

Pressure-Freezing of Dodecane: Exploring the Crystal Structures, Formation Kinetics and Phase Diagrams for Colossal Barocaloric Effects in *n*-Alkanes

Tomasz Poręba* [a], Inga Kicior [a][b]

[a] European Synchrotron Radiation Facility. 71 Avenue des Martyrs, 38000 Grenoble, France

[b] School of Chemical and Process Engineering, University of Leeds. Leeds LS2 9JT, United Kingdom

Contents

1. Selected crystallographic information for <i>n</i> -undecane at 0.17(1) GPa	2
2. Selected crystallographic information for <i>n</i> -dodecane at 0.15(1) GPa	7
3. Effect of data completeness on the C-C bond distances	10
4. Lattice energy calculations for <i>n</i> -alkanes.....	11
5. Pressure-freezing of pentadecane: coexistence of solid phases	12
6. Thermal expansivity of <i>n</i> -dodecane close to its melting point.....	13
7. Bulk modulus calculation and comparison with entropy change.....	13
8. References.....	14

1. Selected crystallographic information for *n*-undecane at 0.17(1) GPa

Table S1 Crystal data and structure refinement for undecane.

Identification code	undecane
Empirical formula	C ₁₁ H ₂₄
Formula weight	156.30
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
<i>a</i> /Å	4.1808(5)
<i>b</i> /Å	4.7113(3)
<i>c</i> /Å	29.53(2)
α /°	93.609(19)
β /°	90.41(2)
γ /°	107.274(9)
Volume/Å ³	554.1(4)
<i>Z</i>	2
$\rho_{\text{calc}}/\text{cm}^3$	0.937
μ/mm^{-1}	0.025
<i>F</i> (000)	180.0
Crystal size/mm ³	0.21 × 0.04 × 0.05
Radiation	synchrotron ($\lambda = 0.410$)
2 Θ range for data collection/°	5.236 to 29.604
Index ranges	-5 ≤ <i>h</i> ≤ 4, -5 ≤ <i>k</i> ≤ 5, -12 ≤ <i>l</i> ≤ 16
Reflections collected	867
Independent reflections	586 [<i>R</i> _{int} = 0.0054, <i>R</i> _{sigma} = 0.0122]

Data/restraints/parameters 586/80/102
 Goodness-of-fit on F^2 0.995
 Final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0539$, $wR_2 = 0.1564$
 Final R indexes [all data] $R_1 = 0.1045$, $wR_2 = 0.1951$
 Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 0.07/-0.07

Table S2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for undecane. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U_{eq}
C6	2606(8)	5578(7)	7458(2)	53(4)
C4	4489(8)	5739(7)	6639(2)	58(4)
C8	760(8)	5453(8)	8278(2)	57(4)
C3	5915(8)	7619(7)	6250(2)	55(4)
C9	335(8)	7221(7)	8703(3)	57(4)
C10	-1029(10)	5371(9)	9097(3)	69(4)
C7	2156(8)	7317(7)	7886(2)	53(4)
C5	4011(7)	7449(7)	7069(2)	54(4)
C1	7868(11)	7822(8)	5427(3)	74(5)
C2	6384(9)	5917(8)	5815(2)	63(4)
C11	-1419(12)	7158(9)	9527(3)	84(5)

Table S3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for undecane. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C6	65(2)	48.8(15)	42(12)	-2(4)	-3(4)	14.4(13)
C4	71(2)	48.9(17)	51(13)	-5(3)	0(4)	15.1(14)
C8	67(2)	51.0(16)	49(13)	2(3)	16(4)	13.6(13)
C3	67(2)	49.5(16)	47(13)	-2(4)	-1(5)	15.5(14)

