



# The 5-(isopropylidene)-2-thiobarbituric acid: Preparation, crystal structure, thermal stability and IR-characterization



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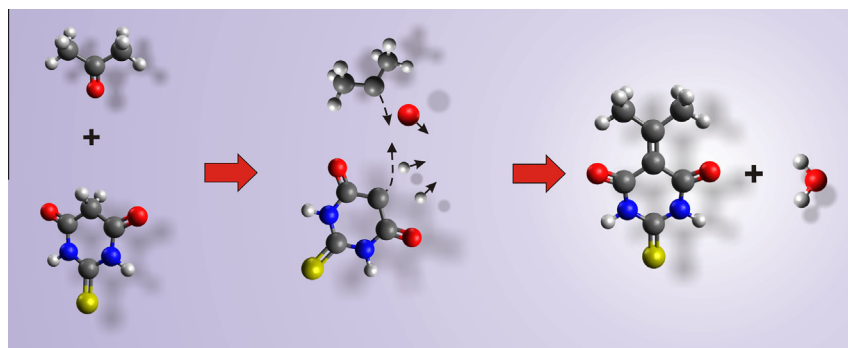
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## HIGHLIGHTS

- A novel 5-(isopropylidene)-2-thiobarbituric acid was prepared.
- XRD, XRPD, DSM, TG and IR spectroscopy were used for the compound characterization.
- The heterocyclic ring of C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S corresponded to the thionedicarbonyl structure.
- There are two different chain-forming intermolecular N—H...O bonds.
- C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S is thermally stable up to 230.0 °C and melts with decomposition at 261.4 °C.

## GRAPHICAL ABSTRACT



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## ABSTRACT

5-(Isopropylidene)-2-thiobarbituric acid (**1**), C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>S, has been crystallized by reacting 2-thiobarbituric acid with excessing acetone for 5–6 days under ambient conditions. The pale yellow crystals have been investigated using X-ray single crystal and powder techniques and characterized by differential scanning calorimetry, thermogravimetry and infrared spectroscopy. The compound crystallizes in the monoclinic system with  $a = 8.8268(19)$  Å,  $b = 12.044(3)$  Å,  $c = 8.0998(19)$  Å,  $\beta = 105.388(6)^\circ$ ,  $Z = 4$ ,  $V = 830.2(3)$  Å<sup>3</sup>, space group  $P2_1/c$ . The geometric parameters of the heterocycle of the molecule **1** are similar to those found previously for the molecule of thionedicarbonyl tautomer in polymorphic modifications of 2-thiobarbituric acid. Infrared spectroscopy also evidences the thionedicarbonyl structure of the **1** heterocyclic ring. Intermolecular N—H...O hydrogen bonds join the molecules in the chains along  $b$  axis. The **1** compound is thermally stable up to 230.0 °C and melts with decomposition at 261.4 °C. The results of mass spectrometric analysis are consistent with the structural parameters found by X-ray diffraction methods.

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## Introduction

2-Thiobarbituric acid (2-thioxodihydropyrimidine-4,6(1H,5H)-dione, H<sub>2</sub>TBA) is a simplest representative of the class of thiobarbituric acids (Fig. 1). It is a key compound used in the synthesis of a

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number of its derivatives which have an important therapeutic value, such as sodium thiopental [1], thiobarbital (5,5-diethyl-2-thiobarbituric acid) and thiobutabarbital (5-(2-butyl)-5-ethyl-2-thiobarbituric acid) [2]. In the general class of depressants, the 2-thiobarbituric acid derivatives are known as thiobarbiturates [1,2], and they are used as antihyperthyroid and anesthetic agents. Complexes of 2-thiobarbituric acid with metals can possess anti-cancer activity [3], antibacterial activity [4–6] and interesting structural features [7–14].

Typically, synthesis using thiobarbituric acid is conducted in organic solvents [15,16], and it is necessary to account for their possible interaction. Since 2-thiobarbituric acid contains an active methylene group, it can enter into a condensation reaction with aldehydes and ketones (Knoevenagel reaction) to form ethylene derivatives. Thus, it was found that, in this way, acetone reacted with the C5 carbon atom (Fig. 1) of 1-N-aryl substituted derivatives of 2-thiobarbituric acid. The resulting products were identified by NMR  $^{13}\text{C}$  and mass spectroscopy [17]. In the present study, 5-(isopropylidene)-2-thiobarbituric acid is obtained by the reaction of 2-thiobarbituric acid with acetone, and the crystal structure, thermal decomposition parameters and IR spectroscopic characteristics are found.

