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Research Article

Catalytic Effect of Catocene on the Thermal Decomposition Kinetic of NTO and NTO/TNT Explosives

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ABSTRACT

The catalytic effect of catocene was studied on the kinetic of thermal decomposition of NTO (3-Nitro-1, 2, 4-triazol-5-one) and NTO/TNT (Trinitrotoluene) explosives. NTO is an insensitive explosive and can use as an alternative of many nitramine explosives and thus composite explosive of NTO/TNT shows the properties of an insensitive explosive. FT-IR spectra show the minor changes in molecular bonds of NTO and TNT with addition of catocene. SEM-EDS (Scanning Electron Microscopy-Energy Dispersive X-ray Spectroscopy) analysis indicates the morphology of prepared samples and presence of catalyst in the matrix of samples. TG/DSC (Thermal Gravimetry/Differential Scanning Calorimetery) method is used to study the thermal behaviour of NTO and NTO/TNT in absence and presence of 3% wt. of catocene. A decrease ~5 ºC in exothermic peak temperature of DSC curves and a decrease ~50 kJ/mol in activation energy (E_a) of thermal decomposition reactions of NTO and NTO/TNT are seen in presence of catocene. The activation energies are calculated by model-free methods of Ozawa–Flynn–Wall (OFW), and Kissinger–Akahira–Sunose (KAS). Tests of sensitivity to impact, friction, and electric discharge show the stability of NTO and NTO/TNT against external stimuli in the presence of catalyst.

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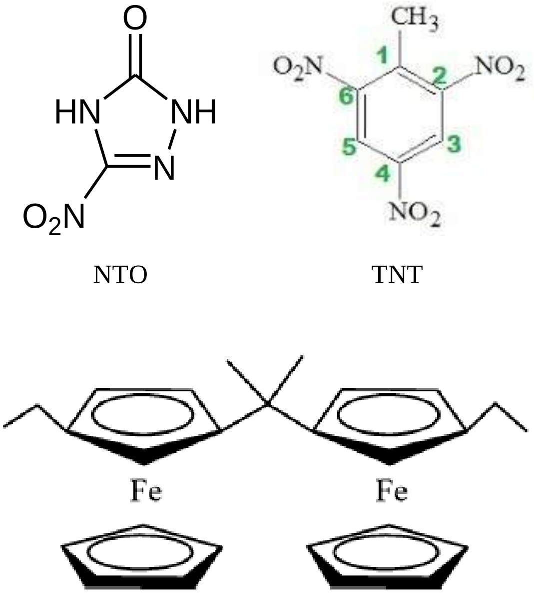
1. Introduction

Catocene (2, 2′-Bis (ethylferrocenyl) propane, scheme 1) with formula of $C_{27}H_{32}Fe_2$ is used as a catalyst for increasing the burning rate of solid propellants of fuel-rich [1]. The weight percent of catocene in a solid propellant is usually < 5%. Also, catocene catalyst can increase the kinetic of thermal decomposition reaction of explosives including ammonium perchlorate [2, 3]. Thermal analysis methods including TG, and DSC are the main methods in studying the thermal behaviour and thermal decomposition reactions of energetic materials such as explosives. Thermal methods give information concerning thermal stability, melting, evaporation, decomposition etc. In fact, any reaction or transformation involving absorption or release of heat can be detected with these techniques. The decrease of the peak temperature in DSC curves and onset temperature in TG curves show the reduction of thermal stability of explosives that is due to increase of kinetic of thermal decomposition reaction [4-6]. Thermal analysis techniques have the advantage of using a small amount of sample, and rapidly often yield sufficient information for the accurate determination of the kinetic parameters of the reactions. The kinetic parameters such as the activation energy, the pre-exponential factor, and the reaction model are calculated from data through thermal analysis techniques using both model-fitting approaches and model-free (Isoconversional) kinetic approaches.

TNT (2, 4, 6-trinitrotoluene, scheme 1) is a molecular explosive widely used in various military systems as well as commercial civilian boosters. TNT is a relatively strong explosive material that exhibits a detonation rate of 6900 m/s during explosion. Normally, molecular explosives are very sensitive to external stimuli such as impact, friction, and thermal shock, and their use without desensitization can lead to unwanted explosions during production, storage, and transportation [7, 8]. Explosive of NTO (scheme 1) was first synthesized by Manchot and Nolle in 1905, but its explosive properties were identified and developed in the mid-1980s. NTO shows explosion rate 8550 m/s and density of 1.911 g/cm^3. NTO explosive is used to increase safety and to reduce the sensitivity of most explosives to external stimuli including impact, friction, heat, spark and shock waves. Its thermal stability is also high and decomposes exothermically at around 272 °C [9]. NTO explosive is more stable and less sensitive to temperature than other known explosives. So researchers have tried to use NTO in composite explosives.



