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Thermal Decomposition Study of Trichloroisocyanuric Acid

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Abstract: Trichloroisocyanuric acid (TCCA) is widely used as a disinfectant, bactericide and bleaching agent, yet frequent safety accidents occur during its lifecycle, with its thermal stability and decomposition mechanisms unclear. This work investigated thermal hazards of TCCA using simultaneous thermal analysis, differential scanning calorimetry and accelerating rate calorimetry for samples with varied moisture under open- and closed-system conditions. Decomposition pathways were predicted via Gaussian 16W, and non-condensable gaseous products were identified by gas chromatography-mass spectrometry. No obvious exothermicity was detected in open systems, whereas violent exothermic decomposition took place in closed systems. Samples containing 10%, 20%, 30%, and 40% moisture showed lower initial decomposition temperatures and higher heat decomposition release, raising thermal-runaway risks. Molecular simulations and GC-MS jointly confirmed major gaseous products including NO_x, CO_x, Cl_2 and trace cyanogen. This study clarifies TCCA decomposition mechanisms and moisture-dependent thermal stability, offering theoretical and experimental support for its safe production, storage and transportation.

Keywords: Trichloroisocyanuric acid; Thermal stability; Molecular simulation

1 Introduction

Trichloroisocyanuric acid (TCCA) is a chlorine-containing organic compound with strong oxidizing properties. It exhibits significant bactericidal and bleaching effects and can slowly release active chlorine in aqueous solutions, resulting in long-lasting performance and good chemical stability[1]-[2]. Therefore, TCCA has been widely applied in municipal drinking water purification, swimming pool disinfection, sterile assurance in medical institutions, microbial control in food processing, disease prevention in aquaculture[3]-[5], and public space disinfection. In recent years, its application scope has further expanded to emerging fields such as fine chemical synthesis [6], organic reaction catalysis[7], and oxidative decomposition of ores [8], with global demand growing at an annual rate of approximately 8%.

TCCA exhibits significant reaction hazards during use: when mixed with nitrogen-containing compounds such as ammonium salts, ammonia, or urea, it may generate highly explosive nitrogen trichloride (NCl_3), and contact with flammable or organic substances can easily trigger combustion [9]. Studies have shown that TCCA has caused multiple accidents during production, storage, and application. Given its potential risks and the lessons learned from past accidents, the current understanding and research on the thermal stability of TCCA are insufficient to support effective safety practices. Therefore, a systematic investigation of its thermal stability, including a clear determination of the boundary conditions and mechanisms of its thermal decomposition, is a critical and urgent task.

Our previous work investigated the thermal stability of neat TCCA with multiple heating rates by DSC and ARC experiments [10]. Heat–Cool–Reheat Experiment were adopted to confirm the autocatalytic behavior of TCCA decomposition. Subsequent decomposition kinetic calculations yielded a T_{D24} of 216.8 °C.

However, in actual production processes, TCCA undergoes moisture-involved operations

such as crystallization, centrifugation, and filtration, making it essential to study its safety under moisture conditions. Therefore, thermogravimetry (TG)–differential scanning calorimetry (DSC), accelerating rate calorimetry (ARC) and GC-MS were employed in this study to systematically investigate the difference of thermal stability between TCCA and its moisture-containing systems, and an innovative observation indicated that neat TCCA and its hydrous systems possess drastically different thermal behaviors under open and closed conditions. Its thermal decomposition boundary conditions and influencing factors were clarified, and the Gaussian software was used to predict the thermal decomposition pathways of TCCA. Meanwhile, the gases released during the ARC testing were collected and analized via GC-MS for product composition. The findings will provide a theoretical basis for establishing and optimizing safety boundary conditions and risk prevention technologies for TCCA operation, use, and storage, with significant implications.

2 Materials and Experiments

2.1 Materials

The TCCA used in the experiments was purchased from Adamas-beta, with a purity ≥95.0%. The samples were always stored in a desiccator. All experiments were conducted independently at least three times to ensure reproducibility and accuracy of the results.

2.2 Experimental Methods

2.2.1 Simultaneous Thermal Analysis (STA)

Simultaneous thermal analysis (STA) was used to study the thermal decomposition and weight loss characteristics of TCCA[11]-[12]. The experiments were conducted in an open system: approximately 10 mg of sample was placed in a ceramic crucible and heated from 30°C to 450°C at a heating rate of 5°C/min under an air flow of 50 mL/min, yielding thermogravimetric (weight

loss) curves and corresponding heat flow curves.

