Experimental Enthalpy Increments from the Solid Phases to the Liquid Phase of Homologous *n*-Alkane Series (C_{18} to C_{38} and C_{41}, C_{44}, C_{46}, C_{50}, C_{54}, and C_{60})

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Measurements of enthalpy increments from the temperature of the ordered phases of low temperatures at 293.4 K and 298.3 K up to the liquid phase above the melting point were carried out by differential scanning calorimetry using a discontinuous mode of temperature programming on the *n*-alkanes from C_{18} to C_{38} and C_{41}, C_{44}, C_{46}, C_{50}, C_{54}, and C_{60}. The temperatures and enthalpies of the solid−solid transitions and of the fusion were also determined and compared with the values of the literature.

Introduction

Because of the importance of the *n*-alkanes (hereafter denoted by C_n), numerous studies[1−83] have been carried out to determine their thermodynamic properties and their structural behavior. Although numerous values of the temperatures and enthalpies of solid−solid and solid−liquid transitions of C_n's are available in the literature,[1−85] only some authors (Messerly et al.;[7] Finke et al.;[10] Schaerer et al.;[16,40] Barbillon et al.;[19] Parks et al.;[34] Andon and Martin;[46] Jin and Wunderlich;[57] Van Miltenburg[85]) have carried out measurements of the variations of thermodynamic properties (enthalpies, entropies) of light C_n's (n < 27) with respect to the temperature from the ordered solid phases of low temperatures up to the liquid phase above the melting point: these data types are still less numerous for the heavy C_n's (n > 26). The aim of this article is to determine the enthalpy increments of the *n*-alkanes from C_{18} to C_{38} and C_{41}, C_{44}, C_{46}, C_{50}, C_{54}, and C_{60}, as a function of the increasing temperature by differential scanning calorimetry.

Structural Behavior−Literature Results

C_n Crystalline Structures of Low Temperatures. The crystallographic structures of ordered phases at low temperatures have been studied by Craig et al.,[64] who identified the crystallographic space groups, and Chevallier et al.,[72] who correlated the crystalline long *c*-parameter with the number of carbon atoms of pure C_n chains: (i) odd-numbered C_{2p+1}'s have an orthorhombic structure, described by Smith[66] for the C_{23} with the crystallographic space group *Pbcm*;[64] (ii) even-numbered C_{2p}'s with $14 \leq 2p \leq 26$ have the triclinic structure described by Müller[67] and Nyburg et al.[65,68] for the C_{18} whose space group is $P\bar{1}$; C_{2p}'s with $28 \leq 2p \leq 36$ have a monoclinic structure, determined by Shearer and Vand[69] for the C_{36} with the $P2_1/a$ crystallographic space group; C_{2p}'s with $2p = 38$, 40, and 44 have a *Pbca* orthorhombic structure, described by Boistelle et al.;[70] and C_{2p}'s with $2p$ > 44 have a $Pca2_1$ orthorhombic structure, determined by Shearer and Vand[69] and Teare.[71]

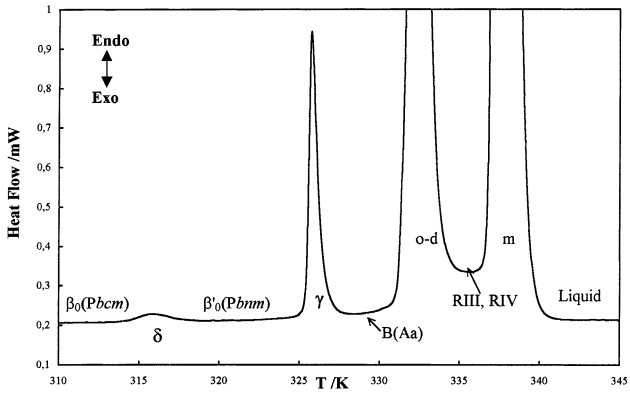

Figure 1. DSC curve of the *n*-alkane C_{29} with increasing temperature: observation of δ and γ order−order transitions below the order−disorder transition and the melting.

C_n Structural Behavior versus Temperature. Müller[73,74] was the first to observe polymorphism by X-ray diffraction in C_n, over a range of temperature, particularly in disordered phases below the melting point. From the literature data,[50−80] Chevallier et al.[83] and Dirand et al.[84] classified these polymorphic transitions according to the following behavior (Scheme 1) with respect to the increasing temperature:

For the pure C_n's, it is possible to distinguish two categories of polymorphic phases: (i) the ordered phases of low temperatures, observed below the order−disorder transition temperature, T_{o-d}, and (ii) the disordered phases of high temperatures that can present molecular movements of the Rotator type: orthorhombic β-RI ($Fmmm$), rhombohedral α-RII ($R\bar{3}m$), triclinic RIII, and monoclinic RIV disordered structures.

The order−disorder solid−solid transition (hereafter named the o−d transition) is characterized by the higher thermal effect observed at the solid state below the melting point (Figure 1). Other polymorphic transitions, with which

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Scheme 1[a]

odd-numbered C_{2p+1}

9 to 21	β_o (Pbcm)	$\xrightarrow{o-d}$ β(Fmmm)⇒β-RI(Fmmm)		→liquid
23	β_o (Pbcm) $\xrightarrow{\delta}$ β'_o (Pbnm)	$\xrightarrow{o-d}$ β(Fmmm)⇒β-RI(Fmmm)→αRII ($R\bar{3}m$)		→liquid
25	β_o(Pbcm) $\xrightarrow{\delta}$ β'_o(Pbnm) $\xrightarrow{\gamma}$ B(Aa)	$\xrightarrow{o-d}$ β(Fmmm)⇒β-RI(Fmmm)→αRII ($R\bar{3}m$)		→liquid
27-29	β_o (Pbcm) $\xrightarrow{\delta}$ β'_o (Pbnm) $\xrightarrow{\gamma}$ B(Aa)	$\xrightarrow{o-d}$ RIII → RIV		→liquid
31,33,37	β_o(Pbcm) $\xrightarrow{\gamma}$ B (Aa) $\xrightarrow{\beta}$ C(A2)	$\xrightarrow{o-d}$ RIII		→liquid
45	β_o(Pbcm) $\xrightarrow{\gamma}$ B (Aa) $\xrightarrow{\beta}$ C(A2)			→liquid
61,65,69	β_o(Pbcm) $\xrightarrow{\beta}$ C(A2)			→liquid

even-numbered C_{2p}

10 to 20	γ_o ($P\bar{1}$)			→liquid
22 to 26	γ_o ($P\bar{1}$)	$\xrightarrow{o-d}$ α-RII ($R\bar{3}m$)		→liquid
28,30	δ_o ($P2_1/a$)	$\xrightarrow{o-d}$ RIII → RIV		→liquid
32→36	δ_o ($P2_1/a$)	$\xrightarrow{o-d}$ RIII		→liquid
38→44	β_o(Pbca)	$\xrightarrow{o-d}$ RIII		→liquid
48,60	β_o($Pca2_1$)	$\xrightarrow{\beta}$ C(A2)		→liquid

[a] → corresponds to first-order transitions. ⇒ corresponds to second- or higher-order transitions. The o−d transition disappears from C_{45}.[53,54,77]

lower thermal effects are associated, appear in each category:[83,84] (i) order−order transitions below the o−d transition [δ-transition,[75] which corresponds to the phase change β_0 (orthorhombic *Pbcm*) → β'_0 (orthorhombic *Pbnm*); γ-transition,[83,75] corresponding to β_0 (orthorhombic *Pbcm*) → B (monoclinic *A*a); and β-transition,[55,56,75] corresponding to B (monoclinic *Aa*) → C (monoclinic *A*2)]; (ii) disorder ↔ disorder transitions between the o−d transition temperature and the melting point (Scheme 1).

The temperatures and enthalpies of solid−solid and solid−liquid transitions of C_n's were reported as a function of the carbon atom number of the C_n chain from the methane up to the C_n with n equal to 390 by Dirand et al.[84]

Experimental Section

Principle of Measurement and Operating Conditions. The measurement of the enthalpy increments was deduced from differential thermal analyses, performed with a differential scanning calorimeter of the Tian-Calvet type,[86] using a discontinuous mode of temperature programming. The calorimeter principle has been described before.[86−89] The calorimeter temperature is programmed as shown in Figure 2, it increases linearly between T_1 and T_2 during time t_i and is then constant at T_2 during time t_l. Thus, the calorimeter temperature increases step by step from room temperature up to the maximum temperature of the experiment.

The device measures the difference in heat flows that are exchanged between the two cells and the calorimeter block; it is evaluated by measurement of the electromotive force, ΔE, developed in two thermopiles surrounding the two calorimeter cells and connected together in opposition.

ΔE, measured in the course of a temperature jump from T_1 to T_2 during time $t_i + t_l$, is related to the difference in heat, Q, exchanged between the two cells and the calorimeter block, by means of the sensitivity coefficient, $S(T)$,

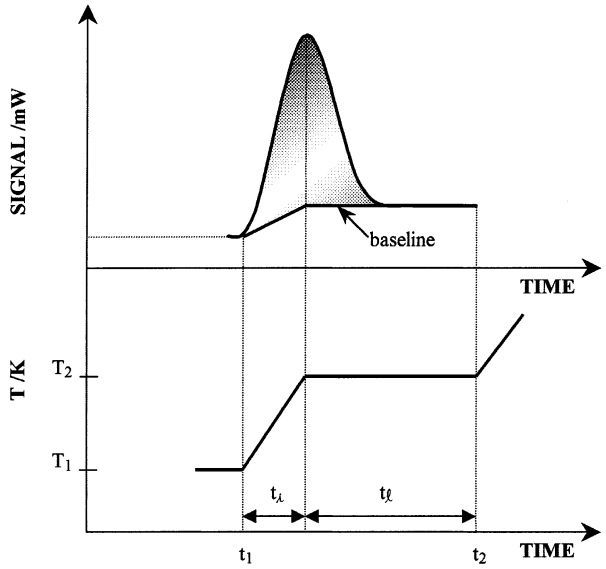

Figure 2. Calorimetric signal and temperature jump.

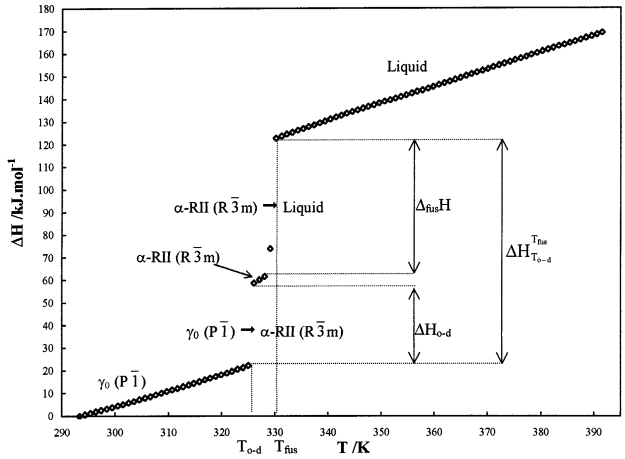

Figure 3. Enthalpy curve for the even *n*-alkane C_{26}: $\Delta H_{tot} = \Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$.

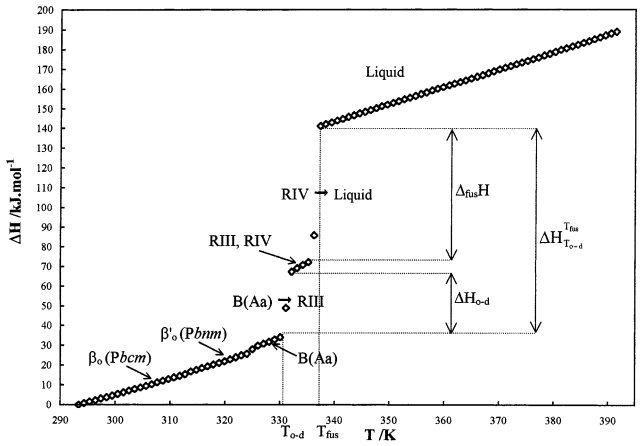

Figure 4. Enthalpy curve for the odd *n*-alkane C_{29}: $\Delta H_{tot} = \Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$.

determined by calibration.

$$Q = \frac{1}{S(T)} \int_{t_1}^{t_2} \Delta E \, dt$$

The sensitivity coefficient, $S(T)$, was obtained with respect to temperature variations by calibration with the help of the thermodynamic data on alumina, reported in the N.B.S. Table,[90] and on the two metals gallium and indium. The change in enthalpy of the sample was obtained as the difference in heat transfer in two experiments. In the blank experiment both cells were empty. The observed heat is the asymmetric term, Q_a. In the other experiment a sample is placed in one of the cells. It gives the total heat transferred, Q_0. The difference is the heat transferred to the sample, Q_s.

$$Q_s = Q_0 - Q_a$$

Table 1. Purity of the *n*-Alkanes Used in This Study

name	symbol	purity/%
octadecane	$C_{18}H_{38}$	≈99
nonadecane	$C_{19}H_{40}$	≈98
eïcosane	$C_{20}H_{42}$	≥97
heneicosane	$C_{21}H_{44}$	≥98
docosane	$C_{22}H_{46}$	≥98
tricosane	$C_{23}H_{48}$	≥98
tetracosane	$C_{24}H_{50}$	≥99
pentacosane	$C_{25}H_{52}$	≥98
hexacosane	$C_{26}H_{54}$	≥99
heptacosane	$C_{27}H_{56}$	≥98
octacosane	$C_{28}H_{58}$	≥98
nonacosane	$C_{29}H_{60}$	≥99.5
triacontane	$C_{30}H_{62}$	≥98
hentriacontane	$C_{31}H_{64}$	≥99.5
dotriacontane	$C_{32}H_{66}$	≈98
tritriacontane	$C_{33}H_{68}$	>97
tetratriacontane	$C_{34}H_{70}$	≥97
pentatriacontane	$C_{35}H_{72}$	≥99.5
hexatriacontane	$C_{36}H_{74}$	≈98
heptatriacontane	$C_{37}H_{76}$	≥99
octatriacontane	$C_{38}H_{78}$	>98
hentetracontane	$C_{41}H_{84}$	≥99
tetratetracontane	$C_{44}H_{90}$	≈99
hexatetracontane	$C_{46}H_{94}$	≥98
pentacontane	$C_{50}H_{102}$	≥97
tetrapentacontane	$C_{54}H_{110}$	≈99
hexacontane	$C_{60}H_{122}$	>98

Table 2. Comparison of the Experimental Enthalpy Increments ($H_{293.4}^T$) versus Temperature of the *n*-Alkane $C_{18}H_{38}$ with the Literature Data[7] ($H_{293.4}^T$ (lit.)[7])

T^a / K	$H_{293.4}^T$ / kJ·mol^{-1}	$H_{293.4}^T$(lit.)[7] / kJ·mol^{-1}	% diff
293.4 (s)	0	0	
319.9 (l)	76.7	74.9	2.3
330.2 (l)	82.2	81.0	1.4
340.4 (l)	88.0	87.1	1.0
350.6 (l)	93.7	93.3	0.5
360.8 (l)	99.3	99.4	0.1

[a] In parentheses is the state of the *n*-alkane at that temperature: l, liquid; s, solid.

