



Low-Temperature Heat Capacities and Thermodynamic Properties of 2-Aminopyridine

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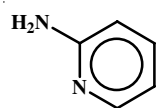
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Low-temperature heat capacities of 2-aminopyridine have been measured by a precision automatic adiabatic calorimeter over the temperature range from 78 to 370 K. A solid-liquid phase transition was observed from 315 to 335 K. The peak temperature, molar enthalpy and entropy of the solid-liquid phase transition were determined to be: (330.09 ± 0.01) K, (18.33 ± 0.05) kJ mol⁻¹ and (55.53 ± 0.14) J K⁻¹ mol⁻¹, respectively. In addition, the mole fraction purity, the melting temperature of the given sample and that of pure sample were calculated to be (99.54 ± 0.06) %, (330.20 ± 0.01) K and (330.43 ± 0.01) K by means of fractional melting method. The results showed that the melting temperature of the sample from adiabatic calorimetry agreed basically with that from theoretical analysis of the purity.

Keywords: 2-Aminopyridine, Adiabatic calorimetry, Heat capacity, Melting process, Thermodynamic function, Purity analysis.

INTRODUCTION

2-Aminopyridine (C₅H₆N₂) (CAS registry number, 504-29-0) is an important alkaloid and starting material in the production of many intermediates of medicine, such as sulfanilyl pyridine. 2-Aminopyridine is not only an important intermediate of common synthesized medicine, agricultural chemicals and dyes, but also a chemical reagent which can be used in medicine, chemical analysis and environment monitoring [1]. For instance, it is used to detect the existence of elements such as stilbium, bismuth and gold, because both the nitrogen atom of the amino group and the pyridyl nitrogen atom in the 2-aminopyridine have the ability of forming strong coordination bonds with some metallic ions to give stable coordination compounds. The nitrogen atom of the pyridine ring in the 2-aminopyridine has a certain alkalinity and nucleophilicity, so it is also widely used to prepare the fine ultra-nucleophilic catalysts [1]. Its molecular formula is C₅H₆N₂, molar mass is 94.1146 g mol⁻¹ and the chemical structure is:



Many papers have reported the properties of 2-aminopyridine [2-6], such as Bickerton *et al.* reported the enthalpies of combustion of 2-aminopyridine in 1984 [2] and Brostow *et al.* reported the enthalpies of sublimation of 2-aminopyridine

in 1985 [3]. Heat capacity of a substance is one of the most fundamental thermodynamic properties and closely related to other physical, biological, physiological and chemical properties. The purpose of this paper is to report the low temperature heat capacities and other derived thermodynamic properties of 2-aminopyridine measured by an improved adiabatic calorimeter.

EXPERIMENTAL

The sample used in the calorimetric experiments was of analytical grade. It was purchased from Neimenggu Pharmaceutical Factory, China. The labeled purity was higher than 99.5 % (mass percentage). The melting temperature was measured by using a micro-melting point device to be $T = 329.0$ K to 330.6 K, which agreed with the literature value [7]. But after purification by recrystallization from petroleum ether three times, the average purity of the sample was calculated by means of an adiabatic calorimetric approach to be higher than 99.54 % (molar percentage). This result was identical with the value of purity (> 99.5 %) obtained from HPLC. The structure of 2-aminopyridine was verified by FTIR and ¹H NMR. In addition, crystal structure is measured by a X ray single crystal diffraction technique. The molecular structure of the compound is shown in the Fig. 1.

X-ray crystallography: A colour-less flaky crystal suitable for X-ray analysis is glued to fine glass fiber and then mounted on the Bruker Smart-1000 CCD diffractometer with

