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Research paper

Preparation and Characterization of a Novel Energetic Cocrystal RDX:TNT (1:2)

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Abstract: In this work, a new cocrystal named RDX:TNT is introduced and characterized. The DSC profile of the cocrystal exhibits a decomposition temperature of 217.71°C, a melting point of 78.30 °C, and the thermal behaviour of melt-cast formulations. The results confirmed that the performance properties of the cocrystal are improved compared to TNT. The SEM images revealed that the cocrystal has a different morphology to its individual components. Furthermore, the existence of intermolecular hydrogen bonding is proven according to transitions in the FT-IR spectrum. The powder X-ray diffraction pattern verified the different crystal structure of the cocrystal by comparison to the individual components.

Keywords: energetic material, cocrystallization, RDX, TNT

Nomenclature

ADN	Ammonium dinitramide
DNAN	2,4-Dinitroanisole
QSPR	Quantitative structure property relationship
RDX	1,3,5-Trinitroperhydro-1,3,5-triazine
TNAZ	1,3,3-Trinitroazetidine
TNT	2,4,6-Trinitrotoluene

1 Introduction

The role of chemistry in providing day to day needs and expanding technologies that utilize existing components to produce new materials and consequently new challenges and opportunities, cannot be ignored. A class of significant energetic materials (EMs), categorized into three groups (explosives, propellants and pyrotechnics) by their applications, perform self-redox reactions under adequate stimulation and release a vast amount of heat [1-3].

In order to achieve better and safer transportation, storage and handling of high energy materials a desirable balance between sensitivity and performance is required. To achieve this goal several strategies have been examined, as follows: designing new EMs, modifying crystal quality, coating and polymer bonding explosives, *etc*. However, the high cost and time-consuming processes limit the application of these strategies [4-6]

Recently, the cocrystallization technique has appeared as an approach to modify the properties of EMs and to alleviate the safety-performance contradiction. On the other hand, a cocrystal is defined as a crystalline solid, composed of two or more components in a defined stoichiometric ratio. The application of the cocrystallization approach is present in other fields of science and technology, such as: pharmaceuticals, green chemistry, electronics, luminescent materials, solar cells, and energy storage. Experimental strategies for the preparation of energetic cocrystals have been demonstrated as follows [7-10]:

– solvent evaporation (SE),
– spray drying (SD),
– vacuum freeze drying (VFD),
– solvent/non solvent (S/NS),
– cooling crystallization (CCM),
– grinding method (GM),
– melting crystallization method (MCM),
– resonant acoustic mixing (RAM).

According to available references, many energetic cocrystals have been reported and some of them are listed in Table 1.

Table 1. Reported energetic cocrystals

Cocrystal	Molar ratio	Method	Purpose	Ref.
RDX:CL-20	1:1	SE	Sensitivity reduction of CL-20	[11]
CL-20:TNT	1:1	S/NS	Sensitivity reduction of CL-20 and improving the detonation properties of TNT	[12]
HMX:TNT	3:1	SD	Sensitivity reduction of HMX	[13]
TNT:TNB	1:1	SE	Performance improvement of TNT and TNB	[14]
DAF:ADNP	1:1	SE	Thermal stability improvement of ADNP	[15, 16]
DNAN:NA	1:1	SE	Thermal stability improvement of DNAN	[17]
DNAN:DNB	1:1	SE	Thermal stability improvement of DNAN	[17]
BTF:DNAN	2:1	SE	Sensitivity reduction of BTF	[18]
BTNEN:HMX	1:2	S/NS	Sensitivity reduction of BTNEN	[19]
PETN:TKX-50	1:1	S/NS	Decreasing the sensitivity of PETN	[20]
HNTO:AN	1:1	SE	Improving the performance of AN and HNTO	[21]
HMX:CL-20	1:2	SE	Modifying sensitivity of CL-20 and detonation performance of HMX	[22]
NTO:TZTN	1:1	SE	Sensitivity reduction of TZTN	[23]
HMX:NTO	1:1	S/NS	Sensitivity reduction of HMX	[24]
HMX:NQ	1:1	VFD	Sensitivity reduction of HMX	[25]
HNIW:TNT	1:1	GM	Sensitivity reduction of CL-20	[26]

The current melt-cast technology is based on TNT, DNAN, TNAZ and ADN. Actually, melt-cast explosives have some specific characteristics, *e.g.*:

– a melting point 70 to 120 °C,
– enough separation between melting point and decomposition temperatures,
– high performance as well as high density.

