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Crystal Structure and Thermodynamic Properties of *N, N*-dimethylnorephedrine Hydrochloride ($C_{11}H_{18}NOCl$) (s)

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Abstract

Crystal structure of *N, N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (s) has been determined by an X-ray crystallography. The compound is orthorhombic $P2_12_12_1$. Unit cell parameters are a = 7.2486(19) Å, b = 9.674(3) Å, c = 16.952(5) Å; $\alpha = 90°$, $\beta = 90°$, $\gamma = 90°$, and $Z = 4$. Low-temperature heat capacities of the compound were measured by a precision automated adiabatic calorimeter over the temperature range from 80 to 390 K. A polynomial equation of heat capacities as a function of the temperature in the region of 80–390 K was fitted by least square method. Based on the fitted polynomial equation, the smoothed heat capacities and thermodynamic functions of the compound relative to the standard reference temperature 298.15 K were calculated with 5 K step. In addition, DSC technique was used to determine the melting process of the compound.

Keywords: *N*, *N*-dimethylnorephedrine hydrochloride; X-ray crystallography; adiabatic calorimetry; low-temperature heat capacity; thermodynamic function

1. Introduction

N, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$)(s) (CAS and EINECS registry numbers are 18760-80-0 and 242-557-4, respectively) is an important intermediate in medicine industry, which is often used to prepare a drug to treat the asthma.[1] The asthma is a common disease especially for weaker and older people, which makes it necessary for manufacturing some efficacious medicines treating the illness. 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.[2,3] However, crystal structure and thermodynamic properties of the title compound have not been reported in the literature. These results are instructive and urgently needed in order to develop its new application fields, to improve the techniques of chemical synthesis in which it participates, and carry out relevant theoretical research.[4] For these purposes, in the present work, crystal structure of the substance has been determined by an X-ray crystallography, low-temperature heat capacities were measured by a precision automated adiabatic calorimeter over the temperature range from 80 to 390 K, and the melting process was tested by DSC technique.

2. Experimental

2. 1. Sample

The sample used in the measurements of X-ray crystallography and calorimetric experiments was commercially purchased from Neimenggu pharmaceutical factory (China). The content of the chloride in the compound was

determined by chemical analysis. Elemental analyses (C, H and N) were carried out on a Vario EL III CHNOS instrument made in Germany. These results showed that purity of the sample was higher than 99.6%. A micro melting point device was used for measuring the melting point of the substance, and DSC technique was applied to measure the onset point, peak temperature, and enthalpy of melting process.

2. 2. X-ray Crystallography

All diffraction data for the compound were collected on a Bruker Smart-1000 CCD area – detector diffractometer with graphite monochromated MoK_α radiation (λ = 0.71073) at 293(2) K using the program SMART and processed by SAINT-plus.[5] Absorption corrections were applied by SADABS. The structure was solved by direct methods and refined with full-matrix least-squares technique using SHELXTL. All non-hydrogen atoms were refined anisotropically. All H-atoms were located theoretically and refined. The structural plots were drawn using the SHELXTL and OLEX programs.

2. 3. Adiabatic Calorimetry

A fully automatic adiabatic calorimeter is used to measure heat capacities over the temperature range 78 ≤ (T /K) ≤ 400. The calorimeter is established in the Thermochemistry Laboratory in the College of Chemistry and Chemical Engineering, Liaocheng University, China. The principle and structure of the adiabatic calorimeter are described in detail elsewhere.[6–8] 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) is applied to measure the temperature of the sample. The thermometer is 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 are 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 ≤ (T /K) ≤ 390. 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}. 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[9] over the whole temperature range.

Heat-capacity measurements are 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 are generally controlled at (0.1 to 0.4) K min^{-1} and (1 to 3) K. The heating duration is 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}) Kmin^{-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.[6] The sample mass used for calorimetric measurements was 3.3156 g, which was equivalent to 0.01537 mol in terms of its molar mass, M = 215.72 g mol^{-1}.

2. 4. Differential Scanning Calorimetry (DSC)

DSC analysis was carried out in a Perkin-Elmer diamond DSC. Sample with the mass of 4.67 mg was weighed in a closed pan, placed in the DSC cell, and heated at the rate of 5 K min^{-1} under the high-purity nitrogen with a flow rate of 30 mL min^{-1}.

