Vol 17 No 8, August 2008
1674-1056/2008/17(08)/2859-08

Chinese Physics B

© 2008 Chin. Phys. Soc.
and IOP Publishing Ltd

Low-temperature heat capacities and standard molar enthalpy of formation of N-methylnorephedrine $C_{11}H_{17}NO(s)$*

Di You-Ying(邸友莹)[a)†], Wang Da-Qi(王大奇)[a)],
Shi Quan(史 全)[b)], and Tan Zhi-Cheng(谭志诚)[b)]

[a)] *College of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng* 252059, *China*

[b)] *Thermochemistry Laboratory, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian* 116023, *China*

(Received 13 October 2007; revised manuscript received 13 November 2007)

This paper reports that low-temperature heat capacities of N-methylnorephedrine $C_{11}H_{17}NO(s)$ have been measured by a precision automated adiabatic calorimeter over the temperature range from T=78 K to T=400 K. A solid to liquid phase transition of the compound was found in the heat capacity curve in the temperature range of T=342–364 K. The peak temperature, molar enthalpy and entropy of fusion of the substance were determined. The experimental values of the molar heat capacities in the temperature regions of T=78–342 K and T=364–400 K were fitted to two polynomial equations of heat capacities with the reduced temperatures by least squares method. The smoothed molar heat capacities and thermodynamic functions of N-methylnorephedrine $C_{11}H_{17}NO(s)$ relative to the standard reference temperature 298.15 K were calculated based on the fitted polynomials and tabulated with an interval of 5 K. The constant-volume energy of combustion of the compound at T=298.15 K was measured by means of an isoperibol precision oxygen-bomb combustion calorimeter. The standard molar enthalpy of combustion of the sample was calculated. The standard molar enthalpy of formation of the compound was determined from the combustion enthalpy and other auxiliary thermodynamic data through a Hess thermochemical cycle.

Keywords: N-methylnorephedrine $C_{11}H_{17}NO(s)$, heat capacity, constant-volume energy of combustion, standard molar enthalpy of formation

PACC: 0570, 8260

1. Introduction

N-methylnorephedrine ($C_{11}H_{17}NO$) (CAS registry number, 299-42-3) is an important alkaloid used in medicine and a rude material in manufacturing the drugs for curing the tracheitis, rheum and so on, all of which are the common diseases all over the world. Chemical name of the compound is (1R, 2S)-2-dimethylamino-1-phenylpropanol. Recently, it was found that the coordination compounds of N-methylnorephedrine with some transition or biologically active metals can greatly enhance the curing effect of the drugs. The compound medicines synthesized as the complexes have the wide application perspectives since they have no toxicity, high efficiency and no side effect in the human body. For the purpose of the application development and relevantly theoretical study of the substance, the data of its thermodynamic properties are urgently needed. Heat capacity and standard molar enthalpy of formation are the fundamental thermodynamic properties of substances and are closely related to other physical and chemical properties.[1−4] However, up to now, no report about thermodynamic properties of N-methylnorephedrine was found in literature.

This paper investigates low-temperature heat capacities, standard molar enthalpy of formation and thermodynamic properties of N-methylnorephedrine by adiabatic calorimetry and combustion calorimetry.

2. Experimental

2.1. Sample

The sample used in these calorimetric measurements was produced by the pharmaceutical factory of Inner Mongolia, China. Labelled purity is more than 99.0%. The melting point was measured to be 357–360 K by micro melting point device. The ac-

*Project supported by the National Natural Science Foundation of China (Grant No 20673050).

†E-mail: yydi@lcu.edu.cn; diyouying@126.com

tual purity of the sample was determined to be more than 99.5% by high performance liquid chromatography. At last, fourier transform infrared spectrometer and H^1 nuclear magnetic resonance spectroscopy were applied to verify the structure of the compound.