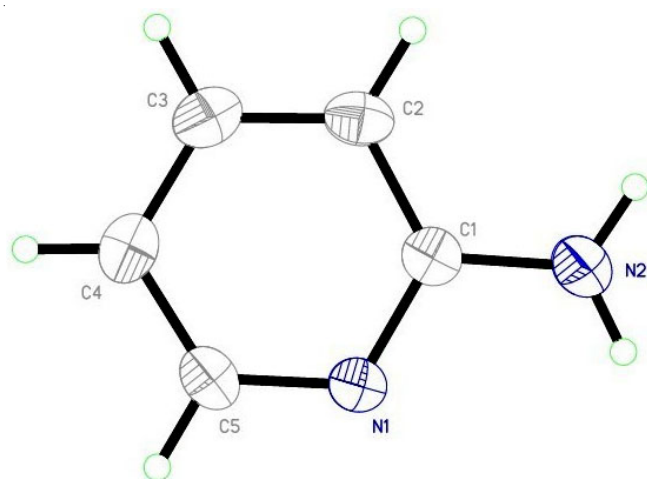


Fig. 1. Molecular structure of 2-aminopyridine

MoK α radiation, $\lambda = 0.071073$ nm. The intensity data are collected at $T = (298 \pm 2)$ K using the program SMART and processed by SAINT-plus. The structure is solved by direct method and expanded using Fourier technique with SHELXL-97 program. The non-hydrogen atoms are refined anisotropically by full-matrix least-squares calculation on F^2 . The hydrogen atoms are added theoretically, riding on the concerned atoms and not refined. Crystal data and refinement details are summarized in Table-1.

TABLE-1
CRYSTAL DATA AND STRUCTURE
REFINEMENT FOR 2-AMINOPYRIDINE

Empirical formula	C ₅ H ₅ N ₂ O ₂
Formula weight	344.40
Temperature	298(2) K
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	$a = 11.740(2)$ Å, $\alpha = 90^\circ$ $b = 5.6804(16)$ Å, $\beta = 5.4950(10)^\circ$ $c = 7.6003(16)$ Å, $\gamma = 90^\circ$
Volume	$504.5(2)$ Å ³
Z, Calculated density	1, 1.134 Mg/m ³
Absorption coefficient	0.073 mm ⁻¹
F(000)	182
θ range for data collection	3.49 to 24.99°
Limiting indices	$-13 \leq h \leq 13$, $-6 \leq k \leq 6$, $-9 \leq l \leq 8$
Collected/unique	1590/890 [R(int) = 0.0477]
Data/restraints/parameters	890/0/65
Goodness-of-fit on F^2	1.006
Final R indices [I > 2 σ (I)]	R1 = 0.0558, wR2 = 0.0830
R indices (all data)	R1 = 0.1338, wR2 = 0.1270

Adiabatic calorimetry: A precision automatic adiabatic calorimeter was used to measure heat capacities of the compound over the temperature range $78 \leq (T/K) \leq 370$. The calorimeter was established in the Thermochemistry Laboratory of the College of Chemistry and Chemical Engineering, Liaocheng University, China. The principle and performance of the

adiabatic calorimeter and the procedures of heat capacity measurements have already been described [8,9]. 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. Liquid nitrogen was used as the coolant. 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 kept within $\pm 10^{-3}$ K min⁻¹ during the acquisition of all heat-capacity data. The data of heat capacities and the corresponding equilibrium temperature have been corrected for heat exchange of the sample cell with its surroundings [10]. The reliability of the calorimeter was confirmed by the measurement of the heat capacities of the reference standard material (α -Al₂O₃) over the temperature range $78 \leq (T/K) \leq 400$. Deviations of the experimental results within ± 0.20 %, while the uncertainty is from those of the smoothed curve lie ± 0.30 %, as compared with the values given by the former National Bureau of Standards [11] over the whole temperature range.

The mass of the sample of 2-aminopyridine used in the heat capacity measurement was 1.71803 g, which is equivalent to 0.01825 mol, based on the molar mass $M(C_5H_5N_2O_2) = 94.11$ g mol⁻¹.

RESULTS AND DISCUSSION

Crystal structure: The molecular structure of 2-aminopyridine is shown in Fig. 1. The crystal system of the compound is monoclinic, space group is P2(1)/c, unit cell dimensions are $a = 1.1740(2)$ nm, $b = 0.56804(16)$ nm, $c = 0.76003(16)$ nm, $\alpha = 90^\circ$, $\beta = 95.4950(10)^\circ$, $\gamma = 90^\circ$ and $Z = 1$. The selected bond lengths and angles of 2-aminopyridine are listed in Table-2. The information on the hydrogen bonds is given in Table-3.