TNT was initially synthesized in 1863 through nitration of toluene in two or three steps, since the direct nitration of toluene to TNT is not industrially possible. Its moderate sensitivity, high chemical stability and low melting point makes TNT a great candidate for munitions [27].

Cyclotrimethylenetrinitramine (RDX), was initially prepared by Henning in 1899 through nitric acid and the di-nitrate of hexamethylenetetramine. It has been utilized in oil-drilling industries, military applications and mining, and has

two crystal structures: α-RDX and β-RDX. However, β-RDX is unstable and has the tendency to convert to α-RDX [28].

The purpose of the present work is to improve the performance of TNT and to provide a melt-cast explosive through cocrystallization.

2 Experimental Section

2.1 Materials

RDX and TNT were gifts from the Chemical Industries Department of Defence Industries (Iran), and other materials utilized in this research were purchased from Merck.

2.2 Preparation of RDX and TNT cocrystal

RDX (0.50 g) and TNT (1.02 g) in 1:2 molar ratio were added to acetone (30 mL) in order to dissolve completely, then the solution was stirred for 30 min at 30 °C. Thereafter water (10 mL), as an anti-solvent, was slowly added to the solution from a dropping funnel during 10 min. After complete addition, the solution was stirred for 15 min at the same temperature, the resulting precipitate was then filtered off and dried at room temperature to give colorless plates, yield 90%.

2.3 Characterization

The morphologies of the RDX:TNT cocrystals and the initial materials were investigated with a VEGA3 TESCAN scanning electron microscope (SEM) operating at an accelerating voltage of 20 kV. The powder X-Ray diffraction (PXRD) was performed at room temperature using a Philips analytical X-Ray-PW1800 instrument (CuKα, λ = 1.5406 nm, 40 kV). Fourier transform infrared spectroscopy (FT-IR) was characterized using a Thermos Fisher Nicolet 800 FT-IR spectrometer, and the FT-IR data were obtained in the range of 400-4000 cm^{-1}.

2.4 Performance tests

DSC analysis was performed with using a model TA-1 differential scanning calorimeter. The sample (4.66 mg) was placed in aluminum pans under an argon atmosphere and the thermal behaviour of the sample was investigated at a heating rate of 10 °C·min^{-1}.

The impact sensitivity test was performed in accordance with the GJB-772-97 Standard method. The conditions of the test were as follows: a drop weight of 2.5 kg with a sample mass of 60 mg. The impact sensitivity of each test sample was defined by the drop height of 50% explosion probability (H_{50}).

The density was measured using a "Micrometrics Occupy 1330 instrument". The detonation properties were calculated by computational methods.

3 Results and Discussion

3.1 FT-IR spectrum

The FT-IR spectra of the cocrystals and the intial materials are shown in Figure 1. The wave numbers of the characteristic bonds of RDX, TNT and the cocrystal are listed in Table 2. In the spectrum of the RDX:TNT cocrystal, some of the characteristic peaks of RDX and TNT have been shifted. For instance, RDX has a band at 1467.40 cm^{-1}, corresponding to the absorption peak of the methylene functional groups. However, this band has shifted to 1461.68 cm^{-1} in the cocrystal. RDX and TNT have absorption peaks at 1532.27 cm^{-1} and 1538.18 cm^{-1}, correlating to the NO_2 functional groups, however, this has shifted to 1543.48 cm^{-1} in the cocrystal. Furthermore, the NO_2 aromatic conjugation of TNT at 1618.26 cm^{-1} has shifted to 1620.37 cm^{-1} and, as illustrated in Table 2, there are some other differences between the wavenumbers of the cocrystal in comparison to pure initial components, which suggest the generation of intermolecular hydrogen bonding, leading to variations of electron density in the crystal lattice.

