

# Synthesis and thermal behavior of 2,4-diaryl-3H-1,2,4-triazole-3-ones

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## Abstract

1,2,4-Triazole-3-one derivatives with 2,4-aryl groups (ArTOs) were synthesized and their thermal behavior was investigated using thermogravimetry / differential thermal analysis (TG/DTA), sealed cell differential scanning calorimetry (SC-DSC), and flash pyrolysis FT-IR. In addition, semiempirical molecular orbital (MO) calculations were carried out using the AM1 method to estimate the strength of bonds and two-center energies in the ArTOs. The ArTOs were obtained in good yields by the heating of semicarbazidomethylenemalonic acid derivatives. The TG/DTA and SC-DSC results showed that the introduction of electron-releasing substituents on the 2,4-aryl groups of ArTOs influenced their thermal characteristics. No residue was observed after TG/DTA was performed on the ArTOs. Since decomposition of ArTOs showed endothermic peaks without residue under open pan conditions, but exothermic peaks with residue under closed pan conditions, it was considered that the decomposition of ArTOs proceeds in the gas phase. Flash pyrolysis FT-IR measurements indicated the formation of isocyanate and hydrogen cyanate. This suggested that thermal decomposition of 2,4-diphenyl-3H-1,2,4-triazole-3-one was mainly initiated at either the N2-C3 and N4-C5 bonds, or the N1-N2 and C3-N4 bonds. The calculated two-center energies of the N1-N2 and N2-C3 bonds, which correspond to the bond energies, were lower than those of the other bonds. This result supports, and is consistent with, our experimental results.

**Keywords:** 2,4-diaryl-3H-1,2,4-triazole-3-one, semicarbazidomethylenemalonic acid, pyrolysis mechanism, flash pyrolysis FT-IR, molecular orbital calculations.

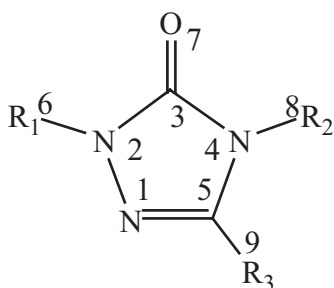
## 1. Introduction

In recent years, the uses of energetic materials have become quite diverse and widespread and include air-bag systems, synthesis technology and medical technology. Therefore, it is essential to ensure that the properties of such energetic materials are investigated and utilized in a safe and controlled manner. In particular, from a safety point of view, it is important to acquire a better understanding of the stability and reactivity of energetic materials during the course of their lifetimes. Additionally, the development of new energetic materials will enable the expansion and improvement of their performance in each device.

Gas-generating agents have recently received considerable attention due to their possible applications in air-bag

systems. These agents require specialized control in order to operate effectively. The essential features of these agents are thermal stability, release of large volumes of gas, high combustion speed, non-explosiveness, non-toxicity (both agents and generated gas), and long-term stability.

1,2,4-Triazole-3-ones (TOs) (see Fig.1), which contain a carbonyl group attached to a five-membered ring, are anticipated to be useful as next generation energetic materials and gas-generating agents. In previous work, researchers have studied 5-nitro-3H-1,2,4-triazole-3-one (NTO), which is equivalent in energy to 1,3,5-trinitroperhydro-1,3,5-triazine (RDX) or 1,3,5,7-tetranitroperhydro-1,3,5,7-tetrazocine (HMX), but with greater thermal stability<sup>1)-5)</sup>. Based on these characteristics, NTO is used



**Fig. 1** 1,2,4-triazole-3-one derivatives (TOs).

TO:  $R_1, R_2, R_3 = H$

NTO:  $R_1, R_2 = H, R_3 = NO_2$

ArTO:  $R_1, R_2 = \text{aryl group}, R_3 = H$

as a propellant powder for military explosives. TOs, which have a framework identical to NTO, are anticipated to exhibit higher stability and reactivity. Additionally, since three nitrogen atoms are contained in the framework of the triazole, their derivatives are expected to generate nitrogen gases during decomposition.

However, there have been few detailed studies of the thermal behavior of TOs. To obtain a better understanding of the thermal substituent effects in TOs, the synthesis, thermal behavior, and thermal decomposition mechanisms of TOs with three types of electron-releasing substituents at positions 2 and 4 (ArTOs) were investigated.