TABLE-2
BOND LENGTHS (nm) AND ANGLES (°)
FOR 2-AMINOPYRIDINE

Bonds	Bond lengths	Bonds	Bond angles
N(1)-C(5)	0.1335(4)	C(5)-N(1)-C(1)	117.3(3)
N(1)-C(1)	0.1339(4)	N(1)-C(1)-N(2)	116.2(3)
N(2)-C(1)	0.1353(4)	N(1)-C(1)-C(2)	122.0(3)
C(1)-C(2)	0.1404(4)	N(2)-C(1)-C(2)	121.8(3)
C(4)-C(5)	0.1377(4)	C(3)-C(4)-C(5)	117.1(3)
C(2)-C(3)	0.1367(4)	N(1)-C(5)-C(4)	124.7(3)
C(3)-C(4)	0.1377(5)	C(3)-C(2)-C(1)	118.5(3)
—	—	C(2)-C(3)-C(4)	120.4(3)

Fig. 1 shows that pyridine ring (C1, C2, C3, C4, C5, N1) and N2 are almost co-planar. The packing diagrams of 2-aminopyridine are shown in Fig. 2. There are two hydrogen bonds (N2-H2A...N1 and N2-H2B...N1) exist between amino nitrogen atom (N1) and pyridine nitrogen atom (N2), which join two 2-aminopyridine molecules together.

TABLE-3
HYDROGEN BONDS (nm AND °) FOR 2-AMINOPYRIDINE

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(DHA)$	Symmetry code
N2-H2A...N1	0.0860	0.2229	3.080	170.43	$[-x, -y+2, -z+1]$
N2-H2B...N1	0.0860	0.2695	3.415	142.22	$[x, -y+3/2, z+1/2]$

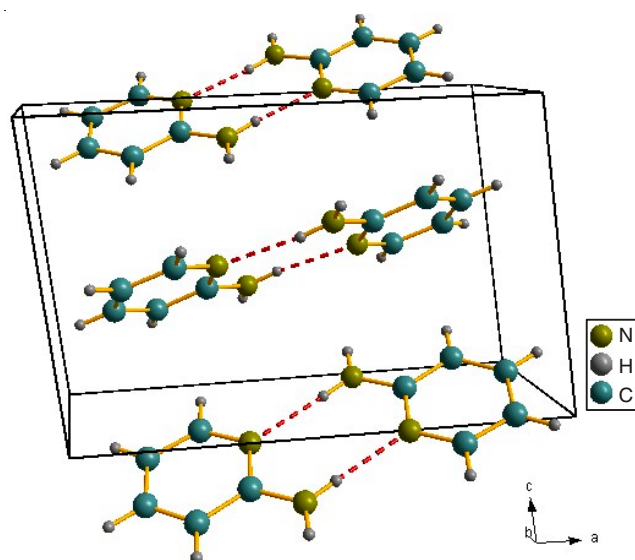


Fig. 2. Packing of the molecule in the crystal lattice

Low-temperature heat capacities: The experimental results of low-temperature heat capacities are listed in Table-4

and plotted in Fig. 3, which shows that an obvious endothermic peak appeared in the temperature range between $T = 315$ and 335 K, which is a solid-liquid phase transition process. Because the melting temperature of the compound is $T = 330$ to 331 K [7], as indicated in the previous experiment by a micro melting point device.