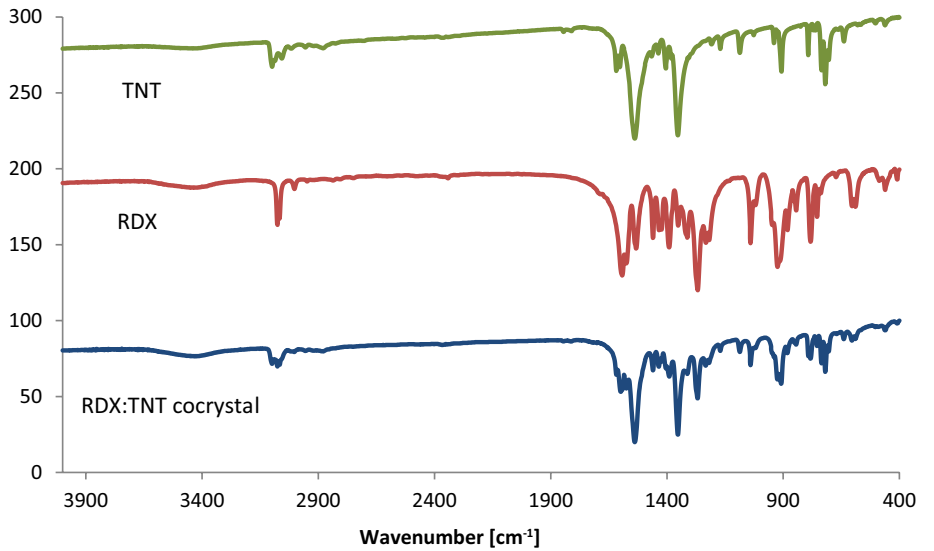


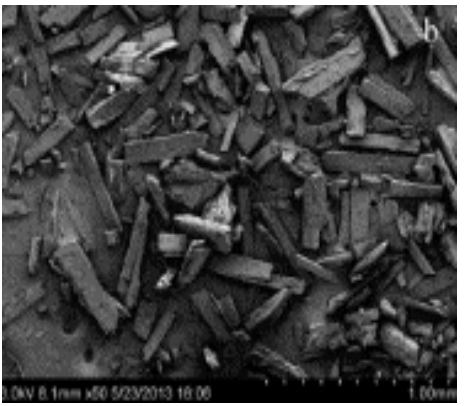
Figure 1. FT-IR spectra of RDX, TNT and the RDX:TNT cocrystal

Table 2. IR frequencies of the RDX:TNT cocrystal and the initial materials

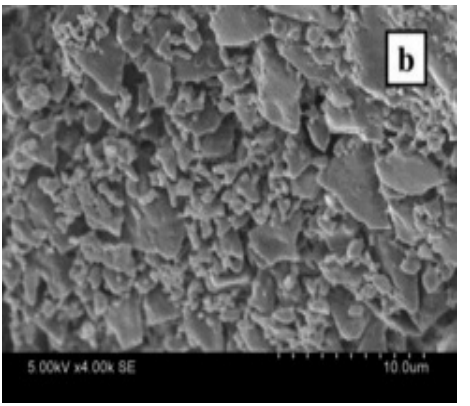
Assignment	RDX [cm^{-1}]	Cocrystal [cm^{-1}]	TNT [cm^{-1}]
CH_2 Asymmetric stretch	3075.75	3083.25	3099.17
NO_2 Aromatic conjugation	–	1620.37	1618.26
NO_2 Asymmetric stretch	1532.27	1543.48	1538.18
CH_2 Bending	1467.40	1461.68	–
NO_2 Symmetric stretch	1267.14	1273.38	–
H–C–C in plane bend	–	1218.12	1208.68
NO_2 out of plane deformation	755.63	760.78	–
C–H out of plane and C–N bend	–	782.48	792.46