2.2.2 Differential Scanning Calorimetry (DSC)

To determine the exothermic characteristics of the samples during decomposition, DSC was used for testing[13]-[14]. All experiments were conducted under an air atmosphere, with a heating rate of 5.0°C/min and a temperature range from 30°C to 450°C, to compare the thermal behaviors of samples in open and closed systems. The instrument detection sensitivity was 0.04 μW. Both the sample and reference pans were high-pressure sealed gold-plated crucibles with a capacity of 25 μL and a maximum pressure resistance of 20 MPa.

2.2.3 Accelerating Rate Calorimetry (ARC)

To study the thermal stability of TCCA with different moisture contents under adiabatic conditions[15]-[16], ARC was conducted, with an instrumental detection sensitivity of 0.02°C/min. The sample vessel was made of Hastelloy with a volume of 10 mL and a maximum pressure resistance of 20 MPa.

Samples with moisture contents of 0%, 10%, 20%, 30%, and 40% were selected. Approximately 2.1±0.05 g of each sample was accurately weighed and placed in the sample vessel. Under an air atmosphere, “Heat–Wait–Search” (H-W-S) mode was used, with a temperature range of 180°C–300°C and a heating step of 5.0°C/min. Each temperature step was held for 15 min to determine whether self-heating reactions occurred.

2.2.4 Gaussian Simulation of Decomposition Pathways

To investigate the thermal decomposition mechanism of TCCA at the molecular level, density functional theory (DFT) was performed using the Gaussian16 software, employing the B3LYP functional and 6-311G(d,p) basis set to perform structural optimization and frequency calculations for TCCA molecules, intermediates, and product molecules involved in the potential

decomposition pathways to determine their stable configurations. Subsequently, higher-precision single-point energy calculations were conducted to obtain relevant thermodynamic data. Furthermore, bond dissociation energies of key chemical bonds were calculated to evaluate the bond cleavage difficulty in order to provide a theoretical basis for studying TCCA thermal decomposition pathways[17]-[18].

2.2.5 Gas Chromatography–Mass Spectrometry (GC-MS) Analysis of Evolved Gas Components

To determine the gaseous products of TCCA during adiabatic thermal decomposition, the evolved gases were analyzed [19]. A 50 mL gas bag was used to collect the gases generated from pure TCCA after ARC testing, and a Clarus 590/SQ 8 S gas chromatography–mass spectrometry (GC-MS) system was used for detection. To eliminate interference from air components, high-purity helium (99.999%) was used as the carrier gas in both the GC-MS analysis and ARC testing. The GC-MS conditions were set as follows: chromatographic column Agilent HP-PLOT/Q (30 m × 0.320 mm × 20.0 μm), an injector temperature of 220°C, an EI ion source temperature of 230°C, and a helium carrier gas flow rate of 1.2 mL/min. The temperature program was as follows: the initial temperature of 40°C was maintained for 5 min, after which the temperature was increased to 220°C at 15°C/min, where it was held for 5 min.

3 Results and Discussion

3.1 STA

The thermal decomposition and weight loss characteristics of TCCA were studied using STA. For a heating rate of 5°C/min, the mass loss and heat flow curves of TCCA are shown in Figure 1.

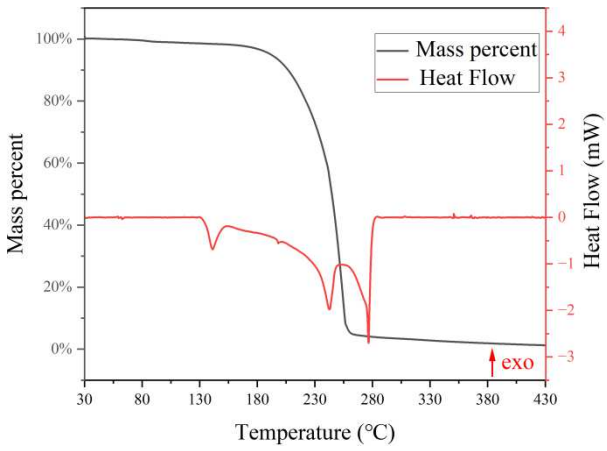

Fig. 1 Thermogravimetry (TG)–differential scanning calorimetry (DSC) curves of trichloroisocyanuric acid (TCCA).

In the open system, the TCCA sample exhibited a very high rate of mass loss in the temperature range of 180°C–250°C. During the mass loss process, the heat flow generally showed endothermic behavior. However, within the temperature range of 230°C–280°C, the rate of thermal mass loss remained nearly unchanged, while the heat flow signal showed a trend of first increasing, then decreasing, and then increasing again. It was inferred that the TCCA underwent exothermic decomposition during this process, while the endothermic evaporation of volatile components partially masked or reduced the actual exothermic effect[20].

Previous studies have shown that the thermal decomposition behavior of pure TCCA in closed systems is significantly different from that in open systems: in closed systems, pure TCCA decomposes violently with a large amount of heat release and exhibits autocatalytic characteristics. Therefore, to comprehensively evaluate its thermal hazard, it is particularly important to conduct more in-depth studies on its decomposition process in different systems.