2.2. Adiabatic calorimetry

We applied a high-precision automatic adiabatic calorimeter with a small sample size to measure the heat capacities in the temperature range from T=78 K to T=400 K. The principle and design of the adiabatic calorimeter were described in detail elsewhere.[5,6] Briefly, the calorimeter mainly comprised a sample cell, a platinum resistance thermometer, an electric heater, the inner and the outer adiabatic shields, and a vacuum can. Two sets of six-junction chromel-constantan thermopiles installed between the calorimetric cell and the inner shield and between the inner and outer shields, respectively. We applied the miniature platinum resistance thermometer (IPRT No.2, produced by Shanghai Institute of Industrial Automatic Meters, 16 mm in length, 1.6 mm in diameter and a nominal resistance of 100 Ω) to measure the temperature of the sample. The thermometer was calibrated on the basis of ITS-90 by the Station of Low-temperature Metrology and Measurements, Chinese Academy of Sciences. The thermometer was inserted into the copper sheath which was silver-soldered closely at the bottom of the sample cell. The temperature differences between the sample cell and the inner shield and between the inner and outer shields were monitored by two sets of thermopiles, and controlled by two sets of DWT-702 precision temperature controllers (manufactured by Shanghai No.6 Automated Instrumentation Works). The vacuum can was evacuated to 100 Pa during the heat capacity measurements so as to eliminate heat transfer by convection. The electrical energy introduced into the sample cell and the equilibrium temperature of the cell after the energy input were automatically picked up by using the Data Acquisition / Switch Unit (Model 34970A, Agilent, USA), and processed on line by a computer.

To verify the accuracy of the calorimeter, the heat-capacity measurements of the reference standard material, α-Al_2O_3, were made in the temperature range from T=78 K to T=370 K. The sample mass used was 1.6382 g, which was equivalent to 0.0161 mol based on its molar mass, $M(Al_2O_3)$=101.9613 g·mol^{-1}. The results indicated that deviations of the experimental data from those of the former National Bureau of Standards in the same temperature range were within ±0.3%.[7]

The sample mass used for the calorimetric measurements was 2.7992 g, which was equivalent to 0.01562 mol in terms of molar mass of the sample, *N*-methylnorephedrine $C_{11}H_{17}NO$(s), M=179.26 g·mol^{-1}.

Heat-capacity measurements were continuously and automatically carried out by means of the standard method of intermittently heating the sample and alternately measuring the temperature. The heating rate and the temperature increments were generally controlled at 0.1–0.4 K·min^{-1} and 1–3 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·min^{-1} during the acquisition of all heat-capacity data.

2.3. Isoperibol oxygen-bomb combustion calorimetry

The constant-volume energy of combustion of the sample was measured by means of a homemade precision oxygen-bomb combustion calorimeter. It was an isoperibolic macrocalorimeter with a static oxygen bomb and set up in our thermochemistry laboratory. The structure and principle of the calorimeter have been described in detail previously elsewhere.[6] It consisted of a static oxygen bomb, inner calorimetric vessel, outer thermostatic bath, platinum resistance thermometer, precision temperature controller, ignition system and temperature measurement system. The system of controlling the temperature was composed of a thermostatic bath, an electric stirrer, an electric heater, a precision temperature controller and a Cu 50 resistance thermometer. The precision of controlling the temperature for the thermostatic system can reach ±0.001 K.

The temperature measurement system consisted of a precision platinum resistance thermometer (PTΦ5×40, 40 mm in length, 5 mm in diameter; R_0=196.9865Ω, made by the Instrument Manufacture Co. of Yunnan, China) and a Data Acquisition / Switch Unit (Model 34970A, Agilent, USA). The thermometer was calibrated on the basis of ITS-90 by the National Institute of Metrology.

The correction of the temperature rise (ς) was obtained from the following formula described in Refs.[6, 8, 9].

The sample was pressed into pellets of (0.6 to 1.0) g for each combustion and burned under an oxy-

