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Molar Heat Capacity and Thermodynamic Properties of 4-Methyl-4-cyclohexene-1,2-dicarboxylic Anhydride [$C_9H_{10}O_3$]

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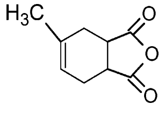
The molar heat capacity $C_{p,\mathrm{m}}$ of 4-methyl-4-cyclohexene-1,2-dicarboxylic anhydride was measured over the temperature range from $T = 80$ K to $T = 361$ K with a small-sample automated adiabatic calorimeter. The melting point T_m and the molar enthalpy $\Delta_\mathrm{fus}H_\mathrm{m}$ and entropy $\Delta_\mathrm{fus}S_\mathrm{m}$ of fusion for the compound were determined to be (335.54±0.41) K, (17.67±0.04) kJ·mol^{-1}, and (52.65±0.04) J·K^{-1}·mol^{-1}, respectively. Thermodynamic functions $[H_\mathrm{T} - H_{298.15}]$ and $[S_\mathrm{T} - S_{298.15}]$ were derived in the temperature range from $T = 80$ K to $T = 361$ K with a temperature interval of 5 K. The purity of the sample in mole fraction used in the adiabatic calorimetry study was determined to be 0.9940 by using the fractional melting technique. The thermal stability of the compound was investigated by differential scanning calorimetry (DSC) and a thermogravimetric (TG) technique, and the process of the mass loss of the sample was due to evaporation instead of thermal decomposition.

Introduction

The molar heat capacities $C_{p,\mathrm{m}}$ of the compound as a function of temperature are basic physical data from which many other thermodynamic properties such as the enthalpy, entropy, and Gibbs free energy, which are important for both theoretical and practical purposes, can be calculated.[1,2] Adiabatic calorimetry at low temperature is a classical method for heat capacity measurement, from below 1 K to temperatures approaching the limits imposed by the materials themselves.[3−5] In the present paper, an adiabatic low-temperature calorimeter for small samples, of which the structure, working principle, and reliability have been described in our previous works,[2,4,6,11] was used to measure the molar heat capacities $C_{p,\mathrm{m}}$ of the studied compound in the temperature range from $T = 80$ K to $T = 361$ K. Moreover, the molar enthalpy and entropy of fusion and thermodynamic functions $[H_\mathrm{T} - H_{298.15}]$ and $[S_\mathrm{T} - S_{298.15}]$ were derived from the measured heat capacity data. The mass fraction purity of the sample was determined by the fractional melting technique.

4-Methyl-cyclohex-4-ene-1, 2-dicarboxylic acid anhydride (CAS number 3425-89-6, Beilstein registry number 135751) is also named 4-methyltetrahydrophthalic anhydride (abbreviated 4-MTHPA). Its molecular formula is $C_9H_{10}O_3$, the molar mass is 166.18 g·mol^{-1}, and the structural formula is

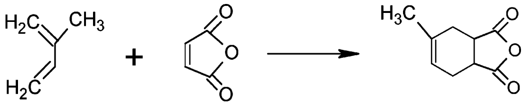


4-MTHPA is an anhydride-like curing agent for epoxy resins. Curing agents for epoxy resins promote attractive characteristics of high tensile strength and modulus, low shrinkage on curing, high resistance to chemicals and corrosion, excellent dimensional stability, and superior electrical properties.[7] Although epoxy resin can be cured with different hardeners, most studies performed up to now have been devoted to different aspects related to epoxy resins cured with amine curing agents, and few papers have been devoted to epoxy + anhydride mixtures. In fact, anhydride-like curing agents are preferred for electrical and electronic applications or when chemical safety has to be taken into account.[8] Anhydride-like curing agents mainly include tetrahydrophthalic anhydride (THPA), 3,4,5,6-tetrahydrophthalic anhydride (3,4,5,6-THPA), 4-methyltetrahydrophthalic anhydride (4-MTHPA), and hexahydrophthalic acid anhydride (HHPA). Besides being used as a curing agent for epoxy resins, some of them are used as intermediates in the preparation of many pesticides and herbicides, such as 3,4,5,6-THPA and 4-MTHPA; some of them are used as adhesives and plasticizers, such as THPA and HHPA.

