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Thermodynamics of the thallium alkanoates. IX. Thermodynamics of thallium(I) *n*-octanoate from temperatures of 6 to 490 K [☆]

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Abstract

The heat capacity of thallium(I) *n*-octanoate has been measured from 5 to 350 K by equilibrium adiabatic calorimetry and, taken together with DSC data determined earlier by a subset of the present authors, represents the thermodynamic behaviour in the liquid phase at about 500 K. Transitions occur at 269.8, 290.0, and 293.5 K, melting at 411 K, and clearing at 495 K. Except for a small $\Delta_{trs}S^\circ_m$, the lowest temperature (269.2 K) phase transition (crystal IV/crystal III) has $\Delta_{trs}S^\circ = 0.62R$, the higher temperature transitions (approx. 293.5 and 290 K) have $\Delta_{trs}S^\circ_m$ values for III/II/I of $3.97R$ ((approximate partial resolution) III/II $\cong 1.7R$ and II/I $= 2.25R$), for crystal I/mesophase (411 K) of $1.66R$, and for mesophase/isotropic liquid (495 K) of $0.73R$.

Keywords: Entropy; Heat capacity; Melting; Thallium alkanoates; Thermophysics; Transition

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[☆] Dedicated to Hiroshi Suga on the Occasion of his 65th Birthday.

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1. Introduction

The initial incentive for the examination of the heat capacity morphology of thallium(I) *n*-octanoate (Chemical Abstracts registry number [18993-50-5]), hereafter Tl8C, was occasioned by the observation that the total $\Sigma_i \Delta_{\mathrm{trs}} S^{\circ}_{\mathrm{m},i}$ from the DSC data was lower than the expected value in terms of the even-odd alternations existing at the time of the initiation of these studies [2]. That morphology was seen for other members of the series [1] and shows evidence of a non-cooperative energy effect taking place in a very wide temperature range as a "hump". Vibration spectroscopy (FTIR and Raman) study [3] enabled us to interpret this anomaly as due to the energy evolved in a trans–gauche conformational transition of the $-CH_2-$ groups. With the aid of these studies and a comparison of the adiabatic data together with the DSC values [4] garnered here, it was possible to give an interpretation of the step-wise melting process from the ordered crystal at very low temperatures to the isotropic liquid, for all the members of the series [5].

2. Experimental

Tl(I) octanoate was obtained by the method already reported elsewhere [11], by using Tl(I) carbonate in slight excess over the *n*-octanoic acid to prevent contamination of octanoate with the corresponding acid-salt molecular complex [6]. Essentially, *n*-octanoic acid (Fluka puriss, > 99.5% pure by GC) and Tl_2CO_3 (Fluka puriss, > 99% purity) were dissolved in dry methanol and brought to reflux with stirring. After a reaction time of two hours, the ethyl-ether-precipitated thallium(I) *n*-octanoate was filtered, crystallized twice in ethanol, and vacuum-dried at room temperature. Its purity was then assessed by the usual DSC method [7].

A Perkin-Elmer DSC-2C with a 3700 Data Acquisition System, provided with an Intracooler II accessory for subambient temperature was used in the temperature range 250–500 K. The temperature response was calibrated by the melting points of high-purity standard chemicals (*n*-undecane, *n*-tridecane, and *n*-pentadecane, and lauric, stearic, and benzoic acids, as well as indium and tin). The calibration constant for energy was obtained by the melting enthalpy of high-purity indium (> 99.999 mol% pure).

The purity of the alkanoate was determined on three samples, weighing around 5 mg (± 0.002, by an electronic Perkin-Elmer AD-4 microbalance) by employing a low heating rate of 0.3 K min^{-1}. The mean value was 99.76 mol%.

Enthalpy increment determinations were carried out on six 15 mg samples scanned at a 10 K min^{-1} heating rate.

Heat capacity measurements were also made on several samples of about 15–20 mg at 10 K min^{-1} heating rate between 300 and 500 K, by successive determinations of about 30 K each, overlapping with each other in order to minimize baseline uncertainties.

Solid pans were normally used except for the high-temperature region where the sample was encapsulated in hermetically sealed pans to minimize thermal decomposition of the samples.

