Always a Step Ahead

ARDEC ARMAMENTS

Characterization of MTNP (1-methyl-3,4,5-trinitro-1,2-pyrazole)

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UNPARALLELED COMMITMENT & SOLUTIONS

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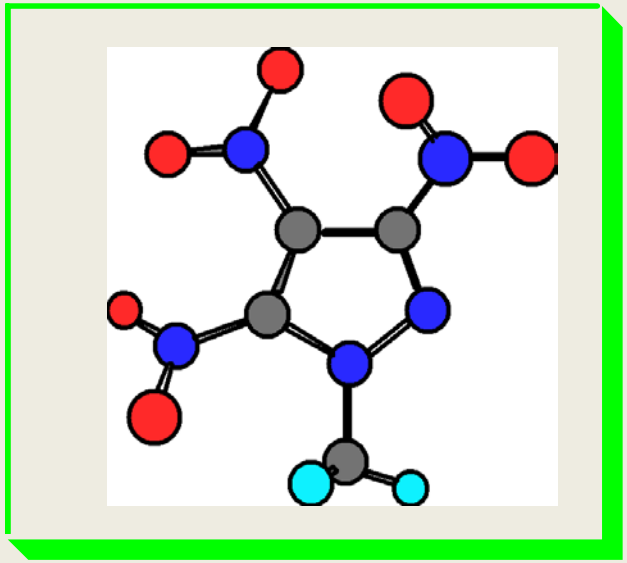
MTNP OVERVIEW



Molecular Formula	$C_4H_3N_5O_6$
Molecular Weight	217
Melting Point	91 C
Exotherm	256 C
Density	1.839 g/cc
Heat of Formation	50.7 kJ/mol

OBJECTIVE

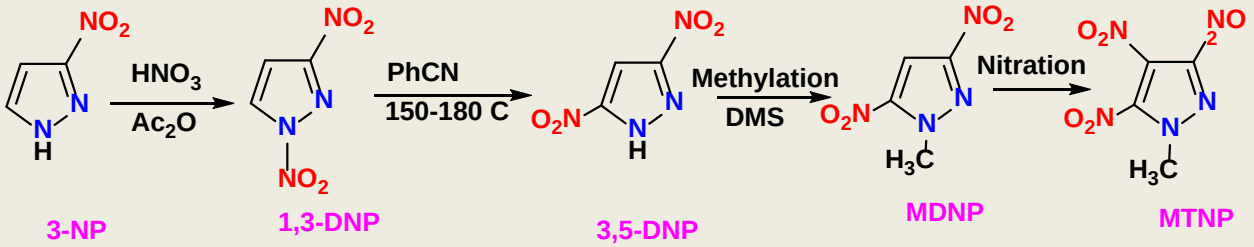
SYNTHESIZE AND PROVIDE MTNP FOR INITIAL EVALUATION EFFORTS

- UP TO DATE LITERATURE SEARCH AND ANALYSIS OF LITERATURE
- IDENTIFICATION OF SUITABLE ROUTES
- CONDUCT EXPERIMENTS TO DETERMINE THE SUITABILITY OF IDENTIFIED METHODS FOR LAB SCALE PREPARATION – DOWN SELECT THE RIGHT METHOD
- ANALYSIS, CHARACTIZATION AND PROPERTIES DETERMINATION
- DEVELOP PROCESSES AND METHODS FOR LAB SCALE SCALE-UP PROCESS
    - ENVIRONMENTALLY FRIENDLY
    - LEAST NUMBER OF STEPS
    - BETTER YIELDS
    - REPRODUCEABLE METHODS
    - LESS HAZARDOUS WASTE
- DEMONSTRATE THE VIABILITY OF THE DEVELOPED PROCESS BY PRODUCING SIGNIFICANT QUANTITY OF MTNP
- PROVIDE MTNP FOR PERFORMANCE EVALUATION

