Membrane Technology
ISSN (online): 1873-4049

Thermal Decomposition and Stability of CL-20/TNT Co-crystal

Jianyu Zhu[1], Xiaoyu Sun[2], Xiangdong Li[1], Wentao Liang[1], Hao Wang[1], Zengming Zhang[2,*]

[1]*Department of Physics, School of Physical Sciences, University of Science and Technology of China, Hefei 230026, Anhui, China*

[2]*The Center for Physical Experiments, School of Physical Sciences, University of Science and Technology of China, Hefei 230026, Anhui, China*

**Corresponding Author.*

Abstract:

2, 4, 6, 8, 10, 12-hexanitro-2, 4, 6, 8, 10, 12-hexaazaisowurtzitane, commonly referred to as CL-20, is among the most potent explosives in existence, but it can't be generally applied due to its extremely high sensitivity. However, it has been found that CL-20 can be passivated by TNT within the co-crystal structure. In the current work, many testing methods such as DSC-TG and Raman spectroscopy, etc., were utilized to study the thermally induced decomposition of the CL-20/TNT co-crystal. Results show that the CL-20/TNT co-crystal can no longer maintain over 90 ℃, but its thermal decomposition process is severely retarded by the co-crystal structure, with a sharp increase in decomposition rate at around 127 ℃. The activation energies of the thermal decomposition of the co-crystal below and above 127 ℃ are 141 kJ·mol^{-1} and 167 kJ·mol^{-1}, respectively. In the region from 90°C to 127°C, the intermolecular hydrogen bonds between TNT and CL-20 molecules gradually weaken and break, leading to the decomposition of the CL-20/TNT co-crystal; above 127°C, CL-20 within the co-crystal tends to recrystallize into γ-phase CL-20, accelerating the decomposition of the co-crystal. This study discovered a slow decomposition process preceding the rapid decomposition of the CL-20/TNT co-crystal, re-determined the thermal decomposition products and the decomposition temperature of this explosive, and found that the thermal stability of the co-crystal explosive is influenced by the phase transitions of its components.

Keywords: CL-20/TNT co-crystal, thermal stability, decomposition products, decomposition mechanism, activation energy.

INTRODUCTION

CL-20 is one of the most power explosives with its outstanding detonation velocity and pressure (9580 m·s-1, 45.2 GPa [1]). However, the military and engineering applications of such an excellent explosive are severely limited [2,3] by its extremely high mechanical sensitivity [4,5]. Multiple attempts [6,7] have been taken over the past few years in order to enhance its stability and it turned out that CL-20 can be effectively passivated when co-crystallized with other insensitive explosives [8]. TNT is well recognized for its high mechanical stability [9], whose co-crystal with CL-20 has proven to possess markedly lower friction and impact sensitivity than pure CL-20 [10,11]. Hang et al. [12] found with molecular dynamics simulation that CL-20/TNT co-crystal has double intermolecular binding energy of CL-20&TNT mixture, which means co-crystal structure can provide explosives with higher stability and security. Guo et al. [11] reached the same conclusion with ReaxFF reactive dynamics that the co-crystal has a higher energy barrier with slower decomposition behavior than the mixture and pure CL-20. Ren et al. [13] indicated that the CL-20/TNT co-crystal structure can considerably slow down the breakage of N−NO2 and C−N bonds of CL-20 via ReaxFF MD simulation. Moreover, Hang et al. [14] figured out with molecular dynamic simulations again that surface defects result in up to 15% loss of intermolecular binding energy of the CL-20/TNT co-crystal, which means intact co-crystal structure can further enhance its own stability. In terms of experimental investigations, Hu et al. [15] examined the impact sensitivity of CL-20/TNT co-crystal and raw CL-20 with the characteristic drop height criterion and tested the friction sensitivity of the two explosives with the explosion probability criterion (both according to GJB772A-97 601.2 standard), finding that the co-crystal prevails raw CL-20 to a large extent in both sides (39 cm, 68% compared with 13 cm, 100%). Bolton et al. [10] demonstrated with fast heating differential scanning calorimetry tests (DSC) that CL-20/TNT co-crystal converts to TNT liquid and β-CL-20 at 136 ℃. Yang et al. [16,17] obtained a similar result with the same experimental method that the CL-20/TNT co-crystal structure raised the melting point of TNT by 54 ℃. In conclusion, according to all the theoretical calculations and experimental results, the CL-20/TNT co-crystal structure can not only increase the mechanical and thermal stability of the interior CL-20 but maintain the solid form of TNT at a temperature much higher than its melting point as well. However, seeing that the decomposition temperature judged by DSC is dramatically affected by the heating rate [18-20], it has become quite necessary to reconsider the thermal stability and decomposition temperature of CL-20/TNT co-crystal. In that case, decomposition experiments at different heating rates or fixed temperatures were carried out in order to reinvestigate its thermal stability within different temperature ranges. Those efforts would provide solid proofs for the security of CL-20/TNT co-crystal and shed light on the thermal decomposition mechanisms of this promising co-crystal explosive.