## 2. Experimental

### 2.1 Agents

Triethyl orthoformate (Kanto Chemical Co., Inc.) and semicarbazide hydrochloride (Kanto Chemical Co., Inc.) were used to synthesize TO. Phenylhydrazine hydrochloride (Tokyo Kasei Kogyo Co., Ltd.), 4-methylphenylhydrazine hydrochloride (Tokyo Kasei Kogyo Co., Ltd.), 4-methoxyphenylhydrazine hydrochloride (Tokyo Kasei Kogyo Co., Ltd.), 4-methoxyphenylisocyanate (Tokyo Kasei Kogyo Co., Ltd.), phenylisocyanate (Kanto Chemical Co., Inc.) and 4-methylphenylisocyanate (Kanto Chemical Co., Inc.) were used to synthesize the ArTOs. Benzene (Kanto Chemical Co., Inc.) and triethylene glycol dimethyl ether (Nacalai Tesque Co., Inc.) were used as solvents.

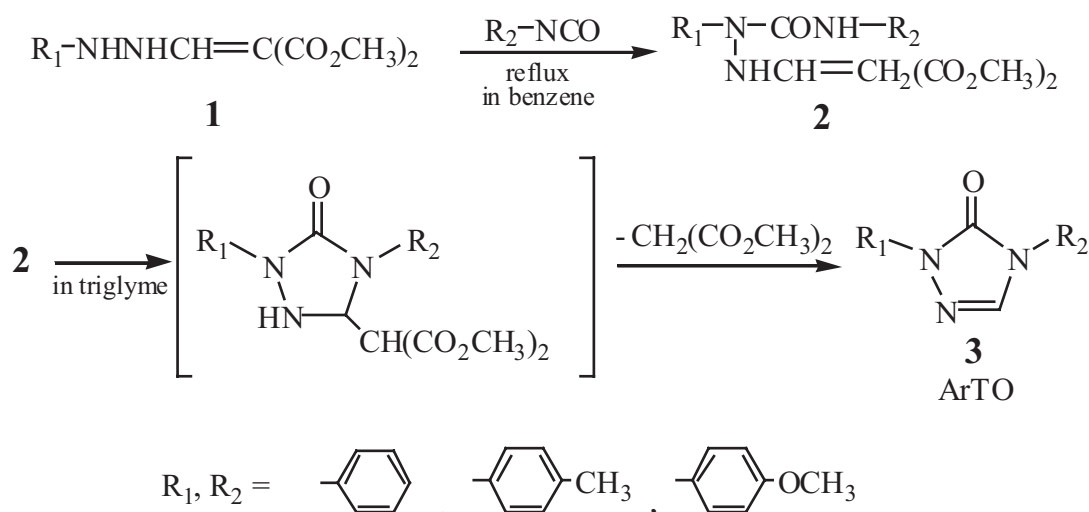
### 2.2 Instruments

All compounds were characterized by elemental analysis (Perkin Elmer: PE 2400 series CHNS/O analyzer), FT-IR measurements using the KBr method, and  $^1H$ -NMR (JEOL Ltd.) spectroscopy with  $CDCl_3$  as the solvent and TMS as an internal reference at temperatures of 30 °C. The thermal properties of the products were analyzed by TG/DTA (Seiko Instruments, Inc.: TG/DTA 220) under  $N_2$  gas at a flow rate of 200 mL  $min^{-1}$ , with the sample in an aluminum pan, at a heating rate of 10 K  $min^{-1}$  over a measurement range of 25–450 °C. SC-DSC (Mettler Toledo, HP DSC827e) was carried out in a stainless steel sealed cell (Seiko Instruments, Inc.) at a heating rate of 10 K  $min^{-1}$  over a measurement range of 25–500 °C. Flash pyrolysis FT-IR was used to analyze gases evolved from TOs. The apparatus consisted of two parts: a pyroprobe (CDS Analytical, Inc.: Pyroprobe 2000) and an IR spectrometer (MAGNA-IR 850, Nicolet Instrument Corporation). The gases evolved after rapid pyrolysis of the samples by the pyroprobe in a Brill cell were analyzed by IR measurements. Flash pyrolysis FT-IR was carried out in a quartz tube under  $N_2$  gas, under the following conditions: heating rate, 100 K  $s^{-1}$ ; measurement range, RT–1000 °C; measurement time, 3 min; scanning resolution, 4  $cm^{-1}$ . The spectra were integrated 4 times.

Two-center energies and ionization energies for the ArTOs were calculated via energy partition analysis<sup>6)</sup> by the AM1 method<sup>7)</sup> using the program MOPAC 2002<sup>8)</sup>.