gen pressure of 3.01 MPa in the presence of 0.001 dm^3 of distilled water in the bomb to ensure equilibrium in the final state after the combustion. The purity of the oxygen used in the experiment was of research grade, mole fraction 0.99998. The mass of the sample has been calibrated from the air buoyancy on the basis of the determination of the density for a pellet of the sample. At the T=(298.15 ± 0.001) K, the differential quotient of the constant-volume energy of combustion with the oxygen pressure, $(\partial U/\partial P)_T$, for the solid was assumed to be –0.21 $J\cdot g^{-1}\cdot MPa^{-1}$, a typical value for organic solids. The standard energy of combustion of the nickel fuse for ignition has been determined previously to be $\Delta_c U^\circ$=2.929$J\cdot cm^{-1}$. The real energy of combustion of the nickel fuse (Q_{Ni}) was calculated from the formula, Q_{Ni}=2.929·ΔLJ, in which ΔL/cm was the length of the combusted nickel wire. The correction for the energy of formation of aqueous nitric acid, produced by oxidation of a trace of nitrogen contained in the oxygen bomb, was determined by the neutral titration with a 0.1000 $mol\cdot dm^{-3}$ of sodium hydroxide solution by using the methyl orange as the indicator. We can derive the heat of formation of the aqueous nitric acid in the oxygen bomb from the equation, Q_{HNO_3}=59.8·N·VJ, where $N/mol\cdot dm^{-3}$ is the concentration of the sodium hydroxide solution and V/cm^3 is the volume of the consumed sodium hydroxide solution, based on the molar energy of formation of HNO_3(aq) from N_2(g), O_2(g) and H_2O(l), $\Delta_f H^0_m$=59.8 $kJ\cdot mol^{-1}$, for 0.1 $mol\cdot dm^{-3}$ of HNO_3(aq).[6,8,9]

After each combustion test, the combustion products were analysed mainly for carbon dioxide by the Rossini method.[6] No soot was observed in the sample crucible after each of combustion experiments for N-methylnorephedrine ($C_{11}H_{17}NO$). Qualitative tests for CO with indicator tubes were negative within the limits of their sensitivity {mole fraction x (CO) $<10^{-6}$}.

The energy equivalent of the calorimeter, ε_{calor}, has been determined from 10 combustion experiments using about 0.7 g of NIST 39i benzoic acid with a certified energy of combustion under experimental conditions of $\Delta_c U = -(26434\pm3)\,J\cdot g^{-1}$ to be: ε_{calor}=(13572.22 ± 0.98)$J\cdot K^{-1}$. The uncertainty of the results was the standard deviation of the mean value from the respective measurements.

3. Results and discussion

3.1. Low-temperature heat capacity

All experimental heat-capacity values are tabulated in Table 1 and plotted in Fig.1. It was seen that an obvious endothermic peak appeared in the temperature range of 342–364 K. The melting point of the compound is about 357–359 K, as measured by a micro melting point device. The area corresponding to the peak in the heat capacity curve is the sum of enthalpy of the fusion of the substance.

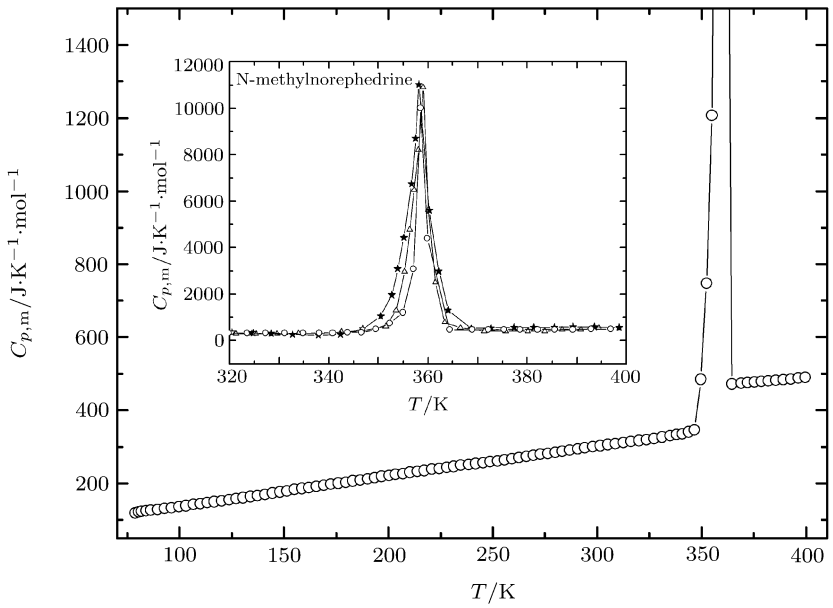


Fig.1. The curve of the experimental molar heat capacities of N-methylnorephedrine $C_{11}H_{17}NO$(s) (○ is the first series of measurements, △ is the second series of measurements, and ★ is the third series of heat capacity measurements).