3. Results and Discussion

3. 1. Structural Description

The molecular structure of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) is plotted in Figure 1. The dimensions of the crystal used for X-ray diffraction data collection are given in Table 1. It is found out from Table 1 that the crystal system of the compound is orthor-

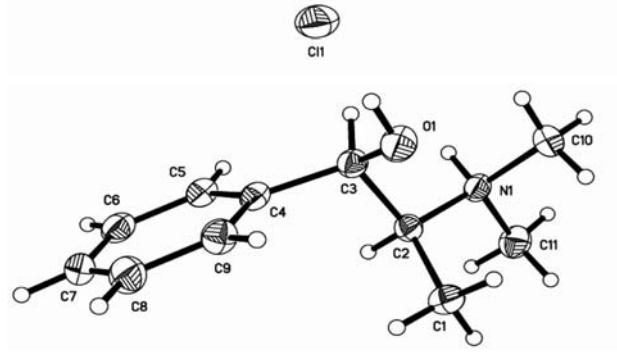

Figure 1. Structure of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (s)

hombic, the space group is $P2_12_12_1$, unit cell parameters are a = 7.2486(19) Å, b = 9.674(3) Å, c = 16.952(5) Å; α = 90°, β = 90°, γ = 90°, and Z = 4. Table 2 give non-hydrogen atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3). U (eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor, which is equal to thermal parameters relative to the structure of the compound. Selected bond lengths and angles are listed in Table 3. The geometries of the hydrogen bonding are listed in Table 4.

Table 1. Crystallographic data and structure refinement for the title compound

Crystallographic data	structure refinement
Empirical formula	$C_{11}H_{18}NOCl$
Formula weight	215.72
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
space group	$P2_12_12_1$
Unit cell dimensions	a = 7.2486(19) Å, b = 9.674(3) Å, c = 16.952(5) Å; α = 90°, β = 90°, γ = 90°
Volume	1188.7(5) Å^3
Z	4
Calculated density	1.205 mg/m^3
Absorption coefficient	0.292 mm^{-1}
F(000)	464
Crystal size	0.32 × 0.27 × 0.25 mm
θ range for data collection	2.40 to 25.00°
Limiting indices	–8 ≤ h ≤ 7, –11 ≤ k ≤ 11, –15 ≤ l ≤ 20
Reflections collected / unique	4940/2080 [R (int.) = 0.0220]
Completeness to theta = 25.00	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2080 / 0 / 131
Goodness-of-fit on F^2	0.996
Final R indices [I > 2 sigma (I)]	R_1=0.0318, wR_2 = 0.0797
R indices (all data)	R_1= 0.0389, wR_2 = 0.0848
Absolute structure parameter	–0.03(7)
Largest diff. peak and hole	0.115 and –0.196 e Å^{-3}

Table 2. Non-hydrogen atomic coordinates (×10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3)

Atoms	x	y	z	U (eq)
Cl(1)	–159(1)	3409(1)	1205(1)	51(1)
N(1)	3744(2)	6792(2)	3558(1)	37(1)
O(1)	2934(2)	5119(1)	2005(1)	49(1)
C(1)	6010(3)	6651(2)	2427(1)	45(1)
C(2)	4098(3)	7091(2)	2692(1)	35(1)
C(3)	2523(3)	6519(2)	2177(1)	37(1)
C(4)	2333(3)	7416(2)	1445(1)	35(1)
C(5)	1425(3)	8679(2)	1501(1)	40(1)
C(6)	1378(3)	9568(2)	854(1)	47(1)
C(7)	2223(3)	9201(2)	159(1)	52(1)
C(8)	3079(3)	7946(2)	95(1)	55(1)
C(9)	3134(3)	7050(2)	734(1)	45(1)
C(10)	3657(3)	5299(2)	3776(1)	51(1)
C(11)	5044(4)	7555(2)	4085(1)	51(1)

As shown in Figure 2, the symmetric unit consists of four N, N-dimethylnorephedrine chlorides. Two different kinds of hydrogen bonds N1-H1...Cl1 and O1-H1A...Cl1 exist in the packing structure of *N*, *N*-dimethylnorephedrine hydrochloride form a network structure. The bond distances of N1-C2(1.518 Å), N1-C10(1.492 Å), N1-C11 (1.494 Å), O1-C3(1.417 Å), N1-H1(0.910 Å), and O1-H1 A(0.820 Å) are shorter than the normal mean bond distances of N-C(1.52 Å), O-C(1.43 Å), N-H(1.04 Å) and O-H(0.96 Å), respectively. This can be ascribed to the formation of the intermolecular hydrogen bonds, which makes these chemical bonds involved in the formation of the hydrogen bonds slightly move towards the centralization of electron clouds, shortening of bond lengths and strengthening of bond energies.

