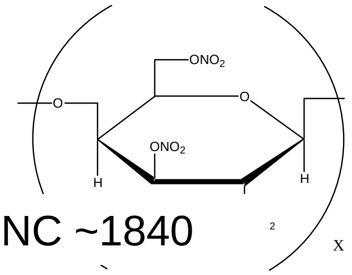
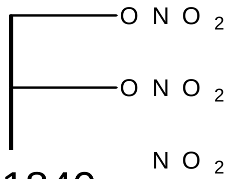
Center of Excellence for Explosives

Detection, Mitigation & Response



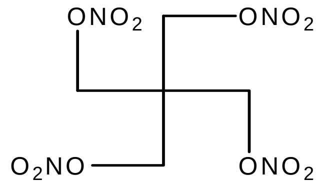
NC ~1840

NC
1846

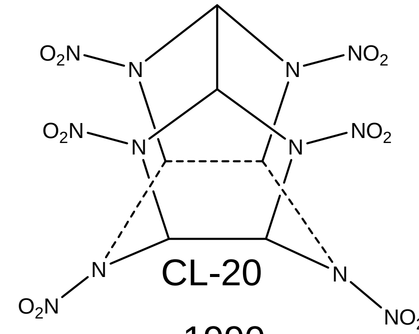


NG ~1840

N G
1 8 4 6

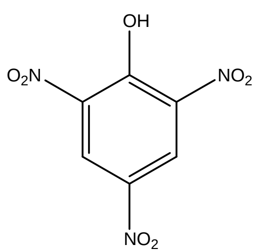


PETN
~1930

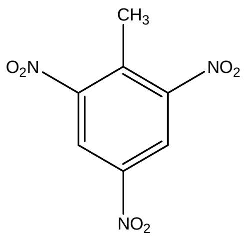


CL-20

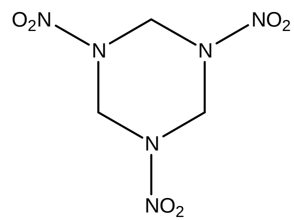
~1990



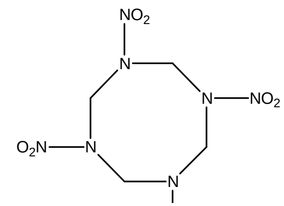
picric acid
1870



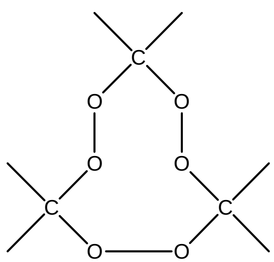
TNT
~1900



RDX
~1940



HMX
~1950



TATP

H-O-O-H

CH_3NO_2

NH_4^+
NO_3^-

$NH_4^+ NO_2^-$

NH_4^+
ClO_4^-

NH_4^+
ClO_3^-

Most explosives are not new;
they are 60 to 100 years old.