Table 1. Experimental molar heat capacities of *N*-methylnorephedrine $C_{11}H_{17}NO$(s) (M=179.26 g·mol^{-1}).

T/K	$C_{p,m}$ /J·K^{-1}·mol^{-1}	T/K	$C_{p,m}$ /J·K^{-1}·mol^{-1}	T/K	$C_{p,m}$ /J·K^{-1}·mol^{-1}
78.896	118.85	186.608	208.64	301.522	302.36
80.318	120.81	190.034	211.88	305.192	305.69
81.827	122.53	193.459	215.47	308.863	308.06
84.196	124.55	196.885	218.10	312.533	311.29
86.211	126.13	200.228	221.08	316.203	314.36
89.555	128.15	203.572	224.06	319.873	316.99
92.981	130.69	206.916	226.34	323.624	319.53
96.243	133.21	210.423	229.14	327.294	322.69
99.705	135.39	213.848	231.85	331.128	326.01
103.257	138.16	217.355	234.92	334.879	329.78
106.682	141.23	220.943	237.72	338.142	332.76
110.026	144.03	224.451	239.82	340.833	335.47
113.371	146.59	227.958	242.80	343.769	340.20
116.795	148.82	231.302	245.43	346.624	346.42
120.302	151.53	234.809	248.76	349.526	484.45
123.809	154.51	238.397	250.59	352.333	747.47
127.235	157.40	241.904	253.23	355.024	1206.7
130.660	160.03	245.329	255.85	357.103	3090.2
134.004	163.18	248.836	258.74	358.530	10018
137.511	166.16	252.343	261.02	359.897	4396.9
141.099	168.88	255.769	263.74	364.403	471.36
144.606	172.38	259.194	266.98	368.970	473.60
148.195	176.23	262.621	269.87	372.151	475.22
151.702	179.04	266.045	273.46	375.332	476.78
155.209	182.54	269.552	276.18	378.594	478.27
158.716	185.52	272.977	279.24	382.101	480.02
162.141	188.32	276.403	281.34	385.608	481.38
165.648	191.21	279.828	284.15	389.196	483.39
169.237	194.10	283.335	287.12	392.948	485.36
172.662	196.99	287.005	290.19	396.781	487.35
176.087	199.97	290.594	293.52	399.689	489.46
179.594	202.77	294.264	296.41		
183.101	205.58	297.852	299.91		

The experimental molar heat capacities (J·K^{-1}·mol^{-1}) in the temperature range of 78–342 K were fitted to the polynomial:

$$C_{p,m} = 228.3298 + 109.06016X - 8.39642X^2 - 0.45574^3 + 8.07264X^4,$$

in which, $X = (T-210)/132$. $X=f(T) = \left[T-\frac{1}{2}(T_1+T_2)\right] \Big/ \left[\frac{1}{2}(T_1-T_2)\right]$ (where T_1=342 K and T_2=78 K). The equation is valid in the temperature range from T=78 to T=342 K, and gives out the relative deviations of experimental molar heat capacities within ±0.3% from smoothed heat capacities.

The experimental molar heat capacities (J·K^{-1}·mol^{-1}) in the temperature range of 364–400 K were fitted to:

$$C_{p,m} = 479.85089 + 8.52275X + 0.57023X^2 + 0.77219X^3 - 0.03788X^4,$$

in which, $X = (T-382)/18$. $X = f(T) = \left[T-\frac{1}{2}(T_3+T_4)\right] \Big/ \left[\frac{1}{2}(T_3-T_4)\right]$ (where T_3=400 K and T_4=364 K). The equation is valid in the temperature range from T=364 to T=400 K, and gives out the relative deviations of experimental molar heat-capacities within ±0.25% from smoothed heat-capacities.

