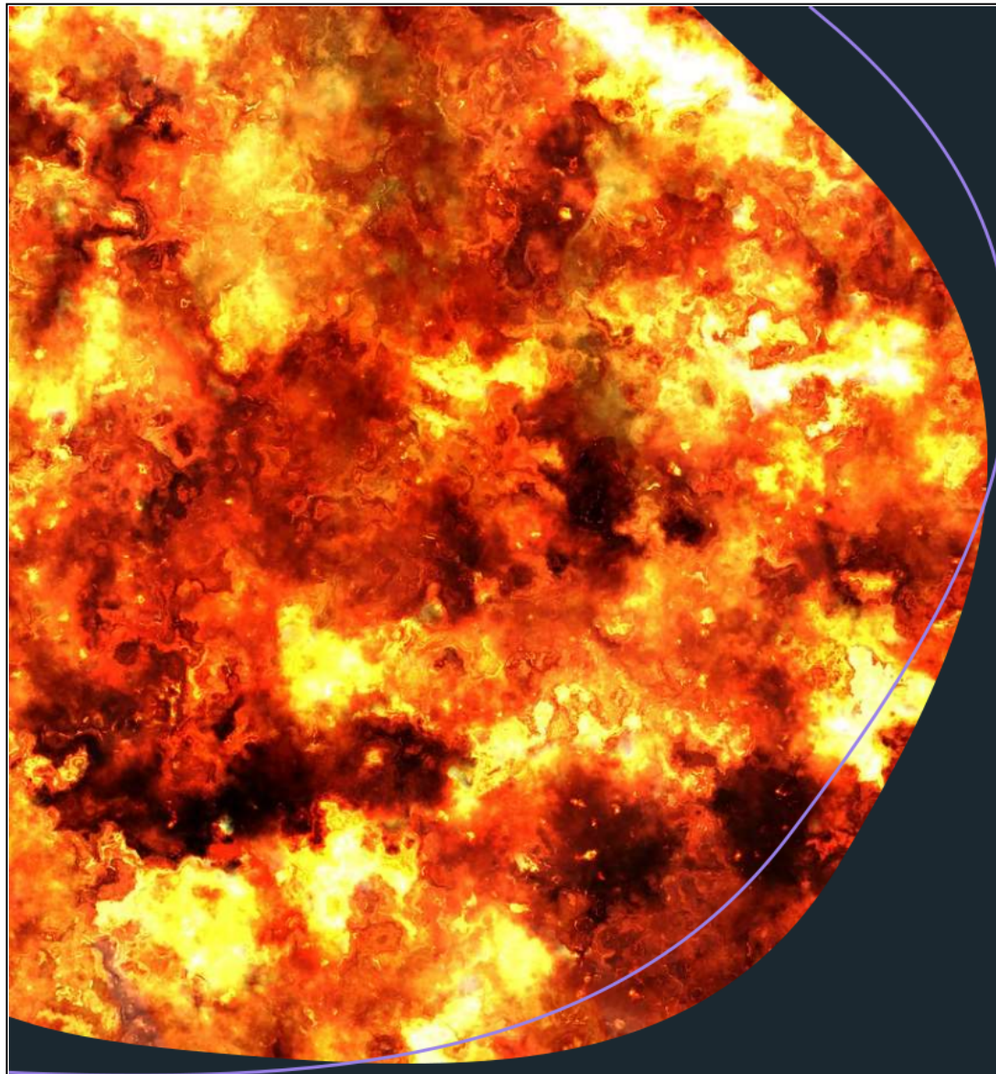
Final Presentation

by Joshua Ede

Submission date: 04-Dec-2023 01:39AM (UTC+0000)
Submission ID: 217722298
File name: 27258_Joshua_Ede_Final_Presentation_544928_1444411300.pptx (13.35M)
Word count: 3279
Character count: 18457



Explosive Materials in OME

Thermodynamic analysis, Reaction Chemistry, and Lifecycle Assessment

Part 1: Thermodynamic Analysis

- What is an explosive?
- Why do they explode?
- What makes an explosive?
- What makes a good explosive?

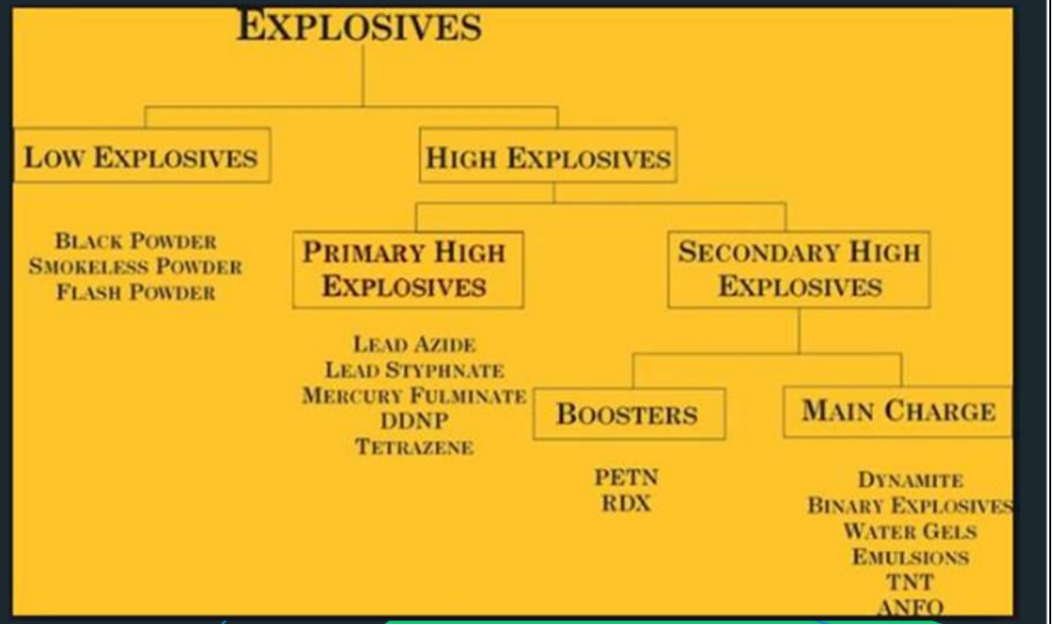


What is an explosive?

Chemical capable of reacting suddenly to release vast quantities of gas and heat



Classified by: High or Low, Military or civilian, functional group, use case etc.

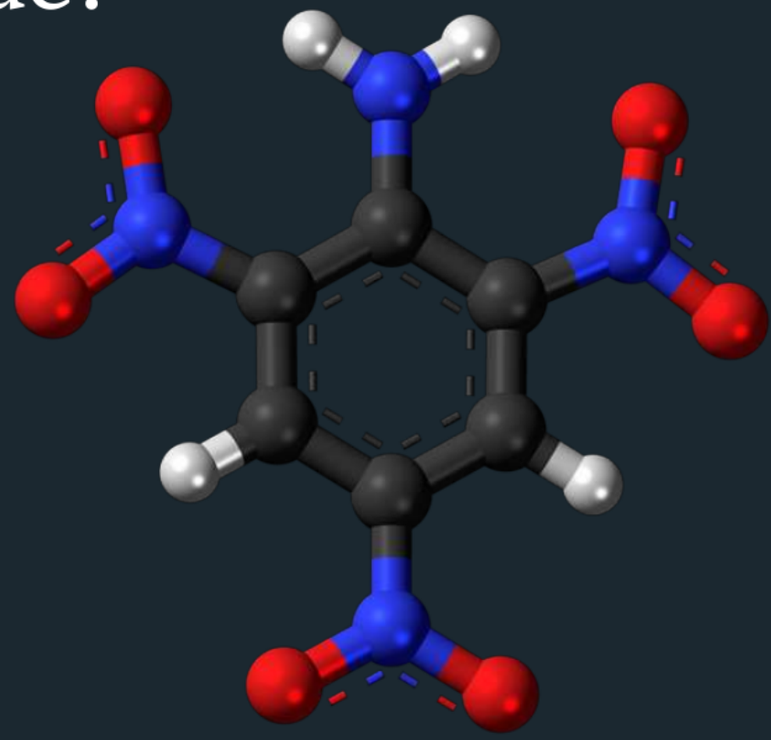


J. Agrawal, High Energy Materials: Propellants, Explosives and Pyrotechnics, Wiley, 2010

Why Do Explosives Explode?

Gibb's Free Energy:

$$\Delta G = \Delta H - T\Delta S$$

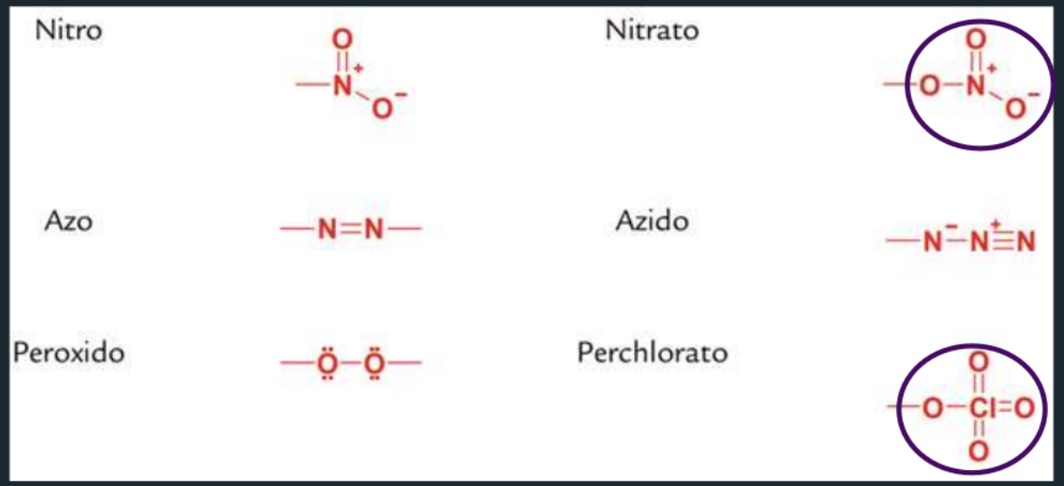


An Explosion is massively exothermic **(big -ΔH)**

Explosions release large amounts of gaseous products **(big ΔS)**

S. Venugopalan, Demystifying Explosives, Elsevier, 2015

What makes an explosive… explosive?



- It's Functional groups!
- Similar electronegativities make weak bonds, which are easily broken.

Oxidation Number: Cl = +7, N = +5

S. Venugopalan, Demystifying Explosives, Elsevier, 2015
D. Kumar & A. Elias, "The Explosive Chemistry of Nitrogen", *Resonance*, 24, 2019

Thermodynamics, Maths and other scary words

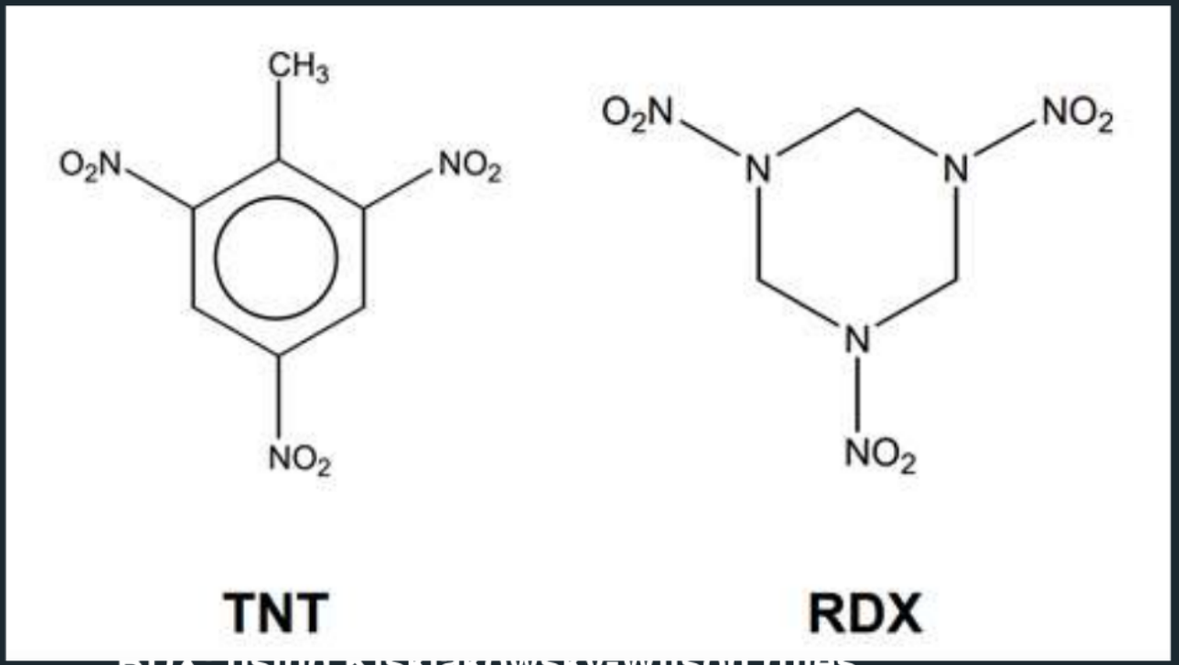
TNT:

