Low-temperature heat capacities and standard molar enthalpy of formation of pyridine-2,6-dicarboxylic acid*

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This paper reports that the low-temperature heat capacities of pyridine-2,6-dicarboxylic acid were measured by a precision automatic calorimeter over a temperature range from 78 K to 380 K. A polynomial equation of heat capacities as a function of temperature was fitted by the 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 intervals of 5 K. The constant-volume energy of combustion of the compound was determined by means of a precision rotating-bomb combustion calorimeter. The standard molar enthalpy of combustion of the compound was derived from the constant-volume energy of combustion. The standard molar enthalpy of formation of the compound was calculated from a combination of the datum of the standard molar enthalpy of combustion of the compound with other auxiliary thermodynamic quantities through a Hess thermochemical cycle.

Keywords: pyridine-2,6-dicarboxylic acid, adiabatic calorimetry, low-temperature heat capacity, standard molar enthalpy of formation

PACC: 0570, 8260

1. Introduction

Pyridine-2,6-dicarboxylic acid (H_2DPC) is a water-soluble, commercially available, versatile N, O-chelator possessing diverse coordination modes, with a recognized biological function in body metabolism, namely as a major component of bacterial spores, and in a variety of processes as an enzyme inhibitor plant preservative, food sanitizer, etc.[1] It has the ability to build stabilizing structures with divalent metals[2] and also can form bridging hydrogen bonds making it useful for self-assembly. H_2DPC or its salts are usually added to food, especially fresh fruit juices, to reduce the oxidation of vitamin C; H_2DPC is the precursor of L-lysine, which is an indispensable nutrient in organisms and the basic units that constitute the proteins demanded for life activity. In addition, metal complexes formed between H_2DPC and various biological metal elements have attracted interest from inorganic and bioinorganic chemists.[3] For instance, the coordination of Ni(II) with H_2DPC can reduce the surface contact between Ni(II) and cells, which will abate the toxic action of the nickel ion to microorganisms. The complex of iron with H_2DPC can be used as an electron carrier applied in imitation of an organism; it is also a special molecular device in the division of DNA.

The heat capacity and standard molar enthalpy of formation of a substance are the most fundamental thermodynamic properties and closely related to other physical, biological, physiological and chemical properties.[4−10] However, up to now, low-temperature heat capacities and standard molar enthalpy of formation of H_2DPC have not been found in the literature, which has restricted the progress of relevant theoretical study and application development of the title compound. In view of the significance of its derivatives and complexes in the fields of three-dimensional chemicals, structural chemistry, magnetism, spectral dynamics and reaction mechanisms, biochemical simulation systems and analytical chemistry, etc., low-temperature heat capacities and the constant volume energy of combustion of H_2DPC were measured by adiabatic calorimetry and combustion calorimetry in the present work. Finally, smoothed heat capacities and thermodynamic functions, the standard molar enthalpy of combustion and the standard molar enthalpy of formation of the compound were derived from these experimental results.

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2. Experimental

2.1. Sample

The sample used in these calorimetric measurements was of analytical grade. It was purchased from J & K SCIENTIFIC LTD. The labelled purity is more than 99.0 %. The melting point was measured to be 249–250 °C, as measured by a micro melting point device. Fourier transform infrared spectroscopy (FTIR) and hydrogen-1 nuclear magnetic resonance spectroscopy (HNMR) were used to verify the structure of the compound, elementary analysis was used to confirm the composition of the compound, and high performance liquid chromatography (HPLC) was used to determine the purity of the sample.

2.2. Adiabatic calorimetry

A precision automatic adiabatic calorimeter was used to measure the heat capacities of the compound over the temperature range $78 \leq (T/\mathrm{K}) \leq 400$. The calorimeter was established in the Thermochemistry Laboratory of the College of Chemistry and Chemical Engineering, Liaocheng University, China. The principle and structure of the adiabatic calorimeter have been described in detail elsewhere.[11,12] 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 were installed between the sample cell and the inner shield, between the inner and middle shields, and between the middle and outer shields — and a high vacuum can. The miniature platinum resistance thermometer (IPRT No.2, produced by the Shanghai Institute of Industrial Automatic Meters, 16 mm in length, 1.6 mm in diameter and a nominal resistance of 100 Ω) was used 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 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 a reference standard material (α-Al_2O_3) were measured over the temperature range $78 \leq (T/\mathrm{K}) \leq 400$. The sample mass was 1.71431 g, which was equivalent to 0.0168 mol based on its molar mass, $M(Al_2O_3) = 101.9613$ g·mol^{-1}. 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[13] 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 to 0.4) K·min^{-1} and (1 to 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 for heat capacities and corresponding equilibrium temperatures have been corrected for heat exchange of the sample cell with its surroundings.[11]