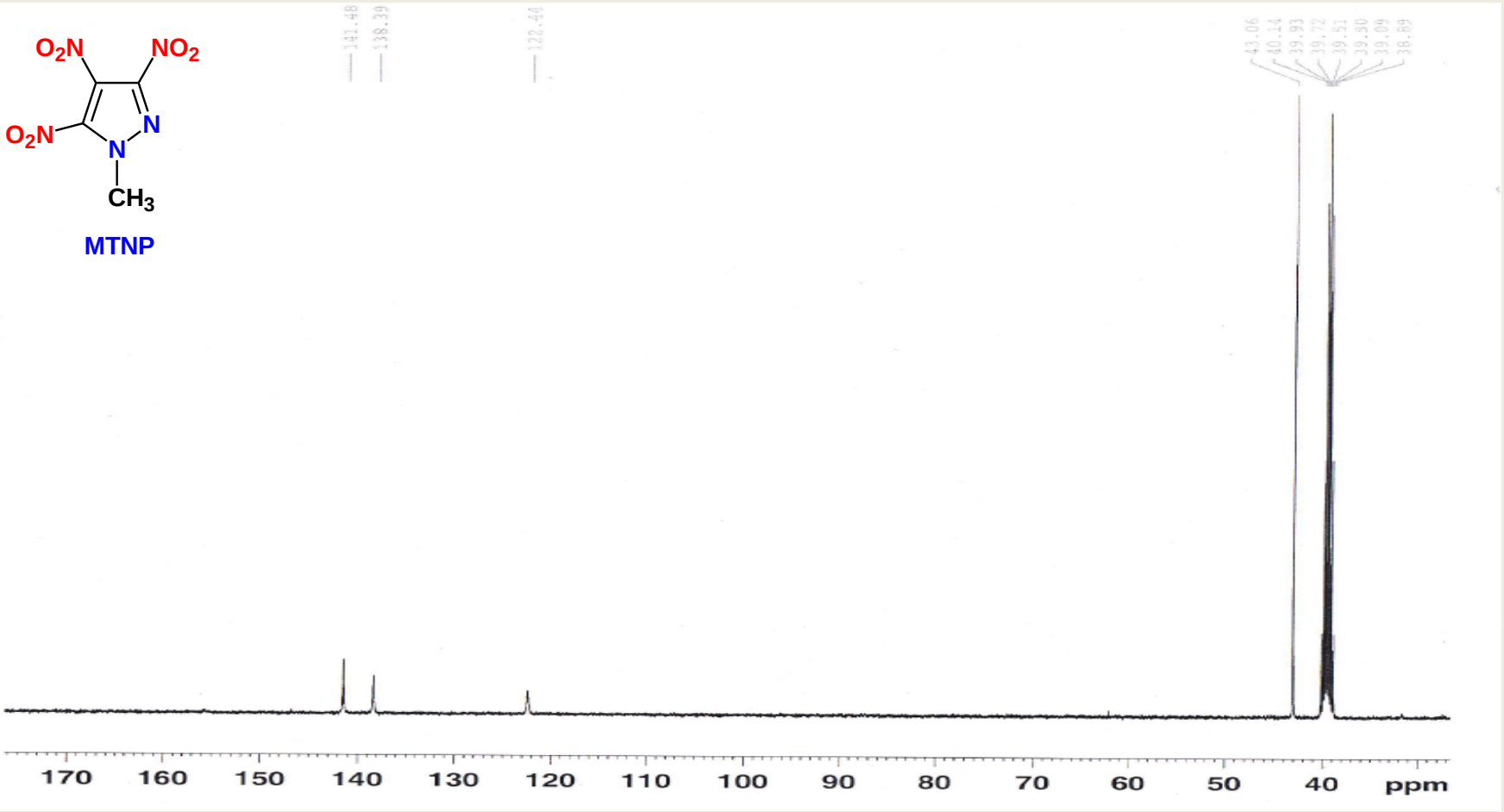
JAGUAR CALCULATIONS

Explosive	Formula	Density	DH_f	Det Vel	C-J P	Gurn Vel(3)	Gurn Vel(7)	OB
		g/cm^3	kJ/mol	km/s	GPa	km/s	km/s	%
DNAN	C7H6N2O5	1.546	-186.5	6.14	14.8	1.88	2.10	-96.9
3,4 DNP	C3H2N4O4	1.791	120.5	8.31	30.9	2.63	2.86	-30.4
MTNP	C4H3N5O6	1.82	4.53	8.36	31.1	2.59	2.82	-25.8
PrNQ	C4H10N4O2	1.335	-217.3	6.45	14.4	1.95	2.10	-120