$$C_7H_5N_3O_6$$

RDX:

$$C_3H_6N_6O_6$$

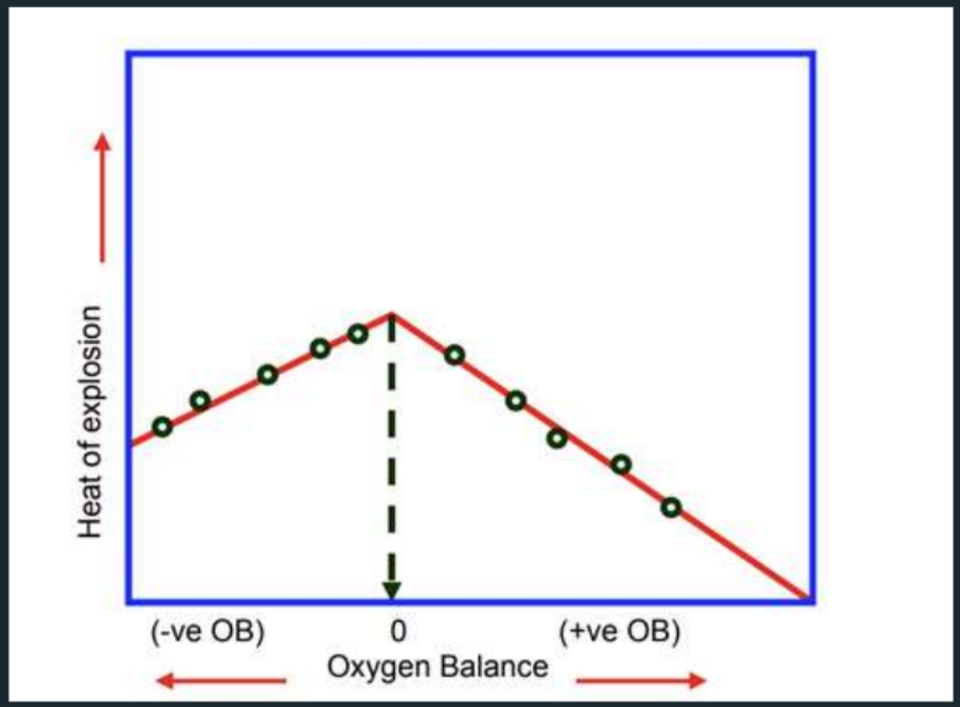
Oxygen Balance Calculations:



RDX: using Kiskiakowsky-Wilson rules

$$C_3H_6N_6O_6 \rightarrow 3CO + 3H_2O + 3N_2$$

Thermodynamics 2: The way of water



Volume of Gaseous Products:

TNT:

$$C_7H_5N_3O_6 \rightarrow \frac{7}{2}CO + \frac{7}{2}C + \frac{5}{2}H_2O + \frac{3}{2}N_2$$

Gaseous products = $0.740\ dm^3 g^{-1}$

RDX:

$$C_3H_6N_6O_6 \rightarrow 3CO + 3H_2O + 3N_2$$

Gaseous products = $0.908\ dm^3 g^{-1}$

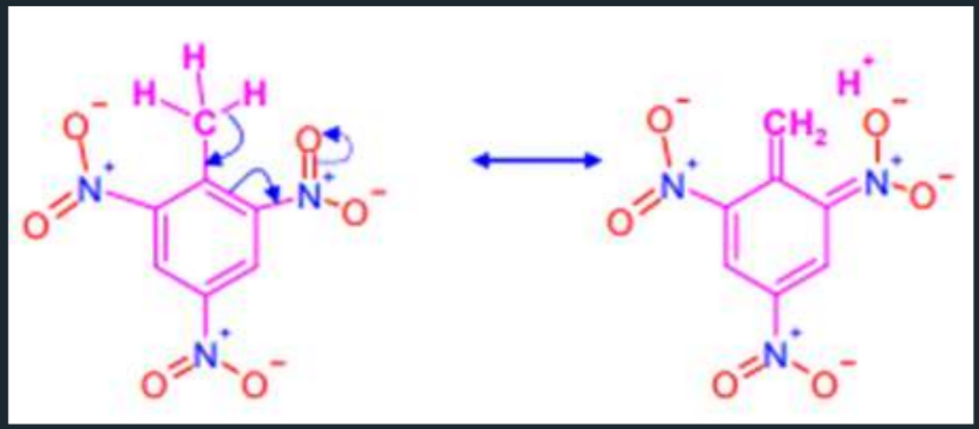
Is TNT just worse at everything?

Property	TNT	RDX
OB	-73.96%	-21.61%
ΔH_f – heat of formation	-62.07 kJ/mol	+70.29 kJ/mol
ΔH_d – heat of explosion	-929.34 kJ/mol	-1838.37 kJ/mol
Volume of Gaseous products	739.65 dm^3/kg	907.63 dm^3/kg
VOD	6900 m/s	8750 m/s
H_{50}	220 cm	19 cm
Melting point	80.35° C	205° C
Auto-Detonation temp	240° C	217° C

- Assessment of key detonation properties suggests so, but RDX has one major downside, it cannot be melt cast in munitions!

M. Cawkwell et al., "Understanding Explosive Sensitivity with Effective Trigger Linkage Kinetics," ACS Physical Chemistry, no. 2, pp. 448-458, 2022
P. Ravi, D. Badgujar, G. Gore, S. Tewari and A. Sikder, "Review on Melt Cast Explosives," *Propellants, Explosives, Pyrotechnics,* vol. 36, no. 5, pp. 393-403, 2011

What causes the differences?



Resonance-stability: Why TNT is more stable than RDX

- RDX has a weak '**Trigger Linkage**', which is the bond that first breaks to set off the explosive reaction

S. Venugopalan, Demystifying Explosives, Elsevier, 2015
M. Cawkwell et al., "Understanding Explosive Sensitivity with Effective Trigger Linkage Kinetics," ACS Physical Chemistry, no. 2, pp. 448-458, 2022

Sensitivity – the future of OME

- IMX-104 is comparable to Comp B, but why bother replacing Comp B?

It's all about sensitivity! Worse performance is worth an improvement in safety.

Property	Comp B	IMX - 104
Melting point	80° C	89° C
Temperature of detonation	3939 K	3428 K
H_{50}	33.9 cm	114.4 cm
VOD	8172 m/s	7811 m/s
Critical diameter	1.9 – 6.7mm	22 - 30mm

D. Frem, "A Review on IMX-101and IMX-104 Melt-Cast Explosives: Insensitive Formulations for the Next-Generation Munition Systems", *Propellants, Explosives, Pyrotechnics*, 2023

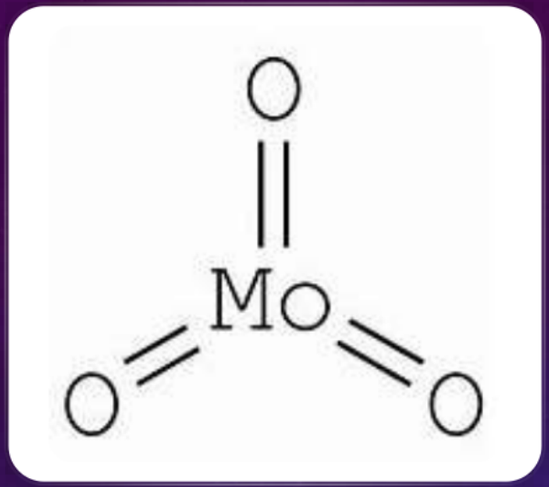


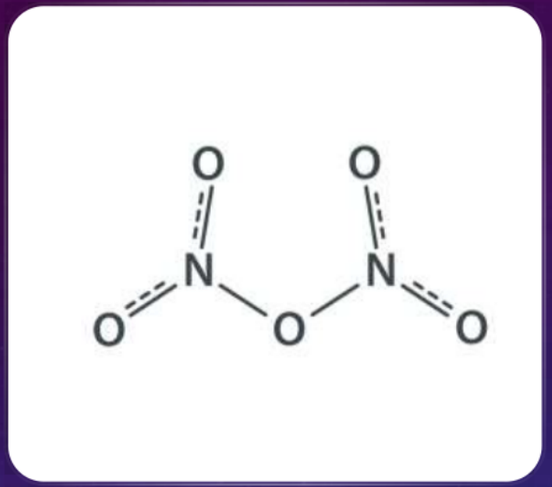
Thermodynamics: What makes a good explosive?

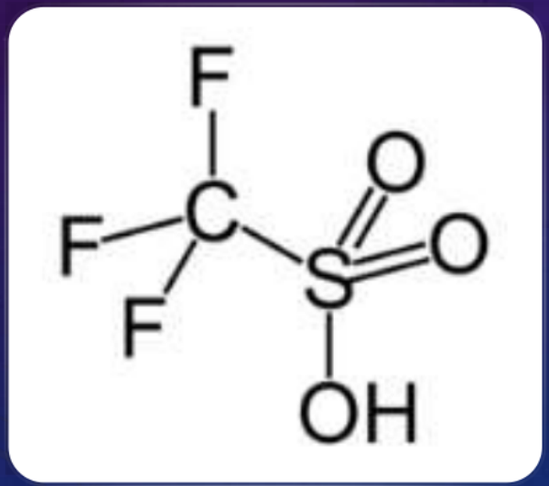
- Thermodynamics of explosives is simple, but gets very complicated

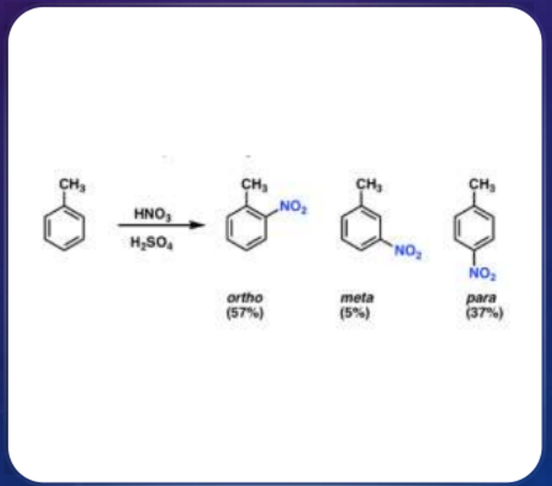
- Detonation properties are only one aspect of what makes a good explosive

SECTION: II
EXPLOSIVE SYNTHESIS





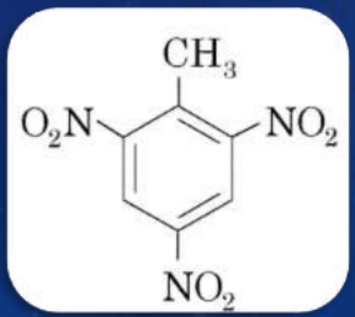




TNT

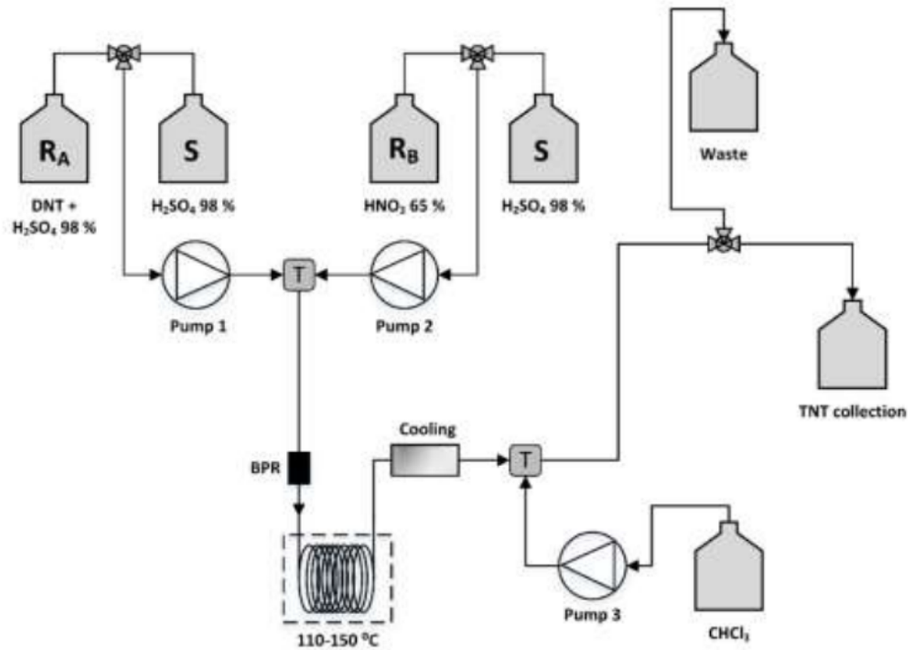
(2,4,6-Trinitrotoluene)

- Synthesised in 1860s
- Nitration of toluene via electrophilic aromatic substitution
- Traditionally synthesised by treating 2,4 and 2,6 DNT with 100% HNO3 and oleum
- Other methods of synthesis have been used e.g. N205 with H2SO4, NaNO3/ MoO3 and HNO3 with trifluoromethanesulfonic acid.
- Different synthetic methods used to try and improve safety, which flow synthesis and the following study shows



FLOW

Flow synthesis in a nutshell



D. Kyprianou and e. al, "Synthesis of 2,4,6-Trinitrotoluene (TNT) Using Flow Chemistry," Molecules, vol. 25, pp. 1-15, 2020.