Temperature, enthalpy and heat capacity values ascertained by the DSC method are estimated to have standard deviations ± 0.5 K, 2% and 3%, respectively, The calorimetric measurements were made in the Mark XIII cryostat described previously [8]. This calorimeter uses intermittent-heating adiabatic equilibrium methods. The programming, data logging, and calorimetry were done by automated computerization described elsewhere [9]. All measurements of mass, time, resistance, etc., were referred to calibrations of the U.S. National Bureau of Standards (formerly NBS, currently NIST). The sample loaded into the gold-plated OFHC copper calorimeter W-62 had a mass of 42.9304 g, which corresponds to an amount-of-substance factor of 8.0965 samples mol^{-1}, on the basis of the 1992 IUPAC relative atomic masses. The molar mass was 347.5892 g mol^{-1}. The buoyancy corrections were calculated on the assumed density of 3.5 g cm^{-3}. No crystallographic information is available for this compound nor for adjacent members of the homologous series. The closest member of the series for which the density is available is that of thallium acetate which has a density of 3.6 g cm^{-3}. Following evacuation, 2.6 kPa of purified helium was added to the calorimeter to enhance thermal equilibration; the calorimeter was then sealed via a screw cap which pressed a gold gasket against the circular knife edge on the stainless-steel neck of the calorimeter. The calorimeter was sealed within the vacuum chamber by a remotely operating hexagonal wrench.

The thermal history of the thallium *n*-octanoate sample is shown by the linear array below, (solid arrows indicate cooling and dashed arrows indicate data acquisition ranges for various series)

$$310\,\mathrm{K} \xrightarrow{21\,\mathrm{h}} 92\,\mathrm{K} \underset{\text{Series I}}{\overset{15\,\mathrm{h}}{\dashrightarrow}} 300\,\mathrm{K} \xrightarrow{17\,\mathrm{h}} 240\,\mathrm{K} \underset{\text{Series II}}{\overset{31\,\mathrm{h}}{\dashrightarrow}} 350\,\mathrm{K}$$

$$\xrightarrow{7\,\mathrm{h}} 130\,\mathrm{K} \underset{\text{Series III}}{\overset{24\,\mathrm{h}}{\dashrightarrow}} 350\,\mathrm{K} \xrightarrow{12\,\mathrm{h}} 190\,\mathrm{K} \underset{\text{Series IV}}{\overset{4\,\mathrm{h}}{\dashrightarrow}} 310\,\mathrm{K}$$

$$\xrightarrow{2\,\mathrm{h}} 233\,\mathrm{K} \underset{\text{Series V}}{\overset{4\,\mathrm{h}}{\dashrightarrow}} 303\,\mathrm{K} \xrightarrow{23\,\mathrm{h}} 5\,\mathrm{K} \underset{\text{Series IV}}{\overset{19\,\mathrm{h}}{\dashrightarrow}} 127\,\mathrm{K}$$

$$\xrightarrow{3\,\mathrm{h}} 260\,\mathrm{K} \underset{\text{Series VII}}{\overset{27\,\mathrm{h}}{\dashrightarrow}} 340\,\mathrm{K} \xrightarrow{18\,\mathrm{h}} 155\,\mathrm{K} \underset{\text{Series VIII}}{\overset{18\,\mathrm{h}}{\dashrightarrow}} 300\,\mathrm{K}$$

The values of C_p measured have a standard deviation varying from 6% at 6 K to 0.5% at 10 K, and 0.12% above this temperature to 350 K. The values of the smoothed integrated thermophysical properties are more reliable and have a standard deviation of 0.10% above 100 K.

The heat capacity of the sample varied between 59 and 68% of the total (sample + calorimeter + heater + thermometer) over the measurement range of the adiabatic calorimeter, except, of course, in the transition regions. The precision indices (standard deviations) are about 2–5% below 12 K and diminish to 0.2% above about 30 K.