The sample mass used for the calorimetric measurement was 1.79816 g, which was equivalent to 0.01076 mol in terms of its molar mass, $M(C_7H_5NO_4) = 167.12$ g·mol^{-1}.

2.3. Rotating-bomb combustion calorimetry

The constant-volume combustion energy of the compound was measured by a precision rotating-bomb combustion calorimeter (model: RBC-type II, made in China). The structure and principle of the calorimeter have previously been described in detail elsewhere.[14] It mainly consists of a thermostatic trough with an outer casing, a calorimetric tube and a system for the temperature measurement. The volume of the thermostatic trough was about 25.0 dm^3 and was equipped with two interior agitators. The temperature of the thermostatic water in the bath was automatically maintained at $T = (298.15 \pm 0.001)$ K by means of a precise thermosistor. The volume of the calorimetric tube was 4.5 dm^3. The temperature gauge from the digital indicator with integrated circuit was used to measure the temperature of the calorimetric tube. The bicyclic structure of the crucible support in the oxygen bomb was constructed so that the bomb can make a compound rotation about an axis perpendicular to the bomb axis (i.e., end-over-end rotation) and about the bomb axis (axial rotation) at the same time.

The thermostatic water bath of the outer casing was controlled at $T = (298.15 \pm 0.001)$ K, then the water temperature in the calorimetric tube was adjusted to a temperature lower than that of the water bath of the outer casing, and it was ensured that the range of the temperature change in the calorimetric tube was half of the total temperature rise of the calorimeter after the combustion was completed. When adding a known amount of pure water to the calorimetric tube, laying the sample into the crucible fixed onto the support in the rotating bomb but not fallen into the solution, fastening the combustion fuse in the support pillars of the bomb, injecting the initial bomb solution into the rotating bomb, and filling the bomb with 2.5 MPa of oxygen were completed, subsequently the bomb was sealed. In addition, it was important for the temperature change of the calorimeter to remain constant at the beginning of every experiment. In the initial stage of the experiment, the temperature reading was recorded every 30 s until the tenth one had been recorded. From the eleventh reading, the sample was ignited and the temperature reading was recorded once per minute till the rate of the temperature change remained invariable. It was assumed that the main period (15 minutes) of the combustion reaction was finished at this stage. During the final state of the experiment, a temperature reading was taken every 30 s and recorded 10 times.

The temperature rise must be corrected on the basis of the heat exchange between the calorimetric tube and its surroundings. The corrected value of the heat exchange was calculated by means of the Linio–Pyfengdelel–Wsava equation:[15]

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

where $\Delta(\Delta T)$/K denotes the corrected value of the heat exchange; n, the number of readings for the main (or reaction) stage; V_n and V_0/K·min^{-1}, the temperature drift rates in the final and initial stages, respectively (V is positive when the temperature decreases); $\overline{T_n}$ and $\overline{T_0}$/K, the average temperatures of the calorimeter during the final and initial stages, respectively; 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; $(V_n - V_0)/(\overline{T_n} - \overline{T_0})$, a constant related to the calorimeter performance.