STUDY



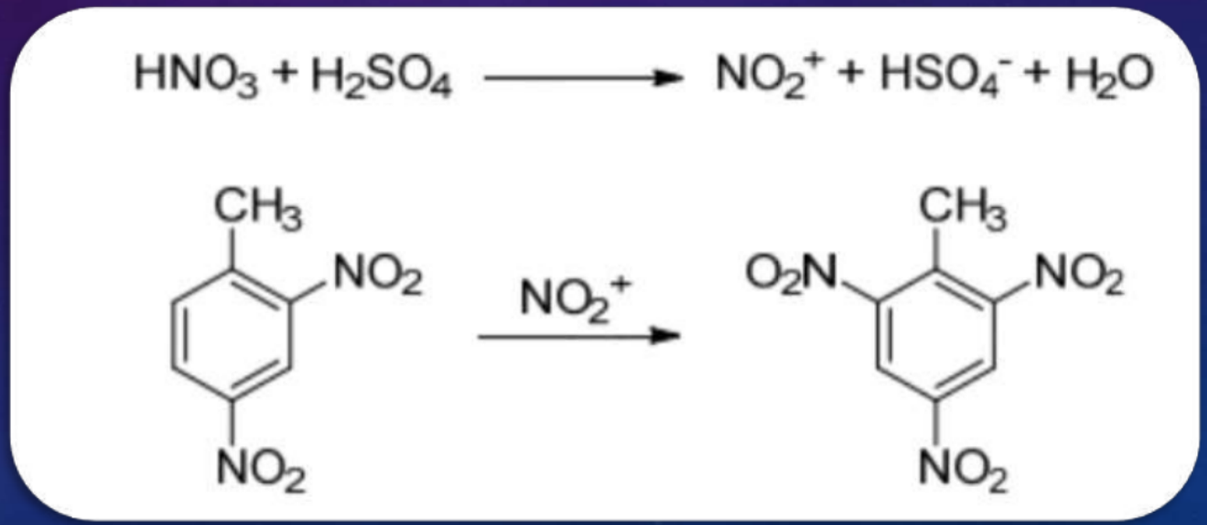
2,4-DNT to TNT with 98% H2SO4 and 65% HNO3, but in a flow synthesis set up.



Why focus on the third step?



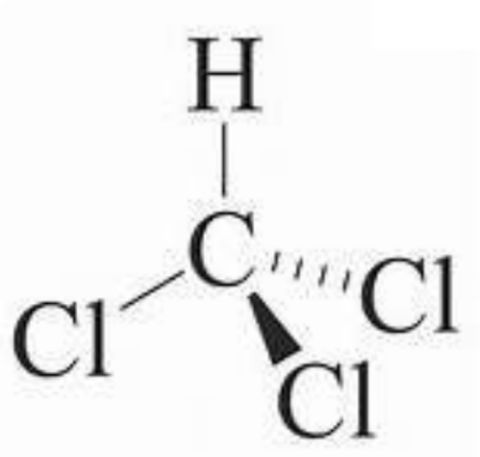
One variable at a time approach.

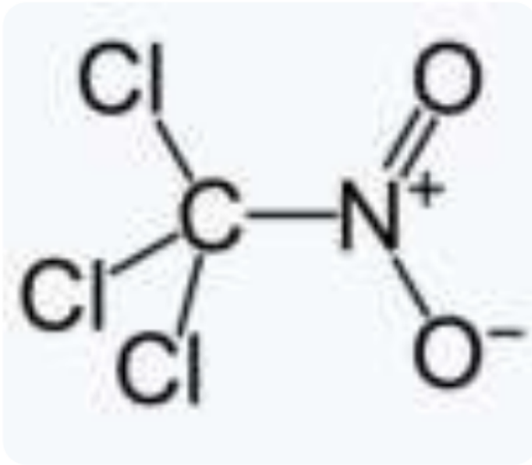


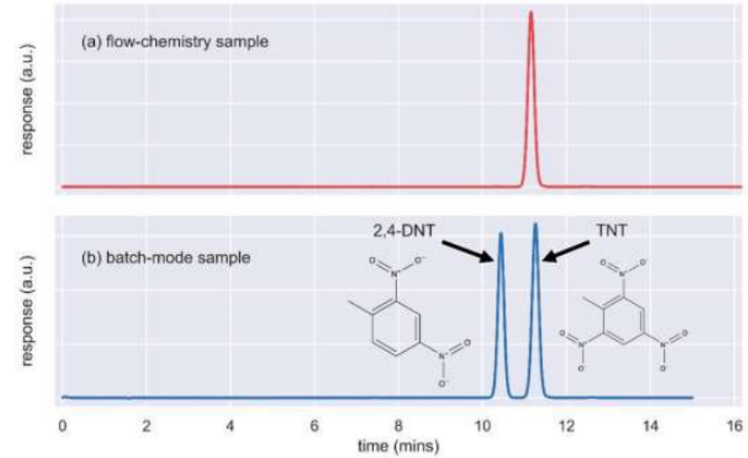
D. Kyprianou and e. al, "Synthesis of 2,4,6-Trinitrotoluene (TNT) Using Flow Chemistry," Molecules, vol. 25, pp. 1-15, 2020.

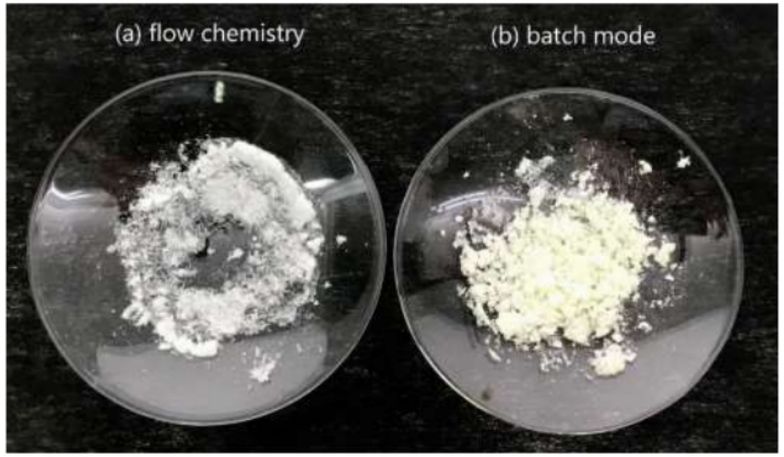
ISSUES FACED IN FLOW

- TNT forms as a solid under the reaction conditions.
- Chloroform added.
- Using chloroform had advantages.









- The main factors investigated for the study were the:
    a) Effect of the HNO3: DNT ratio
    b) Effect of residence time
    c) Effect of temperature

- With optimum conditions they were able to repeatedly achieve conversion rates in excess of 99% via analysis using High Pressure Liquid Chromatography – Diode Array Detection.

- They also compared their flow synthesis with batch synthesis.

- Flow chemistry does however benefit from the following factors:
    a) Shorter reaction times
    b) Safety at higher temps, ability to use less hazardous reagents
    c) Highly reproducible

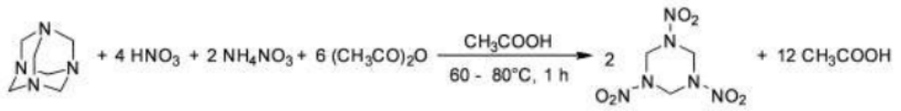
D. Kyprianou and e. al, "Synthesis of 2,4,6-Trinitrotoluene (TNT) Using Flow Chemistry," Molecules, vol. 25, pp. 1-15, 2020.

RDX

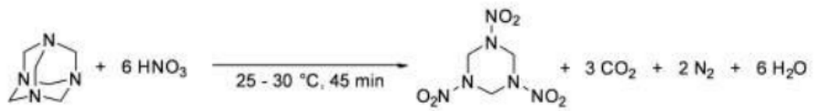
(1,3,5-TRINITROPERHYDRO-1,3,5-TRIAZINE)

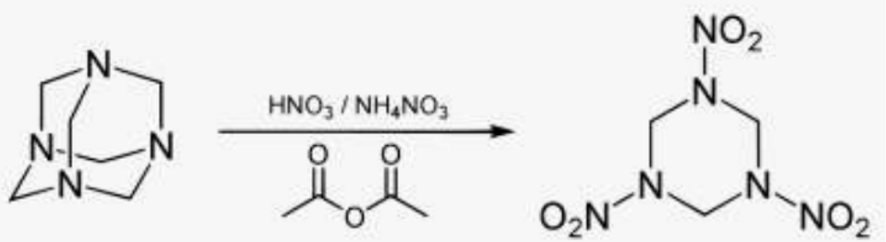
- First used as an explosive in the 1930s, but first synthesised in 1899 by the reaction of hexamine with nitric acid.
- Industrial processes shown.

Bachmann process for RDX synthesis:



Woolwich process for RDX synthesis:

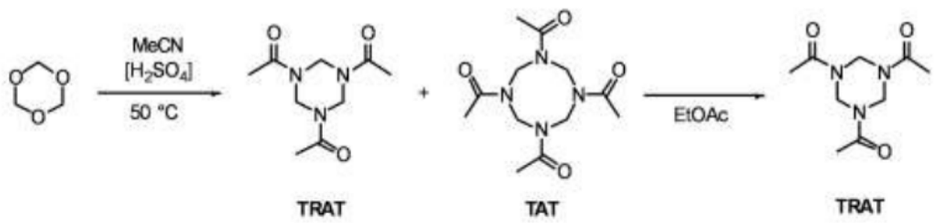




T. Klapotke, "Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT)," *Propellants, Explosives, Pyrotechnics,* p. e202300062, 2023.

ALTERNATIVE SYNTHESIS

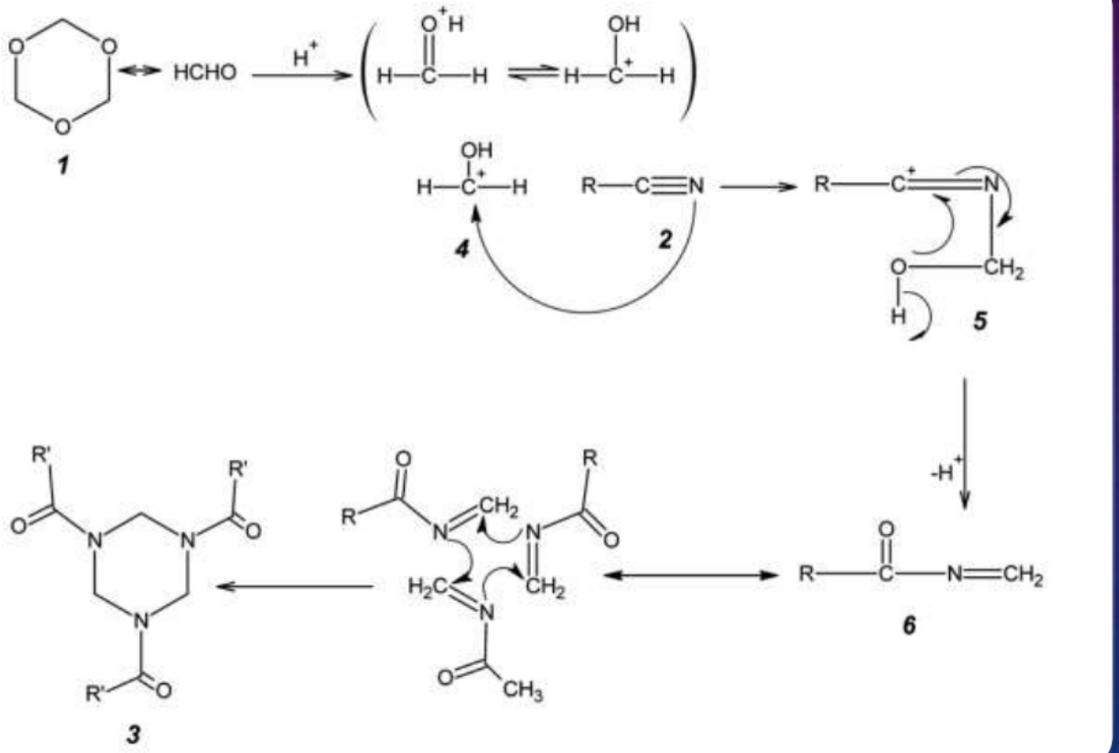
Thomas Klapotke in his Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT)



- TAT is a precursor for another explosive HMX. RDX and HMX are usually very difficult to separate, but TRAT and TAT are very easily separatable.
- This is useful for industrial application as starting with these precursors will lead to greater selectivity for large scale production, and therefore less waste.
- It is also important to note that starting materials for synthesis in this way are cheap, which is vital for industrial application.

T. Klapotke, “Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT),” *Propellants, Explosives, Pyrotechnics,* p. e202300062, 2023.

