Scientific paper

Low Temperature Heat Capacities and Standard Molar Enthalpy of Formation of 2-Pyrazinecarboxylic Acid ($C_5H_4N_2O_2$)(s)

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Received: 28-09-2009

Abstract

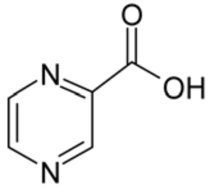
Low-temperature heat capacities of 2-pyrazinecarboxylic acid ($C_5H_4N_2O_2$)(s) were measured by a precision automated adiabatic calorimeter over the temperature range from 78 to 400 K. A polynomial equation of heat capacities as a function of temperature was fitted by least squares method. Based on the fitted polynomial, the smoothed heat capacities and thermodynamic functions of the compound relative to the standard reference temperature 298.15 K were calculated and tabulated at 10 K intervals. The constant-volume energy of combustion of the compound at $T = 298.15$ K was measured by a precision rotating-bomb combustion calorimeter to be $\Delta_c U = -(17839.40 \pm 7.40)$ J g^{-1}. The standard molar enthalpy of combustion of the compound was determined to be $\Delta_c H_m^0 = -(2211.39 \pm 0.92)$ KJ mol^{-1}, according to the definition of combustion enthalpy. Finally, the standard molar enthalpy of formation of the compound was calculated to be $\Delta_f H_m^0 = -(327.82 \pm 1.13)$ kJ mol^{-1} in accordance with Hess law.

Keywords: 2-pyrazinecarboxylic acid; adiabatic calorimetry; low temperature heat capacity; rotating-bomb combustion calorimeter; standard molar enthalpy of formation

1. Introduction

2-Pyrazinecarboxylic acid ($C_5H_4N_2O_2$) (CAS registry number, 98-97-5), which is also called the pyrazine-2-carboxylic acid and pyrazinoic acid, has a melting point of 222 ~ 225 °C, and is soluble in hot water, while insoluble in ethyl ether, chloroform and benzene. In medicine industry, it is an important pharmaceutical intermediate to synthesis the medicament oltipraz, which is often used for treating schistosomiasis and preventing liver cancer. When 2-pyrazinecarboxylic acid[1, 2] coordinates to some transition or biologically active metals, it acts as a bridging ligand which can produce electron coupling with metals via orbital overlap, hence it has been extensively studied as a potential transmitter in the course of electron-transfer and magnetochemistry research.

Its molecular structure is,



For the purpose of the application development and relevant theoretical study of the substance, the data of its thermodynamic properties are urgently needed. Heat capacity and standard molar enthalpy of formation of a substance are some of the most fundamental thermodynamic properties,[3, 4] and closely related to other physical, biological, physiological and chemical properties. The standard molar enthalpy of formation of a substance is one of the important data that is used when calculating enthalpy changes, equilibrium constants, and theoretical yields of the reactions in which the substance is involved. However, up to now, no report about thermodynamic properties of the title compound was found in the literature. In the present work, heat capacities, thermodynamic properties and standard molar enthalpy of formation of the title compound were investigated by adiabatic calorimetry and combustion calorimetry.

2. Experimental Section

2. 1. Sample

The sample used in these calorimetric measurements was purchased from J&K chemical ltd. (Beijing, China). The labeled purity was 99.0%. Its melting point is determined to be 222 ~ 225 °C by a micro melting point device. The actual purity of the sample was determined to be more than 99.5% by HPLC. FTIR and H^1 NMR were applied to verify the structure of the compound. These results have confirmed the reliability of the sample used in these calorimetric researches.

2. 2. Adiabatic Calorimetry

A precision automatic adiabatic calorimeter was used to measure heat capacities of the compound over the temperature range $78 \leq (T/\mathrm{K}) \leq 400$. The calorimeter was established in the Thermochemistry Laboratory in the College of Chemistry and Chemical Engineering, Liaocheng University, China. The principle and structure 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, inner, middle and outer adiabatic shields, three sets of six-junction chromel-constantan thermopiles installed between the calorimetric cell and the inner shield, between the inner and middle shields, and between the middle and outer shields, respectively, and a high vacuum can. 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) was applied 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, Academia Sinica. The electrical energy introduced into the sample cell and the equilibrium temperature of the cell after the energy input were automatically recorded by use of a Data Acquisition / Switch Unit (Model 34970A, Agilent, USA), and processed on line by a computer.

