6-((2H-tetrazol-5-yl)-amino)-1,2,4,5-tetrazin-3(2H)-one: High-nitrogen Insensitive Energetic Compound Stabilized by π-stacking and Hydrogen-bonding Interactions

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Abstract: 6-((2H-tetrazol-5-yl)-amino)-1,2,4,5-tetrazin-3(2H)-one (TATzO) was synthesized and characterized by FT-IR, elemental analysis, 1H NMR and 13C NMR and single crystal X-ray diffraction. The single crystal structure solution indicates that a hydrate forms (TATzO·H2O) and it crystallizes in the orthorhombic Pnma space group with a density of 1.730 g·cm⁻³ and 296 K. The thermal behavior and thermal decomposition kinetic of TATzO·H2O were studied by differential scanning calorimetry (DSC) and thermogravimetry-derivative thermogravimetry (TG-DTG) methods. The thermal decomposition peak temperature is determined to be 230.46°C, indicating a similar thermal stability to cyclotrimethylenetetranitramine (RDX). The apparent activation energies (E) and pre-exponential constant (A) of the compound are 169.03 kJ·mol⁻¹ and 15.65 s⁻¹, respectively. The thermal ignition temperature (Tₗ) and the critical temperature of thermal explosion (Tₜₑ) are 213.75°C and 223.03°C, respectively. The enthalpy of formation was theoretically calculated by Gaussian03, and the detonation velocity (D) and detonation pressure (p) were calculated by the Kamlet-Jacobs (K-J) equation. The obtained D and p are 7757m·s⁻¹ and 25.74 GPa, respectively. The impact sensitivity is larger than 24 J.

Key words: energetic material; 6-((2H-tetrazol-5-yl)-amino)-1,2,4,5-tetrazin-3(2H)-one; crystal structure; thermal behavior; detonation properties

CLC number: TJ55; O64

1 Introduction

The energetic materials (EMs) used at present are mainly nitro (−NO₂), nitrate (−ONO₂), and nitramine (−NHNO₂) containing compounds, such as 2,4,6-trinitrotoluene (TNT), Hexogone (RDX) and Octagon (HMX). These materials, however, have drawbacks of sensitive to external stimulus, high toxicity and high environmental contamination during production. Herein, it is essential to exploit alternative environmentally friendly and insensitive energetic materials[1]. High-nitrogen heterocycle compounds, including tetrazine, tetrazole and triazole, exhibit excellent properties such as high positive heats of formation (HOF), high density, low sensitivity, good thermal stability, and releasing environment-friendly decomposition products[2-5]. The 1,2,4,5-tetrazine heterocycle with four nitrogen atoms in the six-member ring, is electron-deficient at positions 3 and 6, at which nucleophilic aromatic substitution is extremely easy to take place[6-7]. Therefore, the oxygen balance and density of tetrazine derivatives could be further improved by introducing various explosophores at these two positions.

As high nitrogen content heterocycles, 1,2,4,5-
tetrazine derivatives have shown great potential in the design of EMs and several related compounds have been reported. However, to the best of our knowledge, most of these studies focused on the synthesis and characterization of symmetrical tetrazine compounds. The unsymmetrical 1,2,4,5-tetrazine derivatives, such as 3-amino-6-nitroamino-tetrazine (ANAT) and 3-(3,3′-dinitroacetidine)-6-(3,5-dimethylpyrazole)-tetrazine (DNAZTzDMP), also have high positive HOF, good thermal stability, excellent detonation performance and mechanical stability for the applications of EMs. Probably due to the need for more synthetic steps, the derivatives of unsymmetrical 1,2,4,5-tetrazine are seldom studied. Therefore, it is worthy of taking effort to explore novel unsymmetrical 1,2,4,5-tetrazine based materials.

Hydrogen bonding interaction plays an important role in reducing sensitivity and increasing density of EMs. The introduction of hydrogen bonding donor and acceptor to a main moiety is good strategy for design EMs. In addition, the crystal packing within a lattice has been shown a great influence on the sensitivity of EMs. Explosives that have parallel layers are generally less sensitive to mechanical stimuli due to the ability of the layers to freely slide and disperse energy upon external stimuli. A co-planar molecular structure combining with multiple hydrogen bonding interactions may result in insensitive EMs.