The experimental heat capacity values in the temperature range between $T = 78$ K and $T = 315$ K and between $T = 336$ K and $T = 370$ K were respectively fitted by means of the least squares method and two polynomial equations of the experimental molar heat capacities ($C_{p,m}$) vs. reduced temperature (X), $X = f(T)$, have been obtained:

(i) In the range before the solid-liquid phase transition from $T = 78$ K to $T = 315$ K:

$$C_{p,m} (\text{J K}^{-1} \text{mol}^{-1}) = 97.659 + 46.883X + 6.419X^2 - 8.123X^3 + 1.301X^4 + 10.040X^5 \quad (1)$$

where $X = (T - 196.5)/118.5$, in which 196.5 is half of the upper limit 315 K plus the lower limit 78 K over the temperature range from $T = 78$ to 315 K, while 118.5 is half of the upper limit 315 K minus the lower limit 78 K. The correlation coefficient for the fitting R^2 equals 0.9999. The reduced

TABLE-4
THREE SERIES OF EXPERIMENTAL MOLAR HEAT CAPACITIES OF 2-AMINOPYRIDINE ($M = 94.1146 \text{ g mol}^{-1}$)

T (K)	$C_{p,m}$ ($\text{J K}^{-1} \text{mol}^{-1}$)	T (K)	$C_{p,m}$ ($\text{J K}^{-1} \text{mol}^{-1}$)	T (K)	$C_{p,m}$ ($\text{J K}^{-1} \text{mol}^{-1}$)	T (K)	$C_{p,m}$ ($\text{J K}^{-1} \text{mol}^{-1}$)
Series 1							
78.250	57.49	158.591	83.92	244.608	117.56	321.620	171.42
81.845	58.71	162.231	84.99	248.347	118.94	324.570	195.65
85.228	59.64	165.940	86.22	252.085	120.95	327.280	319.58
88.583	60.95	169.513	87.46	255.824	122.67	329.080	1289.74
91.895	62.06	173.288	88.68	259.654	124.35	329.810	6537.43
95.203	63.16	176.929	90.10	263.227	125.77	330.020	19058.70
98.366	64.18	180.705	91.54	267.003	127.44	330.080	34950.10
102.536	65.61	184.480	92.77	270.711	129.18	330.110	43817.40
106.994	67.19	188.391	94.25	274.689	130.71	331.020	1395.52
110.301	68.31	192.099	95.72	278.397	132.44	335.060	214.10
113.752	69.43	195.874	97.10	282.375	134.18	339.615	215.06
117.347	70.37	200.459	98.86	286.083	135.78	342.600	215.83
120.798	71.51	205.043	100.72	289.926	137.87	345.615	216.53
124.393	72.69	208.819	102.34	293.634	139.89	348.649	217.24
127.701	73.63	212.733	103.96	297.410	141.72	351.680	218.00
131.296	74.69	216.424	105.28	300.983	143.93	354.690	218.71
134.891	75.99	220.249	107.21	303.430	145.84	357.684	219.43
138.485	77.46	224.008	108.83	306.510	147.79	360.718	220.12
142.141	78.57	227.927	110.24	309.500	150.20	363.684	220.84
145.736	79.65	231.810	111.86	312.530	153.09	366.651	221.51
150.277	81.20	235.773	113.69	315.610	156.57	369.700	222.21
154.883	82.52	240.150	115.60	318.660	161.31	—	—
Series 2							
306.516	147.96	321.375	172.53	330.007	23475.30	339.704	214.57
309.104	149.97	324.298	201.56	330.067	36281.20	342.673	216.06
312.377	152.82	326.980	324.85	330.080	44605.00	345.702	216.67
315.376	156.45	328.895	1496.93	331.030	1261.77	348.732	217.37
318.406	161.36	329.732	14541.00	335.150	213.53	—	—
Series 3							
295.200	143.86	315.574	156.19	329.946	19387.70	345.916	216.54
297.660	141.26	318.589	161.71	330.007	31179.30	348.915	217.20
300.746	143.31	321.557	172.31	330.067	43883.80	351.929	217.99
303.730	146.34	324.420	209.87	331.150	1064.78	354.928	218.69
306.699	147.96	327.010	361.74	335.396	213.83	—	—
309.667	150.41	328.804	1855.18	339.933	214.53	—	—
312.610	152.49	329.656	11108.90	342.886	215.49	—	—