3.2 Morphology

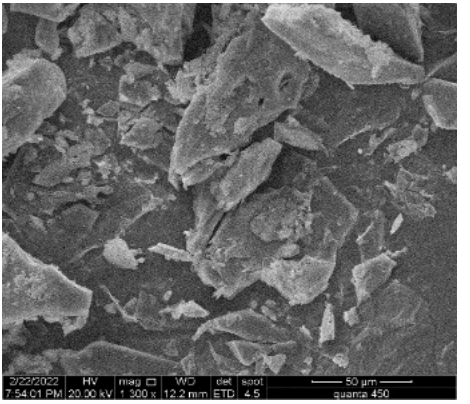
After succesfully preparing the cocrystal, the SEM was utilized to determine the morphological features of the cocrystal and the initial materials. As illustrated in Figure 2, there are obvious differences between the morphologies of the cocrystal and its initial materials. The TNT has a rod-like morphology and RDX exhibits hexagonal shaped plates. In contrast, the cocrystal exhibits a variant morphology. According to SEM results it can be concluded that cocrystallization can alter the morphological features of energetic materials.



(a)



(b)



(c)

Figure 2. SEM images of TNT (a), RDX (b) and the RDX:TNT cocrystal (c)

3.3 Thermal analysis

Figure 3 illustrates the thermal behaviour of the RDX:TNT cocrystal using the DSC thermogram. With reference to the DSC profile, there is an endothermic peak at 78.30 °C, attributed to the melting point of the cocrystal, which is lower than the melting point of RDX (205 °C) and TNT (80.35 °C) [29, 30]. In addition, there is an exothermic peak at 217.71 °C, corresponding to the decomposition temperature of the cocrystal, which is lower than the decomposition temperatures of each of the initial materials (TNT: 290 °C, RDX: 234 °C) [31, 32].

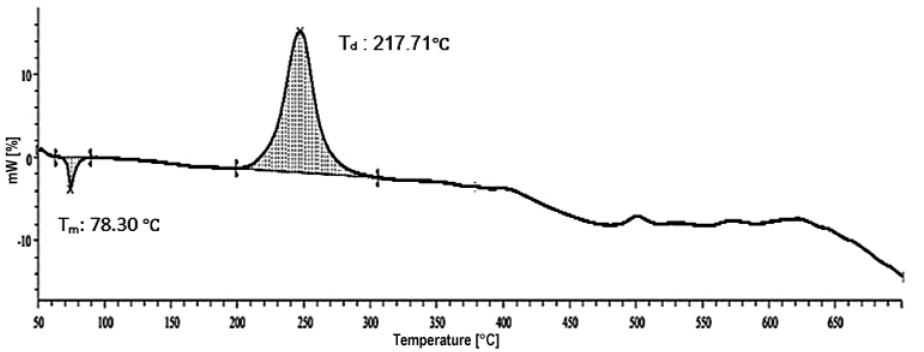


Figure 3. DSC curve of the RDX:TNT cocrystal

3.4 PXRD

The structure of the RDX:TNT cocrystal and its initial materials were determined through PXRD patterns and the results are shown in Figure 4. According to the PXRD profile, some new peaks have arisen after cocrystallization, which are located at 12.5°, 16.5° and 20.5° while there are no corresponding peaks in the pure components. In addition, there are some peaks with a more or less transition from those of the initial materials. In consequence, the differences in the PXRD patterns of the cocrystal and the pure materials, verify the formation of a new compound with a different crystal structure to those of the pure components.