In view of the above considerations, we designed and synthesized a novel unsymmetrical tetrazine derivative 6-((2H-tetrazol-5-yl)-amino)-1,2,4,5-tetrazin-3(2H)-one (TATZo) using BTATz (3,6-Bis(1H-1,2,3,4-tetrazol-5-yl-amino)-1,2,4,5-tetrazine) as a raw material. In the structure, three NH act as hydrogen donors while unprotonated N atoms and ketone O atom act as hydrogen acceptors. The crystal structure and thermal behavior of TATZo were investigated by single crystal X-ray diffraction, DSC and TG-DTG. The thermal explosion critical temperature (Texp) was also estimated to evaluate the thermal safety performance. Besides, the detonation properties, including the detonation velocity (D) and pressure (P), were calculated based on Kamlet-Jacobs (K-J) equation, and the impact sensitivity (IS) was determined.

2 Experimental Part

2.1 Experimental Measurements

3,6-bis(3,5-dimethylpyrazolyl)-1,2,4,5-tetrazine (BT) and 3,6-bis(1H-1,2,3,4-tetrazol-5-ylamino)-1,2,4,5-tetrazine was prepared according to the Ref[7]. Sodium hydroxide and hydrochloric acid were purchased from Aladdin and used without further purification.

IR spectra were determined using an IRAffinity-1S spectrometer with ATR (Shimadzu). Elemental analysis was performed on a VarioEL III analyzer (Elementar Co.). 1H and 13C NMR spectra were recorded on 600 MHz NMR spectrometer (Bruker) at 25 °C, respectively. TG-DTG and DSC measurements were performed on SDT-Q600 (TA) and Q2000 (TA) apparatus under nitrogen atmosphere at a heating rate of 10 °C min⁻¹ with the nitrogen flowing rate of 50 ml/min⁻¹. The HOF of the title compound was theoretically calculated using Gaussian 03 program package[12].

The impact sensitivity test was performed on a ZBL-B impact sensitivity instrument (Nachcn). The mass of drop hammer was 2.0 kg, and the sample mass for test was 30 mg.

2.2 Synthesis of TATZo

BTATz (0.9 g, 4 mmol) was immersed in 1.0 mol/L NaOH solution (5mL) for 10 h at 25 °C with stirring. After that, the obtained solution was neutralized with 3 mol/L HCl aqueous solution until the bright orange precipitate formed. The precipitate was filtered, washed with H₂O and dried under vacuum to give TATZo as orange solid or powder (Scheme 1). Elemental analysis: calcd (%) for C₉H₈N₂O₂: C 19.82, H 1.84, N 70.21; found: C 19.89, H 1.67, N 69.90. IR (ATR, ν/cm⁻¹): 3498(w), 3433(w), 3252(m), 3184(m), 1693(s), 1573(s), 1514(s), 1406(s), 1357(m), 1155(m), 1103(s), 1043(s), 993(s). 1H NMR (600 MHz, DMSO-d₆): δ 12.13(s, 1H); 13C NMR (600 MHz, DMSO-d₆): δ 151.2, 151.7, 155.6.

2.3 Crystal Structure Determination

The crystal of TATZo was chosen for X-ray de-
termination. The data were collected on a Bruker SMART APEX CCD X-ray diffractometer (Bruker, Germany) with graphite-monochromatized Mo-Kα radiation (λ = 0.071073 nm). The structure was solved by the direct methods and refined by the full-matrix least-squares method on F2 with anisotropic thermal parameters for all nonhydrogen atoms (SHELXS-97 and SHELXL2014)\textsuperscript{11,14}. The hydrogen positions for water molecules were calculated by Fourier syntheses and hydrogen atoms of TATzO were added to their geometrically ideal positions and refined isotropically using a riding model. Crystal data and refinement results were summarized in Table 1 (CCDC 1873209).

3 Results and Discussion

3.1 Synthesis of the Title Compound

We initially tried to prepare the target compound through path 1 (Scheme 1), and successfully obtained intermediate compound 6-((3,5-dimethylpyrazol-1-yl)-1,2,4,5-tetrazin-3(2H)-one(DPTzO))\textsuperscript{15}. Then we attempted to synthesize TATzO involved the reaction of DPTzO and 5-amino-tetrazole(5-AT) in refluxing methanol. However, no product was obtained even after long reaction time. The reason was speculated to be that the strong electron-withdrawing effect of the ketone group reduces nucleophilic substitution ability of the para-carbon position of the tetrazine. After considering the reactivity of the tetrazine moiety, we switched the synthetic route to path 2 and successfully obtained the target compound.