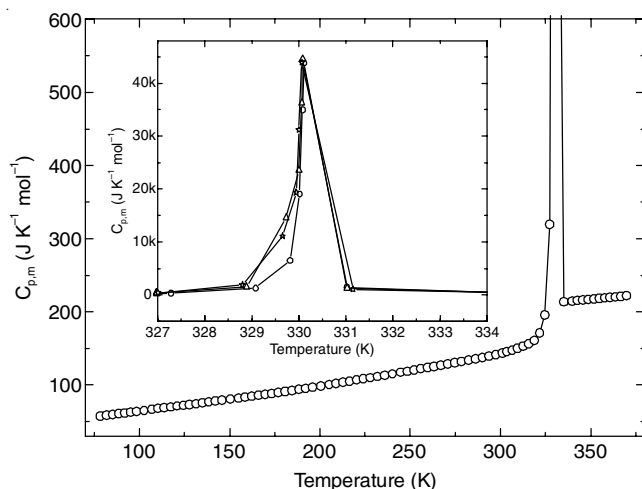


Fig. 3. Curves of experimental molar heat capacities of 2-aminopyridine (s) (○, Δ and ☆ denote the first, second and third series of measurements, respectively)

temperature (X) obtained using the method is placed between +1 and -1. The above equation (1) has an uncertainty of $\pm 0.3\%$.

(ii) In the range after the solid-liquid phase transition from $T = 336\text{ K}$ to $T = 370\text{ K}$:

$$C_{p,m} (\text{J K}^{-1} \text{mol}^{-1}) = 218.308 + 4.083X - 0.109X^2 - 0.076X^3 + 0.078X^4 \quad (2)$$

where $X = (T - 353)/17$. The correlation coefficient for the fitting R^2 is 0.99999. The above eqn. 2 has an uncertainty of $\pm 0.2\%$.

Melting temperature, molar enthalpy and entropy of fusion: Three series of repeated experiments in the solid-liquid phase transition region with different cooling rates for the sample were carried out so that the reversibility and repeatability of the solid-liquid phase transition of the sample were verified. The cooling rate of series 1 was about 15 K min^{-1} (liquid nitrogen as the cooling agent), that of series 2 was about 2.5 K min^{-1} (ice-water cooling) and that of series 3 was about 0.5 K min^{-1} (natural cooling). It can be seen from the inset that there are some slight differences in heights and widths of peaks corresponding to each series of heat-capacity measurements during solid-liquid phase transition of the sample. However, the solid-liquid phase transition basically exhibited good reversibility and repeatability and different cooling rates did not affect the experimental results. A close agreement in $C_{p,m}$

values of each series of repeated experiment is obtained. The molar enthalpy of the fusion ($\Delta_{\text{fus}}H_m$) in the $C_{p,m}$ - T curve is obtained from eqn. 3. The molar entropy ($\Delta_{\text{fus}}S_m$) of the fusion is calculated with the following thermodynamic eqn. 4 [12]:

$$\Delta_{\text{fus}}H_m = [Q - n \cdot \int_{T_i}^{T_{\text{peak}}} C_{p(s)} dT - n \cdot \int_{T_{\text{peak}}}^{T_f} C_{p(l)} dT - \int_{T_i}^{T_f} H_0 dT] / n \quad (\text{kJ mol}^{-1}) \quad (3)$$

$$\Delta_{\text{fus}}S_m = \frac{\Delta_{\text{fus}}H_m}{T_{\text{peak}}} (\text{J K}^{-1} \text{mol}^{-1}) \quad (4)$$

where T_i in eqn. 3 is the temperature slightly smaller than the starting solid-liquid phase transition temperature; T_f is the temperature slightly higher than the finishing solid-liquid phase transition temperature; $C_{p(s)}$ is the heat capacity at the temperature T_i ; $C_{p(l)}$ is the heat capacity at the temperature T_f ; Q is the total heat quantity introduced to the calorimeter from temperature T_i to T_f ; T_{peak} is the peak temperature of the solid-liquid phase transition of the sample; n is the molar number of the sample; H_0 is the average heat capacity of the empty sample cell. The values of Q and H_0 are calculated with the program stored in the computer linked with the adiabatic calorimetric system and printed along with experimental results of heat capacities. The details of three repeated experiments are listed in Table-5.