TNT	C7H5N3O6	1.654	-63	6.89	19.8	2.20	2.43	-74.0
RDX	C3H6N6O6	1.816	70	8.76	34.8	2.73	3.01	-21.6
HMX	C4H8N8O8	1.905	75	9.09	38.7	2.76	3.04	-21.6

MTNP Starting from 3-NP



Spectral analysis of MTNP



^{13}C-NMR of 1-methyl-3,4,5-trinitropyrazole in DMSO-d_6

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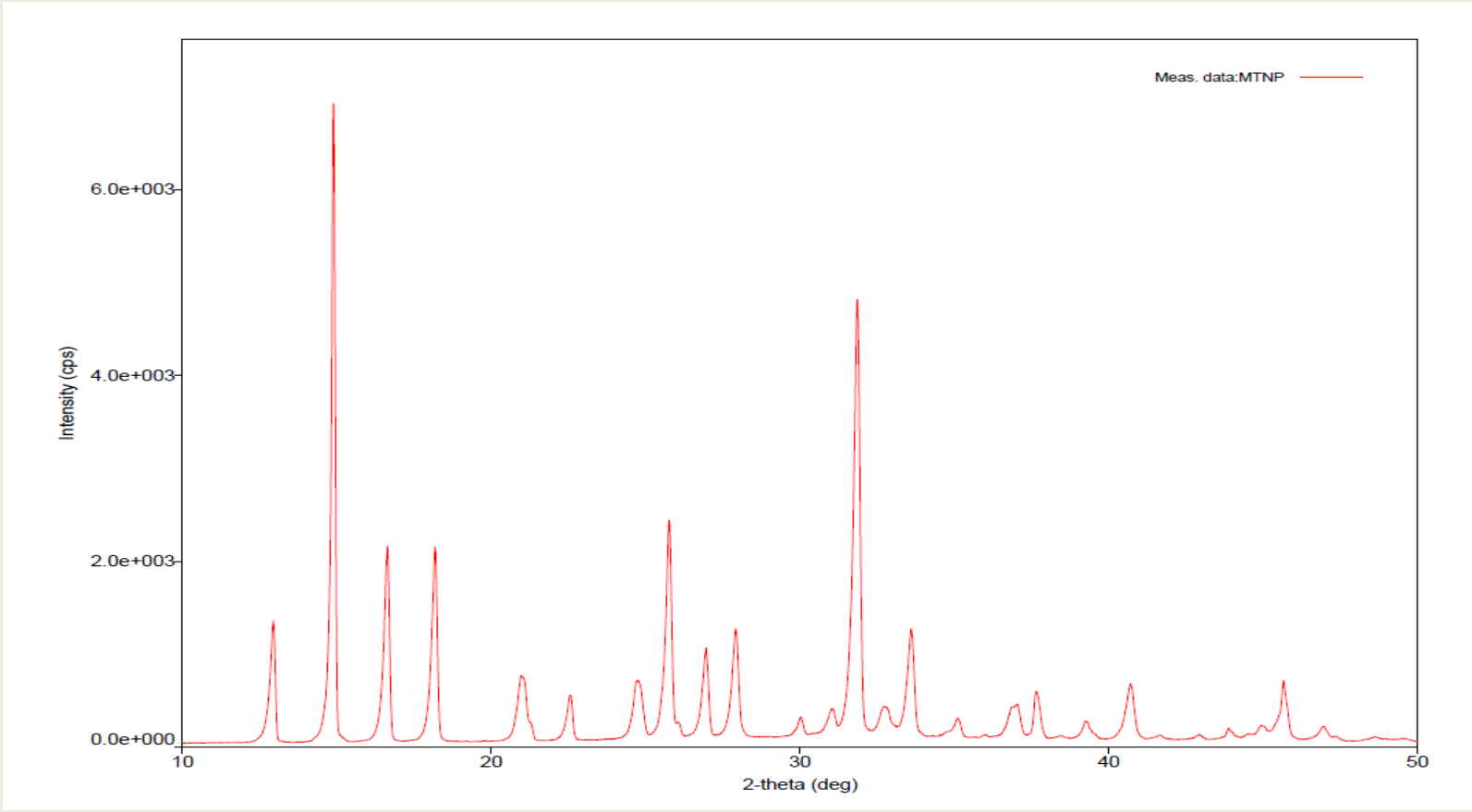
Spectral analysis of MTNP