Table 3. Comparison of the Experimental Enthalpy Increments ($H_{293.4}^T$) versus Temperature of the *n*-Alkane $C_{26}H_{54}$ with the Literature Data[46] ($H_{293.4}^T$ (lit.)[46])

T / K	$H_{293.4}^T$ / kJ·mol^{-1}	$H_{293.4}^T$(lit.)[46] / kJ·mol^{-1}	% diff
293.4 (s)	0	0	
300.5(s)	4.6	4.6	0.6
309.7(s)	10.7	10.7	0.3
319.9(s)	17.7	17.9	1.1
330.1 (l)	124.3	121.9	1.9
340.4 (l)	132.7	130.7	1.5
350.6 (l)	140.5	139.5	0.7
360.8 (l)	147.7	148.4	0.5

Table 4. Thermodynamic Data of C_{18}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	γ_0 ($P\bar{1}$)	313.8	73.4	L	334.3	84.5	L	353.7	95.4	L	373.1	105.9	L
294.4	0.6	γ_0 ($P\bar{1}$)	314.8	74.0	L	335.3	85.1	L	354.7	95.9	L	374.1	106.4	L
295.4	1.3	γ_0 ($P\bar{1}$)	315.9	74.5	L	336.3	85.7	L	355.7	96.5	L	375.1	107.0	L
296.4	2.1	γ_0 ($P\bar{1}$)	316.9	75.1	L	337.3	86.3	L	356.8	97.0	L	376.2	107.5	L
297.4	2.9	γ_0 ($P\bar{1}$)	317.9	75.6	L	338.4	86.9	L	357.8	97.6	L	377.2	108.1	L
298.5	4.1	γ_0 ($P\bar{1}$)	318.9	76.2	L	339.4	87.4	L	358.8	98.1	L	378.2	108.6	L
299.5	6.4	γ_0 ($P\bar{1}$)	320.0	76.7	L	340.4	88.0	L	359.8	98.7	L	379.2	109.2	L
300.5	19.6	L	321.0	77.2	L	341.4	88.6	L	360.9	99.3	L	380.3	109.8	L
301.5	66.5	L	322.0	77.7	L	342.4	89.2	L	361.9	99.8	L	381.3	110.4	L
302.5	67.1	L	323.0	78.3	L	343.5	89.8	L	362.9	100.4	L	382.3	111.0	L
303.6	67.6	L	324.0	78.8	L	344.5	90.3	L	363.9	100.9	L	383.3	111.6	L
304.6	68.2	L	325.1	79.4	L	345.5	90.9	L	364.9	101.4	L	384.4	112.2	L
305.6	68.8	L	326.1	79.9	L	346.5	91.5	L	365.9	102.0	L	385.4	112.9	L
306.7	69.4	L	327.1	80.5	L	347.6	92.0	L	367.0	102.5	L	386.4	113.5	L
307.7	69.9	L	328.1	81.0	L	348.6	92.6	L	368.0	103.1	L	387.5	114.1	L
308.7	70.5	L	329.1	81.6	L	349.6	93.2	L	369.0	103.6	L	388.5	114.7	L
309.7	71.1	L	330.2	82.2	L	350.6	93.7	L	370.0	104.2	L	389.5	115.4	L
310.8	71.7	L	331.2	82.8	L	351.7	94.3	L	371.1	104.7	L	390.6	116.0	L
311.8	72.2	L	332.2	83.4	L	352.7	94.8	L	372.1	105.3	L	391.6	116.6	L
312.8	72.8	L	333.2	83.9	L									

Table 5. Thermodynamic Data of C_{19}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	β-RI ($Fmmm$)	313.8	72.5	L	334.2	85.8	L	354.6	99.7	L	374.0	113.6	L
294.4	0.8	β-RI ($Fmmm$)	314.8	73.2	L	335.2	86.4	L	355.6	100.5	L	375.0	114.3	L
295.4	10.6	β-RI ($Fmmm$)	315.8	73.8	L	336.3	87.1	L	356.6	101.2	L	376.1	115.1	L
296.4	13.6	β-RI ($Fmmm$)	316.8	74.5	L	337.3	87.8	L	357.7	101.9	L	377.1	115.8	L
297.4	14.7	β-RI ($Fmmm$)	317.8	75.1	L	338.3	88.5	L	358.7	102.7	L	378.1	116.6	L
298.4	15.8	β-RI ($Fmmm$)	318.9	75.8	L	339.3	89.2	L	359.7	103.4	L	379.2	117.3	L
299.5	17.1	β-RI ($Fmmm$)	319.9	76.4	L	340.3	89.9	L	360.7	104.1	L	380.2	118.1	L
300.5	18.5	β-RI ($Fmmm$)	320.9	77.1	L	341.4	90.6	L	361.7	104.8	L	381.2	118.8	L
301.5	20.1	β-RI ($Fmmm$)	321.9	77.8	L	342.4	91.3	L	362.8	105.5	L	382.2	119.6	L
302.5	22.1	β-RI ($Fmmm$)	323.0	78.4	L	343.4	92.0	L	363.8	106.3	L	383.2	120.4	L
303.5	25.4	β-RI ($Fmmm$)	324.0	79.1	L	344.4	92.7	L	364.8	107.0	L	384.3	121.1	L
304.6	43.6	L	325.0	79.7	L	345.5	93.4	L	365.8	107.7	L	385.3	121.9	L
305.6	67.3	L	326.0	80.4	L	346.5	94.1	L	366.9	108.4	L	386.3	122.6	L
306.6	67.9	L	327.0	81.1	L	347.5	94.8	L	367.9	109.2	L	387.3	123.4	L
307.6	68.6	L	328.1	81.7	L	348.5	95.6	L	368.9	109.9	L	388.4	124.2	L
308.7	69.2	L	329.1	82.4	L	349.5	96.3	L	369.9	110.7	L	389.4	124.9	L
309.7	69.9	L	330.1	83.1	L	350.5	97.0	L	370.9	111.4	L	390.4	125.7	L
310.7	70.5	L	331.1	83.8	L	351.6	97.6	L	372.0	112.1	L	391.5	126.5	L
311.7	71.2	L	332.2	84.4	L	352.6	98.3	L	373.0	112.9	L	392.5	127.3	L
312.8	71.8	L	333.2	85.1	L	353.6	99.0	L						

Table 6. Thermodynamic Data of C_{20}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	γ_0 ($P\bar{1}$)	313.8	85.5	L	334.2	99.8	L	354.7	114.8	L	374.1	129.7	L
294.4	0.6	γ_0 ($P\bar{1}$)	314.8	86.2	L	335.2	100.5	L	355.7	115.6	L	375.1	130.5	L
295.4	1.1	γ_0 ($P\bar{1}$)	315.8	86.9	L	336.3	101.2	L	356.7	116.3	L	376.1	131.3	L
296.4	1.7	γ_0 ($P\bar{1}$)	316.9	87.6	L	337.3	102.0	L	357.7	117.1	L	377.2	132.1	L
297.4	2.3	γ_0 ($P\bar{1}$)	317.9	88.3	L	338.3	102.7	L	358.8	117.9	L	378.2	132.9	L
298.5	2.8	γ_0 ($P\bar{1}$)	318.9	89.0	L	339.3	103.4	L	359.8	118.7	L	379.2	133.7	L
299.5	3.4	γ_0 ($P\bar{1}$)	319.9	89.8	L	340.4	104.2	L	360.8	119.4	L	380.2	134.5	L
300.5	4.0	γ_0 ($P\bar{1}$)	321.0	90.5	L	341.4	104.9	L	361.8	120.2	L	381.2	135.3	L
301.5	4.7	γ_0 ($P\bar{1}$)	322.0	91.2	L	342.4	105.6	L	362.9	121.0	L	382.3	136.1	L
302.5	5.3	γ_0 ($P\bar{1}$)	323.0	91.9	L	343.4	106.4	L	363.9	121.7	L	383.3	136.9	L
303.6	5.9	γ_0 ($P\bar{1}$)	324.0	92.6	L	344.5	107.1	L	364.9	122.5	L	384.3	137.8	L
304.6	6.5	γ_0 ($P\bar{1}$)	325.0	93.3	L	345.5	107.9	L	365.9	123.3	L	385.4	138.6	L
305.6	7.1	γ_0 ($P\bar{1}$)	326.1	94.0	L	346.5	108.6	L	366.9	124.1	L	386.4	139.4	L
306.6	7.8	γ_0 ($P\bar{1}$)	327.1	94.7	L	347.5	109.4	L	368.0	124.9	L	387.4	140.2	L
307.7	8.6	γ_0 ($P\bar{1}$)	328.1	95.4	L	348.5	110.1	L	369.0	125.7	L	388.4	141.0	L
308.7	9.7	L	329.1	96.2	L	349.6	110.9	L	370.0	126.5	L	389.4	141.9	L
309.7	82.7	L	330.1	96.9	L	350.6	111.7	L	371.0	127.3	L	390.5	142.7	L
310.7	83.4	L	331.2	97.6	L	351.6	112.4	L	372.1	128.1	L	391.5	143.6	L
311.8	84.1	L	332.2	98.3	L	352.6	113.2	L	373.1	128.9	L	392.5	144.4	L
312.8	84.8	L	333.2	99.0	L	353.7	114.0	L						

Table 7. Thermodynamic Data of C_{21}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 298.3 K ($H^T_{298.3}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{298.3}$		T	$H^T_{2938.3}$		T	$H^T_{298.3}$		T	$H^T_{2938.3}$		T	$H^T_{2938.3}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
298.3	0.0	β_0 (*Pbcm*)	327.0	88.6	L	354.6	106.6	L	382.2	125.2	L	409.9	144.4	L
299.4	0.6	β_0 (*Pbcm*)	328.0	89.2	L	355.6	107.3	L	383.2	125.9	L	411.0	145.1	L
300.4	1.2	β_0 (*Pbcm*)	329.0	89.9	L	356.6	108.0	L	384.2	126.6	L	412.0	145.8	L
301.4	1.8	β_0 (*Pbcm*)	330.0	90.5	L	357.6	108.6	L	385.3	127.3	L	413.0	146.6	L
302.4	2.5	β_0 (*Pbcm*)	331.0	91.2	L	358.6	109.3	L	386.3	128.0	L	414.0	147.3	L
303.4	3.1	β_0 (*Pbcm*)	332.1	91.8	L	359.7	110.0	L	387.3	128.7	L	415.1	148.1	L
304.5	3.9	β-RI (*Fmmm*)	333.1	92.5	L	360.7	110.6	L	388.3	129.4	L	416.1	148.8	L
305.5	20.5	β-RI (*Fmmm*)	334.1	93.2	L	361.7	111.3	L	389.4	130.1	L	417.1	149.6	L
306.5	21.9	β-RI (*Fmmm*)	335.1	93.8	L	362.7	112.0	L	390.4	130.9	L	418.2	150.3	L
307.5	23.5	β-RI (*Fmmm*)	336.2	94.5	L	363.8	112.7	L	391.4	131.6	L	419.2	151.1	L
308.6	25.2	β-RI (*Fmmm*)	337.2	95.2	L	364.8	113.3	L	392.4	132.3	L	420.2	151.8	L
309.6	27.0	β-RI (*Fmmm*)	338.2	95.9	L	365.8	114.0	L	393.5	133.0	L	421.2	152.5	L
310.6	28.9	β-RI (*Fmmm*)	339.2	96.5	L	366.8	114.7	L	394.5	133.7	L	422.3	153.3	L
311.6	30.6	β-RI (*Fmmm*)	340.2	97.2	L	367.8	115.4	L	395.5	134.4	L	423.3	154.1	L
312.6	32.3	L	341.3	97.9	L	368.9	116.1	L	396.5	135.1	L	424.3	154.8	L
313.7	79.9	L	342.3	98.6	L	369.9	116.8	L	397.6	135.8	L	425.4	155.6	L
314.7	80.6	L	343.3	99.3	L	370.9	117.5	L	398.6	136.5	L	426.4	156.3	L
315.7	81.2	L	344.3	99.9	L	371.9	118.2	L	399.6	137.2	L	427.4	157.1	L
316.7	81.9	L	345.4	100.6	L	373.0	118.9	L	400.7	137.9	L	428.5	157.9	L
317.8	82.5	L	346.4	101.2	L	374.0	119.5	L	401.7	138.6	L	429.5	158.7	L
318.8	83.2	L	347.4	101.9	L	375.0	120.2	L	402.7	139.3	L	430.5	159.5	L
319.8	83.9	L	348.4	102.6	L	376.0	120.9	L	403.7	140.0	L	431.6	160.2	L
320.8	84.5	L	349.4	103.2	L	377.1	121.6	L	404.8	140.8	L	432.6	161.0	L
321.9	85.2	L	350.5	103.9	L	378.1	122.4	L	405.8	141.5	L	433.6	161.8	L
322.9	85.9	L	351.5	104.6	L	379.1	123.1	L	406.8	142.2	L	434.7	162.7	L
323.9	86.5	L	352.5	105.2	L	380.1	123.8	L	407.9	142.9	L	435.7	163.5	L
324.9	87.2	L	353.5	105.9	L	381.2	124.5	L	408.9	143.6	L	436.7	164.3	L
325.9	87.9	L												

Table 8. Thermodynamic Data of C_{22}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 298.3 K ($H^T_{298.3}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{298.3}$		T	$H^T_{2938.3}$		T	$H^T_{298.3}$		T	$H^T_{2938.3}$		T	$H^T_{2938.3}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
298.3	0.0	γ_0 ($P\bar{1}$)	326.9	99.5	L	354.5	120.7	L	382.2	142.1	L	409.9	164.2	L
299.4	0.7	γ_0 ($P\bar{1}$)	328.0	100.3	L	355.6	121.5	L	383.2	142.9	L	410.9	165.1	L
300.4	1.3	γ_0 ($P\bar{1}$)	329.0	101.1	L	356.6	122.3	L	384.2	143.7	L	412.0	165.9	L
301.4	2.0	γ_0 ($P\bar{1}$)	330.0	101.9	L	357.6	123.1	L	385.3	144.6	L	413.0	166.8	L
302.4	2.6	γ_0 ($P\bar{1}$)	331.0	102.7	L	358.6	123.9	L	386.3	145.4	L	414.0	167.7	L
303.4	3.3	γ_0 ($P\bar{1}$)	332.1	103.5	L	359.7	124.6	L	387.3	146.2	L	415.0	168.5	L
304.5	3.9	γ_0 ($P\bar{1}$)	333.1	104.2	L	360.7	125.4	L	388.3	147.1	L	416.1	169.4	L
305.5	4.6	γ_0 ($P\bar{1}$)	334.1	105.0	L	361.7	126.2	L	389.4	147.9	L	417.1	170.2	L
306.5	5.2	γ_0 ($P\bar{1}$)	335.1	105.8	L	362.7	127.0	L	390.4	148.7	L	418.1	171.1	L
307.5	5.9	γ_0 ($P\bar{1}$)	336.1	106.6	L	363.8	127.8	L	391.4	149.5	L	419.2	172.0	L
308.6	6.6	γ_0 ($P\bar{1}$)	337.2	107.3	L	364.8	128.6	L	392.4	150.4	L	420.2	172.8	L
309.6	7.3	γ_0 ($P\bar{1}$)	338.2	108.1	L	365.8	129.4	L	393.5	151.2	L	421.2	173.7	L
310.6	7.9	γ_0 ($P\bar{1}$)	339.2	108.9	L	366.8	130.2	L	394.5	152.0	L	422.2	174.5	L
311.6	8.6	α-RII ($R\bar{3}m$)	340.2	109.7	L	367.8	131.0	L	395.5	152.9	L	423.3	175.4	L
312.7	9.3	α-RII ($R\bar{3}m$)	341.3	110.5	L	368.9	131.8	L	396.5	153.7	L	424.3	176.2	L
313.7	10.1	α-RII ($R\bar{3}m$)	342.3	111.3	L	369.9	132.6	L	397.6	154.6	L	425.3	177.1	L
314.7	10.8	α-RII ($R\bar{3}m$)	343.3	112.1	L	370.9	133.4	L	398.6	155.5	L	426.4	178.0	L
315.7	11.7	L	344.3	112.9	L	371.9	134.2	L	399.6	156.3	L	427.4	178.9	L
316.7	43.4	L	345.3	113.6	L	373.0	134.9	L	400.7	157.1	L	428.4	179.8	L
317.7	92.5	L	346.4	114.4	L	374.0	135.7	L	401.7	157.9	L	429.5	180.7	L
318.8	93.3	L	347.4	115.2	L	375.0	136.5	L	402.7	158.7	L	430.5	181.5	L
319.8	94.1	L	348.4	116.0	L	376.0	137.3	L	403.7	159.5	L	431.5	182.4	L
320.8	94.8	L	349.4	116.8	L	377.1	138.1	L	404.8	160.3	L	432.6	183.3	L
321.8	95.6	L	350.5	117.6	L	378.1	138.9	L	405.8	161.1	L	433.6	184.2	L
322.9	96.4	L	351.5	118.4	L	379.1	139.7	L	406.8	161.8	L	434.6	185.1	L
323.9	97.2	L	352.5	119.1	L	380.1	140.5	L	407.8	162.6	L	435.7	186.0	L
324.9	98.0	L	353.5	119.9	L	381.1	141.4	L	408.9	163.4	L	436.7	186.9	L
325.9	98.7	L												

For each temperature jump, j, the molar enthalpy increment of the sample is as follows:

$$\Delta H_{T_1}^{T_2} = H°(T_2) - H°(T_1) = \frac{M}{m}(Q_s)_j$$

where M and m are the molar mass and the mass of the sample, respectively. The molar enthalpy increment above T_0 of the sample heating at temperature T, with T_0 equal to 293.4 K or 298.3 K, is as follows:

$$H_{T_0}^{T} = H(T) - H(T_0) = \sum_j \frac{M}{m}(Q_s)_j$$

where $H(T)$ and $H(T_0)$ are the enthalpies at T and T_0, respectively.