To verify the accuracy of the calorimeter, the heat capacities of the reference standard material (α-Al_2O_3) were measured over the temperature range $78 \leq (T/\mathrm{K}) \leq 400$. The sample mass used was 1.7143 g, which was equivalent to 0.0168 mol based on its molar mass, M (Al_2O_3) = 101.9613 g mol^{-1}. Relative deviations of the experimental results from those of the smoothed curve lie within ± 0.2%, while the uncertainty is ± 0.3%, as compared with the values given by the former National Bureau of Standards [7] over the whole temperature range.

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 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. The data of heat capacities and corresponding equilibrium temperature have been corrected for heat exchange of the sample cell with its surroundings.[5] The sample mass used for calorimetric measurements was 3.66005 g, which was equivalent to 0.0295 mol in terms of its molar mass, M = 124.10 g mol^{-1}.

2. 3. Rotating-bomb Combustion Calorimetry

The constant-volume energy of combustion of the sample was measured by means of a precise rotating-bomb combustion calorimeter (RBC-type II). The structure and principle of the calorimeter has been described in detail previously elsewhere.[8, 9] It mainly consisted of a water thermostat, a caloritube, and the system for temperature measurement. The bicyclical structure was used as the holder for the crucible support in the oxygen bomb, which facilitates the crucible stable relative to the bomb when the bomb was rotated in crosswise direction and vertically, assuring that the stable final state is attained in a short time.

The temperature of the water thermostat was maintained at T = (298.15 ± 0.001) K, and the initial oxygen pressure was 2.5MPa. The corrected value of the heat exchange was calculated according to *Linio-Pyfengdelel-Wsava* equation. [10]

$$\Delta(\Delta T) = nV_0 + \left(\frac{V_n - V_0}{\bar{\bar{T}}_n - \bar{\bar{T}}_0}\right)\left(\frac{T_0 + T_n}{2} + \sum_{i=1}^{n-1} T_i - n\bar{T}_0\right) \quad (1)$$

Where $\Delta(\Delta T)$(K) denotes the correction value of the heat exchange; n, the number of readings for the main (or reaction) stage; V_n (K min^{-1}) and V_0 (K min^{-1}), the temperature drift rates in the final and initial stages, respectively (V is positive when the temperature decrease); $\bar{T}_0$ (K) and $\bar{T}_n$ (K), the average temperature of the calorimeter during the initial and final stages, respectively (average temperature for first and last readings); T_0 (K), the last reading of the initial stage; T_n (K), the first reading of the final stage; $\sum_{i=1}^{n-1} T_i$, the sum of all the temperature readings, except for the last one of the main stage; $(V_n - V_0)/(\bar{T}_n - \bar{T}_0)$, a constant relative to the calorimeter performance.

The energy equivalent of the calorimeter was calibrated with benzoic acid of 99.999% purity, which has an isothermal heat of combustion of (–26434 ± 3) J g^{-1} at 298.15 K.[11] It was calculated according to the following equation,

$$W = \frac{Qa + Gb + 5.97c}{\Delta T} = \frac{Qa + Q_{\mathrm{Ni}} + Q_{\mathrm{HNO_3}}}{\Delta T} \qquad (2)$$

Where W(J K^{-1}) is the energy equivalent of the calorimeter; Q(J g^{-1}), the combustion enthalpy of benzoic acid; a(g), the mass of benzoic acid; G(0.9 J cm^{-1}), the combustion enthalpy of Ni–Cr wire for ignition; b(cm), the length of actual Ni–Cr wire consumed; 5.97 (J cm^{-3}), the formation enthalpy and solution enthalpy of nitric acid corresponding to 1 cm^{-3} of 0.1000 mol dm^{-3} solution of NaOH; c(cm^3), the volume of consumed 0.1000 mol dm^{-3} solution of NaOH; ΔT (K), the corrected value of the temperature rise. The calibrated experimental result was (18604.99 ± 8.14) J K^{-1}, which were summarized in Table 1.

