Explosive Compounds using GC/MS

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Outline

- Compounds tested
- Methods tested
- Results
- Problematic compounds
- future work

Compounds Tested

- Toluenes
  - TNT
  - 2,4 DNT; 2,6 DNT; 3,4 DNT
  - 2 NT, 3 NT; 4 NT
  - 2 Amino DNT; 4 Amino DNT
- Benzenes
  - TNB
  - 1,2 DNB; 1,3 DNB
- Nitroglycerins
  - 1,2 DNG; 1,3 DNG
  - 1MNG; 2MNG
- Dinitrophenylamines (DNDP)
  - 2,2' DNDP; 2,4 DNDP; 2,4' DNDP; 4,4' DNDP
- RDX
- HMX
- PETN
- Tetryl
- Picric acid
- Ammonium picrate
- Nitroguanadine
- EGDN
- PGDN
- Ethyl Centralite
- Butanetriol trinitrate
- Butanetriol dinitrate

Starting Method using a 6890/5973 Fast Oven GC/MS

Initial oven temp	40°C
Oven ramp	
Inlet mode	split
Inlet temp	80°C; 150°C; 250°C
Inlet pressure	2.13 psi
Split ratio	10:1
Injection volume	1 uL
Column	DB-5ms 15m x .25cm x .25um
Column flow	1.2 mL/min Helium
Transfer line temp	220°C
MS source	230°C
MS Quad	150°C
Mass scan range	30.0 - 500.0

Method Changes

	80oC inlet	150oC inlet	250oC inlet
Oven ramp	40oC to 150oC @ 10oC/min; to 250oC @ 15oC/min		
Inlet mode	splitless		
Injection volume	5uL (splitless)		
Mode and oven ramp	Splitless and above ramping		

Resulting in a total of 15 methods tested.

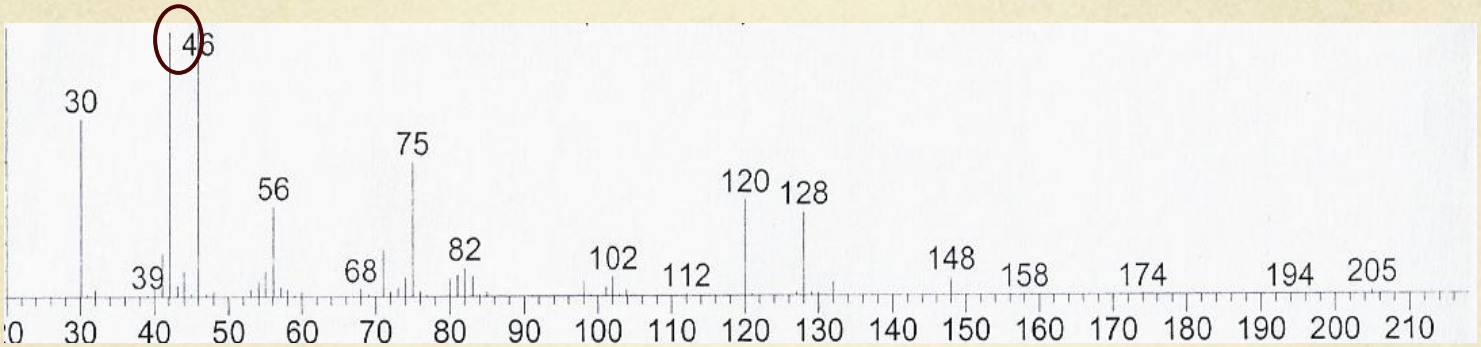
General Results

- Inlet temperatures
  - Different compounds showed improved chromatography at different inlet temperatures
- Inlet mode change
  - Improved some compound chromatography
- Injection volume
  - Samples over blown
- Oven ramping
  - Improved chromatography of early eluting compounds
  - Improved separating of RTs of isomers such as the DNTs