Melting temperature and purity: The purity of the sample was evaluated from a set of equilibrium melting temperatures and melting fractions corresponding to these temperatures. According to the law of ideal solution, the relation between the mole fraction x ($x < 1$) of a small amount of impurities in the sample and the melting temperature of the sample can be expressed as follows [12-14]:

$$x = \frac{\Delta_{\text{fus}}H_m (T_{\text{fus}}^0 - T_{\text{fus}})}{RT_{\text{fus}}^2} \quad (5)$$

in which T_{fus}^0 is the melting temperature of an absolutely pure substance; T_{fus} is the melting temperature of the given sample (strictly speaking, T_{fus}^0 and T_{fus} should be the triple points under the experimental adiabatic condition); $\Delta_{\text{fus}}H_m$ is the mole enthalpy of fusion of the sample; R is the molar gas constant. If x' is the mole fraction of the impurities in the liquid solution formed by the melting of part of sample and T is the melting temperature, then,

TABLE-5
SOLID-LIQUID PHASE TRANSITION OBTAINED FROM THE THREE
SERIES OF REPEATED EXPERIMENTS OF 2-AMINOPYRIDINE^a

Thermodynamic properties	Series 1: x_1	Series 2 x_1	Series 3 x_1	Mean value ($\bar{x} \pm \sigma_a$) ^a
T_i (K)	315.610	315.376	315.576	(315.52 $\pm$ 0.073)
$C_{p(s)}$ ($\text{J K}^{-1} \text{mol}^{-1}$)	156.570	156.358	156.190	(156.37 $\pm$ 0.11)
T_f (K)	335.060	335.150	335.396	(335.20 $\pm$ 0.10)
$C_{p(l)}$ ($\text{J K}^{-1} \text{mol}^{-1}$)	214.100	213.530	213.825	(213.82 $\pm$ 0.16)
T_{peak} (K)	330.110	330.080	330.067	(330.09 $\pm$ 0.013)
Q (J)	499.45	499.50	502.53	(500.49 $\pm$ 1.02)
$H_0(T_f - T_i)$ (J)	103.198	104.901	105.179	(104.43 $\pm$ 0.62)
H_{fus} (kJ mol^{-1})	18.38	18.24	18.37	(18.33 $\pm$ 0.05)
$\Delta_{\text{fus}}S_m$ ($\text{J K}^{-1} \text{mol}^{-1}$)	55.69	55.26	55.66	(55.53 $\pm$ 0.14)

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

$$x' = \frac{\Delta_{\text{fus}} H_m (T_{\text{fus}}^0 - T)}{RT_{\text{fus}}^0} \quad (6)$$

Assuming that the impurities are solid-insoluble, namely, no solid-solution would be formed and all of the impurities could transfer completely into the liquid phase when the melting started, the relative amount of the sample in the liquid phase would increase in the process of the melting. On the other hand, since the total amount of the impurities in the sample is constant, the mole fraction of the impurities in the liquid phase would gradually decrease with the melting process. Given that F is the ratio of the sample melted in the liquid phase to the total amount, then,

$$F = \frac{q}{Q} \quad (7)$$

in which F is also designated as the melting fraction and its value is the ratio of the partial heat (q) required for melting a part of the sample to the total heat, the value of Q (equates $n \cdot \Delta_{\text{fus}} H_m$, n is the mole number of the sample, $n = 0.01825$ mol) is the total heat required for melting the whole sample. Obviously, F is inversely proportional to the mole fraction of the impurities in the liquid phase, that is,

$$x' = \frac{1}{F} x \quad (8)$$

$$T_{\text{fus}}^0 - T = \frac{T_{\text{fus}}^0 - T_{\text{fus}}}{F} \quad (9)$$

Eqn. 9 suggested that the relationship between the equilibrium melting temperature ' T ' and the reciprocal of melting fraction $1/F$ is linear. The observed equilibrium temperature and corresponding melting fractions during the melting process are tabulated in Table-6. Plotting T versus $1/F$ and extrapolating the straight line, we can obtain T_{fus}^0 and T_{fus} at $1/F = 0$ and $1/F = 1$, respectively. The every series of repeated experimental results are plotted in Fig. 4 and listed in Table-7.