However, few thermodynamic data of anhydride-like curing agents have been reported up to now, except for the reaction thermochemistry data of THPA by Ghitat et al. [9] in 1983; the boiling temperature of 3,4,5,6-THPA was measured to be from $T = 441$ K to $T = 443$ K by Frinton Laboratories Inc. in 1986. Because these compounds are very useful in many fields, for the sake of its application, in this paper a thermodynamic study was performed to measure the low-temperature heat capacity and thermal stability of 4-MTHPA.

Experimental Section

Sample. The compound used in these experiments was provided by Huicheng Chemicals Co. of China with a purity >99% and a melting point of 62−63 °C. It was synthesized by the following procedure. Briefly, C (4-MTHPA) is



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synthesized with A (Me-butadiene) and B (maleic acid anhydride) in terms of the Diels−Alder reaction.

Adiabatic Calorimetry. A precision automatic adiabatic calorimeter was used to measure the heat capacity of the compound. The calorimeter was located in the Thermochemistry Laboratory of the Dalian Institute of Chemical Physics, Chinese Academy of Sciences. The principles of operation and structure of the instrument have been described in detail elsewhere.[2,4,6,10−12] Briefly, the automatic adiabatic calorimeter was composed of a sample cell, a miniature platinum resistance thermometer, an electric heater, inner and the outer adiabatic shields, two sets of six-junction chromel−constantan thermopiles installed between the calorimetric cell and the inner shield and between the inner and the outer shields, and a high-vacuum can.[2] Its working temperature range is from T = 78 K to T = 400 K, and it is cooled by liquid nitrogen. Prior to the heat capacity measurement of the sample, the molar heat capacities of α-Al_2O_3, the standard reference material, were measured from T = 78 K to T = 400 K to verify the reliability of the adiabatic calorimeter. The results showed that the deviation of our calibration data from those of NIST[13] was within ±0.3% over the whole temperature range.

The heat capacity measurements were conducted by the standard procedure of intermittently heating the sample and alternately measuring the temperature. The heating rate and the temperature increments of the experimental points were generally controlled from (0.1 to 0.4) $K{\cdot}min^{-1}$ and (1 to 4) K. The heating duration was 10 min, and the temperature drift rates of the sample cell measured in an equilibrium period were always kept within (10^{-3} to 10^{-4}) $K{\cdot}min^{-1}$ during the acquisition of all heat capacity data.

The mass of 4-MTHPA used for the measurement was 3.8321 g, which was equivalent to 0.0231 mol on the basis of the molar mass M = 166.18 $g{\cdot}mol^{-1}$.

DSC and TG Techniques. Thermal analysis of 4-MTHPA was performed using a differential scanning calorimeter (DSC-141, Setaram, France) at the heating rate of 10 $K{\cdot}min^{-1}$ under pure nitrogen with a flow rate of 50 $mL{\cdot}min^{-1}$. The mass of the sample used in the experiment was (2.30 ± 0.01) mg (Mettler Toledo AB135-S Balances, Switzerland). A thermogravimetric analyzer (model DT-20B, Shimadzu, Japan) was used to carry out the TG measurement of the compound at the heating rate of 10 $K{\cdot}min^{-1}$ under pure nitrogen with a flow rate of 30 $mL{\cdot}min^{-1}$. The mass of the sample used in the experiment was (9.80 ± 0.01) mg.

Results and Discussion

Molar Heat Capacity and Thermodynamic Functions. The experimental molar heat capacities $C_{p,\mathrm{m}}/R$ and temperaure T from T = 80 K to T = 361 K for 4-MTHPA are presented in Table 1 and plotted in Figure 1. It can be seen from the Figure that the heat capacity curve is continuous and smooth except in the melting-temperature range from T = 330 K to T = 338 K, which means that the structure of the sample was stable: no phase change occurred in the solid phase from T = 80 K to T = 330 K, and neither association nor thermal decomposition occurred in the liquid phase from T = 338 K to T = 361 K. The compound melted from T = 330 K to T = 338 K with a peak temperature of T = 335.29 K.