Bond angle of O1-C3-C2 is 107.72° and deviates from regular tetrahedron angle 109.28°, which may also result from the forming of intermolecular hydrogen bonds. In addition, the bond length of C-C in the benzene ring of *N*, *N*-dimethylnorephedrine hydrochloride is slightly lower than that of normal value 1.396 Å in the regular benzene ring , the difference may be assigned to the benzene ring in the title compound placing in a distinctly different surroundings from a regular benzene ring and the influence of tertary ammonium ion, chloride ion and hydroxyl group with polarity on the whole molecule structure. These results reveal that interactions of hydrogen bonds between the molecules play a critical role in formation, stability and crystallization of the cluster.

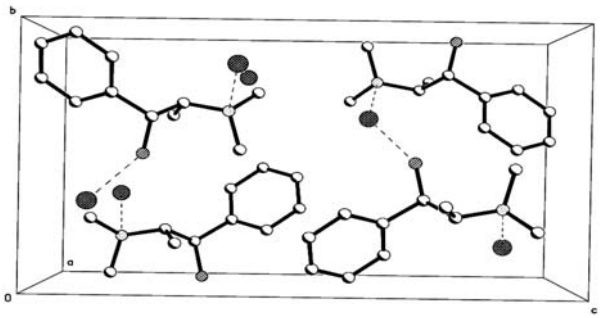

Figure 2. Packing of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (s) in unit cell

3. 2. Heat Capacity

All experimental results were listed in Table 5 and plotted in Figure 3. It can be seen from Figure 3 that the heat capacity curve was smooth and continuous in the temperature region from 80 to 390 K and no thermal anomaly appeared. Experimental molar heat capacities in the temperature region of 80–390 K were fitted by the least square method and a polynomial equation of heat ca-

Table 3. Bond lengths [Å] and angles [°]

N(1)-C(10)	1.492(2)	C(2)-H(2)	0.9800	C(8)-C(9)	1.388(3)
N(1)-C(11)	1.494(3)	C(3)-C(4)	1.519(3)	C(8)-H(8)	0.9300
N(1)-C(2)	1.518(2)	C(3)-H(3)	0.9800	C(9)-H(9)	0.9300
N(1)-H(1)	0.9100	C(4)-C(9)	1.385(3)	C(10)-H(10A)	0.9600
O(1)-C(3)	1.417(2)	C(4)-C(5)	1.390(3)	C(10)-H(10B)	0.9600
O(1)-H(1A)	0.8200	C(5)-C(6)	1.395(3)	C(10)-H(10C)	0.9600
C(1)-C(2)	1.518(3)	C(5)-H(5)	0.9300	C(11)-H(11A)	0.9600
C(1)-H(1B)	0.9600	C(6)-C(7)	1.375(3)	C(11)-H(11B)	0.9600
C(1)-H(1C)	0.9600	C(6)-H(6)	0.9300	C(11)-H(11C)	0.9600
C(1)-H(1D)	0.9600	C(7)-C(8)	1.368(3)		
C(2)-C(3)	1.540(3)	C(7)-H(7)	0.9300		
C(10)-N(1)-C(11)	110.87(16)	C(3)-C(2)-H(2)	106.2	C(7)-C(8)-C(9)	120.3(2)
C(10)-N(1)-C(2)	115.57(15)	O(1)-C(3)-C(4)	113.41(16)	C(7)-C(8)-H(8)	119.9
C(11)-N(1)-C(2)	112.20(15)	O(1)-C(3)-C(2)	107.72(15)	C(9)-C(8)-H(8)	119.9
C(10)-N(1)-H(1)	105.8	C(4)-C(3)-C(2)	108.93(15)	C(4)-C(9)-C(8)	120.6(2)
C(11)-N(1)-H(1)	105.8	O(1)-C(3)-H(3)	108.9	C(4)-C(9)-H(9)	119.7
C(2)-N(1)-H(1)	105.8	C(4)-C(3)-H(3)	108.9	C(8)-C(9)-H(9)	119.7
C(3)-O(1)-H(1A)	109.5	C(2)-C(3)-H(3)	108.9	N(1)-C(10)-H(10A)	109.5
C(2)-C(1)-H(1B)	109.5	C(9)-C(4)-C(5)	118.84(19)	N(1)-C(10)-H(10B)	109.5
C(2)-C(1)-H(1C)	109.5	C(9)-C(4)-C(3)	121.78(18)	H(10A)-C(10)-H(10B)	109.5
H(1B)-C(1)-H(1C)	109.5	C(5)-C(4)-C(3)	119.27(17)	N(1)-C(10)-H(10C)	109.5
C(2)-C(1)-H(1D)	109.5	C(4)-C(5)-C(6)	119.99(19)	H(10A)-C(10)-H(10C)	109.5
H(1B)-C(1)-H(1D)	109.5	C(4)-C(5)-H(5)	120.0	H(10B)-C(10)-H(10C)	109.5
H(1C)-C(1)-H(1D)	109.5	C(6)-C(5)-H(5)	120.0	N(1)-C(11)-H(11A)	109.5
C(1)-C(2)-N(1)	112.74(16)	C(7)-C(6)-C(5)	120.2(2)	N(1)-C(11)-H(11B)	109.5
C(1)-C(2)-C(3)	114.09(16)	C(7)-C(6)-H(6)	119.9	H(11A)-C(11)-H(11B)	109.5
N(1)-C(2)-C(3)	110.75(16)	C(5)-C(6)-H(6)	119.9	N(1)-C(11)-H(11C)	109.5
C(1)-C(2)-H(2)	106.2	C(8)-C(7)-C(6)	120.0(2)	H(11A)-C(11)-H(11C)	109.5
N(1)-C(2)-H(2)	106.2	C(8)-C(7)-H(7)	120.0	H(11B)-C(11)-H(11C)	109.5