Table S3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for undecane. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U_{11}+2hka*b*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C9	73(2)	56.9(17)	40(13)	6(4)	9(5)	15.9(15)
C10	86(3)	75(2)	48(14)	9(4)	20(5)	25.3(19)
C7	66(2)	48.5(16)	41(12)	2(3)	5(4)	15.0(13)
C5	65(2)	48.0(16)	46(13)	-3(4)	6(5)	13.9(14)
C1	91(2)	79(2)	52(15)	3(4)	17(5)	23.1(16)
C2	76(2)	60.0(19)	51(14)	-1(4)	-3(5)	16.6(15)
C11	113(3)	115(3)	34(14)	25(5)	19(7)	47(2)

Table S4 Bond Lengths for undecane.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
C6	C7	1.506(5)	C8	C7	1.510(5)
C6	C5	1.508(5)	C3	C2	1.516(5)
C4	C3	1.512(5)	C9	C10	1.510(5)
C4	C5	1.508(5)	C10	C11	1.514(5)
C8	C9	1.505(5)	C1	C2	1.519(5)

Table S5 Bond Angles for undecane.

Atom	Atom	Atom	Angle/ $^\circ$	Atom	Atom	Atom	Angle/ $^\circ$
C7	C6	C5	114.8(3)	C9	C10	C11	114.5(4)
C5	C4	C3	115.3(3)	C6	C7	C8	115.0(3)
C9	C8	C7	114.4(3)	C6	C5	C4	115.4(3)
C4	C3	C2	115.7(3)	C3	C2	C1	115.4(3)
C8	C9	C10	114.6(3)				

Table S6 Torsion Angles for undecane.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C4	C3	C2	C1	-179.1(3)	C7	C6	C5	C4	179.8(3)
C8	C9	C10	C11	179.4(4)	C7	C8	C9	C10	-179.4(3)
C3	C4	C5	C6	-179.7(3)	C5	C6	C7	C8	-179.8(3)
C9	C8	C7	C6	179.8(3)	C5	C4	C3	C2	-179.6(3)

Table S7 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for undecane.

Atom	x	y	z	U(eq)
H6A	451.31	4195.85	7362.54	63
H6B	4088.19	4411.9	7526.88	63
H4A	2339.64	4357.3	6540.53	69
H4B	5968.29	4569.97	6707.34	69
H8A	-1401.21	4071.67	8183.78	68
H8B	2240.4	4286.23	8346.38	68
H3A	8069.55	8992.92	6347.83	66
H3B	4442.9	8798.19	6182.96	66
H9A	-1162.63	8372.85	8635.03	69
H9B	2492	8616.96	8795.14	69
H10A	455.1	4203.34	9163.75	83
H10B	-3197.81	3991.08	9006.94	83
H7A	670.3	8478.94	7817.85	63
H7B	4310.74	8703.78	7981.45	63
H5A	6158.58	8838	7166.53	65
H5B	2522.84	8609.6	7000.97	65
H1A	8160.59	6563.39	5172.42	112
H1B	9998.74	9188.53	5523.48	112
H1C	6381.23	8917	5341.41	112

Table S7 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for undecane.

Atom	x	y	z	U(eq)
H2A	4223.97	4567.27	5713.45	76
H2B	7828.6	4714.2	5882.02	76
H11A	-2892.79	8317.77	9466.11	126
H11B	732.57	8461.19	9628.89	126
H11C	-2342.53	5826.36	9757.83	126

Experimental

Refinement model description

Number of restraints - 80, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2. Restrained distances