Table 9. Thermodynamic Data of C_{23}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	313.8	36.4	β-RI (*Fmmm*)	334.2	110.5	L	354.6	126.9	L	374.1	143.9	L
294.4	0.6	β_0 (*Pbcm*)	314.8	38.9	β-RI (*Fmmm*)	335.2	111.3	L	355.7	127.8	L	375.1	144.7	L
295.4	1.2	β_0 (*Pbcm*)	315.8	41.1	β-RI (*Fmmm*)	336.2	112.1	L	356.7	128.7	L	376.1	145.6	L
296.4	1.9	β_0 (*Pbcm*)	316.8	43.0	α-RII ($R\bar{3}m$)	337.3	113.0	L	357.7	129.6	L	377.1	146.5	L
297.4	2.5	β_0 (*Pbcm*)	317.9	44.6	α-RII ($R\bar{3}m$)	338.3	113.8	L	358.7	130.4	L	378.2	147.4	L
298.5	3.2	β_0 (*Pbcm*)	318.9	45.8	α-RII ($R\bar{3}m$)	339.3	114.6	L	359.8	131.3	L	379.2	148.3	L
299.5	3.9	β_0 (*Pbcm*)	319.9	47.4	L	340.3	115.4	L	360.8	132.2	L	380.2	149.2	L
300.5	4.5	β_0 (*Pbcm*)	320.9	100.3	L	341.4	116.2	L	361.8	133.1	L	381.2	150.1	L
301.5	5.2	β_0 (*Pbcm*)	321.9	101.1	L	342.4	117.0	L	362.8	134.0	L	382.3	151.0	L
302.5	5.9	β_0 (*Pbcm*)	323.0	101.9	L	343.4	117.8	L	363.8	134.9	L	383.3	151.9	L
303.6	6.6	β_0 (*Pbcm*)	324.0	102.7	L	344.4	118.6	L	364.9	135.8	L	384.3	152.8	L
304.6	7.3	β_0 (*Pbcm*)	325.0	103.5	L	345.4	119.4	L	365.9	136.7	L	385.3	153.7	L
305.6	8.0	β_0 (*Pbcm*)	326.0	104.2	L	346.5	120.3	L	366.9	137.5	L	386.4	154.6	L
306.6	8.7	β_0 (*Pbcm*)	327.0	105.0	L	347.5	121.1	L	367.9	138.4	L	387.4	155.4	L
307.7	9.5	β_0 (*Pbcm*)	328.0	105.8	L	348.5	121.9	L	368.9	139.3	L	388.4	156.4	L
308.7	10.2	β_0 (*Pbcm*)	329.1	106.6	L	349.5	122.7	L	370.0	140.2	L	389.4	157.3	L
309.7	10.9	β_0 (*Pbcm*)	330.1	107.4	L	350.5	123.6	L	371.0	141.1	L	390.5	158.2	L
310.7	11.7	β'_0 (*Pbnm*)	331.1	108.2	L	351.6	124.4	L	372.0	142.0	L	391.5	159.1	L
311.8	12.5	β'_0 (*Pbnm*)	332.1	108.9	L	352.6	125.2	L	373.0	143.0	L	392.5	160.0	L
312.8	13.8	β-RI (*Fmmm*)	333.2	109.7	L	353.6	126.1	L						

Table 10. Thermodynamic Data of C_{24}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	γ_0 ($P\bar{1}$)	313.8	13.5	γ_0 ($P\bar{1}$)	334.2	118.5	L	353.6	134.2	L	373.0	150.4	L
294.4	0.6	γ_0 ($P\bar{1}$)	314.8	14.2	γ_0 ($P\bar{1}$)	335.3	119.4	L	354.7	135.0	L	374.1	151.3	L
295.4	1.3	γ_0 ($P\bar{1}$)	315.9	14.9	γ_0 ($P\bar{1}$)	336.3	120.2	L	355.7	135.8	L	375.1	152.2	L
296.4	1.9	γ_0 ($P\bar{1}$)	316.9	15.7	γ_0 ($P\bar{1}$)	337.3	121.0	L	356.7	136.6	L	376.1	153.1	L
297.4	2.5	γ_0 ($P\bar{1}$)	317.9	16.4	γ_0 ($P\bar{1}$)	338.3	121.9	L	357.7	137.5	L	377.1	154.0	L
298.5	3.2	γ_0 ($P\bar{1}$)	318.9	17.2	γ_0 ($P\bar{1}$)	339.4	122.7	L	358.7	138.3	L	378.2	154.9	L
299.5	3.8	γ_0 ($P\bar{1}$)	319.9	18.1	α-RII ($R\bar{3}m$)	340.4	123.5	L	359.8	139.1	L	379.2	155.8	L
300.5	4.5	γ_0 ($P\bar{1}$)	321.0	47.8	α-RII ($R\bar{3}m$)	341.4	124.4	L	360.8	140.0	L	380.2	156.7	L
301.5	5.1	γ_0 ($P\bar{1}$)	322.0	51.1	α-RII ($R\bar{3}m$)	342.4	125.2	L	361.8	140.8	L	381.2	157.6	L
302.6	5.8	γ_0 ($P\bar{1}$)	323.0	53.0	L	343.4	126.0	L	362.8	141.7	L	382.3	158.6	L
303.6	6.5	γ_0 ($P\bar{1}$)	324.0	110.3	L	344.5	126.9	L	363.9	142.5	L	383.3	159.5	L
304.6	7.1	γ_0 ($P\bar{1}$)	325.0	111.1	L	345.5	127.7	L	364.9	143.4	L	384.3	160.4	L
305.6	7.8	γ_0 ($P\bar{1}$)	326.0	111.9	L	346.5	128.5	L	365.9	144.2	L	385.4	161.3	L
306.6	8.5	γ_0 ($P\bar{1}$)	327.1	112.7	L	347.5	129.3	L	366.9	145.1	L	386.4	162.2	L
307.7	9.2	γ_0 ($P\bar{1}$)	328.1	113.6	L	348.5	130.1	L	367.9	146.0	L	387.4	163.1	L
308.7	9.9	γ_0 ($P\bar{1}$)	329.1	114.4	L	349.6	130.9	L	369.0	146.8	L	388.5	164.1	L
309.7	10.6	γ_0 ($P\bar{1}$)	330.1	115.2	L	350.6	131.7	L	370.0	147.7	L	389.5	165.0	L
310.7	11.3	γ_0 ($P\bar{1}$)	331.2	116.0	L	351.6	132.6	L	371.0	148.6	L	390.5	166.0	L
311.8	12.0	γ_0 ($P\bar{1}$)	332.2	116.9	L	352.6	133.4	L	372.0	149.5	L	391.5	167.0	L
312.8	12.7	γ_0 ($P\bar{1}$)	333.2	117.7	L									

Table 11. Thermodynamic Data of C_{25}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}, % diff: 1.5%); Phase Name

T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$		T	$H^T_{293.4}$	
K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase	K	kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	313.8	15.1	β'_0 (*Pbcm*)	334.2	119.6	L	353.6	137.3	L	373.1	154.7	L
294.4	0.7	β_0 (*Pbcm*)	314.8	16.0	β'_0 (*Pbcm*)	335.2	120.5	L	354.7	138.3	L	374.1	155.6	L
295.4	1.3	β_0 (*Pbcm*)	315.8	17.0	β'_0 (*Pbcm*)	336.3	121.4	L	355.7	139.2	L	375.1	156.6	L
296.4	1.9	β_0 (*Pbcm*)	316.8	18.0	B (*Aa*)	337.3	122.3	L	356.7	140.2	L	376.2	157.5	L
297.4	2.6	β_0 (*Pbcm*)	317.9	19.1	B (*Aa*)	338.3	123.2	L	357.7	141.1	L	377.2	158.5	L
298.4	3.3	β_0 (*Pbcm*)	318.9	20.6	β-RI (*Fmmm*)	339.3	124.1	L	358.8	142.1	L	378.2	159.5	L
299.5	4.0	β_0 (*Pbcm*)	319.9	37.9	β-RI (*Fmmm*)	340.4	125.0	L	359.8	113.3	L	379.2	160.5	L
300.5	4.7	β_0 (*Pbcm*)	320.9	48.1	β-RI (*Fmmm*)	341.4	125.9	L	360.8	143.1	L	380.2	161.5	L
301.5	5.4	β_0 (*Pbcm*)	321.9	50.4	α-RII ($R\bar{3}m$)	342.4	126.9	L	361.8	144.0	L	381.3	162.4	L
302.5	6.1	β_0 (*Pbcm*)	323.0	52.9	α-RII ($R\bar{3}m$)	343.4	127.8	L	362.9	145.0	L	382.3	163.4	L
303.5	6.9	β_0 (*Pbcm*)	324.0	56.5	α-RII ($R\bar{3}m$)	344.4	128.7	L	363.9	145.8	L	383.3	164.4	L
304.6	7.6	β_0 (*Pbcm*)	325.0	63.2	L	345.5	129.7	L	364.9	146.8	L	384.3	165.4	L
305.6	8.4	β_0 (*Pbcm*)	326.0	89.0	L	346.5	130.7	L	365.9	147.8	L	385.4	166.4	L
306.6	9.1	β_0 (*Pbcm*)	327.0	113.3	L	347.5	131.6	L	366.9	148.8	L	386.4	167.4	L
307.6	9.9	β_0 (*Pbcm*)	328.1	114.2	L	348.5	132.5	L	368.0	149.8	L	387.4	168.4	L
308.7	10.6	β_0 (*Pbcm*)	329.1	115.1	L	349.6	133.5	L	369.0	150.8	L	388.4	169.4	L
309.7	11.4	β_0 (*Pbcm*)	330.1	116.0	L	350.6	134.5	L	370.0	151.8	L	389.5	170.4	L
310.7	12.2	β'_0 (*Pbcm*)	331.1	116.9	L	351.6	135.4	L	371.0	152.8	L	390.5	171.4	L
311.7	13.2	β'_0 (*Pbcm*)	332.2	117.8	L	352.6	136.4	L	372.1	153.7	L	391.5	172.4	L
312.8	14.2	β'_0 (*Pbcm*)	333.2	118.7	L									

Table 12. Thermodynamic Data of C_{26}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	γ_0 ($P\bar{1}$)	313.8	13.5	γ_0 ($P\bar{1}$)	334.2	127.7	L	353.7	142.6	L	373.1	156.7	L
294.4	0.7	γ_0 ($P\bar{1}$)	314.8	14.2	γ_0 ($P\bar{1}$)	335.3	128.6	L	354.7	143.3	L	374.1	157.5	L
295.4	1.3	γ_0 ($P\bar{1}$)	315.8	14.9	γ_0 ($P\bar{1}$)	336.3	129.4	L	355.7	144.1	L	375.1	158.2	L
296.4	2.0	γ_0 ($P\bar{1}$)	316.8	15.5	γ_0 ($P\bar{1}$)	337.3	130.2	L	356.7	144.8	L	376.2	159.0	L
297.4	2.6	γ_0 ($P\bar{1}$)	317.9	16.3	γ_0 ($P\bar{1}$)	338.3	131.0	L	357.7	145.5	L	377.2	159.8	L
298.5	3.2	γ_0 ($P\bar{1}$)	318.9	17.0	γ_0 ($P\bar{1}$)	339.3	131.9	L	358.8	146.2	L	378.2	160.6	L
299.5	3.9	γ_0 ($P\bar{1}$)	319.9	17.7	γ_0 ($P\bar{1}$)	340.4	132.7	L	359.8	146.9	L	379.2	161.4	L
300.5	4.6	γ_0 ($P\bar{1}$)	320.9	18.5	γ_0 ($P\bar{1}$)	341.4	133.5	L	360.8	147.7	L	380.2	162.2	L
301.5	5.2	γ_0 ($P\bar{1}$)	322.0	19.2	γ_0 ($P\bar{1}$)	342.4	134.3	L	361.8	148.4	L	381.3	163.0	L
302.5	5.9	γ_0 ($P\bar{1}$)	323.0	19.9	γ_0 ($P\bar{1}$)	343.4	135.1	L	362.9	149.2	L	382.3	163.7	L
303.6	6.6	γ_0 ($P\bar{1}$)	324.0	20.7	γ_0 ($P\bar{1}$)	344.5	135.9	L	363.9	149.9	L	383.3	164.5	L
304.6	7.3	γ_0 ($P\bar{1}$)	325.0	21.6	α-RII ($R\bar{3}m$)	345.5	136.8	L	364.9	150.6	L	384.3	165.3	L
305.6	7.9	γ_0 ($P\bar{1}$)	326.0	44.3	α-RII ($R\bar{3}m$)	346.5	137.5	L	365.9	151.3	L	385.4	166.0	L
306.6	8.6	γ_0 ($P\bar{1}$)	327.0	59.1	α-RII ($R\bar{3}m$)	347.5	138.3	L	366.9	152.0	L	386.4	166.8	L
307.6	9.3	γ_0 ($P\bar{1}$)	328.1	60.7	α-RII ($R\bar{3}m$)	348.5	139.0	L	368.0	152.8	L	387.4	167.5	L
308.7	10.0	γ_0 ($P\bar{1}$)	329.1	73.8	L	349.6	139.7	L	369.0	153.5	L	388.5	168.3	L
309.7	10.7	γ_0 ($P\bar{1}$)	330.1	124.3	L	350.6	140.5	L	370.0	154.4	L	389.5	169.1	L
310.7	11.4	γ_0 ($P\bar{1}$)	331.2	125.1	L	351.6	141.2	L	371.0	155.2	L	390.5	169.9	L
311.7	12.1	γ_0 ($P\bar{1}$)	332.2	126.0	L	352.6	141.9	L	372.1	156.0	L	391.5	170.6	L
312.8	12.7	γ_0 ($P\bar{1}$)	333.2	126.9	L									

Table 13. Thermodynamic Data of C_{27}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	313.8	16.6	β'_0 (*Pbcm*)	334.3	138.9	L	353.7	158.8	L	373.1	179.7	L
294.4	0.8	β_0 (*Pbcm*)	314.8	17.5	β'_0 (*Pbcm*)	335.3	140.0	L	354.7	159.9	L	374.2	180.8	L
295.4	1.5	β_0 (*Pbcm*)	315.8	18.4	β'_0 (*Pbcm*)	336.3	141.0	L	355.7	160.9	L	375.2	181.9	L
296.4	2.3	β_0 (*Pbcm*)	316.9	19.4	β'_0 (*Pbcm*)	337.3	142.1	L	356.8	161.9	L	376.2	183.0	L
297.4	3.1	β_0 (*Pbcm*)	317.9	20.3	β'_0 (*Pbcm*)	338.3	143.1	L	357.8	163.0	L	377.2	184.1	L
298.5	3.9	β_0 (*Pbcm*)	318.9	21.3	β'_0 (*Pbcm*)	339.3	144.2	L	358.8	164.1	L	378.2	185.2	L
299.5	4.7	β_0 (*Pbcm*)	319.9	22.6	B (*Aa*)	340.4	145.2	L	359.8	165.2	L	379.3	186.4	L
300.5	5.5	β_0 (*Pbcm*)	321.0	24.6	B (*Aa*)	341.4	146.3	L	360.9	166.4	L	380.3	187.5	L
301.5	6.3	β_0 (*Pbcm*)	322.0	25.7	B (*Aa*)	342.4	147.3	L	361.9	167.5	L	381.3	188.7	L
302.5	7.1	β_0 (*Pbcm*)	323.0	28.6	B (*Aa*)	343.5	148.4	L	362.9	168.6	L	382.4	189.9	L
303.6	7.9	β_0 (*Pbcm*)	324.0	28.6	B (*Aa*)	344.5	149.5	L	363.9	169.7	L	383.4	191.0	L
304.6	8.7	β_0 (*Pbcm*)	325.0	30.0	RIV	345.5	150.5	L	365.0	170.8	L	384.4	192.1	L
305.6	9.6	β_0 (*Pbcm*)	326.1	51.7	RIV	346.5	151.6	L	366.0	171.9	L	385.4	193.3	L
306.6	10.4	β_0 (*Pbcm*)	327.1	61.0	RIV	347.5	152.6	L	367.0	173.0	L	386.5	194.4	L
307.6	11.2	β_0 (*Pbcm*)	328.1	62.9	RIV	348.6	153.7	L	368.0	174.1	L	387.5	195.5	L
308.7	12.1	β_0 (*Pbcm*)	329.1	64.5	RIV	349.6	154.7	L	369.0	175.3	L	388.5	196.6	L
309.7	13.0	β_0 (*Pbcm*)	330.1	66.1	RIV	350.6	155.8	L	370.0	176.3	L	389.5	197.7	L
310.7	13.9	β_0 (*Pbcm*)	331.2	67.9	L	351.6	156.8	L	371.1	177.5	L	390.6	198.9	L
311.8	14.8	β_0 (*Pbcm*)	332.2	136.8	L	352.7	157.8	L	372.1	178.6	L	391.6	200.1	L
312.8	15.7	β'_0 (*Pbcm*)	333.2	137.9	L									