OBJECTIVES

CL-20 and TNT samples were provided by Institute of Chemical Materials while the CL-20/TNT co-crystal sample were provided by the North University of China. Powder samples were ground from particle samples before used in experiments. The CL-20&TNT mixture in a control group was prepared by grinding CL-20 and TNT compound with 1: 1 molar ratio.

METHODS

X-Ray Diffractometer (XRD) with CuKα radiation source, SmartLab (9kW) XG, produced by Rigaku. Thermal Gravimetric Analyzer (TGA) and Differential Scanning Calorimeter, Discovery, produced by TA. Raman spectrometer with excitation wavelength of 632.8 nm, LabRAM HR800, produced by Horiba. Scanning Electron Microscopy (SEM), SU8000, produced by Hitachi.

EXPERIMENT RESULTS

Lattice Parameters Influenced by Temperature

Figure 1 shows XRD pattern and refinement result of the CL-20/TNT co-crystal sample at room temperature 294 K. The lattice constants are a = 9.735 Å, b = 19.900 Å and c = 24.682 Å, with α = β = γ = 90 °, compared with the data acquired at 95 K: a = 9.674 Å, b = 19.369 Å and c = 24.690 Å, with α = β = γ = 90 ° provided by Bolton et al. [21] (CSD reference code: 826174). We can see from this contrast that with temperature rising from 95 K to 293 K, the CL-20/TNT co-crystal expanded by 0.63%, 2.74% and -0.03% in a, b and c direction, respectively. Notice that b direction exactly corresponds to the way that CL-20 and TNT layers stack alternately.

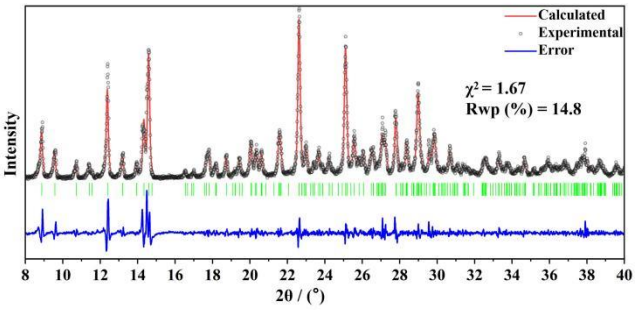
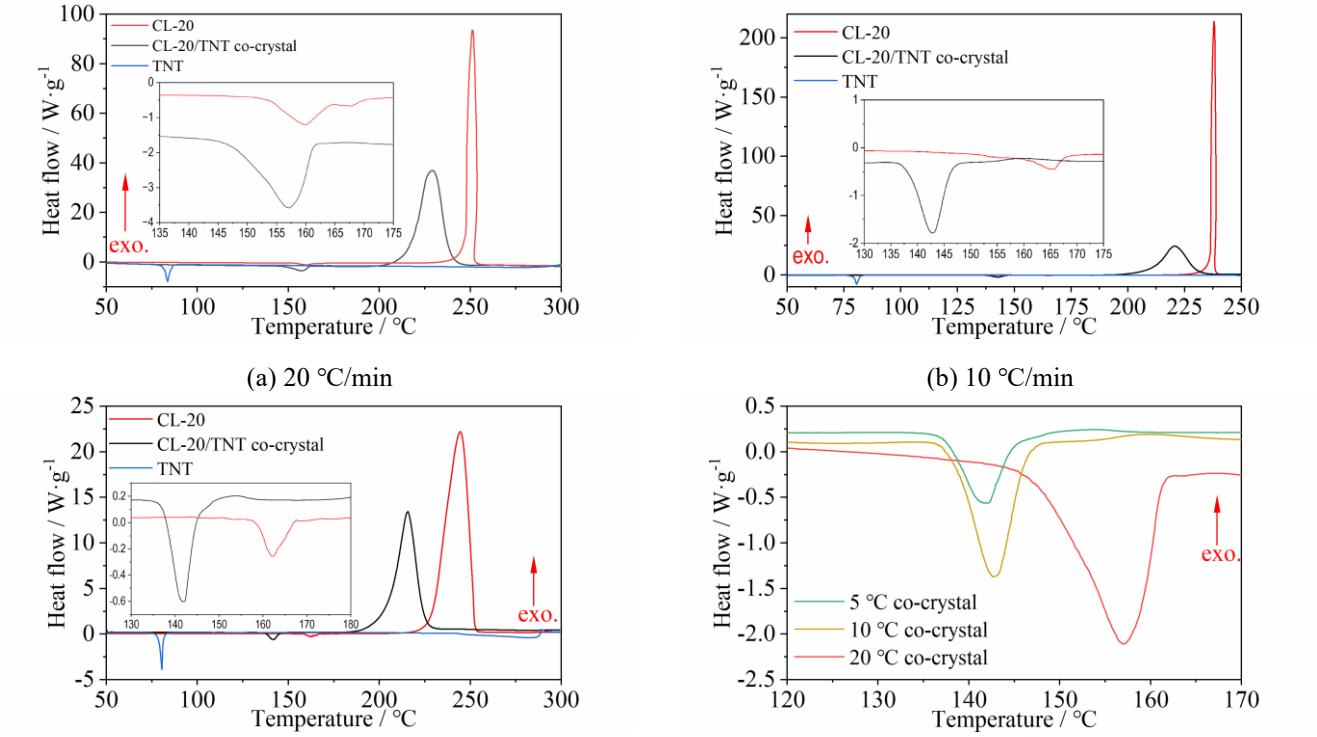