C11-C10 = C9-C10 = C9-C8 = C8-C7 = C7-C6 = C6-C5 = C5-C4 = C4-C3 = C3-C2 = C2-C1

1.52 with sigma of 0.005

C1-C2 \approx C2-C3

with sigma of 0.02

C9-C10 \approx C10-C11

with sigma of 0.02

C3-C4 \approx C4-C5

with sigma of 0.02

C5-C6 \approx C6-C7

with sigma of 0.02

C7-C8 \approx C8-C9

with sigma of 0.02

C9-C8 \approx C8-C7

with sigma of 0.02

C7-C6 \approx C7-C8

with sigma of 0.02

C10-C9 \approx C9-C8

with sigma of 0.02

C5-C6 \approx C5-C4

with sigma of 0.02

C3-C4 \approx C2-C3

- with sigma of 0.02
3. Rigid bond restraints
C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11
with sigma for 1-2 distances of 0.01 and sigma for 1-3 distances of 0.01
4. Uiso/Uanis restraints and constraints
Unis(C11) \approx Ueq: with sigma of 0.01 and sigma for terminal atoms of 0.02
- 5.a Secondary CH2 refined with riding coordinates:
C6(H6a,H6b), C4(H4a,H4b), C8(H8a,H8b), C3(H3a,H3b), C9(H9a,H9b), C10(H10a, H10b), C7(H7a,H7b), C5(H5a,H5b), C2(H2a,H2b)
- 5.b Idealised Me refined as rotating group:
C1(H1a,H1b,H1c), C11(H11a,H11b,H11c)

2. Selected crystallographic information for *n*-dodecane at 0.15(1) GPa

Table S8 Crystal data and structure refinement for *n*-dodecane.

Identification code	n-dodecane
Empirical formula	C ₁₂ H ₂₆
Formula weight	170.33
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
<i>a</i> /Å	4.2522(9)
<i>b</i> /Å	4.7701(11)
<i>c</i> /Å	15.904(6)
α /°	88.90(3)
β /°	84.67(2)
γ /°	73.309(19)
Volume/Å ³	307.64(16)
Z	1
ρ_{calc} /cm ³	0.919
μ /mm ⁻¹	0.025

F(000)	98.0
Crystal size/mm ³	0.31 × 0.08 × 0.10
Radiation	? (λ = 0.410)
2Θ range for data collection/°	4.452 to 36.75
Index ranges	-6 ≤ h ≤ 6, -5 ≤ k ≤ 4, -24 ≤ l ≤ 23
Reflections collected	1339
Independent reflections	834 [R _{int} = 0.0329, R _{sigma} = 0.0498]
Data/restraints/parameters	834/0/56
Goodness-of-fit on F ²	1.075
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0662, wR ₂ = 0.2262
Final R indexes [all data]	R ₁ = 0.0953, wR ₂ = 0.2574
Largest diff. peak/hole / e Å ⁻³	0.07/-0.07

TableS9 Fractional Atomic Coordinates (×10⁴) and Equivalent Isotropic Displacement Parameters (Å²×10³) for *n*-dodecane. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
C5	2185(3)	3604(5)	3880.4(7)	58.2(8)
C6	442(3)	5767(5)	4593.0(7)	58.4(8)
C4	3059(3)	5133(5)	3068.8(8)	60.0(8)
C3	4813(3)	3000(5)	2355.9(8)	59.1(9)
C1	7443(4)	2356(6)	844.3(9)	83.8(11)
C2	5674(4)	4506(6)	1545.3(8)	70.3(9)

Table S10 Anisotropic Displacement Parameters (Å²×10³) for *n*-dodecane. The Anisotropic displacement factor exponent takes the form: -2π²[h²a*²U₁₁+2hka*b*U₁₂+...].

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C5	67.0(9)	54(2)	47.3(8)	-5.3(12)	4.6(7)	-10.9(8)
C6	65.4(8)	56(2)	48.0(9)	-7.7(13)	5.6(7)	-11.2(7)

Table S10 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for *n*-dodecane. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4	67.1(8)	58(2)	48.3(8)	-5.1(12)	5.3(7)	-10.4(8)
C3	67.9(9)	56(2)	47.6(8)	-3.8(13)	4.7(6)	-11.8(8)
C1	91.7(11)	96(3)	54.3(9)	-8.2(15)	15.0(7)	-17.9(12)
C2	78.5(9)	74(2)	50.9(8)	-2.7(12)	8.0(7)	-14.8(9)

Table S11 Bond Lengths for *n*-dodecane.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA
C5	C6	1.532(2)	C4	C3	1.526(2)
C5	C4	1.538(3)	C3	C2	1.530(3)
C6	C6 ¹	1.544(4)	C1	C2	1.518(2)

¹-X,1-Y,1-Z

Table S12 Bond Angles for *n*-dodecane.