3.2 DSC of Trichloroisocyanuric Acid (TCCA) with Different Moisture Contents

Because TCCA is prone to mixing with water and other impurities during production, storage, and transportation, and because historical accidents have indicated a high risk of thermal runaway when it is exposed to water or moisture, the effect of the moisture content on its thermal stability was further investigated using DSC. Based on the method described in Section 2.2.2, samples with moisture contents of 10%, 20%, 30%, and 40% were prepared by adding the corresponding amounts of water to TCCA, and the thermal decomposition behaviors were systematically tested to determine the influence of the moisture content on the thermal decomposition process of TCCA.

3.2.1 DSC in Open Systems with Different Moisture Contents

DSC tests were conducted under open conditions on TCCA samples with different moisture contents using the experimental method described in Section 2.2.2, and the resulting DSC curve is shown in Figure 2.

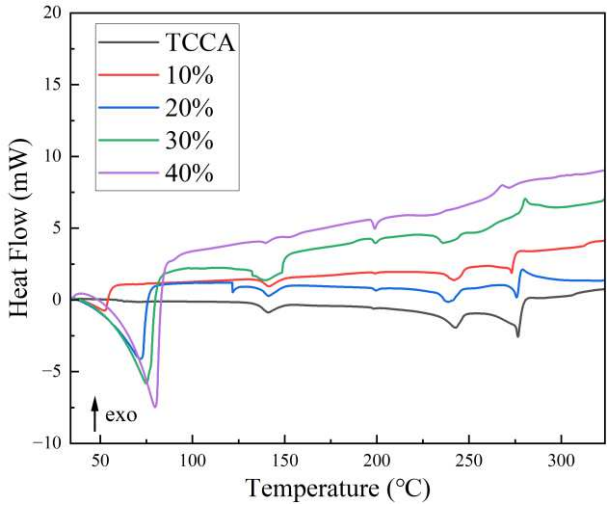

Fig. 2 DSC curves for different moisture contents in open systems.

Within the test range of 30°C to 450°C, none of the samples exhibited exothermic peaks. This phenomenon was consistent with the exothermic behavior of pure TCCA. During the heating

process up to 100°C, the endothermic effect increased significantly with increasing moisture content, which was inferred to be due to the endothermic evaporation of water.

3.2.2 DSC in Closed Systems with Different Moisture Contents

Given that pure TCCA exhibited significantly different thermal behavior in open versus closed systems, to systematically investigate the effect of the moisture content on its thermal stability, DSC tests under closed conditions were conducted on samples with different moisture contents. The experimental results are presented in a three-dimensional diagram showing the heat flow, temperature, and moisture content in Figure 3, and the corresponding experimental data are listed in Table 1.