Figure 1. XRD pattern and refinement result of the CL-20/TNT co-crystal sample

Thermal Decomposition Behavior Influenced by Heating Rate

In order to verify the effect that the heating rate may have on DSC curves, DSC measurements under different heating rates were carried out on CL-20 co-crystal, CL-20 and TNT samples, 1 mg each, as shown in Figure 2. In Figure 2(d), the CL-20/TNT co-crystal was clearly observed to decompose at 147 ℃, 136 ℃ and 134 ℃ under heating rate of 20, 10 and 5 ℃·min^{-1}, respectively. Previously, Bolton et al. [10] found with the fast heating DSC test that CL-20/TNT co-crystal converts to TNT liquid and β-CL-20 at 136 ℃, while Yang et al. [16] used the same experimental method finding that CL-20/TNT co-crystal structure raises the melting point of TNT by 54 ℃ (134 ℃). Those precedent conclusions accord well with Figure 2(b), but Figure 2(d) shows that decomposition temperatures determined by DSC tests are critically affected by the heating rate. The faster the co-crystal is heated, the higher decomposition temperature should be acquired. With temperature rising fast the decomposition behavior at relatively low temperature can hardly be observed, which results in an apparent lag in the endothermic peak, leading to overestimation of the decomposition temperature. In that case, the temperature where CL-20/TNT co-crystal disintegrates should be reconfirmed.



(a) 20 °C/min

(b) 10 °C/min

(c) 5 °C/min

(d) endothermic peaks of the co-crystal at different heating rates

Figure 2. DSC and TGA curves of CL-20/TNT co-crystal, ε-CL-20 and TNT with heating rate (a) 20 °C/min, (b) 10 °C/min, (c) 5 °C/min and (d) Endothermic peaks of the co-crystal at different heating rates

In Figures 2(a), 2(b) and 2(c), the exothermic peak of CL-20 oxidation in pure CL-20 is later than that of CL-20/TNT co-crystal, because the CL-20 product of the co-crystal decomposition has far more defects (as shown in Figure 3) and far less thermal stability than pure CL-20. It means that CL-20 molecules have better thermal stability in intact CL-20/TNT co-crystal [11,12], but much worse stability in decomposition product than in pure CL-20. What's more, CL-20/TNT co-crystal will no longer provide CL-20 molecules with higher mechanical stability as well after co-crystal breaking down [15]. In conclusion, keeping the CL-20/TNT co-crystal structure intact is a crucial precondition of its safety in applications.

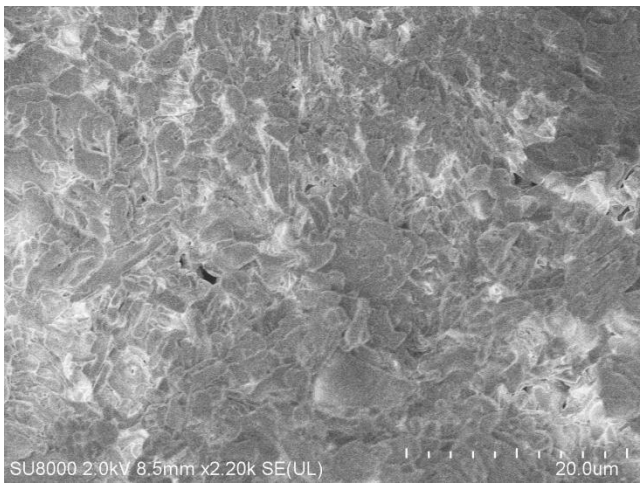


Figure 3. SEM image of decomposition residue of CL-20/TNT co-crystal

Decomposition Temperature Reconfirmation

It has become of great importance to verify the thermal stability of CL-20/TNT co-crystal lower than the announced 136 °C [10] and 134 °C [16], and to avoid the affection that the heating rate has on the detection of decomposition temperature. That being the case, a staged insulation experiment was carried out on a 2.1 mg CL-20/TNT co-crystal block sample. The subject was kept

at 90 ℃, 95 ℃ and 100 ℃ in sequence, as shown in Fig. 4. It can be observed from this figure that the co-crystal sample lost 1% mass over three hours at 90 ℃, 3% at 95 ℃ and 6% at 100 ℃, which manifests that the thermolysis temperature of CL-20/TNT co-crystal can be no higher than 90 ℃. There exists a slow decomposition period before the well recognized fast decomposition period, which can't be effectively detected by fast heating DSC tests.