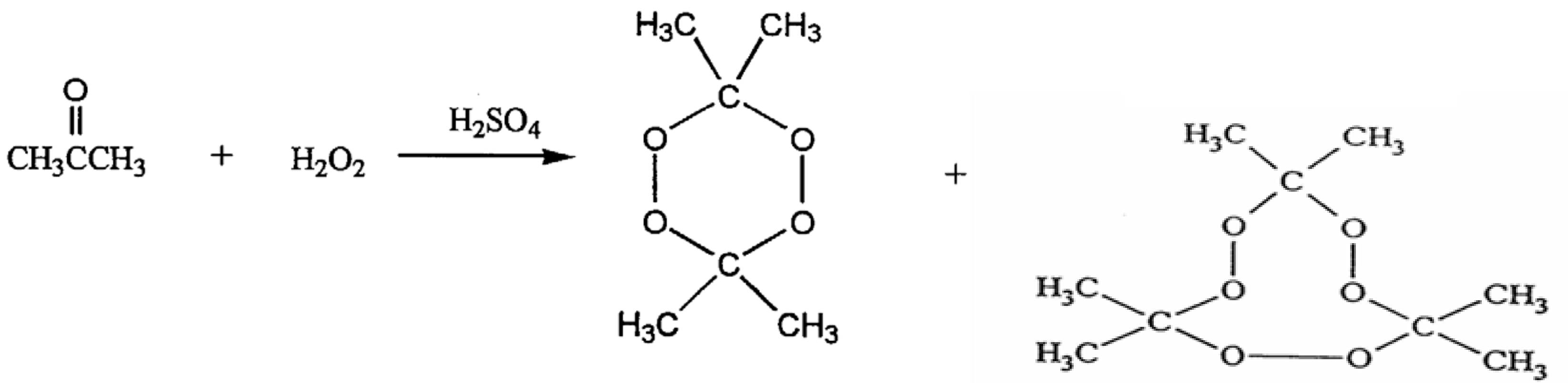
Characterization of Energetic Materials

What’s its density?
What’s its performance?
What’s its signature? vapor pressure?
What are its decomposition products?
What are its safety parameters?
Is it an explosive? at what scale?

Edward AFB 1999

13,700lb propellant with 1700 lb C4 booster

TATP (triacetone triperoxide)



DADP

mp = 126-128°C

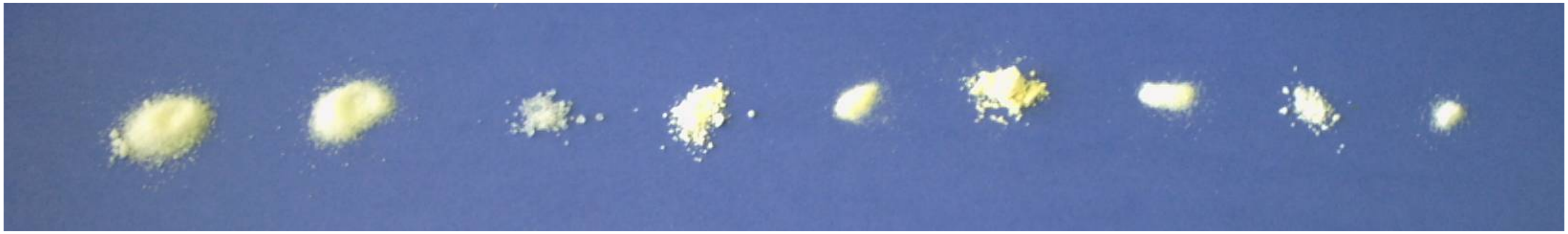
TATP

mp = 93-95°C

(3,3,6,6,9,9-hexamethyl-[1,2,4,5,7,8]hexaoxocyclononane)

- ***High explosive*** discovered in 1895
- Detonation velocity ~5290 m/s
- Density ~1.20 g/cc
- Highly sensitive to heat, friction and mechanical shock [drop height (5 kg) = 10 cm]
- **ENERGETIC without nitrogen**

crystalline TATP



sugar salt AN HMX RDX TNT PETN TATP HMTD

Flame Test is a quick method of assessing hazard on small quantity

RDX

Sugar

TATP

Physical properties are noted, but most explosives have such low vapor pressures that they are not measured routinely.