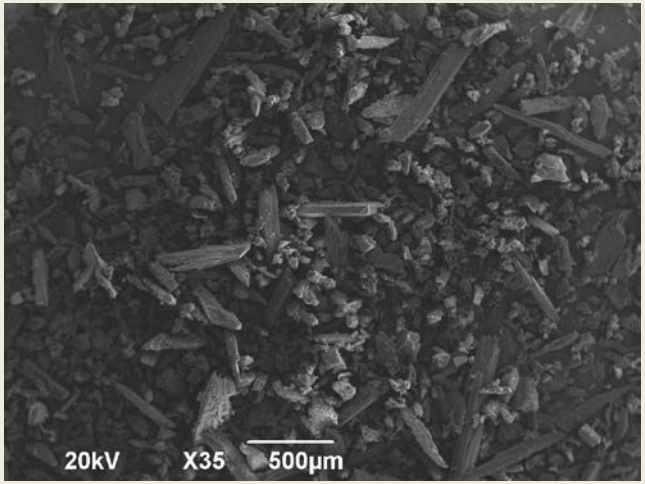


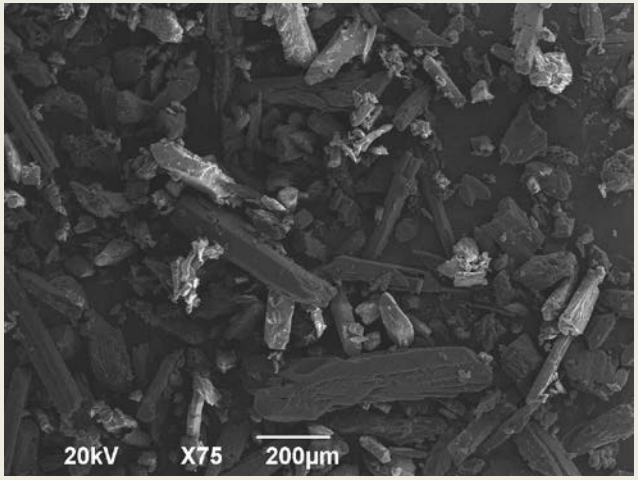
XRD of MTNP

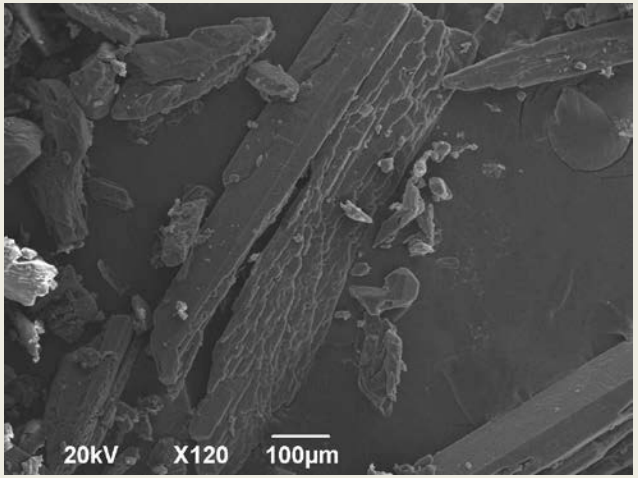
Properties of 1-methyl-3,4,5-trinitropyrazole (MTNP)