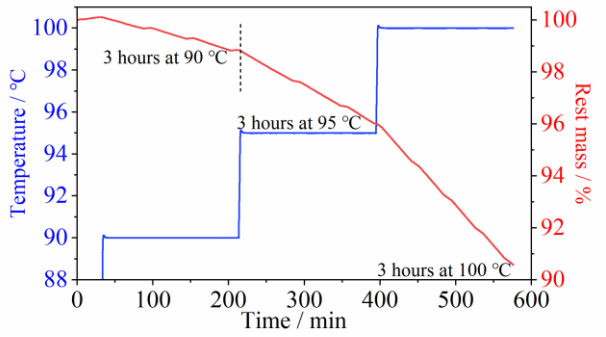
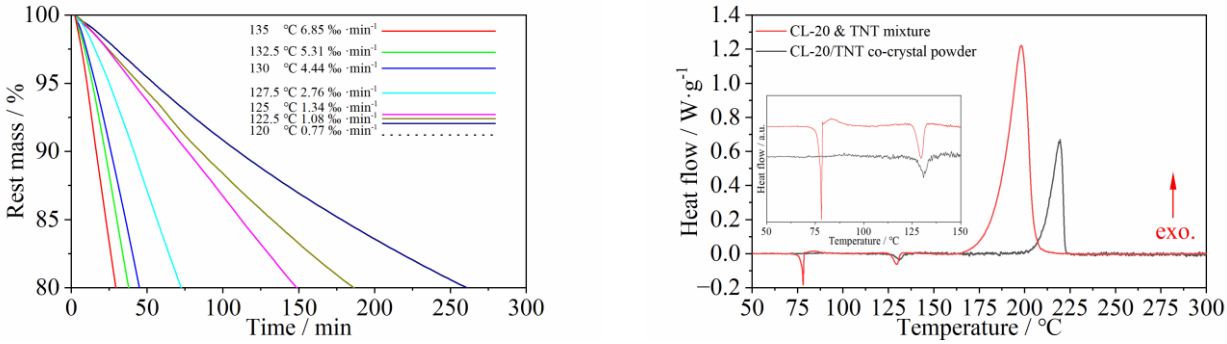


Figure 4. TGA curve of CL-20/TNT co-crystal held for three hours at 90 ℃, 95 ℃ and 100 ℃, respectively

The Critical Temperature between the Slow and Fast Decomposition Period

Insulation TGA and slowly heating DSC tests were carried out in order to make clear the temperature where CL-20/TNT co-crystal switches from slow to fast decomposition. In Fig. 5a, 1 mg co-crystal powder was kept at certain temperatures within the range from 120 ℃ to 135 ℃ and the distances between the colored lines in the figure represent the different decomposition rates. It's obvious in Fig. 5a that when the temperature exceeded approximately 127 ℃, the decomposition rate of the co-crystal suddenly lifts up. Besides, it can be seen from Fig. 5b that the endothermic peak of the co-crystal decomposition emerged at about 127 ℃ with the sample heated at a rather low rate of 0.5 ℃·min^{-1}. The results above both suggest that the co-crystal enters the fast decomposition period at around 127 ℃. What's more, Figure 5(b) shows that the endothermic peak of CL-20 phase transition in the CL-20&TNT mixture appear at the same temperature. It's supposed that the acceleration of the co-crystal decomposition is relevant to CL-20's phase transformation tendency to γ phase [3].

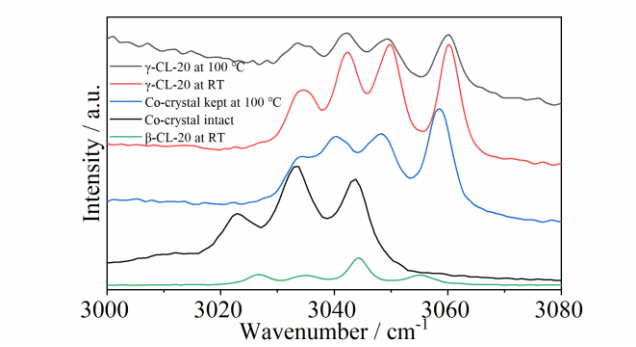


(a) TGA curves (b) DSC curve (0.5 ℃/min)