### 2.3 Synthesis

The reaction scheme for the synthesis of ArTOs containing phenyl groups, 4-methylphenyl groups, or 4-methoxyphenyl groups at positions 2 and 4 is shown in Fig. 2. Dimethyl hydrazinomethylenemalonates (1) was obtained using the Crombie method<sup>9)</sup>. Semicarbazidomethylenemalononic acid derivatives (2) were synthesized by reactions of 1 with arylisocyanates. Nine ArTOs (3a–3j) were synthesized via cyclization reactions of 2a–2j. 3a–3j were recrystallized from a mixed solvent of benzene and hexane.



**Fig. 2** Preparation of ArTOs.

**Table 1** Preparation conditions, yields, and results of structure confirmation of TOs.

Compounds	Temp./		Yield	Elemental Analyses			IR measure- ment	<sup>1</sup> H-NMR (CDCl <sub>3</sub> , TMS)
	R <sub>1</sub>	R <sub>2</sub>		Time	Found (Calcd)			
			(°C/h)	(%)	C	H	N	cm <sup>-1</sup>
3a	Ph	Ph	130/6	77	70.89 (70.87)	4.86 (4.67)	17.71 (17.71)	vC=O : 1697 δ : 7.32–7.32 (1H, m), 7.40 (1H, dd, <i>J</i> =7.3, 7.6), 7.46 (2H, t, <i>J</i> =7.3), 7.52 (2H, dd, <i>J</i> =7.8, 8.1), 7.60 (2H, d, <i>J</i> =7.3), 7.85 (1H, s), 8.02 (2H, d, <i>J</i> =7.6)
3b	Ph	4-Me-Ph	150/8	92	71.53 (71.70)	5.33 (5.21)	16.83 (16.72)	vC=O : 1693 δ : 2.47 (3H, s), 7.25 (1H, dd, <i>J</i> =7.3, 7.6), 7.30 (2H, d, <i>J</i> =8.1), 7.44 (2H, d, <i>J</i> =7.8), 7.46 (2H, d, <i>J</i> =7.8), 7.80 (1H, s), 8.01 (2H, d, <i>J</i> =7.6)
3c	Ph	4-MeO-Ph	140/5	93	67.45 (67.40)	4.95 (4.90)	15.70 (15.72)	vC=O : 1687 δ : 3.85 (3H, s), 7.01 (2H, d, <i>J</i> =9.0), 7.25 (1H, t, <i>J</i> =7.3), 7.44 (2H, d, <i>J</i> =8.5), 7.47 (2H, d, <i>J</i> =9.0), 7.77 (1H, s), 8.01 (2H, d, <i>J</i> =7.8)
3d	4-Me-Ph	Ph	130/5	70	71.56 (71.70)	5.33 (5.21)	16.82 (16.72)	vC=O : 1698 δ : 2.38 (3H, s), 7.25 (2H, d, <i>J</i> =8.1), 7.36–7.52 (3H, m), 7.59 (2H, d, <i>J</i> =8.3), 7.80 (1H, s), 7.87 (2H, d, <i>J</i> =8.5)
3e	4-Me-Ph	4-Me-Ph	110/5	60	72.12 (72.43)	5.68 (5.70)	15.79 (15.84)	vC=O : 1697 δ : 2.37 (3H, s), 2.40 (3H, s), 7.25 (2H, d, <i>J</i> =8.3), 7.30 (2H, d, <i>J</i> =8.1), 7.46 (2H, d, <i>J</i> =8.3), 7.79 (1H, s), 7.87 (2H, d, <i>J</i> =8.5)
3f	4-Me-Ph	4-MeO-Ph	130/5	71	68.33 (68.31)	5.34 (5.37)	14.99 (14.94)	vC=O : 1681 δ : 2.37 (3H, s), 3.85 (3H, s), 7.00–7.26 (4H, m), 7.47 (2H, d, <i>J</i> =5.9), 7.75 (1H, s), 7.87 (2H, d, <i>J</i> =5.7)
3g	4-MeO-Ph	Ph	120/9	89	67.56 (67.40)	4.98 (4.90)	15.80 (15.72)	vC=O : 1685 δ : 3.85 (3H, s), 7.01 (2H, d, <i>J</i> =8.8), 7.25 (1H, dd, <i>J</i> =7.3, 7.6), 7.42–7.50 (4H, m), 7.77 (1H, s), 8.01 (2H, d, <i>J</i> =7.8)
3h	4-MeO-Ph	4-Me-Ph	120/4	84	68.37 (68.31)	5.58 (5.37)	14.05 (15.94)	vC=O : 1684 δ : 2.40 (3H, s), 3.84 (3H, s), 6.97 (2H, d, <i>J</i> =9.3), 7.30 (2H, d, <i>J</i> =8.1), 7.46 (2H, d, <i>J</i> =8.3), 7.78 (1H, s), 7.88 (2H, d, <i>J</i> =9.3)
3i	4-MeO-Ph	4-MeO-Ph	120/5	86	64.41 (64.64)	5.18 (5.09)	14.11 (14.13)	vC=O : 1684 δ : 3.84 (3H, s), 3.85 (3H, s), 6.97 (2H, d, <i>J</i> =9.0), 7.00 (2H, d, <i>J</i> =9.0), 7.47 (2H, d, <i>J</i> =8.8), 7.74 (1H, s), 7.88 (2H, d, <i>J</i> =9.0)
TO	H	H	90/3	90	28.54 (28.24)	3.56 (3.55)	49.65 (49.40)	vC=O : 1700 δ : 7.71 (1H, s), 11.26 (1H, s), 11.39 (1H, s)