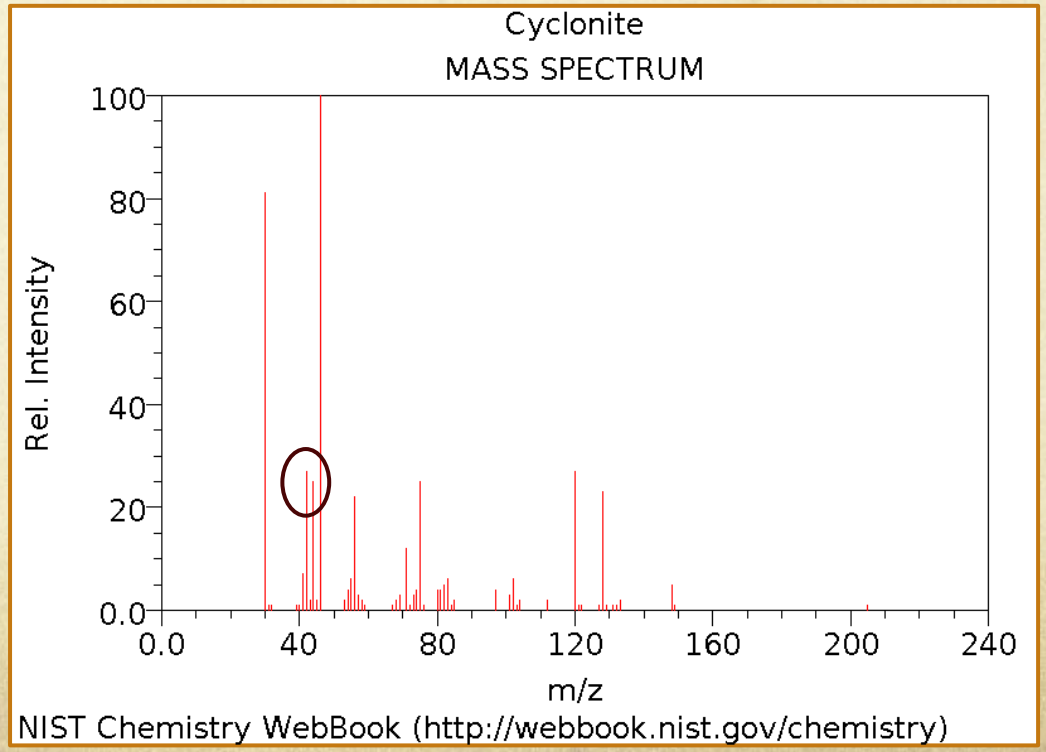
Problematic compounds

- Chromatography
  - HMX, Nitroguanadine, MNGs, BTDN
    - Low abundances when present
    - HMX difficult to get
    - Nitroguanadine gives low abundance and broad peak width
- Mass Spectra
  - RDX, HMX, PETN, BTTN, MNGs, 1,2 DNB
    - Variations in abundances of masses compared to published
  - Tetryl analysis produces a hydrolysis product
  - EGDN and PGDN are difficult to distinguish
  - DNDPs have same chromatography but still different RTs