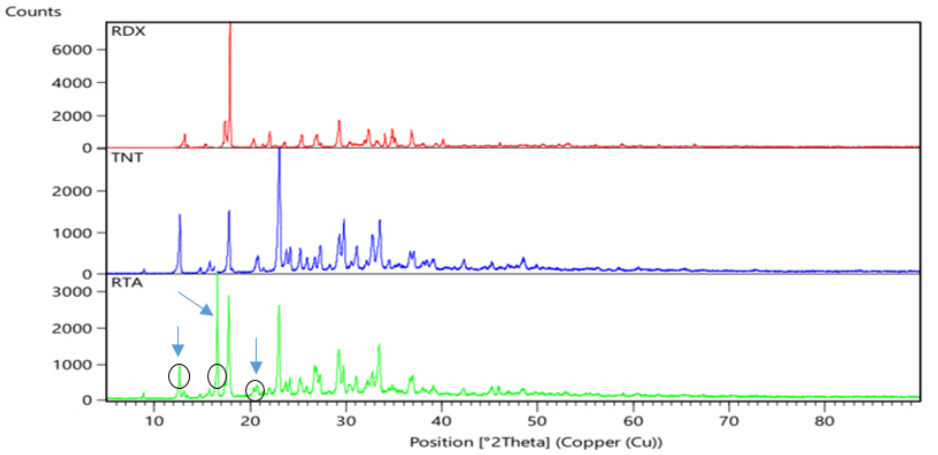


Figure 4. PXRD patterns of RDX, TNT and the RDX:TNT cocrystal

3.5 Impact sensitivity

In order to assess the safety of explosives and determine their susceptibility under external stimuli, the measurement of their impact sensitivity is vital. The impact sensitivity of the RDX:TNT cocrystal was measured by the drop height of 50% explosion probability. The cocrystal has H_{50} 30 cm which is between that of TNT (154 cm) and RDX (28 cm), demonstrating enhancement of sensitivity in comparison to pure RDX. Consequently, cocrystallization of explosives can affect their sensitivity.

3.6 Density, oxygen balance and detonation properties

The detonation characteristics of energetic materials have a dependence on density according to the Kamlet-Jacob equation. Actually, higher or lower values of this parameter may affect the detonation properties and provide a chance to synthesize and design new explosives [33]. The oxygen balance is another key property in the field of energetic materials and is defined as the degree to which an explosive can be oxidized. As a matter of fact, compounds may have positive, negative or zero oxygen balance depending on the oxygen content. The more positive this quantity is, the more oxygen will be available in the energetic material. When the substance burns or explodes, it has more internal oxygen to convert its combustible elements into products. For example, in the presence of sufficient oxygen, the combustion of the energetic material would be complete and its carbon content could be converted to carbon dioxide instead of carbon monoxide.

The densities of the RDX:TNT cocrystal and the pure components were measured at room temperature. The results are listed in Table 3. Furthermore, Rothstein and Petersen's equations were utilized to calculate the detonation performance, including detonation velocity and detonation pressure [34]. The results confirmed that the detonation properties of TNT have been enhanced. These detonation properties have been calculated to be 7.25 km·s^{-1} and 23.15 GPa, respectively by two QSPR models, which connect the structure and properties of a compound [35, 36].

Table 3. Density and detonation properties of the RDX:TNT cocrystal and the initial materials

Sample	Density [g·cm^{-3}]	Detonation velocity [km·s^{-1}]		Detonation pressure [GPa]		Oxygen balance [%]
		Rothstein Petersen method	QSPR method	Rothstein Petersen method	QSPR method	
RDX	1.81	8.92		37.44		–21.60
TNT	1.65	6.40		27.10		–74.00
RDX:TNT	1.67	7.47	7.25	22.20	23.15	–56.77

4 Conclusions

- A new cocrystal with RDX:TNT in a 1:2 molar ratio was prepared and characterized successfully.
- The DSC profile provides a melt-cast cocrystal according to its melting point and decomposition temperatures, which are consistent with the properties of the melt-cast compositions. The varied morphological features of the cocrystal in comparison to its initial materials was determined through SEM images. Moreover, the diverse spectroscopicpatterns of the cocrystal, including FT-IR and PXRD, compared to its initial materials verify the formation of a new compound.
- Rothstein and Petersen's equations were applied for the calculation of the detonation velocity (7.47 km·s^{-1}) and the detonation pressure (22.20 GPa), which are also the basis of the calculated density value (1.67 g·cm^{-3}). Moreover, QSPR models were used for estimating the detonation velocity of the cocrystal (7.25 km·s^{-1}) as well as its detonation pressure (23.15 GPa). These results confirm that the performance properties of the cocrystal are improved compared to TNT.