Atom	Atom	Atom	Angle/ $^\circ$	Atom	Atom	Atom	Angle/ $^\circ$
C6	C5	C4	112.8(2)	C4	C3	C2	113.5(2)
C5	C6	C6 ¹	112.8(3)	C1	C2	C3	112.9(2)
C3	C4	C5	113.3(2)				

¹-X,1-Y,1-Z

Table S13 Torsion Angles for *n*-dodecane.

A	B	C	D	Angle/ $^\circ$	A	B	C	D	Angle/ $^\circ$
C5	C4	C3	C2	179.70(10)	C4	C5	C6	C6 ¹	179.87(12)
C6	C5	C4	C3	179.68(9)	C4	C3	C2	C1	179.52(11)

¹-X,1-Y,1-Z

Table S14 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for *n*-dodecane.

Atom	x	y	z	U(eq)
H5A	768.05	2424.49	3754.98	70
H5B	4190.03	2300.54	4070.29	70
H6A	-1560.21	7073.76	4402.63	70
H6B	1861.25	6943.74	4719.31	70
H4A	1050.24	6430.07	2878.54	72
H4B	4462.08	6323.28	3196.22	72
H3A	3413.83	1802.83	2231.39	71
H3B	6825.85	1709.85	2545.93	71
H1A	9416.83	1061.22	1036.12	126
H1B	8004.48	3410.51	360.64	126
H1C	6026.52	1238.15	693.01	126
H2A	3661.37	5781.87	1350.84	84
H2B	7061.67	5714.56	1669.19	84

Refinement model description

Number of restraints - 0, number of constraints - unknown.

Details:

1. Fixed Uiso

At 1.2 times of:

All C(H,H) groups

At 1.5 times of:

All C(H,H,H) groups

2.a Secondary CH₂ refined with riding coordinates:

C5(H5A,H5B), C6(H6A,H6B), C4(H4A,H4B), C3(H3A,H3B), C2(H2A,H2B)

2.b Idealised Me refined as rotating group:

C1(H1A,H1B,H1C)

3. Effect of data completeness on the C-C bond distances

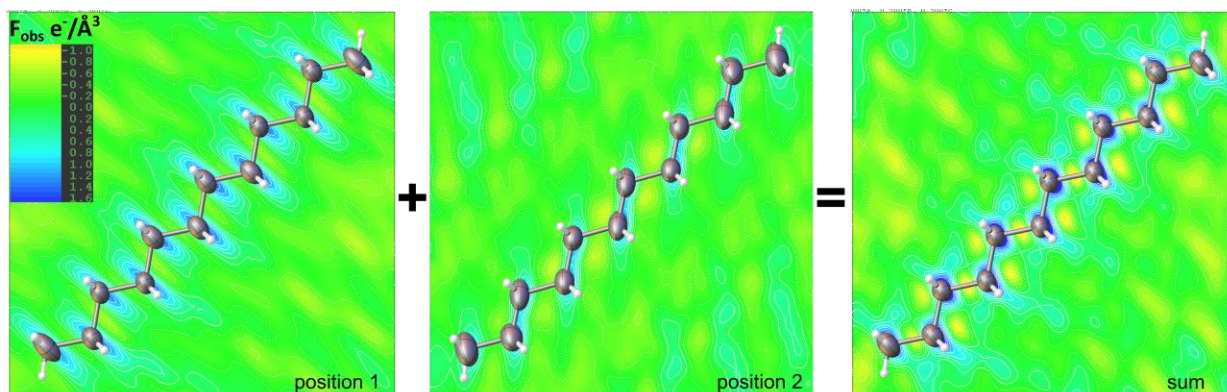


Figure S1. Result of merging of the XRD data collected from two different orientations of *n*-dodecane in DAC visible in total electron density map (F_{obs}).