## Experimental section

### Chemical and reagents

2-Thiobarbituric acid was purchased from Sigma–Aldrich with  $\geq 98.0\%$  of purity and used without further purification. Acetone and KBr of analytical grade were supplied by Acros. All the chemicals were used as received.

### Synthesis

5-(Isopropylidene)-2-thiobarbituric acid (**1**) was prepared by mixing 5 mL of acetone and 200 mg of 2-thiobarbituric acid. Pale-yellow needle-like crystals precipitated after the solution being kept for 5 days in ambient conditions. The crystals were separated from the solution by filtration, washed by a small amount of acetone and dried in the air at ambient temperature. Crystals suitable for X-ray analysis were grown by continuous evaporation of the filtrate. The product output was about 80%. The powder product was hardly soluble in water and acetone.

The chemical analysis was carried out with an HCNS-0 EA 1112 Flash Elemental Analyser. The elemental analysis for  $\text{C}_7\text{H}_8\text{N}_2\text{O}_2\text{S}$ : Calc.: C, 45.6%; H, 4.38%; N, 15.2%; S, 17.4%. Found: C, 45.4%; H, 4.52%; N, 14.9%; S, 17.3%.

### Physical measurements

IR spectra were recorded for the powder samples packed into KBr pellets on a Bruker Vector-22 Fourier spectrometer over the

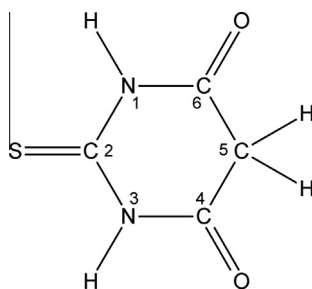


Fig. 1. Scheme and atom nomenclature in a 2-thiobarbituric acid molecule ( $\text{H}_2\text{TBA}$ ).

spectral range of  $400\text{--}4000\text{ cm}^{-1}$ . The spectral resolution during measurements was  $5\text{ cm}^{-1}$ . Thermal behavior was studied by simultaneous thermal analysis using a Netzsch STA Jupiter 449C with an on-line Aeolos QMS 403C mass spectrometer under dynamic argon atmosphere at the temperature ramp rate of  $10^\circ\text{ min}^{-1}$ . The sample mass was 4.54 mg and 6.18 mg for **1** and  $\text{H}_2\text{TBA}$ , respectively. Powder X-ray diffraction data were obtained using the diffractometer D8 ADVANCE (Bruker) equipped with a VANTEC detector with a Ni filter. The measurements were made using  $\text{Cu K}\alpha$  radiation.

### X-ray diffraction analysis

The intensities of a single crystal of  $0.4 \times 0.4 \times 0.2\text{ mm}$  dimensions were collected at 300 K using the SMART APEX II X-ray single crystal diffractometer (Bruker AXS) equipped with a CCD-detector, graphite monochromator and  $\text{Mo K}\alpha$  radiation source.

The crystal was twinned. Cell parameter search procedure using standard APEX II program was failed. Therefore, Cell\_Now (Version 2008/2) program supplied as a part of APEX II software was used. It analyses a list of reflections to find a cell and orientation matrix despite the presence of several twin domains. In our case, from total 147 reflections only 122 were indexed by first domain. The unit cell corresponds to monoclinic symmetry. 115 from 147 reflections including all previously unindexed reflections were indexed by second domain. The cell parameters of second domain were the same as those of the first domain but matrix of orientation was another. The analysis shows that second domain is rotated in reference to first domain by  $180^\circ$  about axis *a*.

Integration of intensities were carried out considering the two domains by APEX II program. The absorption corrections were applied using TWINABS program, and corrected intensities of the two domains were saved in one file. Space group  $P2_1/c$  was determined from the statistical analysis of the intensities of all the reflections. The structure was solved by the direct methods using package SHELXS. Intensities of the first domain were used for this purpose. Structure was refined in anisotropic approach for non-hydrogen atoms using SHELXL program [19] using intensities of the two domains. The volume percentage of the first and second domains was 58.1(2)% and 41.9(2)%, respectively. All the hydrogen atoms were refined in a constrained mode. The structure test for the presence of other missing elements of symmetry and possible voids was produced using the program PLATON [20]. The main crystal data are shown in Table 1. The crystallographic data are deposited in Cambridge Crystallographic Data Centre (CCDC # 989216). The data can be downloaded from the site ([www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif)). The main bond lengths are shown in Table 2. The DIAMOND program is used for the crystal structure plotting [21].