Explosive & Propellant Properties		MW g/mol	m.p. C	vapor pres torr @25C	state
AN, NH4NO3		80	169	salt	S
HMX		296	280d	3E-09*	S
RDX		222	204d	2E-09	S
Picric acid		229	122	1E-09	S
PETN		316	141	3E-08	S
Tetryl		287	129	3.5E-05*	S
TNT		227	81	4.5E-06	S
NG, nitroglycerin	**AN** →	227	13	2.3E-04	L
DMNB^, 2,3-dimethyl-2,3-dinitrobutane	**UN** →	176		2.1E-03	L
2,4-DNT, 2,4-dinitrotoluene		182	69	1.9.E-02	S
EGDN^, ethylene glycol dinitrate	**TATP** →	152	-23	4.8E-02	L
p-MNT^, 4-nitrotoluene	**DADP** →	137	55	4.1E-02	S
o-MNT^, 2-nitrotoluene		137	-3	1.5E-01	L
Nitromethane, CH3NO2		61	-29	37	L

^ ICAO taggants

*100C, ** 150C

Decomposition Mechanism of Explosives

Provide graduate students publishable projects

Determine at what point reaction can be modified—slowing it (making explosive more stable) or accelerating it (making it less stable)

e.g. would an additive to acetone prevent its use in TATP manufacture?