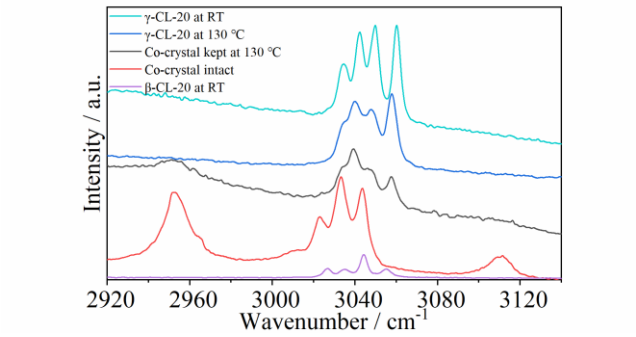
Figure 5. Isothermal TGA curves and DSC curve of CL-20/TNT co-crystal

Solid Product of Thermal Decomposition

In order to verify that the tendency of CL-20 to transit to γ phase has something to do with the thermolysis rate of CL-20/TNT co-crystal, it has become of great importance to make sure the phase of the CL-20 product of the decomposition. Two samples of co-crystal powder, 1 mg each, were held at 100 ℃ and 130 ℃, respectively, whose solid products were identified by Raman spectrum. Figure 6 indicates that after whether fast or slow decomposition period, the Raman characteristic peaks of the co-crystal converted to characteristic peaks of γ-CL-20. This testifies from another prospective that the sharp increase in the co-crystal decomposition rate is connected with the phase transformation of CL-20.



(a) C-H stretching vibrations of CL-20/TNT co-crystal held at 100 ℃



(b) C-H stretching vibrations of CL-20/TNT co-crystal held at 130 ℃

Figure 6. C-H stretching vibrations of (a) CL-20/TNT co-crystal kept at 100 ℃ and (b)130 ℃ compared with those of γ-CL-20.

β-CL-20 is a metastable phase [22], which has almost the same molecular morphology with CL-20 within CL-20/TNT co-crystal structure [23]. However, CL-20 of *β* phase converts to γ phase at around 129 ℃ (Figure 7), so the 100 ℃ insulation experiment exhibited in Figure 6(a) wipes out the possibility that the decomposition of the co-crystal produces *β*-CL-20 before it finally converts to γ phase.

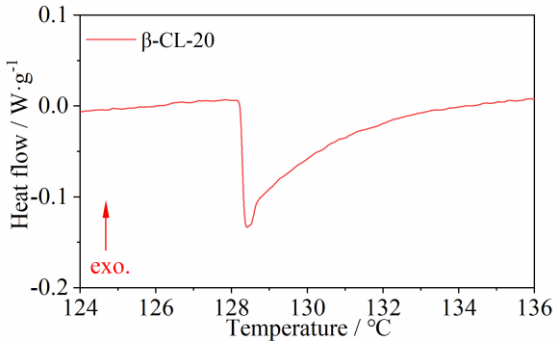


Figure 7. DSC curve of β-CL-20 heated at a rate of 10 ℃·min^{-1}

Activation Energy of CL-20/TNT Co-crystal Thermal Decomposition

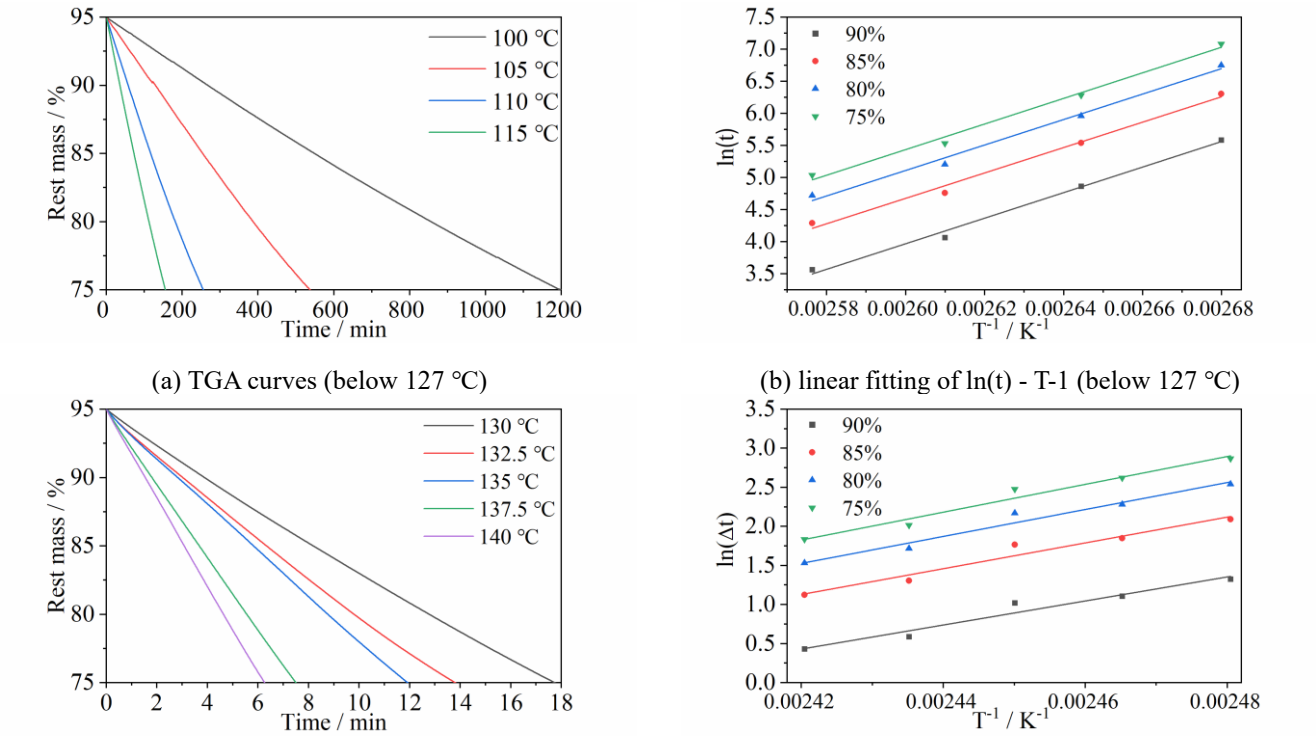
In order to investigate the mechanism differences between the fast and slow decomposition, a series of insulated TGA tests were carried out to figure out the activation energy below and above 127 ℃, as shown in Fig. 8a, c. Arrhenius equation [24,25] was employed as follow:

$$k = Ae^{-\frac{E_a}{RT}} \quad (1)$$

In Eq. (1), k (min^{-1}) represents the decomposition rate of CL-20/TNT co-crystal, which is in this context the mass loss percentage per unit time. A represents Arrhenius constant; E_a (J·mol^{-1}) activation energy; R (8.314 J·mol^{-1}·K^{-1}) gas constant; T (K) temperature. After some certain mathematical manipulation, we get:

$$\ln t = \frac{E_a}{RT} + const \quad (2)$$

In Eq. (2), t (min) represents the time consumed by the same mass percentage loss at different temperatures. Due to the fact that TGA curves fluctuate when heated to the supposed temperatures, we took the points where there are 95% mass percentage left as the beginning of the curves. $\ln t$ - $\frac{1}{T}$ curves were plotted as shown in Figure 8(b), (d), and $\frac{E_a}{R}$ was obtained by linear fitting with the least squares method. The activation energies of CL-20/TNT co-crystal below and above 127 ℃ are 167 kJ·mol^{-1} and 141 kJ·mol^{-1} in sequence.



(a) TGA curves (below 127 ℃)

(b) linear fitting of ln(t) - T-1 (below 127 ℃)

(c) TGA curves (above 127 ℃)

(d) linear fitting of ln(t) - T-1 (above 127 ℃)

Figure 8. TGA curves of CL-20/TNT co-crystal kept at various temperature points and their ln(t) - T^{-1} linear fitting results

Results and Discussions

CL-20/TNT co-crystal decomposes slowly within the temperature range from 90 ℃ to 127 ℃, which can't be effectively detected by the generally adopted DSC test. However, insulation TGA is able to observe the weight loss of TNT during the co-crystal decomposition procedure. The existence of the slow decomposition period means that the CL-20/TNT co-crystal structure can't maintain the solid form of TNT inside it at a temperature much higher than its melting point [10][16], but it can greatly slow down the melting period of TNT above its melting point. Co-crystals have long-range orders just like average crystals, and the decomposition of CL-20/TNT co-crystal is a pure physical process. Considering this, it appears quite fascinating to see CL-20/TNT co-crystal even needs five hours to decompose completely at a temperature 35 ℃ higher than its own decomposition temperature, which behaves like an amorphous body. This phenomenon indicates that there are still much left to explore in the CL-20/TNT co-crystal.

Above 127 ℃, the co-crystal steps into the fast decomposition period. The two decomposition procedures have different activation energies and of course, different mechanisms. 127 ℃ accords well with the temperature where the CL-20 in CL-20&TNT mixture transforms to γ phase, the temperature where pure CL-20 transits from ε or β phase to γ phase (125 ℃ and 129 ℃ respectively), and the temperature where CL-20/DNB co-crystal starts to decompose [26]. Besides, the solid decomposition product of CL-20/TNT co-crystal has been confirmed as γ-CL-20. With all those evidences, the tendency that CL-20 tries to convert to γ phase above 127 ℃ is supposed to have great relations with the co-crystal decomposition acceleration.