The structural parameters of **1** defined by single crystal analysis were used as a basis in Rietveld refinement of the powder pattern. The refinement was produced using program TOPAS 4.2 [18]. Low *R*-factors and good refinement shown in Fig. 2a indicate the crystal structure of the powder sample to be a representative of the bulk structure. A thionedicarbonyl tautomer of  $\text{H}_2\text{TBA}$  was obtained by recrystallization of the acid from  $\text{CH}_3\text{COOH}$ . Its powder pattern well corresponds to pure III polymorphic modification as it is evident from Fig. 2b.

## Results and discussion

### Crystal structure of 5-(isopropylidene)-2-thiobarbituric acid

The independent part of the **1** unit cell contains one molecule of  $\text{C}_7\text{H}_8\text{N}_2\text{O}_2\text{S}$  (Fig. 3). The X-ray data analysis verifies the thionedicarbonyl type structure of 5-(isopropylidene)-2-thiobarbituric acid.

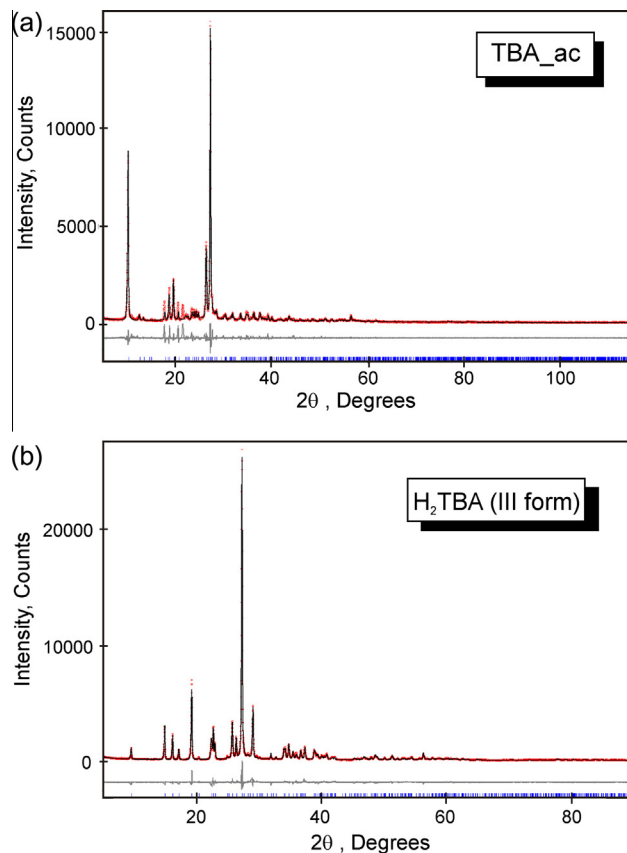
**Table 1**  
The crystal structure parameters of compound **1**.

Formula moiety	C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S
Molecular weight	184.21
Temperature (K)	298
Space group, Z	P2 <sub>1</sub> /c, 4
a (Å)	8.8268(19)
b (Å)	12.044(3)
c (Å)	8.0998(19)
β (°)	105.388(6)
V (Å <sup>3</sup> )	830.2(3)
ρ <sub>calc</sub> (g/cm <sup>3</sup> )	1.474
μ (mm <sup>-1</sup> )	0.348
Reflections measured	5102
Independent reflections	4008
Reflections with F > 4σ(F)	2121
2θ <sub>max</sub> (°)	59.3
h, k, l - limits	-12 ≤ h ≤ 11; 0 ≤ k ≤ 16; 0 ≤ l ≤ 11
R <sub>int</sub>	0.0431
<b>Refinement results</b>	
The weighed refinement of F <sup>2</sup>	w = 1/[σ <sup>2</sup> (F <sub>o</sub> <sup>2</sup> ) + (0.0667P) <sup>2</sup> + 1.064P] where P = max(F <sub>o</sub> <sup>2</sup> + 2F <sub>c</sub> <sup>2</sup> )/3
Number of refinement parameters	110
R1 [F <sub>o</sub> > 4σ(F <sub>o</sub> )]	0.0865
wR2	0.1821
Goof	1.041
Δρ <sub>max</sub> (e/Å <sup>3</sup> )	0.450
Δρ <sub>min</sub> (e/Å <sup>3</sup> )	-0.407
(Δ/σ) <sub>max</sub>	0.006