3.2. The peak temperature, molar enthalpy and entropy of phase change

Three series of heat-capacity experiments in the temperature region of the fusion and first dehydration of the compound were carried out so that the repeatability of the fusion was verified. Before each series of measurements, the sample was cooled from T=400 K to T=300 K by using different cooling rates. In the first series, the sample was quenched into liquid nitrogen (about 20 K·min^{-1}); in the second series, the sample was naturally cooled (about 0.5 K·min^{-1}); and in the third series, the ice water was used as coolant (about 5 K·min^{-1}). The results of the three series of repeated experiments were plotted in the inset of Fig.1 and also given in Table 2. It can be seen from the inset of Fig.1 that the phase transition is repeatable, no supercooling and other thermal anomaly are caused by the different cooling rates.

The peak temperature T_{fus} and molar enthalpy $\Delta_{\mathrm{fus}}H_{\mathrm{m}}$ of the phase transition of the sample were determined by the method described in Ref.[6]. The molar entropy of the transition, using $\Delta_{\mathrm{fus}}S_{\mathrm{m}} = \Delta_{\mathrm{fus}}H_{\mathrm{m}}/T_{\mathrm{fus}}$, was calculated.

The results of the phase transition of the sample obtained from three series of repeated heat-capacity measurements are listed in Table 2.

Table 2. Results of the phase transition of the compound obtained from three series of heat capacity measurements.

Thermodynamic properties	Series 1 x_1	Series 2 x_2	Series 3 x_3	$(\overline{x} \pm \sigma_{\mathrm{a}})^*$
T_{fus} /K	358.530	359.026	358.156	(358.571±0.252)
$\Delta_{\mathrm{fus}}H_{\mathrm{m}}$/kJ·mol^{-1}	21.568	21.698	22.124	(21.797 ± 0.168)
$\Delta_{\mathrm{fus}}S_{\mathrm{m}}$ /J·K^{-1}·mol^{-1}	60.157	60.436	61.772	(60.788 ± 0.498)

$^*\sigma_{\mathrm{a}} = \sqrt{\sum_{i=1}^{3}(x_i - \overline{x})^2/n(n-1)}$, in which n is the experimental number; x_i, a single value obtained from a series of heat capacity measurements; $\overline{x}$, the mean value of results obtained from three series of heat capacity measurement.

3.3. Thermodynamic functions of the compound

The smoothed molar heat capacities and thermodynamic functions of N-methylnorephedrine ($C_{11}H_{17}NO$) were calculated based on two fitted polynomials of the heat capacities as a function of the reduced temperature (X) according to the following thermodynamic equations:

$$(H_T - H_{298.15}) = \int_{298.15}^{T} C_p \mathrm{d}T, \qquad (1)$$

$$(S_T - S_{298.15}) = \int_{298.15}^{T} C_p \cdot T^{-1}\mathrm{d}T, \qquad (2)$$

$$(G_T - G_{298.15}) = \int_{298.15}^{T} C_p \mathrm{d}T - T \cdot \int_{298.15}^{T} C_p \cdot T^{-1}\mathrm{d}T. \qquad (3)$$

The polynomial fitted values of the molar heat capacities and fundamental thermodynamic functions of the sample relative to the standard reference temperature 298.15 K were tabulated in Table 3 with the interval of 5 K.

Table 3. Thermodynamic functions of N-methylnorephedrine $C_{11}H_{17}NO$(s).

T/K	$C_{p,\mathrm{m}}$ /J·K^{-1}·mol^{-1}	$(H_T - H_{298.15\mathrm{K}})$ /kJ·mol^{-1}	$(S_T - S_{298.15\mathrm{K}})$ /J·K^{-1}·mol^{-1}	$(G_T - G_{298.15\mathrm{K}})$ /kJ·mol^{-1}
80	120.71	–45.82	–251.0	–25.74
85	124.40	–45.20	–243.6	–24.50
90	128.10	–44.57	–236.4	–23.30
95	131.89	–43.92	–229.4	–22.13
100	135.77	–43.25	–222.5	–21.01
105	139.73	–42.56	–215.7	–19.91
110	143.75	–41.86	–209.1	–18.86
115	147.83	–41.13	–202.6	–17.83
120	151.96	–40.38	–196.2	–16.84
125	156.13	–39.61	–189.9	–15.87
130	160.34	–38.81	–183.7	–14.94
135	164.58	–38.00	–177.5	–14.04
140	168.84	–37.17	–171.5	–13.16
145	173.12	–36.31	–165.5	–12.32

Table 3. (*Continued*).