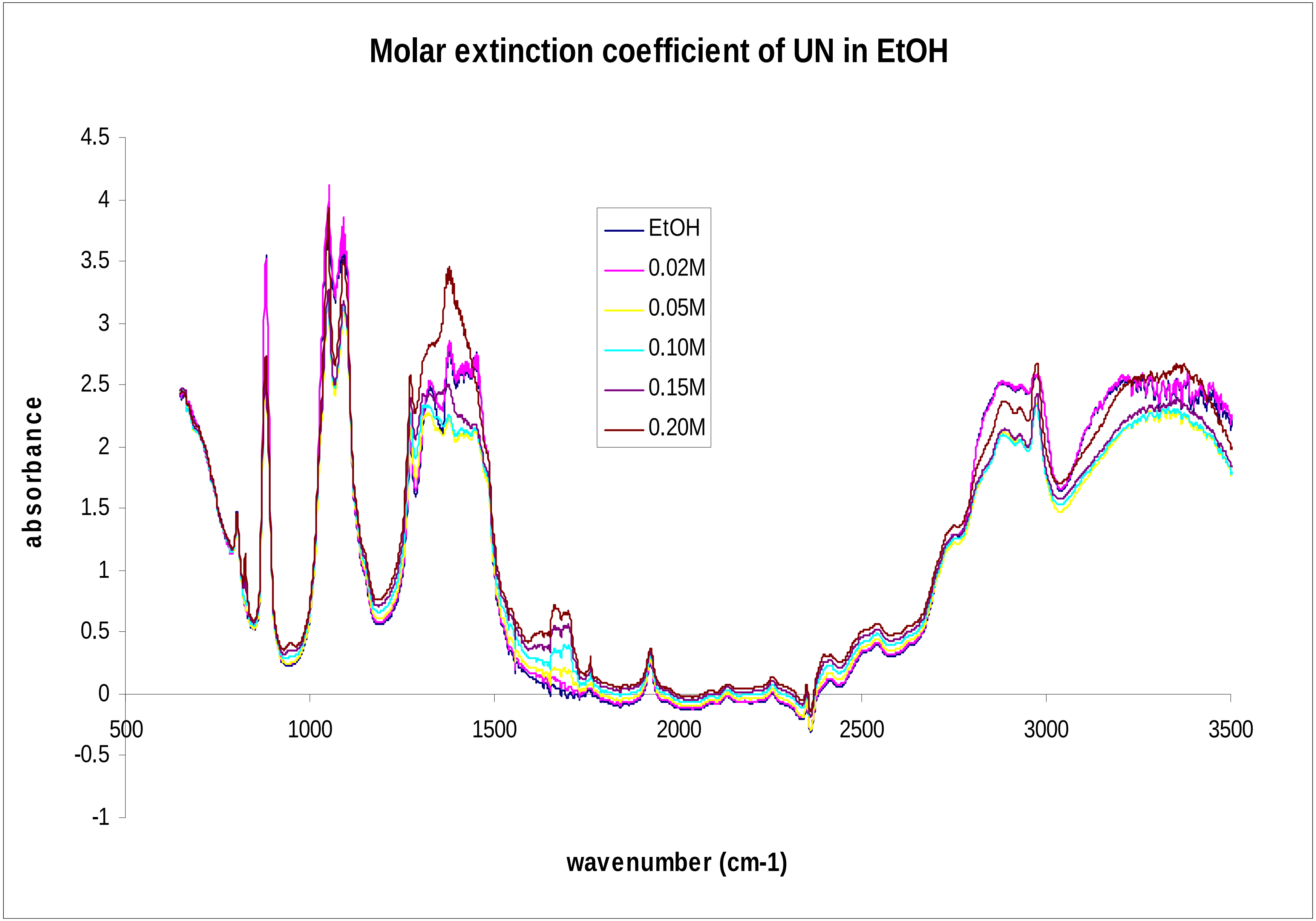
Aid design of “interruptors” in the synthesis chain