NTO TNT

Catocene

Scheme 1. Molecular structure of NTO and TNT explosives and catocene as a catalyst.

NTO is currently widely employed in several formulations such as melt-cast, cast-cured plastic bonded explosives (PBX), composite explosives, co-crystal explosives and gas generators. The composite explosives based on NTO are insensitive explosives [10-12]. It displays performance characteristics comparable to those of the currently commonly employed secondary explosives and possesses an appropriate potential to be used as an explosive and propellant ingredient. This compound has been shown to be less harmful to human health than traditional explosives.

Catalysts could affect the rate of a chemical reaction using an alternative and lower energy profile or pathway. Therefore, they decrease the activation energies thorough the effects on the transition state and activation path [13-15]. The complexing of the catalyst with one of the reagents is a new pathway for the catalytic reactions. Transition metals with a wide variety of oxidation states are the suitable candidates for complexation process. The properties of electron-donor and electron-acceptor indicate the ability of complexation of transition metals. The transition metals play as an electron-acceptor if the transition state is electron rich. Also, the transition metals might undergo formal oxidation/reduction process to achieve electron transfer to a substrate which is due to a reaction [16, 17]. NTO explosive as an insensitive explosive is a good option for adding to TNT-containing compounds and producing insensitive composite explosive. But, the desensitizing composite explosive can lead to a decrease in its performance. This limitation is related to reduction of sensitivity to the detonator or ammunition activity. Therefore, the use of various additives such as catalysts is a solution for modification and improvement of the composite explosives. The catalysts used are mainly solid, and therefore preparing a homogeneous mixture is limited. But, catocene is a liquid substance and it can be easily added to explosives (NTO and NTO/TNT) and get a homogeneous mixture. Review of previous literature shows that the effect of Catocene and Its Influence on the Mechanical Sensitivities of a Fine AP/Catocene Mixture [18]. Thermal decomposition of cured GAP-AP propellants containing catocene investigated by Shin-Ming Shen and etal.The results revealed that catocene plays an important role in catalyzing the decomposition of both AP and GAP [19]. In this research, the catalytic effect of catocene on the insensitive explosive of NTO and NTO/TNT is studied by TG/DSC thermal methods. The interaction of catalyst with host materials, the morphology of prepared samples and the sensitivity to external stimuli were studied.

2. Experimental

2.1. Materials and Instrumentations

TNT explosive (solidification point of 80.40°C) and NTO explosive (melting point of 268°C, purity of 99%, and grain size of 60-100 micron) were obtained from Iran Chemical Industries. Catocene (molecular weight of 468.25 g/mol) with purity of 99.5% was prepared from Iran Chemical Industries. The technical indexes of catocene are collected in Table 1.

Table 1. The technical indexes of catocene

Item	Index
Iron content,%(m/m)	23.3-24.3
Viscosity, Pa·s (25℃)	< 2.8
Density, g/cm^3 (20℃)	1.2910-1.2960
Volatilization loss, % (80±1℃, 20±1*102Pa,12h）	< 2.0
Insoluble, %(m/m)	< 0.10
Acidity, mmol/100 g	< 0.30
Moisture content, %(m/m)	<0.08
Ethylferrocene content,%(m/m)	<3.0
Appearance	Brown red viscous liquid

A PerkinElmer thermal analyzer, model STA 6000TG/DSC, used to study the thermal behaviour of samples. The thermal analyzer was calibrated by a standard material of indium metal with phase transition temperature at 156.6 ºC. The conditions TG/DSC analysis were sample weight of ~2.50 mg, an alumina pan, heating rates of 5, 10, 15, and 20 $°C\cdot min^{-1}$, temperature range of 25 – 400 °C, and N_2 atmosphere at a rate 20 $cm^3\cdot min^{-1}$. The FT–IR spectrums of prepared samples were obtained by a LUMEX INFRALUM FT-08 spectrometer with KBr pellets in the range of 400–4000 cm^{-1}. The SEM – EDS analysis was done by a VEGA-Mira 3-XMU FE-SEM.

The sensitivity to impact was taken by a drop-weight tester with varying the drop-weight over 0 – 50 cm (interval 0.5 cm) and from 1 – 5 kg (interval 0.1 kg). A large BAM (Bundesanstalt fur Materialprufung, Germany) tester was applied for testing of sensitivity to friction. Nine different positions on the arm of tester give a weight charge 0.5 – 36 kg. The samples were analyzed between a porcelain pin and a porcelain plate of standardized roughness by a path of 10 mm length. Electrostatic discharge sensitivity of samples was measured by an ABL ESD machine in calibrated engineering units (Joules). An applied voltage used in range 0 – 10,000 volts with direct current (VDC). The calibration of ABL ESD machine was used in rang $0.10 \times 10^{-4} - 0.75$ microfarads (µF) with output 0.001 – 37.5 Joules (J) for discharge energies. Vacuum thermal stability (VTS) of samples was studied by vacuum stability tester STABIL VI (OZM Company).