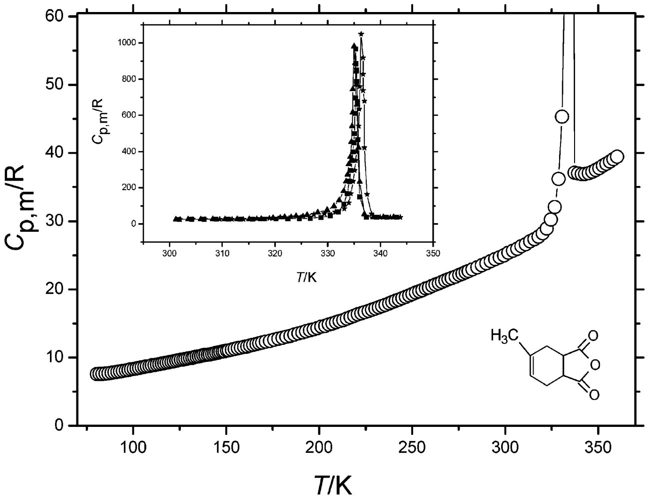

Figure 1. Experimental molar heat capacity plotted against temperature for the 4-MTHPA sample: ▲, first time; ■, second time; ★, third series of heat capacity measurements.

Table 1. Experimental Molar Heat Capacities of 4-MTHPA (M = 166.18 $g{\cdot}mol^{-1}$) (R = 8.314427 $J{\cdot}mol^{-1}{\cdot}K^{-1}$)[17]

T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$
80.446	7.598	140.138	10.426	216.903	15.914	301.806	25.365
81.951	7.608	141.268	10.460	218.837	16.112	304.158	25.671
83.525	7.624	142.478	10.542	220.750	16.323	306.510	25.957
85.169	7.655	143.599	10.611	222.697	16.493	308.807	26.316
86.782	7.704	144.723	10.692	224.578	16.667	311.132	26.612
88.377	7.752	145.848	10.738	226.557	16.836	313.434	27.050
89.948	7.832	146.978	10.815	228.408	17.001	315.718	27.367
91.497	7.894	148.097	10.875	230.190	17.182	317.980	27.701
93.028	7.969	149.216	10.925	232.007	17.367	320.221	28.229
94.537	8.038	150.433	11.023	233.858	17.552	322.437	28.916
96.029	8.117	151.552	11.062	235.737	17.729	324.603	30.219
97.509	8.196	153.011	11.154	237.587	17.947	326.702	32.072
98.968	8.283	154.666	11.259	239.369	18.132	328.697	36.197
100.412	8.345	156.320	11.383	241.155	18.316	330.500	45.330
101.842	8.411	158.040	11.457	242.939	18.501	331.985	66.038
103.257	8.476	159.694	11.541	244.818	18.697	333.040	108.490
104.66	8.566	161.348	11.640	246.540	18.894	333.684	167.667
106.051	8.64	162.970	11.763	248.356	19.111	334.098	235.051
107.429	8.703	164.625	11.886	250.173	19.311	334.385	295.509
108.796	8.77	166.247	11.985	251.990	19.511	334.606	350.858
110.151	8.858	167.804	12.087	253.806	19.713	334.787	399.180
111.495	8.909	169.458	12.189	255.536	19.888	334.938	449.326
112.828	8.980	171.372	12.327	257.364	20.120	335.069	499.897
114.152	9.042	173.611	12.453	259.094	20.282	335.166	611.333
115.465	9.125	175.849	12.605	260.824	20.506	335.242	696.366
116.77	9.180	178.120	12.762	262.608	20.688	335.292	967.014
118.066	9.250	180.277	12.906	264.313	20.873	335.353	884.527
119.353	9.326	182.434	13.057	266.122	21.085	335.422	849.729
120.631	9.403	184.607	13.202	267.825	21.291	335.489	786.862
121.901	9.474	186.684	13.371	269.529	21.471	335.567	674.709
123.163	9.538	188.841	13.526	271.280	21.670	335.681	466.063
124.418	9.592	190.917	13.693	273.313	21.883	336.034	150.149
125.66	9.661	192.993	13.843	275.346	22.107	337.337	37.105
126.903	9.726	195.069	14.002	277.030	22.304	339.252	36.996
128.136	9.784	197.135	14.159	278.733	22.503	341.155	36.895
129.358	9.854	199.146	14.310	280.363	22.692	343.057	36.918
130.58	9.915	201.222	14.527	282.450	22.931	344.964	37.052
131.834	9.977	203.201	14.643	284.970	23.216	346.864	37.242
132.964	10.076	205.180	14.849	287.457	23.537	348.764	37.493
134.164	10.121	207.191	15.002	289.884	23.811	350.672	37.797
135.381	10.174	209.137	15.171	292.312	24.128	352.571	38.125
136.592	10.257	211.090	15.336	294.669	24.435	354.471	38.428
137.716	10.336	213.030	15.499	297.102	24.720	356.364	38.729
138.927	10.368	214.965	15.690	299.373	24.974	358.256	39.083
						360.133	39.437