4. Lattice energy calculations for *n*-alkanes

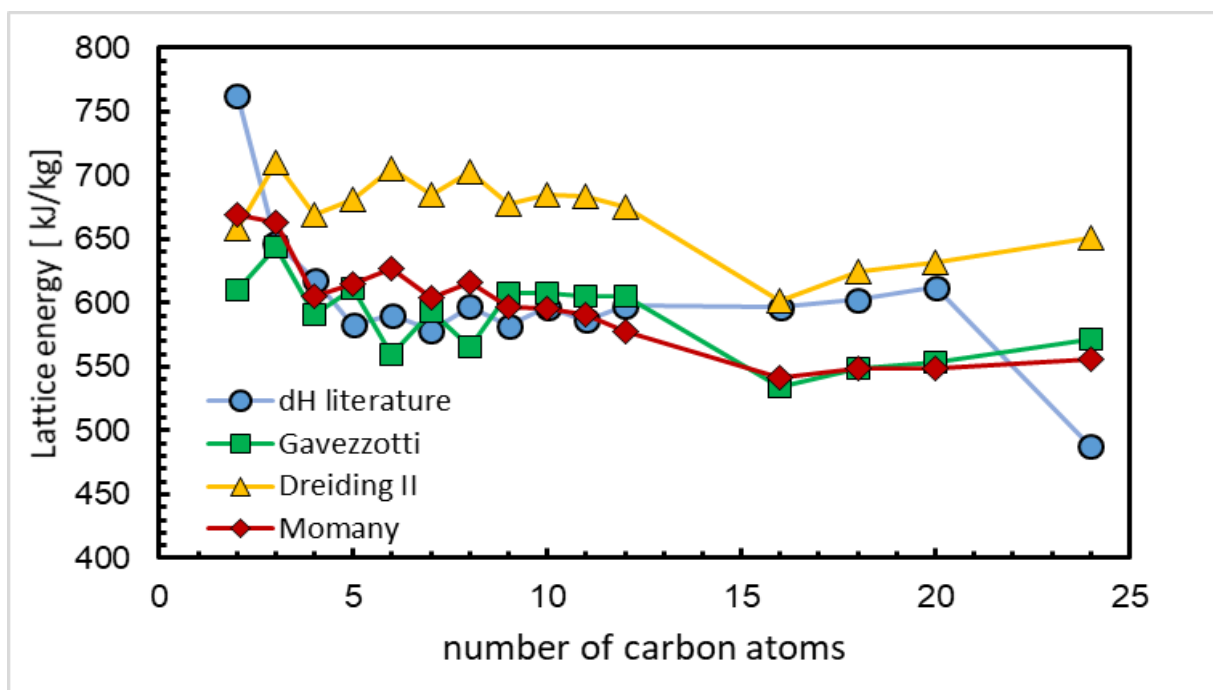


Figure S2. Comparison of the lattice energies for *n*-alkanes calculated with DREIDING II (triangles)¹⁻³, “Momany” (diamonds)⁴ and “Gavezzotti” (squares)^{5,6} potentials as implemented in Mercury 4.0.⁷ with the experimental values of the heat of sublimation (dH).

5. Pressure-freezing of pentadecane: coexistence of solid phases

n-pentadecane (Sigma, >99%) was loaded into DAC in a way described in the experimental section in the main text. We found that it crystallizes around 0.11(3) GPa in form of the round-edged plates. Further pressure increase also caused formation of multiple needle-like crystals. After careful heating-decompression cycling, we have managed to isolate two phases coexisting at 0.17(3) GPa (Figure S3). PXRD patterns from the crystals were collected at ID27 beamline (ESRF, France) using a monochromatic synchrotron beam ($\lambda = 0.3738 \text{ \AA}$). The data was collected through $\pm 32^\circ$ ω -scan. The samples poorly scattered X-ray and were highly mosaic, which precluded structure solution and refinement using single-crystal XRD methods. Nevertheless, indexing of the primitive orthorhombic cell (PO) of the needle-like crystals yielded the following crystallographic parameters: $a = 4.9320(9)$, $b = 7.361(8)$, $c = 41.672(7) \text{ \AA}$, space group $Pbcm$, consistent with the other odd-numbered members of the homologous series. For the plate-like crystal, rotator phase face-centered orthorhombic (FCO) unit cell was found. Determined lateral reticular distances are: $a = 7.534(5)$ and $b = 5.035(5) \text{ \AA}$, in accordance to the literature values for low-temperature plastic (rotator) phase of pentadecane⁸.