3. Results

The experimental molar heat capacity data taken by equilibrium adiabatic calorimetry are presented in Table 1 and the morphology of the heat capacity curves

Table 1

Experimental molar heat capacity of thallium octanoate ($R = 8.31451$ J K^{-1} mol^{-1})

T/K	$C_{p,m}/R$	T/K	$C_{p,m}/R$	T/K	$C_{p,m}/R$	T/K	$C_{p,m}/R$	T/K	$C_{p,m}/R$	T/K	$C_{p,m}/R$
Series I		Series II		161.52	21.37	293.59	300	20.36	3.204	280.55	37.70
98.09	15.861	257.26	32.62	167.06	22.00	293.82	132	22.08	3.580	282.51	39.54
100.69	16.27	262.78	33.14	172.50	22.37	294.41	53.7	23.83	4.019	284.46	40.84
105.68	16.62	266.66	35.44	177.86	22.83	295.36	56.8	25.61	4.440	286.14	40.10
110.80	17.17	268.58	37.98	183.12	23.48	296.36	50.4	27.35	4.976	287.54	69.1
116.05	17.69	274.14	36.25	188.31	23.77	300.66	38.94	29.11	5.181	288.66	89
121.51	18.201	281.98	38.27	193.43	24.12	305.93	37.30	31.05	5.735	289.41	175
127.02	18.70	283.83	38.63	198.14	24.88	326.87	36.27	33.15	5.824	289.82	260
132.49	19.24	285.39	60.6	202.43	25.27	332.04	36.26	35.21	6.900	290.04	185
137.83	19.67	288.55	76.7	206.69	25.97	337.22	36.09	37.32	7.114	290.25	160
143.06	19.97	289.39	159.3	210.89	26.43	347.57	36.20	39.46	7.541	290.50	130
148.21	20.44	289.82	304	219.06	27.16			41.59	7.853	290.99	57.5
153.61	20.84	290.05	308	224.17	27.67	Series IV		43.73	8.352	291.49	66.5
159.27	21.27	290.65	87.6			216.70	26.87	45.86	8.717	292.13	41.92
164.84	21.88	291.94	53.2	230.22	28.84	251.48	32.48	48.21	9.168	293.43	1180
170.32	22.19	293.06	120	236.12	29.57	269.80	40.79	50.78	9.421	293.74	350
175.72	22.54	293.39	272	241.92	31.00	278.01	38.78	53.14	9.977	295.40	51.1
181.04	23.15	293.50	620	247.57	31.77	285.46	44.18	55.78	10.380	297.84	51.1
186.27	23.61	293.52	1190	253.10	32.85	292.81	107.38	58.58	10.956	299.89	40.5
191.50	24.08	293.56	390	258.49	34.49	300.11	42.64	61.72	11.407	312.33	36.42
196.73	24.62	293.60	510	262.40	32.54			65.36	11.890	314.45	36.330
201.19	25.10	293.76	150	264.84	35.82	Series V		68.02	12.348	316.54	36.595
205.61	25.75	294.32	58.9	267.22	35.61	249.98	31.78	71.44	12.767	318.65	36.464
210.67	26.32	295.33	44.0	269.43	42.50	268.12	37.46	75.13	13.651	331.34	36.225
215.68	26.59	296.37	44.40	271.56	39.78	276.05	38.2	78.76	13.767		
220.79	27.30	297.40	44.42	273.79	37.81	283.37	45.4	82.44	14.233	Series VIII	
225.97	27.95	300.80	39.03	278.29	38.94	291.06	110	86.41	14.538	194.98	24.05
231.06	28.59	306.32	36.93	280.57	36.92	300.06	39.26	90.55	15.14	201.27	24.99
236.06	30.04	311.62	36.64	282.79	40.54			94.76	15.63	207.40	25.80
241.04	30.82	316.86	36.59	284.88	42.10	Series VI		98.98	16.23	213.43	26.31

245.99	31.65	322.05	36.22	286.64	56.77	5.61	0.248	103.63	16.42	219.34	27.26
251.21	32.51	327.17	36.44	288.02	85.6	6.71	0.355	108.68	17.04	225.13	27.92
256.65	32.82	332.38	36.04	289.06	116	7.85	0.519	113.72	17.55	230.78	29.08
262.00	34.21	337.58	36.11	289.65	270	9.05	0.698	118.78	17.90	236.31	29.91
267.10	38.54	342.59	36.37	290.07	125	10.30	0.912	123.84	18.40	241.74	30.43
271.98	38.96	347.73	36.26	290.83	98.8	11.62	1.190			247.07	31.69
277.47	37.90			292.04	52.40	13.01	1.452	Series VIII		252.27	32.68
283.38	43.08	Series II		293.11	150	14.48	1.704	264.17	34.33	257.35	33.98
287.48	113	138.37	19.51	293.42	660	15.93	2.105	268.41	39.87	262.37	33.58
290.18	221	144.32	20.31	293.46	590	17.42	2.371	270.37	40.19	267.18	38.49
292.21	119	150.15	20.62	293.47	510	17.15	2.408	271.68	42.00	271.71	39.23
296.65	88	155.88	21.02	293.52	460	18.77	2.731	276.43	37.65	276.29	37.07
								278.50	36.97	280.89	39.14