3.2 Structural Characterization

It crystallizes with a calculated density of 1.730 g·cm\textsuperscript{-3} at 296 K in the orthorhombic Pnma space group. A water molecule co-crystallize in the single crystal so that the structure can be described as TATzO·H\textsubscript{2}O (Fig.1). For the tetrazine and tetrazole rings, the N—C bond lengths are within the range between 1.276 Å to 1.410 Å and an average value of 1.351 Å, which is longer than normal N—C bond (1.22 Å) and shorter than normal N—C bond (1.47 Å) (Table 2). The N—N bond lengths have a minimum of 1.276 Å for N(1)—N(2) and a maximum of 1.355 Å for N(3)—N(4), which is longer than that of the normal N≡N bond (1.20 Å) and

![Scheme 1 Synthesis of TATzO](Image)

**Table 1** X-ray diffraction data collection and refinement parameters for TATzO·H\textsubscript{2}O

<table>
<thead>
<tr>
<th>Chemical formula</th>
<th>C\textsubscript{21}H\textsubscript{18}N\textsubscript{9}O·H\textsubscript{2}O</th>
</tr>
</thead>
<tbody>
<tr>
<td>M/ g·mol\textsuperscript{-1}</td>
<td>199.16</td>
</tr>
<tr>
<td>Crystal system</td>
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</tr>
<tr>
<td>Space group</td>
<td>Pnma</td>
</tr>
<tr>
<td>V/ Å\textsuperscript{3}</td>
<td>764.6(7)</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>D\textsubscript{calc} / g·cm\textsuperscript{-3}</td>
<td>1.730</td>
</tr>
<tr>
<td>F(000)</td>
<td>408.0</td>
</tr>
<tr>
<td>a / Å</td>
<td>14.217(8)</td>
</tr>
<tr>
<td>b / Å</td>
<td>6.209(3)</td>
</tr>
<tr>
<td>c / Å</td>
<td>8.662(5)</td>
</tr>
<tr>
<td>a / (°)</td>
<td>90.0</td>
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<td>90.0</td>
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<tr>
<td>θ / (°)</td>
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</tr>
<tr>
<td>R\textsubscript{int}</td>
<td>0.1098</td>
</tr>
<tr>
<td>Goodness-of-fit on F\textsuperscript{2}</td>
<td>1.002</td>
</tr>
<tr>
<td>R indices (I &gt; 2σ(I))</td>
<td>R\textsubscript{I}=0.0603, wR\textsubscript{I}=0.1279</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>R\textsub{2}=0.1275, wR\textsub{2}=0.1511</td>
</tr>
<tr>
<td>Index ranges</td>
<td>18≤h≤18,-6≤k≤6,-11≤l≤11</td>
</tr>
<tr>
<td>Reflections collected/unique</td>
<td>945/4147</td>
</tr>
<tr>
<td>T/K</td>
<td>296</td>
</tr>
</tbody>
</table>

![Fig.1 The asymmetric unit of TATzO·H\textsubscript{2}O, with displacement ellipsoids drawn at the 30% probability level.](Image)
axis hydrogen-bond interactions are shown as dashed

It is reported that the intensive

The tetrazine ring and the tetrazole moiety connect-
ed by amino group located on a crystallographic mirror plane. Thus, the whole molecule is a plane structure. The TATzO and solvent molecules bring about six types of hydrogen bonds in the crystal (Table 3).

 shorter than that of the normal N—N bond (1.41 Å)\(^{[16]}\).

The tetrazine ring and the tetrazole moiety connected by amino group located on a crystallographic mirror plane. Thus, the whole molecule is a plane structure. The TATzO and solvent molecules bring about six types of hydrogen bonds in the crystal (Table 3), including five intermolecular hydrogen bonds (O(2) —H(2)…N(9)\(^{[1]}\), O(2) —H(2)A…N1\(^{[8]}\), N(3) —H(3)…N(8)\(^{[8]}\), N(5) —H(5)…O(1)\(^{[8]}\), N(6) —H(6)…O(2)\(^{[2]}\) and one intramolecular hydrogen bond (N(6) —H(6)…N(4)).