**Table 2**  
The main bond lengths (Å) of compound **1**.

S–C2	1.645 (3)	N3–C4	1.379 (4)
O1–C4	1.224 (4)	C4–C5	1.478 (4)
O2–C6	1.223 (4)	C5–C7	1.364 (4)
N1–C2	1.360 (4)	C5–C6	1.476 (4)
N1–C6	1.377 (4)	C7–C8	1.490 (5)
N3–C2	1.355 (4)	C7–C9	1.495 (5)

The bond length d(C5–C7) = 1.363(4) Å in **1** is noticeably shorter than that of the single bond d(C5–C7) = 1.551(4) Å between similar atoms in 5-(isopropyl)-2-thiobarbituric acid [22]. Thus, this bond in the **1** compound should be classified as a double one. The valence angles in **1** are better fitted by sp<sup>2</sup> hybridization of atom C5: ∠C4–C5–C6 = 116.3(3)°, ∠C6–C5–C7 = 121.6(3)°, ∠C7–C5–C4 = 122.1(3)°. Comparatively, in 5-(isopropyl)-2-thiobarbituric acid, the related angles are significantly different and are closer to sp<sup>3</sup> hybridization of the C5 atom: ∠C4–C5–C6 = 115.2(2)°, ∠C6–C5–C7 = 112.0(3)°, ∠C7–C5–C4 = 111.7(3)° [22]. Moreover, ∠C4–C5–C6 angles in heterocycle are similar in both compounds, unlike the other two angles. The value of 116.3° is in better agreement with the thionedicarbonyl structure of pyrimidine heterocycle shown in Fig. 1. Our analysis of structural data available from CSD [23] shows that in this case the valence angle ∠C4–C5–C6 is approximately equal to 116°. The average values of bond lengths C4–C5 and C5–C6 (1.48 Å) in **1** and (1.50 Å) in 5-(isopropyl)-2-thiobarbituric acid are closer to single bond. Other bond lengths C–O, C–N and C–C and the corresponding heterocycle valence angles in the **1** molecule were similar to those found previously for the molecules of thionedicarbonyl isomer in five polymorph modifications of 2-thiobarbituric acid (H<sub>2</sub>TBA) [24] and in 5-(isopropyl)-2-thiobarbituric acid [23] close in composition and structure to **1**. Thus, the insertion of the isopropylidene substituent in thiobarbituric acid at position 5 leads to the formation of thionedicarbonyl structure of the modified compound.



**Fig. 2.** Experimental (dots) and theoretical (lines) X-ray diffraction patterns of (a) 5-(isopropylidene)-2-thiobarbituric acid **1** (TBA-ac) and (b) H<sub>2</sub>TBA (III polymorph form).

Analysis of the structure reveals two intermolecular hydrogen bonds N–H...O (Table 3), which form a chain along *b* axis (Figs. 4 and 5). There are no hydrogen bonds between the chains. Also, the π–π interaction between heterocyclic rings is absent because the minimal distance between centers of the rings is as long as 4.807(2) Å. There is structural motif R<sub>2</sub><sup>2</sup>(8) [25] in the structure due to hydrogen bonding.