2.2. Work safety

Using small amounts of explosives reduces their risk of danger. Also, wear a mask or proper ventilation to protect your lungs from inhaling toxic fumes. In addition, wear safety glasses to protect your eyes and special work clothes to prevent chemicals from entering your body.

2.3. Preparation of samples

The pure TNT and NTO were used as received. For preparation of NTO/Catocene (97:3), a 0.3 g of catocene catalyst was added to 9.7 g of NTO explosive into a 100 ml beaker. Then, 20 ml chloroform solvent was added and mixed by a mechanical stirrer in time of 10 min for obtaining a uniform mixture. Finally, the chloroform solvent was evaporated using a hot water bath.

The composite explosives of NTO/TNT and NTO/TNT/Catocene were prepared in ratios 50:50 and 48.5:48.5:3, respectively. TNT explosive was used as the base component because the low melting point. TNT explosive was melted using a double-wall bath with hot water circulation (95–98 °C) and indirect heat. Then, NTO and or NTO/Catocene were added to melt TNT and the samples were mixed for 30 minutes. The obtained mixtures were transferred to a plate of aluminium foil using a wooden spoon for formation a thin layer. The solidified samples were separated from the foil and ground in a Chinese mortar to obtain a uniform powder.

3. Results and discussion

3.1. Characterization of samples

The FT-IR spectra of TNT, NTO, catocene, and NTO/TNT, NTO/Catocene, NTO/TNT/Catocene are given in Fig. 1 and Fig. 2, respectively.