<table>
<thead>
<tr>
<th>Table 3</th>
<th>Hydrogen-bond geometry of TATzO·H(_2)O</th>
</tr>
</thead>
<tbody>
<tr>
<td>D—H···A</td>
<td>d(D—H)</td>
</tr>
<tr>
<td>O(2) —H(2)A…N(1)(^{[8]})</td>
<td>0.86(19)</td>
</tr>
<tr>
<td>O(2) —H(2)B…N(9)(^{[1]})</td>
<td>0.84(19)</td>
</tr>
<tr>
<td>N(3) —H(3)…N(8)(^{[8]})</td>
<td>0.86</td>
</tr>
<tr>
<td>N(5) —H(5)…O(1)(^{[8]})</td>
<td>0.86</td>
</tr>
<tr>
<td>N(6) —H(6)…O(2)</td>
<td>0.86</td>
</tr>
<tr>
<td>N(6) —H(6)…N(4)</td>
<td>0.86</td>
</tr>
</tbody>
</table>

Note: Symmetry codes: (i) 0.5+x, 0.5-y, 0.5-z; (ii) x, y, -1+z; (iii) -0.5+x, 0.5-y, 1.5-z.

Besides, those hydrogen bonds also form hydrogen - bond graph - set motifs (R\(_1\)(8), R\(_1\)(10) and R(6)) , according to the definition of Bernstein\(^{[17]}\).

The extensive inter- and intramolecular hydrogen bonds link the molecules into two-dimensional layer like structure (Fig.2). It is reported that the intensive hydrogen - bonding interactions make an important contribution to improving the thermal stability and decreasing the sensitivity of EMs. On the other hand, the crystal structure of TATzO·H\(_2\)O features face-to-face geometries with the interlayer distance of 3.104 Å and the π-stacked sheets are arranged in a layer-like structure (Fig.3). In the case of external mechanical stimulation, the π-stacked structures can cause slippage between the layers, thereby counteracting external stimuli and reducing sensitivity: \(^{[18]}\)

To further understand the interactions between the molecules contained in TATzO·H\(_2\)O, the Hirshfeld surface and the 2D fingerprint spectrum were analyzed. \(^{[19-21]}\) Fig.4 shows an approximately plate-like surface, indicating that the planar molecule of TATzO·H\(_2\)O. Besides, the red dots showing the intermolecular close contacts are located on the side faces of the plate. It suggests that the intermolecular interactions in the crystal occur through the oxygen

![Fig. 2](image-url) The two-dimensional structure of TATzO·H\(_2\)O along the b axis hydrogen-bond interactions are shown as dashed lines.
and nitrogen atoms encompassing the molecules. From fingerprint spectra of TATzO·H₂O in Fig. 5, it was observed that two sharp spikes exist in the bottom left of the spectra, indicating the interactions of O···H and N···H. Among them, the interaction of N···H (44.5%) was much higher than that of O···H (16.8%), showing the main interactions of the energetic molecules were N···H interactions.

![Crystal packing of TATzO·H₂O along the c axis.](image)

**Fig. 3** Crystal packing of TATzO·H₂O along the c axis.

![Hirshfeld surface of TATzO·H₂O.](image)

**Fig. 4** Hirshfeld surface of TATzO·H₂O.

![Fingerprint spectra of TATzO·H₂O.](image)

**Fig. 5** Fingerprint spectra of TATzO·H₂O.

### 3.3 Thermal Behavior Analysis

The typical DSC and TG-DTG curves of TATzO·H₂O measured at heating rate of 10.0 K·min⁻¹ are shown in Fig. 6 and Fig. 7. Both DSC and TG-DTG curves show two reaction processes. On the DSC curve, the first stage is an endothermic decomposition process with the peak temperature of 136.34 °C due to the dehydration of crystalline water. The second stage is an intense exothermic decomposition process with the peak temperature of 230.46 °C, which is higher than 1,1-diamino-2,2-dinitroethylene FOX-7 (221.9 °C) and lower than BTATz (320.5 °C). Meanwhile, the first stage of decomposition process on TG curve between 129.18 to 138.94 °C with a mass loss of 9.14% corresponds to the releasing of crystalline water (cal: 9.05%). The second stage ranges from 213.59 °C to 234.05 °C with a mass loss of 35.49%.

![DSC curve for TATzO·H₂O at 10 °C·min⁻¹](image)

**Fig. 6** DSC curve for TATzO·H₂O at 10 °C·min⁻¹

![TG-DTG curves for TATzO·H₂O at 10 °C·min⁻¹](image)

**Fig. 7** TG-DTG curves for TATzO·H₂O at 10 °C·min⁻¹

### 3.4 Non-isothermal Kinetics and Thermal Explosion Critical Temperature

In order to estimate the thermal kinetics of the intense exothermic process of TATzO·H₂O during the decomposition process, the kinetic parameters (the apparent activation energy (E) and pre-exponential constant (A)) have been calculated through Kissinger method and Ozawa method at different T_p (maximum peak temperature) and T_o (the extrapolated onset temperature). All the data are listed in Table 4. The value of E_o obtained by Ozawa method is in agreement with E_o obtained by Kissinger method, and the linear correlation coefficient shows that the result is convincible.