TO was obtained by employing the method used in the previous studies<sup>10</sup>. A suspension of semicarbazide hydrochloride in an excess of triethyl orthoformate was heated at reflux for 3.0 h. The precipitate was filtered and recrystallized from ethanol.

The structures of **3a–3j** and TO were confirmed by elemental analysis, IR measurement, and <sup>1</sup>H-NMR spectroscopy. Table 1 summarizes the preparation conditions, yields, and results of structure confirmation **3a–3j** and TO. The results of elemental analysis for **3a–3j** were within 0.3 % of the calculated value. The signals observed for **3a–3j** by IR measurement were vC=O : 1681–1700 cm<sup>-1</sup>. Synthetic methods for TOs which utilize the reaction of semicarbazide or semicarbazone with triethyl orthoformate have been reported<sup>11–14</sup>, and compound **3a** has been synthesized<sup>14, 15</sup>. However, all of the **3a–3j** synthesized using semicarbazidomethylenemalonic acid derivatives were obtained in good yields (60–93 %). TO was obtained in good yield (90 %) by the method used in the previous studies<sup>10</sup>.

### 3. Results and discussion

#### 3.1 Thermal behavior of TOs

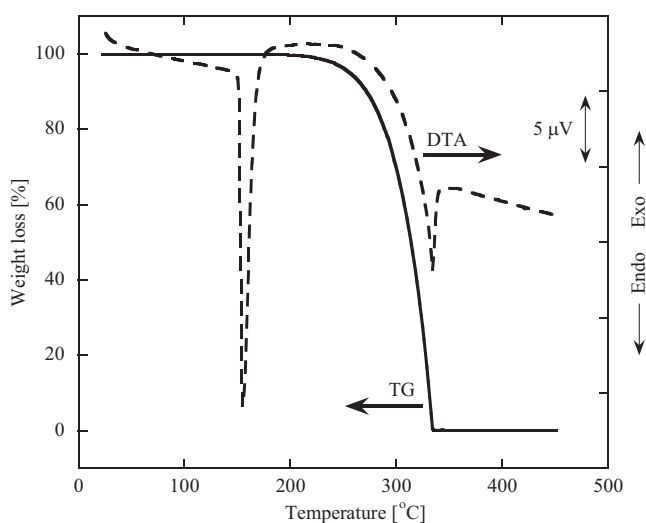
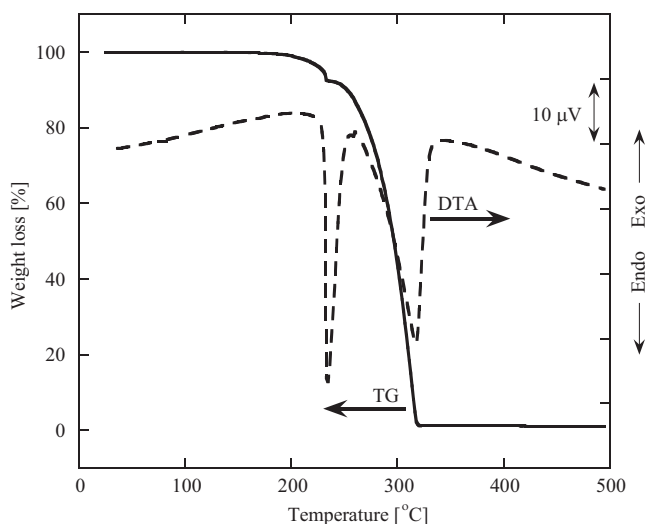
Figure 3 shows the TG/DTA curves of **3c**. Compound **3c** showed an endothermic peak (158 °C) that corresponded to melting, a broad endothermic DTA curve (251–330 °C), and a weight loss TG curve. TG/DTA curves for TO are shown in Fig.4. At 228 °C, an endothermic peak in the DTA curve and a weight loss TG curve were observed. The melting point (Mp) for TO was also found to be around 228 °C using a melting point measurement appara-