Targeted molecules

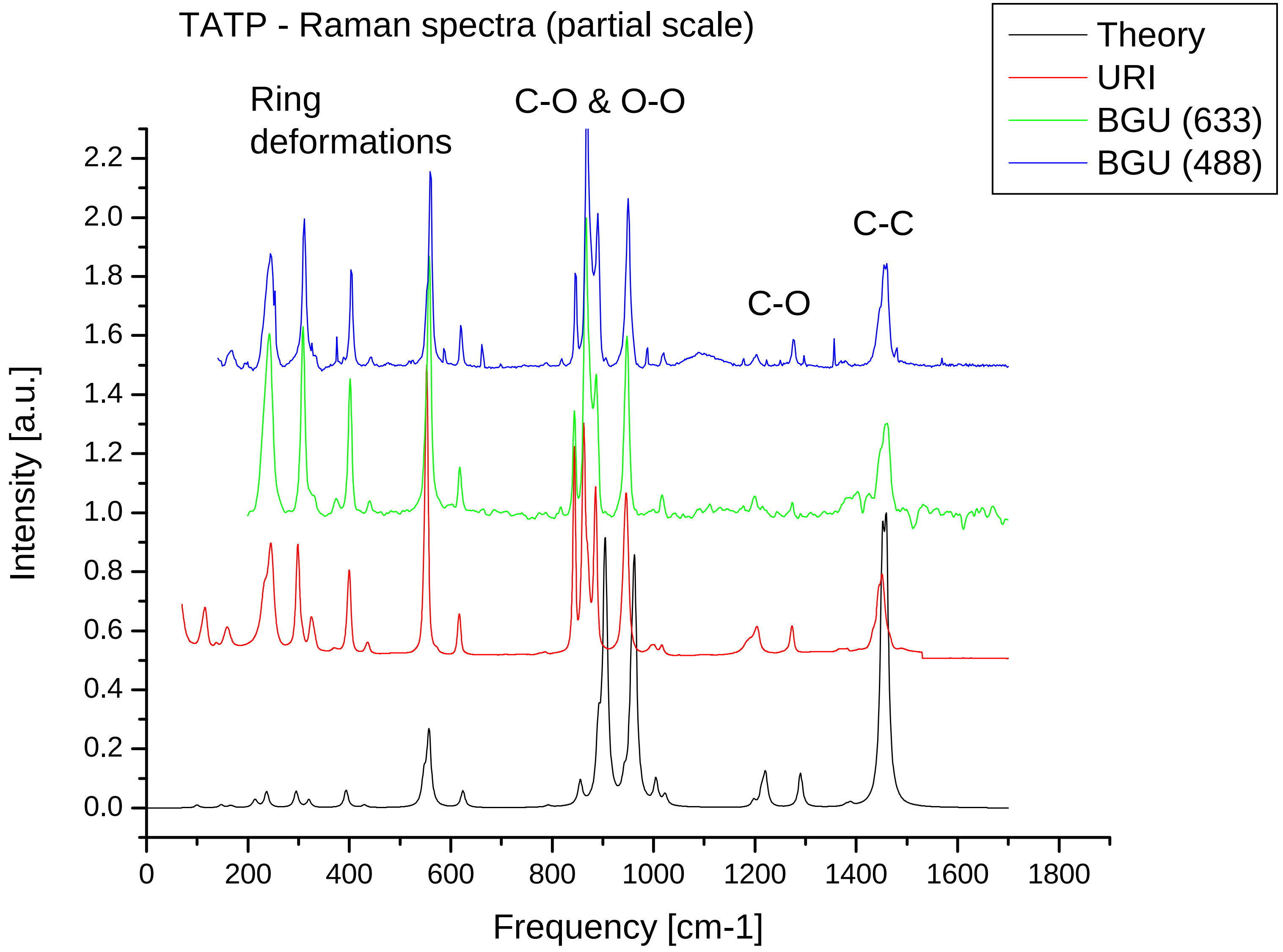
- Urea nitrate
- TATP
- HMTD

$$[NH_2CONH_3]^+NO_3^- \Leftrightarrow O{=}C(NH_2)_2 + HNO_3$$

$$[NH_2CONH_3]^+NO_3^- \rightarrow NH_2CONHNO_2 + H_2O$$



Molar extinction coefficient of UN in EtOH
EtOH
0.02M
0.05M
0.10M
0.15M
0.20M
absorbance
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
-1
500
1000
1500
2000
2500
3000
3500
wavenumber (cm-1)



TATP Raman spectra—theoretical & found

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What Makes a Good Chemical Explosive?

They undergo sustained **exothermic** (heat releasing) **reaction**, usually that reaction is oxidation:

$$4\ TNT\ [C_7H_5N_3O_6] \rightarrow 10\ H_2O + 7\ CO_2 + 6\ N_2 + 21\ C$$

The volume of products is much greater than reactants, providing a fluid to do work. This requires high density materials which make a **lot of gas.**

One liter of explosives will expand to ~1000 liters in milliseconds. When confined this causes extreme stress

Exothermic decomposition of explosive is very ***fast***.

Are chemicals with a **TNT equivalence** of 20-30% detonable at some size of material or booster?

TNT equivalence

PETN	170%
HMX	160%
RDX	160%
tetryl	144%
picric acid	105%
TNT	100%
ANFO	60%
TATP	88%
HMTD	60%
AN	**30-25%**
dibenzoyl peroxide	**25%**
di-t-butyl peroxide	**30%**
2,4-DNT	**30%**
chlorate/vasoline	**45%**