TRAT SYNTHESIS



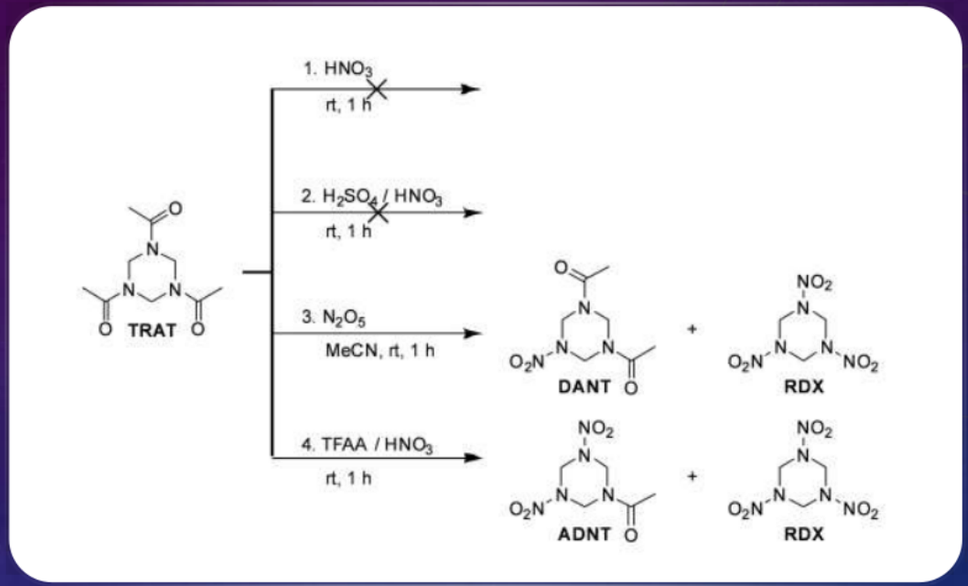
J. Yang, "Triacylperhydro-1,3,5-triazines over Phenylsulfonic Acid Functionalized Mesoporous Silica," *Synthetic Communications,* vol. 41, no. 23, pp. 3455-3461, 2011.

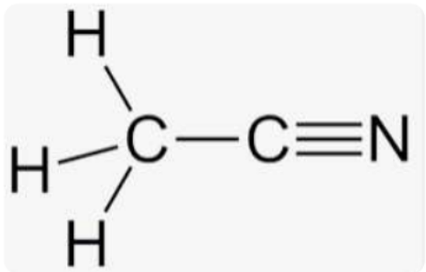
T. Klapotke, "Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT)," *Propellants, Explosives, Pyrotechnics,* p. e202300062, 2023.

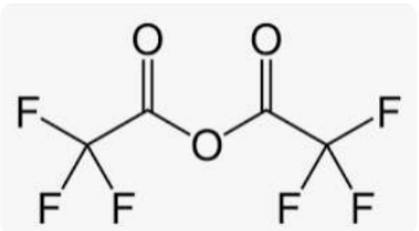
RDX FROM TRAT

•They tried 4 different routes for RDX synthesis from TRAT, which were:

- Nitration with HNO3.
- Nitration with conc H2SO4 and HNO3 (as seen previously with TNT).
- Nitration with N2O5*.
- Nitration with trifluoroacetic anhydride and HNO3*.







T. Klapotke, "Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT)," *Propellants, Explosives, Pyrotechnics,* p. e202300062, 2023.

APPLICABLE?

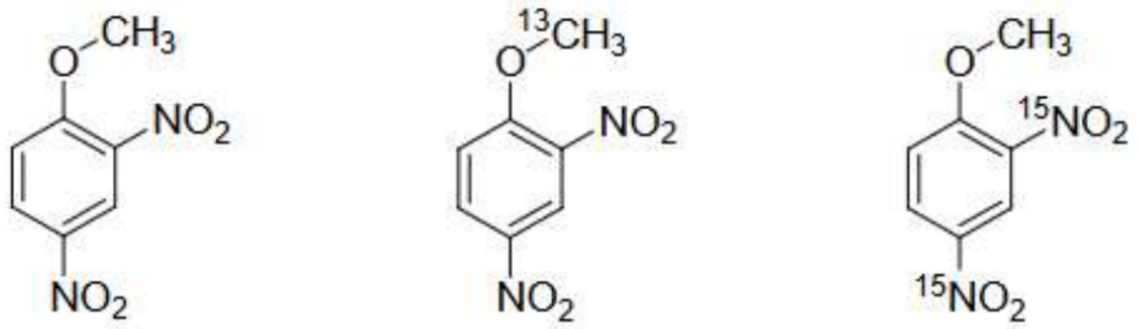
- Reaction scheme 3 yielded 5% RDX, and therefore it was said not to be suitable for industrial synthesis.
- Scheme 4 yielded 29% RDX, so better than scheme 3, but still not good enough for industrial application.
- To summarise, under the conditions that have been used the synthesis of RDX using TRAT is ready for industrial scale up, and further method development is needed.
- Process still highly desirable for better separation of RDX and HMX.

T. Klapotke, "Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT)," *Propellants, Explosives, Pyrotechnics,* p. e202300062, 2023.

DNAN

(2,4-DINITROANISOLE)

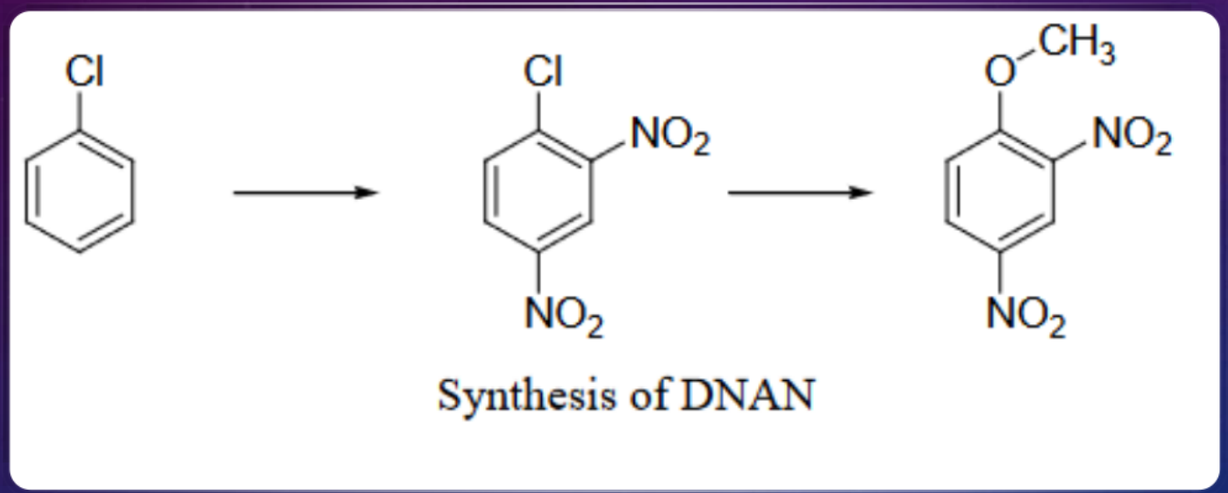
- Next synthesis covered is going to be of DNAN, one of the components of IMX 104, along with other insensitive munitions.
- Joseph Mannion for the Naval and Surface Warfare Center in the U.S. has used an industrial synthesis process, but included isotopic labelling.
- What is an isotope?



DNAN, ^{13}C-Labeled DNAN, and ^{15}N-Labeled DNAN

J. Mannion, "SYNTHESIS OF 13C- AND 15N-LABELED DNAN," United States Navy, Indian Head, 2014.

DNAN SYNTHESIS



Synthesis of DNAN

- DNAN is synthesized in high yield and high purity by first nitrating chlorobenzene to yield 2,4-dinitrochlorobenzene
- Cl is then displaced with methoxide to form DNAN. This was done using methanol and sodium hydroxide.
- 6 theoretical isomers of the dinitrochlorobenzene
- Regioselectivity can be controlled by the temperature of the reaction

J. Mannion, "SYNTHESIS OF 13C- AND 15N-LABELED DNAN," United States Navy, Indian Head, 2014.

^{15}N DNAN, ^{13}C DNAN & ISOTOPIC LABELLING

- Isotopic labelling is an important process for sample analysis
- This is a technique used extensively in complex chemical structures like proteins, but also is important for OME because it allows you to more accurately see how the molecule degrades, and the potentially toxic products that it will form.

$$2\,NaNO_3 + H_2SO_4 \rightleftharpoons 2\,HNO_3 + Na_2SO_4$$

$$C_6H_5Cl_1 + 2\,HNO_3 \rightleftharpoons C_6H_5N_2O_4Cl_1 + 2\,H_2O$$

$$Na_2SO_4 + 2\,H_2O \rightleftharpoons Na_2SO_4{\bullet}2H_2O$$

J. Mannion, "SYNTHESIS OF 13C- AND 15N-LABELED DNAN," United States Navy, Indian Head, 2014.

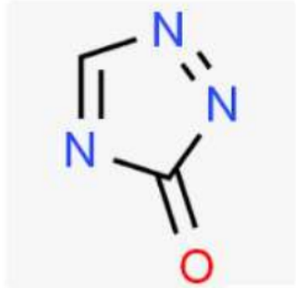
NTO - NITROTRIAZOLONE

(5-NITRO-1,2-DIHYDRO-3*H*-1,2,4-TRIAZIN-3-ONE)

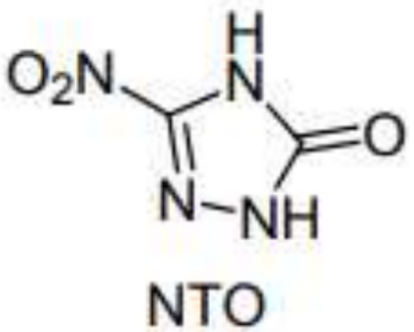
•A comprehensive study into various aspects if NTO has been carried out by Sardar Patel University.

•The most common route for synthesising NTO comes from the nitration of 1,2,4-triazol-5-one (intermediate, TO)

•A key part of this process being suitable for industry, is that if TO can be produced relatively cheaply, and in good yield.



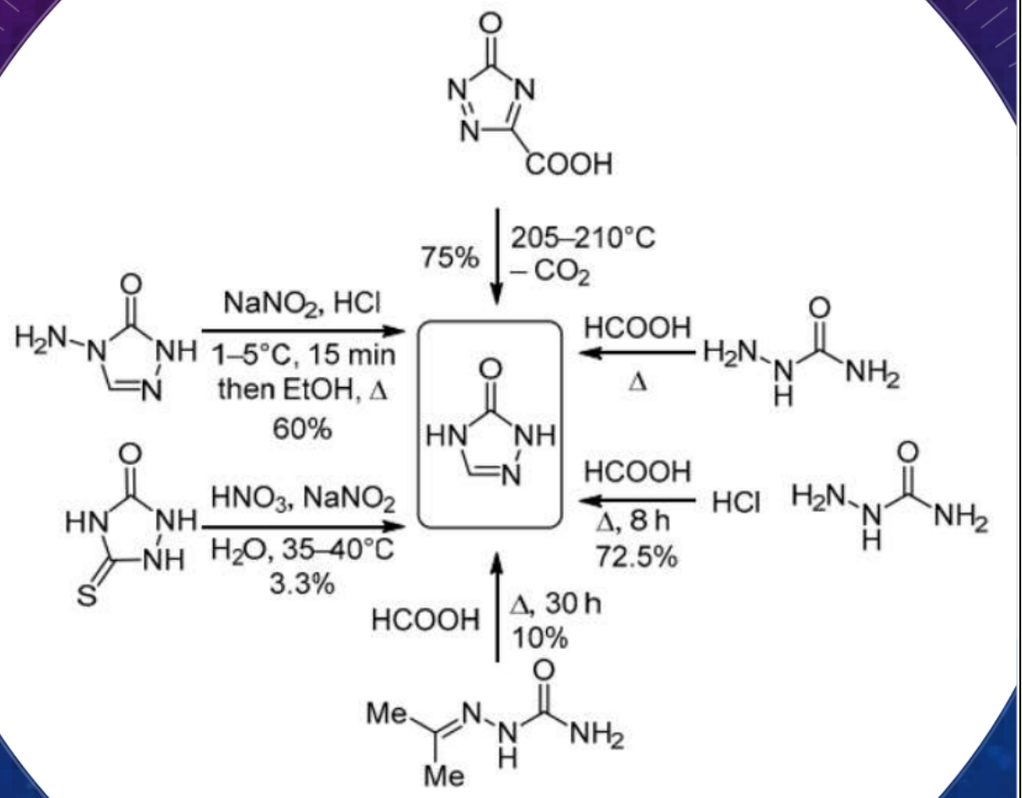
1,2,4-triazol-5-one



NTO

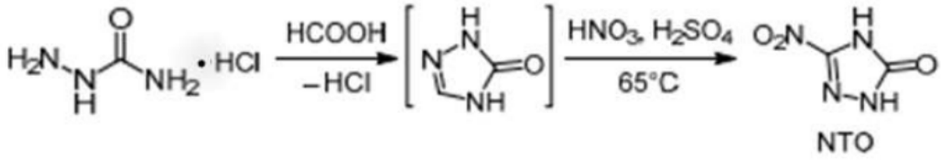
R. Sirach and D. Pragnesh, "3-Nitro-1,2,4-triazol-5-one (NTO): high explosive insensitive energetic material," *Chemistry of Heterocyclic Compounds,* vol. 57, no. 7, pp. 720-730, 2021.