The analyses for the final products (gas and liquid) which resulted from the combustion reaction were the same as those reported in the reference, [8] and the analytical results indicated that the combustion reaction was complete. The methods of determination and calculation of the constant-volume combustion energy for the title compound are similar to that for benzoic acid.

means of the least squares method and a polynomial equation of the experimental molar heat-capacities ($C_{p,\mathrm{m}}$) vs. reduced temperature (X), $X = f(T) = [T/\mathrm{K} - \frac{1}{2}(T_1 + T_2)]/[\frac{1}{2}(T_1 - T_2)]$ (where T_1 = 400 K and T_2 = 78 K), has been obtained, and the experimental molar heat capacities in the temperature range of 78 to 400 K were fitted to:

$$C_{p,\mathrm{m}}/(\mathrm{J\ K^{-1}\ mol^{-1}}) = 120.992 + 61.646X - 3.401X^2 + 0.489X^3 - 1.464X^4 \qquad (3)$$

in which, $X = \frac{T - 239}{161}$.

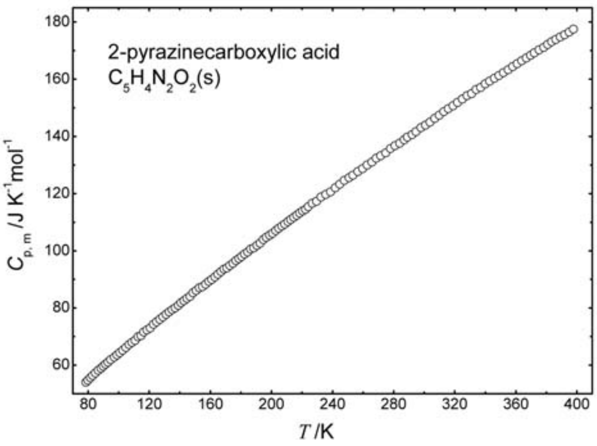


Figure 1. The curve of experimental molar heat capacities of 2-pyrazinecarboxylic acid ($C_5H_4N_2O_2$)(s).

Table 1. The calibrated experimental results of the energy equivalent of rotating-bomb combustion calorimeter

No.	Mass of benzoic acid a (g)	Calibrated ΔT(K)	Calibrated heat of nitric acid $Q_{\mathrm{HNO_3}}$	Calibrated heat of combustion wire Q_{Ni}(J)	Energy equivalent of calorimeter W (J K^{-1})
1	0.98450	1.4004	25.90	12.60	18610.95
2	0.86320	1.2301	19.96	12.60	18576.04
3	1.10295	1.5658	19.49	12.60	18640.61
4	1.11940	1.5924	25.99	12.60	18606.39
5	0.82615	1.1764	23.82	12.60	18594.75
6	0.93520	1.3317	19.31	11.70	18586.83
7	0.84385	1.1999	22.46	12.60	18619.38
Avg. W = (18604.99 ± 8.14) J K^{-1}					

3. Results and Discussion

3. 1. Low-temperature Heat Capacity

All experimental heat-capacity values were tabulated in Table 2, and plotted in Figure 1, showed that the structure of the compound was stable over the temperature range between T = 78 K and T = 400 K, that is, no phase change, association nor thermal decomposition occurred. The 135 experimental points in the temperature region between T = 78 K and T = 400 K were fitted by means of the least squares method (see above)

The standard deviations of experimental molar heat capacities from the smoothed heat capacities calculated by the polynomial equation were within ± 0.35%. The coefficient of determination for the fitting R^2 equals 0.99998.