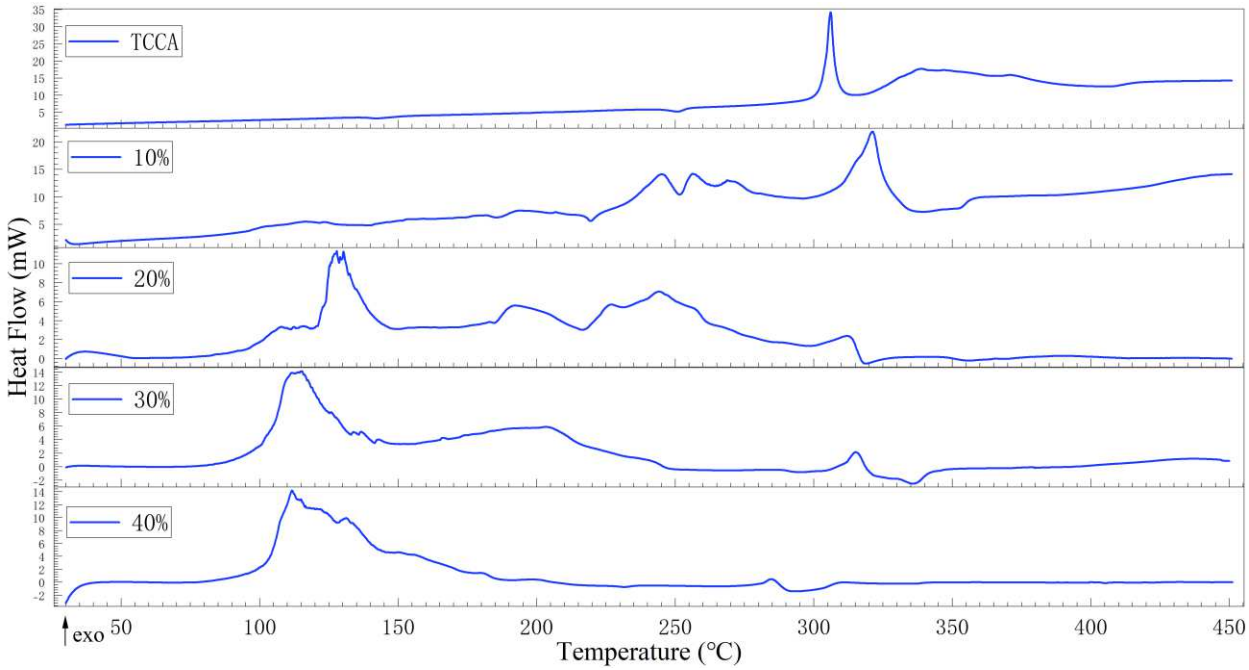

Fig. 3 DSC curves for different moisture contents in closed systems.

Table 1 Characteristic thermal decomposition parameters of TCCA with different moisture

contents in closed systems.

Moisture content	m (mg)	β (°C/min)	T_o (°C)	T_p (°C)	ΔH_d (J/g) (based on sample mass)	ΔH_d (J/g) (based on TCCA mass)
0	2.510	5	283.60	306.00	2619.04	2619.04
10%	2.331	5	85.14	321.15	2799.15	3110.17
20%	3.657	5	74.41	127.83	3074.69	3843.36
30%	3.833	5	71.41	115.34	2554.00	3648.57
40%	3.067	5	70.95	111.68	2106.90	3511.50

As shown in Figure 3, the thermal decomposition behavior of TCCA with different moisture contents in closed systems exhibited significant differences. At low moisture contents, two adjacent exothermic peaks appeared during the thermal decomposition process of TCCA, with weak coupling between the two peaks, and the exothermic temperature range was wide, at approximately 300°C–400°C. With increasing moisture content, the exothermic region shifted toward the lower temperature range, and both the onset temperature (T_{onset}) and peak temperature (T_p) gradually decreased. When the moisture content exceeded 20%, the exothermic onset temperature remained essentially unchanged.

Table 1 shows that as the moisture content increased, the exothermic onset temperature of the sample first decreased and then tended to stabilize, while the heat release first increased and then tended to stabilize. When the moisture content reached 20% or above, both the heat release and exothermic onset temperature showed little change, indicating that the presence of water significantly reduced the thermal stability of TCCA. In addition, the heat release of the moisture-containing TCCA was above 2000 J/g, indicating a relatively intense decomposition reaction.

According to the standard “Safety Risk Assessment Specification for Fine Chemical Reactions” (GB/T 42300-2022), this material would be classified as level 3 for explosion hazards, with a large amount of decomposition heat release and a high potential explosion risk. Therefore, further in-depth research on the thermal decomposition process of this substance was necessary.

3.3 ARC of TCCA with Different Moisture Contents

Because TCCA production involves crystallization, centrifugation, filtration, and other process steps in which water is used as the solvent, and because thermal runaway under actual industrial-scale conditions approaches adiabatic conditions, ARC was conducted under the experimental conditions described in Section 2.2.3 to test TCCA samples with different moisture contents. The exothermic curves from the ARC for different moisture content conditions are shown in Figures 4, 5, 6, and 7.

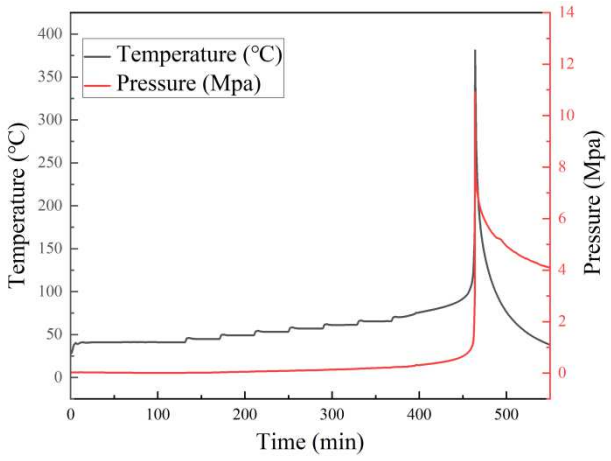

Fig. 4 Accelerating rate calorimetry (ARC) curve for a moisture content of 10%.