RESEARCH INTO INTERMEDIATE



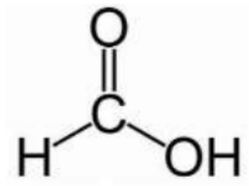
R. Sirach and D. Pragnesh, "3-Nitro-1,2,4-triazol-5-one (NTO): high explosive insensitive energetic material," *Chemistry of Heterocyclic Compounds,* vol. 57, no. 7, pp. 720-730, 2021.

NTO SYNTHESIS



3·HCl, g	HCOOH, ml	Concd HNO_3, ml	Concd H_2SO_4, ml	Time, min	Yield of NTO, %*
33.45	34.5	125	20	90	77.0
33.45	34.5	125	20	135	73.4
33.45	34.5	100	20	100	77.4
33.45	34.5	100	10	150	72.3
133.8	138.0	500	80	480	56.3
33.45	34.5	75	0	90	69.9

- Now that we have the intermediate production, we can focus on NTO synthesis
- Spear et al devised a ‘one pot reaction’.



R. Spear, “A PRELIMINARY ASSESSMENT OF NTO AS AN INSENSITIVE HIGH EXPLOSIVE,” DSTO Materials Research Laboratory, Victoria, 1989.

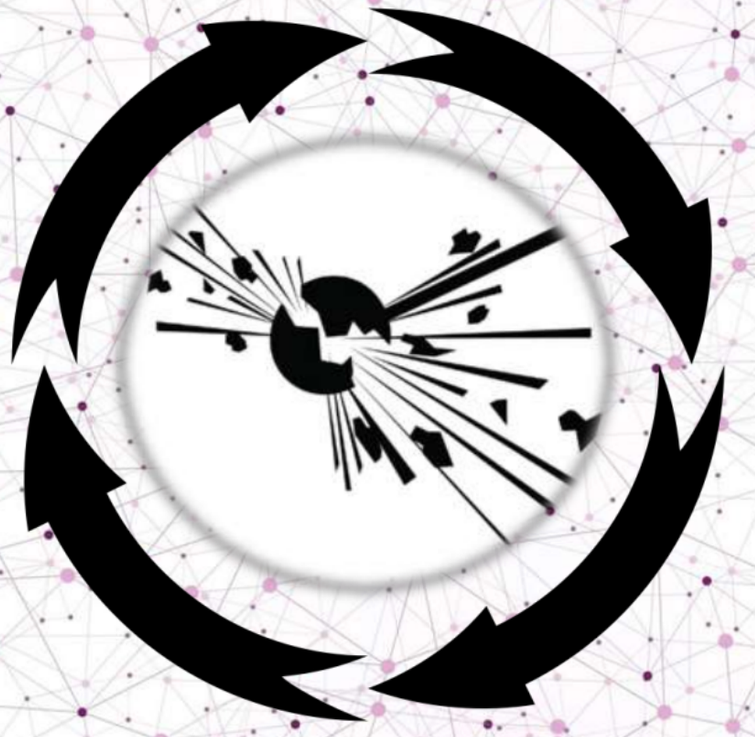
R. Sirach, “3-Nitro-1,2,4-triazol-5-one (NTO): high explosive insensitive energetic material,” *Chemistry of Heterocyclic Compounds,* vol. 57, no. 7, pp. 720-730, 2021.

CLOSING SYNTHESIS THOUGHTS

- Optimisation
- Post synthesis processing

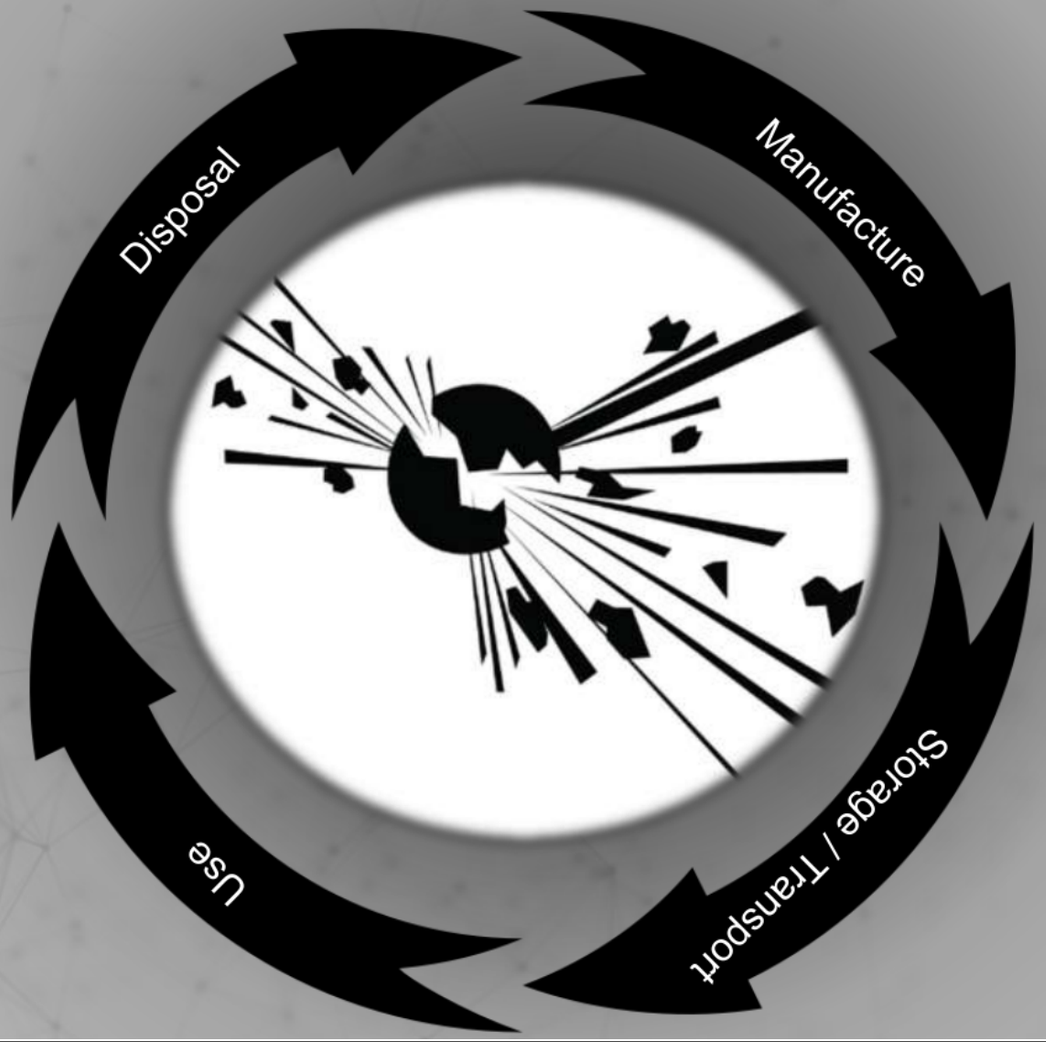


EXPLOSIVE MATERIALS IN OME: THERMODYNAMIC ANALYSIS, REACTION CHEMISTRY, AND LIFECYCLE ASSESSMENT

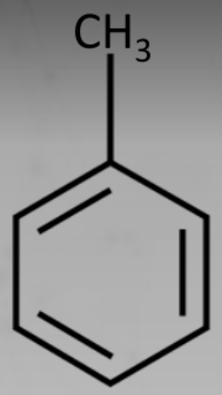


Episode C Lifecycle Assessment by Josh Ede

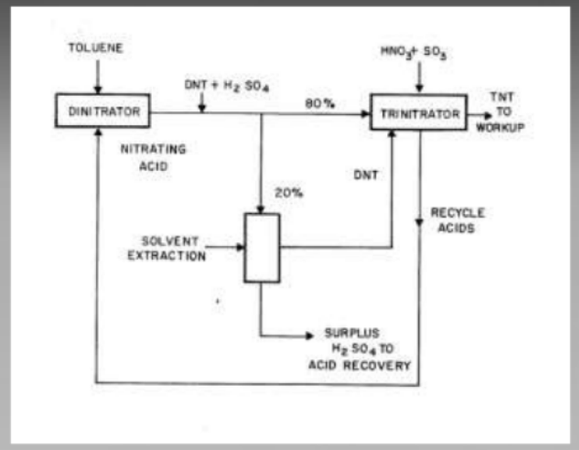
Overview & Importance of the Lifecycle Approach



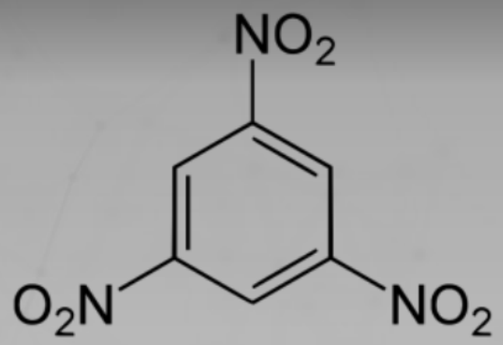
Production of TNT



[1]



[1] M. E. Hill, W. E. Tolberg and G. J. McDonald, "Process for the manufacture of trinitrotoluene". United States of America Patent 3,799.993, 26 03 1974.



[2]



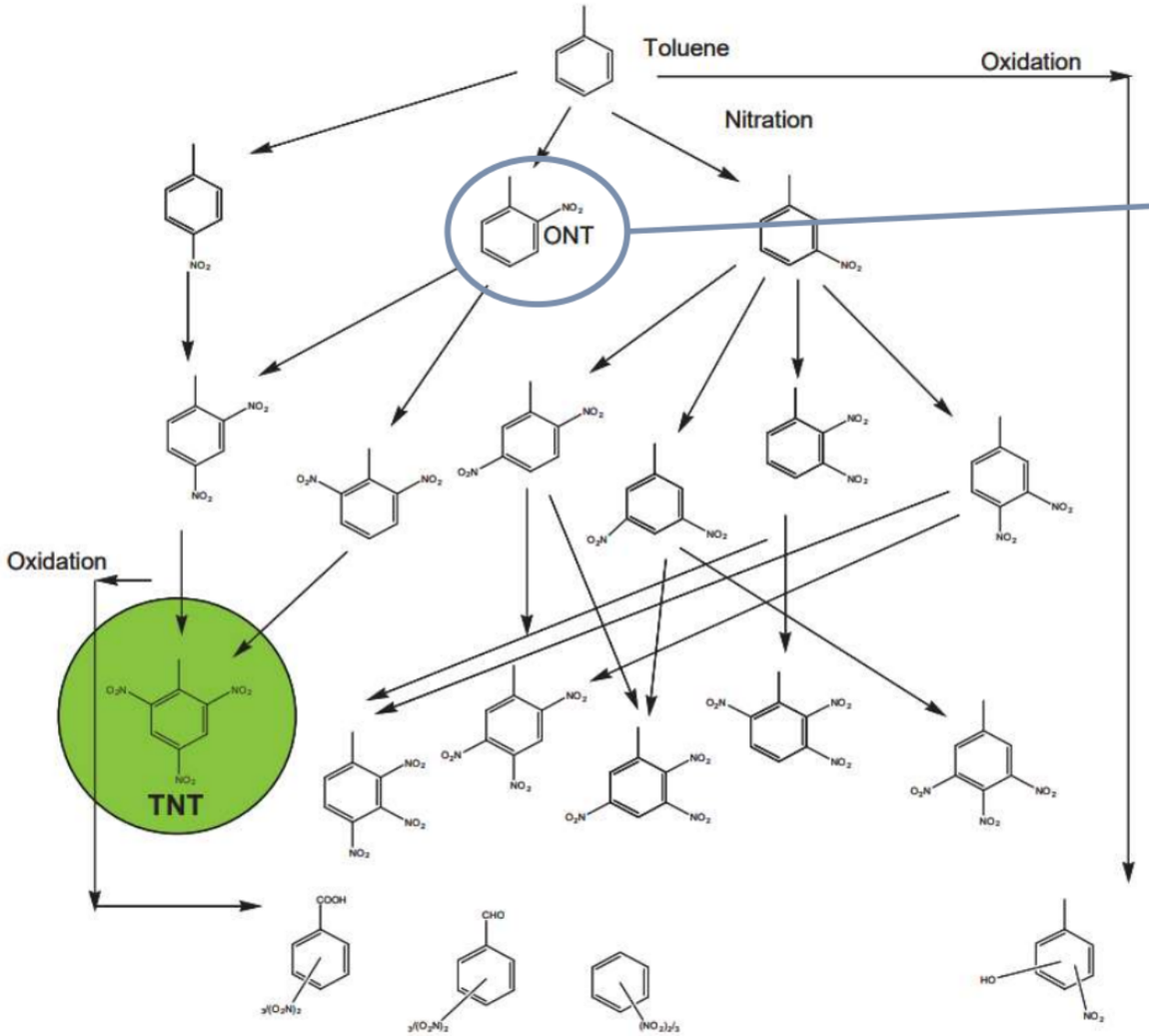
[2] Environmental Protection Agency, "Contaminated Site Clean Up Division," Environmental Protection Agency , 07 09 2018. [Online]. Available: https://clu-in.org/characterization/technologies/exp.cfm. [Accessed 23 11 2023].