Table 2
DSC determined heat capacities for thallium(I) *n*-octanoate ($R = 8.31451\ \mathrm{J\,K^{-1}\,mol^{-1}}$)

T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$	T/K	$C_{p,\mathrm{m}}/R$
Crystal I		330	35.0	355	36.2	380	37.3	Mesophase		470	52.4
305	35.4	335	35.1	360	36.4	385	37.5	430	48.4	480	53.1
310	35.3	340	35.3	365	36.6	390	37.7	440	49.5	490	54.1
315	35.0	345	35.8	370	36.9	395	38.0	450	50.3		
320	34.9	350	36.0	375	37.0	400	38.2	460	51.2	Isotropic liquid	
325	34.9										

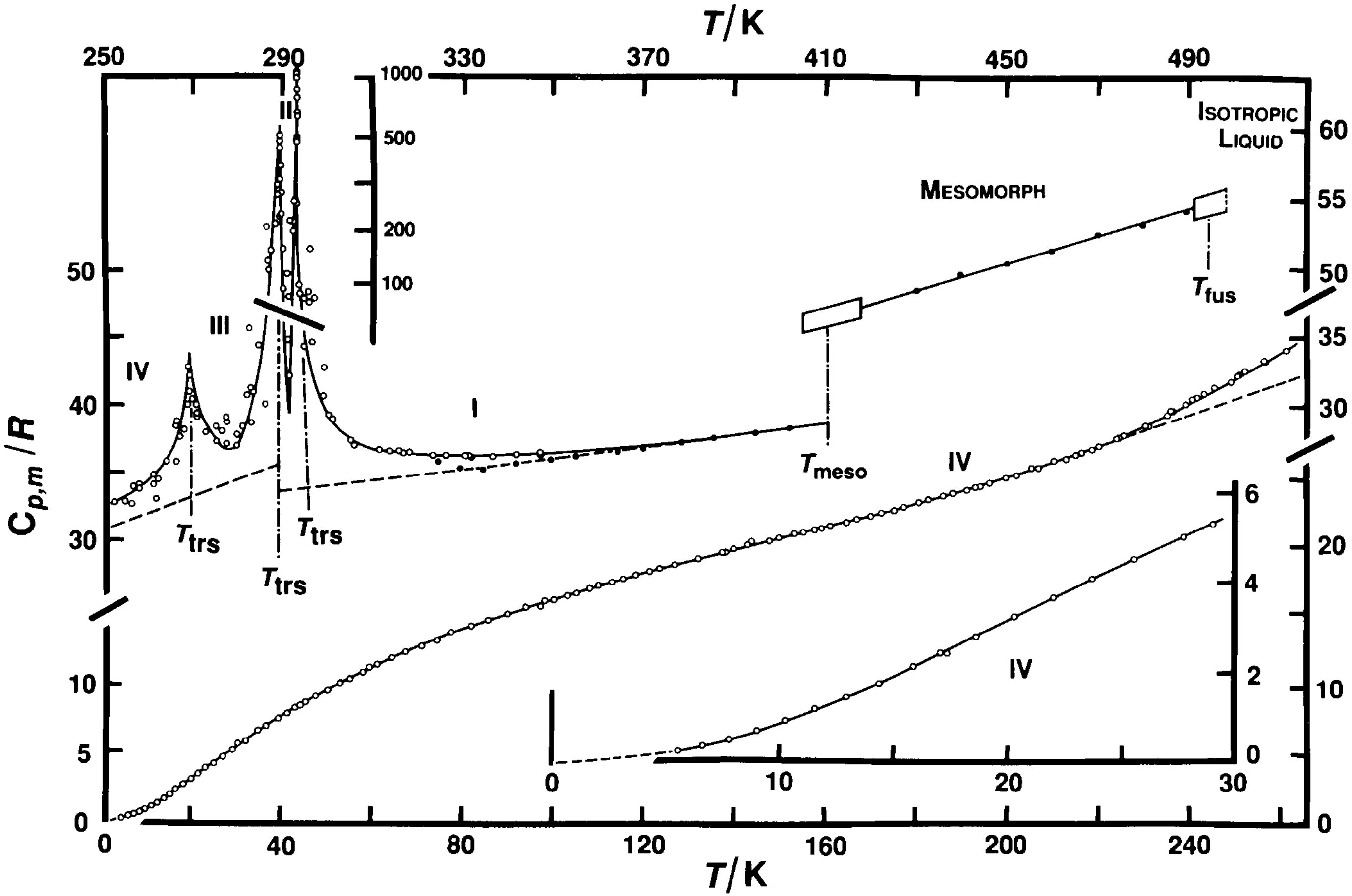

Fig. 1. Composite representation of the heat capacity of $TlO_2C_8H_{15}$ (Tl8C); this work plus $\Delta_{trs}H_m^\circ$ at higher temperatures by DSC [4].

with the transitions are shown in Fig. 1. Heat capacities determined by differential scanning calorimetry (DSC) are compiled in Table 2. The transitional behaviour determined by this technique by a subset of the present authors [4] is summarized in Table 3 together with other literature values mainly on the transition temperatures associated with the thermotropic mesophase.

Table 3
Experimental molar transition enthalpy determinations for thallium(I) octanoate ($R = 8.31451$ J K^{-1} mol^{-1})

N[a]	n[b]	T_i/K	T_f/K	T_{trs}/K	$\Delta_{260K}^{280K}H_m{}^c/(R\,K)$	$\Delta_{trs}H_m{}^d/(R\,K)$
For transition IV/III by adiabatic calorimetry						
I	3	259.35	274.34	269.8 ± 0.2	$738.8 \pm {}^e$	144.9
II	7	260.06	275.15		710.7^e	116.9