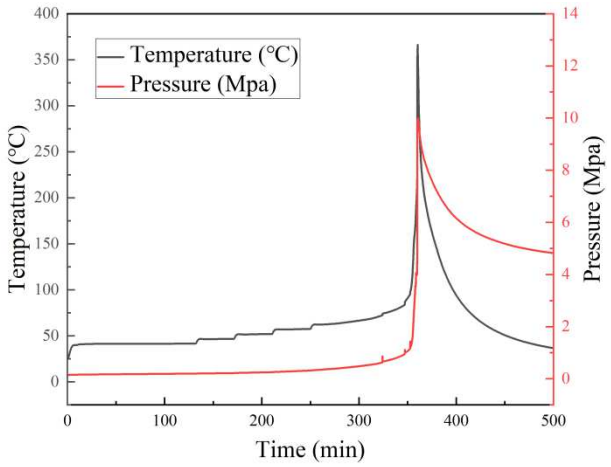

Fig. 5 ARC curve for a moisture content of 20%.

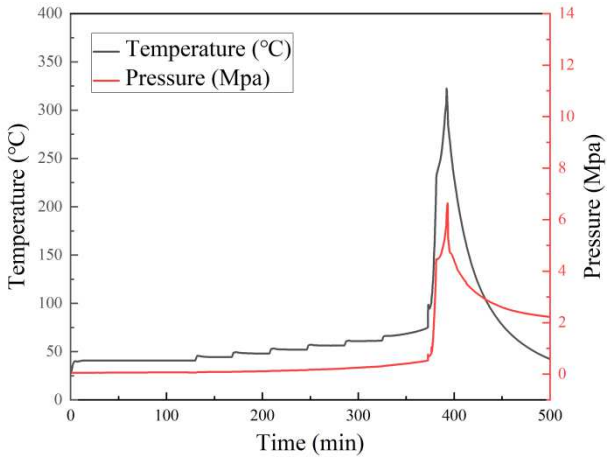

Fig. 6 ARC curve for a moisture content of 30%.

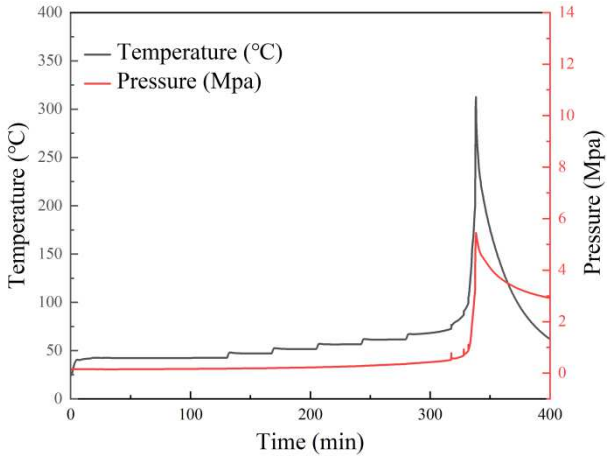

Fig. 7 ARC curve for a moisture content of 40%.

The resulting safety data of these ARC samples, along with the safety data of pure TCCA, are shown in Table 2.

Table 2 ARC data for different moisture contents.

Item	0	10%	20%	30%	40%
Sample mass (g)	2.1014	2.1083	1.9435	2.0261	1.9512
Φ	2.71	2.46	2.46	2.23	2.14
Onset decomposition temperature (°C)	237.81	70.26	62.34	66.31	67.11
Heat release (J g^{-1}) (based on sample mass)	940	1570	1710	1440	1450
Heat release (J·g^{-1}) (based on TCCA mass)	940	1744	2137	2057	2416
Adiabatic temperature rise (°C)	191.16	310.98	303.85	256.16	245.45
Maximum rate of temperature rise (°C·min^{-1})	761.56	6201.92	5885.17	769.23	913.46
Maximum rate of pressure rise (MPa·min^{-1})	27.74	652.88	625.84	40.30	45.19

During the experiment, part of the heat generated by sample decomposition was absorbed by the test pan, and the adiabatic test data were corrected using the thermal inertia factor Φ [10]. As shown in Figures 4, 5, 6, and 7 and Table 2, TCCA with different moisture contents exhibited significant thermal instability in the adiabatic calorimetry tests. The decomposition process was violent, releasing a large amount of heat accompanied by gas generation, resulting in a rapid increase in the system pressure. After cooling, the pressure did not return, indicating that the sample decomposed during the test and released a large volume of gas that could not be condensed at room temperature. As the moisture content increased, the onset decomposition temperature first decreased and then stabilized, while the decomposition heat release first increased and then stabilized. When the moisture content reached 20% or above, the variation in both became

significantly smaller, indicating that the presence of water significantly reduced the thermal stability of the TCCA. When the moisture content reached a certain level, further increases in the moisture had little additional effect on reducing the thermal stability. This phenomenon was consistent with the DSC results described above.