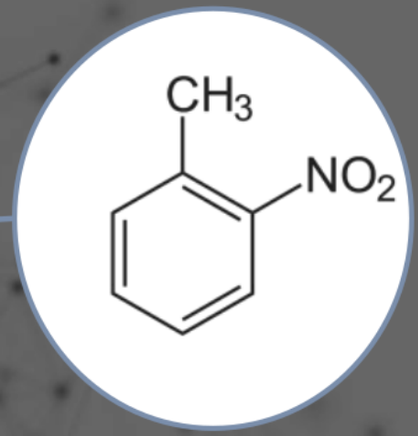
- **TNT is water soluble at a rate of approximately 100 milligrams per litre mgL^{-1} at 25 C° [3]**
- **TNT in water undergoes photolysis**
- **Trinitrobenzene – common and toxic [4]**

[3] K. Dontsova, "Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils," Strategic Environmental Research and Development Program, Alexandria, Virginia, 2018.

[4] U.S. Department of Health and Human Services, "Toxicological profile for 2,4,6 trinitrotoluene," Public Health Service, Atlanta, Georgia, 1995

Production of TNT continued



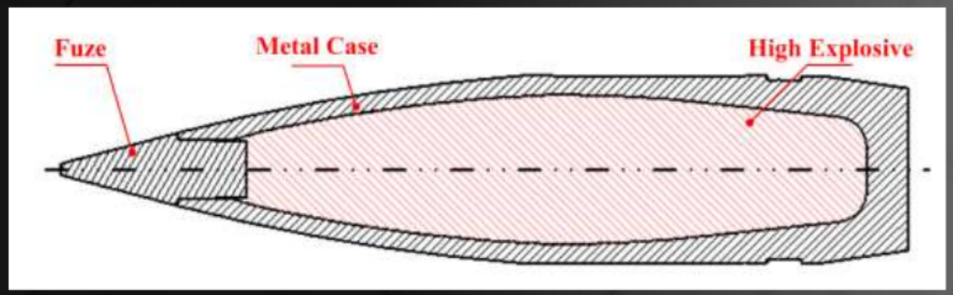


- Ortho-nitrotoluene



[1] Radford Army Ammunition Plant Pollution Prevention Team , "Secretary of Defense Environmental Awards," Radford Army Ammunition Plant Pollution Prevention Team , Virginia, Maryland, 2006.

Warhead filling and issues

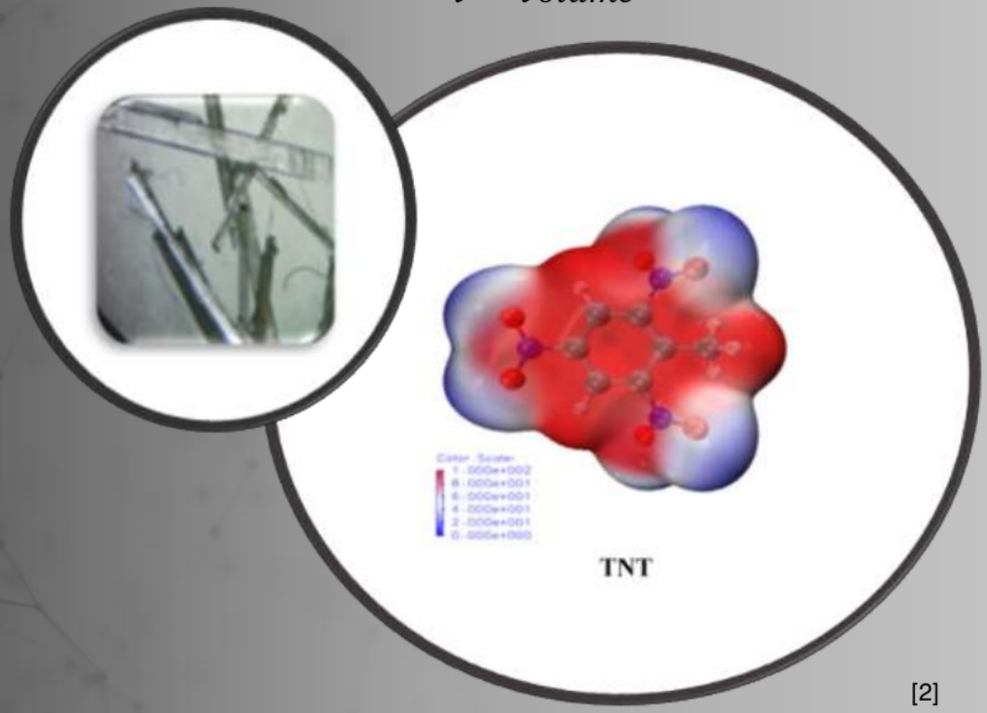


[1]

[1] M. Khalil, H. Abdalla and O. Kamal, "Dispersion Analysis for Spinning Artillery Projectile," in *13th International Conference on Aerospace Sciences and Aviation Technology, ASAT 13*, Cairo, Egypt, 2009.

$$\rho = \frac{m}{v}$$

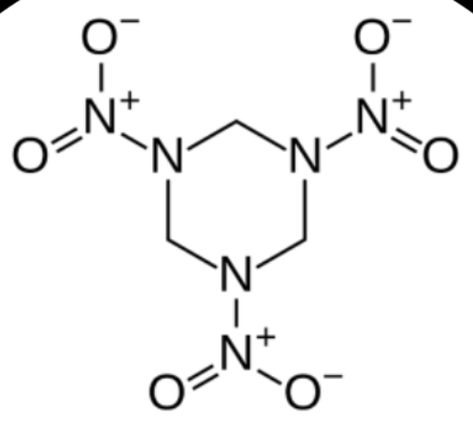
$\rho =$ density
$m = mass$
$v = volume$



[2]

- **Red shaded area shows the optimum filling of a 120mm shell**
- **Crystal structure of TNT, can be by heating to 80C°**
- **UXO**

[2] N. Şen, N. Aslan, B. Yüksel and I. Teciman, "Characterization and properties of a new insensitive explosive co-crystal composed of trinitrotoluene and pyrene," *Structural Chemistry*, 2023



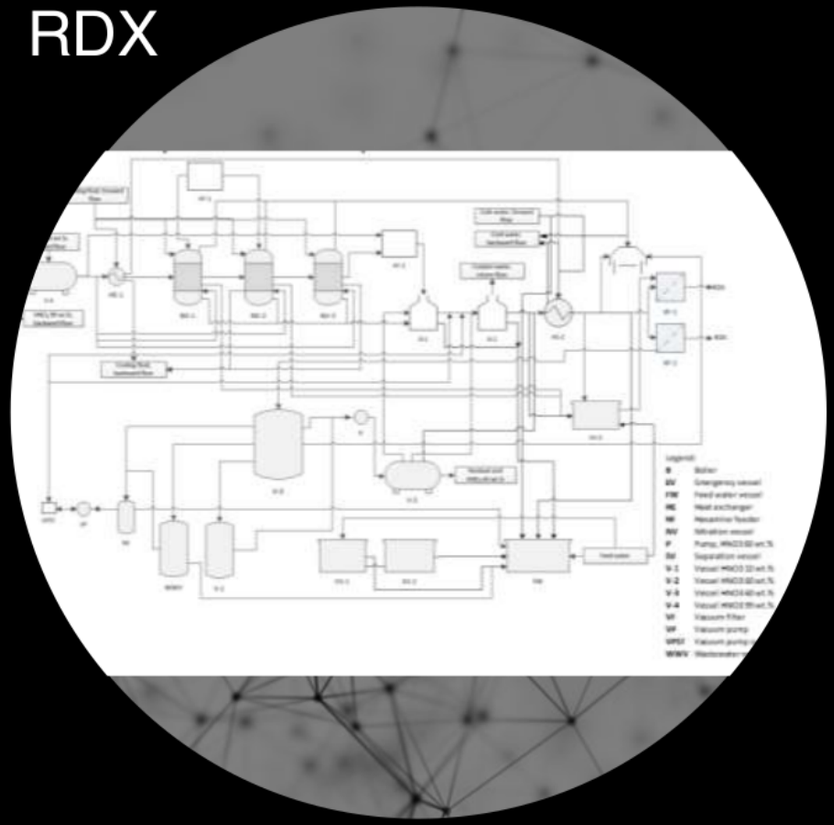
RDX

Research Demolition Explosive

Royal Demolition Explosive

Cyclotrimethylene trinitramine

Manufacturing process of RDX



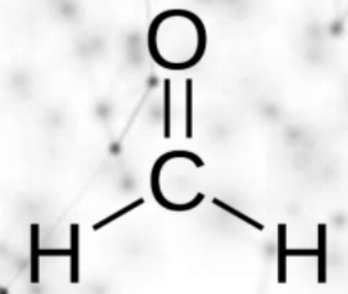
D. Costa, E. Galante, I. Andrade and J. Cunha, "Environmental life-cycle assessment of a military explosive production unit: a preliminary approach," *University of Porto Journal of Engineering,* vol. 1, pp. 2-10, 2015.

96%

$(CH_2)6N_4 + 4HNO_3 \longrightarrow C_3H_6N_6O_6 + 3HCOH + NH_4NO_3$

4%

$(CH2)6N4 + 6HNO_3 \longrightarrow C_3H_6N_6O_6 + 6H_2O + 3CO_2 + 2N_2$



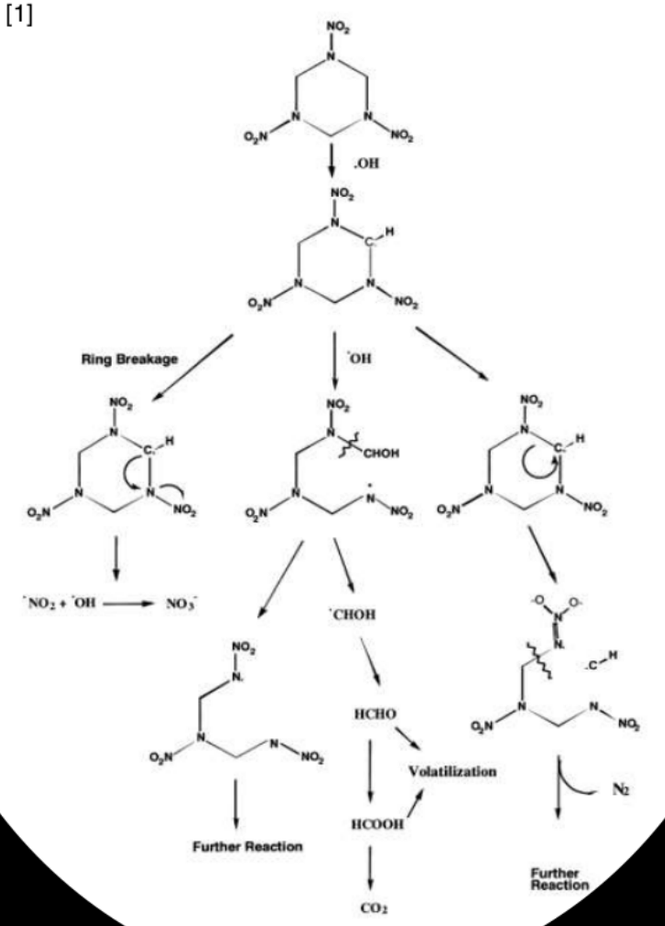
- **Formaldehyde, highly toxic substance!**

- **RDX is more toxic than TNT attacking the central nervous system!** [2]
- **It lasts in soils longer, due to its lower solubility in water around 59.9 mgL^{-1} at 25 C^o** [3]
- **Traditional methods for disposal are incineration and composting** [2]

Fenton's Reagent

$$H_2O_2 + Fe^{2+} \longrightarrow Fe^{3+} + OH^- + OH$$

[1]



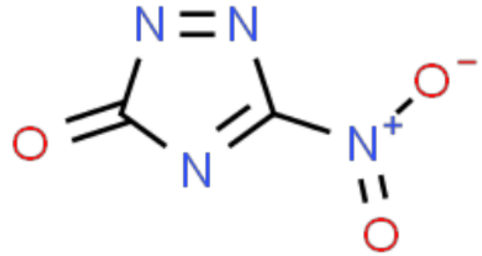
[1] K.-D. Zoha and M. K. Stenstrom, "Fenton oxidation of hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) and octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)," *Water Research,* vol. 36, pp. 1331-1341, 2002.

[2] U.S. Department of Health and Human Services , "Toxicological profile for RDX," Public Health Service, Atlanta, Georgia, 2012.