Kissinger method:

\[
\ln \frac{\beta}{T_p^2} = \ln \frac{AR}{E} - \frac{E}{RT_p} \quad (1)
\]

Flynn-Wall-Ozawa method:

\[
\log \beta + \frac{0.4567E}{RT} = C \quad (2)
\]
The thermal stability of the EMs can be evaluated through the thermal ignition temperature ($T_{\text{on}}$) and the thermal explosion critical temperature ($T_{\text{e}}$). $T_{\text{on}}$ and $T_{\text{e}}$ were obtained by third order polynomial fit of the extrapolated onset decomposition temperature ($T_o$) and the extrapolated peak temperature ($T_p$) corresponding to $\beta \to 0$ based on Eqs. (3) and (4) [26-27].

The parameters $a$, $b$, and $c$ are coefficients. The values of $T_{\text{on}}$ and $T_{\text{e}}$ of the compound are 213.75 °C and 223.03 °C, respectively, which are higher than the typical explosive FOX-7 (206.0, 207.1 °C) and lower than BTATz (262.5, 272.1 °C), indicating good thermal stability of the title compound [23]. We speculate that high thermal stability is caused by the presence of a conjugation in the molecular structure and the introduction of amino groups to the structure.

$$T_{\text{on}} = T_{\text{on}} + a\beta_i + b\beta_i^2 + c\beta_i^3 + d\beta_i^4; \quad i = 1 \sim 6 \quad (3)$$

$$T_{e} = T_{e} - \frac{E_{\text{corr}} - \sqrt{E_{\text{corr}}^2 - 4E_{\text{corr}}RT_{\text{corr}}}}{2R} \quad (4)$$

### 3.5 Heats of Formation and Detonation Properties

The HOF of TATzO was calculated by designing an isodesmic reaction (Scheme 2). For the involved compounds, geometric optimization and frequency were calculated using the B3LYP functional with the 6-311+G** basis set and the HOF of C₅H₆N₄O (1, 2, 4, 5-tetrazin-3 (2H)-one) was obtained by G3 method. All of the optimized structures were characterized to be local energy minima on the potential-energy surface without any imaginary frequency. On the basis of the energy properties of the reference compounds (Table 5), the HOF of C₅H₆N₄O calculated by G3 theory is 459.92 kJ·mol⁻¹, and the HOF of TATzO was predicted to be 777.09 kJ·mol⁻¹.

![Scheme 2 Designed isodesmic reaction for the prediction of the HOF of TATzO.](image)

Then, the heat of formation of TATzO (677.8 kJ·mol⁻¹) in solid state was estimated with Trouton’s rule (Eq. 5), in which $T_d$ represents the decomposition temperature [28].

$$\Delta H_f(s) = \Delta H_f(g) + \Delta H_{\text{m}} = \Delta H_f(g) - 188 \times T_d \quad (5)$$

The performance of EMs is evaluated by its detonation velocity ($D$) and detonation pressure ($p$). And the empirical Kamlet-Jacobs (K-J) equation (Eqs. (6) - (8)) are widely applied to estimate the values of $D$ and $p$ for the explosives containing C, H, O, and N as follows [11]:

$$D = 1.01(\text{NM}_{\text{av}}^{1/2}Q^{1/2})^{1/2} (1 + 1.30p) \quad (6)$$

$$p = 1.558 \rho^{1/2} \text{NM}_{\text{av}}^{1/2} \quad (7)$$

$$Q = \frac{\Delta H_d + \Delta H_e}{\text{mass of energetic complex}} \quad (8)$$
where $D$ is detonation velocity (m·s$^{-1}$), $p$ is detonation pressure (GPa), $N$ is moles of gaseous detonation products per gram of explosives, $M_{\text{mole}}$ is average molecular weights of gaseous products, $Q$ is chemical energy of detonation (J·g$^{-1}$), and $\rho$ is the density of explosive (g·cm$^{-3}$).