3. 2. Thermodynamic Functions of the Compound

The smoothed molar heat capacities and thermodynamic functions of the sample were calculated based on

Table 2. Experimental molar heat capacities of 2-pyrazinecarboxylic acid ($C_5H_4N_2O_2$)(s)

T (K)	$C_{p,\mathrm{m}}$ (J K^{-1} mol^{-1})	T (K)	$C_{p,\mathrm{m}}$ (J K^{-1} mol^{-1})	T (K)	$C_{p,\mathrm{m}}$ (J K^{-1} mol^{-1})
78.504	54.06	164.95	91.79	268.62	132.3
79.909	54.77	166.94	92.75	271.65	133.2
81.462	55.60	168.94	93.62	274.75	134.3
83.014	56.41	170.86	94.01	277.86	135.8
84.789	57.25	172.78	94.83	280.89	136.7
86.638	58.20	174.78	95.66	283.92	137.6
88.486	58.92	176.70	96.57	286.96	138.9
89.965	59.64	178.63	97.31	289.03	139.8
91.370	60.29	180.47	98.02	292.06	140.6
93.071	61.01	182.40	98.85	294.65	141.6
94.846	61.88	184.39	99.57	297.83	143.1
97.138	62.75	186.39	100.6	300.86	143.9
98.913	63.55	188.39	101.0	303.81	144.9
100.76	64.35	190.46	101.8	306.85	146.3
102.61	65.22	192.53	102.7	309.88	147.4
104.68	66.13	194.60	103.9	312.84	148.6
106.75	67.16	196.59	104.7	315.79	149.7
108.75	67.95	198.74	105.4	318.83	150.7
110.74	68.71	200.74	106.1	321.86	151.9
112.67	69.94	202.73	107.0	324.96	153.1
114.59	70.33	204.73	107.8	327.99	154.3
116.44	71.63	206.72	108.6	330.95	155.0
118.51	72.30	208.72	109.4	333.98	156.4
120.65	73.05	210.72	110.2	336.94	157.1
122.80	74.31	212.57	110.9	339.90	158.3
124.87	75.18	214.56	111.7	342.86	159.3
126.94	76.01	216.49	112.4	345.89	160.3
129.01	76.91	218.41	113.2	348.92	161.3
131.00	77.74	220.33	113.9	351.88	162.3
133.00	78.61	222.25	114.5	354.91	163.3
135.00	79.40	224.03	115.4	357.87	164.4
136.99	80.02	226.76	116.6	360.83	165.5
138.99	80.90	229.57	117.3	363.78	166.5
140.84	81.84	232.53	118.8	366.74	167.4
142.76	82.57	235.56	119.6	369.63	168.4
144.68	83.33	238.74	120.6	372.07	169.2
146.68	84.01	241.77	122.0	375.25	170.3
148.68	85.31	244.73	123.3	378.28	171.2
150.67	86.13	247.76	124.7	380.79	172.2
152.74	87.04	250.80	125.6	383.45	173.1
154.82	87.46	253.38	126.4	386.12	173.9
156.89	88.34	256.71	127.7	389.07	174.8
158.96	89.21	259.74	128.8	391.96	175.6
160.95	89.97	262.78	130.0	394.84	176.5
162.95	90.84	265.73	131.0	397.73	177.5

the fitted polynomial of the heat capacities as a function of the reduced temperature (X), too. The polynomial fitted values relative to the standard reference temperature 298.15 K were listed in Table 3 at an interval of 10 K.

3. 3. 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 the formula,

$$-\Delta_c U = \left(\frac{W\Delta T - Q_{\mathrm{Ni}} - Q_{\mathrm{HNO_3}}}{m} \right) \tag{4}$$

Table 3. Smoothed heat capacities and thermodynamic functions of 2-pyrazinecarboxylic acid ($C_5H_4N_2O_2$)(s)

T (K)	$C_{p,\mathrm{m}}$ ($\mathrm{J\ K^{-1}\ mol^{-1}}$)	$H_T–H_{298.15\ \mathrm{K}}$ [a] ($\mathrm{kJ\ mol^{-1}}$)	$S_T–S_{298.15\ \mathrm{K}}$ [b] ($\mathrm{J\ K^{-1}\ mol^{-1}}$)
80	54.93	–21.91	–121.3
90	59.57	–21.36	–114.2
100	64.11	–20.75	–107.5
110	68.56	–20.10	–110.0
120	72.94	–19.40	–94.66
130	77.24	–18.65	–88.55
140	81.48	–17.86	–82.60
150	85.66	–17.03	–76.79
160	89.78	–16.16	–71.11
170	93.86	–15.24	–65.54
180	97.90	–14.28	–60.06
190	101.9	–13.28	–54.66
200	105.9	–12.24	–49.34
210	109.8	–11.16	–44.09
220	113.7	–10.05	–38.89
230	117.5	–8.890	–33.76
240	121.4	–7.696	–28.67
250	125.2	–6.463	–23.64
260	129.0	–5.192	–18.65
270	132.7	–3.884	–13.70
280	136.5	–2.538	–8.798
290	140.2	–1.155	–3.935
298.15	143.2	0	0
300	143.9	0.265	0.890
310	147.5	1.722	5.681
320	151.1	3.214	10.44
330	154.7	4.741	15.17
340	158.2	6.303	19.89
350	161.7	7.898	24.59
360	165.1	9.527	29.28
370	168.5	11.19	33.98
380	171.8	12.88	38.70
390	175.1	14.60	43.46
400	178.3	16.35	48.26