Analysis of the Thermal Decomposition Mechanism

The comparison between the XRD refinement result (Figure 1) and the data from CSD indicates that with temperature rising, CL-20/TNT co-crystal expands primarily in b direction, which is exactly the way CL-20 and TNT layers stack alternately.

Therefore, the hydrogen bonds linking the two kinds of molecules, which serve as the main cohesion force of the co-crystal [10], extends greatly when heated. Within the temperature range from 90 ℃ to 127 ℃, the distance between CL-20 and TNT layers increases and the hydrogen bonds between the two kinds of molecules weaken and slowly break. TNT molecules gradually free themselves from the CL-20 layers and volatilize fast, before CL-20 layers lose their core confinement becoming almost free. The CL-20 molecules need far less activation energy without restriction of the co-crystal structure [27] to recrystallize to γ phase, so such a process can't take place before the collapse of the co-crystal and thus have no influence on the decomposition procedure. Over 127 ℃ the mechanism mentioned above still exists and becomes stronger. What's more, CL-20 molecules in this temperature range already have enough activation energy to directly transit to γ phase. In this process, CL-20 molecules rearrange and rupture their hydrogen bonds with TNT molecules, forcing the later to escape the co-crystal structure faster. That explains why the co-crystal speeds up to decompose and the activation energy for co-crystal structure collapsing shrinks above 127 ℃.

CONCLUSIONS

(1) CL-20/TNT co-crystal undergoes a slow decomposition period before the well recognized fast decomposition behavior, which can't be effectively detected by the generally adopted DSC tests. Although the CL-20/TNT co-crystal can't raise the melting temperature of TNT to such a large extent as some articles declared, it can greatly slow down the melting behavior, manifested as the explosive responding slowly to temperature increase. Insulation TGA tests are able to accurately identify the weight loss caused by decomposition.

(2) The slow decomposition period exists between 90 ℃ and 127 ℃, while the fast period starts above 127 ℃. Their mechanisms are not accurately the same, with different activation energies of 141 $kJ \cdot mol^{-1}$ and 167 $kJ \cdot mol^{-1}$, respectively. The solid products of both fast and slow decomposition periods are γ-CL-20.

(3) CL-20 has a strong tendency to transform to γ phase above 127 ℃, which significantly accelerates the thermal decomposition of the co-crystal. The same mechanism may take effect on CL-20/DNB co-crystal and other CL-20 based co-crystals.

(4) Between 90 ℃ and 127 ℃, the distance between CL-20 and TNT layers increases, leading to gradual breakage of the hydrogen bonds between the two kinds of molecules. TNT molecules slowly escape and the co-crystal structure collapse at a quite low rate. Above 127 ℃, CL-20 molecules already have enough activation energy to recrystallize in γ phase, which further reduces the activation energy it takes for TNT molecules to free themselves from the co-crystal structure. In that case, the decomposition process accelerates.

ACKNOWLEDGMENT

This work was supported by the Fund of National Key Laboratory of Shock Wave and Detonation Physics (No. JCKYS2022212008), the Fundamental Research Funds for the Central Universities (No. WK2030000058), infrared spectroscopy and micro spectroscopy at National Synchrotron Radiation Laboratory (NSRL, Hefei).

REFRENCES

[1] Sun Kang-bo, Zhang Shu-hai, Hao Yong-ping, et al. Preparation and Characterization of CL-20/DMMD Co-crystal Explosive. Chinese Journal of Energetic Materials (Hanneng Cailiao), 2021, 29 (9): 790-797.

[2] An Chong-wei, Li He-qun, Ye Bao-yun, et al. Nano-CL-20/HMX Cocrystal Explosive for Significantly Reduced Mechanical Sensitivity. Journal of Nanomaterials, 2017, 2017 (1): 3791320.

[3] Doblas D, Rosenthal M, Burghammer M, et al. Smart energetic nanosized co-crystals: exploring fast structure formation and decomposition. Crystal Growth & Design, 2016, 16 (1): 432-439.

[4] Pi Zheng-di, Chen Lang, Wu Jun-ying. Temperature-dependent shock initiation of CL-20-based high explosives. Central European Journal of Energetic Materials, 2017, 14 (2): 361-374.

[5] Guo Chang-ping, Wang Dun-ju, Gao Bing, et al. Solid–solid phase transition study of ε-CL-20/binder composites. RSC advances, 2016, 6 (2): 859-865.

[6] Huang Ye-ming, Wang Xin, Zhang Jing-xuan, et al. Preparation and Performance of Low Sensitivity CL-20@ GO Core-shell Composites by Electrostatic Assembly. Chinese Journal of Explosives & Propellants, 2024, 47 (1).

[7] Mao Xiao-xiang, Li Yan-chun, Li Yi-fan, et al. Thermal properties of decomposition and explosion for CL-20 and CL-20/n-Al. Journal of Energetic Materials, 2020, 38 (1): 98-110.