Table 14. Thermodynamic Data of C_{28}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	δ_0 ($P2_1/a$)	313.8	14.9	δ_0 ($P2_1/a$)	334.3	122.3	L	353.7	149.8	L	373.1	167.5	L
294.4	0.7	δ_0 ($P2_1/a$)	314.8	15.7	δ_0 ($P2_1/a$)	335.2	133.3	L	354.7	150.6	L	374.1	168.5	L
295.4	1.5	δ_0 ($P2_1/a$)	315.8	16.5	δ_0 ($P2_1/a$)	336.3	134.2	L	355.7	151.5	L	375.1	169.4	L
296.4	2.2	δ_0 ($P2_1/a$)	316.9	17.2	δ_0 ($P2_1/a$)	337.3	135.1	L	356.7	152.4	L	376.1	170.4	L
297.4	2.9	δ_0 ($P2_1/a$)	317.9	18.0	δ_0 ($P2_1/a$)	338.3	136.0	L	357.7	153.3	L	377.2	171.3	L
298.5	3.7	δ_0 ($P2_1/a$)	318.9	18.8	δ_0 ($P2_1/a$)	339.3	137.0	L	358.8	154.2	L	378.2	172.3	L
299.5	4.3	δ_0 ($P2_1/a$)	319.9	19.5	δ_0 ($P2_1/a$)	340.4	137.9	L	359.8	155.1	L	379.3	173.2	L
300.5	5.1	δ_0 ($P2_1/a$)	320.9	20.3	δ_0 ($P2_1/a$)	341.4	138.8	L	360.8	156.8	L	380.2	174.2	L
301.5	5.8	δ_0 ($P2_1/a$)	321.9	21.2	δ_0 ($P2_1/a$)	342.4	139.8	L	361.8	157.7	L	381.3	175.1	L
302.5	6.5	δ_0 ($P2_1/a$)	323.0	22.0	δ_0 ($P2_1/a$)	343.4	140.7	L	362.9	158.6	L	382.3	176.1	L
303.6	7.2	δ_0 ($P2_1/a$)	324.0	22.8	δ_0 ($P2_1/a$)	344.4	141.7	L	363.9	159.5	L	383.3	177.0	L
304.6	8.0	δ_0 ($P2_1/a$)	325.0	23.6	δ_0 ($P2_1/a$)	345.5	142.6	L	364.9	160.4	L	384.3	178.0	L
305.6	8.7	δ_0 ($P2_1/a$)	326.0	24.4	δ_0 ($P2_1/a$)	346.5	143.6	L	365.9	161.3	L	385.4	179.0	L
306.6	9.4	δ_0 ($P2_1/a$)	327.0	25.3	δ_0 ($P2_1/a$)	347.5	144.5	L	367.0	162.2	L	386.4	179.9	L
307.6	10.1	δ_0 ($P2_1/a$)	328.1	26.2	δ_0 ($P2_1/a$)	348.5	145.3	L	368.0	163.1	L	387.4	180.9	L
308.7	10.9	δ_0 ($P2_1/a$)	329.1	27.0	δ_0 ($P2_1/a$)	349.6	146.3	L	369.0	163.9	L	388.5	181.8	L
309.7	11.7	δ_0 ($P2_1/a$)	330.1	28.0	RIII	350.6	147.2	L	370.0	164.8	L	389.5	182.8	L
310.7	12.5	δ_0 ($P2_1/a$)	331.1	61.1	RIII	351.6	148.0	L	371.1	165.7	L	390.5	183.3	L
311.7	13.3	δ_0 ($P2_1/a$)	332.2	66.2	RIV	352.6	148.9	L	372.1	166.6	L	391.5	156.8	L
312.8	14.0	δ_0 ($P2_1/a$)	333.2	67.9	L									

Table 15. Thermodynamic Data of C_{29}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	313.8	16.3	β_0 (*Pbcm*)	334.2	70.5	RIII	353.7	33.8	L	373.1	164.7	L
294.4	0.8	β_0 (*Pbcm*)	314.8	17.1	β'_0 (*Pbcm*)	335.3	71.9	RIII	354.7	48.5	L	374.1	165.7	L
295.4	1.6	β_0 (*Pbcm*)	315.8	18.1	β'_0 (*Pbcm*)	336.3	85.7	L	355.7	67.1	L	375.1	166.6	L
296.4	2.3	β_0 (*Pbcm*)	316.9	19.0	β'_0 (*Pbcm*)	337.3	141.0	L	356.7	68.8	L	376.1	167.6	L
297.4	3.1	β_0 (*Pbcm*)	317.9	19.9	β'_0 (*Pbcm*)	338.3	142.0	L	357.8	70.5	L	377.2	168.5	L
298.5	3.9	β_0 (*Pbcm*)	318.9	20.7	β'_0 (*Pbcm*)	339.3	142.9	L	358.8	71.9	L	378.2	169.5	L
299.5	4.7	β_0 (*Pbcm*)	319.9	21.7	β'_0 (*Pbcm*)	340.4	143.9	L	359.8	85.7	L	379.2	170.5	L
300.5	5.4	β_0 (*Pbcm*)	321.0	22.6	β'_0 (*Pbcm*)	341.4	144.8	L	360.8	153.4	L	380.2	171.5	L
301.5	6.3	β_0 (*Pbcm*)	322.0	23.6	β'_0 (*Pbcm*)	342.4	145.8	L	361.8	154.4	L	381.3	172.4	L
302.5	7.1	β_0 (*Pbcm*)	323.0	24.5	β'_0 (*Pbcm*)	343.4	146.7	L	362.9	155.3	L	382.3	173.3	L
303.6	7.9	β_0 (*Pbcm*)	324.0	25.5	B (*Aa*)	344.5	147.6	L	363.9	156.3	L	383.3	174.3	L
304.6	8.6	β_0 (*Pbcm*)	325.0	27.7	B (*Aa*)	345.5	148.6	L	364.9	157.2	L	384.3	175.2	L
305.6	9.5	β_0 (*Pbcm*)	326.1	29.6	B (*Aa*)	346.5	149.5	L	365.9	158.2	L	385.3	176.2	L
306.6	10.3	β_0 (*Pbcm*)	327.1	30.6	B (*Aa*)	347.5	150.5	L	366.9	159.1	L	386.4	177.2	L
307.7	11.2	β_0 (*Pbcm*)	328.1	31.6	B (*Aa*)	348.5	151.5	L	368.0	160.1	L	387.4	178.2	L
308.7	12.0	β_0 (*Pbcm*)	329.1	32.6	B (*Aa*)	349.6	152.4	L	369.0	161.0	L	388.4	179.2	L
309.7	12.8	β_0 (*Pbcm*)	330.1	33.8	B (*Aa*)	350.6	30.6	L	370.0	161.9	L	389.5	180.2	L
310.7	13.7	β_0 (*Pbcm*)	331.1	48.5	RIII	351.6	31.6	L	371.0	162.9	L	390.5	181.2	L
311.8	14.5	β_0 (*Pbcm*)	332.2	67.1	RIII	352.6	32.6	L	372.1	163.7	L	391.5	182.1	L
312.8	15.3	β_0 (*Pbcm*)	333.2	68.8	RIII									

Table 16. Thermodynamic Data of C_{30}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	δ_0 ($P2_1/a$)	313.8	18.8	δ_0 ($P2_1/a$)	334.2	72.8	RIII	353.7	171.0	L	373.1	189.4	L
294.4	1.0	δ_0 ($P2_1/a$)	314.8	19.7	δ_0 ($P2_1/a$)	335.3	81.6	RIII	354.7	171.9	L	374.1	190.3	L
295.4	2.0	δ_0 ($P2_1/a$)	315.8	20.8	δ_0 ($P2_1/a$)	336.3	83.8	RIV	355.7	172.9	L	375.2	191.3	L
296.4	2.9	δ_0 ($P2_1/a$)	316.9	21.9	δ_0 ($P2_1/a$)	337.3	87.0	RIV	356.7	173.8	L	376.2	192.3	L
297.4	3.8	δ_0 ($P2_1/a$)	317.9	22.9	δ_0 ($P2_1/a$)	338.3	117.1	L	357.8	174.8	L	377.2	193.2	L
298.5	4.7	δ_0 ($P2_1/a$)	318.9	24.1	δ_0 ($P2_1/a$)	339.3	157.3	L	358.8	175.7	L	378.2	194.3	L
299.5	5.6	δ_0 ($P2_1/a$)	319.9	25.1	δ_0 ($P2_1/a$)	340.4	158.3	L	359.8	176.7	L	379.3	195.3	L
300.5	6.5	δ_0 ($P2_1/a$)	321.0	26.2	δ_0 ($P2_1/a$)	341.4	159.4	L	360.8	177.7	L	380.3	196.3	L
301.5	7.5	δ_0 ($P2_1/a$)	322.0	27.1	δ_0 ($P2_1/a$)	342.4	160.4	L	361.8	178.7	L	381.3	197.3	L
302.6	8.4	δ_0 ($P2_1/a$)	323.0	28.0	δ_0 ($P2_1/a$)	343.4	161.4	L	362.9	179.7	L	382.3	198.4	L
303.6	9.3	δ_0 ($P2_1/a$)	324.0	29.0	δ_0 ($P2_1/a$)	344.5	162.4	L	363.9	180.6	L	383.3	199.5	L
304.6	10.3	δ_0 ($P2_1/a$)	325.0	30.1	δ_0 ($P2_1/a$)	345.5	163.4	L	364.9	181.6	L	384.4	200.5	L
305.6	11.3	δ_0 ($P2_1/a$)	326.0	31.1	δ_0 ($P2_1/a$)	346.5	164.4	L	366.0	182.5	L	385.4	201.6	L
306.6	12.2	δ_0 ($P2_1/a$)	327.1	32.2	δ_0 ($P2_1/a$)	347.5	165.3	L	367.0	183.5	L	386.4	202.7	L
307.7	13.1	δ_0 ($P2_1/a$)	328.1	33.3	δ_0 ($P2_1/a$)	348.6	166.2	L	368.0	184.4	L	387.5	203.8	L
308.7	14.0	δ_0 ($P2_1/a$)	329.1	34.6	δ_0 ($P2_1/a$)	349.6	167.2	L	369.0	185.4	L	388.5	204.8	L
309.7	15.0	δ_0 ($P2_1/a$)	330.1	35.9	δ_0 ($P2_1/a$)	350.6	168.2	L	370.0	186.4	L	389.5	205.9	L
310.7	15.9	δ_0 ($P2_1/a$)	331.2	37.3	δ_0 ($P2_1/a$)	351.6	169.1	L	371.1	187.4	L	390.5	207.1	L
311.8	16.9	δ_0 ($P2_1/a$)	332.2	39.5	RIII	352.6	170.0	L	372.1	188.4	L	391.6	208.2	L
312.8	17.8	δ_0 ($P2_1/a$)	333.2	58.2	RIII									

Table 17. Thermodynamic Data of C_{31}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.3 K ($H^T_{293.3}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase
293.3	0.0	β_0 (*Pbcm*)	319.9	22.6	β_0 (*Pbcm*)	346.5	164.7	L	372.1	191.8	L	397.7	221.1	L
294.4	0.8	β_0 (*Pbcm*)	320.9	23.7	β_0 (*Pbcm*)	347.5	165.8	L	373.1	193.0	L	398.8	222.3	L
295.4	1.6	β_0 (*Pbcm*)	322.0	24.7	β_0 (*Pbcm*)	348.5	166.9	L	374.1	194.1	L	399.8	223.4	L
296.4	2.4	β_0 (*Pbcm*)	323.0	25.7	β_0 (*Pbcm*)	349.5	168.0	L	375.2	195.3	L	400.8	224.6	L
297.4	3.2	β_0 (*Pbcm*)	324.0	26.7	β_0 (*Pbcm*)	350.6	169.1	L	376.2	196.4	L	401.9	225.7	L
298.5	4.0	β_0 (*Pbcm*)	325.0	27.7	β_0 (*Pbcm*)	351.6	170.2	L	377.2	197.6	L	402.9	226.8	L
299.5	4.8	β_0 (*Pbcm*)	326.0	28.7	β_0 (*Pbcm*)	352.6	171.3	L	378.2	198.8	L	403.9	228.0	L
300.5	5.6	β_0 (*Pbcm*)	327.1	29.8	β_0 (*Pbcm*)	353.6	172.3	L	379.3	200.0	L	405.0	229.3	L
301.5	6.4	β_0 (*Pbcm*)	328.1	31.5	B (*Aa*)	354.7	173.4	L	380.3	201.1	L	406.0	230.5	L
302.5	7.3	β_0 (*Pbcm*)	329.1	34.2	B (*Aa*)	355.7	174.5	L	381.3	202.3	L	407.0	231.6	L
303.6	8.1	β_0 (*Pbcm*)	330.1	35.4	B (*Aa*)	356.7	175.7	L	382.3	203.4	L	408.0	232.8	L
304.6	9.0	β_0 (*Pbcm*)	331.2	36.6	B (*Aa*)	357.7	176.9	L	383.4	204.5	L	409.1	234.1	L
305.6	9.8	β_0 (*Pbcm*)	332.2	37.7	B (*Aa*)	358.8	178.0	L	384.4	205.8	L	410.1	235.3	L
306.6	10.7	β_0 (*Pbcm*)	333.2	38.9	B (*Aa*)	359.8	179.1	L	385.4	207.0	L	411.2	236.5	L
307.7	11.6	β_0 (*Pbcm*)	334.2	40.1	B (*Aa*)	360.8	180.1	L	386.4	208.2	L	412.2	237.7	L
308.7	12.5	β_0 (*Pbcm*)	335.2	41.6	RIII	361.8	181.1	L	387.5	209.4	L	413.2	238.9	L
309.7	13.3	β_0 (*Pbcm*)	336.3	78.1	RIII	362.9	182.2	L	388.5	210.6	L	414.2	240.1	L
310.7	14.2	β_0 (*Pbcm*)	337.3	80.3	RIII	363.9	183.3	L	389.5	211.7	L	415.3	241.3	L
311.8	15.0	β_0 (*Pbcm*)	338.3	82.3	RIII	364.9	184.4	L	390.5	212.9	L	416.3	242.5	L
312.8	15.9	β_0 (*Pbcm*)	339.3	84.2	RIII	365.9	185.6	L	391.6	214.1	L	417.3	243.6	L
313.8	16.9	β_0 (*Pbcm*)	340.4	104.5	L	366.9	186.6	L	392.6	215.3	L	418.3	244.8	L
314.8	17.8	β_0 (*Pbcm*)	341.4	159.1	L	368.0	187.7	L	393.6	216.4	L	419.4	246.0	L
315.8	18.7	β_0 (*Pbcm*)	342.4	160.2	L	369.0	188.8	L	394.7	217.6	L	420.4	247.2	L
316.9	19.6	β_0 (*Pbcm*)	343.4	161.3	L	370.0	189.8N	L	395.7	218.7	L	421.4	248.4	L
317.9	20.6	β_0 (*Pbcm*)	344.4	162.4	L	371.1	190.8	L	396.7	219.9	L	422.5	249.7	L
318.9	21.6	β_0 (*Pbcm*)	345.5	163.5	L									

Table 18. Thermodynamic Data of C_{32}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	δ_0 ($P2_1/a$)	313.8	17.4	δ_0 ($P2_1/a$)	334.2	37.3	δ_0 ($P2_1/a$)	354.6	178.5	L	374.0	198.2	L
294.4	0.8	δ_0 ($P2_1/a$)	314.8	18.3	δ_0 ($P2_1/a$)	335.2	38.6	δ_0 ($P2_1/a$)	355.6	179.5	L	375.0	199.2	L
295.4	1.7	δ_0 ($P2_1/a$)	315.8	19.2	δ_0 ($P2_1/a$)	336.2	39.8	δ_0 ($P2_1/a$)	356.6	180.5	L	376.0	200.3	L
296.4	2.5	δ_0 ($P2_1/a$)	316.8	20.1	δ_0 ($P2_1/a$)	337.2	41.3	δ_0 ($P2_1/a$)	357.7	181.5	L	377.1	201.4	L
297.4	3.3	δ_0 ($P2_1/a$)	317.9	21.0	δ_0 ($P2_1/a$)	338.3	48.0	RIII	358.7	182.6	L	378.1	202.5	L
298.4	4.2	δ_0 ($P2_1/a$)	318.9	21.9	δ_0 ($P2_1/a$)	339.3	85.1	RIII	359.7	183.6	L	379.1	203.5	L
299.5	5.0	δ_0 ($P2_1/a$)	319.9	22.8	δ_0 ($P2_1/a$)	340.3	87.1	RIII	360.7	184.6	L	380.1	204.6	L
300.5	5.9	δ_0 ($P2_1/a$)	320.9	23.7	δ_0 ($P2_1/a$)	341.3	89.0	RIII	361.7	185.7	L	381.2	205.7	L
301.5	6.7	δ_0 ($P2_1/a$)	321.9	24.5	δ_0 ($P2_1/a$)	342.4	114.9	L	362.8	186.8	L	382.2	206.8	L
302.5	7.6	δ_0 ($P2_1/a$)	322.9	25.4	δ_0 ($P2_1/a$)	343.4	167.2	L	363.8	187.8	L	383.2	207.9	L
303.5	8.5	δ_0 ($P2_1/a$)	324.0	26.3	δ_0 ($P2_1/a$)	344.4	168.3	L	364.8	188.8	L	384.2	209.0	L
304.6	9.4	δ_0 ($P2_1/a$)	325.0	27.2	δ_0 ($P2_1/a$)	345.4	169.3	L	365.8	189.9	L	385.3	210.1	L
305.6	10.3	δ_0 ($P2_1/a$)	326.0	28.2	δ_0 ($P2_1/a$)	346.4	170.4	L	366.8	190.9	L	386.3	211.2	L
306.6	11.2	δ_0 ($P2_1/a$)	327.0	29.3	δ_0 ($P2_1/a$)	347.5	171.4	L	367.9	192.0	L	387.3	212.3	L
307.6	12.0	δ_0 ($P2_1/a$)	328.0	30.4	δ_0 ($P2_1/a$)	348.5	172.4	L	368.9	193.0	L	388.3	213.4	L
308.7	12.9	δ_0 ($P2_1/a$)	329.1	31.6	δ_0 ($P2_1/a$)	349.5	173.4	L	369.9	194.1	L	389.4	214.6	L
309.7	13.8	δ_0 ($P2_1/a$)	330.1	32.8	δ_0 ($P2_1/a$)	350.5	174.5	L	370.9	195.1	L	390.4	215.6	L
310.7	14.7	δ_0 ($P2_1/a$)	331.1	33.8	δ_0 ($P2_1/a$)	351.5	175.5	L	372.0	196.2	L	391.4	216.7	L
311.7	15.6	δ_0 ($P2_1/a$)	332.1	35.0	δ_0 ($P2_1/a$)	352.6	176.5	L	373.0	197.2	L	392.4	217.8	L
312.7	16.5	δ_0 ($P2_1/a$)	333.1	36.1	δ_0 ($P2_1/a$)	353.6	177.5	L						