#### IR absorption spectrum of 5-(isopropylidene)-2-thiobarbituric acid

The following bands were found in the IR absorption spectrum of **1** shown in Fig. 6a (cm<sup>-1</sup>): 3317 vw., 3138 m., 3072 m., 2928 m., 2827 w., 2619 w., 1701 s., 1650 vs., 1547 s., 1446 s., 1403 m., 1338 m., 1256 m., 1216 m., 1174 s., 1061 vw., 1024 vw., 863 m., 797 w., 681w., 643 vw., 523 s., 435 vw. (vs. – very strong, s. – strong, m. – medium, w. – weak, vw. – very weak). The IR absorption spectrum of III polymorph modification of 2-thiobarbituric acid (Fig. 6b) is similar to the spectrum of **1** that indirectly confirms a thionedicarbonyl type of the **1** structure. Other bands, for example at 1740 and 1665 cm<sup>-1</sup>, however, were observed in the IR absorption spectra of 5-(isopropyl)-2-thiobarbituric acid, the compound with the structure and composition close to **1** [22], and the bands were referred to ν(C=O). The analysis of IR spectra of 2-thiobarbituric acid [26–30] shows that: (1) lines of ν(C=S) are usually in the frequency range of 1145–1185 cm<sup>-1</sup>; (2) the most high-frequency ν(C=O) band lies in the range from 1705 to 1750 cm<sup>-1</sup>; (3) the ν(N–H) values are generally not very informative since they vary over the wide range of ~3100–3450 cm<sup>-1</sup> that appeared due to their participation in the formation of various hydrogen bonds. Using this generalization, the strong band at 1701 cm<sup>-1</sup> in IR

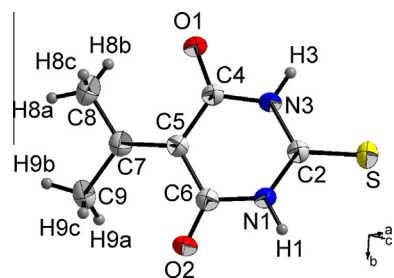


Fig. 3. The independent part of the **1** unit cell. Ellipsoids are drawn at the 50% probability level, except for the hydrogen atoms represented by spheres.

spectra of **1** can be attributed to  $\nu(\text{C}=\text{O})$ , very strong band at  $1650\text{ cm}^{-1}$  –  $\nu(\text{C}=\text{O}) + \nu(\text{C}=\text{C})$ , strong band at  $1174\text{ cm}^{-1}$  with a shoulder at the low-frequency region –  $\nu(\text{C}=\text{S})$ , very weak band at  $3317\text{ cm}^{-1}$  –  $\nu(\text{NH})$ . The absence of the characteristic bands over the range of  $2300\text{--}2500\text{ cm}^{-1}$  in the IR absorption spectra of **1** and the presence of a signal of cyclic thioamide structure – $\text{NH}(\text{C}=\text{S})$  at  $1567\text{ cm}^{-1}$  indicate that thione structure dominates in the solid state. Therefore, the results of IR spectroscopy confirm the thionedicarbonyl type structure obtained by X-ray investigation.

#### Thermal analysis of 5-(isopropylidene)-2-thiobarbituric acid

There are three endothermic effects observed at the differential scanning calorimetry (DSC) curve for **1** as it is shown in Fig. 7. The first significant endoeffect at  $261.4\text{ }^\circ\text{C}$  corresponds to the melting process with the decomposition. The other two effects at  $357.8$  and  $446.6\text{ }^\circ\text{C}$  are associated with some thermal degradation compounds. Initially,  $\text{H}_2\text{TBA}$  also melts with decomposition at  $250.6\text{ }^\circ\text{C}$ . In general features, the heating behavior of  $\text{H}_2\text{TBA}$  and its derivative **1** are similar. The dynamics of mass changes of these compounds on heating, however, is different. The results of thermogravimetric analysis of the compounds are summarized in Table 4.

The TG curves are shown in Fig. 8. At the initial stage ( $40\text{--}275\text{ }^\circ\text{C}$ ), the degradation of **1** proceeds with a higher speed than that of  $\text{H}_2\text{TBA}$ , and the degradation is accompanied by a greater mass loss. The most significant difference in the behavior of these two compounds occurs over the temperature range of  $275\text{--}335\text{ }^\circ\text{C}$ . In this temperature interval, the degradation of **1** continues at the rate of  $2.6\%/ \text{min}$  with the mass loss of  $18\%$ . Comparatively,  $\text{H}_2\text{TBA}$  in this range exhibits the induction period and the mass remains almost persistent ( $<1\%$ ).

As a result, at the end of the second stage of thermal degradation ( $335\text{ }^\circ\text{C}$ ), the **1** sample mass loss is nearly twice as much ( $39.7\%$ ) as that of 2-thiobarbituric acid ( $15.0\%$ ). At stages 3 and 4 (Table 4), the process is enhanced and the degradation of  $\text{H}_2\text{TBA}$  proceeds at nearly two times higher rate than that found for the decomposition of its derivative **1**. At the stages, the mass loss is  $43.3\%$  and  $29.0\%$  for thiobarbituric acid and **1**, respectively. Thus, the thermal stability of these compounds over different temperature ranges is significantly different. At  $T < 335\text{ }^\circ\text{C}$ , the **1** sample is significantly less stable than  $\text{H}_2\text{TBA}$ . At  $T > 335\text{ }^\circ\text{C}$ , the destruction of **1** becomes slow.