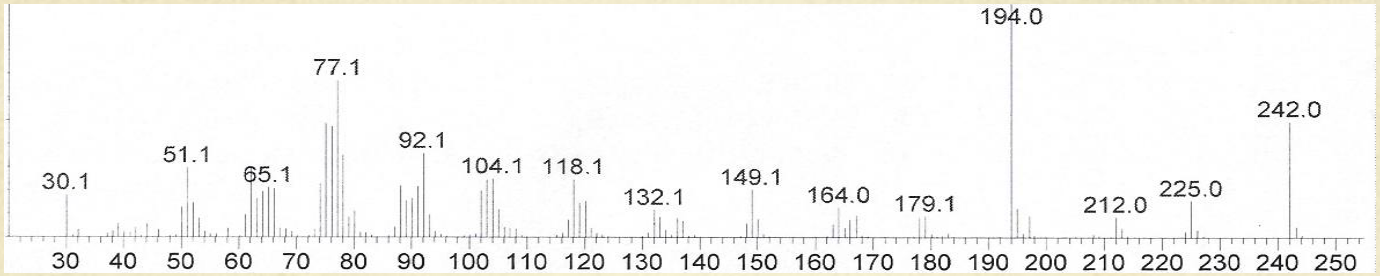
RDX

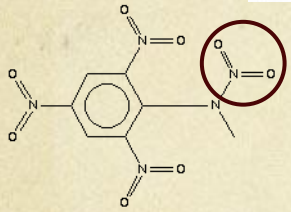


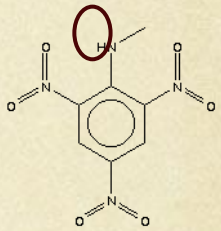
m/z 42 shows unusually high abundance compared to published mass spectra. This may suggest a possible separation of the six membered ring.