Table 19. Thermodynamic Data of C_{33}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	319.9	26.9	β_0 (*Pbcm*)	346.5	177.8	L	372.1	205.5	L	397.7	232.3	L
294.4	1.0	β_0 (*Pbcm*)	321.0	28.0	β_0 (*Pbcm*)	347.5	179.0	L	373.1	206.6	L	398.8	233.3	L
295.4	2.0	β_0 (*Pbcm*)	322.0	29.2	β_0 (*Pbcm*)	348.6	180.1	L	374.2	207.7	L	399.8	234.4	L
296.4	2.9	β_0 (*Pbcm*)	323.0	30.3	β_0 (*Pbcm*)	349.6	181.2	L	375.2	208.8	L	400.8	235.6	L
297.4	3.8	β_0 (*Pbcm*)	324.0	31.5	β_0 (*Pbcm*)	350.6	182.4	L	376.2	209.7	L	401.9	236.7	L
298.5	4.7	β_0 (*Pbcm*)	325.0	32.7	β_0 (*Pbcm*)	351.6	183.5	L	377.2	210.7	L	402.9	237.8	L
299.5	5.7	β_0 (*Pbcm*)	326.1	33.9	β_0 (*Pbcm*)	352.7	184.6	L	378.2	211.7	L	403.9	238.9	L
300.5	6.7	β_0 (*Pbcm*)	327.1	35.2	β_0 (*Pbcm*)	353.7	185.7	L	379.3	212.8	L	404.9	240.0	L
301.5	7.6	β_0 (*Pbcm*)	328.1	36.4	β_0 (*Pbcm*)	354.7	186.8	L	380.3	213.8	L	406.0	241.2	L
302.5	8.6	β_0 (*Pbcm*)	329.1	37.7	β_0 (*Pbcm*)	355.7	187.9	L	381.3	214.8	L	407.0	242.4	L
303.6	9.7	β_0 (*Pbcm*)	330.1	39.0	B (*Aa*)	356.8	189.1	L	382.3	215.8	L	408.0	243.6	L
304.6	10.7	β_0 (*Pbcm*)	331.2	40.2	B (*Aa*)	357.8	190.2	L	383.4	216.9	L	409.1	244.8	L
305.6	11.7	β_0 (*Pbcm*)	332.2	41.6	B (*Aa*)	358.8	191.2	L	384.4	218.0	L	410.1	246.1	L
306.6	12.8	β_0 (*Pbcm*)	333.2	43.1	B (*Aa*)	359.8	192.4	L	385.4	219.1	L	411.1	247.3	L
307.7	13.9	β_0 (*Pbcm*)	334.2	44.6	B (*Aa*)	360.8	193.6	L	386.4	220.1	L	412.2	248.7	L
308.7	14.9	β_0 (*Pbcm*)	335.3	46.1	C (*A2*)	361.9	194.7	L	387.5	221.2	L	413.2	250.0	L
309.7	15.9	β_0 (*Pbcm*)	336.3	47.9	C (*A2*)	362.9	195.8	L	388.5	222.3	L	414.2	251.4	L
310.7	17.0	β_0 (*Pbcm*)	337.3	50.3	C (*A2*)	363.9	196.9	L	389.5	223.4	L	415.3	252.6	L
311.8	18.0	β_0 (*Pbcm*)	338.3	55.6	RIII	364.9	198.1	L	390.6	224.6	L	416.3	253.9	L
312.8	19.1	β_0 (*Pbcm*)	339.4	77.9	RIII	366.0	199.2	L	391.6	225.7	L	417.3	255.3	L
313.8	20.2	β_0 (*Pbcm*)	340.4	85.2	RIII	367.0	200.3	L	392.6	226.8	L	418.4	256.7	L
314.8	21.3	β_0 (*Pbcm*)	341.4	87.2	RIII	368.0	201.4	L	393.6	227.9	L	419.4	258.0	L
315.9	22.4	β_0 (*Pbcm*)	342.4	89.2	RIII	369.0	202.4	L	394.7	228.9	L	420.4	259.3	L
316.9	23.5	β_0 (*Pbcm*)	343.5	93.9	L	370.1	203.5	L	395.7	230.0	L	421.5	260.7	L
317.9	24.7	β_0 (*Pbcm*)	344.5	175.5	L	371.1	204.5	L	396.7	231.1	L	422.5	262.1	L
318.9	25.8	β_0 (*Pbcm*)	345.5	176.7	L									

Table 20. Thermodynamic Data of C_{34}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	δ_0 ($P2_1/a$)	319.9	24.5	δ_0 ($P2_1/a$)	346.5	181.7	L	372.1	211.4	L	397.7	242.6	L
294.4	0.8	δ_0 ($P2_1/a$)	321.0	25.7	δ_0 ($P2_1/a$)	347.5	182.9	L	373.1	212.6	L	398.8	243.7	L
295.4	1.6	δ_0 ($P2_1/a$)	322.0	26.8	δ_0 ($P2_1/a$)	348.6	184.0	L	374.1	213.8	L	399.8	245.0	L
296.4	2.3	δ_0 ($P2_1/a$)	323.0	27.9	δ_0 ($P2_1/a$)	349.6	185.2	L	375.2	215.0	L	400.8	246.1	L
297.4	3.2	δ_0 ($P2_1/a$)	324.0	29.1	δ_0 ($P2_1/a$)	350.6	186.3	L	376.2	216.2	L	401.9	247.3	L
298.5	4.0	δ_0 ($P2_1/a$)	325.0	30.2	δ_0 ($P2_1/a$)	351.6	187.4	L	377.2	217.5	L	402.9	248.5	L
299.5	4.8	δ_0 ($P2_1/a$)	326.1	31.3	δ_0 ($P2_1/a$)	352.7	188.6	L	378.2	218.8	L	403.9	249.7	L
300.5	5.7	δ_0 ($P2_1/a$)	327.1	32.4	δ_0 ($P2_1/a$)	353.7	189.8	L	379.3	220.0	L	405.0	250.9	L
301.5	6.6	δ_0 ($P2_1/a$)	328.1	33.6	δ_0 ($P2_1/a$)	354.7	191.0	L	380.3	221.2	L	406.0	252.1	L
302.5	7.5	δ_0 ($P2_1/a$)	329.1	34.8	δ_0 ($P2_1/a$)	355.7	192.3	L	381.3	222.5	L	407.0	253.4	L
303.6	8.4	δ_0 ($P2_1/a$)	330.1	36.1	δ_0 ($P2_1/a$)	356.7	193.4	L	382.3	223.8	L	408.1	254.5	L
304.6	9.3	δ_0 ($P2_1/a$)	331.2	37.4	δ_0 ($P2_1/a$)	357.8	194.6	L	383.4	225.1	L	409.1	255.8	L
305.6	10.2	δ_0 ($P2_1/a$)	332.2	38.7	δ_0 ($P2_1/a$)	358.8	195.8	L	384.4	226.4	L	410.1	257.0	L
306.6	11.1	δ_0 ($P2_1/a$)	333.2	40.0	δ_0 ($P2_1/a$)	359.8	197.0	L	385.4	227.7	L	411.1	258.2	L
307.7	12.0	δ_0 ($P2_1/a$)	334.2	41.4	δ_0 ($P2_1/a$)	360.8	198.1	L	386.5	228.9	L	412.2	259.4	L
308.7	13.0	δ_0 ($P2_1/a$)	335.3	42.8	δ_0 ($P2_1/a$)	361.9	199.3	L	387.5	230.2	L	413.2	260.7	L
309.7	13.9	δ_0 ($P2_1/a$)	336.3	44.3	δ_0 ($P2_1/a$)	362.9	200.5	L	388.5	231.5	L	414.2	261.9	L
310.7	14.9	δ_0 ($P2_1/a$)	337.3	45.9	δ_0 ($P2_1/a$)	363.9	201.7	L	389.5	232.8	L	415.3	263.2	L
311.8	15.8	δ_0 ($P2_1/a$)	338.3	47.5	δ_0 ($P2_1/a$)	364.9	202.8	L	390.6	234.1	L	416.3	264.4	L
312.8	16.8	δ_0 ($P2_1/a$)	339.4	49.3	δ_0 ($P2_1/a$)	366.0	204.0	L	391.6	235.4	L	417.3	265.7	L
313.8	17.8	δ_0 ($P2_1/a$)	340.4	51.2	δ_0 ($P2_1/a$)	367.0	205.2	L	392.6	236.6	L	418.3	266.9	L
314.8	18.8	δ_0 ($P2_1/a$)	341.4	54.0	RIII	368.0	206.4	L	393.6	237.8	L	419.4	268.2	L
315.8	19.9	δ_0 ($P2_1/a$)	342.4	90.0	RIII	369.0	207.6	L	394.7	239.0	L	420.4	269.4	L
316.9	21.1	δ_0 ($P2_1/a$)	343.5	92.3	RIII	370.0	208.8	L	395.7	240.2	L	421.4	270.7	L
317.9	22.3	δ_0 ($P2_1/a$)	344.5	95.1	RIII	371.1	210.1	L	396.7	241.4	L	422.5	271.9	L
318.9	23.4	δ_0 ($P2_1/a$)	345.5	111.9	L									

Table 21. Thermodynamic Data of C_{35}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	326.1	33.6	β_0 (*Pbcm*)	358.8	204.3	L	391.6	241.5	L
294.4	0.9	β_0 (*Pbcm*)	327.1	34.7	β_0 (*Pbcm*)	359.8	205.6	L	392.6	242.8	L
295.4	1.8	β_0 (*Pbcm*)	328.1	36.0	β_0 (*Pbcm*)	360.8	206.7	L	393.6	244.0	L
296.4	2.8	β_0 (*Pbcm*)	329.1	37.2	B (*Aa*)	361.8	208.0	L	394.6	245.3	L
297.4	3.7	β_0 (*Pbcm*)	330.1	38.8	B (*Aa*)	362.9	209.3	L	395.7	246.5	L
298.5	4.6	β_0 (*Pbcm*)	331.2	40.4	B (*Aa*)	363.9	210.4	L	396.7	247.8	L
299.5	5.6	β_0 (*Pbcm*)	332.2	41.7	B (*Aa*)	364.9	211.7	L	397.7	249.1	L
300.5	6.6	β_0 (*Pbcm*)	333.2	43.0	B (*Aa*)	365.9	212.9	L	398.7	250.3	L
301.5	7.6	β_0 (*Pbcm*)	334.2	44.3	B (*Aa*)	367.0	214.1	L	399.8	251.6	L
302.5	8.6	β_0 (*Pbcm*)	335.3	45.5	B (*Aa*)	368.0	215.4	L	400.8	252.9	L
303.6	9.6	β_0 (*Pbcm*)	336.3	46.9	B (*Aa*)	369.0	216.7	L	401.8	254.1	L
304.6	10.6	β_0 (*Pbcm*)	337.3	48.2	B (*Aa*)	370.0	217.7	L	402.8	255.4	L
305.6	11.7	β_0 (*Pbcm*)	338.3	50.2	C (*A2*)	371.1	218.9	L	403.9	256.6	L
306.6	12.7	β_0 (*Pbcm*)	339.3	53.0	C (*A2*)	372.1	220.1	L	404.9	257.9	L
307.7	13.7	β_0 (*Pbcm*)	340.4	54.9	C (*A2*)	373.1	221.2	L	405.9	259.2	L
308.7	14.8	β_0 (*Pbcm*)	341.4	56.7	C (*A2*)	374.1	222.2	L	407.0	260.5	L
309.7	15.8	β_0 (*Pbcm*)	342.4	58.6	C (*A2*)	375.1	223.3	L	408.0	261.8	L
310.7	16.9	β_0 (*Pbcm*)	343.4	60.7	C (*A2*)	376.2	224.3	L	409.0	263.1	L
311.8	17.9	β_0 (*Pbcm*)	344.5	63.3	RIII	377.2	225.4	L	410.1	264.4	L
312.8	19.0	β_0 (*Pbcm*)	345.5	98.8	RIII	378.2	226.4	L	411.1	265.7	L
313.8	20.2	β_0 (*Pbcm*)	346.5	102.6	L	379.2	227.6	L	412.1	267.0	L
314.8	21.2	β_0 (*Pbcm*)	347.5	185.5	L	380.3	228.6	L	413.1	268.3	L
315.8	22.3	β_0 (*Pbcm*)	348.6	192.3	L	381.3	229.8	L	414.2	269.6	L
316.9	23.5	β_0 (*Pbcm*)	349.6	193.6	L	382.3	231.0	L	415.2	270.9	L
317.9	24.5	β_0 (*Pbcm*)	350.6	194.7	L	383.3	232.1	L	416.2	272.2	L
318.9	25.6	β_0 (*Pbcm*)	351.6	195.9	L	384.4	233.3	L	417.3	273.6	L
319.9	26.8	β_0 (*Pbcm*)	352.6	197.0	L	385.4	234.4	L	418.3	274.9	L
321.0	27.9	β_0 (*Pbcm*)	353.7	198.2	L	386.4	235.4	L	419.3	276.3	L
322.0	29.0	β_0 (*Pbcm*)	354.7	199.4	L	387.4	236.6	L	420.3	277.6	L
323.0	30.1	β_0 (*Pbcm*)	355.7	200.6	L	388.5	237.7	L	421.4	279.0	L
324.0	31.2	β_0 (*Pbcm*)	356.7	201.8	L	389.5	238.9	L	422.4	280.3	L
325.0	32.4	β_0 (*Pbcm*)	357.8	203.1	L	390.5	240.2	L			