Table 3  
Hydrogen-bond geometry in the **1** structure ( $\text{\AA}$ ,  $^\circ$ ).

D–H	d(D–H)	d(H···A)	$\angle\text{D–H}\cdots\text{A}$	D···A	A	Transformation for A atom
N1–H1	0.86	2.01	176	2.863(3)	O1	$1 - x, y - \frac{1}{2}, 3/2 - z$
N3–H3	0.86	2.00	172	2.856(4)	O2	$1 - x, \frac{1}{2} + y, 3/2 - z;$

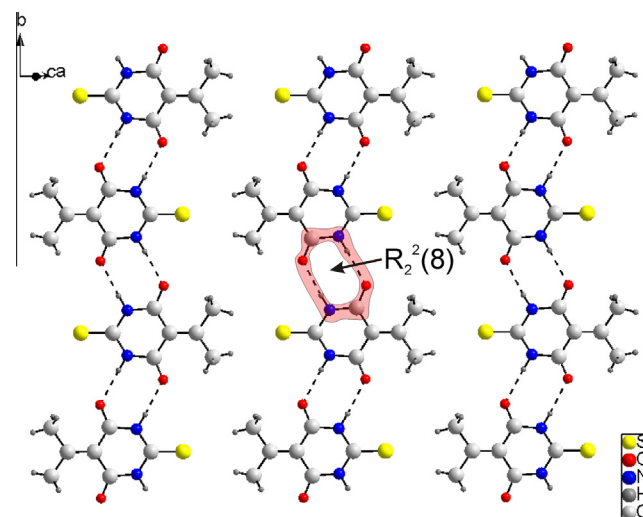


Fig. 4. Part of the **1** structure with molecules within one layer. Hydrogen bonds are shown by dashed lines. The symbols used for the structural motif are taken from [25].

#### Mass spectrometric analysis of 5-(isopropylidene)-2-thiobarbituric acid

In parallel with the thermal analysis, the mass spectrometric analysis of gaseous degradation products of **1** and  $\text{H}_2\text{TBA}$  was conducted. The basic elements of the cyclic structure of the compounds are the amide  $\text{C}(=\text{O})\text{NH}$ – and monothioimide  $\text{C}(=\text{S})\text{N}(\text{H})\text{C}(=\text{O})$ –groups, and specifically for **1** – the isopropylidene group at position 5. The profiles of functional groups evolution during the thermal degradation of these compounds are shown in Fig. 9. The temperature and ion current (I) values obtained for the peaks of the functional group evolution are reported in Table 5.

As it is evident from the mass spectrometric results, the formation of an amide group  $\text{C}(=\text{O})\text{NH}$ – ( $m/z = 43$ ) in the products of **1** degradation is more intensive and occurs at much lower temperatures ( $275.4\text{ }^\circ\text{C}$ ) than that of  $\text{H}_2\text{TBA}$  ( $471.0\text{ }^\circ\text{C}$ ). Furthermore, at the initial stage of the **1** degradation in the range of  $T = 275\text{--}335\text{ }^\circ\text{C}$ , structural fragments  $(\text{CH}_3)_2\text{C}=\text{C}(\text{C}=\text{O})_2$ – ( $m/z = 110$ ) and isopropylidene groups  $(\text{CH}_3)_2\text{C}(\text{C}=\text{O})$ – ( $m/z = 54$ ) are revealed, and these evolved due to a rupture of the amide bonds in the cyclic structure of the molecule. This well agrees with the X-ray structure investigation results. Thus, the substitution of two hydrogen atoms in 2-thiobarbituric acid by isopropylidene groups results in a drastic variation of the thermal behavior and decreases the thermal stability at  $T < 335\text{ }^\circ\text{C}$ . Also, at a rupture of the cyclic amide bond, the structural group  $\text{HNC}(=\text{S})\text{NH}$ – ( $m/z = 74$ ) is formed. Its fragmentation to  $\text{C}(=\text{S})\text{NH}$ – ( $m/z = 59$ ) proceeds at higher temperatures with a maximum at  $T \sim 376.0\text{ }^\circ\text{C}$ . Thus, on the basis of the thermoanalysis results, it is found that **1** compound is thermally stable up to  $230.0\text{ }^\circ\text{C}$ , melts with decomposition at  $261.4\text{ }^\circ\text{C}$ , and undergoes further degradation with the total mass loss of  $73\%$  at  $T \sim 1000\text{ }^\circ\text{C}$ .