Table 4. Hydrogen bonding data [Å.and deg.]

D–H	d(D–H)/Å	d(H···A)/Å	<DHA/deg.	d(D···A)/Å	A
N1–H1	0.910	2.167	166.59	3.060	Cl1[x, y + 1/2, z + 1/2]
O1–H1A	0.820	2.289	169.63	3.099	Cl1

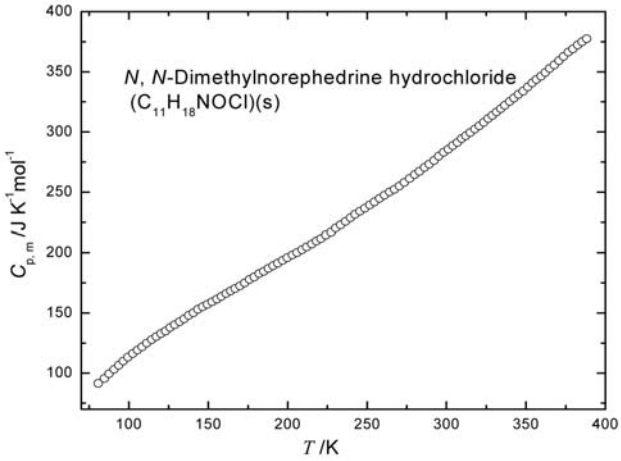

Figure 3. Experimental molar heat capacity curve of the title compound with the temperature (K)

pacities versus the reduced temperature(x) has been obtained as follows:

$$C_{p,\mathrm{m}} = 224.289 + 129.719\,x + 27.966\,x^2 + \\ + 14.412\,x^3 - 16.837\,x^4 \qquad (1)$$

in which R-Square (COD) = 0.99998, x was the reduced temperature, and $x = (T - 235) / 155$. The relative deviations of the smoothed heat capacities obtained by the above equation from the experimental heat capacities were within 0.30% except for several points around the lower and upper temperature limits.

3. 3. Thermodynamic Functions of the Compound

The smoothed molar heat capacities and thermodynamic functions of *N, N*-dimethylnorephedrine hy-