Table 22. Thermodynamic Data of C_{36}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	δ_0 ($P2_1/a$)	326.1	38.5	δ_0 ($P2_1/a$)	358.8	209.7	L	391.5	247.8	L
294.4	1.1	δ_0 ($P2_1/a$)	327.1	39.9	δ_0 ($P2_1/a$)	359.8	211.0	L	392.6	249.0	L
295.4	2.1	δ_0 ($P2_1/a$)	328.1	41.5	δ_0 ($P2_1/a$)	360.8	212.3	L	393.6	250.1	L
296.4	3.2	δ_0 ($P2_1/a$)	329.1	43.0	δ_0 ($P2_1/a$)	361.9	213.6	L	394.6	251.3	L
297.4	4.3	δ_0 ($P2_1/a$)	330.2	44.7	δ_0 ($P2_1/a$)	362.9	214.8	L	395.6	252.5	L
298.5	5.3	δ_0 ($P2_1/a$)	331.2	46.4	δ_0 ($P2_1/a$)	363.9	216.1	L	396.7	253.7	L
299.5	6.4	δ_0 ($P2_1/a$)	332.2	48.1	δ_0 ($P2_1/a$)	364.9	217.3	L	397.7	254.9	L
300.5	7.6	δ_0 ($P2_1/a$)	333.2	49.9	δ_0 ($P2_1/a$)	366.0	218.6	L	398.7	256.1	L
301.5	8.7	δ_0 ($P2_1/a$)	334.2	51.8	δ_0 ($P2_1/a$)	367.0	219.9	L	399.7	257.3	L
302.5	9.8	δ_0 ($P2_1/a$)	335.3	53.4	δ_0 ($P2_1/a$)	368.0	221.1	L	400.8	258.4	L
303.6	11.0	δ_0 ($P2_1/a$)	336.3	55.0	δ_0 ($P2_1/a$)	369.0	222.5	L	401.8	259.7	L
304.6	12.2	δ_0 ($P2_1/a$)	337.3	56.8	δ_0 ($P2_1/a$)	370.0	223.6	L	402.8	260.9	L
305.6	13.4	δ_0 ($P2_1/a$)	338.3	58.5	δ_0 ($P2_1/a$)	371.1	224.7	L	403.9	262.2	L
306.6	14.6	δ_0 ($P2_1/a$)	339.4	60.5	δ_0 ($P2_1/a$)	372.1	225.9	L	404.9	263.5	L
307.7	15.7	δ_0 ($P2_1/a$)	340.4	62.6	δ_0 ($P2_1/a$)	373.1	227.1	L	405.9	264.8	L
308.7	16.8	δ_0 ($P2_1/a$)	341.4	64.9	δ_0 ($P2_1/a$)	374.1	228.2	L	406.9	266.2	L
309.7	18.0	δ_0 ($P2_1/a$)	342.4	67.4	δ_0 ($P2_1/a$)	375.1	229.3	L	408.0	267.5	L
310.7	19.2	δ_0 ($P2_1/a$)	343.4	70.0	RIII	376.2	230.4	L	409.0	268.9	L
311.8	20.4	δ_0 ($P2_1/a$)	344.5	73.1	RIII	377.2	231.5	L	410.0	270.3	L
312.8	21.6	δ_0 ($P2_1/a$)	345.5	76.9	RIII	378.2	232.6	L	411.1	271.6	L
313.8	22.9	δ_0 ($P2_1/a$)	346.5	94.5	L	379.2	233.7	L	412.1	273.0	L
314.8	24.1	δ_0 ($P2_1/a$)	347.5	118.1	L	380.3	234.8	L	413.1	274.4	L
315.9	25.4	δ_0 ($P2_1/a$)	348.6	156.1	L	381.3	235.9	L	414.2	275.7	L
316.9	26.5	δ_0 ($P2_1/a$)	349.6	198.0	L	382.3	237.2	L	415.2	277.1	L
317.9	27.8	δ_0 ($P2_1/a$)	350.6	199.2	L	383.3	238.3	L	416.2	278.5	L
318.9	29.1	δ_0 ($P2_1/a$)	351.6	200.5	L	384.4	239.5	L	417.2	279.9	L
319.9	30.3	δ_0 ($P2_1/a$)	352.7	201.7	L	385.4	240.7	L	418.3	281.3	L
321.0	31.6	δ_0 ($P2_1/a$)	353.7	203.1	L	386.4	241.8	L	419.3	282.7	L
322.0	32.9	δ_0 ($P2_1/a$)	354.7	204.3	L	387.4	242.9	L	420.3	284.1	L
323.0	34.2	δ_0 ($P2_1/a$)	355.7	205.6	L	388.4	244.1	L	421.4	285.5	L
324.0	35.6	δ_0 ($P2_1/a$)	356.7	207.0	L	389.5	245.3	L	422.4	286.9	L
325.0	37.0	δ_0 ($P2_1/a$)	357.8	208.4	L	390.5	246.6	L			

Table 23. Thermodynamic Data of C_{37}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	326.1	34.8	B(Aa)	358.8	213.0	L	391.6	255.5	L
294.4	1.0	β_0 (*Pbcm*)	327.1	36.6	B(Aa)	359.8	214.2	L	392.6	256.7	L
295.4	2.1	β_0 (*Pbcm*)	328.1	37.9	B(Aa)	360.8	215.6	L	393.6	258.0	L
296.4	3.1	β_0 (*Pbcm*)	329.1	39.2	B(Aa)	361.9	216.9	L	394.6	259.2	L
297.4	4.0	β_0 (*Pbcm*)	330.1	40.5	B(Aa)	362.9	218.3	L	395.7	260.3	L
298.5	5.0	β_0 (*Pbcm*)	331.2	41.7	B(Aa)	363.9	219.6	L	396.7	261.7	L
299.5	6.0	β_0 (*Pbcm*)	332.2	42.9	B(Aa)	364.9	220.9	L	397.7	262.9	L
300.5	7.0	β_0 (*Pbcm*)	333.2	44.1	B(Aa)	365.9	222.3	L	398.7	264.1	L
301.5	8.0	β_0 (*Pbcm*)	334.2	45.4	B(Aa)	367.0	223.6	L	399.8	265.3	L
302.5	9.0	β_0 (*Pbcm*)	335.3	46.7	B(Aa)	368.0	225.0	L	400.8	266.5	L
303.6	10.0	β_0 (*Pbcm*)	336.3	48.1	B(Aa)	369.0	226.3	L	401.8	267.8	L
304.6	11.1	β_0 (*Pbcm*)	337.3	49.5	C(A2)	370.0	227.6	L	402.8	268.9	L
305.6	12.1	β_0 (*Pbcm*)	338.3	52.6	C(A2)	371.1	228.8	L	403.9	270.1	L
306.6	13.2	β_0 (*Pbcm*)	339.4	54.3	C(A2)	372.1	230.2	L	404.9	271.3	L
307.7	14.2	β_0 (*Pbcm*)	340.4	56.0	C(A2)	373.1	231.6	L	405.9	272.6	L
308.7	15.3	β_0 (*Pbcm*)	341.4	57.7	C(A2)	374.1	233.0	L	407.0	273.9	L
309.7	16.4	β_0 (*Pbcm*)	342.4	59.5	C(A2)	375.2	234.3	L	408.0	275.1	L
310.7	17.5	β_0 (*Pbcm*)	343.5	61.3	C(A2)	376.2	235.6	L	409.0	276.3	
311.8	18.6	β_0 (*Pbcm*)	344.5	63.2	C(A2)	377.2	236.9	L	410.0	277.6	L
312.8	19.7	β_0 (*Pbcm*)	345.5	65.2	C(A2)	378.2	238.2	L	411.1	278.8	L
313.8	21.0	β_0 (*Pbcm*)	346.5	67.3	C(A2)	379.2	239.5	L	412.1	280.1	L
314.8	22.2	β_0 (*Pbcm*)	347.5	69.6	RIII	380.3	240.8	L	413.1	281.3	L
315.8	23.2	β_0 (*Pbcm*)	348.6	72.4	RIII	381.3	242.2	L	414.2	282.7	L
316.9	24.5	β_0 (*Pbcm*)	349.6	109.6	L	382.3	243.6	L	415.2	283.9	L
317.9	25.5	β_0 (*Pbcm*)	350.6	193.5	L	383.4	244.9	L	416.2	285.3	L
318.9	26.6	β_0 (*Pbcm*)	351.6	203.7	L	384.4	246.3	L	417.2	286.7	L
319.9	27.8	β_0 (*Pbcm*)	352.7	205.0	L	385.4	247.6	L	418.3	288.0	L
321.0	28.9	β_0 (*Pbcm*)	353.7	206.4	L	386.4	249.0	L	419.3	289.2	L
322.0	30.0	β_0 (*Pbcm*)	354.7	207.7	L	387.4	250.3	L	420.3	290.5	L
323.0	31.2	β_0 (*Pbcm*)	355.7	209.1	L	388.5	251.7	L	421.4	291.8	L
324.0	32.4	β_0 (*Pbcm*)	356.7	210.4	L	389.5	253.0	L	422.4	293.1	L
325.0	33.5	β_0 (*Pbcm*)	357.8	211.7	L	390.5	254.3	L			

Table 24. Thermodynamic Data of C_{38}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbca*)	326.1	35.5	β_0 (*Pbca*)	358.8	218.1	L	391.6	261.1	L
294.4	1.0	β_0 (*Pbca*)	327.1	36.8	β_0 (*Pbca*)	359.8	219.4	L	392.6	262.5	L
295.4	2.0	β_0 (*Pbca*)	328.1	38.1	β_0 (*Pbca*)	360.8	220.8	L	393.6	263.9	L
296.4	2.9	β_0 (*Pbca*)	329.1	39.3	β_0 (*Pbca*)	361.8	222.1	L	394.7	265.4	L
297.4	3.9	β_0 (*Pbca*)	330.2	40.6	β_0 (*Pbca*)	362.9	223.4	L	395.7	266.8	L
298.5	4.8	β_0 (*Pbca*)	331.2	42.0	β_0 (*Pbca*)	363.9	224.8	L	396.7	268.2	L
299.5	5.8	β_0 (*Pbca*)	332.2	43.4	β_0 (*Pbca*)	364.9	226.1	L	397.8	269.6	L
300.5	6.8	β_0 (*Pbca*)	333.2	44.8	β_0 (*Pbca*)	366.0	227.5	L	398.8	271.0	L
301.5	7.9	β_0 (*Pbca*)	334.3	46.2	β_0 (*Pbca*)	367.0	228.8	L	399.8	272.4	L
302.5	8.9	β_0 (*Pbca*)	335.3	47.7	β_0 (*Pbca*)	368.0	230.2	L	400.8	273.8	L
303.6	9.9	β_0 (*Pbca*)	336.3	49.2	β_0 (*Pbca*)	369.0	231.5	L	401.9	275.2	L
304.6	11.0	β_0 (*Pbca*)	337.3	50.8	β_0 (*Pbca*)	370.0	232.8	L	402.9	276.6	L
305.6	12.0	β_0 (*Pbca*)	338.3	52.4	β_0 (*Pbca*)	371.1	234.2	L	403.9	278.0	L
306.6	13.1	β_0 (*Pbca*)	339.4	54.1	β_0 (*Pbca*)	372.1	235.5	L	405.0	279.5	L
307.7	14.1	β_0 (*Pbca*)	340.4	55.8	β_0 (*Pbca*)	373.1	236.8	L	406.0	280.9	L
308.7	15.2	β_0 (*Pbca*)	341.4	57.6	β_0 (*Pbca*)	374.1	238.2	L	407.0	282.4	L
309.7	16.3	β_0 (*Pbca*)	342.4	59.5	β_0 (*Pbca*)	375.2	239.5	L	408.0	283.9	L
310.7	17.5	β_0 (*Pbca*)	343.5	61.6	β_0 (*Pbca*)	376.2	240.8	L	409.1	285.3	L
311.8	18.6	β_0 (*Pbca*)	344.5	63.8	β_0 (*Pbca*)	377.2	242.1	L	410.1	286.7	L
312.8	19.8	β_0 (*Pbca*)	345.5	66.1	β_0 (*Pbca*)	378.2	243.5	L	411.1	288.2	L
313.8	20.9	β_0 (*Pbca*)	346.5	68.7	β_0 (*Pbca*)	379.2	244.8	L	412.2	289.7	L
314.8	22.2	β_0 (*Pbca*)	347.5	71.7	β_0 (*Pbca*)	380.3	246.1	L	413.2	291.1	L
315.8	23.4	β_0 (*Pbca*)	348.6	75.5	RIII	381.3	247.5	L	414.2	292.6	L
316.9	24.6	β_0 (*Pbca*)	349.6	81.6	RIII	382.3	248.8	L	415.2	294.0	L
317.9	25.8	β_0 (*Pbca*)	350.6	122.0	L	383.4	250.1	L	416.3	295.5	L
318.9	26.9	β_0 (*Pbca*)	351.6	208.8	L	384.4	251.5	L	417.3	297.0	L
319.9	28.1	β_0 (*Pbca*)	352.6	210.2	L	385.4	252.9	L	418.3	298.5	L
321.0	29.3	β_0 (*Pbca*)	353.7	211.5	L	386.4	254.2	L	419.4	300.0	L
322.0	30.5	β_0 (*Pbca*)	354.7	212.8	L	387.5	255.6	L	420.4	301.5	L
323.0	31.7	β_0 (*Pbca*)	355.7	214.2	L	388.5	257.0	L	421.4	303.0	L
324.0	33.0	β_0 (*Pbca*)	356.7	215.5	L	389.5	258.4	L	422.4	304.6	L
325.0	34.3	β_0 (*Pbca*)	357.8	216.8	L	390.6	259.7	L			

Table 25. Thermodynamic Data of C_{41}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 (*Pbcm*)	326.0	36.6	β_0 (*Pbcm*)	358.7	223.8	L	390.4	267.3	L
294.4	1.0	β_0 (*Pbcm*)	327.0	37.9	β_0 (*Pbcm*)	359.7	225.2	L	391.4	268.7	L
295.4	2.1	β_0 (*Pbcm*)	328.1	39.2	β_0 (*Pbcm*)	360.7	226.5	L	392.4	270.1	L
296.4	3.1	β_0 (*Pbcm*)	329.1	40.5	β_0 (*Pbcm*)	361.7	227.9	L	393.5	271.6	L
297.4	4.1	β_0 (*Pbcm*)	330.1	41.8	β_0 (*Pbcm*)	362.8	229.2	L	394.5	273.2	L
298.5	5.2	β_0 (*Pbcm*)	331.1	43.1	β_0 (*Pbcm*)	363.8	230.6	L	395.5	274.7	L
299.5	6.3	β_0 (*Pbcm*)	332.2	44.4	β_0 (*Pbcm*)	364.8	231.9	L	396.5	276.3	L
300.5	7.4	β_0 (*Pbcm*)	333.2	45.8	β_0 (*Pbcm*)	365.8	233.4	L	397.6	277.8	L
301.5	8.5	β_0 (*Pbcm*)	334.2	47.1	β_0 (*Pbcm*)	366.8	234.7	L	398.6	279.4	L
302.5	9.5	β_0 (*Pbcm*)	335.2	48.6	β_0 (*Pbcm*)	367.9	235.9	L	399.6	281.0	L
303.6	10.6	β_0 (*Pbcm*)	336.2	50.0	β_0 (*Pbcm*)	368.9	237.2	L	400.7	282.6	L
304.6	11.7	β_0 (*Pbcm*)	337.3	51.4	B(Aa)	369.9	238.6	L	401.7	284.2	L
305.6	12.8	β_0 (*Pbcm*)	338.3	52.9	B(Aa)	370.9	239.9	L	402.7	285.7	L
306.6	13.9	β_0 (*Pbcm*)	339.3	54.4	B(Aa)	371.9	241.3	L	403.8	287.3	L
307.7	15.0	β_0 (*Pbcm*)	340.3	56.0	B(Aa)	373.0	242.6	L	404.8	288.9	L
308.7	16.2	β_0 (*Pbcm*)	341.3	57.6	B(Aa)	374.0	243.9	L	405.8	290.5	L
309.7	17.4	β_0 (*Pbcm*)	342.4	59.2	B(Aa)	375.0	245.2	L	406.9	292.1	L
310.7	18.5	β_0 (*Pbcm*)	343.4	60.9	B(Aa)	376.0	246.6	L	407.9	293.6	L
311.7	19.7	β_0 (*Pbcm*)	344.4	62.6	B(Aa)	377.1	247.9	L	408.9	295.3	L
312.8	20.9	β_0 (*Pbcm*)	345.4	64.5	B(Aa)	378.1	249.2	L	410.0	296.8	L
313.8	22.1	β_0 (*Pbcm*)	346.4	66.3	C(A2)	379.1	250.5	L	411.0	298.4	L
314.8	23.3	β_0 (*Pbcm*)	347.5	68.3	C(A2)	380.1	251.9	L	412.0	300.0	L
315.8	24.4	β_0 (*Pbcm*)	348.5	70.3	C(A2)	381.2	254.6	L	413.1	301.6	L
316.9	25.6	β_0 (*Pbcm*)	349.5	72.4	C(A2)	382.2	256.0	L	414.1	303.2	L
317.9	26.8	β_0 (*Pbcm*)	350.5	74.6	C(A2)	383.2	257.3	L	415.1	304.8	L
318.9	28.0	β_0 (*Pbcm*)	351.5	76.8	C(A2)	384.2	258.7	L	416.1	306.5	L
319.9	29.2	β_0 (*Pbcm*)	352.6	79.1	RIII	385.3	260.0	L	417.2	308.1	L
320.9	30.4	β_0 (*Pbcm*)	353.6	81.4	RIII	386.3	261.3	L	418.2	309.7	L
322.0	31.7	β_0 (*Pbcm*)	354.6	83.9	L	387.3	262.8	L	419.2	311.4	L
323.0	32.9	β_0 (*Pbcm*)	355.6	155.1	L	388.3	264.3	L	420.3	313.0	L
324.0	34.2	β_0 (*Pbcm*)	356.6	220.9	L	389.3	265.8	L	421.3	314.7	L
325.0	35.4	β_0 (*Pbcm*)	357.7	222.4	L						