When using K-J equation, for the compound of $C_9H_9N_9O_9$, TATzO ($C_9H_9N_9O_9$) suites $b/2c$, thus, the equation of explosion reaction is Equation (9):

$$C_9H_9O_9N_9 \rightarrow H_2O + (3/2 - 1) H_2 + 3C + 9/2N_2 + Q \quad (9)$$

Where $\Delta H_m^n(H_2O, l) = -241.8$ kJ·mol$^{-1}$,

$$\Delta H_m^n(H_2, g) = 0$ kJ·mol$^{-1}$,

$$\Delta H_m^n(N_2, g) = 0$ kJ·mol$^{-1}$,

$$\Delta H_m^n(C, s) = 0$ kJ·mol$^{-1}$.

The calculated density of TATzO is 1.71 g·cm$^{-3}$ by the Monte Carlo method, which is almost equal with the density of single crystal of TATzO·H$_2$O. Consequently, the calculated $Q$, $D$ and $p$ are 5082 J·g$^{-1}$, 7757 m·s$^{-1}$ and 25.74 GPa, respectively. The detonation parameters of TATzO are slightly lower than those of BTATZ (8055 m·s$^{-1}$, 25.39 GPa)[7].

### 3.6 Impact Sensitivity

Sensitivity is an important property for EMs in terms of storage and practical application. The impact sensitivity (IS) was determined by fall hammer method using 2-kg drop weight with maximum height of 120 cm. No explosion was detected after 10 time strikes which means the compound has the IS value larger than 24 J. The IS of TATzO is slightly lower than BTATZ (22 J). The reason for the low sensitivity is that there are hydrogen bonds and $\pi$ stacking in the crystal. The $\pi$ stacking in crystal makes it impossible to slide the molecules during impact resistance, resulting in counteracting external stimuli and reducing sensitivity[32].

### 4 Conclusions

1. The unsymmetrical tetrazine derivative 6-((2H-tetrazol-5-yl)-amino)-1, 2, 4, 5-tetrazin-3(2H)-one (TATzO) was synthesized and characterized by IR, EA and NMR. The hydrate with composition of TATzO·H$_2$O was confirmed by single crystal analysis. The adjacent molecules form face-to-face molecular packing diagram with the interlayer distance of 3.104 Å. The $\pi$-stacked sheets are further expanding into layer-like structure through intensive hydrogen-bonding interactions.

2. The thermal decomposition peak temperature is determined to be 230.46 °C, indicating a better thermal stability than the traditional explosive FOX-7. The detonation velocity ($D$) and pressure ($p$) estimated by Eq. of Kamlet-Jacobs (K-J) are 7757 m·s$^{-1}$ and 25.74 GPa, respectively.

### References:


高氮钝感含能化合物 6-(2H-四唑-5-基)-1,2,4,5-四嗪-3(2H)-酮: \( \pi \)-堆积和氢键作用

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摘 要: 合成了 6-(2H-四唑-5-基)-1,2,4,5-四嗪-3(2H)-酮(TATZo)并通过对热分析, 元素分析, 磁谱和单晶 X 射线衍射对其结构进行了验证。单晶结构表明, TATZo·H_2O 属于正交晶系, 空间群是 Pnma, 密度为 1.730 g·cm^{-3}。在非等温条件下, 利用差示扫描量热法 (DSC) 和热重分析 (TG-DTG) 研究了 TATZo 的热分解行为, 并计算得到分解峰温（\( T_d \)）、热安定温度（\( T_m \））和热爆炸临界温度（\( T_{exp} \）），分别为 230.46 °C, 169.03 kJ·mol^{-1}, 15.65 s^{-1}, 213.75 °C 和 223.03 °C。TATZo·H_2O 分解峰温和热爆炸临界温度与传统含能材料 RX 相比, 表明 TATZo 热稳定性较高。通过高斯 03 软件包设计等键反应计算生成焓 (\( \Delta H \))，由 Kamlet-Jacobs (K-J) 方程计算爆炸波速 (\( D \)) 和压缩波 (\( p \)) 以评估爆炸性能。D 和 p 分别为 7757 m·s^{-1} 和 25.74 GPa。撞击法测得 TATZo 爆击感度大于 24 J。

关键词: 含能材料; 6-(2H-四唑-5-基)-1,2,4,5-四嗪-3(2H)-酮; 晶体结构; 热行为; 爆炸性能

中图分类号: TJ55; O64 文献标志码: A DOI: 10.11943/CJEM2019067 (责任编辑: 王祥秀)