[a] $H_{(T)} - H_{(298.15\ \mathrm{K})} = \int_{298.15\mathrm{K}}^{\mathrm{T}} C_{\mathrm{p,m}}\, \mathrm{d}T$

[b] $S_{(T)} - S_{(298.15\ \mathrm{K})} = \int_{298.15\mathrm{K}}^{\mathrm{T}} C_{\mathrm{p,m}} \cdot T^{-1}\, \mathrm{d}T$

The measured result of the constant-volume energy, $\Delta_c U$ ($\mathrm{J\ g^{-1}}$), of combustion of the sample was shown in Table 4.

The standard molar enthalpy of combustion of the sample ($\Delta_c H_m^0$) referred to the enthalpy change of the following reaction at 298.15 K and 100 kPa,

$$C_5H_4N_2O_2(s) + 5O_2(g) = \\ = 5CO_2(g) + 2H_2O(l) + N_2(g) \tag{5}$$

The standard molar enthalpy of combustion of the sample can be derived from the constant-volume energy of combustion by equations (6) and (7),

$$\Delta_c H_m^0 = \Delta_c U + \Delta n RT \tag{6}$$

$$\Delta n = \Sigma n_i\,(\text{products, g}) - \Sigma n_i\,(\text{reactants, g}) \tag{7}$$

Where Σn_i was the total amount (in moles) of the gases present as products or as reactants. The calculated standard molar enthalpy of combustion of the sample was obtained as follows,

$$\Delta_c U = -(17839.40 \pm 7.40)\ \mathrm{J\ g^{-1}} \times 124.10\ \mathrm{g\ mol^{-1}} \times \\ \times\ 0.001 = -(2213.87 \pm 0.92)\ \mathrm{kJ\ mol^{-1}},$$

$$\Delta_c H_m^0 = \Delta_c U + \Delta n RT = -(2213.87 \pm 0.92) + 1 \times 8.314 \times \\ \times 298.15 \times 10^{-3} = -(2213.39 \pm 0.92)\ \mathrm{kJ\ mol^{-1}}.$$

3. 4. Standard Molar Enthalpy of Formation of the Compound

A reaction scheme used to determine the standard molar enthalpy of formation, $\Delta_f H_m^0(C_5H_4N_2O_2, s)$, of the sample was shown in Table 5. $\Delta_f H_m^0(C_5H_4N_2O_2, s)$ was calculated by a designed Hess' thermochemical cycle according to the reaction (8) as follows,

$$\Delta H_4 = \Delta_f H_m^o(C_5H_4N_2O_2,s) = 5\Delta_f H_m^o(CO_2,g) + \\ + 2\Delta_f H_m^o(H_2O,l) - \Delta_c H_m^o(C_5H_4N_2O_2,s) \\ = 5\Delta H_2 + 2\Delta H_3 - \Delta H_1 = -(327.82 \pm 1.13)\,\mathrm{kJ{\cdot}mol^{-1}}.$$

Table 4. The experimental results of the constant-volume energy of combustion for 2-pyrazinecarboxylic acid ($C_5H_4N_2O_2$)(s) at 298.15 K