tus. Thus, it was suggested that TO loses weight upon melting. Figure 5 shows the SC–DSC curves of TOs. After an endothermic peak, compound **3c** also showed an exothermic peak. All of the ArTOs exhibited similar endothermic peaks and broad endothermic curves in the TG/DTA results, and exothermic peaks in the SC–DSC results. After TG/DTA of TOs, there was little residue in the aluminum pan. Since the unsealed cell condition shows endothermic peaks and no residue, whereas the sealed condition shows exothermic peaks, it is thought that TOs decompose in the gas phase.

The thermal analysis results are summarized in Table 2, which shows Mp, weight loss initiation temperatures (T<sub>TG</sub>) of TG, and onset temperatures (T<sub>DSC</sub>) of SC–DSC. The aryl substituents at positions 2 and 4 were found to influence Mp, T<sub>TG</sub>, and T<sub>DSC</sub>. ArTOs containing a phenyl group at position 2 (**3a–3c**) and substituents with a greater electron-releasing effect at position 4 showed increases in Mp and T<sub>TG</sub>. Figure 6 provides a plot of T<sub>TG</sub> against ionization potential for ArTOs. All data points were subjected to least-squares fitting. The ionization potential of ArTOs decreases with increasing T<sub>TG</sub>, and the influence of ionization potential and vaporization has been reported<sup>16</sup>. Therefore, the T<sub>TG</sub> of ArTOs can be related to substituent effects. In addition, the T<sub>DSC</sub> of ArTOs was higher than that of TO, and each substituent influenced the T<sub>DSC</sub> (389–417 °C) of ArTOs. This result indicates that onset temperatures for TOs are affected by substituents at positions 2 and 4. One possible reason for this increased thermal stability may be due to the greater electron density in the triazole ring.

**Table 2** Thermal behaviors of TOs.

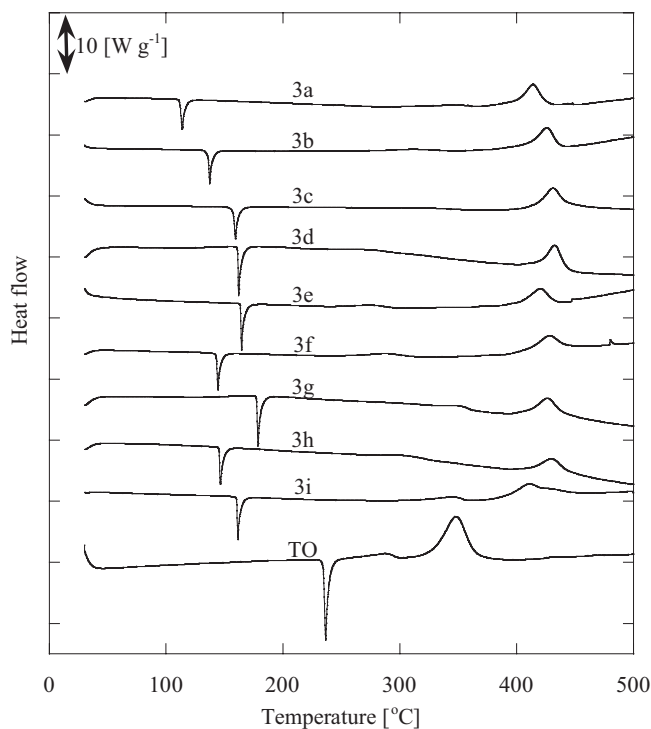
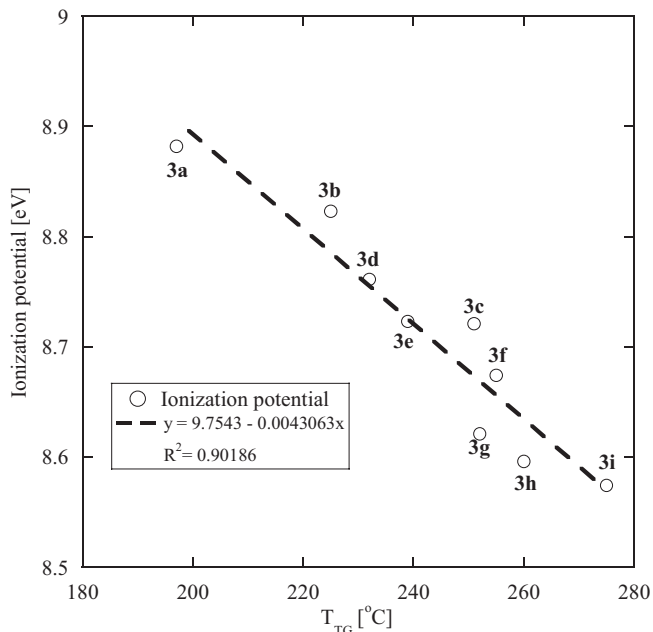
	Compounds		Mp (°C)	T <sub>TG</sub> (°C)	T <sub>DSC</sub> (°C)
	R <sub>1</sub>	R <sub>2</sub>			
3a	Ph	Ph	111–113	197	398
3b	Ph	4-Me-Ph	126–129	225	410
3c	Ph	4-MeO-Ph	158–159	251	415
3d	4-Me-Ph	Ph	160–161	232	417
3e	4-Me-Ph	4-Me-Ph	163–164	239	400
3f	4-Me-Ph	4-MeO-Ph	143–144	255	407
3g	4-MeO-Ph	Ph	146–147	252	408
3h	4-MeO-Ph	4-Me-Ph	145–146	260	410
3i	4-MeO-Ph	4-MeO-Ph	156–158	275	389
TO	H	H	229–230	228	332