Table 26. Thermodynamic Data of C_{44}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 298.3 K ($H^T_{298.3}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{298.3}$/kJ·mol^{-1}	phase
298.3	0.0	β_0 (*Pbca*)	333.0	50.1	β_0 (*Pbca*)	367.7	267.1	L	402.5	316.9	L
299.4	1.3	β_0 (*Pbca*)	334.0	52.0	β_0 (*Pbca*)	368.7	268.5	L	403.6	318.5	L
300.4	2.5	β_0 (*Pbca*)	335.0	54.0	β_0 (*Pbca*)	369.8	269.9	L	404.6	320.0	L
301.4	3.7	β_0 (*Pbca*)	336.0	56.1	β_0 (*Pbca*)	370.8	271.3	L	405.6	321.6	L
302.4	5.0	β_0 (*Pbca*)	337.1	58.3	C(A2)	371.8	272.7	L	406.7	323.1	L
303.4	6.2	β_0 (*Pbca*)	338.1	60.7	C(A2)	372.8	274.0	L	407.7	324.9	L
304.5	7.4	β_0 (*Pbca*)	339.1	63.1	C(A2)	373.8	275.5	L	408.7	326.7	L
305.5	8.6	β_0 (*Pbca*)	340.1	65.8	C(A2)	374.9	276.9	L	409.8	328.5	L
306.5	9.9	β_0 (*Pbca*)	341.2	68.5	C(A2)	375.9	278.5	L	410.8	330.3	L
307.5	11.2	β_0 (*Pbca*)	342.2	71.4	C(A2)	376.9	280.0	L	411.8	332.1	L
308.5	12.5	β_0 (*Pbca*)	343.2	74.0	C(A2)	377.9	281.3	L	412.8	333.8	L
309.5	13.8	β_0 (*Pbca*)	344.2	76.4	C(A2)	379.0	282.8	L	413.9	335.6	L
310.6	15.2	β_0 (*Pbca*)	345.2	78.7	C(A2)	380.0	284.2	L	414.9	337.4	L
311.6	16.5	β_0 (*Pbca*)	346.3	81.2	C(A2)	381.0	285.8	L	415.9	339.3	L
312.6	17.9	β_0 (*Pbca*)	347.3	83.7	C(A2)	382.0	287.3	L	417.0	341.1	L
313.6	19.3	β_0 (*Pbca*)	348.3	86.4	C(A2)	383.1	288.6	L	418.0	342.9	L
314.7	20.7	β_0 (*Pbca*)	349.3	89.1	C(A2)	384.1	290.0	L	419.0	344.7	L
315.7	22.2	β_0 (*Pbca*)	350.3	92.1	C(A2)	385.1	291.5	L	420.0	346.5	L
316.7	23.5	β_0 (*Pbca*)	351.4	95.1	C(A2)	386.1	293.0	L	421.1	348.3	L
317.7	25.0	β_0 (*Pbca*)	352.4	98.4	C(A2)	387.1	294.4	L	422.1	350.0	L
318.7	26.5	β_0 (*Pbca*)	353.4	101.8	C(A2)	388.2	295.8	L	423.1	351.7	L
319.7	28.0	β_0 (*Pbca*)	354.4	105.6	C(A2)	389.2	297.3	L	424.2	353.4	L
320.8	29.6	β_0 (*Pbca*)	355.4	110.2	C(A2)	390.2	298.7	L	425.2	355.2	L
321.8	31.1	β_0 (*Pbca*)	356.5	116.5	C(A2)	391.2	300.3	L	426.2	357.0	L
322.8	32.7	β_0 (*Pbca*)	357.5	127.3	C(A2)	392.3	301.8	L	427.3	358.8	L
323.8	34.3	β_0 (*Pbca*)	358.5	160.9	L	393.3	303.3	L	428.3	360.5	L
324.8	36.0	β_0 (*Pbca*)	359.5	255.8	L	394.3	304.8	L	429.3	362.3	L
325.8	37.6	β_0 (*Pbca*)	360.5	257.2	L	395.4	306.4	L	430.4	364.2	L
326.9	39.3	β_0 (*Pbca*)	361.6	258.7	L	396.4	307.9	L	431.4	366.1	L
327.9	41.0	β_0 (*Pbca*)	362.6	260.1	L	397.4	309.3	L	432.4	367.8	L
328.9	42.8	β_0 (*Pbca*)	363.6	261.6	L	398.4	310.9	L	433.5	369.6	L
329.9	44.6	β_0 (*Pbca*)	364.6	263.0	L	399.5	312.4	L	434.5	371.5	L
330.9	46.4	β_0 (*Pbca*)	365.7	264.4	L	400.5	313.9	L	435.5	373.2	L
332.0	48.2	β_0 (*Pbca*)	366.7	265.8	L	401.5	315.4	L	436.5	375.0	L

Table 27. Thermodynamic Data of C_{46}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^T_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 ($Pca2_1$)	319.9	36.9	β_0 ($Pca2_1$)	345.4	86.4	C(A2)	371.0	292.7	L	396.6	335.0	L
294.4	1.3	β_0 ($Pca2_1$)	320.9	38.5	β_0 ($Pca2_1$)	346.5	89.4	C(A2)	372.0	294.4	L	397.7	336.7	L
295.4	2.7	β_0 ($Pca2_1$)	321.9	39.9	β_0 ($Pca2_1$)	347.5	91.5	C(A2)	373.0	296.1	L	398.7	338.5	L
296.4	4.0	β_0 ($Pca2_1$)	323.0	41.4	β_0 ($Pca2_1$)	348.5	93.9	C(A2)	374.1	297.7	L	399.7	340.2	L
297.4	5.3	β_0 ($Pca2_1$)	324.0	42.9	β_0 ($Pca2_1$)	349.5	96.2	C(A2)	375.1	299.4	L	400.7	341.9	L
298.5	6.6	β_0 ($Pca2_1$)	325.0	44.5	β_0 ($Pca2_1$)	350.6	98.5	C(A2)	376.1	301.0	L	401.8	343.7	L
299.5	7.9	β_0 ($Pca2_1$)	326.0	46.0	β_0 ($Pca2_1$)	351.6	100.9	C(A2)	377.1	302.7	L	402.8	345.4	L
300.5	9.3	β_0 ($Pca2_1$)	327.0	47.5	β_0 ($Pca2_1$)	352.6	103.3	C(A2)	378.2	304.4	L	403.8	347.1	L
301.5	10.7	β_0 ($Pca2_1$)	328.1	49.0	β_0 ($Pca2_1$)	353.6	105.9	C(A2)	379.2	306.1	L	404.9	348.9	L
302.5	12.1	β_0 ($Pca2_1$)	329.1	50.5	β_0 ($Pca2_1$)	354.6	108.3	C(A2)	380.2	307.7	L	405.9	350.7	L
303.5	13.6	β_0 ($Pca2_1$)	330.1	52.1	β_0 ($Pca2_1$)	355.7	110.9	C(A2)	381.2	309.5	L	406.9	352.4	L
304.6	15.1	β_0 ($Pca2_1$)	331.1	53.8	β_0 ($Pca2_1$)	356.7	113.5	C(A2)	382.3	311.2	L	408.0	354.2	L
305.6	16.5	β_0 ($Pca2_1$)	332.2	55.3	β_0 ($Pca2_1$)	357.7	116.1	C(A2)	383.3	312.8	L	409.0	356.0	L
306.6	17.9	β_0 ($Pca2_1$)	333.2	57.0	β_0 ($Pca2_1$)	358.7	118.9	C(A2)	384.3	314.5	L	410.0	357.7	L
307.7	19.4	β_0 ($Pca2_1$)	334.2	58.8	β_0 ($Pca2_1$)	359.7	122.6	C(A2)	385.3	316.2	L	411.0	359.5	L
308.7	20.9	β_0 ($Pca2_1$)	335.2	60.5	β_0 ($Pca2_1$)	360.8	127.0	L	386.4	317.9	L	412.1	361.3	L
309.7	22.3	β_0 ($Pca2_1$)	336.2	64.2	β_0 ($Pca2_1$)	361.8	259.8	L	387.4	319.6	L	413.1	363.1	L
310.7	23.7	β_0 ($Pca2_1$)	337.3	64.2	β_0 ($Pca2_1$)	362.8	279.3	L	388.4	321.2	L	414.1	365.0	L
311.7	25.2	β_0 ($Pca2_1$)	338.3	66.3	β_0 ($Pca2_1$)	363.8	281.0	L	389.4	322.9	L	415.2	366.8	L
312.8	26.6	β_0 ($Pca2_1$)	339.3	68.8	β_0 ($Pca2_1$)	364.9	282.7	L	390.5	324.6	L	416.2	368.6	L
313.8	28.1	β_0 ($Pca2_1$)	340.3	71.1	β_0 ($Pca2_1$)	365.9	284.4	L	391.5	326.3	L	417.2	370.5	L
314.8	29.5	β_0 ($Pca2_1$)	341.4	73.5	C(A2)	366.9	286.0	L	392.5	328.0	L	418.2	372.3	L
315.8	31.0	β_0 ($Pca2_1$)	342.4	76.0	C(A2)	367.9	287.7	L	393.5	329.7	L	419.3	374.1	L
316.8	32.5	β_0 ($Pca2_1$)	343.4	79.0	C(A2)	368.9	289.4	L	394.6	331.4	L	420.3	376.0	L
317.9	33.9	β_0 ($Pca2_1$)	344.4	82.6	C(A2)	370.0	291.1	L	395.6	333.2	L	421.3	377.8	L
318.9	35.4	β_0 ($Pca2_1$)												

Table 28. Thermodynamic Data of C_{50}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.3 K ($H^T_{293.3}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase	T/K	$H^T_{293.3}$/kJ·mol^{-1}	phase
293.3	0.0	β_0 ($Pca2_1$)	319.9	36.2	β_0 ($Pca2_1$)	346.5	85.9	C(A2)	372.0	305.4	L	397.7	352.3	L
294.4	1.3	β_0 ($Pca2_1$)	320.9	37.7	β_0 ($Pca2_1$)	347.5	88.1	C(A2)	373.1	307.3	L	398.7	354.2	L
295.4	2.7	β_0 ($Pca2_1$)	321.9	39.3	β_0 ($Pca2_1$)	348.5	90.2	C(A2)	374.1	309.0	L	399.8	356.1	L
296.4	4.1	β_0 ($Pca2_1$)	323.0	40.8	β_0 ($Pca2_1$)	349.6	92.3	C(A2)	375.1	310.9	L	400.8	358.1	L
297.4	5.4	β_0 ($Pca2_1$)	324.0	42.3	β_0 ($Pca2_1$)	350.6	94.5	C(A2)	376.1	312.8	L	401.8	360.1	L
298.4	6.7	β_0 ($Pca2_1$)	325.0	43.9	β_0 ($Pca2_1$)	351.6	96.7	C(A2)	377.2	314.7	L	402.9	362.0	L
299.5	8.1	β_0 ($Pca2_1$)	326.0	45.4	β_0 ($Pca2_1$)	352.6	98.9	C(A2)	378.2	316.6	L	403.9	364.0	L
300.5	9.5	β_0 ($Pca2_1$)	327.0	47.0	β_0 ($Pca2_1$)	353.6	101.2	C(A2)	379.2	318.5	L	404.9	365.9	L
301.5	11.0	β_0 ($Pca2_1$)	328.1	48.7	β_0 ($Pca2_1$)	354.7	103.5	C(A2)	380.2	320.3	L	405.9	367.9	L
302.5	12.3	β_0 ($Pca2_1$)	329.1	50.4	β_0 ($Pca2_1$)	355.7	105.9	C(A2)	381.3	322.1	L	407.0	369.9	L
303.6	13.7	β_0 ($Pca2_1$)	330.1	52.2	β_0 ($Pca2_1$)	356.7	108.2	C(A2)	382.3	323.9	L	408.0	371.9	L
304.6	15.0	β_0 ($Pca2_1$)	331.2	53.9	β_0 ($Pca2_1$)	357.7	110.6	C(A2)	383.3	325.8	L	409.0	373.9	L
305.6	16.3	β_0 ($Pca2_1$)	332.2	55.7	β_0 ($Pca2_1$)	358.8	113.7	C(A2)	384.4	327.7	L	410.1	375.8	L
306.6	17.6	β_0 ($Pca2_1$)	333.2	57.6	C(A2)	359.8	116.0	C(A2)	385.4	329.7	L	411.1	377.7	L
307.6	18.9	β_0 ($Pca2_1$)	334.2	59.6	C(A2)	360.8	118.3	C(A2)	386.4	331.6	L	412.1	379.7	L
308.7	20.4	β_0 ($Pca2_1$)	335.2	61.9	C(A2)	361.8	120.6	C(A2)	387.4	333.5	L	413.1	381.7	L
309.7	21.9	β_0 ($Pca2_1$)	336.3	64.4	C(A2)	362.8	123.0	C(A2)	388.5	335.4	L	414.2	383.8	L
310.7	23.2	β_0 ($Pca2_1$)	337.3	66.8	C(A2)	363.9	125.5	C(A2)	389.5	337.3	L	415.2	385.9	L
311.7	24.6	β_0 ($Pca2_1$)	338.3	69.3	C(A2)	364.9	129.4	L	390.5	339.1	L	416.2	388.0	L
312.8	25.9	β_0 ($Pca2_1$)	339.3	71.4	C(A2)	365.9	295.2	L	391.5	341.0	L	417.3	390.0	L
313.8	27.5	β_0 ($Pca2_1$)	340.4	73.5	C(A2)	366.9	297.0	L	392.6	342.9	L	418.3	392.0	L
314.8	29.0	β_0 ($Pca2_1$)	341.4	75.6	C(A2)	367.9	298.6	L	393.6	344.8	L	419.3	394.0	L
315.8	30.4	β_0 ($Pca2_1$)	342.4	77.7	C(A2)	369.0	300.3	L	394.6	346.7	L	420.4	396.1	L
316.9	31.9	β_0 ($Pca2_1$)	343.4	79.8	C(A2)	370.0	302.0	L	395.6	348.5	L	421.4	398.1	L
317.9	33.3	β_0 ($Pca2_1$)	344.4	81.8	C(A2)	371.0	303.7	L	396.7	350.4	L	422.4	400.2	L
318.9	34.7	β_0 ($Pca2_1$)	345.5	83.9	C(A2)									

The measurements were carried out by sequential programming of the temperature as a function of the time: (i) the rising temperature period, t_i, was set at 200 s and corresponded to a temperature jump equal to $T_2 - T_1 = 1$ K (Figure 2); (ii) the temperature level length, t_l, depends on a computer test, checking that the calorimeter signal returned to a constant value, corresponding to a steady state.

The C_n's were obtained from Fluka and had the stated purities reported in Table 1. First the samples were melted in stainless steel crucibles which were sealed before their introduction into the calorimeter cell. Figures 3 and 4 show the enthalpy increment through curves as a function of the increasing temperature, obtained for the even C_{28} and the odd C_{29}, respectively. The repeatability and the accuracy of temperature and enthalpy measurements were determined by using C_{18} and C_{26}, for which the experimental enthalpy variations in relation to the temperature were compared with the literature data[7,46] (Tables 2 and 3): experimental data are in good agreement with the literature results, and this agreement justifies the experimental method used (percent difference < 1.5%); the accuracy of temperature measurements is equal to ±0.5 K.

Results

The enthalpy ($H^T_{T_0}$/kJ·mol^{-1}; T_0 = 293.4 K or 298.3 K) variations with respect to the temperature are listed for each C_n (from C_{18} to C_{38}, C_{41}, C_{44}, C_{46}, C_{50}, C_{54}, and C_{60}) in Tables 4−30, where the phase type and the transition temperatures are specified.