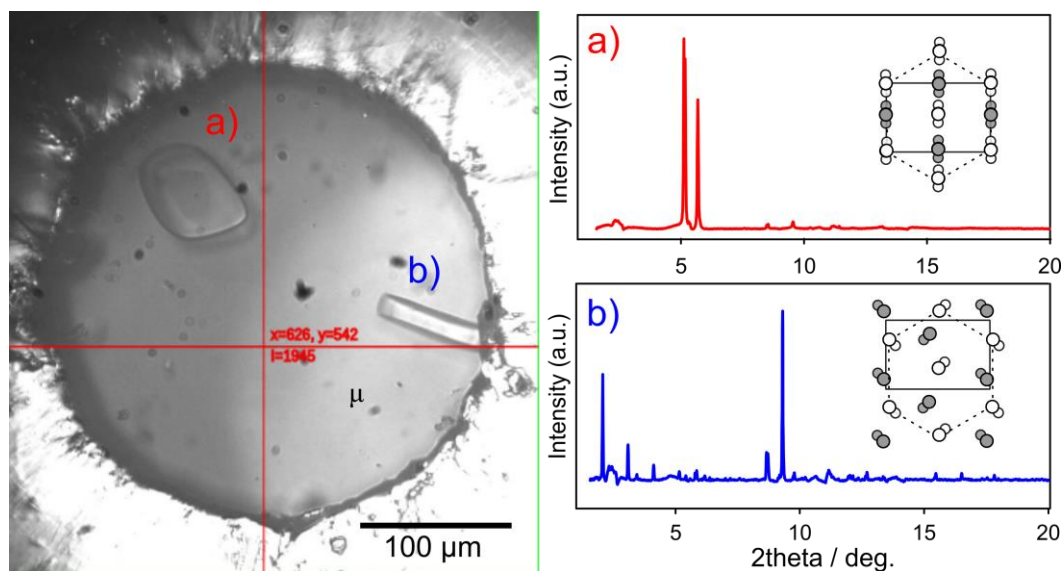


Figure S3. Two polymorphic forms of *n*-pentadecane grown at 0.17(3) GPa and 295 K: FCO plastic phase (a) and crystalline PO phase (b) with the corresponding PXRD patterns ($\lambda = 0.3738 \text{ \AA}$).