Table 5. Experimental molar heat capacities of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (M = 215.72 gmol^{-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})
80.68	91.35	184.89	184.60	292.15	276.31
84.57	95.63	187.83	187.09	295.09	279.80
87.52	99.54	190.76	189.27	298.17	283.08
90.69	103.22	193.70	191.34	301.10	285.59
93.59	106.60	196.78	193.83	303.89	288.65
96.46	110.06	199.71	195.91	306.83	291.27
99.41	113.26	202.94	198.29	309.47	294.43
102.44	116.23	205.87	200.16	312.11	296.83
105.38	119.14	208.96	202.54	314.90	299.45
108.27	121.87	211.89	204.93	317.83	302.29
111.23	124.95	215.12	207.21	320.62	305.02
114.27	127.86	218.05	209.70	323.41	307.97
117.25	130.42	220.84	211.77	326.19	311.14
120.17	132.84	224.07	214.57	328.84	313.76
123.05	135.11	227.30	217.06	331.48	316.59
125.91	137.91	230.23	220.20	334.12	319.21
128.84	140.25	233.31	222.71	336.76	322.27
131.87	142.70	236.39	225.55	339.69	325.33
134.70	145.05	239.48	228.71	342.48	328.17
137.71	147.97	242.41	231.55	345.27	331.22
140.58	150.17	245.49	234.06	348.20	333.89
143.37	152.97	248.57	236.57	351.14	337.31
146.45	155.15	251.65	239.30	353.93	340.74
149.38	157.22	254.59	241.92	356.57	343.62
152.32	159.40	257.82	244.65	359.47	346.38
155.40	161.47	260.90	247.49	362.14	349.39
158.19	163.86	264.13	250.11	364.97	352.74
161.27	166.25	267.21	252.29	367.81	355.72
164.06	168.42	270.29	255.02	370.81	359.21
166.84	170.29	273.37	257.97	373.64	362.80
169.92	172.47	276.75	261.25	376.65	366.29
172.86	175.01	279.97	264.63	379.65	369.00
175.94	177.96	282.91	267.25	382.48	372.23
178.88	179.93	286.14	270.42	385.32	375.02
181.96	182.74	289.07	273.25	388.32	377.56

drochloride were calculated based on a polynomial of the heat capacities as a function of the reduced temperature (x) according to the following thermodynamic equations:

$$(H_T\text{-}H_{298.15}) = \int_{298.15}^{T} C_p \mathrm{d}T \quad (2)$$

$$(S_T\text{-}S_{298.15}) = \int_{298.15}^{T} C_p \cdot T^{-1} \mathrm{d}T \quad (3)$$

$$(G_T\text{-}G_{298.15}) = \int_{298.15}^{T} C_p \mathrm{d}T - T \cdot \int_{298.15}^{T} C_p \cdot T^{-1} \mathrm{d}T \quad (4)$$

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 6 at the interval of 5 K.

3. 4. Results of DSC Analysis of the Compound

The onset point, peak temperature and molar enthalpy of the endothermic phase change were determined to be 464.63 K, 466.04 K and 34.223 kJmol^{-1}, respectively, by the analysis of DSC curve, as shown in Figure 4. The melting point of the compound was determined to be 464.7–465.7 K by the micro melting point device, which was in conformity with the results in literature,[1] so, the endothermic peak appearing in DSC curve is in correspondence with the melting process of the substance.

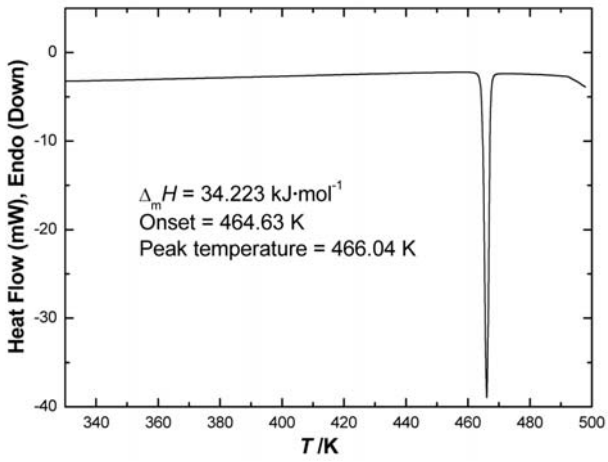

Figure 4. DSC curve of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (s)

4. Conclusions

The paper reported crystal structure and low temperature heat capacities measured by X-ray crystallography and adiabatic calorimetry. The data and geometries of the structure, the smoothed heat capacities and thermodynamic functions of the title compound were derived from these experimental results. In addition, the onset point, peak temperature and enthalpy of fusion of the compound have been measured by DSC technique.