$T(K)$	$Q(J)$	$q(J)$	$F = \frac{q}{(n \cdot \Delta_{\text{fus}} H_m)}$	$1/F$
Series 1				
329.08	160.32	50.462	0.15042	6.6480
329.81	216.85	101.015	0.30111	3.3218
330.02	273.38	155.814	0.46446	2.1530
330.08	329.90	211.830	0.63144	1.5837
330.11	386.42	268.094	0.79916	1.2498
$T = 330.404 - 0.1953 (1/F)$				
Series 2				
328.89	160.33	50.165	0.15070	6.6357
329.74	216.87	99.748	0.29965	3.3372
330.00	273.40	154.137	0.46304	2.1596
330.06	329.93	210.162	0.63134	1.5839
330.09	386.46	266.434	0.80039	1.2494
$T = 330.441 - 0.2289 (1/F)$				
Series 3				
328.81	163.42	55.611	0.16588	6.0285
329.65	219.94	105.263	0.31398	3.1849
329.94	276.46	159.401	0.47547	2.1032
330.01	332.99	215.347	0.64234	1.5568
330.06	389.51	271.448	0.80968	1.2351
$T = 330.445 - 0.2663 (1/F)$				

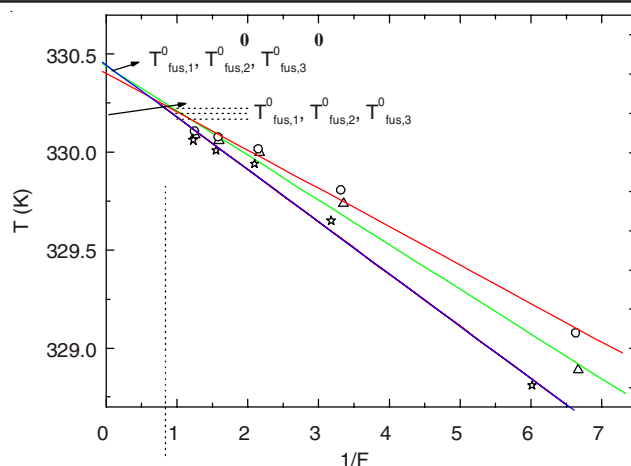


Fig. 4. A plot of temperature versus reciprocal of melting fraction during the fusion of 2-aminopyridine, (Δ , $\circ$ and $\star$ denote the first, second and third series of measurements, respectively)

Series	$T_{\text{fus}}^0 (K)$	$T_{\text{fus}} (K)$	X_2	$1 - x_2$
1	330.40	330.21	0.00395	99.61 %
2	330.44	330.21	0.00460	99.54 %
3	330.45	330.18	0.00539	99.46 %
Mean value	(330.43 ± 0.01)	(330.20 ± 0.01)		$(99.54 \pm 0.06) \%$

Smoothed molar heat capacities and thermodynamic functions of the compound: The smoothed molar heat capacities and thermodynamic functions were calculated based on the fitted polynomial equations of the heat capacities as a function of the reduced temperature (X) according to the following thermodynamic equations

$$(H_T - H_{298.15}) = \int_{298.15}^T C_{p,m} dT \quad (10)$$

$$(S_T - S_{298.15}) = \int_{298.15}^T C_{p,m} \cdot T^{-1} dT \quad (11)$$

$$(G_T - G_{298.15}) = \int_{298.15}^T C_{p,m} dT - T \cdot \int_{298.15}^T C_{p,m} \cdot T^{-1} dT \quad (12)$$

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 shown in Table-8 at 5 K intervals. The uncertainties of $(H_T - H_{298.15})$, $(S_T - S_{298.15})$ and $(G_T - G_{298.15})$ were evaluated to be $\pm 0.45 \%$, $\pm 0.50 \%$ and $\pm 0.60 \%$, respectively, mainly resulted from uncertainties in the temperature, experimental heat capacities and relative deviations of the experimental heat capacities from the smoothed values.