In summary, the thermal decomposition reaction of TCCA with different moisture contents in closed systems is highly destructive. It not only releases a large amount of heat but also generates a large volume of gas, with extremely high rates of temperature and pressure rise. Once the thermal decomposition reaction is initiated, it can easily develop into uncontrollable thermal runaway, ultimately leading to severe safety accidents. Therefore, during the production, storage, and transportation of TCCA, strict control of the temperature and moisture content is required. During the drying process of wet products, it is necessary to ensure smooth ventilation of the drying system and timely removal of moisture to avoid the thermal decomposition of moisture-containing TCCA and the resulting safety accidents.

3.4 Decomposition Mechanism of TCCA Based on Molecular Simulation

To investigate the thermal decomposition mechanism of TCCA at the theoretical level, the Gaussian 16 software was used to optimize the structure of the TCCA molecule with the B3LYP functional and the 6-311G(d,p) basis set. Figure 8 shows the optimized molecular structure of TCCA on the lowest potential energy surface. Based on this, the energy parameters of TCCA and its possible decomposition structures, including the zero-point energy, internal energy, enthalpy, and Gibbs free energy, were calculated. The bond dissociation energies were also computed to determine the relative ease of bond cleavage and thereby infer the thermodynamically plausible fragmentation scheme of TCCA.

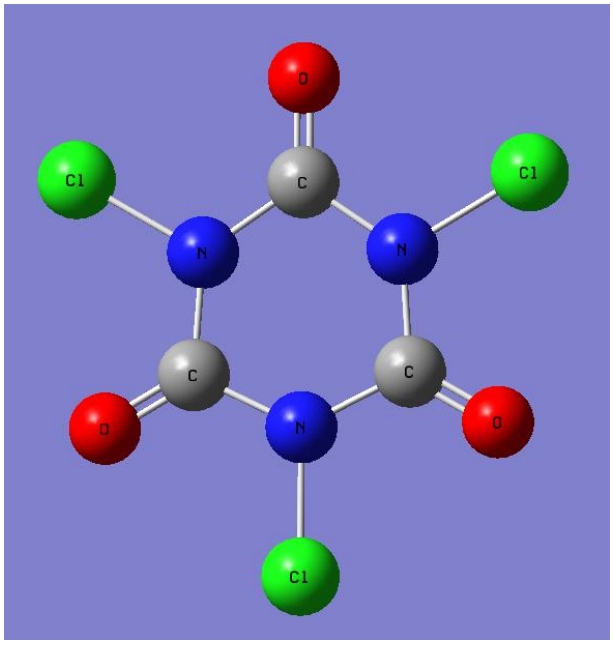

Fig. 8 Molecular structure of TCCA on the lowest potential energy surface.

Due to the symmetry of the TCCA structure, three different initial decomposition pathways were predicted, yielding five types of radicals, as shown in Figure 9. M1 represents the TCCA molecule. Cleavage of bond 1 produced the radicals M2 and M3, cleavage of bond 2 produced the radicals M5 and M6, and cleavage of bond 3 produced the radical M4. By performing structural optimization, frequency calculations, and single-point energy calculations, the single-point energy, Gibbs free energy, and other energy parameters of each radical were obtained, as listed in Table 3.

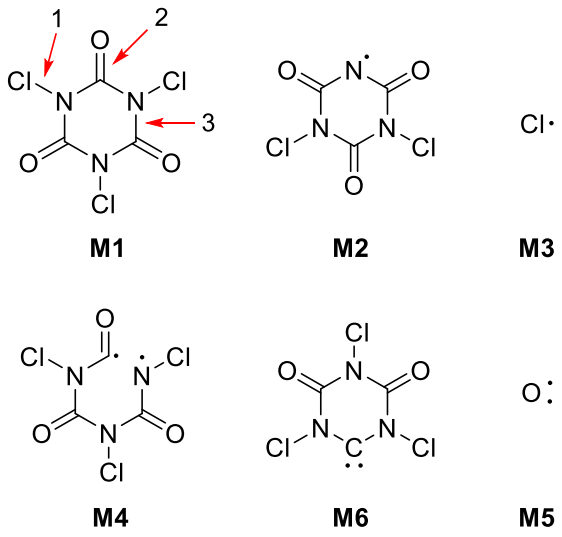

Fig. 9 Predicted structures after initial decomposition.

Table 3 Thermodynamic parameters of corresponding structures after the first decomposition step.

Structure	Internal energy	Enthalpy	Gibbs free energy	Single-point energy	Enthalpy correction term
M1	-1884.89	-1884.89	-1884.94	-1884.95	0.06
M2	-1424.64	-1424.64	-1424.69	-1424.69	0.06
M3	-460.17	-460.16	-460.18	-460.17	0.01
M4	-1884.70	-1884.69	-1884.76	-1884.75	0.06
M5	-74.98	-74.98	-74.99	-74.98	0.01
M6	-1809.59	-1809.59	-1809.63	-1809.64	0.05

Note: All parameters in the table are in Hartree; 1 Hartree = 2,625.5 kJ/mol.