After the end of the experiment, the final products of the combustion reaction were analysed.[14] The gases formed in the combustion were collected in a gas-collecting bag. They were measured by a gas meter which was fitted between the bag and the bomb. The gaseous carbon dioxide produced in the combustion was absorbed by a weighted absorption tube containing alkali asbestos. The amount of CO_2 (g) was determined through the weight increment of the tube after absorbing the carbon dioxide. The amount of CO_2 (g) dissolved in the final solution was neglected. Four absorption tubes were connected in series with each other for the measurement. The first was filled with P_4O_{10} and $CaCl_2$ (anhydrous) to absorb the water vapour contained in the gas, the second was filled with active MnO_2 in order to absorb the nitrogen oxides, the third was filled with alkali asbestos to absorb the CO_2, and the fourth was full of solid P_4O_{10} and $CaCl_2$ (anhydrous) to absorb the water formed in the determination. The nitrogen oxides (NO_x) produced from oxidation of a trace of nitrogen contained in the bomb mainly existed in the form of NO_2 due to the excess of oxygen in the bomb, and no NO_2 appeared in the gas phase because it was readily dissolved in the water poured into the bottom of the bomb to form the aqueous nitric acid.

The fittings and the inside wall of the bomb were washed three times by using distilled water at first, then the bomb solution including the washing solution was completely transferred to a conical bottle and heated to boiling to remove a small amount of CO_2 dissolved in the bomb solution. The total amount of nitric acid was obtained from titrating the solution to a phenothalin end-point with a standard solution of NaOH.

From 6 combustion experiments using about 0.9 g of NIST (National Institute of Standards and Technology) 39i benzoic acid with an isothermal heat of combustion of $Q = -(26434 \pm 3)$ J·g^{-1} under the same experimental conditions the energy equivalent of the RBC-type II calorimeter, W, was determined to be (18604.99 ± 8.14) J·K^{-1} by the formula:

$$W = \frac{Q \cdot a + G \cdot b + 5.97 \cdot c}{\Delta T}, \quad (2)$$

where W/J·K^{-1} is the energy equivalent of the calorimeter, Q/J·g^{-1} is the combustion enthalpy of benzoic acid, a/g is the mass of determined benzoic acid, G/J·cm^{-1} is the combustion enthalpy of Ni–Cr wire for ignition ($G = 0.9$ J·cm^{-1}), b/cm is the

length of the actual Ni–Cr wire consumed in ignition, 5.97/J·mL^{-1} is the formation enthalpy and solution enthalpy of nitric acid corresponding to 1 mL 0.1000 mol·dm^{-3} solution of NaOH, c/cm^3 is the volume of consumed 0.1000 mol·dm^{-3} NaOH (aq) in the final bomb solution, ΔT is the corrected value of the temperature rise.

3. Results and discussion

3.1. Low-temperature heat capacities

All experimental results, plotted in Fig. 1 and listed in Table 1, show that the structure of the compound was stable over the temperature range between $T = 78$ K and 380 K, namely, no phase change, association or thermal decomposition occurred.

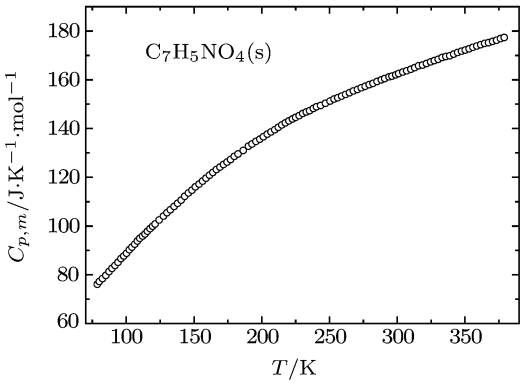


Fig. 1. The experimental molar heat capacity curve of the solid compound $C_7H_5NO_4$(s) with temperature (K).