The temperatures and enthalpies of the order−disorder transition and of the fusion as well as the total enthalpy variation from the order−disorder temperature up to the

Table 29. Thermodynamic Data of C_{54}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 293.4 K ($H^{T}_{293.4}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^{T}_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{293.4}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{293.4}$/kJ·mol^{-1}	phase
293.4	0.0	β_0 ($Pca2_1$)	319.9	40.4	β_0 ($Pca2_1$)	346.5	98.0	C(A2)	372.1	344.7	L	397.7	396.4	L
294.4	1.5	β_0 ($Pca2_1$)	321.0	42.1	β_0 ($Pca2_1$)	347.5	102.5	C(A2)	373.1	346.6	L	398.7	398.6	L
295.4	2.7	β_0 ($Pca2_1$)	322.0	43.9	β_0 ($Pca2_1$)	348.6	105.3	C(A2)	374.1	348.6	L	399.8	400.8	L
296.4	4.1	β_0 ($Pca2_1$)	323.0	45.4	β_0 ($Pca2_1$)	349.6	108.1	C(A2)	375.1	350.8	L	400.8	402.9	L
297.4	5.5	β_0 ($Pca2_1$)	324.0	46.9	β_0 ($Pca2_1$)	350.6	110.8	C(A2)	376.2	352.9	L	401.8	404.9	L
298.5	7.1	β_0 ($Pca2_1$)	325.0	48.7	β_0 ($Pca2_1$)	351.6	113.6	C(A2)	377.2	355.0	L	402.9	407.0	L
299.5	8.5	β_0 ($Pca2_1$)	326.1	50.5	β_0 ($Pca2_1$)	352.7	116.3	C(A2)	378.2	357.1	L	403.9	409.1	L
300.5	10.1	β_0 ($Pca2_1$)	327.1	52.3	β_0 ($Pca2_1$)	353.7	119.1	C(A2)	379.2	359.2	L	404.9	411.2	L
301.5	11.7	β_0 ($Pca2_1$)	328.1	54.2	β_0 ($Pca2_1$)	354.7	122.1	C(A2)	380.3	361.3	L	405.9	413.2	L
302.5	13.2	β_0 ($Pca2_1$)	329.1	56.0	β_0 ($Pca2_1$)	355.7	124.9	C(A2)	381.3	363.6	L	407.0	415.3	L
303.6	14.6	β_0 ($Pca2_1$)	330.1	57.9	β_0 ($Pca2_1$)	356.7	127.8	C(A2)	382.3	365.6	L	408.0	417.5	L
304.6	16.1	β_0 ($Pca2_1$)	331.2	59.8	β_0 ($Pca2_1$)	357.8	130.9	C(A2)	383.3	367.8	L	409.0	419.5	L
305.6	17.7	β_0 ($Pca2_1$)	332.2	61.7	β_0 ($Pca2_1$)	358.8	134.0	C(A2)	384.4	369.9	L	410.1	421.6	L
306.6	19.4	β_0 ($Pca2_1$)	333.2	63.5	β_0 ($Pca2_1$)	359.8	137.1	C(A2)	385.4	372.1	L	411.1	423.6	L
307.7	21.0	β_0 ($Pca2_1$)	334.2	65.5	β_0 ($Pca2_1$)	360.8	140.0	C(A2)	386.4	374.1	L	412.1	425.8	L
308.7	22.5	β_0 ($Pca2_1$)	335.3	67.6	β_0 ($Pca2_1$)	361.9	142.8	C(A2)	387.4	376.0	L	413.1	427.9	L
309.7	24.0	β_0 ($Pca2_1$)	336.3	69.6	β_0 ($Pca2_1$)	362.9	145.8	C(A2)	388.5	378.0	L	414.2	430.0	L
310.7	25.7	β_0 ($Pca2_1$)	337.3	71.7	β_0 ($Pca2_1$)	363.9	148.7	C(A2)	389.5	380.1	L	415.2	432.2	L
311.8	27.3	β_0 ($Pca2_1$)	338.3	73.8	β_0 ($Pca2_1$)	364.9	151.8	C(A2)	390.5	382.4	L	416.2	434.2	L
312.8	28.9	β_0 ($Pca2_1$)	339.4	76.0	β_0 ($Pca2_1$)	365.9	154.8	C(A2)	391.5	384.4	L	417.3	436.3	L
313.8	30.5	β_0 ($Pca2_1$)	340.4	78.3	β_0 ($Pca2_1$)	367.0	158.0	C(A2)	392.6	386.4	L	418.3	438.4	L
314.8	32.1	β_0 ($Pca2_1$)	341.4	80.5	β_0 ($Pca2_1$)	368.0	162.1	L	393.6	388.4	L	419.3	440.5	L
315.9	33.8	β_0 ($Pca2_1$)	342.4	83.0	β_0 ($Pca2_1$)	369.0	304.7	L	394.6	390.4	L	420.4	442.7	L
316.9	35.4	β_0 ($Pca2_1$)	343.4	85.7	β_0 ($Pca2_1$)	370.0	340.9	L	395.7	392.4	L	421.4	444.9	L
317.9	37.0	β_0 ($Pca2_1$)	344.5	88.5	C(A2)	371.1	342.8	L	396.7	394.4	L	422.4	447.1	L
318.9	38.7	β_0 ($Pca2_1$)	345.5	92.2	C(A2)									

Table 30. Thermodynamic Data of C_{60}: Temperature ($T \pm 0.5$)/K; Enthalpy Values Referred to 298.3 K ($H^{T}_{298.3}$/kJ·mol^{-1}; % diff: 1.5%); Phase Name

T/K	$H^{T}_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{298.3}$/kJ·mol^{-1}	phase	T/K	$H^{T}_{298.3}$/kJ·mol^{-1}	phase
298.3	0.0	β_0 ($Pca2_1$)	326.9	45.7	β_0 ($Pca2_1$)	354.5	103.0	C(A2)	382.1	344.5	L	409.9	405.0	L
299.4	1.7	β_0 ($Pca2_1$)	327.9	47.4	β_0 ($Pca2_1$)	355.5	105.2	C(A2)	383.2	346.8	L	410.9	407.2	L
300.4	3.4	β_0 ($Pca2_1$)	328.9	49.1	β_0 ($Pca2_1$)	356.6	107.6	C(A2)	384.2	349.0	L	411.9	409.5	L
301.4	5.1	β_0 ($Pca2_1$)	330.0	50.8	β_0 ($Pca2_1$)	357.6	110.0	C(A2)	385.2	351.3	L	413.0	411.7	L
302.4	6.7	β_0 ($Pca2_1$)	331.0	52.4	β_0 ($Pca2_1$)	358.6	112.2	C(A2)	386.2	353.5	L	414.0	413.9	L
303.4	8.4	β_0 ($Pca2_1$)	332.0	54.2	β_0 ($Pca2_1$)	359.6	114.5	C(A2)	387.3	355.7	L	415.0	416.2	L
304.5	10.0	β_0 ($Pca2_1$)	333.0	55.9	β_0 ($Pca2_1$)	360.6	116.6	C(A2)	388.3	358.0	L	416.1	418.5	L
305.5	11.7	β_0 ($Pca2_1$)	334.1	57.7	β_0 ($Pca2_1$)	361.7	119.0	C(A2)	389.3	360.2	L	417.1	420.8	L
306.5	13.4	β_0 ($Pca2_1$)	335.1	59.3	β_0 ($Pca2_1$)	362.7	121.3	C(A2)	390.4	362.5	L	418.1	423.1	L
307.5	15.0	β_0 ($Pca2_1$)	336.1	61.2	β_0 ($Pca2_1$)	363.7	123.7	C(A2)	391.4	364.8	L	419.2	425.4	L
308.6	16.7	β_0 ($Pca2_1$)	337.1	63.1	C(A2)	364.7	126.1	C(A2)	392.4	367.0	L	420.2	427.8	L
309.6	18.3	β_0 ($Pca2_1$)	338.2	65.1	C(A2)	365.8	128.6	C(A2)	393.4	369.3	L	421.2	430.1	L
310.6	19.9	β_0 ($Pca2_1$)	339.2	67.1	C(A2)	366.8	131.3	C(A2)	394.5	371.5	L	422.3	432.4	L
311.6	21.5	β_0 ($Pca2_1$)	340.2	69.3	C(A2)	367.8	134.3	C(A2)	395.5	373.8	L	423.3	434.6	L
312.6	23.1	β_0 ($Pca2_1$)	341.2	71.7	C(A2)	368.8	137.5	C(A2)	396.5	376.0	L	424.3	436.9	L
313.6	24.6	β_0 ($Pca2_1$)	342.2	75.0	C(A2)	369.8	141.5	C(A2)	397.5	378.3	L	425.3	439.2	L
314.7	26.3	β_0 ($Pca2_1$)	343.3	79.7	C(A2)	370.9	146.9	C(A2)	398.6	380.6	L	426.4	441.4	L
315.7	27.9	β_0 ($Pca2_1$)	344.3	81.9	C(A2)	371.9	158.4	C(A2)	399.6	382.8	L	427.4	443.7	L
316.7	29.5	β_0 ($Pca2_1$)	345.3	83.8	C(A2)	372.9	233.3	L	400.6	385.0	L	428.4	446.0	L
317.7	31.1	β_0 ($Pca2_1$)	346.3	85.9	C(A2)	373.9	339.6	L	401.7	387.2	L	429.5	448.2	L
318.7	32.8	β_0 ($Pca2_1$)	347.3	87.9	C(A2)	375.0	341.7	L	402.7	389.5	L	430.5	450.5	L
319.8	34.4	β_0 ($Pca2_1$)	348.4	90.1	C(A2)	376.0	344.0	L	403.7	391.7	L	431.5	452.8	L
320.8	36.0	β_0 ($Pca2_1$)	349.4	92.1	C(A2)	377.0	346.2	L	404.8	393.9	L	432.6	455.0	L
321.8	37.6	β_0 ($Pca2_1$)	350.4	94.2	C(A2)	378.0	348.5	L	405.8	396.0	L	433.6	457.3	L
322.8	39.2	β_0 ($Pca2_1$)	351.4	96.4	C(A2)	379.1	337.8	L	406.8	398.3	L	434.6	459.6	L
323.8	40.8	β_0 ($Pca2_1$)	352.5	98.6	C(A2)	380.1	340.1	L	407.8	400.5	L	435.7	461.9	L
324.9	42.4	β_0 ($Pca2_1$)	353.5	100.8	C(A2)	381.1	342.3	L	408.9	402.7	L	436.7	464.2	L
325.9	44.1	β_0 ($Pca2_1$)												

melting temperature ($\Delta H^{T_{fus}}_{T_{o-d}}$) are reported in Table 31 and compared to literature data.[84] The experimental results are in agreement with those of the literature,[84] especially for the C_n's whose carbon atom numbers are lower than or equal to 26. For the C_n's, whose carbon atom numbers are higher than 26, the experimental results are slightly higher than those of the literature (Figure 5, Table 31); however, the literature data of those C_n's are determined by differential thermal analyses, using a continuous mode of temperature programming. In this last case, it is more difficult to determine with accuracy the baseline of the calorimetric signal in the course of the solid−solid or solid−liquid transitions. Moreover, for the heavy C_n's ($n > 40$), a higher enthalpy consumption in relation to that of light C_n's is observed, certainly due to the progressive appearance of a higher quantity of conformation defects[75] in the course of the heating.

The $\Delta H^{T_{fus}}_{T_{o-d}}$ enthalpy variations from the T_{o-d} order−disorder transition temperature up to the T_{fus} melting temperature are shown in Figure 5, where the mean values of the literature[84] and the new experimental data are also shown. All these values increase linearly with respect to the n_c carbon atom number from $n_c = 4$ to $n_c = 60$ in a manner independent of the n_c parity.

The linear equation of the variations of $\Delta H^{T_{fus}}_{T_{o-d}}$ enthalpy values as a function of the n_c carbon number is established by linear least-squares fitting, and the result is as follows:

$$4 \le n_c \le 60: \quad \Delta H^{T_{fus}}_{T_{o-d}}/\text{kJ·mol}^{-1} = 4.10 n_c - 10.98$$

Table 31. Comparison of Transition Enthalpy between the Experimental Results and the Mean Values of the Literature[83] (lit.)[a]

		melting				order/disorder				total	
nc.	molar mass	T_{fus}(lit.)[83] K	T_{fus} K	$\Delta_{fus}H$(lit.)[83] kJ·mol^{-1}	$\Delta_{fus}H$ kJ·mol^{-1}	T_{o-d}(lit.)[83] K	T_{o-d} K	ΔH_{o-d}(lit.)[83] kJ·mol^{-1}	ΔH_{o-d} kJ·mol^{-1}	ΔH_{tot}(lit.)[83] kJ·mol^{-1}	ΔH_{tot} kJ·mol^{-1}
18	254.50	301.2	300.2	61.3	61.5	*b*				61.3	61.5
19	268.53	304.9	303.7	45.6	44.5	295.5	294.4	13.7	11.8	65.5	66.5
20	282.55	309.5	308.7	69.7	73.5	*b*				69.7	73.5
21	296.58	313.2	312.6	47.7	47.5	305.6	304.4	16.3	16.6	73.0	75.8
22	310.60	316.8	314.9	48.8		315.2	314.9	29.0		77.6	80.5
23	324.63	320.4	319.9	53.1	52.9	315.6	312.8	21.7	22.4	82.5	86.5
24	338.66	323.6	323.0	54.4	57.2	320.7	319.9	31.7	29.9	88.3	92.4
25	352.69	326.3	324.7	57.1	58.7	320.3	318.8	26.7	28.6	90.7	92.8
26	366.71	329.2	328.9	60.0	61.4	326	325.0	33.8	36.5	97.5	100.6
27	380.74	331.7	331.2	61.1	68.9	326.3	325.0	26.8	29.5	96.6	107.6
28	394.77	334.2	333.2	65.1	63.5	330.5	330.1	35.1	36.9	102.2	104.7
29	408.79	336.2	336.0	68.2	67.8	330.8	330.3	30.8	33.0	103.8	106.9
30	422.82	338.2	337.5	68.3	69.8	332.2	332.1	37.0	40.8	108.9	118.9
31	436.85	341.1	340.0		73.3	336.5	335.2		36.6		117.4
32	450.87	342.5	341.9	75.8	77.0	337.2	338.0	40.8	44.2		126.5
33	464.90	344.3	343.4	79.5	80.7	340.9	337.9	31.2	37.9		125.8
34	478.93	345.6	345.3	79.4	84.5	342.2	341.1	48.0	45.4		137.0
35	492.95	347.7	346.5	86.3	86.4	344.2	344.2	41.1	44.1		136.4
36	506.98	348.9		87.7		347	346.1	31.1		134.0	136.1
37	521.01	349.8				348.8	349.0				140.0
38	535.03	351.7		133.2		350.2	349.9			133.2	146.5
41	577.11	354.8					354.3				149.2
44	619.20	358.7	358.0	149.6	143.1	357.7		18.2		167.8	167.3
46	647.25	360.7	360.7	176.0	156.6					176.0	180.5
50	703.36	365.2	364.9	162.4	167.1					171.1	191.6
54	759.46	368.1	368.0		177.2						216.2
60	843.62	372.4	372.0	193.2	204.1					193.2	225.3

[a] T_{fus} (±0.5)/K and $\Delta_{fus}H$/kJ·mol^{-1} (% diff: 3%), temperature and enthalpy of fusion; T_{o-d} (±0.5)/K and ΔH_{o-d}/kJ·mol^{-1} (% diff: 3%), temperature and enthalpy of order−disorder transition; $\Delta H_{tot} = \Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$/kJ·mol^{-1} (% diff: 3%). [b] No solid/solid transition.

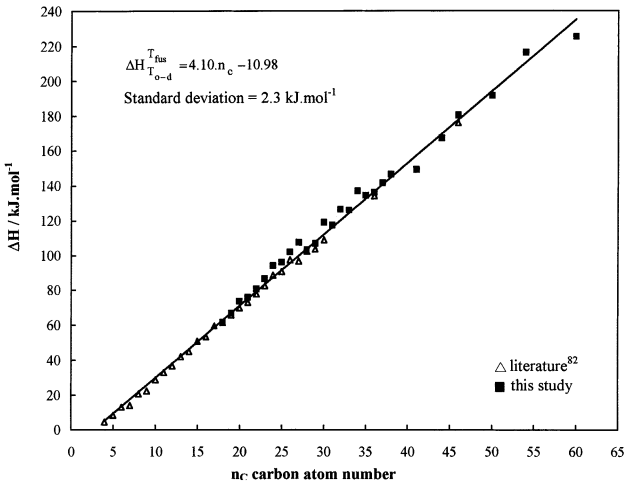

Figure 5. $\Delta H_{T_{o-d}}^{T_{fus}}$ variations in relation to the carbon atom number of the C_n chain: $\Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$ (Figures 3 and 4).

with a standard deviation $\sigma = 2.3$ kJ·mol^{-1} and $\Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$.

Conclusion

The calorimetric measurement method, using a discontinuous mode of temperature programming, allows us to determine the enthalpy variations with respect to the increasing temperature in the thermodynamic equilibrium state. For the light C_n's ($18 \le n \le 26$), the experimental results are in agreement with those of the literature and justify the measurement method for the thermodynamic data variations of heavier C_n's ($27 \le n \le 38$, 41, 44, 46, 50, 54, and 60). These new thermodynamic data will enable us to establish new predictive models about the behavior of multi-C_n mixtures and solid−liquid equilibria of crude oil cuts.

Notation

Crystallographic Structure

Ordered Phases of n-Alkanes at "Room Temperature"

$\beta_0(C_{2p+1})$ = orthorhombic phase *Pbcm* of odd-numbered C_{2p+1} ($n_c = 2p + 1$)

$\gamma_0(C_{2p})$ = triclinic phase $P\bar{1}$ of even-numbered C_{2p} ($n_c = 2p \le 26$)

$\delta_0(C_{2p})$ = monoclinic phase $P2_1/a$ of even-numbered C_{2p} ($28 \le n_c = 2p \le 36$)

$\beta_0(C_{2p})$ = orthorhombic phase *Pbca* of even-numbered C_{2p} ($38 \le n_c = 2p \le 44$)

$\beta_0(C_{2p})$ = orthorhombic phase $Pca2_1$ of even-numbered C_{2p} ($46 \le n_c = 2p$)

Disordered Phases at "High Temperature"

$\beta(Fmmm)$ = orthorhombic phase; this phase presents the "Rotator" state, called β-RI

α-RII = rhombohedral Rotator phase ($R\bar{3}m$)

RIII = triclinic disorder phase

RIV = monoclinic disorder phase

Thermodynamic Data

T_{o-d}/K, ΔH_{o-d}/kJ·mol^{-1} = temperature and enthalpy of the order−disorder transition (o−d transition)

T_{fus}/K, $\Delta_{fus}H$/kJ·mol^{-1} = temperature and enthalpy of the melting (disordered phase → liquid)

$\Delta H_{T_{o-d}}^{T_{fus}}$/kJ·mol^{-1} = enthalpy variation from the order−disorder transition temperature (T_{o-d}) to the melting temperature (T_{fus}) (ordered phase → liquid): $\Delta H_{T_{o-d}}^{T_{fus}} = \Delta H_{o-d} + \int_{T_{o-d}}^{T_{fus}} C_p \, dT + \Delta_{fus}H$

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