**Fig. 3** TG/DTA curves of 3c.

**Fig. 4** TG/DTA curves of TO.

The presence of methylphenyl and methoxyphenyl groups, which are electron-releasing substituents, contributes to the electronic state in the triazole ring, thus increasing thermal stability.

### 3.2 Generated gases

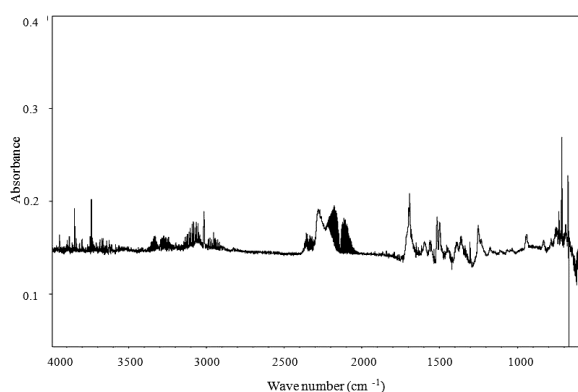
The flash pyrolysis FT-IR spectrum of 3c is shown in Fig.7. The signals observed among the gases generated


**Fig. 5** DSC curves of TOs.

**Fig. 6** Relation between T<sub>TG</sub> and Ionization potential of Ar-TOs.

from 3c were  $\nu_{\text{CO}}$ : 2050–2200  $\text{cm}^{-1}$ ,  $\nu_{\text{CO}_2}$ : 2300–2400  $\text{cm}^{-1}$ ,  $\nu_{\text{NCO}}$ : 2250–2275  $\text{cm}^{-1}$ ,  $\nu_{\text{HCN}}$ : 3200–3350  $\text{cm}^{-1}$ ,  $\delta_{\text{HCN}}$ : 710  $\text{cm}^{-1}$ ,  $\nu_{\text{CH}}(\text{CH}_4)$ : 2900–3150  $\text{cm}^{-1}$ ,  $\nu_{\text{CH}}$  (benzene ring): 3030–3080  $\text{cm}^{-1}$ ,  $\nu_{\text{C=C}}$  (the vibration of the benzene frame work): 1600 and 1500  $\text{cm}^{-1}$ , and  $\nu_{\text{C=O}}$ : 1700  $\text{cm}^{-1}$ . The flash pyrolysis FT-IR results for the TOs are listed in Table 3. Signals due to CO, CO<sub>2</sub>, isocyanate, and benzene were observed in the gases generated from ArTOs. For the generated gases of 3a, absorption bands for CH<sub>4</sub> were not observed. It was expected that methane gas was generated from methyl and methoxy groups in the substituents of ArTOs.