Table 1. The experimental molar heat capacities of the compound ($M_{C_7H_5NO_4} = 167.12$ 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}
78.62	76.05	166.6	123.2	273.5	156.7
80.17	77.20	169.1	124.1	276.4	157.3
82.54	78.45	171.8	125.2	279.3	158.0
84.98	79.74	174.4	126.2	282.2	158.6
87.35	81.31	177.0	127.3	285.2	159.3
89.55	82.62	179.8	128.6	288.3	160.0
91.75	83.81	182.5	129.6	290.8	160.5
93.95	85.11	186.4	131.0	293.9	161.2
96.08	86.62	190.2	132.7	296.1	161.5
98.20	87.66	192.9	133.7	298.9	162.0
100.2	88.83	195.7	134.7	301.2	162.6
102.3	90.29	198.6	135.6	304.1	163.1
104.3	91.31	201.3	136.6	307.0	163.7
106.3	92.51	204.1	137.7	310.0	164.3
108.2	93.80	206.8	138.5	312.9	165.0
110.1	94.99	209.6	139.5	315.8	165.7
112.1	95.91	212.3	140.4	318.7	166.1
113.9	96.68	214.9	141.4	321.6	166.7
115.7	97.84	217.5	142.3	324.6	167.3
117.6	98.89	220.1	143.1	327.4	167.9
119.5	99.86	222.6	143.9	330.3	168.4
121.3	100.8	225.1	144.6	333.2	169.1
124.3	102.5	227.7	145.3	336.0	169.6
127.5	104.1	230.3	146.2	338.9	169.8
130.1	105.5	232.8	146.8	341.7	170.5
132.6	106.6	235.4	147.3	344.5	171.2
135.4	108.0	238.1	148.2	347.4	171.7
138.0	109.3	240.4	148.9	350.2	172.1
140.6	110.6	243.5	149.4	353.1	172.7
143.2	112.2	247.0	150.3	355.8	173.3
145.9	113.6	250.5	151.3	358.7	173.9
148.5	114.7	253.4	152.1	361.7	174.3
151.0	116.0	256.2	152.6	364.5	174.9
153.7	117.2	259.0	153.3	367.4	175.2
156.3	118.4	261.9	154.0	370.4	175.8
158.9	119.6	264.8	154.7	373.3	176.2
161.5	120.9	267.7	155.4	376.2	176.9
164.0	122.0	270.7	156.0	379.0	177.3

The 114 experimental points in the temperature region were fitted by the least-square method, and a polynomial equation of experimental molar heat-capacities ($C_{p,m}$) vs. reduced temperature (X),

$$X = f(T) = \left[T - \frac{(T_1 + T_2)}{2}\right] \Big/ \left[\frac{(T_1 - T_2)}{2}\right]$$

(where $T_1 = 380$ K and $T_2 = 78$ K), was obtained:

$$\begin{aligned} & C_{p,m}/(\mathrm{J \cdot mol^{-1} \cdot K^{-1}}) \\ &= 145.504 + 44.571X - 21.910X^2 \\ &\quad + 6.734X^3 + 3.116X^4, \end{aligned} \tag{3}$$

in which $X = (T - 229)/151$. This equation is valid between $T = 78$ K and $T = 380$ K. The standard deviations of experimental molar heat capacities from the smoothed heat capacities calculated by the polynomial equation were within ±0.3% except for several points around the lower temperature limit. The coefficient of determination for the fitted R^2 was equal to 0.99996.

3.2. Thermodynamic functions of the compound

The smoothed molar heat capacities and thermodynamic functions were calculated based on the fitted polynomial of the heat capacities as a function of the reduced temperature (X). The relations between molar heat capacities and thermodynamic functions of the sample relative to the standard reference temperature 298.15 K are shown as follows:

$$(H_T - H_{298.15}) = \int_{298.15}^{T} C_p \mathrm{d}T, \tag{4}$$

$$(S_T - S_{298.15}) = \int_{298.15}^{T} C_p \cdot T^{-1} \mathrm{d}T. \tag{5}$$

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 are tabulated in Table 2 at 5 K intervals.

Table 2. The smoothed heat capacities and thermodynamic functions of the compound ($M_{\mathrm{C_7H_5NO_4}} = 167.12$ g·mol^{-1}).