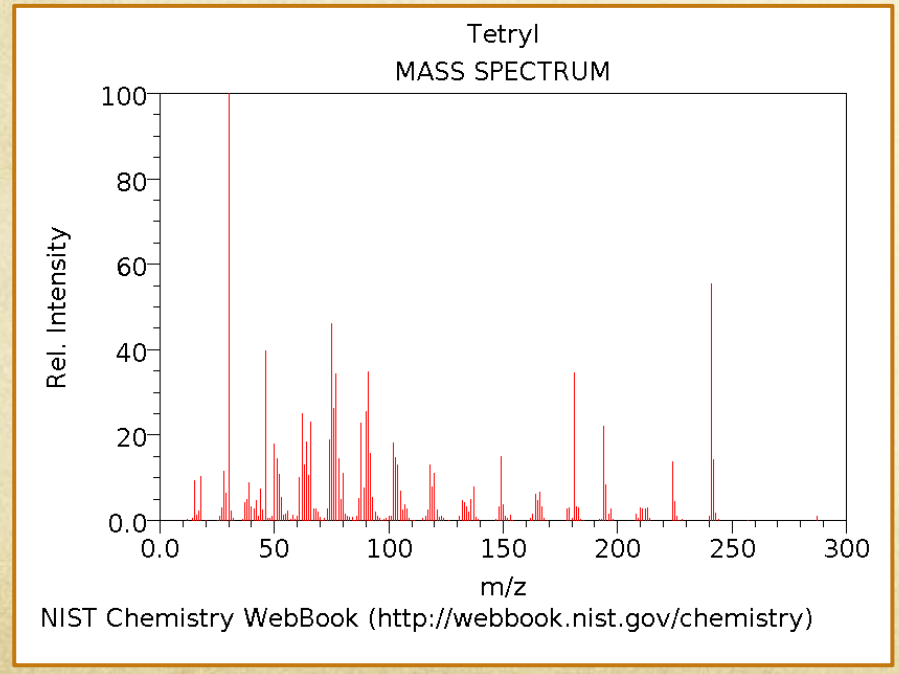


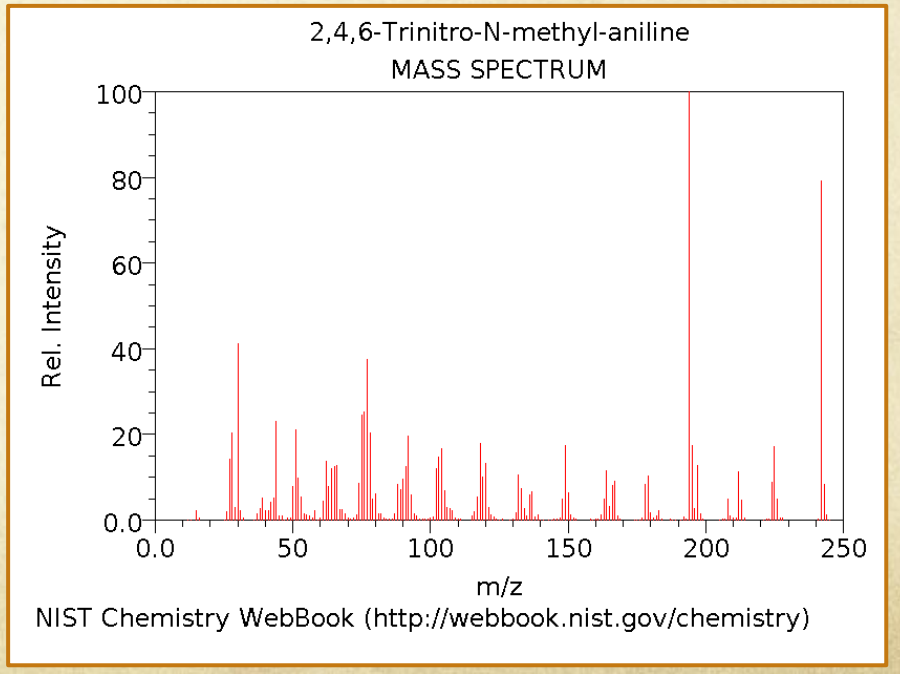
Tetryl


194.0
77.1
242.0
92.1
51.1
104.1
118.1
65.1
149.1
30.1
132.1
164.0
179.1
212.0
225.0
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250

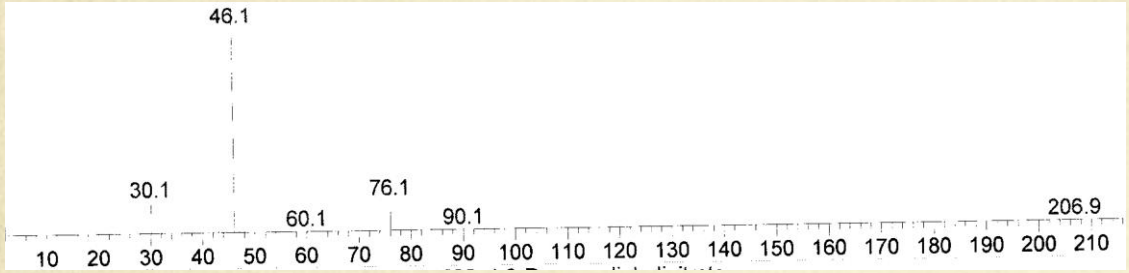





Tetryl
MASS SPECTRUM
Rel. Intensity
m/z
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

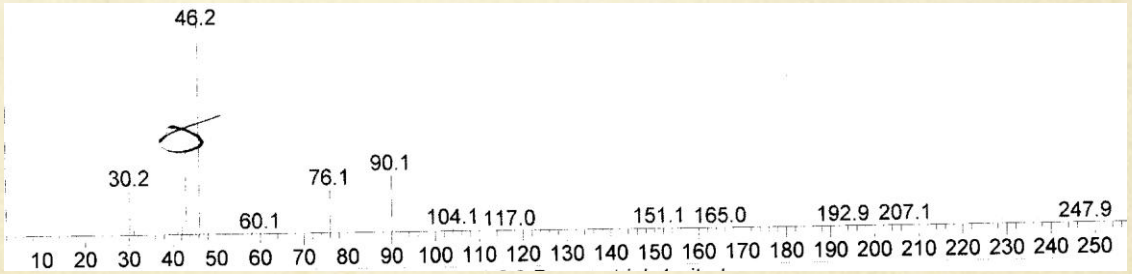

2,4,6-Trinitro-N-methyl-aniline
MASS SPECTRUM
Rel. Intensity
m/z
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

EGDN vs. PGDN



EGDN

Major differences are the larger 42 and 90 m/z seen in PGDN but these differences are not observed in



PGDN

Future Work

- Standard mixtures
- Analysis of Post blast C4 samples
- Possible analysis of trace C4 or TNT on paper or clothing
- Run standards on a direct probe TOF MS to determine if the differences are occurring in GC