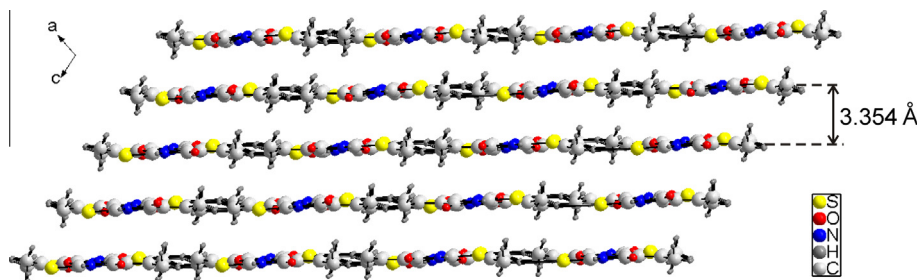


Fig. 5. View of the **1** structure along the molecule layers.

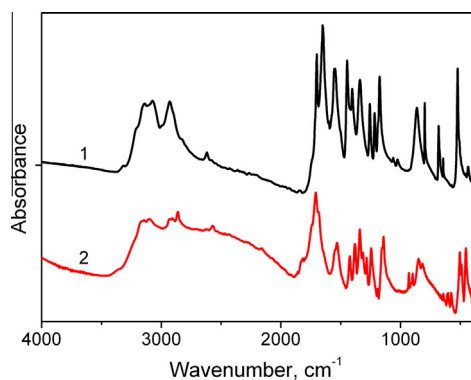


Fig. 6. IR spectra of (1) 5-(isopropylidene)-2-thiobarbituric acid and (2) III polymorph modification of 2-thiobarbituric acid.

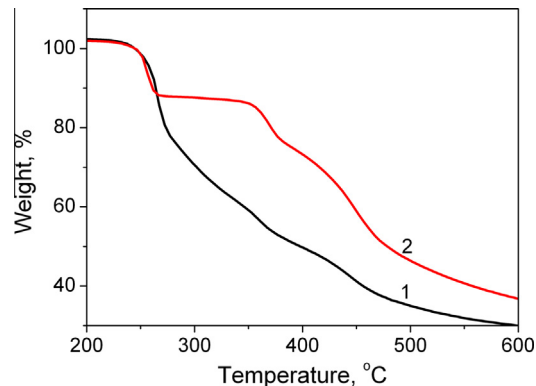


Fig. 8. TG-curves recorded from (1) 5-(isopropylidene)-2-thiobarbituric acid and (2) H<sub>2</sub>TBA.

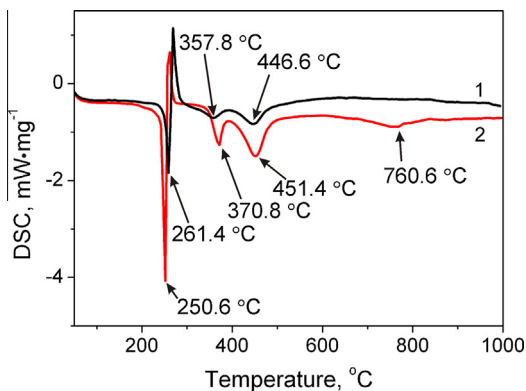


Fig. 7. DSC-curves of (1) 5-(isopropylidene)-2-thiobarbituric acid and (2) H<sub>2</sub>TBA.

