

Chemical Science

Electronic supplementary material for:

Thermal expansion properties of organic crystals: a CSD study

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Fig. S1: Fraction of observations that originates from the same study per number of temperatures used to determine the thermal expansion properties of a crystal structure. (lower) Global number of observations per number of temperatures used to determine the thermal expansion properties of a crystal structure

Fig. S2a-b: Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in in the CSD (version 5.41). Complete dataset

Fig. S3: Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in in the CSD (version 5.41). Only observations with $R^2 > 0.75$ were used.

Fig. S4: Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in in the CSD (version 5.41). Only observations with $R^2 > 0.80$ were used.

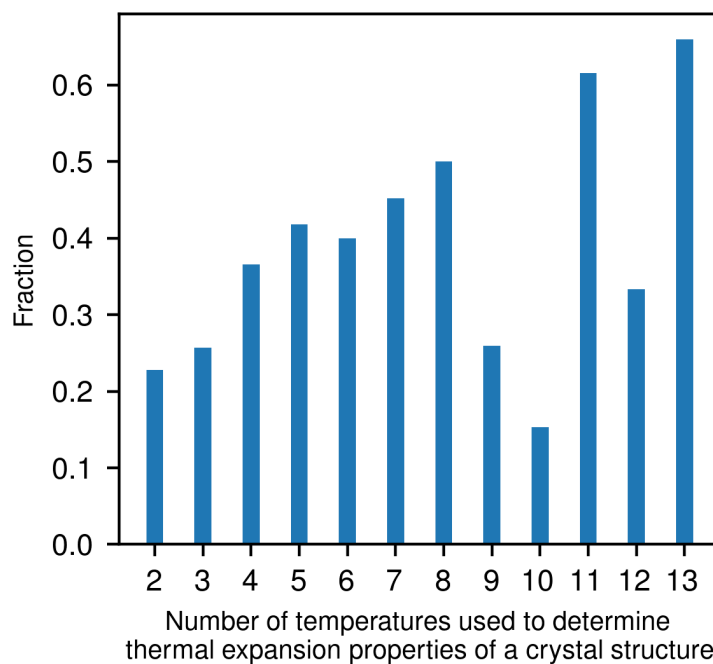
Fig. S5: Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in in the CSD (version 5.41). Only observations with $R^2 > 0.85$ were used.

Fig. S6: Best overlay of the structures with *refcodes* VERMAG and VERMAG01

Table S1: Mean, median, and standard deviations of distributions of volumetric (α_V), uniaxial thermal expansion (α), and indicatrix anisotropy (IAC) coefficients as a function of R^2 .

Table S2: Possible organic compounds with negative volumetric thermal expansion

Fraction of observations that originates from the same study per number of temperatures used to determine thermal expansion properties of a crystal structure



Number of observations per number of temperatures used to determine thermal expansion properties of a crystal structure

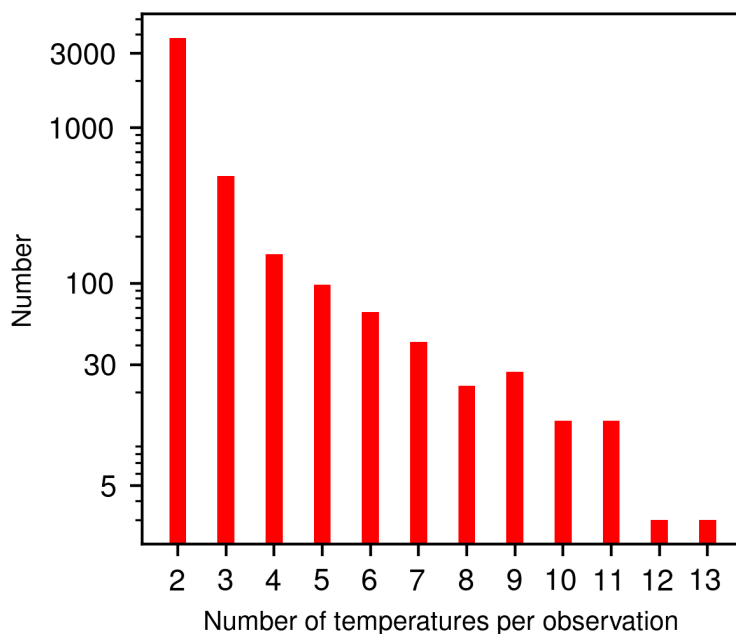


Fig. S1: (upper) Fraction of observations that originates from the same study per number of temperatures used to determine the thermal expansion properties of a crystal structure. (lower) Global number of observations per number of temperatures used to determine the thermal expansion properties of a crystal structure. An 'observation' is a set of thermal expansion coefficients for a particular compound.