Conclusion

This paper mainly reported the low temperature heat capacities and thermodynamic properties of 2-aminopyridine. The data of the smoothed heat capacities, the thermodynamic properties of the fusion transition and thermodynamic functions relative to reference temperature 298.15 K of the compound were derived from these experimental results. In

TABLE-8
SMOOTHED HEAT CAPACITIES AND THERMODYNAMIC
FUNCTIONS OF 2-AMINOPYRIDINE

T (K)	$C_{p,m}$ (J K ⁻¹ mol ⁻¹)	$H_T-H_{298.15}$ (kJ mol ⁻¹)	$S_T-S_{298.15}$ (J K ⁻¹ mol ⁻¹)	$G_T-G_{298.15}$ (kJ mol ⁻¹)
80.00	58.149	-21.10	-115.9	-11.83
85.00	59.684	-20.80	-112.3	-11.26
90.00	61.305	-20.50	-108.9	-10.70
95.00	62.978	-20.19	-105.5	-10.17
100.00	64.675	-19.87	-102.2	-9.647
105.00	66.377	-19.54	-99.01	-9.142
110.00	68.069	-19.20	-95.89	-8.653
115.00	69.742	-18.86	-92.83	-8.180
120.00	71.393	-18.50	-89.83	-7.723
125.00	73.022	-18.14	-86.88	-7.281
130.00	74.630	-17.77	-83.99	-6.855
135.00	76.223	-17.40	-81.15	-6.443
140.00	77.807	-17.01	-78.35	-6.046
145.00	79.390	-16.62	-75.59	-5.663
150.00	80.980	-16.22	-72.87	-5.293
155.00	82.586	-15.82	-70.19	-4.937
160.00	84.215	-15.40	-67.54	-4.594
165.00	85.874	-14.98	-64.92	-4.264
170.00	87.571	-14.54	-62.33	-3.947
175.00	89.310	-14.10	-59.76	-3.642
180.00	91.096	-13.65	-57.22	-3.349
185.00	92.930	-13.19	-54.70	-3.068
190.00	94.815	-12.72	-52.19	-2.800
195.00	96.748	-12.24	-49.71	-2.543
200.00	98.728	-11.75	-47.23	-2.299
205.00	100.75	-11.25	-44.77	-2.068
210.00	102.82	-10.74	-42.32	-1.848
215.00	104.91	-10.21	-39.88	-1.641
220.00	107.03	-9.684	-37.44	-1.446
225.00	109.18	-9.143	-35.02	-1.264
230.00	111.33	-8.592	-32.60	-1.095
235.00	113.49	-8.031	-30.18	-0.9381
240.00	115.65	-7.459	-27.77	-0.7940
245.00	117.81	-6.876	-25.36	-0.6625
250.00	119.96	-6.283	-22.96	-0.5435
255.00	122.11	-5.680	-20.56	-0.4367
260.00	124.25	-5.066	-18.17	-0.3421
265.00	126.40	-4.441	-15.78	-0.2593
270.00	128.57	-3.804	-13.39	-0.1881
275.00	130.78	-3.157	-11.01	-0.1283
280.00	133.05	-2.497	-8.634	-0.07967
285.00	135.42	-1.825	-6.258	-0.04199
290.00	137.93	-1.141	-3.881	-0.01528
295.00	140.63	-0.4428	-1.502	0.0003155
298.15	142.47	0	0	0
300.00	143.60	0.2695	0.8839	0.004383
305.00	146.89	0.9972	3.282	-0.00383
310.00	150.61	1.741	5.699	-0.02551
315.00	Phase change			
320.00	Phase change			
325.00	Phase change			
330.00	Phase change			
335.00	Phase change			
340.00	215.17	21.69	66.22	-0.8215
345.00	216.39	22.77	69.37	-1.160
350.00	217.59	23.86	72.49	-1.515
355.00	218.78	24.95	75.59	-1.885
360.00	219.97	26.04	78.65	-2.271
365.00	221.13	27.15	81.70	-2.672
370.00	222.28	28.26	84.71	-3.088

addition, the melting temperatures of the absolutely pure and the given sample were calculated from the theoretical analysis of the purity and fractional melting method.

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