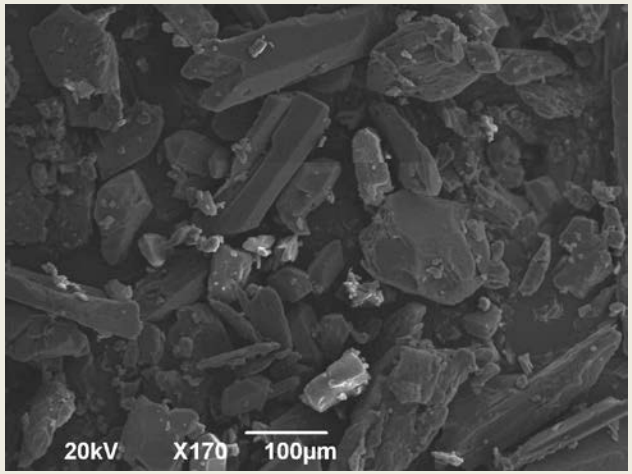
Molecule	Impact (cm)	BAM Friction (N)	ABL ESD (J)
MTNP	54.1	No Reaction in 10 trials @ 360N	Reacted @ 0.063J, did not react in 20 trails @ 0.051J
RDX Class I Type II	18	Reacted @ 216N, did not react in 10 trials at 192N	Reacted @ 0.063J, did not react in 20 trails @ 0.051J
RDX Class V Type II	>100	Reacted @ 324N, did not react in 10 trials at 288N	Reacted @ 0.051J, did not react in 20 trails @ 0.040J
DNP	>100	No Reaction in 10 trials @ 360N	Reacted @ 0.063J, did not react in 20 trails @ 0.051J
TNT	88.3	Reacted @ 240N, did not react in 10 trials at 216N	Did not react in 20 trials @ 0.25J (Old Test Method)