T/K	$C_{p,\mathrm{m}}$ /J·K^{-1}·mol^{-1}	$(H_T - H_{298.15\mathrm{K}})$ /kJ·mol^{-1}	$(S_T - S_{298.15\mathrm{K}})$ /J·K^{-1}·mol^{-1}	$(G_T - G_{298.15\mathrm{K}})$ /kJ·mol^{-1}
150	177.41	–35.44	–159.6	–11.50
155	181.71	–34.54	–153.7	–10.72
160	186.01	–33.62	–147.9	–9.960
165	190.30	–32.68	–142.1	–9.231
170	194.59	–31.72	–136.4	–8.531
175	198.87	–30.73	–130.7	–7.860
180	203.14	–29.73	–125.1	–7.217
185	207.39	–28.70	–119.5	–6.603
190	211.62	–27.65	–113.9	–6.018
195	215.83	–26.59	–108.3	–5.460
200	220.02	–25.50	–102.8	–4.932
205	224.19	–24.39	–97.34	–4.431
210	228.33	–23.25	–91.88	–3.959
215	232.45	–22.10	–86.45	–3.514
220	236.54	–20.93	–81.05	–3.098
225	240.62	–19.74	–75.68	–2.709
230	244.66	–18.52	–70.33	–2.347
235	248.69	–17.29	–65.01	–2.013
240	252.70	–16.04	–59.71	–1.705
245	256.69	–14.76	–54.44	–1.424
250	260.66	–13.47	–49.20	–1.169
255	264.62	–12.16	–43.98	–0.9401
260	268.58	–10.82	–38.79	–0.7368
265	272.52	–9.470	–33.63	–0.5589
270	276.47	–8.098	–28.49	–0.4059
275	280.42	–6.705	–23.37	–0.2776
280	284.37	–5.293	–18.28	–0.1738
285	288.34	–3.861	–13.22	–0.09428
290	292.33	–2.409	–8.174	–0.03886
295	296.34	–0.9376	–3.153	–0.00746
298.15	298.89	0	0	0
300	300.39	0.5544	1.848	0.00007
305	304.47	2.067	6.831	–0.01677
310	308.59	3.600	11.80	–0.05776
315	312.77	5.153	16.75	–0.1233
320	317.01	6.728	21.69	–0.2140
325	321.32	8.324	26.63	–0.3302
330	325.71	9.942	31.56	–0.4730
335	330.18	11.58	36.49	–0.6431
340	334.75	13.25	41.43	–0.8419
345	Phase change	–	–	–
350	Phase change	–	–	–
355	Phase change	–	–	–
360	Phase change	–	–	–
365	471.63	36.18	104.2	–2.320
370	474.19	38.55	105.5	–2.863
375	476.58	40.93	111.9	–3.437
380	478.91	43.32	118.3	–4.044
385	481.29	45.72	124.6	–4.683
390	483.82	48.13	130.9	–5.354
395	486.58	50.55	137.1	–6.056
400	489.68	52.99	143.3	–6.788

3.4. Constant-volume energy of combustion and standard molar enthalpy of combustion of the compound

The method for determining the constant-volume energy of combustion of the sample was the same as that used in the calibration of the combustion calorimeter with benzoic acid. The constant-volume energy of combustion of the sample can be calculated according to Refs.[6] and [9].

The measured result of the constant-volume energy ($\Delta_c U$) of combustion of the sample is indicated in Table 4.

Table 4. The experimental results of the constant-volume energy of combustion for *N*-methylnorephedrine $C_{11}H_{17}NO$(s) at 298.15 K and 0.1 MPa.