The bond dissociation energy (BDE) is an important parameter affecting the chemical

reactivity of free radicals. It refers to the energy consumed when a covalent bond in a compound undergoes homolytic cleavage, i.e., the enthalpy change during bond breaking (for a single bond). A lower bond dissociation energy indicates that the bond is more likely to break during thermal decomposition. Researchers commonly use BDE values to evaluate the structural stability. The BDE is calculated as follows:

$$\Delta H = H(A\cdot) + H(B\cdot) - H(A-B),$$

where the enthalpy values are obtained through high-precision calculations. The single-point energy calculation results were combined with the enthalpy correction terms obtained from frequency analysis. Based on this, BDE values were calculated, and the data are shown in Table 4.

Table 4 Bond dissociation energies of chemical bonds potentially cleaved in the first decomposition step of TCCA.

Chemical bond	Bond dissociation energy (kJ/mol)
1	230.16
2	512.51
3	855.44

The results indicated that bond 1 (N–Cl bond) was the easiest to break, with a BDE of 230.16 kJ/mol. After cleavage, radicals M2 and M3 were generated. The BDE calculation provided a basis for the subsequent inference of the thermal decomposition pathways. Following the above method, the thermodynamically plausible fragmentation scheme of TCCA were deduced, and the results are shown in Figure 10.

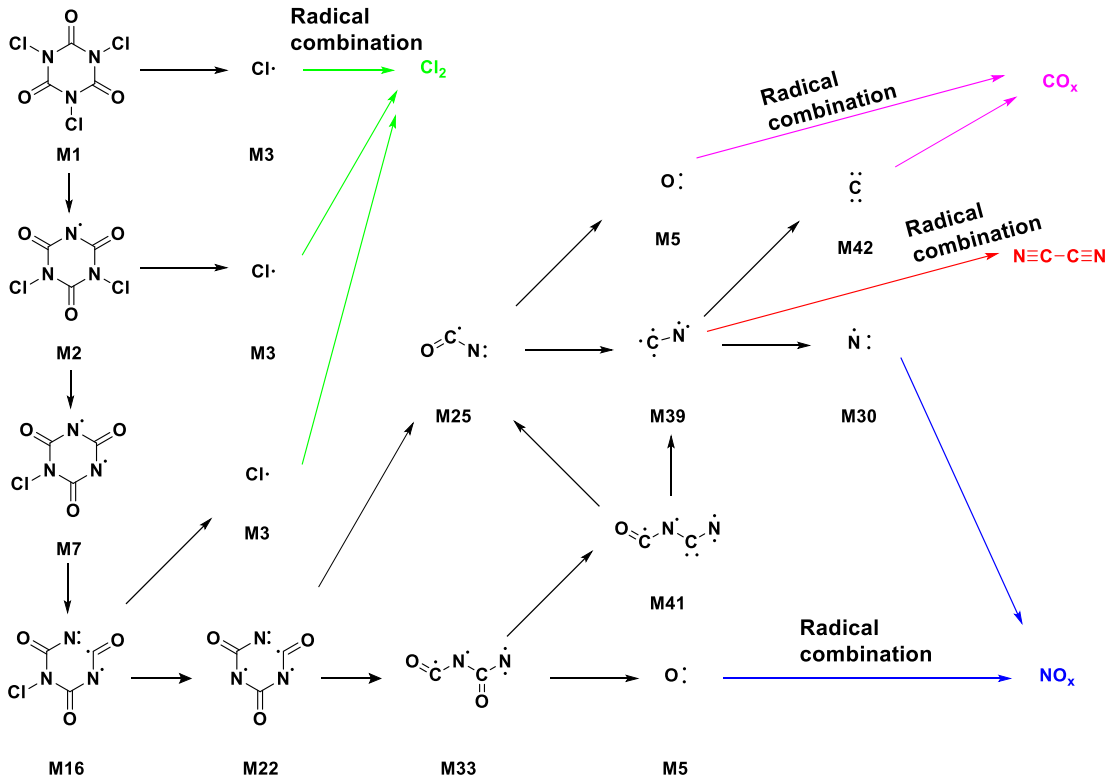

Fig. 10 Thermodynamically plausible fragmentation scheme of TCCA.

The molecular simulation revealed the thermodynamically plausible fragmentation scheme of TCCA. At high temperatures, TCCA underwent successive homolytic cleavage of two N–Cl bonds, generating chlorine radicals. These radicals mainly combined with each other to form chlorine gas. The triazine skeleton then decomposed at high temperatures, and the remaining radical fragments were eventually converted into nitrogen oxides, carbon oxides, and a small amount of cyanogen.