SEM Images of MTNP

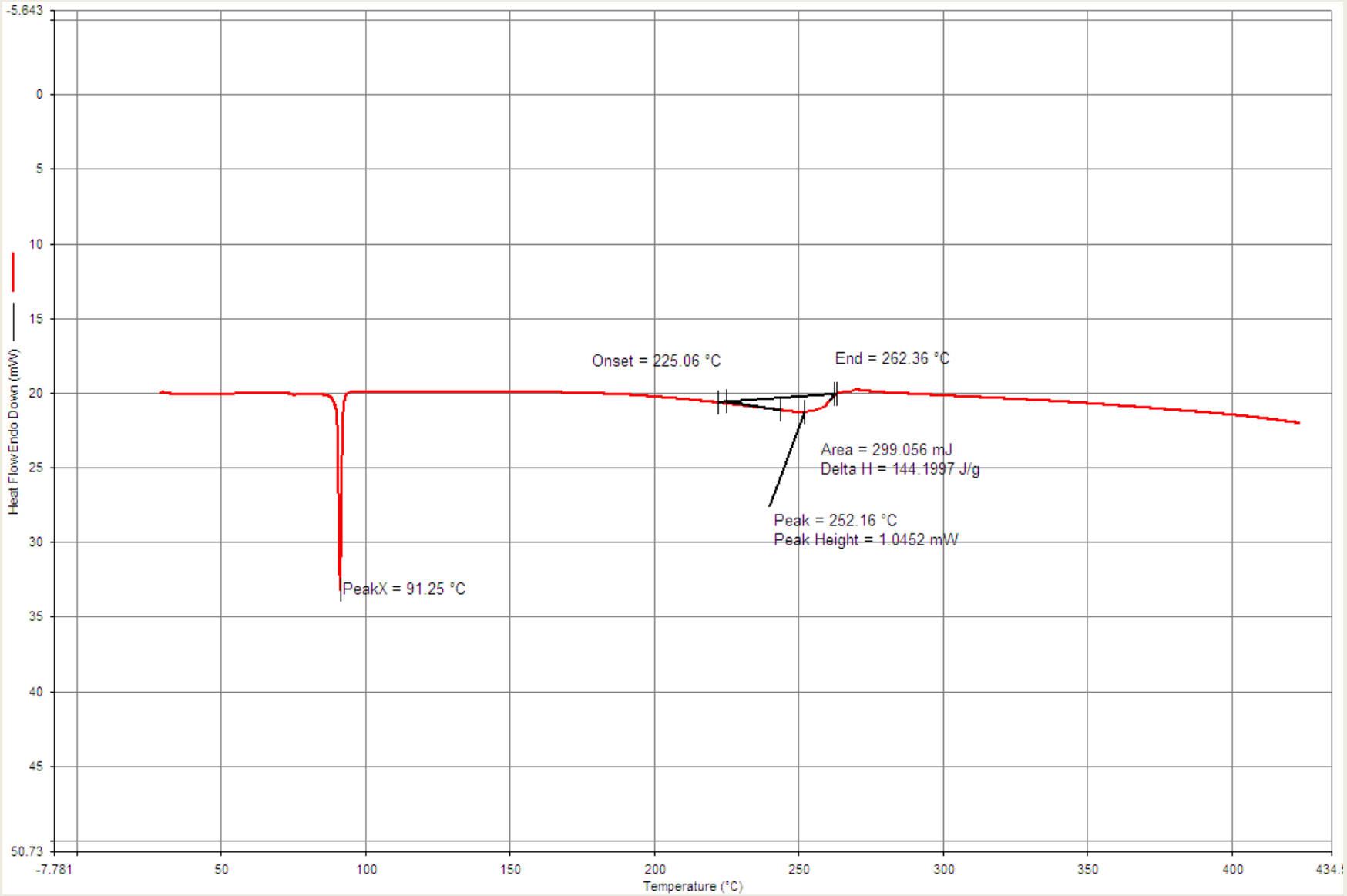




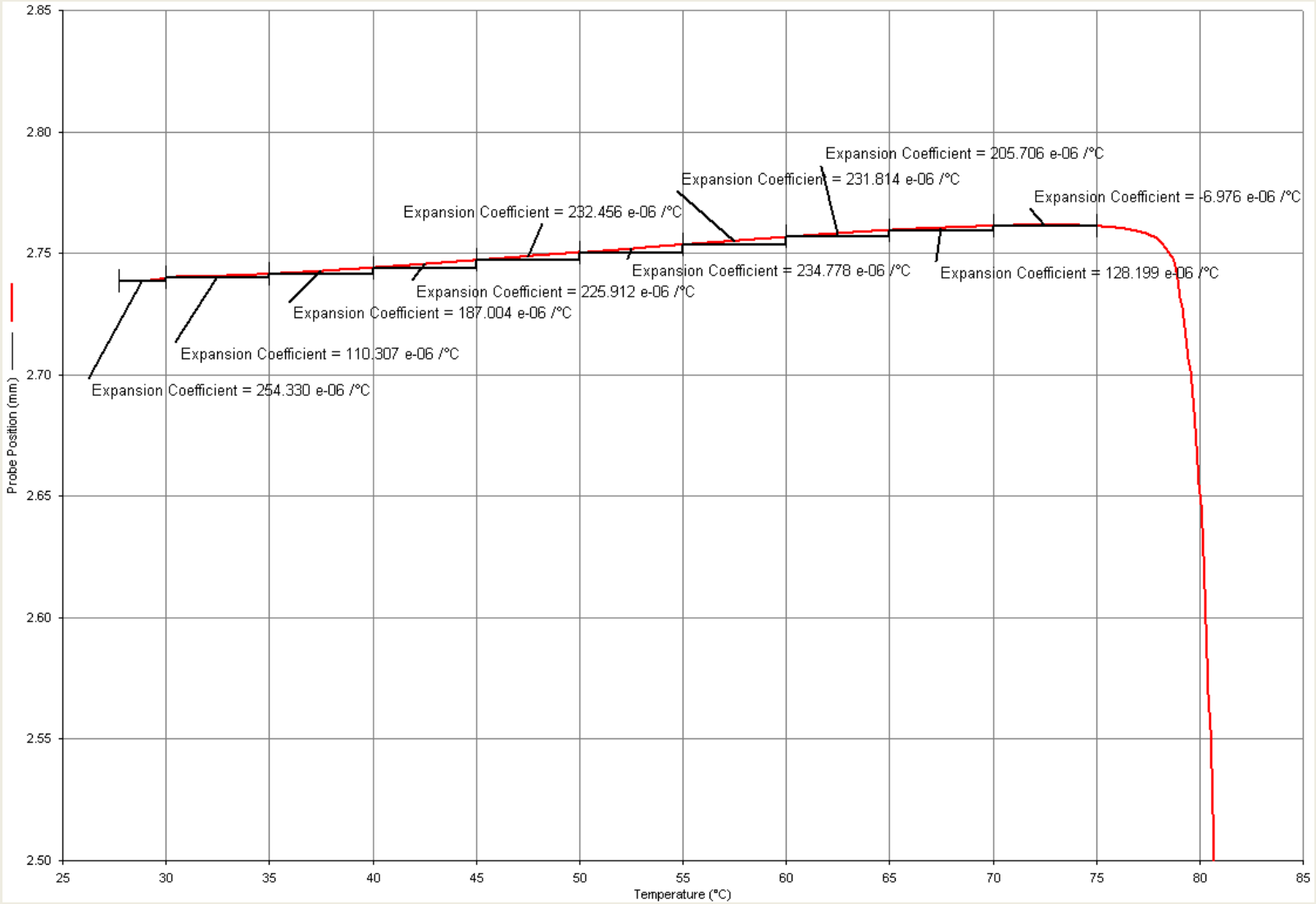




DSC of MTNP


-5.643
0
5
10
15
20
25
30
35
40
45
50.73
Heat Flow Endo Down (mW)
-7.781
50
100
150
200
250
300
350
400
434.
Temperature (°C)
Onset = 225.06 °C
End = 262.36 °C
Area = 299.056 mJ
Delta H = 144.1997 J/g
Peak = 252.16 °C
Peak Height = 1.0452 mW
PeakX = 91.25 °C

TMA analysis of MTNP



DSC Compatibility Testing

- Performed compatibility testing in accordance to STANAG 4147 ED.2
- A DSC for each individual explosive, test material and mixture shall be run in duplicate
- Explosives and test materials are mixed in a 1:1 (w/w) ratio
- Samples are heated at a rate of 5°C/min from room temperature to 300°C or more for each sample
- The reactivity (compatibility) is then determined by comparing the decomposition profiles of the individual components to the mixture

Compatibility Results for MTNP

- MTNP is compatible with Al.
- MTNP requires VTS testing with NTO, FOX-7, HMX and O-ring since DSC compatibility showed more than 10C exotherm shift
- MTNP requires VTS testing with brass and 304/316 stainless steel to determine compatibility due to the appearance of a new exotherm
- VTS testing is also needed with copper and A2 Steel due to earlier onset of the decomposition (around 250°C)
- VTS testing with Copper: Pass

Conclusions

- Performed Literature Search and Analyzed Reported Methods
- Made attempts to synthesize MTNP in one pot process from Pyrazole
- Will Investigate Preparing MTNP Using Sequential Nitration Process
- Looking to Reduce the Amount of Required Reagents
- Characterized and Determined Small Scale Safety and Handling and Thermal Properties of MTNP
- Developed Scale up process
- FUTURE WORK:
    - Continue Investigating Alternate Nitrating Agents/Reagents