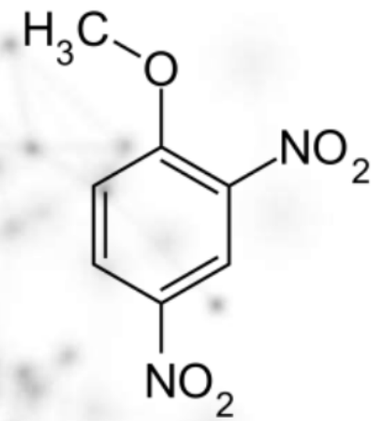
[3] K. Dontsova, S. Taylor, R. Pesce-Rodriguez, M. Brusseau, J. Arthur, N. Mark, M. Walsh, J. Lever and J. Šimůnek, "Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils," US Army Corps of Engineers, Alexandria, Virginia, 2014.

IMX104 AN INTRO

NTO & DNAN



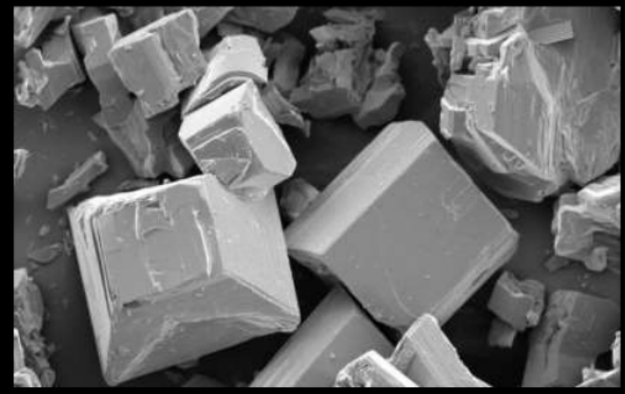
- NTO or 3-nitro-1,2,4 -triazol-5-one



- DNAN or 2,4 dinitroanisole

- **Industrial process is fairly close to the synthesis in terms of complexity.**
- **Same issues as TNT and RDX but also…**
- **NTO solubility in water is 16642.0 mgL^{-1} significantly higher than any of the explosives looked at so far!** [3]
- **Treatment routes using UV/H_2O_2 to oxidise NTO**

NTO



[1] NTO Class 1 Crystals

[2]

$$C_2H_2N_4O_3 + 8OH^{\bullet} \longrightarrow 2CO_2 + 2HNO_3 + 2NH_3 + H_2O$$

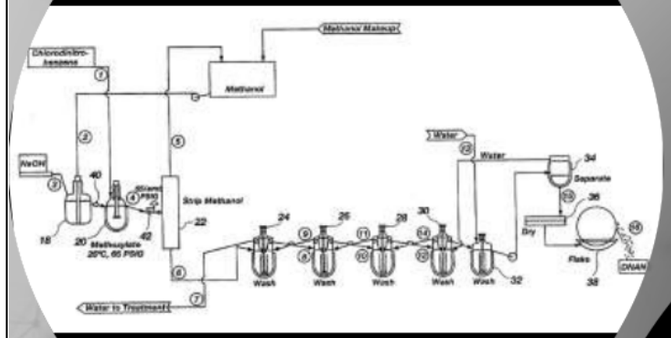
$$H_2O_2 \xrightarrow{UV} 2OH^{\bullet}$$

[1] D. Price, J. Morris and A. Carrill, *Development and Production of a New Class of NTO,* Holston, Texas: BAE systems, 2013.

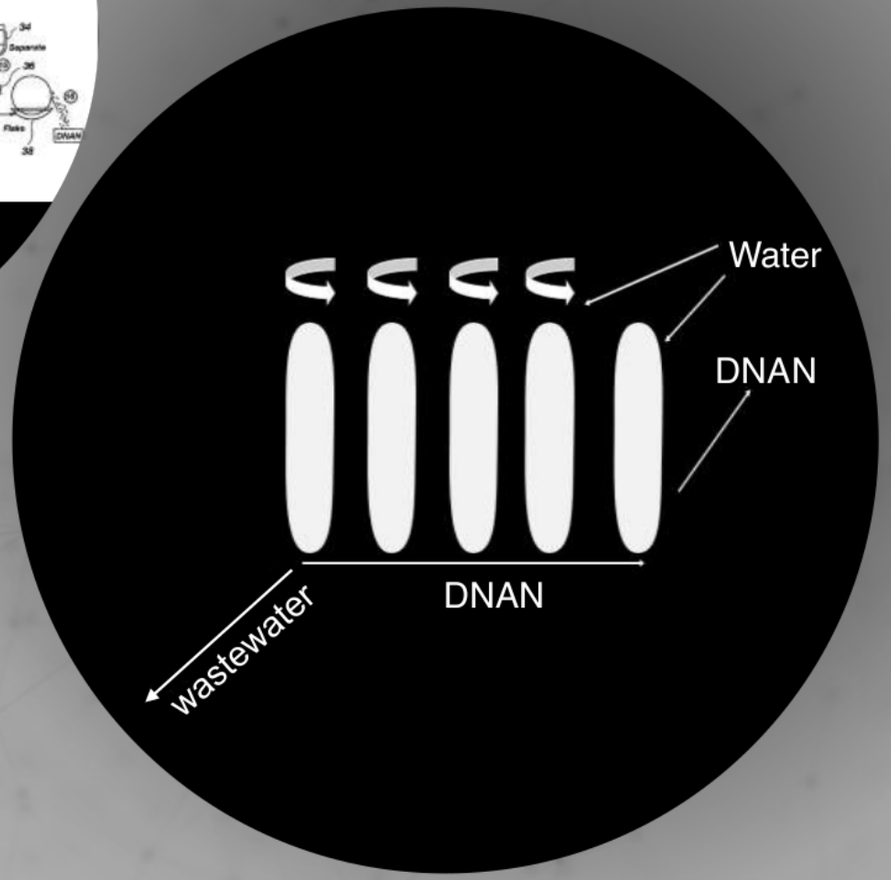
[2] A. Terraccianoa, C. Christodoulatos, A. Koutsospyros, Z. Zheng, T.-L. Su, B. Smolinski, P. Arienti and X. Meng, "Degradation of 3-nitro-1,2,4-trizole-5-one (NTO) in wastewater with UV/ H2O2 oxidation.," *Chemical Engineering Journal,* vol. 354, pp. 481-491, 2018.

[3] K. Dontsova, S. Taylor, R. Pesce-Rodriguez, M. Brusseau, J. Arthur, N. Mark, M. Walsh, J. Lever and J. Šimůnek, "Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils," US Army Corps of Engineers, Alexandria, Virginia, 2014.

DNAN Production



[1]



- More soluble than TNT at 276.2mgL^{-1} at 25 C^{o} [2]
- More toxic than TNT when ingested and can be broken down to dinitrophenol (DNP)



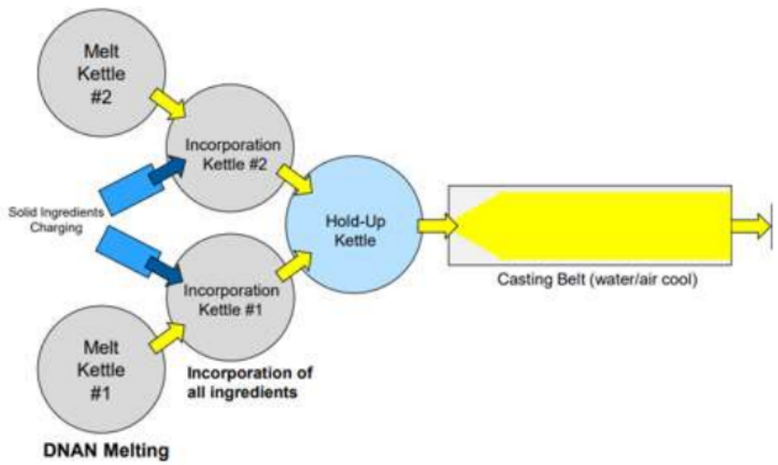
[3]

[1] T. K. Highsmith and H. E. Johnston, "Continuous process for preparing alkoxynitroarenes". United States of America Patent 10/338,767, 8 07 2004

[2] K. Dontsova, S. Taylor, R. Pesce-Rodriguez, M. Brusseau, J. Arthur, N. Mark, M. Walsh, J. Lever and J. Šimůnek, "Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils," US Army Corps of Engineers, Alexandria, Virginia, 2014.

3] W. Fawcett-Hirst, T. J. Temple, M. K. Ladyman and F. Coulon, "A review of treatment methods for insensitive high explosive contaminated wastewater," *Heliyon,* vol. 7, pp. 1-13, 2021.

IMX104 manufacture



- **The ingredients for IMX104 are DNAN, NTO and RDX.**
- **The DNAN is heated in the melt kettles and the NTO and RDX are added, dissolving into the mixture.**
- **The final product is cooled using a mixture of air and water.**
- **This can be used to fill the 120mm shell**

V. Fung, "A Modernized IM Melt Pour Explosive Manufacturing Facility at Holston Army Ammunition Plant," in *Insensitive Munitions & Energetic Material Technology Symposium 2015*, Rome, Italy, 2015.

Issues with IMX104

[1]

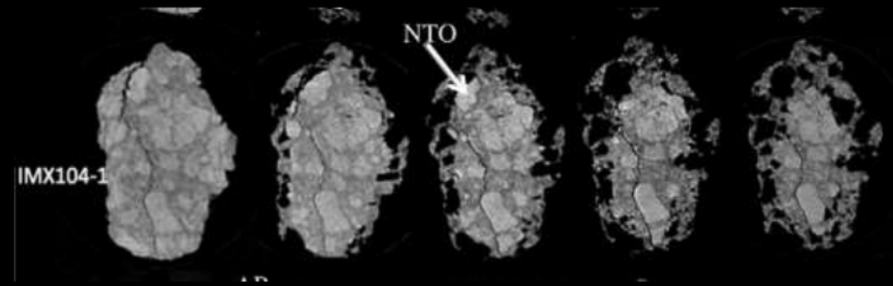
Situation	Explosive fill Detonations	Plume area (m2)	Explosive material	Estimated total mass (mg)	% or original material mass
Live Firing	Comp B	230	RDX + HMX	8.5	0.00014%
	IMX-104	350	RDX + HMX	16	0.001%
			DNAN	27	0.001%
			NTO	1,900	0.4%
In situ	Comp-B	820	RDX +HMX	150	0.0014%
	IMX-104	590	RDX + HMX	11,000	1.6%
			DNAN	29,000	11%
			NTO	193,000	45%

[2]



- DNAN is more prone to photolysis than TNT
- DNP!

[3]

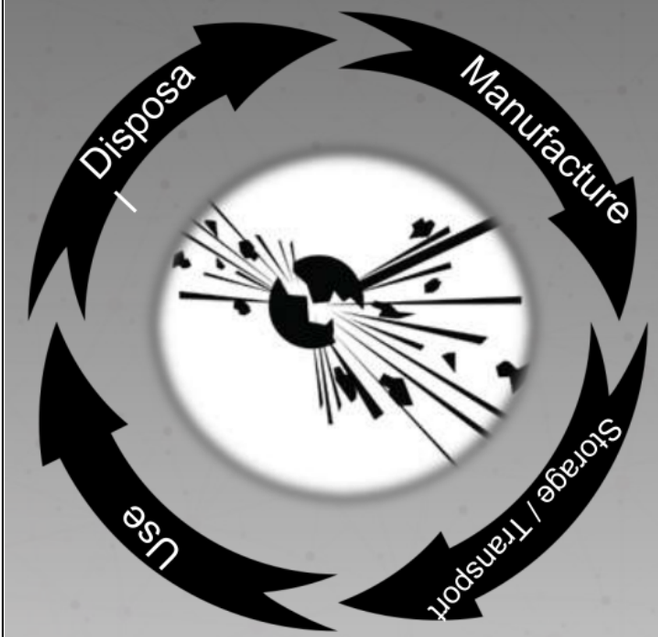


[1] M. R. Walsh, M. E. Walsh, C. A. Ramsey, S. Thiboutot, G. Ampleman, E. Diaz and J. E. Zufelt, "Energetic Residues from the Detonation of IMX-104 Insensitive Munitions," *Propellants, Explosives and Pyrotechnics,* vol. 39, pp. 243-250, 2014.

[2] K. Dontsova, "Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils," Strategic Environmental Research and Development Program, Alexandria, Virginia, 2018.

[3] S. Taylor, E. Park, K. Bullion and K. Dontsova, "Dissolution of three insensitive munitions formulations," *Chemosphere,* vol. 119, pp. 342-348, 2015.