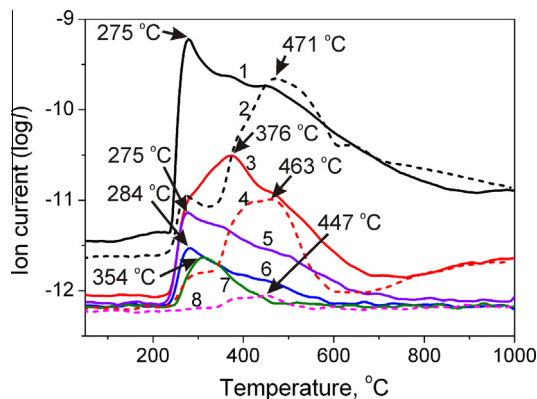


Fig. 9. The fragment of mass spectrum of **1** (solid lines: (1)  $m/z = 43$ ; (3)  $m/z = 59$ ; (5)  $m/z = 54$ ; (6)  $m/z = 74$ ; (7)  $m/z = 110$ ) and H<sub>2</sub>TBA (dashed lines: (2)  $m/z = 43$ ; (4)  $m/z = 59$ ; (8)  $m/z = 74$ ).

Table 4

Details of the thermal behavior stability of **1** and H<sub>2</sub>TBA on heating in an inert atmosphere.

Stages of thermal destruction	Temperature range, °C	<b>1</b>			H <sub>2</sub> TBA		
		$T_{\max}$ , °C	$V_{\max}$ , %/min	$\Delta m$ , %	$T_{\max}$ , °C	$V_{\max}$ , %/min	$\Delta m$ , %
1	40–275	266.9	10.5	21.7	256.3	8.0	14.0
2	275–335	298.0	2.6	18.0	–	–	1.0
3	335–395	358.6	2.7	12.0	369.3	4.1	12.5
4	395–520	444.6	2.1	17.0	449.6	4.0	30.8

$V_{\max}$  – maximal decomposition rate (mass percent per minute).

Table 5

Temperature and the ion current ( $I$ ) values.

Structure element	$m/z$	<b>1</b>		H <sub>2</sub> TBA	
		$T$ , °C	$I$ , $\times 10^{-10}$ , A	$T$ , °C	$I$ , $\times 10^{-10}$ , A
–C(=O)NH–	43	275.4	58.7	471.0	21.9
–HNC(=S)NH–	74	283.5	0.29	447.3	0.088
–C(=S)NH–	59	376.0	3.10	463.1	1.0
(CH <sub>3</sub> ) <sub>2</sub> C=C(C=O) <sub>2</sub> –	110	314.2	0.23	–	–
(CH <sub>3</sub> ) <sub>2</sub> C(=C)–	54	275.4	0.73	–	–

## Conclusions

Thus, a novel 2-thiobarbituric acid derivative, 5-(isopropylidene)-2-thiobarbituric acid, was synthesized. X-ray diffraction analysis, differential scanning calorimetry, thermogravimetric analysis and infrared spectroscopy were carried out for the compound characterization. The results obtained by these techniques are well consistent. The product obtained by crystallization from the acetone solution was the single phase compound. The X-ray phase analysis verified a high purity of obtained 5-(isopropylidene)-2-thiobarbituric acid.

The structure of the heterocyclic ring in **1** corresponds to the thionedicarbonyl structure. The bond length  $d(\text{C5}–\text{C7})$  in the **1** structure is noticeably shorter than the similar bond in 5-(isopropyl)-2-thiobarbituric acid. Thus the bond in **1** should be considered as a double one. The valence angles in **1** are better fitted by  $\text{sp}^2$  hybridization of atom C5, and this is also consistent with the existence of the above mentioned double C5–C7 bond. Analysis of the structure revealed two intermolecular hydrogen bonds that resulted in the chain formation. There are no hydrogen bonds between the chains. Also, there is no  $\pi$ – $\pi$  interaction between the heterocyclic rings.

As it is defined by thermoanalysis, the **1** compound is thermally stable up to 230.0 °C, melts with decomposition at 261.4 °C, and it undergoes further degradation with the total mass loss of 73% at the temperature increase up to 1000 °C. The mass spectrometric analysis reveals the formation of  $(\text{CH}_3)_2\text{C}=\text{C}(\text{C}=\text{O})_2$ –,  $(\text{CH}_3)_2\text{C}(\text{C}=\text{O})$ –,  $-\text{HNC}(\text{S})\text{NH}-$ ,  $-\text{C}(\text{O})\text{NH}-$  and  $-\text{C}(\text{S})\text{NH}-$  groups in keeping with the structure obtained by X-ray diffraction. The results of IR spectroscopy also gave evidence of the thionedicarbonyl structure of the heterocyclic ring.

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