No.	Mass of sample W/g	Corrected heat of ignition wire Q_c/J	Corrected heat of nitric acid Q_N/J	Corrected temperature rise $\Delta_c T$/K	Combustion energy of sample $-\Delta_c U$ /J·g^{-1}
1	0.36027	39.54	53.49	0.9157	34239.2
2	0.26391	27.82	48.97	0.6690	34114.7
3	0.36527	42.47	51.41	0.9257	34122.2
4	0.33232	29.29	49.33	0.8395	34047.9
5	0.37326	42.47	56.76	0.9495	34258.0
6	0.38629	40.42	59.20	0.9876	34440.1
			Mean	$\Delta_c U$=–(34203.7 ± 17.5)J·g^{-1}	

The standard molar enthalpy of combustion of the sample ($\Delta_c H^o_m$) referred to the enthalpy change of the following reaction at 298.15 K and 100 kPa,

$$C_{11}H_{17}NO(s) + \frac{59}{4}O_2(g) = \frac{1}{2}N_2(g) + 11CO_2(g) + \frac{17}{2}H_2O(l). \quad (4)$$

The standard molar enthalpy of combustion of the sample can be derived from the constant-volume energy of combustion by Eqs.(5) and (6):

$$\Delta_c H^o_m = \Delta_c U^o_m + \Delta n \cdot RT, \quad (5)$$

$$\Delta n = \Sigma n_i(\text{products, g}) - \Sigma n_i(\text{reactants, g}), \quad (6)$$

where Σn_i was the total amount (in moles) of the gases present as products or as reactants. The calculated standard molar enthalpies of combustion of the samples were calculated to be $\Delta_c H^o_m = -(6139.4 \pm 3.1)$ kJ·mol^{-1}.

3.5. Standard molar enthalpy of formation of the compound

The standard molar enthalpy of formation of the compound, $\Delta_f H^o_m$, was calculated by a designed Hess's thermochemical cycle according to the reaction Eq.(4) as follows:

$$\Delta_f H^o_m[C_{11}H_{17}NO, s] = [11\Delta_f H^o_m(CO_2, g) + \frac{17}{2}\Delta_f H^o_m(H_2O, s) - \Delta_c H^o_m[C_{11}H_{17}NO, s]. \quad (7)$$

In Eq.(7), the standard molar enthalpies of formation of CO_2 (g) and H_2O (l), recommended by CODATA,[10,11] $\Delta_f H^o_m$ (CO_2, g)=−(393.51± 0.13) kJ·mol^{-1} and $\Delta_f H^o_m$ (H_2O, l)=−(285.83± 0.04) kJ·mol^{-1}, were employed in the calculation of $\Delta_f H^o_m$ [$C_{11}H_{17}NO$, s]. Finally, The standard molar enthalpy of formation of the compound can be derived to be $\Delta_f H^o_m$ [$C_{11}H_{17}NO$, s]=−(618.8± 3.4) kJ·mol^{-1}.

4. Conclusion

This paper reports low-temperature heat capacities and constant-volume energy of combustion of N-methylnorephedrine measured by adiabatic calorimetry and isoperibol oxygen-bomb combustion calorimetry. Additionally, thermodynamic parameters of the phase transition, the thermodynamic functions and standard molar enthalpy of formation of the compound were derived from these experimental results.

References

[1] Zhou S Q 2007 *Chin. Phys.* **16** 1167

[2] Chen X R, Liu K, Zhou X L and Zhu J 2006 *Chin. Phys.* **15** 3014

[3] Cai Y D, Li G and Yao X 2006 *Acta Phys. Sin.* **55** 844 (in Chinese)

[4] Wu D C, Huang L J and Liang G Y 2008 *Acta Phys. Sin.* **57** 1813 (in Chinese)

[5] Tan Z C, Liu B P, Yan J B and Sun L X 2003 *J. Comput. Appl. Chem.* **20** 265 (in Chinese)

[6] Di Y Y, Tan Z C, Sun X H, Wang M H, Xu F, Liu Y F, Sun L X and Zhang H T 2004 *J. Chem. Thermodyn.* **36** 79

[7] Donald G A 1993 *J. Phys. Chem. Ref. Data* **22** 1441

[8] Yang X W, Chen S P and Gao S L 2002 *Instrument. Sci. & Technol.* **30** 311

[9] Popov M W 1954 *Thermometry and Calorimetry* (in Russ.) (Moscow: Moscow Univ. Publishing House) p331

[10] Report of the CODATA task group on key values for thermodynamics 1978 *J. Chem. Thermodyn.* **10** 903

[11] Cox J D, Wagman D D and Medvedev V A 1984 *CODATA Key Values for Thermodynamics* (New York: Hemisphere Publishing) p1