Two polynomial equations were obtained by least-squares fitting by using the experimental molar heat capacities ($C_{p,\mathrm{m}}$) and the experimental temperatures (T). From T = 80 K to T = 330 K (solid phase),

$$C_{p,\mathrm{m}}/\mathrm{J{\cdot}K{\cdot}mol^{-1}} = 122.4 + 97.263x + 66.425x^2 - 54.12x^3 - 130.4x^4 + 64.302x^5 + 114.25x^6 \quad (1)$$

where x is the reduced temperature $x = [(T/K) - 205]/125$,

Table 2. Thermodynamic Parameters of the Melting Process Obtained from Three Series of Heat Capacity Measurements

thermodynamic properties	series 1, x_1	series 2, x_2	series 3, x_3	$(\bar{x} \pm \sigma_a)^a$
T_{fus}/K	334.99	335.29	336.33	335.54 ± 0.41
$\Delta_{fus}H_m$/kJ·mol^{-1}	17.61	17.66	17.73	17.67 ± 0.04
$\Delta_{fus}S_m$/J·K^{-1}·mol^{-1}	52.57	52.66	52.72	52.65 ± 0.04
H_0/J·K^{-1}	6.50	6.49	6.48	
Q/J	547.71	508.58	537.08	

[a] $\sigma = \sqrt{\sum_{i=1}^{3}(x_i - \bar{x})^2/n(n-1)}$,

in which n is the experimental number, x_i is a single value in a set of heat capacity measurements, and $\bar{x}$ is the mean value of a set of measurements.

T is the experimental temperature, 205 is obtained from the polynomial $(T_{max} + T_{min})/2$, 125 is obtained from the polynomial $(T_{max} - T_{min})/2$, T_{max} is the upper limit (330 K) of the above temperature region, and T_{min} is the lower limit (80 K) of the above temperature region. The correlation coefficient R^2 of the least-squares fit is 0.9968. The relative deviations of the smoothed heat capacities from those obtained from the experiment were within ±0.3%.

From $T = 337$ K to $T = 361$ K (liquid phase),

$$C_{p,m}/\text{J·K·mol}^{-1} = 312.06 + 14.21x + 6.2326x^2 - 4.2368x^3 + 0.7645x^4 \quad (2)$$

where $x = [(T/K) - 349]/12$ and its correlation coefficient R^2 is also 0.9968. The relative deviations of the smoothed heat capacities from those obtained from the experiment were within ±0.2%.

The molar enthalpy $\Delta_{fus}H_m$ and entropy $\Delta_{fus}S_m$ of fusion of the compound were derived according to eqs 3 and 4

$$\Delta H_m = \frac{Q - n\int_{T_i}^{T_m} C_p(s)\,dT - n\int_{T_m}^{T_f} C_p(L)\,dT - \int_{T_i}^{T_f} H_0\,dT}{n} \quad (3)$$

$$\Delta S_m = \frac{\Delta H_m}{T_m} \quad (4)$$

where T_i is a temperature slightly lower than the initial melting temperature, Q is the total energy introduced into the sample cell from T_i to T_f, T_f is a temperature slightly higher than the final melting temperature, C_p(s) is the heat capacity of the sample in the solid phase from T_i to T_m, C_p(L) is the heat capacity of the sample in the liquid phase from T_m to T_f, and H_0 is the heat capacity of the sample cell from T_i to T_f.