III	6	261.14	274.92		739.6	145.7
IV	2	268.39	271.19		739.8	145.9
V	2	266.50	269.72		739.9	146.1
VII	7	260.83	275.40		739.9	146.1
VIII	3	259.85	273.98		739.8	145.9
		Mean value =			739.8 ± 0.1	166.8 ± 0.2
		Graphical =			740	167
		$\Delta_{trs}S_m/R = 0.062 \pm 0.01$				
For transition III/I by adiabatic calorimetry						
					$\Delta_{280K}^{315K}H_m{}^c/(R\,K)$	
I	4	274.38	299.92	290.0 ± 0.04	2315.9	1147.8
II	13	275.15	314.23	and	2317.2	1149.2
III	26	274.92	313.79	293.47 ± 0.05	2319.7	1151.5
V	24	269.70	302.50		2317.1	1149.1
VII	30	275.39	309.15		2317.8	1149.8
		Mean value =			2317 ± 1	1154 ± 2
		Graphical =			2320	1154
		$\Delta_{trs}S_m/R = 3.97 \pm 0.01$				
For transition III/II by adiabatic calorimetry						
					$\Delta_{280K}^{292K}H_m^{0\,c}/(R\,K)$	
I	7	274.38	290.90	290.0 ± 0.4	924.0	593.7
II	27	275.15	292.67		924.4	594.1
III	9	274.92	291.27		923.9	593.6
VII	15	275.39	291.75		925.0	594.7
		Mean value =			924 ± 0.4	493 ± 2
		Graphical =			926	495
		$\Delta_{trs}S_m/R = 1.70 \pm 0.3$				
For transition II/I by adiabatic calorimetry[f]						
					$\Delta_{292K}^{315K}H_m^{0\,c}/(R\,K)$	
				293.47 ± 0.05		

Table 3 *(continued)*

N [a]	n [b]	T_i/K	T_f/K	T_{trs}/K	$\Delta_{260K}^{280K}H_m$ [c]/(R K)	$\Delta_{trs}H_m$ [d]/(R K)
By the difference between the III/I and III/II integration (see text) we obtain:						
	Mean value =				1393 ± 1	661 ± 2
	Graphical =				1394	663
	$\Delta_{trs}S_m/R = 2.25$					