References

[1] Baumann, M.; Baxendale, I. R. An Overview of the Synthetic Routes to the Best Selling Drugs Containing 6-membered Heterocycles. *Beilstein J. Org. Chem.* **2013**, 9: 2265.

[2] Aakeröy, C.B.; Sinha, A.S. *Co-Crystals: Preparation, Characterization and Applications.* R. Soc. Chem., **2018**, p. 24; ISBN: 978-1-78801-115-0; https://doi.org/10.1039/9781788012874.

[3] Cherukuvada, S.; Kaur, R.; Row, T.N.G. Co-Crystallization and Small Molecule Crystal Form Diversity: from Pharmaceutical to Materials Applications. *CrystEngComm.* **2016**, 18: 8528-8555; https://doi.org/10.1039/C6CE01835A.
[4] Akhavan, J. *The Chemistry of Explosives.* 3rd Ed., R. Soc. Chem., **2011**; ISBN: 9781849733304.
[5] Zohari, N.; Mohammadkhani, F.G. Prediction of the Density of Energetic Co-crystals: a Way to Design High Performance Energetic Materials. *Cent. Eur. J. Energ. Mater.* **2020**, *17*(1): 31-48; https://doi.org/10.22211/cejem/118858.
[6] Xue, Z.H.; Huang, B.; Li, H.; Yan, Q. Design: Nitramine-based Energetic Cocrystals with Improved Stability and Controlled Reactivity. *Cryst. Growth Des.* **2020**, *20*: 8124-8147; https://doi.org/10.1021/acs.cgd.0c01122.
[7] Desiraju, G.R.; Vittal, J.J.; Ramanan, A. *Crystal Engineering: A Textbook.* World Scientific Publishing Co., **2011**.
[8] Aakeröy, C.B.; Beatty, A.M.; Helfrich, B.A. "Total Synthesis" Supramolecular Style: Design and Hydrogen-Bond-Directed Assembly of Ternary Supermolecules. *Angew. Chem., Int. Ed.* **2001**, *40*: 3240-3242; https://doi.org/10.1002/1521-3773(20010903)40:17<3240::AID-ANIE3240>3.0.CO;2-X.
[9] Trask, A.V.; Motherwell, W.D.S.; Jones, W. Solvent-Drop Grinding: Green Polymorph Control of Cocrystallisation. *ChemComm.* **2004**, *7*: 890-891; https://doi.org/10.1039/B400978A.
[10] Plechkova, N.V.; Seddon, K.R. Applications of Ionic Liquids in the Chemical Industry. *Chem. Soc. Rev.* **2008**, *37*: 123-150; https://doi.org/10.1039/B006677J.
[11] Van der Heijden, A.E.D.M.; Bouma, R.H.B. Design: Crystallization and Characterization of RDX, HMX, and CL-20. *Cryst. Growth Des.* **2004**, *4*(5): 999-1007; https://doi.org/10.1021/cg049965a.
[12] Yang, Z.; Zhang, Y.; Li, H.; Zhou, X.; Nie, F.; Li, J.; Huang, H. Preparation, Structure and Properties of CL-20/TNT Cocrystal. *Chin. J. Energ.* **2012**, *20*: 674-679; https://doi.org/10.3969/j.issn.1006-9941.2012.06.003.
[13] Li, H.; An, C.; Guo, W.; Geng, X.; Wang, J.; Xu, W. Explosives, Pyrotechnics: Preparation and Performance of Nano HMX/TNT Cocrystals. *Propellants Explos. Pyrotech.* **2015**, *40*(5): 652-658; https://doi.org/10.1002/prep.201400175.
[14] Guo, C.; Zhang, H.; Wang, X.; Liu, X.; Sun, J. Study on a Novel Energetic Cocrystal of TNT/TNB. *J. Mater. Sci.* **2013**, *48*: 1351-1357; https://doi.org/10.1007/s10853-012-6881-5.
[15] Bennion, J.C.; Siddiqi, Z.R.; Matzger, A. A Melt Castable Energetic Cocrystal. *ChemComm.* **2017**, *53*: 6065-6068; https://doi.org/10.1039/C7CC02636F.
[16] Bennion, J.C.; Matzger, A. Development and Evolution of Energetic Cocrystals. *Acc. Chem. Res.* **2021**, *54*: 1699-1710; https://doi.org/10.1021/acs.accounts.0c00830.
[17] Sun, S.; Zhang, H.; Xu, J.; Wang, S.; Zhu, C.; Wang, H.; Ding, R.; Yu, Z.; Sun, J. Two Novel Melt-Cast Cocrystal Explosives Based on 2,4-Dinitroanisole with Significantly Decreased Melting Point. *Cryst. Growth Des.* **2019**, *19*(12): 6826-6830; https://doi.org/10.1021/acs.cgd.9b00680.
[18] Yuan, M.; Hao, S.L.; Li, H.Z.; Liu, Y.C.; Yang, Z.W. Preparation and Performance