5. Acknowledgements

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Table 6. Thermodynamic functions of *N*, *N*-dimethylnorephedrine hydrochloride ($C_{11}H_{18}NOCl$) (s) (M = 215.72 g mol^{-1})

T (K)	$C_{p,m}$ (J K^{-1} mol^{-1})	$(H_T - H_{298.15K})$ (kJ mol^{-1})	$(S_T - S_{298.15K})$ (J K^{-1} mol^{-1})	$(G_T - G_{298.15K})$ (kJ^{-1} mol^{-1})
80	91.30	–41.02	–221.7	–23.28
85	97.13	–40.54	–216.0	–22.19
90	102.73	–40.04	–210.2	–21.12
95	108.12	–39.52	–204.5	–20.09
100	113.32	–38.96	–198.9	–19.07
105	118.34	–38.38	–193.3	–18.09
110	123.19	–37.78	–187.7	–17.14
115	127.89	–37.15	–182.1	–16.21
120	132.46	–36.50	–176.6	–15.31
125	136.90	–35.83	–171.1	–14.44
130	141.23	–35.13	–165.7	–13.60
135	145.46	–34.42	–160.3	–12.78
140	149.60	–33.68	–154.9	–11.99
145	153.67	–32.92	–149.6	–11.23
150	157.67	–32.14	–144.3	–10.50
155	161.62	–31.34	–139.1	–9.789
160	165.52	–30.53	–133.9	–9.109
165	169.39	–29.69	–128.7	–8.454
170	173.23	–28.83	–123.6	–7.826
175	177.06	–27.96	–118.5	–7.224
180	180.87	–27.06	–113.4	–6.647
185	184.69	–26.15	–108.4	–6.095
190	188.52	–25.22	–103.4	–5.568
195	192.36	–24.26	–98.45	–5.066
200	196.22	–23.29	–93.52	–4.589
205	200.10	–22.30	–88.61	–4.135
210	204.02	–21.29	–83.74	–3.706
215	207.98	–20.26	–78.88	–3.301
220	211.98	–19.21	–74.05	–2.919
225	216.03	–18.14	–69.24	–2.561
230	220.13	–17.05	–64.45	–2.227
235	224.29	–15.94	–59.68	–1.916
240	228.50	–14.81	–54.92	–1.628
245	232.78	–13.65	–50.17	–1.363
250	237.12	–12.48	–45.43	–1.122
255	241.52	–11.28	–40.70	–0.9040
260	245.99	–10.06	–35.98	–0.7094

T (K)	$C_{p,m}$ (J K^{-1} mol^{-1})	$(H_T - H_{298.15}$ K) (kJ^{-1} mol^{-1})	$(S_T - S_{298.15}$ K) (J K^{-1} mol^{-1})	$(GT - G_{298.15}$ K) (kJ^{-1} mol^{-1})
265	250.52	–8.823	–31.26	–0.5381
270	255.13	–7.559	–26.55	–0.3902
275	259.80	–6.272	–21.84	–0.2659
280	264.54	–4.961	–17.13	–0.1652
285	269.34	–3.626	–12.41	–0.0882
290	274.22	–2.268	–7.698	–0.0351
295	279.15	–0.8842	–2.977	–0.0060
298.15	282.29	0	0	0
300	284.14	0.5239	1.750	–0.0010
305	289.20	1.957	6.483	–0.0202
310	294.31	3.416	11.22	–0.0637
315	299.47	4.900	15.97	–0.1317
320	304.69	6.411	20.73	–0.2242
325	309.94	7.947	25.50	–0.3413
330	315.24	9.510	30.28	–0.4831
335	320.57	11.10	35.07	–0.6495
340	325.93	12.72	39.87	–0.8406
345	331.31	14.36	44.68	–1.056
350	336.70	16.03	49.50	–1.296
355	342.11	17.73	54.33	–1.560
360	347.52	19.45	59.16	–1.848
365	352.92	21.20	64.00	–2.160
370	358.31	22.98	68.85	–2.495
375	363.68	24.78	73.70	–2.853
380	369.01	26.62	78.55	–3.232
385	374.30	28.47	83.39	–3.634
390	379.54	30.36	88.24	–4.055

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Povzetek

Z rentgensko kristalografijo smo določili kristalno strukturo spojine *N, N* - dimetilnorefedrin hidroklorid ($C_{11}H_{18}NOCl$) (s). Snov kristalizira v ortorombski obliki $P2_12_12_1$ z naslednjimi dimenzijami osnovne celice: a = 7.2486(19) Å, b = 9.674(3) Å, c = 16.952(5) Å; $\alpha = 90$, $\beta = 90$, $\gamma = 90$, in $Z = 4$. Z adiabatnim kalorimetrom smo v temperaturnem območju med 80 in 390 K izmerili toplotne kapacitete te spojine. Ugotovili smo, da je toplotna kapaciteta v tem območju odvisna od temperature in odvisnost lahko ponazorimo s polinomom. Z metodo DSC smo proučevali tudi taljenje spojin.