Transition thermodynamics by DSC [4]; mean values from 6 determinations of each

Transition designation	T_{trs}/K	$\Delta_{trs}H_m^0$ [c]/(R K)	$\Delta_{trs}S_m^0/R$
Crystals IV → III	268.7 ± 0.4	20 ± 10	0.07 ± 0.04
Crystals III → II	290.0 ± 0.4	455 ± 30	1.57 ± 0.11
Crystals II → I	294.3 ± 0.4	260 ± 20	0.88 ± 0.07
Crystal I → mesophase	411.0 ± 0.5	682 ± 30	1.66 ± 0.08
Mesophase → isotrop. liq.	494.7 ± 0.8	360 ± 20	0.73 ± 0.04

Transitions reported in the literature

Transition designation	T_{trs}/K	$\Delta_{trs}H_m^0$/(R K)	$\Delta_{trs}S_m^o$/(R K)	Method	Ref.
"1st fusion"	408–409			Micr.	[10]
"2nd fusion"	493			Micr. [e]	[10]
Solid → neat	411			Micr.	[11]
Neat → isotropic	495			Micr.	[11]
Fusion	408.9			Micr.	[12]
Clearing	495.7			Micr.	[12]
Solid → mesophase	403	565	1.40	DTA [f]	[13]
Mesophase → isotrop. liq.	494	325	0.66	DTA	[13]

[a] Adiabatic series designation.

[b] Number of heating increments.

[c] $\Delta_{T_i}^{T_f}H_m$ is the molar energy input from the initial temperature T_i to the final temperature T_f adjusted to span the rounded temperature T_1 to T_2 and for quasi-adiabatic drift.

[d] $\Delta_{trs}H_m^0$ is the net molar enthalpy increment of transition relative to the selected lattice curve.

[e] Not included in mean value.

[f] By difference III/I – III/II transition.

Despite their close proximity, transitions III/II and II/I were resolved somewhat arbitrarily into the two components, but it is emphasized that the $\Sigma\Delta_{trs}S_m^o$ over both transitions has been measured far more accurately with respect to $\Delta_{trs}H_m^0$; slightly more uncertainty resides in $\Delta_{trs}S_m^o$ because of the temperature dependence. Differences between adiabatic calorimetry and differential scanning calorimetry values for the standard molar enthalpy and, consequently, the entropy of the transition are occasioned by the "straight baseline" method followed for DSC trace integration, which does not reproduce the lattice heat capacity assignment utilized on adiabatic calorimetry data.

Table 4 lists the smoothed values of the measured heat capacity at selected (rounded) temperatures and the derived thermodynamic properties deduced by integration of the

Table 4
Smoothed heat capacities and derived thermodynamic functions for thallium(I) *n*-octanoate at selected temperatures ($R = 8.31451\ \mathrm{J\,K^{-1}\,mol^{-1}}$)^{a}