Allentown, PA
Feb. 19, 1999
H_2NOH


Manchester, CT 7/01
Phoenix, AZ 8/00
$Ca(OCl)_2$


Port Neal, IA 12/94
aq NH_4NO_3


Danvers, MA 11/06
hexanes

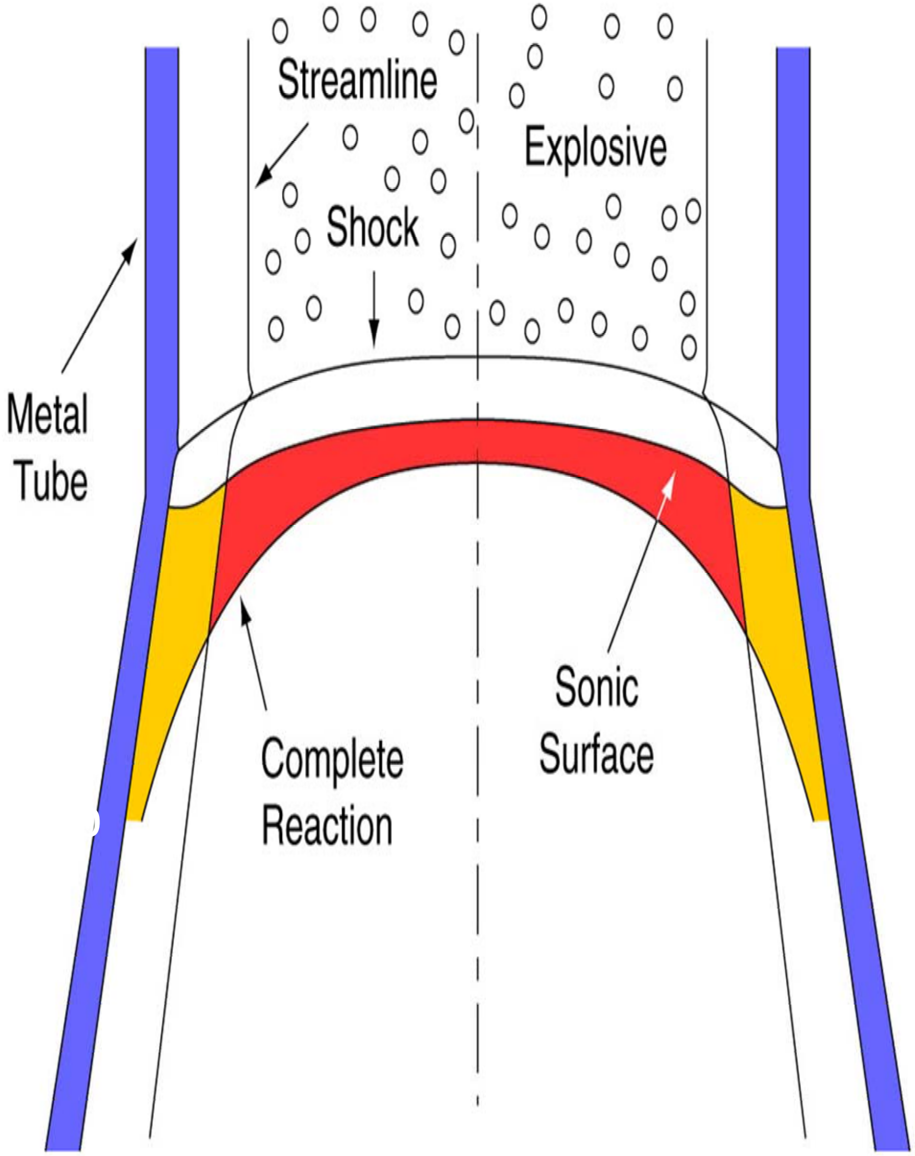
1996-8	Aug. 2006	Nov. 2006	Dec. 2006	Ap 2007	Feb-07
Nation Research Council	Natural Resources Canada	Australia	Singapore	DHS	EU
nitric acid	nitric acid	nitric acid		2000	nitric acid
ammonium nitrate	AN	AN	AN	2000	AN
potassium nitrate	KNO_3	KNO_3	KNO_3 >5%	2000	
calcium nitrate					
mix NaNO3, Ca(CN)2, NH4Cl	$NaNO_3$	$NaNO_3$	$NaNO_3$ >5wt%	2000	
sodium chlorate	$NaClO_3$	$NaClO_3$	$NaClO_3$	2000	$NaClO_3$
potassium chlorate	$KClO_3$	$KClO_3$	$KClO_3$	2000	$KClO_3$
hydrogen peroxide	H_2O_2 >30wt%	H_2O_2	H_2O_2 >20wt%	>30%, 2000	H_2O_2
potassium perchlorate	$KClO_4$	$KClO_4$	$KClO_4$	2000	$KClO_4$
		$NaClO_4$	$NaClO_4$		
		NH_4ClO_4	NH_4ClO_4	2000	NH_4ClO_4
urea				2000	
	nitromethane	nitromethane		2000	
dinitrotoluenes					
nitrobenzene					
$Ca(OCl)_2$					
$Na(OCl)_2$					
$KMnO_4$					
sodium chlorite					
calcium carbide				anhy NH_3 7500	
halogenated biocides				NH_3 >20% 15000	
nitroparaffins					
picric acid					
acetylene				7500	
		sulfuric acid			sulfuric acid
				anhydr any amount	HCl

Government agencies are beginning to worry about chemical precursors, but there is little data to guide choices.