6. Thermal expansivity of *n*-dodecane close to its melting point

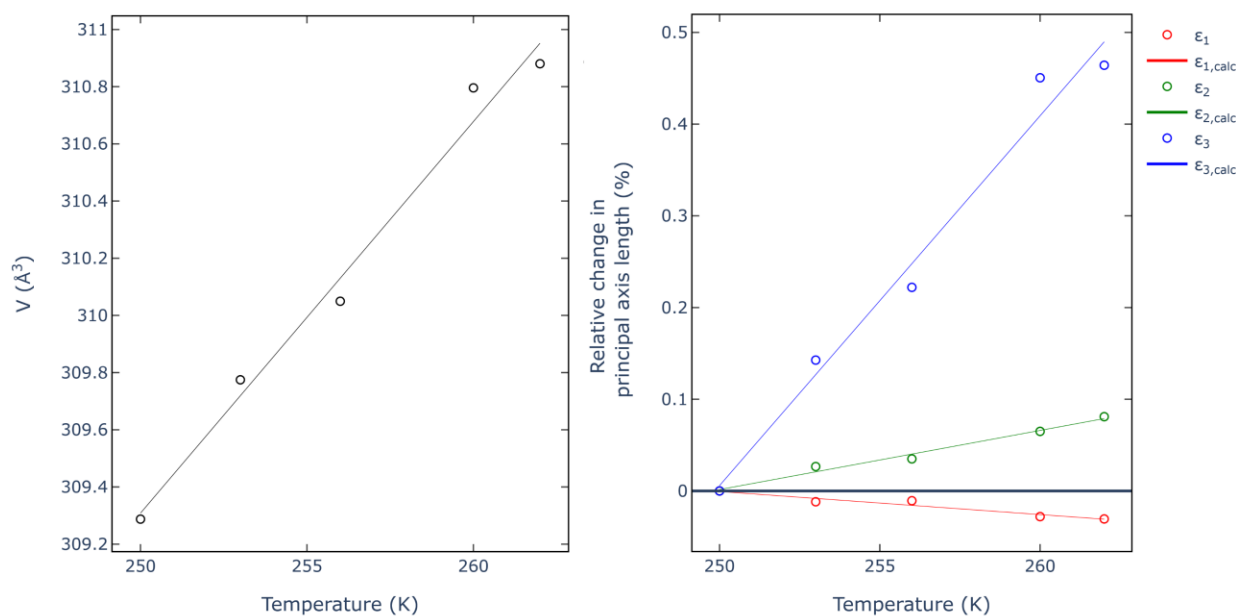


Figure S4. Experimental thermal expansivity data (left) and axial expansivities (right) fitted with linear functions in *n*-dodecane close to the melting point at ambient pressure⁹.

7. Bulk modulus calculation and comparison with entropy change

Density and sound velocity of *n*-dodecane (99%, Sigma Aldrich) was measured using Anton Paar DSA 5000 at 293.15 K. Bulk modulus was calculated from the formula¹⁰:

$$K = d v^2$$

Where: d and v are density ($\text{kg}\cdot\text{m}^{-3}$) and sound velocity ($\text{m}\cdot\text{s}^{-1}$), respectively. Mean results from 5 measurements for *n*-dodecane and chosen literature data are collated in Table S15.

Table S15 Sound velocity and calculated bulk modulus for chosen *n*-alkanes at 293.15 K.

Substance	Density ($\text{kg}\cdot\text{m}^{-3}$)	Sound velocity ($\text{m}\cdot\text{s}^{-1}$)	Bulk modulus (GPa)	Source	ΔS ($\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$)
C₁₀H₂₂	729.87	1253.8 ± 1.1	1.148	11	829^{12}
C₁₂H₂₆	748.79, 746.724 \pm 8.258	1297.9, 1298.122 \pm 0.023	1.261, 1.2583 \pm 0.0139	11, this work	- 778 ^{this work}
C₁₄H₃₀	762.71	1331.2	1.351	11	772^{12}
C₁₆H₃₄	773.52	1357.3	1.425	11	742^{13}

Measurement of sound velocity and density (and calculation of bulk modulus) are important factors in fuel evaluation, therefore literature data are available for different *n*-alkanes, as well as binary and tertiary

mixtures at wide range of temperatures and pressures^{11,14}. The higher number of carbon atoms in the molecule, the higher density and sound velocity of the alkane, and thus the bulk modulus. From the collated literature and experimental data, it can be concluded that entropy change (the measure of the barocaloric effect) is inversely proportional to the bulk modulus. It must be noted that this trend is observed for even-numbered pure n-alkanes, crystallizing according to the mechanism described in this work. However, if this relationship can be observed for mixtures of alkanes with other substances (as it has been reported that crystalline phases can be formed with additives¹⁵), density and sound velocity measurement can be fast and convenient method for preliminary evaluation of barocaloric materials.