[8] Liu Hai., Yang Zhen, He Yuan-hang. Atomistic Simulation on Pyrolysis Mechanism of CL-20/TNT Cocrystal Explosive. Chinese Journal of Explosives & Propellants, 2017, 40(1), 14-20

[9] Rao K S, Ganesh D, Yehya F, et al. A comparative study of thermal stability of TNT, RDX, CL20 and ANTA explosives using UV 266 nm-time resolved photoacoustic pyrolysis technique. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2019, 211: 212-220.

[10] Bolton O, Matzger A J. Improved stability and smart-material functionality realized in an energetic cocrystal. Angewandte Chemie International Edition. 2011.

[11] Guo De-zhou, An Qi, Zybin S V, et al. The co-crystal of TNT/CL-20 leads to decreased sensitivity toward thermal decomposition from first principles based reactive molecular dynamics. Journal of Materials Chemistry A, 2015, 3 (10): 5409-5419.

[12] Hang Gui-yun, Yu Wen-li, Wang Tao, et al. Comparative studies on structures, mechanical properties, sensitivity, stabilities and detonation performance of CL-20/TNT cocrystal and composite explosives by molecular dynamics simulation. Journal of molecular modeling, 2017, 23 (10).

[13] Ren Chun-xing, Li Xiao-xia, Guo Li. Chemical insight on decreased sensitivity of CL-20/TNT cocrystal revealed by ReaxFF MD simulations. Journal of chemical information and modeling, 2019, 59 (5): 2079-2092.

[14] Hang Gui-yun, Yu Wen-li, Wang Tao, et al. Theoretical investigations into effects of adulteration crystal defect on properties of CL-20/TNT cocrystal explosive. Computational Materials Science, 2019, 15677-83.

[15] Hu Yu-bing, Yuan Shuo, Li Xiao-jiang, et al. Preparation and characterization of nano-CL-20/TNT cocrystal explosives by mechanical ball-milling method. ACS omega, 2020, 5 (28): 17761-17766.

[16] Yang Zong-wei, Li Hong-zhen, Huang Hui, et al. Preparation and performance of a HNIW/TNT cocrystal explosive. Propellants, Explosives, Pyrotechnics, 2013, 38 (4): 495-501.

[17] Yang Zong-wei, ZHANG Yan-li, LI Hong-zhen. Preparation, structure and properties of CL-20/TNT cocrystal. Chinese Journal of Energetic Materials (Hanneng Cailiao), 2012, 20 (6): 674-679.

[18] Liang Wen-tao, Sun Xiao-yu, Wang He, et al. Isothermal structural evolution of CL-20/HMX cocrystals under slow roasting at 190° C. Physical Chemistry Chemical Physics, 2023, 25 (23): 15756-15766.

[19] Tompa A S, Bryant Jr W F. Microcalorimetry and DSC study of the compatibility of energetic materials. Thermochimica acta, 2001, 367: 433-441.

[20] Zheng Liang, Liu Yu-feng, Liu Yang, et al. Influencing Factors on Differential Scanning Calorimetry (DSC) Analysis of Superalloy Ⅲ: Alloy State and Heating/Cooling Rate. Rare Metal Materials and Engineering, 48(6):1944

[21] Bolton O, Matzger A J. CCDC 826174: Experimental Crystal Structure Determination, 2011.

[22] Liu Ke, Zhang Gao, Luan Jie-yu, et al. Crystal structure, spectrum character and explosive property of a new cocrystal CL-20/DNT. Journal of Molecular Structure, 2016, 1110: 91-96.

[23] Shi Lu, Duan Xiao-hui, Zhu Li-guo, et al. Directly insight into the inter-and intramolecular interactions of CL-20/TNT energetic cocrystal through the theoretical simulations of THz spectroscopy. The Journal of Physical Chemistry A, 2016, 120 (8): 1160-1167.

[24] Yang Zhen, Xue Yi-jiang, He Yuan-hang. Thermal sensitivity of CL20/DNB co-crystal research via molecular dynamics simulations. Acta Chimica Sinica, 2016, 74 (7): 612-619.

[25] Liu Hong, Li Qi-kai, He Ya-hong. Pyrolysis of CL20-TNT cocrystal from ReaxFF/lg reactive molecular dynamics simulations. Wuli Xuebao/Acta Physica Sinica, 2013, 62 (20): 208202.

[26] Sun Xiao-yu, Liang Wen-tao, Li Xiang-dong, et al. Structural evolution of CL-20/DNB cocrystals at high temperature: Phase transition and kinetics of thermal decomposition. Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2023, 292122436-122436.

[27] Zhang Pu, Xu Jin-jiang, Guo Xue-yong, et al. Effect of addictives on polymorphic transition of ε-CL-20 in castable systems. Journal of Thermal Analysis and Calorimetry, 2014, 117: 1001-1008.