From these equations and the three series of repeated heat capacity measurements, the values of the melting temperature T_m and molar enthalpy $\Delta_{fus}H_m$ and entropy $\Delta_{fus}S_m$ of fusion of the sample were determined to be (335.54±0.41) K, (17.67±0.04) kJ·mol^{-1}, and (52.65±0.04) J·K^{-1}·mol^{-1}, respectively, and are listed in Table 2. The Table also gives Q, which is the total energy introduced into the sample cell, and the empty equivalent H_0 of the sample cell for each of three series of repeated heat capacity measurements during fractional melting.

Thermodynamic functions $[H_T - H_{298.15}]$ and $[S_T - S_{298.15}]$ of the compound were calculated in the temperature range from $T = 80$ K to $T = 361$ K with a temperature interval of 5 K in terms of the polynomials of heat capacity and the thermodynamic relationship and are listed in Table 3.

Table 3. Thermodynamic Functions of 4-MTHPA (R = 8.314427 J·mol^{-1}·K^{-1})^{17}

T/K	$C_{p,m}/R$	$[H_T - H_{298.15}]/R$·K	$[S_T - S_{298.15}]/R$
80	7.845	−3158.2	−15.753
85	7.742	−3119.3	−15.507
90	7.789	−3080.6	−15.258
95	7.944	−3041.3	−15.001
100	8.175	−3001.1	−14.735
105	8.453	−2959.6	−14.459
110	8.757	−2916.6	−14.172
115	9.073	−2872.0	−13.874
120	9.388	−2825.9	−13.566
125	9.696	−2778.2	−13.248
130	9.992	−2729.0	−12.922
135	10.274	−2678.5	−12.589
140	10.545	−2626.3	−12.250
145	10.805	−2572.9	−11.907
150	11.060	−2518.3	−11.559
155	11.313	−2462.4	−11.209
160	11.569	−2405.2	−10.857
165	11.834	−2346.7	−10.505
170	12.112	−2286.8	−10.151
175	12.408	−2225.5	−9.797
180	12.727	−2162.7	−9.443
185	13.070	−2098.2	−9.089
190	13.440	−2032.0	−8.735
195	13.839	−1963.8	−8.380
200	14.267	−1893.5	−8.024
205	14.721	−1821.1	−7.667
210	15.202	−1746.3	−7.307
215	15.704	−1669.0	−6.946
220	16.226	−1589.2	−6.581
225	16.762	−1506.7	−6.212
230	17.307	−1421.6	−5.838
235	17.856	−1333.7	−5.460
240	18.404	−1243.0	−5.076
245	18.946	−1149.7	−4.685
250	19.478	−1053.6	−4.288
255	19.996	−954.9	−3.884
260	20.500	−853.7	−3.473
265	20.990	−749.9	−3.053
270	21.468	−643.8	−2.624
275	21.942	−535.3	−2.186
280	22.420	−424.4	−1.738
285	22.917	−311.1	−1.278
290	23.453	−195.2	−0.805
295	24.052	−76.42	−0.317
298.15	24.476	0.000	0.000
300	24.745	45.53	0.190
305	25.572	171.3	0.717
310	26.580	301.6	1.269
315	27.824	437.5	1.853
320	29.370	580.4	2.474
325	31.296	732.0	3.140
330	33.691	894.3	3.863
335	melting region		
340	36.916	3116.7	10.488
345	37.066	3301.4	11.027
350	37.679	3488.1	11.564
355	38.516	3678.5	12.105
360	39.401	3873.3	12.649

Purity Determination of 4-MTHPA. The plot of the equilibrium melting temperature (T) against the reciprocal of the melting fraction (1/F) is shown in Figure 2. The melting points of the absolutely pure sample (T_0 = 335.67 K) and the present sample (T_1 = 335.35 K) can be obtained from the straight line at 1/F = 0 and 1/F = 1, respectively. The purity of the sample in terms of mole fraction was determined to be 0.9940 according to the van't Hoff equation.

DSC and TG Analysis. The DSC and TG curves of 4-MTHPA are shown in Figure 3 and Figure 4, respectively.