No.	Mass of simple m (g)	Calibrated ΔT (K)	Calibrated heat of nitric acid $Q_{\mathrm{HNO},}$(J)	Calibrated heat of combustion wire Q_{Ni} (J)	Combustion energy of sample $-\Delta_c U$ ($\mathrm{J\ g^{-1}}$)
1	0.60255	0.5809	37.17	12.60	17853.90
2	0.58760	0.5661	36.52	10.80	17843.71
3	0.63105	0.6086	39.93	11.70	17861.29
4	0.64670	0.6219	40.18	12.60	17809.90
5	0.59315	0.5713	37.69	12.60	17834.85
6	0.56975	0.5487	35.75	12.60	17832.75
		Avg. $\Delta_c U = -(17839.40 \pm 7.40)\ \mathrm{J\ g^{-1}}$			

Table 5. Reaction scheme used to determine the standard molar enthalpy of formation of 2-pyrazinecarboxylic acid $(C_5H_4N_2O_2)(s)$

No.	Reactions	$\Delta_f H^o_m$ or $(\Delta_c H^o_m \pm \sigma_a)^*$ (kJ mol^{-1})
1	$C_5H_4N_2O_2(s) + 5O_2(g) = 5CO_2(g) + 2H_2O(l) + N_2(g)$	– (2211.39 ± 0.92), ΔH_1
2	O_2 (g) + C (s) = CO_2 (g)	– (393.51 ± 0.13), ΔH_2
3	H_2 (g) + 1/2O_2 (g) = H_2O (l)	– (285.83 ± 0.04), ΔH_3
4	$5C_5(s) + 2H_2(g) + N_2(g) + O_2(g) = C_5H_4N_2O_2(s)$	– (327.82 ± 1.13), ΔH_4

$\sigma_a = \frac{\sigma}{\sqrt{n}} = \frac{\sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2/(n-1)}}{\sqrt{n}} = \sqrt{\sum_{i=1}^{n}(x_i-\bar{x})^2/n(n-1)}$, in which n is the experimental number; x_i, a single value obtained from a series of measurements; $\bar{x}$, the mean value of the results.

In equation (8), the standard molar enthalpies of formation of CO_2(g) and H_2O(l), recommended by *CODATA*,[12, 13] $\Delta_f H^0_m(CO_2, g) = -(393.51 \pm 0.13)$ kJ mol^{-1} and $\Delta_f H^0_m(H_2O, l) = -(285.83 \pm 0.04)$ kJ mol^{-1}, were employed in the calculation of $\Delta_f H^0_m(C_5H_4N_2O_2, s)$. At last, the standard molar enthalpy of formation of the compound can be derived to be $\Delta_f H^0_m(C_5H_4N_2O_2, s) = -(327.82 \pm 1.13)$ kJ mol^{-1}.

4. Conclusions

In this paper, low-temperature heat capacities from 78 to 400 K and constant-volume energy of combustion at 298.15 K of the compound 2-pyrazinecarboxylic acid were measured by adiabatic calorimetry and rotating-bomb combustion calorimeter, respectively. Moreover, smoothed heat capacities, some relevant thermodynamic parameters, and standard molar enthalpy of formation of the compound were derived from these experimental results.

5. Acknowledgements

This work was financially supported by the National Natural Science Foundations of China under the contract NSFC No. 20673050 and 20973089.

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Povzetek

S preciznim avtomatskim adiabatnim kalorimetrom smo v temperaturnem območju med 78 in 400 K merili toplotne kapacitete 2-pirazinkarboksilne kisline $(C_5H_4N_2O_2)(s)$. Temperaturno odvisnost toplotne kpacitete smo podali s polinomom in z njegogo pomočjo izračunali ostale termodinamske funkcije za spojino pri glede na referenčno temperaturo T = 298.15 K. Pri 298.15 K smo v preciznem rotacijskem bombnem kalorimetru določili tudi sežigno notranjo energijo spojine, $\Delta_c U = -(17839.40 \pm 7.40)$ J g^{-1} ter ocenili standardno molsko sežigno entalpijo $\Delta_c H^0_m$ (298.15 K) = –(2211.39 ± 0.92) kJ mol^{-1}. Z uporabo Hessovega stavka smo izračunali standardno molsko tvorbeno entalpijo 2-pirazinkarboksilne kisline, $\Delta_f H^0_m$ (298.15 K) = – (327.82 ± 1.13) kJ mol^{-1}.