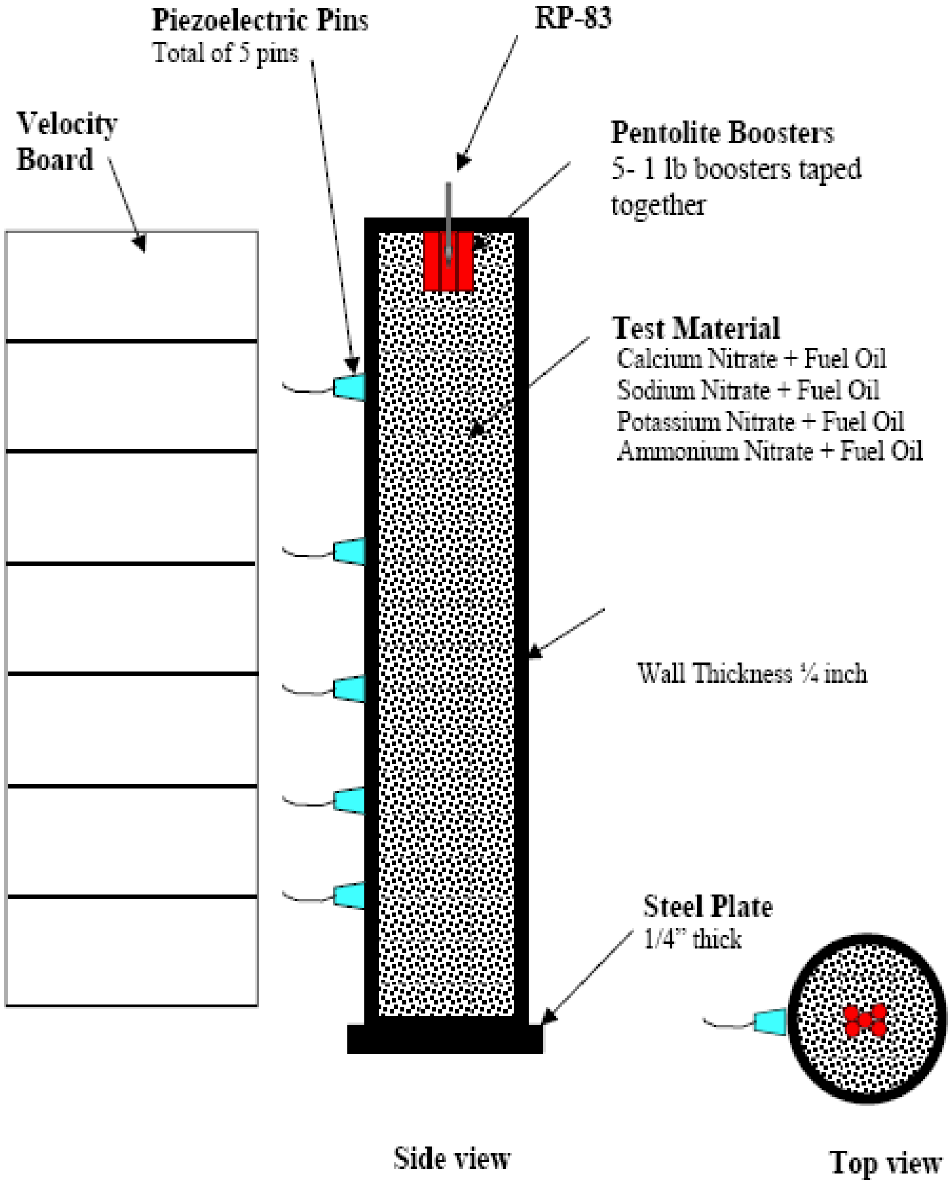
Size Matters

Homemade explosives may not detonate at the small-scales that military HE do. DoT testing may show them inert.

Size is important - especially for potential runaway reactions.



NRC Suggested Detonability Test Scale ~250 lb (12”x60”)



Detonable at 12" x 60" (30 cm x 152 cm)	fuel oil	sugar	nitromethane	aluminum
NH_4NO_3	yes	yes	yes	yes
AN/AS	no	no	yes	yes

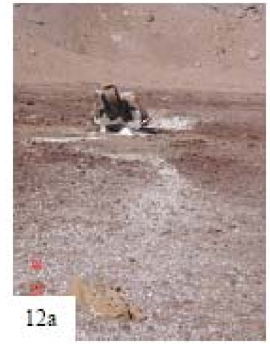
time of arrival pins

Nitrate salts with 2% diesel fuel results of 100 kg detonability test

AN

steel pipe totally fragmented

$Ca(NO_3)_2$



12a

12b

12c

6a

6b

6c

KNO_3

notice unreacted K and Na nitrates

8a

8b

8c

$NaNO_3$

Shock-focusing Test of Detonability

Shock-focusing test will drive a powerful, convergent shock into sample. The shock input will be slightly stronger than ideal detonation could produce in the sample chemical.