**Table 3** Gases generated from TOs.

	Compounds		Generated gases
	R <sub>1</sub>	R <sub>2</sub>	
<b>3a</b>	Ph	Ph	CO CO <sub>2</sub> C <sub>6</sub> H <sub>6</sub> HCN -NCO
<b>3b</b>	Ph	4-Me-Ph	CO CO <sub>2</sub> CH <sub>4</sub> C <sub>6</sub> H <sub>6</sub> HCN -NCO
<b>3c</b>	Ph	4-MeO-Ph	
<b>3d</b>	4-Me-Ph	Ph	
<b>3e</b>	4-Me-Ph	4-Me-Ph	
<b>3f</b>	4-Me-Ph	4-MeO-Ph	
<b>3g</b>	4-MeO-Ph	Ph	
<b>3h</b>	4-MeO-Ph	4-Me-Ph	
<b>3i</b>	4-MeO-Ph	4-MeO-Ph	
<b>TO</b>	H	H	CO CO <sub>2</sub> HCN HNCO

**Fig. 7** IR spectrum of gases generated from **3c** at 2.9 min.

### 3.3 Electronic energy calculations for two-center energy

The results of the two-center energy calculations of **3a**, **3b**, and **3c** are shown in Fig.8. The minimum value of two-center energy in **3a** was the N1–N2 and N2–C3 bonds on the triazole ring (Fig.1). The minimum value of ArTO containing the methyl or methoxy group was that of the C–CH<sub>3</sub> or O–CH<sub>3</sub> bonds in the substituents. The energies corresponded to the binding energy<sup>12)</sup>, and were used as a standard for ease of bond dissociation in the triazole ring. The two-center energy of all ArTOs was determined by MO calculations. Based on these energies and the generated gases, the initial pyrolysis process of ArTOs was examined.

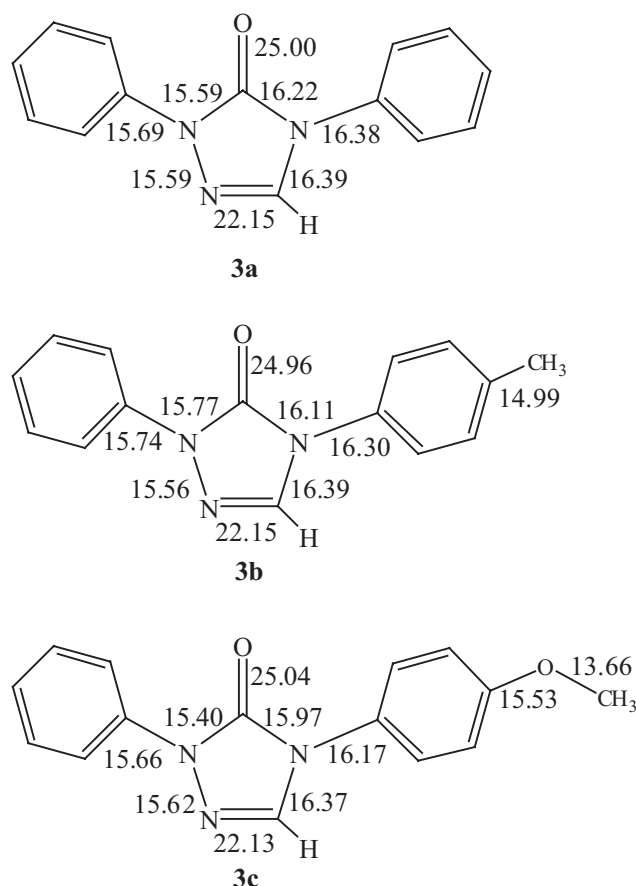
The bond lengths and angles for the geometric structure of TO (see Fig.1) determined by the MO calculations are presented in Table 4. The geometric structure of TO was a planar structure. 1,2,4-Triazoles satisfying Huckel's rule are known to exhibit aromaticity and planar structures. However, TOs which do not satisfy Huckel's rule were also found to have planar structures.

### 3.4 Initial pyrolysis process

The initial pyrolysis process of **3a** was investigated. An important aspect of the experimental results was that isocyanate groups were observed in the gases generated from **3a**. It was assumed that this was the result of cleavage of either the N2–C3 and N4–C5 bonds or the N1–N2

**Table 4** Calculated bond lengths and angles for TO.

	Lengths (Å)		Angles (°)	
	N 1–N 2	1.35	N 1–N 2–C 3	112.2
N 2–C 3	1.43	N 2–C 3–N 4	103.4	
C 3–N 4	1.42	C 5–N 1–N 2	106.6	
N 4–C 5	1.41	H 6–N 2–N 1	121.2	
C 5–N 1	1.34	O 7–C 3–N 2	128.3	
N 2–H 6	0.99	O 7–C 3–N 4	128.3	
N 3–O 7	1.24	H 8–N 4–C 3	125.7	
N 4–H 8	0.98	H 9–C 5–N 4	123.2	
C 5–H 9	1.10			

**Fig. 8** Two-center energies of **3a**, **3b**, and **3c**.

and C3–N4 bonds of the triazole ring. According to the MO calculations for **3a**, the minimum value of the two-center energy was the N1–N2 and N2–C3 bonds, which supported the suggested process.