T/K	$C_{p,\mathrm{m}}/R$	$S^{\mathrm{o}}_{\mathrm{m}}$-$S^{\mathrm{o}}_{\mathrm{m}}(0\ \mathrm{K})/R$	$H^{\mathrm{o}}_{\mathrm{m}}$-$H^{\mathrm{o}}_{\mathrm{m}}(0\ \mathrm{K})/(R\ \mathrm{K})$	$\Phi^{\mathrm{o}}_{\mathrm{m}}/R$
Crystal IV				
0	0	0	0	0
5	(0.162)	(0.057)	(0.213)	(0.015)
10	0.883	0.364	2.629	0.101
15	1.861	0.903	9.438	0.273
20	3.059	1.595	21.614	0.514
25	4.341	2.419	40.197	0.811
30	5.457	3.308	64.66	1.153
35	6.792	4.249	95.29	1.527
40	7.549	5.212	131.38	1.928
45	8.597	6.163	171.78	2.345
50	9.532	7.117	217.12	2.775
60	11.056	8.994	320.31	3.656
70	12.455	10.804	437.87	4.548
80	13.847	12.558	569.4	5.440
90	15.16	14.266	714.6	6.327
100	16.31	15.92	872.1	7.204
110	17.24	17.52	1040.0	8.070
120	17.99	19.06	1216.3	8.924
130	18.83	20.53	1400.4	9.761
140	19.65	21.96	1592.8	10.581
150	20.45	23.34	1793.4	11.386
160	21.26	24.69	2001.9	12.176
170	22.06	26.00	2218.5	12.951
180	22.88	27.28	2443.2	13.711
190	23.73	28.54	2676.3	14.459
200	24.61	29.78	2917.9	15.19
210	25.53	31.01	3168.6	15.92
220	26.51	32.22	3428.7	16.63
230	27.54	33.42	3698.9	17.34
240	28.65	34.61	3979.8	18.03
250	29.84	35.81	4272.2	18.72
260	31.12	37.00	4576.9	19.40
269.80	(32.47)	(38.18)	(4888.3)	(20.06)
Crystal III				
269.80	(32.48)	(38.80)	(5055)	(20.06)
270	32.51	38.82	5062	20.07
280	33.95	40.03	5394	20.76
290.00	(~600)	41.24	5741	21.45
Crystal II				
290.0	(~600)	42.94	6234	21.45
292	32.10	43.16	6298	21.60
293.47	(~1300)	(43.33)	(6345)	(21.71)
Crystal I				
293.47	(~1300)	(45.58)	(7006)	(21.71)
298.15	(32.41)	(46.09)	(7157)	(22.08)

Table 4 *(continued)*

T/K	$C_{p,m}/R$	S^o_m-S^o_m(0 K)/R	H^o_m-H^o_m(0 K)/(R K)	Φ^o_m/R
300	32.50	46.29	7217	22.23
320	33.50	48.42	7877	23.80
340	34.50	50.48	8557	25.31
360	35.50	52.48	9257	26.77
380	36.50	54.43	9977	28.17
400	37.50	56.32	10717	29.53
411.00	(38.05)	(57.35)	(11133)	(30.26)
		Mesophase		
411.00	(46.18)	(59.01)	(11815)	(30.26)
420	(47.28)	(60.02)	(12235)	(30.89)
440	49.44	62.27	13203	32.26
460	51.19	64.51	14210	33.62
480	(52.54)	(66.72)	(15248)	(34.95)
494.70	(53.28)	(68.31)	(16026)	(35.92)
		Isotropic liquid		
494.70	(54.72)	(69.04)	(16386)	(35.92)
Smoothed lattice heat capacities for thallium(I) octanoate at selected temperatures[b]				
120	17.99	19.06	1216.3	8.924
130	18.83	20.53	1400.4	9.761
140	19.65	21.96	1592.8	10.581
150	20.45	23.34	1793.4	11.386
160	21.26	24.69	2001.9	12.176
170	22.06	26.00	2218.5	12.951
180	22.88	27.28	2443.2	13.711
190	23.73	28.54	2676.3	14.459
200	24.61	29.78	2917.9	15.19
210	25.53	31.01	3168.6	15.92
220	26.51	32.22	3428.7	16.63
230	27.54	33.42	3698.9	17.34
240	28.65	34.61	3979.8	18.03
250	29.84	35.81	4272.2	18.72
260	31.12	37.00	4576.9	19.40
270	32.51	38.20	4894.8	20.07
280	33.95	39.41	5227	20.74
290	35.40	40.63	5574	21.41
290	32.00	40.63	5574	21.41
298.15	32.41	41.52	5836	21.94
300	32.50	41.72	5896	22.06
320	33.50	43.85	6556	23.36
340	34.50	45.91	7236	24.63
360	35.50	47.91	7936	25.86
380	36.50	49.86	8656	27.08
400	37.50	51.75	9396	28.26
411	38.05	52.78	9812	28.91

[a] Quantities in parentheses are either C_p values at the peaks or extrapolated C_p transition temperatures, e.g. DSC-determined $\Delta_{trs}H$, and assume the transitions are treated as if they were essentially isothermal.

[b] Assumed to be identical to actual (gross) heat capacity measured outside the range 190–411 K.

heat capacity values and the enthalpies of transition. Our selection of the lattice heat capacities from 190 to 411 K are also given in the table.

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