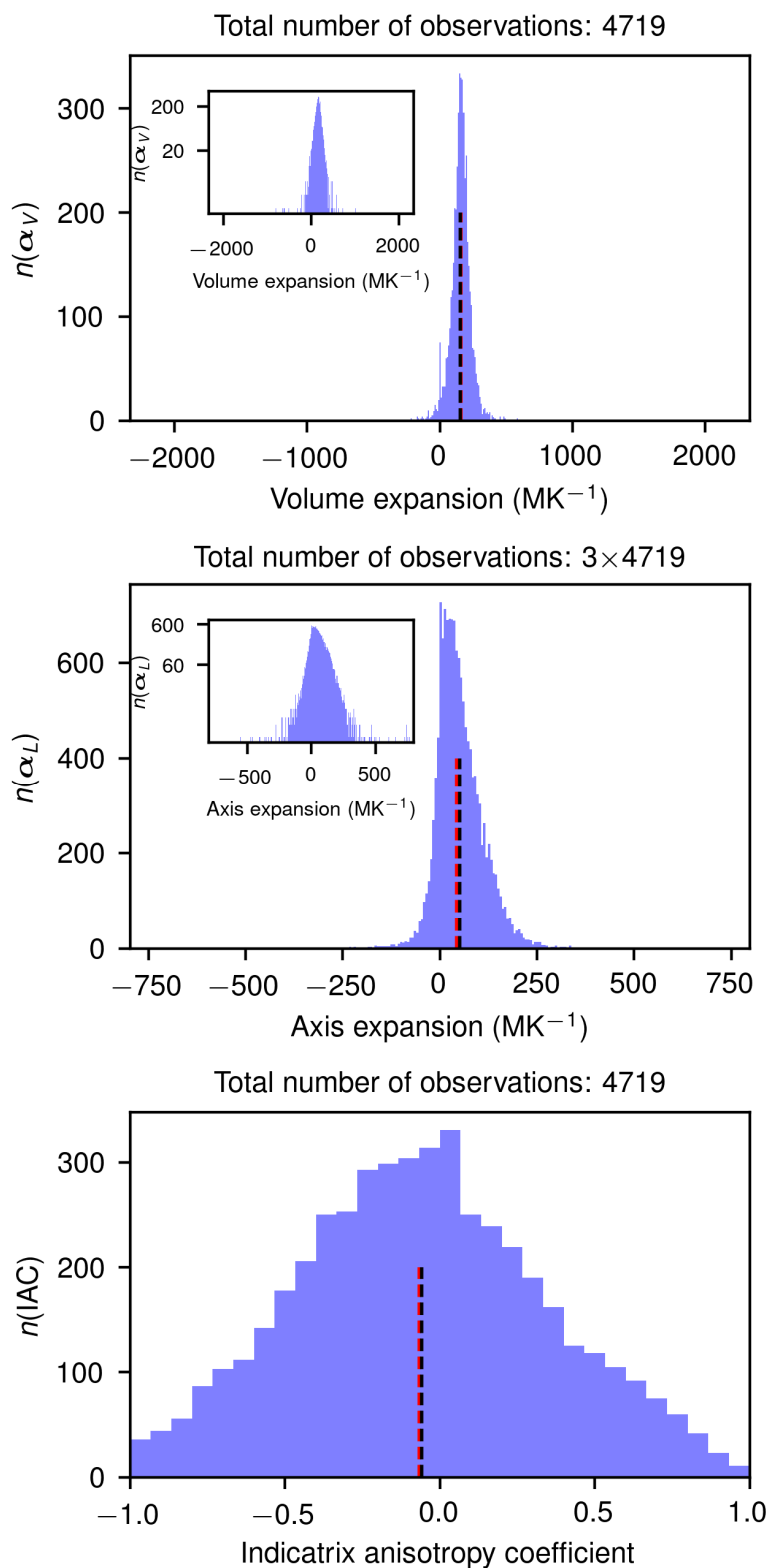


Figure S2a Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in the CSD (version 5.41). The complete data set was used to calculate these histograms.