T/K	$C_{p,m}$ /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}
80	76.674	–27.88	–155.5
85	79.810	–27.48	–150.8
90	82.894	–27.08	–146.2
95	85.923	–26.65	–141.6
100	88.897	–26.22	–137.1
105	91.815	–25.76	–132.7
110	94.677	–25.30	–128.4
115	97.481	–24.82	–124.1
120	100.23	–24.32	–119.8
125	102.91	–23.81	–115.7
130	105.54	–23.29	–111.6
135	108.11	–22.76	–107.5
140	110.62	–22.21	–103.5
145	113.07	–21.65	–99.57
150	115.46	–21.08	–95.68
155	117.79	–20.49	–91.84
160	120.06	–19.90	–88.06
165	122.26	–19.29	–84.33
170	124.41	–18.68	–80.64
175	126.51	–18.05	–77.01
180	128.54	–17.41	–73.42
185	130.51	–16.76	–69.88
190	132.43	–16.11	–66.38
195	134.29	–15.44	–62.93
200	136.09	–14.76	–59.52
205	137.84	–14.08	–56.15
210	139.54	–13.38	–52.82
215	141.18	–12.68	–49.53
220	142.77	–11.97	–46.28
225	144.31	–11.26	–43.08
230	145.80	–10.53	–39.90
235	147.24	–9.797	–36.77
240	148.64	–9.058	–33.67
245	149.99	–8.311	–30.60
250	151.30	–7.558	–27.57
255	152.57	–6.798	–24.58
260	153.79	–6.032	–21.61
265	154.99	–5.260	–18.68
270	156.14	–4.482	–15.78
275	157.27	–3.698	–12.91
280	158.36	–2.909	–10.07
285	159.42	–2.115	–7.257
290	160.46	–1.315	–4.475
295	161.48	–0.5098	–1.721
298.15	162.10	0	0
300	162.47	0.3003	1.006
305	163.45	1.115	3.705
310	164.41	1.935	6.379
315	165.35	2.760	9.026
320	166.29	3.590	11.65
325	167.22	4.424	14.24
330	168.15	5.263	16.82
335	169.08	6.106	19.36
340	170.01	6.955	21.89
345	170.95	7.808	24.39
350	171.90	8.665	26.87
355	172.86	9.528	29.32
360	173.84	10.40	31.76
365	174.85	11.27	34.17
370	175.87	12.15	36.56
375	176.93	13.03	38.92
380	178.02	13.92	41.27
385	179.14	14.81	43.60
390	180.31	15.71	45.90
395	181.52	16.62	48.18
400	182.79	17.53	50.45

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

The constant-volume combustion energy of the sample can be calculated according to the equation derived from Eq. (2):

$$-\Delta_{\rm c}U = \frac{W\cdot\Delta T - G\cdot b - q_{\rm N}}{m} = \frac{W\cdot\Delta T - q_{\rm c} - q_{\rm N}}{m}, \tag{6}$$

where $\Delta_{\rm c}U/{\rm J}\cdot{\rm g}^{-1}$ is the constant-volume combustion energy of the sample, m is the mass of the sample, $q_{\rm N}$ is the calibrated heat of acid. The physical meanings of other symbols are the same as those of Eq. (2).

The measured results of the constant-volume combustion energy of the sample are indicated in Table 3.

Table 3. The constant-volume combustion energy of the compound.

complex	No	mass of complex, m/g	calibrate, ΔT/K	calibrated heat of acid, $q_{\rm N}$/J	calibrated heat of combustion wire, $q_{\rm c}$/J	constant-volume combustion energy, $-\Delta_{\rm c}U/{\rm J}\cdot{\rm g}^{-1}$
H_2DPC	1	0.64385	0.5572	26.02	12.6	16041.13
	2	0.58670	0.5084	23.57	10.8	16063.42
	3	0.54335	0.4707	21.96	12.6	16053.76
	4	0.62590	0.5433	25.48	12.6	16088.85
	5	0.62805	0.5446	25.37	12.6	16072.46
	6	0.57160	0.4953	23.24	12.6	16058.80
Ave. $\Delta_{\rm c}U = -(16063.07 \pm 6.68)$ J·g^{-1}						

The standard molar enthalpy of combustion of the sample ($\Delta_{\rm c}H_m^{\odot}$) is the combustion enthalpy change of the following reaction at $T = 298.15$ K and $P = 100$ KPa:

$$C_7H_5NO_4({\rm s}) + \frac{25}{4}O_2({\rm g}) = \frac{1}{2}N_2({\rm g}) + 7CO_2({\rm g}) + \frac{5}{2}H_2O({\rm l}). \tag{7}$$

The standard molar enthalpies of combustion of the sample can be derived from the constant-volume combustion energy by means of the following formula:

$$\Delta_{\rm c}H_m^{\odot} = \Delta_{\rm c}U_m^{\odot} + \Delta n\cdot RT, \tag{8}$$

$$\Delta n = \sum n_i({\rm products,\ g}) - \sum n_i({\rm reactants,\ g}), \tag{9}$$

where $\Delta_{\rm c}U_m^{\odot}/{\rm J}\cdot{\rm mol}^{-1} = \Delta_{\rm c}U\cdot M$; $\sum n_i$ is the total amount (in moles) of gas present as products or as reactants. The calculated standard molar enthalpy of combustion of the sample is $\Delta_{\rm c}H_m^{\odot} = -(2681.36 \pm 1.12)$ kJ·mol^{-1}.