of BTF-DNAN Cocrystal Explosive. *Chin. J. Energ.* **2015**, *23*: 1228; https://doi.org/10.11943/j.issn.1006-9941.2015.12.015.

[19] Zohari, N.; Mohammadkhani, F.G.; Montazeri, M.; Roosta, S.T.; Hosseini, S.G.; Zaree, M.A. Synthesis and Characterization of a Novel Explosive HMX/BTNEN (2:1) Cocrystal. *Propellants Explos. Pyrotech.* **2021**, *46*(2): 329-333; https://doi.org/10.1002/prep.202000202.

[20] Xiao, L.; Guo, S.; Su, H.; Gou, B.; Liu, Q.; Hao, G.; Hu, Y.; Wang, X.; Jiang, W. Preparation and Characteristics of a Novel PETN/TKX-50 Co-Crystal by a Solvent/Non-Solvent Method. *RSC Adv.* **2019**, *9*: 9204-9210; https://doi.org/10.1039/C8RA10512J.

[21] Hanafi, S.; Trache, D.; Meziani, R.; Boukciat, H.; Mezroua, A.; Tarchoun, A.F.; Derradji, M. Synthesis, Characterization and Thermal Decomposition Behavior of a Novel HNTO/AN Co-Crystal as a Promising Rocket Propellant Oxidizer. *Chem. Eng. J.* **2021**, *417* paper 128010; https://doi.org/10.1016/j.cej.2020.128010.

[22] Fu, Y.; Zhao, P.; Yang, L.; Miao, R.; Zhang, C.; Guo, Z.; Liu, Y. Effect of Cocrystal Behavior on Sensitivity and Thermal Decomposition Mechanisms of CL-20/HMX via Molecular Dynamics Simulations. *ES Mater. Manuf.* **2018**, *1*: 50-56; https://doi.org/10.30919/esmm5f126.

[23] Wu, J.T.; Zhang, J.G.; Li, T.; Li, Z.M.; Zhang, T. A Novel Cocrystal Explosive NTO/TZTN with Good Comprehensive Properties. *Rsc. Adv.* **2015**, *5*: 28354-28359; https://doi.org/10.1039/C5RA01124H.

[24] Li, J.; Jiao, Q.; Gong, Y.; Wang, Y.; Liang, T.; Sun, J. Explosive Performance of HMX/NTO Co-Crystal. *IOP Conf. Ser.: Mater. Sci. Eng.* **2018**, *292* paper 012032; https://doi.org/10.1088/1757-899X/292/1/012032.