8. References

- (1) Mayo, S. L.; Olafson, B. D.; Goddard, W. A. DREIDING: A Generic Force Field for Molecular Simulations. *J. Phys. Chem.* **1990**, *94* (26), 8897–8909. <https://doi.org/10.1021/j100389a010>.
- (2) Williams, D. E. No Title. *J. Chem. Phys.* **1966**, *45*, 3370.
- (3) Allan, N. L.; Rohl, A. L.; Gay, D. H.; Catlow, C. R. A.; Davey, R. J.; Mackrodt, W. C. Calculated Bulk and Surface Properties of Sulfates. *Faraday Discuss.* **1993**, *95*, 273. <https://doi.org/10.1039/fd9939500273>.
- (4) Momany, F. A.; Carruthers, L. M.; McGuire, R. F.; Scheraga, H. A. Intermolecular Potentials from Crystal Data. III. Determination of Empirical Potentials and Application to the Packing Configurations and Lattice Energies in Crystals of Hydrocarbons, Carboxylic Acids, Amines, and Amides. *J. Phys. Chem.* **1974**, *78* (16), 1595–1620. <https://doi.org/10.1021/j100609a005>.
- (5) Gavezzotti, A. Are Crystal Structures Predictable? *Acc. Chem. Res.* **1994**, *27* (10), 309–314. <https://doi.org/10.1021/ar00046a004>.
- (6) Gavezzotti, A.; Filippini, G. Geometry of the Intermolecular X-H.Cntdot..Cntdot..Cntdot.Y (X, Y = N, O) Hydrogen Bond and the Calibration of Empirical Hydrogen-Bond Potentials. *J. Phys. Chem.* **1994**, *98* (18), 4831–4837. <https://doi.org/10.1021/j100069a010>.
- (7) Macrae, C. F.; Sovago, I.; Cottrell, S. J.; Galek, P. T. A.; McCabe, P.; Pidcock, E.; Platings, M.; Shields, G. P.; Stevens, J. S.; Towler, M.; Wood, P. A. Mercury 4.0: From Visualization to Analysis, Design and Prediction. *J. Appl. Crystallogr.* **2020**, *53* (1), 226–235. <https://doi.org/10.1107/S1600576719014092>.
- (8) Ungar, G. Structure of Rotator Phases in N-Alkanes. *J. Phys. Chem.* **1983**, *87* (4), 689–695. <https://doi.org/10.1021/j100227a032>.
- (9) Cliffe, M. J.; Goodwin, A. L. PASCAL: A Principal Axis Strain Calculator for Thermal Expansion and Compressibility Determination. *J. Appl. Crystallogr.* **2012**, *45* (6), 1321–1329. <https://doi.org/10.1107/S0021889812043026>.
- (10) Bansal, R. K. *A Textbook of Fluid Mechanics and Hydraulic Machines*; Laxmi Publications, 2010.
- (11) Luning Prak, D. J.; Lee, B. G.; Cowart, J. S.; Trulove, P. C. Density, Viscosity, Speed of Sound,

- Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of Butylbenzene + Linear Alkanes (n -Decane, n -Dodecane, n -Tetradecane, n -Hexadecane, or n -Heptadecane) at 0.1 MPa. *J. Chem. Eng. Data* **2017**, *62* (1), 169–187. <https://doi.org/10.1021/acs.jced.6b00542>.
- (12) Domalski, E. S.; Hearing, E. D. Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume III. *J. Phys. Chem. Ref. Data* **1996**, *25* (1), 1. <https://doi.org/10.1063/1.555985>.
- (13) Lin, J.; Tong, P.; Zhang, K.; Tao, K.; Lu, W.; Wang, X.; Zhang, X.; Song, W.; Sun, Y. Colossal and Reversible Barocaloric Effect in Liquid-Solid-Transition Materials n-Alkanes. *Nat. Commun.* **2022**, *13* (1), 596. <https://doi.org/10.1038/s41467-022-28229-4>.
- (14) Luning Prak, D. J.; Alexandre, S. M.; Cowart, J. S.; Trulove, P. C. Density, Viscosity, Speed of Sound, Bulk Modulus, Surface Tension, and Flash Point of Binary Mixtures of n -Dodecane with 2,2,4,6,6-Pentamethylheptane or 2,2,4,4,6,8,8-Heptamethylnonane. *J. Chem. Eng. Data* **2014**, *59* (4), 1334–1346. <https://doi.org/10.1021/je5000132>.
- (15) Turner, W. R. Normal Alkanes. *Prod. R&D* **1971**, *10* (3), 238–260. <https://doi.org/10.1021/i360039a003>.