EXPLOSIVE MATERIALS IN OME: THERMODYNAMIC ANALYSIS, REACTION CHEMISTRY, AND LIFECYCLE ASSESSMENT

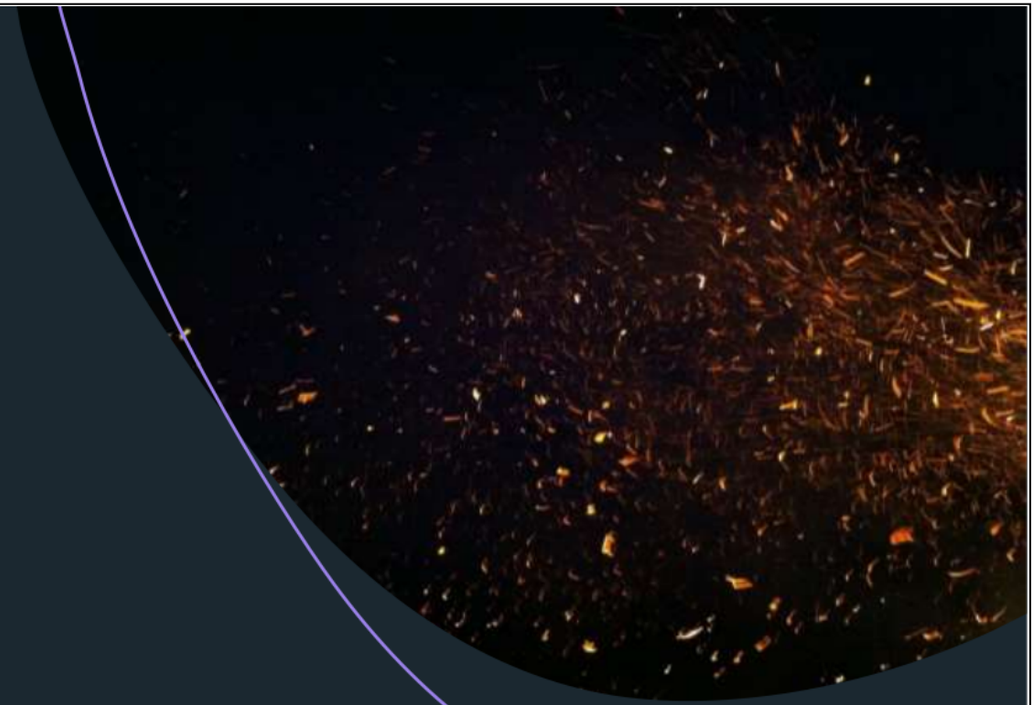


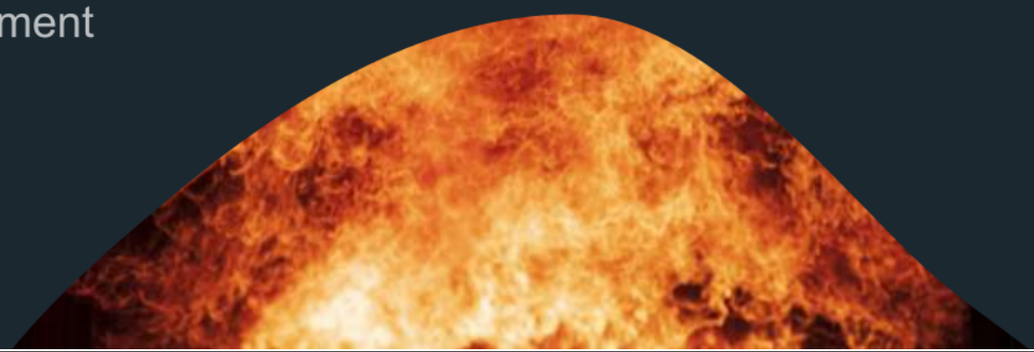
- Explosives are toxic substances DO NOT EAT.
- Manufacturing and processing methods have had to change due to waste contamination: photolysis, dissolution, degradation
- Moving forward there is an opportunity to develop better ways to manufacture and produce munitions.
- Careful that in the pursuit of safety at one end we do not end up creating more problems!

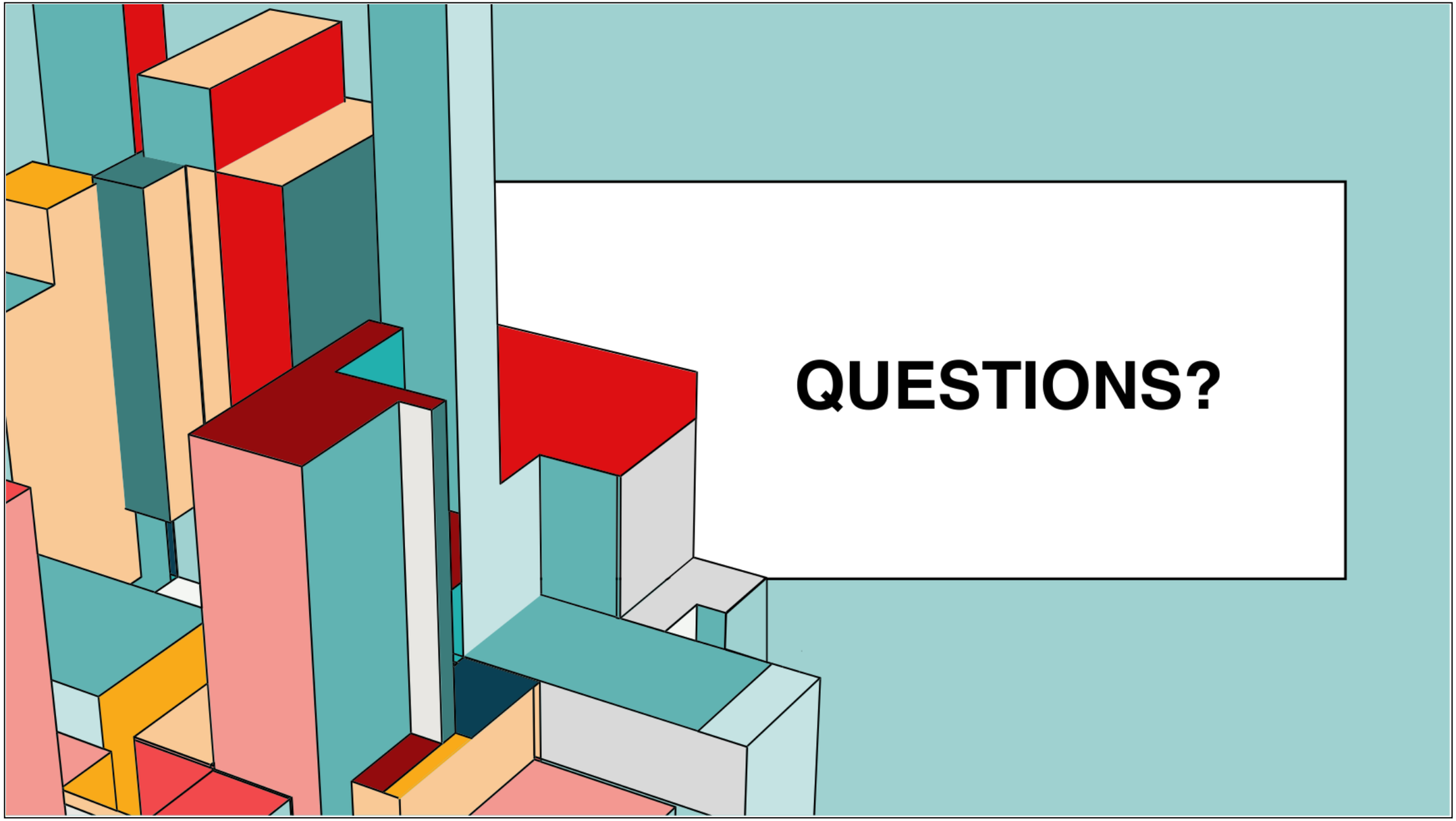
What have we learnt?

Explosive materials cannot simply be defined in a vacuum, rather must be analyzed with respect to all elements of performance, including:

- Detonation properties
- Chemical synthesis
- Lifecycle assessment






QUESTIONS?

References: Thermodynamics

1. J. Agrawal, High Energy Materials: Propellants, Explosives and Pyrotechnics, Wiley, 2010
2. S. Venugopalan, Demystifying Explosives, Elsevier, 2015
3. D. Kumar & A. Elias, “The Explosive Chemistry of Nitrogen”, Resonance, 24, 2019
4. M. Cawkwell et al., “Understanding Explosive Sensitivity with Effective Trigger Linkage Kinetics,” ACS Physical Chemistry, no. 2, pp. 448-458, 2022
5. P. Ravi, D. Badgujar, G. Gore, S. Tewari and A. Sikder, “Review on Melt Cast Explosives,” Propellants, Explosives, Pyrotechnics, vol. 36, no. 5, pp. 393-403, 2011
6. D. Frem, “A Review on IMX-101and IMX-104 Melt-Cast Explosives: Insensitive Formulations for the Next-Generation Munition Systems”, Propellants, Explosives, Pyrotechnics, 2023





References: Synthesis

1. D. Kyprianou and e. al, “Synthesis of 2,4,6-Trinitrotoluene (TNT) Using Flow Chemistry,” Molecules, vol. 25, pp. 1-15, 2020.
2. T. Klapotke, “Investigation of a new promising process for the RDX synthesis via 1,3,5-triacetyl-1,3,5-triazinane (TRAT),” Propellants, Explosives, Pyrotechnics, p. e202300062, 2023.
3. J. Yang, “Triacylperhydro-1,3,5-triazines over Phenylsulfonic Acid Functionalized Mesoporous Silica,” Synthetic Communications, vol. 41, no. 23, pp. 3455-3461, 2011.
4. J. Mannion, “SYNTHESIS OF 13C- AND 15N-LABELED DNAN,” United States Navy, Indian Head, 2014.
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6. R. Spear, “A PRELIMINARY ASSESSMENT OF NTO AS AN INSENSITIVE HIGH EXPLOSIVE,” DSTO Materials Research Laboratory, Victoria, 1989

REFERENCES: LIFECYCLE

1. M. E. Hill, W. E. Tolberg and G. J. McDonald, “Process for the manufacture of trinitrotoluene”. United States of America Patent 3,799.993, 26 03 1974.
2. Environmental Protection Agency, “Contaminated Site Clean Up Division,” Environmental Protection Agency , 07 09 2018. [Online]. Available: https://clu-in.org/characterization/technologies/exp.cfm. [Accessed 23 11 2023].
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6. M. Khalil, H. Abdalla and O. Kamal, “Dispersion Analysis for Spinning Artillery Projectile,” in 13th International Conference on Aerospace Sciences and Aviation Technology, ASAT 13, Cairo, Egypt, 2009.
7. N. Şen, N. Aslan, B. Yüksel and I. Teciman, “Characterization and properties of a new insensitive explosive co-crystal composed of trinitrotoluene and pyrene,” Structural Chemistry, 2023
8. D. Costa, E. Galante, I. Andrade and J. Cunha, “Environmental life-cycle assessment of a military explosive production unit: a preliminary approach,” University of Porto Journal of Engineering, vol. 1, pp. 2-10, 2015.
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10. U.S. Department of Health and Human Services , “Toxicological profile for RDX,” Public Health Service, Atlanta, Georgia, 2012.
11. K. Dontsova, S. Taylor, R. Pesce-Rodriguez, M. Brusseau, J. Arthur, N. Mark, M. Walsh, J. Lever and J. Šimůnek, “Dissolution of NTO, DNAN, and Insensitive Munitions Formulations and Their Fates in Soils,” US Army Corps of Engineers, Alexandria, Virginia, 2014.
12. D. Price, J. Morris and A. Carrill, Development and Production of a New Class of NTO, Holston, Texas: BAE systems, 2013.
13. A. Terraccianoa, C. Christodoulatos, A. Koutsospyros, Z. Zheng, T.-L. Su, B. Smolinski, P. Arienti and X. Meng, “Degradation of 3-nitro-1,2,4-trizole-5-one (NTO) in wastewater with UV/ H2O2 oxidation.,” Chemical Engineering Journal, vol. 354, pp. 481-491, 2018.
14. T. K. Highsmith and H. E. Johnston, “Continuous process for preparing alkoxynitroarenes”. United States of America Patent 10/338,767, 8 07 2004
15. W. Fawcett-Hirst, T. J. Temple, M. K. Ladyman and F. Coulon, “A review of treatment methods for insensitive high explosive contaminated wastewater,” Heliyon, vol. 7, pp. 1-13, 2021.
16. V. Fung, “A Modernized IM Melt Pour Explosive Manufacturing Facility at Holston Army Ammunition Plant,” in Insensitive Munitions & Energetic Material Technology Symposium 2015, Rome, Italy, 2015.
17. M. R. Walsh, M. E. Walsh, C. A. Ramsey, S. Thiboutot, G. Ampleman, E. Diaz and J. E. Zufelt, “Energetic Residues from the Detonation of IMX-104 Insensitive Munitions,” Propellants, Explosives and Pyrotechnics, vol. 39, pp. 243-250, 2014
18. S. Taylor, E. Park, K. Bullion and K. Dontsova, “Dissolution of three insensitive munitions formulations,” Chemosphere, vol. 119, pp. 342-348, 2015.

Final Presentation

GRADEMARK REPORT

FINAL GRADE

85 /100

GENERAL COMMENTS

Engagement with literature (9/10)

You demonstrated excellent engagement with literature referring mainly to journal articles and books; all relevant and credible.

IEEE format applied to all references.

When you show the references within the slides, use only the name and year(e.g. M. Khalil, 2009)

Knowledge and understanding skills (25/30)

Exceptionally good knowledge and understanding of TNT life cycle

Cognitive and intellectual skills (25/30)

You handled the question with confidence.

You demonstrated excellent ability to critically analyse information and draw valuable conclusions.

Practical skills (18/20)

You showed links to industry when discussed the actual yields.

Always look for a way to contextualise your talk.

Transferable skills (8/10)

Excellent team work and very good time management.

Images in slides 36, 37, 40 and 41 are too small

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