A reaction scheme used to determine the standard molar enthalpy of formation of H_2DPC is shown in Table 4, the standard molar enthalpy of formation of the compound, $\Delta_{\rm f}H_m^{\odot}$ is calculated by a designed Hess thermochemical cycle[16,17] according to Eq. (7) as follows:

$$\Delta_{\rm f}H_m^{\odot}(C_7H_5NO_4,{\rm s}) = 7\Delta_{\rm f}H_m^{\odot}(CO_2,{\rm s}) + \frac{5}{2}\Delta_{\rm f}H_m^{\odot}(H_2O,{\rm l}) - \Delta_{\rm c}H_m^{\odot}(C_7H_5NO_4,{\rm s}). \tag{10}$$

In the above formula, the standard molar enthalpies of formation of CO_2(g) and H_2O(l), recommended by CODATA,[18] $\Delta_{\rm f}H_m^{\odot}(CO_2,{\rm g}) = -(393.51 \pm 0.13)$ kJ·mol^{-1} and $\Delta_{\rm f}H_m^{\odot}(H_2O,{\rm l}) = -(285.83 \pm 0.04)$ kJ·mol^{-1}, were employed in the calculation of $\Delta_{\rm f}H_m^{\odot}[C_7H_5NO_4,{\rm s}]$ values. The standard molar enthalpy of formation of the compound can be derived based on these values; the standard molar enthalpy of combustion of the substance is $\Delta_{\rm f}H_m^{\odot}[C_7H_5NO_4,{\rm s}] = -(787.78 \pm 1.45)$ kJ·mol^{-1}.

Table 4. Reaction scheme used to determine the standard molar enthalpy of formation of H_2DPC.

No.	reactions	$\Delta_{\rm f}H_m^{\odot}$ or $(\Delta_{\rm c}H_m^{\odot} \pm \sigma_a)$/(kJ·mol^{-1})
1	$C_7H_5NO_4({\rm s}) + \frac{25}{4}O_2({\rm g}) = \frac{1}{2}N_2({\rm g}) + 7CO_2({\rm g}) + \frac{5}{2}H_2O$ (l)	–(2681.36 ± 1.12)
2	$O_2({\rm g}) + C({\rm s}) = CO_2({\rm g})$	–(393.51 ± 0.13)
3	$H_2({\rm g}) + \frac{1}{2}O_2({\rm g}) = H_2O$ (l)	–(285.83 ± 0.04)
4	$7C({\rm s}) + \frac{5}{2}H_2({\rm g}) + \frac{1}{2}N_2({\rm g}) + 2O_2({\rm g}) = C_7H_5NO_4({\rm s})$	–(787.78 ± 1.45)

Here

$$\sigma_{\mathrm{a}} = \frac{\sigma}{\sqrt{n}} = \frac{\sqrt{\sum_{i=1}^{n}(x_i - \overline{x})^2/(n-1)}}{\sqrt{n}} = \sqrt{\frac{\sum_{i=1}^{n}(x_i - \overline{x})^2}{n(n-1)}},$$

in which n is the experimental number; x_i, a single value in a set of dissolution measurements; $\overline{x}$, the mean value of a set of measurement results.

4. Conclusion

This paper reports low-temperature heat capacities and constant-volume energy of combustion of pyridine-2,6-dicarboxylic acid measured by adiabatic calorimetry and rotating-bomb combustion calorimetry. The standard molar enthalpy of combustion of the compound was derived from the constant-volume energy of combustion. Additionally, some thermodynamic functions, such as $(H_T - H_{298.15})$, $(S_T - S_{298.15})$ and standard molar enthalpy of formation of the compound were derived from the experimentally measured heat capacity data.

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