	: <b>was</b> 🤉
in the range $10^{-6}$ to $10^{-5}$ Tor:					
propellants after pumping dow					
up to mass 100. Unresolved					
spectral signatures are suffic					
cataloguing for purposes of de	eveloping an explo	sive v	vapor dete	ction device bas	sed on
mass spectroscopy.				·	
14. KEY WORDS			•		
Explosive ordnance disposal	Mines (ordnance	e)			
Mass spectra	Powder (ordnan				
Mass spectra Mass spectroscopy	Trinitrotoluene				
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