3.5 Evolved Gas Components

The composition of the gaseous products from the TCCA thermal decomposition was analyzed using ARC combined with GC-MS, and the results are shown in Figure 11. The spectrum contained four main molecular ion peaks, with the following retention times (and corresponding

products in parentheses): 2.81 min (CO_2), 4.03 min (mixture of CO_2, NO_2, and CO), 4.46 min (mixture of CO_2 and NO), and 11.15 min (cyanogen). This indicated that the thermal decomposition products of TCCA mainly included NO_x, CO_x, and a small amount of cyanogen. In addition, moist starch–potassium iodide paper was used to test the gas, and the paper turned blue, confirming the presence of chlorine gas in the decomposition products. The above experimental results were highly consistent with the predictions of the Gaussian theoretical calculations, demonstrating good agreement between the theoretical predictions and the experimental results and further clarifying the main decomposition pathways of TCCA.

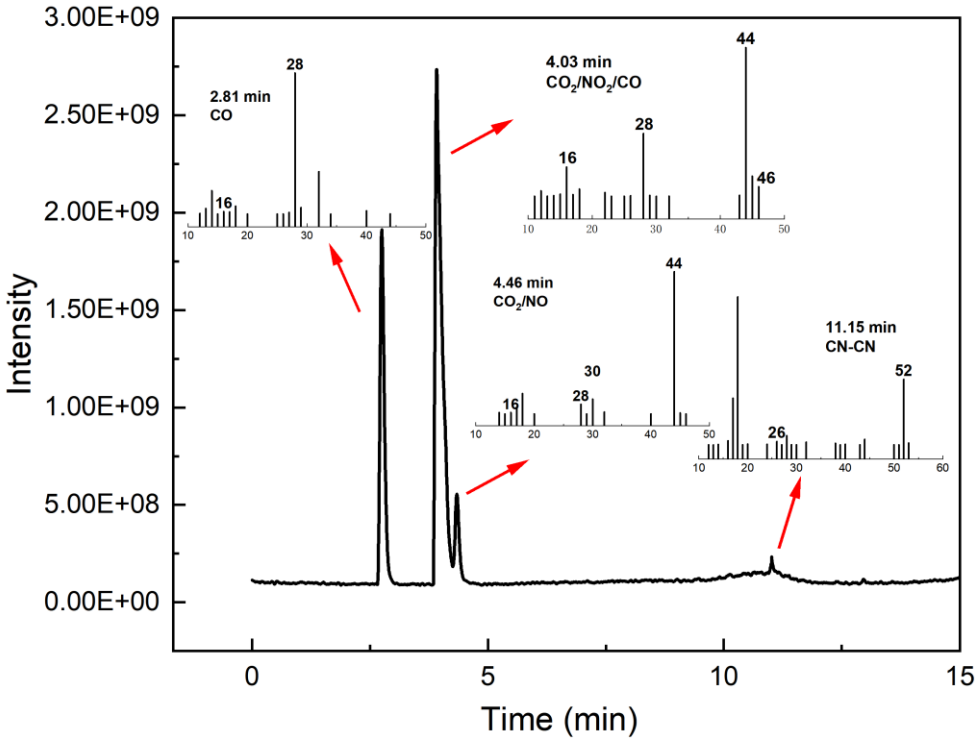

Fig. 11 Chromatogram and mass spectrum of gas products of TCCA thermal decomposition.

4 Conclusion

In this study, the thermal stability and decomposition of TCCA were systematically

investigated by combining experiments and theoretical calculations. The main conclusions are as follows:

In open systems, neither pure TCCA nor moist TCCA with different water contents shows obvious exothermic behavior. In closed systems, moist TCCA presents high thermal sensitivity with highly destructive thermal decomposition. This process releases substantial heat and abundant gas, leading to an extremely rapid rise in system temperature and pressure. Once initiated, the thermal decomposition reaction easily develops into uncontrollable thermal runaway and triggers severe safety accidents.

In closed systems, the presence of water significantly reduces the thermal stability of TCCA and increases the risk of thermal runaway. With the increase in water content, the initial decomposition temperature decreases first and then levels off, while the heat release of decomposition increases initially and then tends to be stable.

Based on density functional theory (DFT-B3LYP), the Gaussian software was used to predict the thermal decomposition pathways of TCCA from a microscopic perspective, and GC-MS analysis of the non-condensable gases confirmed that the main gaseous products of the TCCA thermal decomposition were NO_x, CO_x, Cl_2, and a small amount of cyanogen.

In summary, the thermal decomposition reaction of TCCA with different moisture contents in closed systems is highly destructive. To ensure safety during the production, storage, and transportation of TCCA, strict control of the TCCA temperature is required, and effective measures should be taken to prevent contact between the TCCA and water to avoid thermal decomposition of moisture-containing TCCA and the resulting safety accidents.

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