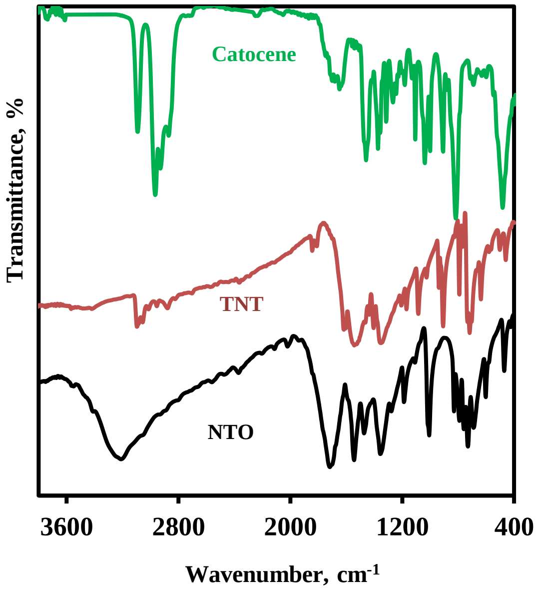


Fig. 1. FT-IR spectra of NTO, TNT, and catocene

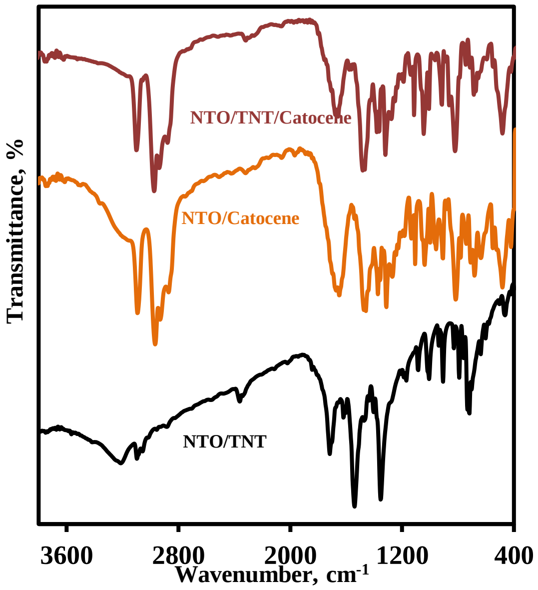
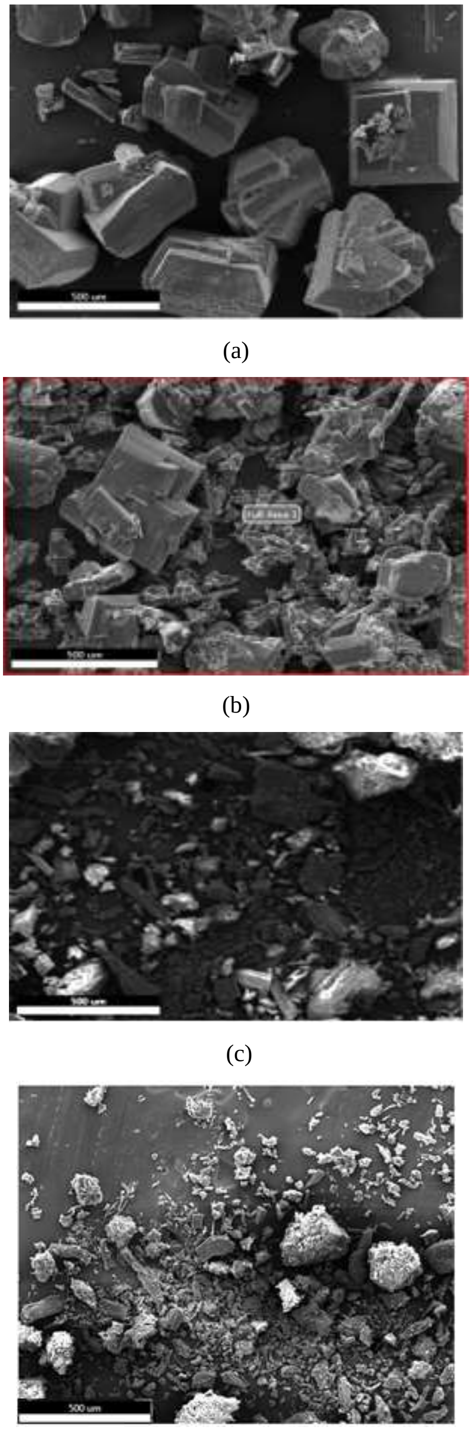


Fig. 2. FT-IR spectra of NTO/TNT, NTO/catocene, and NTO/TNT/Catocene

FT-IR spectra of NTO shows the peak at 3210 cm^{-1} related to the -HN-NH-alkyl, the peak at 1716 cm^{-1} assigned to the C=O functional bond, the peak at 1565 cm^{-1} corresponded to C=N bond, and the peak at 1359 cm^{-1}, specific to the nitro –C-NO$_2$ bond [20, 21]. The most important vibrational frequencies of TNT [22, 23] are peaks of C-H stretch in ring at 3058 and 3096 cm^{-1}, stretch of C-C ring at 1599 cm^{-1}, bend of H-C-C ring in plane at 1619 cm^{-1}, ring torsion at 457 cm^{-1}, C-N bend at 733 cm^{-1}, C-N stretch at 1095 cm^{-1}, C-N-O bend at 625, 677, 718 cm^{-1}, NO$_2$ anti-symmetric stretch at 1539 cm^{-1}, and NO$_2$ symmetric stretch at 1354 cm^{-1}. FT-IR spectra of catocene [24, 25] indicate the vibrational modes at 478 cm^{-1} for symmetric ring metal stretch, 492 cm^{-1} related to anti-symmetric ring, 811 and 1002 cm^{-1} for C-H bending, 1108 cm^{-1} assigned to anti-symmetric ring breathing, 1411 cm^{-1} corresponded anti-symmetric C-C stretch, 3085 cm^{-1} for anti-symmetric C-H stretch, and 3099 cm^{-1} for symmetric C-H stretch.

The comparison of FT-IR spectra of NTO/TNT, NTO/Catocene, and NTO/TNT/Catocene with spectrums of TNT, NTO and catocene confirm the formation of composite explosives. Because the indicator peaks are seen in 1716 cm^{-1} assigned to the C=O functional bond related to NTO. The specified peaks of TNT are observed at 1539 and 1354 cm^{-1} correspond to anti-symmetric stretch and symmetric stretch of NO$_2$, respectively, and at 3085 and 3099 cm^{-1} related to anti-symmetric and symmetric of C-H stretch, respectively. Peak at 478 cm^{-1} for symmetric ring metal stretch are well seen in FT-IR spectra of NTO/Catocene, and NTO/TNT/Catocene. However, the minor shifts in the location of the absorption peaks can be seen due to the presence of the catalyst, which can be related to the interaction of the NTO and NTO/TNT with the catalyst.

The SEM-EDS technique shows the morphology and the elemental analysis of prepared samples. The SEM images and the EDS spectra are shown in Fig. 3 and Fig. 4, respectively. NTO explosive clearly shows the crystalline structure (Fig. 3a). The coating of the NTO crystals by the oily catocene is seen in the Fig. 3b.