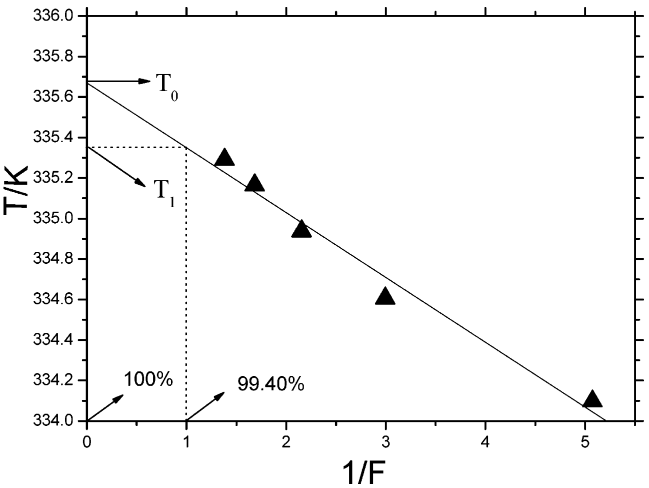

Figure 2. Plot of melting temperature against reciprocal mass fraction melted for 4-MTHPA.

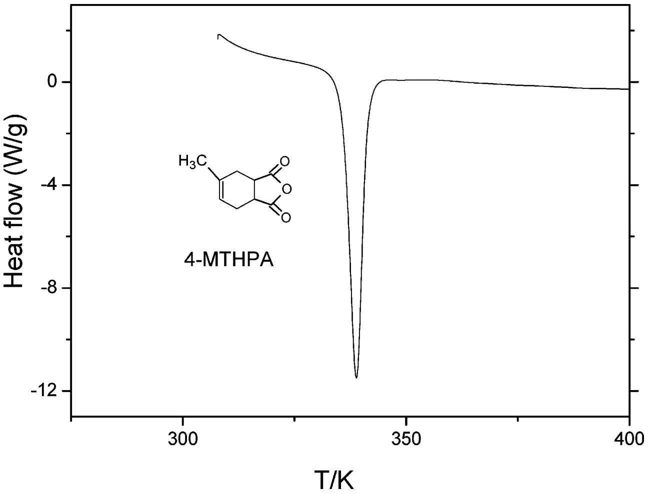

Figure 3. DSC curve of 4-MTHPA.

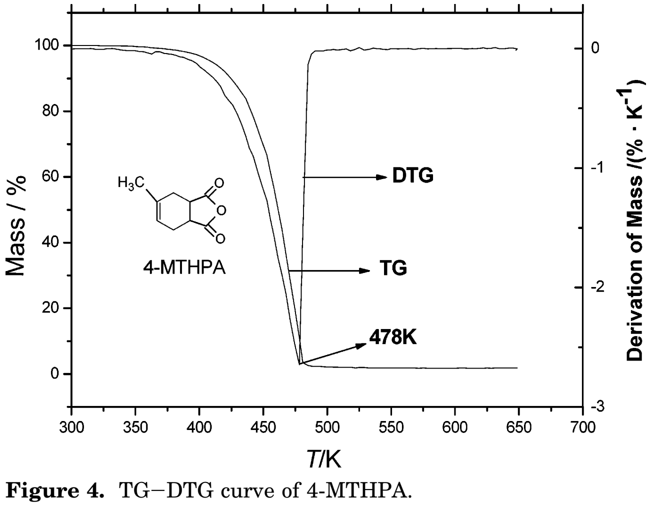

Figure 4. TG−DTG curve of 4-MTHPA.

The DSC curve showed that the compound was stable before and after melting. From the curve, the melting temperature of the sample was determined to be T_m = 335.66 K, which is in agreement with that obtained from the heat capacity measurement, (335.54±0.41) K, and the enthalpy of fusion of the compound was determined to be 17.70 kJ·mol^{-1}, which is consistent with that obtained by adiabatic calorimetry, (17.67±0.04) kJ·mol^{-1}.

Table 4. Experimental Results of Melting Fractions and Equilibrium Temperatures of 4-MTHPA [$F = q/(\Delta H_m n)$]

q/J	F	1/F	T/K
80.37	0.1970	5.076	334.098
136.22	0.3339	2.995	334.606
189.40	0.4643	2.154	334.938
242.30	0.5940	1.684	335.166
295.59	0.7247	1.380	335.292

The TG−DTG curves indicated that the mass loss of 4-MTHPA began at about T = 391 K and ended at about T = 480 K and that the maximum mass loss rate occurred at T = 478 K. The mass loss of the compound may be ascribed to evaporation instead of thermal decomposition because the product collected from the TG experiment was the original compound instead of another.

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