Secondly, for ArTOs (**3b–3i**) containing methyl or methoxy groups in the substituents, we suggest that methane gas was generated from the substituents rather than from the triazole ring itself. There are two experimental results that support this suggestion. First, flash pyrolysis of **3a**, which contained no methyl or methoxy groups, did not generate methane gas, while all ArTOs with methyl or methoxy groups generated methane gas. Second, the minimum values of two-center energies for all ArTOs other than **3a** were the C–CH<sub>3</sub> or O–CH<sub>3</sub> bonds in the substituents. A relationship may be observed between the generated gases in the experimental results and the results of the MO calculations.

In addition, the relationship between the substituent effects on  $T_{DSC}$  and the initial pyrolysis of ArTOs (**3b–3i**) was examined. It was mentioned that the initial pyrolysis process was related to the cleavage of bonds with smaller bond energies. However, it is assumed that  $T_{DSC}$  of ArTOs is not controlled by the strength of its bonds, but by the electronic effects of the substituents. This phenomenon should be observed under the condition that  $T_{DSC}$  does not increase in the order of its bonds' various strengths. However, the experiment demonstrates each  $T_{DSC}$  differs when the substituents at positions 2 and 4 (**3b** and **3d**, **3c** and **3g**, **3f** and **3h**) are exchanged. Since the two different substituents of ArTOs interact with each other and influence the electronic state of a molecule, it is expected that  $T_{DSC}$  of ArTOs is closely related to the state of a given electron.

We therefore propose that the first step in the pyrolysis of **3a** is cleavage of either the N2–C3 and N4–C5 bonds or the N1–N2 and C3–N4 bonds of the triazole ring, while the first step in the pyrolysis of ArTOs containing methyl or methoxy groups (**3b–3i**) is elimination of the methyl or methoxy groups. Since isocyanate was also generated from **3b–3i**, the pyrolysis process of **3b–3i** was considered to be decomposition via triazole ring cleavage reaction with elimination of the methyl or methoxy groups.

#### 4. Conclusions

Based on these experimental investigations on the synthesis and thermal substituent effects in ArTOs, the following conclusions can be drawn :

- (1) ArTOs are synthesized from semicarbazidomethylenemalonic acid derivatives in good to average yields.
- (2) TOs decompose in the gas phase.
- (3) The presence of electron-releasing substituents on the aryl groups at positions 2 and 4 of the ArTOs has a significant influence on thermal stability.
- (4) Exothermic temperatures for TOs are affected by substituents at positions 2 and 4.
- (5) The initial pyrolysis step for **3a** is likely to be cleavage of either the N2–C3 and N4–C5 bonds or N1–N2 and C3–N4 bonds of the triazole ring.
- (6) The initial step in the pyrolysis of ArTOs containing methyl or methoxy groups is elimination of the methyl or methoxy groups.

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## 2,4-ジアリール-3H-1,2,4-トリアゾール-3-オンの 合成と熱的挙動

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2,4位にアリール基を導入した2,4-ジアリール-1,2,4-トリアゾール-3-オン (ArTOs) の合成および熱的挙動の検討, 分解初期過程の推定を行った。熱的挙動の検討に熱重量示差熱同時測定 (TG/DTA) および密封セル-示差熱熱量計 (SC-DSC), 高速熱分解 FT-IR を用いた。半経験的分子軌道計算の AM1 法により ArTOs の結合長および2中心エネルギーを算出した。セミカルバジドメチレンマロン酸誘導体を用いた ArTOs の合成は高収率で得られた。TG/DTA および SC-DSC の結果から, 2,4位の電子供与性置換基は熱特性に影響を及ぼすことが明らかになった。TG/DTA 後のセルに残渣は確認されなかった。解放セル条件では残渣がなく吸熱ピークが確認され, 密閉セル条件では発熱ピークが確認されたことから, ArTO の分解は主に気相反応であると考えられる。高速熱分解 FT-IR の結果から, 生成ガスにイソシアネート化合物およびシアン化水素が確認されたことから, 2,4-ジフェニール-3H-1,2,4-トリアゾール-3-オンの分解初期過程は N2-C3 結合と N4-C5 結合, もしくは N1-N2 結合と C3-N4 結合の解離が考えられる。結合の切れやすさの目安として算出した2中心エネルギー値は, N1-N2 結合および N2-C3 結合が最小値を得られた。この実験結果は分子軌道計算結果と良好な相関が認められた。

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