(a)

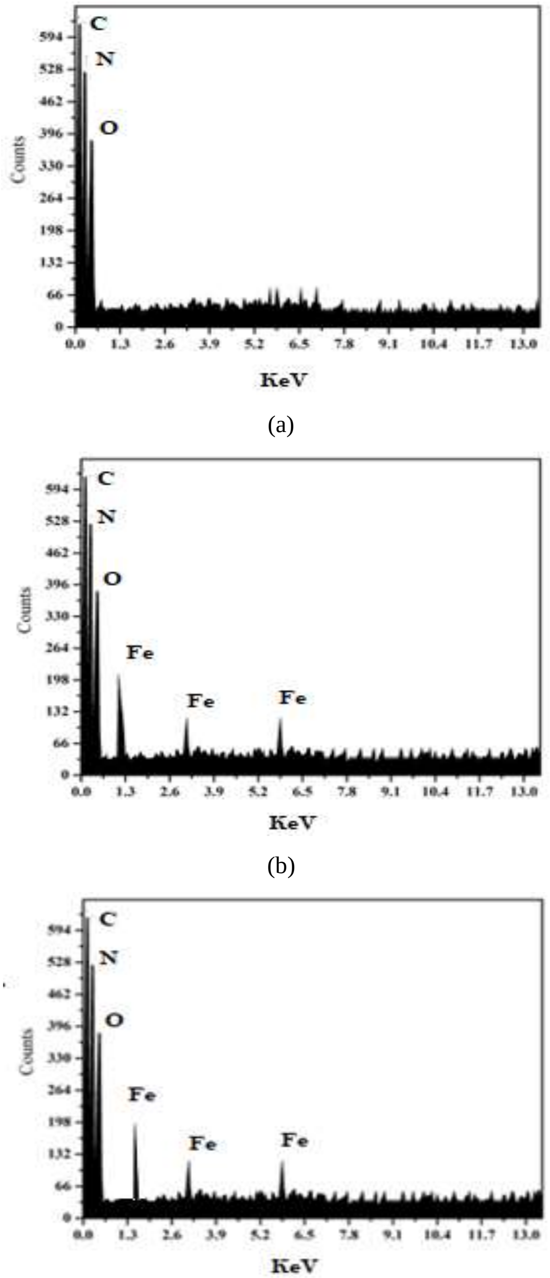
(b)

(c)

(d)

Fig. 3. SEM images of NTO (a), NTO/Catocene (b), NTO/TNT (c) and NTO/TNT/Catocene (d).

TNT explosive is a melt casting type and does not has a crystalline structure. Therefore, composites of NTO/TNT and NTO/TNT/Catocene do not show crystalline morphology and the particles are amorphous (Figs. 3c and 3d). EDS spectra in Fig. 4a and Fig. 4c show the elements C, O and N in the structure of NTO and NTO/TNT. While, the presence of iron of catocene catalyst in the prepared samples of NTO/Catocene and NTO/TNT/Catocene are proved by EDS spectra (Figs. 4b and 4d).



(a)

(b)

(c)

Fig. 4. EDS spectra of NTO (a) ,NTO/Catocene (b), NTO/TNT/Catocene (c).

3.2. Study of thermal decomposition reactions

The TG/DSC thermal curves of NTO, NTO/Catocene, and NTO/TNT, NTO/TNT/Catocene in range 25 – 300 °C at heating rate 10 °C/min (as a common heating rate) are given in Figs. 5 and 6, respectively. As seen, the prepared samples show a thermal decomposition reaction in one step.

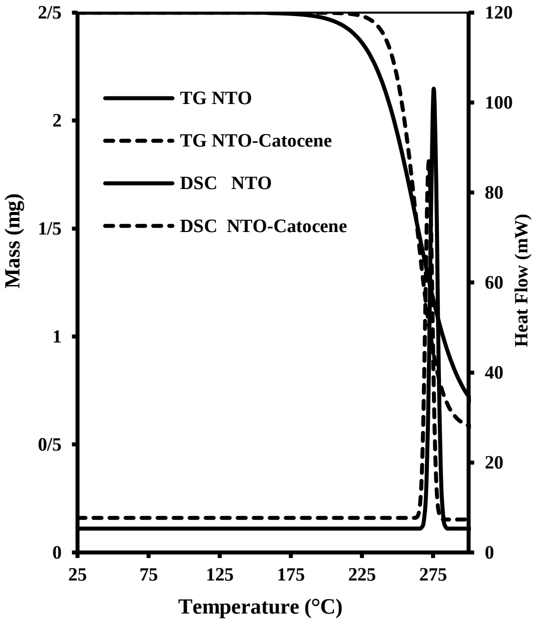


Fig. 5. TG/DSC thermal curves of NTO and NTO/Catocene in range 25 ~ 300 ºC at heating rate10 °C/min.