[25] Gao, H.; Wang, Q.; Ke, X.; Liu, J.; Hao, G.; Xiao, L.; Chen, T.; Jiang, W. Preparation and Characterization of an Ultrafine HMX/NQ Co-Crystal by Vacuum Freeze Drying Method. *Rsc. Adv.* **2017**, *7*: 46229-46235; https://doi.org/10.1039/C7RA06646E.

[26] Sultan, M.; Wu, J.; Haq, I.U.; Imran, M.; Yang, L.; Wu, J.; Lu, J.; Chen, L. Recent Progress on Synthesis, Characterization, and Performance of Energetic Cocrystals: A Review. *Molecules* **2022**, *27*(15) paper 4775; https://doi.org/10.3390/molecules27154775.

[27] Ravi, P.; Badgujar, D.M.; Gore, G.M.; Tewari, S.P.; Sikder, A.K. Review on Melt Cast Explosives. *Propellants Explos. Pyrotech.* **2011**, *36*(5): 393-403; https://doi.org/10.1002/prep.201100047.

[28] Agrawal, J.P.; Hodgson, R. *Organic Chemistry of Explosives.* John Wiley & Sons, **2007**.

[29] Guo, D.; An, Q.; Zybin, S.V.; Goddard III, W.A; Huang, F.; Tang, B. The Co-Crystal of TNT/CL-20 Leads to Decreased Sensitivity toward Thermal Decomposition from First Principles Based Reactive Molecular Dynamics. *J. Mater. Chem.* **2015**, *3*: 5409-5419; https://doi.org/10.1039/C4TA06858K.

[30] Shi, Y.B.; Gong, J.; Hu, X.Y.; Ju, X. Comparative Investigation on the Thermostability, Sensitivity, and Mechanical Performance of RDX/HMX

Energetic Cocrystal and Its Mixture. *J. Mol. Model.* **2020**, *26* paper 176; https://doi.org/10.1007/s00894-020-04426-0.
[31] Millar, D.I.; Oswald, I.D.; Francis, D.J.; Marshall, W.G.; Pulham, C.R.; Cumming, A.S. The Crystal Structure of β-RDX – An Elusive Form of an Explosive Revealed. *Chem. Comm.* **2009**, *5*: 562-564; https://doi.org/10.1039/B817966B.
[32] Miller, G.R.; Garroway, A.N. *A Review of the Crystal Structures of Common Explosives. Part I: RDX, HMX, TNT, PETN, and Tetryl.* Report NRL/MR/6120-01-8585, Naval Research Laboratory, **2001**.
[33] Kamlet, M.J.; Jacobs, S.J. Chemistry of Detonations. I. A Simple Method for Calculating Detonation Properties of C–H–N–O Explosives. *J. Chem. Phys.* **1968**, *48*: 23-35; https://doi.org/10.1063/1.1667908.
[34] Rothstein, L.R.; Petersen, R. Predicting High Explosive Detonation Velocities from their Composition and Structure. *Propellants Explos. Pyrotech.* **1979**, *4*(3): 56-60; https://doi.org/10.1002/prep.19790040305.
[35] Zohari, N.; Montazeri, M.; Hosseini, S.G. Estimation of the Detonation Pressure of Co-crystal Explosives through a Novel, Simple and Reliable Model. *Cent. Eur. J. Energ. Mat.* **2020**, *17*(4): 492-505; https://doi.org/10.22211/cejem/131687.
[36] Zohari, N.; Mohammadkhani, F.G. Detonation Velocity Assessment of Energetic Cocrystals using QSPR Approach. *Z. Anorg. Allg. Chem.* **2020**, *646*: 30-35; https://doi.org/10.1002/zaac.201900202.

Contribution

Narges Zohari: conception, foundations, methods, other contribution to the publication
Faezeh Ghiasvand: performing the experimental part, performing the statistical analysis
Sara Akbari: performing the experimental part, performing the statistical analysis

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