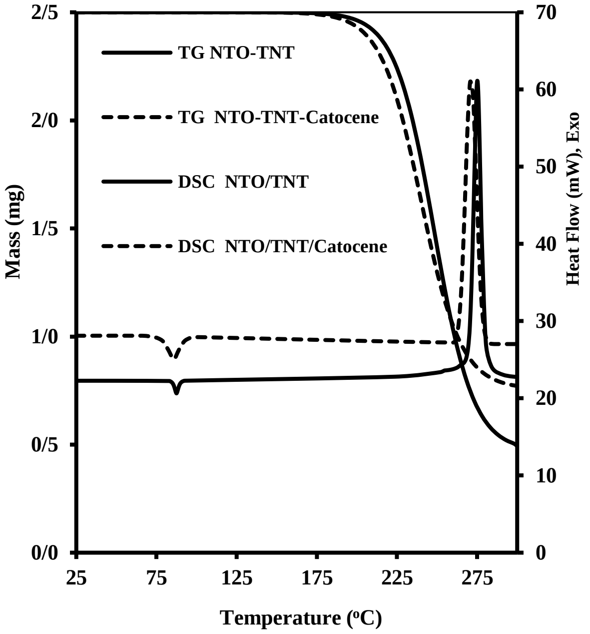
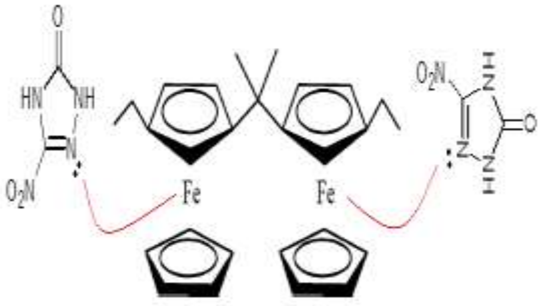


Fig. 6. TG/DSC thermal curves of NTO/TNT and NTO/TNT/Catocene in range 25 ~ 300 ºC at heating rate10 °C/min.

The temperatures of melting point of TNT and NTO are reported at 80 and 270–272 ºC, respectively [26, 27]. Therefore, in Fig. 6., the DSC thermal curves indicate an endothermic peak at 80 ºC which is related to TNT. Various investigators have asserted that NTO thermal decomposition begins with a homolysis of C-NO_2 bond. The sublimation of NTO could compete with decomposition process. Catocence is stable up to 300 ºC and thus there is no peak for it in TG/DSC curves [3]. On the other, NTO/TNT and NTO/TNT/Catocene composite explosives show an exothermic peak in DSC curves [27, 28]. Therefore, the composite explosives are completely homogeneous and give the behavior of a single explosive [29]. The composite explosive of TNT with the other explosives such as NTO is prepared to improve the oxygen balance. TNT has a melting point of about 80 °C and thus is melted with the addition of NTO explosive and poured into chambers of various shapes. Also, TNT is moderately sensitive to impact and friction. Therefore the composite explosive of NTO/TNT becomes insensitive because NTO is an insensitive explosive [1, 30]. However, the effect of catocene catalyst is seen in shift of exothermic peak of thermal decomposition to the lower temperatures for NTO/Catocene and NTO/TNT/Catocene in compared to NTO and NTO/TNT, respectively. The exothermic peak temperatures of NTO, NTO/Catocene, NTO/TNT, and NTO/TNT/Catocene are seen at 275.4, 271.6, 274.2, and 270.6 ºC, respectively. This shift shows that the kinetic of thermal decomposition of samples are increased in presence of catocene catalyst [31]. In the presence of 5 % nickel ferrite, the thermal decomposition peak temperature of NTO was decreased from 276.36 to 260.18 ºC and that of nano NTO was decreased from 261.38 to 258.89 ºC. The DSC peak temperature also suggests the presence of NiZnCoF decreases the nanoparticles of NTO exothermic curve by 5.62°C. The DSC peak curve of NTO in the presence of NiZnCoF was shifted from 276.35 to 272°C [32, 33]. Catocene has iron element in its structure and show an ability to participate in electron donor – electron acceptor interactions. The presence of nitrogen elements in NTO structure and free electron pairs makes it able to interact with an electron-accepting compound such as catocene (see scheme 1). Interaction of Fe atoms of catocene and N atoms of NTO is due to the weakening of the ring in NTO structure and therefore reduces its stability (Scheme 2). Also, the benzene ring in catocene is an electron-rich ring and can interact with electron-lean sites of host molecules.



Scheme 2. Interaction of Fe atoms of catocene and N atoms of NTO.

The decrease of stability of NTO leads to decrease of thermal decomposition temperature of NTO/Catocene and NTO/TNT/Catocene in compared to bear materials [34]. DSC curves at different heating rates of 5, 10, 15 and 20 ºC/min are used to calculate activation energy of thermal decomposition reaction of prepared samples. DSC analysis in different heating rates was repeated twice and the uncertainty of activation energy values was calculated. The obtained DSC thermal curves of NTO, NTO/Catocene, NTO/TNT, and NTO/TNT/Catocene are shown in Figs. 7, 8, 9, and 10, respectively.

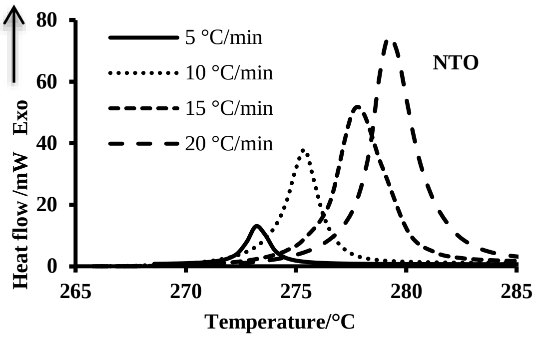


Fig. 7. DSC curves of NTO at heating rates of 5, 10, 15 and 20 °C/min.

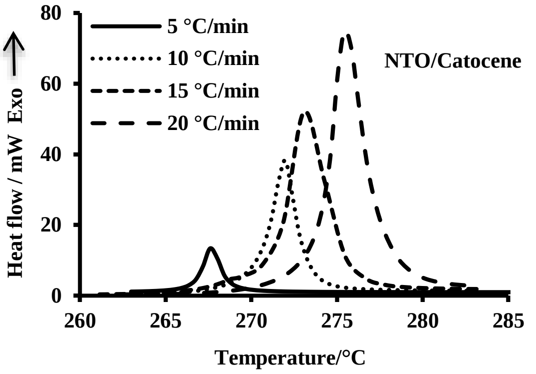


Fig. 8. DSC curves of NTO/Catocene at heating rates of 5, 10, 15 and 20 °C/min.

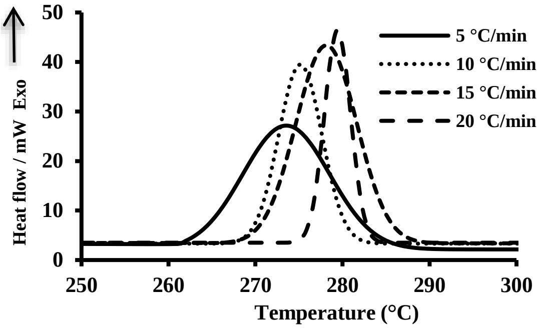


Fig. 9. DSC curves of NTO/TNT at heating rates of 5, 10, 15 and 20 °C/min.

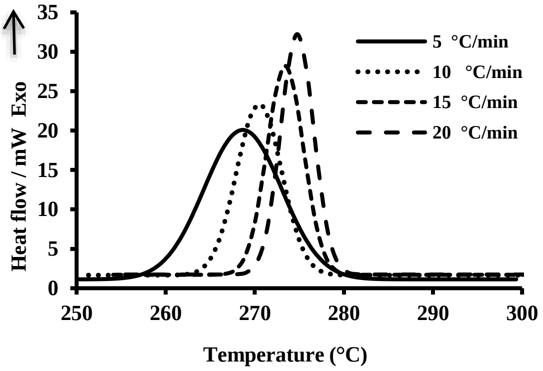


Fig. 10. DSC curves of NTO/TNT/Catocene at heating rates of 5, 10, 15 and 20 °C/min.

The non-isothermal, model-free methods of Ozawa–Flynn–Wall (OFW, Eq. 1), and Kissinger–Akahira–Sunose (KAS, Eq. 2) are used to determine the E_a of thermal decomposition reactions [34-36].

$$\ln(\beta) = Constant - \left(\frac{E_a}{RT_p}\right) \quad (1)$$

$$\ln\left(\frac{\beta}{Tp^{1.92}}\right) = Constant - 1.0008\left(\frac{E_a}{RT_p}\right) \quad (2)$$

Where, β is heating rate (ºC/min), E_a is activation energy (J/mol), T_P is the temperature of exothermic peak in DSC curves, and R is gas constant of 8.314 J/mol·K. The E_a values are calculated by the slope of curves ln(β) vs. ($1/T_P$), and ln($\beta/T_P^{1.92}$) vs. ($1/T_P$) using OFW and KAS equations, respectively. The obtained activation energies are collected in Table 2. Activation energy of thermal decomposition reaction is calculated 556 – 566, 437 – 496, 544 – 554, and 521 – 530 kJ/mol, respectively, for NTO, NTO/Catocene, NTO/TNT, and NTO/TNT/Catocene. In result, the catocene as a catalyst increase the rate of thermal decomposition reaction of NTO/Catocene and NTO/TNT/Catocene versus NTO and NTO/TNT, respectively, through the decrease of activation energy [36, 37]. The thermal heat capacity of samples are obtained from DSC thermal curves and collected in Table 2. Thermal heat capacity shows the heat released from the thermal decomposition reaction. The weight percent of explosive is reduced with addition of catalyst material to prepared samples. Therefore, reduction of thermal heat capacity for NTO/Catocene (1245.72 J/g) versus NTO (1444,95 J/g) and NTO/TNT/Catocene (599.28 J/g) versus NTO/TNT (705.36 J/g) is not far from expected. TNT is a very fuel-rich explosive as indicated by the large negative oxygen balance value of −74% [38]. It means that there is not enough oxygen in its initial chemical compound, and extra oxygen is needed to make the afterburning energy release possible. Therefore, the addition of TNT to NTO and or NTO/Catocene is due to decrease of thermal heat capacity of thermal decomposition reaction from

1444.95 to 1245.72 J/g and from 705.36 to 599.28 J/g. However, the addition of new component to an explosive can be effect on the other characterizations such as sensitivity to external stimuli [12, 39]. The decomposition reaction of explosives can influenced by different external stimuli including impact, friction, heat, static compression, and electric (electrostatic) spark [40].

Table 2 . Activation energy (kJ/mol) of thermal decomposition reaction and thermal heat capacity (J/g) of prepared samples.

Sample	OFW method	KAS method	Thermal Heat Capacity
NTO	566.04±3.45	556.47±3.21	1444.95
NTO/Catocene	496.57±4.66	437.43±5.05	1245.72
NTO/TNT	554.34±4.88	544.75±5.32	705.36
NTO/TNT/Catocene	530.29±3.45	521.82±4.23	599.28

Table 3. Sensitivity to impact, friction, electrostatic discharge, and VTS of prepared samples

Sample	Sensitivity to impact (J)	Sensitivity to friction (N)	Sensitivity to electrostatic discharge (mJ)	VTS at T= 100°C and time=40 hr (ml)
NTO	20	360 <	625 <	0.32
NTO/Catocene	20	360 <	625 <	0.40
NTO/TNT	25	360 <	625 <	0.85
NTO/TNT/Catocene	25	360 <	625 <	0.90

The sensitivity to impact, sensitivity to friction and electrostatic discharge (ESD) are studied and the obtained results for NTO, NTO/Catocene, NTO/TNT and NTO/TNT/Catocene are given in Table 3. Also, the obtained results of VTS (Vacuum Thermal Stability) test are presented in Table 3.

The obtained results show that the addition of catocene catalyst did not affect on the sensitivity of NTO and NTO/TNT samples to external stimuli. All samples indicate the sensitivity to friction and electrostatic discharge (ESD), respectively, more than 360 N and more than 625 mJ. The sensitivity to impact of NTO and NTO/Catocene is 20 J, and also for NTO/TNT and NTO/TNT/Catocene is 25 J. However, VTS results show the reduction of thermal stability of samples with addition of catocene catalyst. Because, the volume of released gases of NTO/Catocene (0.40 ml) and NTO/TNT/Catocene (0.90 ml) is more than NTO (0.32 ml) and NTO/TNT (0.85 ml), respectively. As similar to TG/DSC results, catocene as a catalyst indicates an increase in the kinetic of thermal decomposition reaction of NTO and NTO/TNT explosives.

4. Conclusions

Organometallic compounds such as ferrocene and catocene can have catalytic activity in many chemical reactions including thermal decomposition reactions. Catocene contains ferrous ions shows a catalyst effect on the thermal decomposition reaction of explosives such TNT and NTO/TNT composite which shifts the exothermic peak temperatures in DSC thermal curves to lower temperatures. The presence of ferrous ions in catocene makes it as an effective catalyst due to its electron-accepting properties and ability to change oxidation states. The stable structure and electron-transfer properties of iron, along with the aromatic interactions of the cyclopentadienyl rings, increase the catalytic efficiency of catocene in chemical reactions. The activation energy of thermal reaction is reduced and the kinetic of reaction is increased. Catocene is a liquid substance and it can be easily added to explosives (NTO and NTO/TNT) and get a homogeneous mixture. On the other hand, catocene is an organometallic substance that can have synergistic interactions with organic explosives. The cyclopentadienyl rings in catocene, due to their aromatic properties, can interact with the reactants and provide a suitable environment for their activation. Also, the iron ion, as the catalytic active site, attracts and activates the reactant molecules, which leads to a decrease in the activation energy and an acceleration of the reaction rate.

Acknowledgments

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Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this manuscript. In addition, the authors have entirely observed the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancy.

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