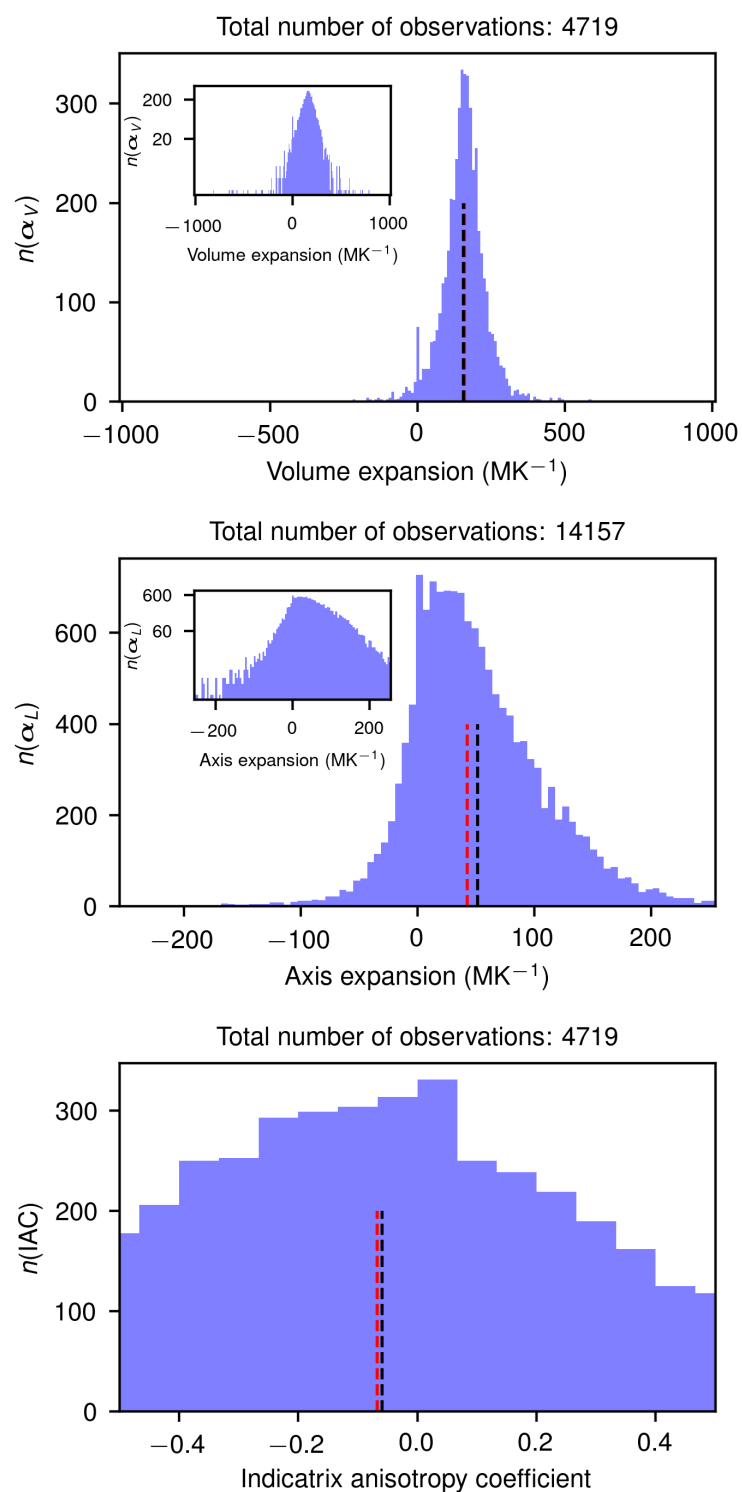


Figure S2b Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in the CSD (version 5.41). This figure is the same as Fig S2a but with different (zoomed) x-axes.

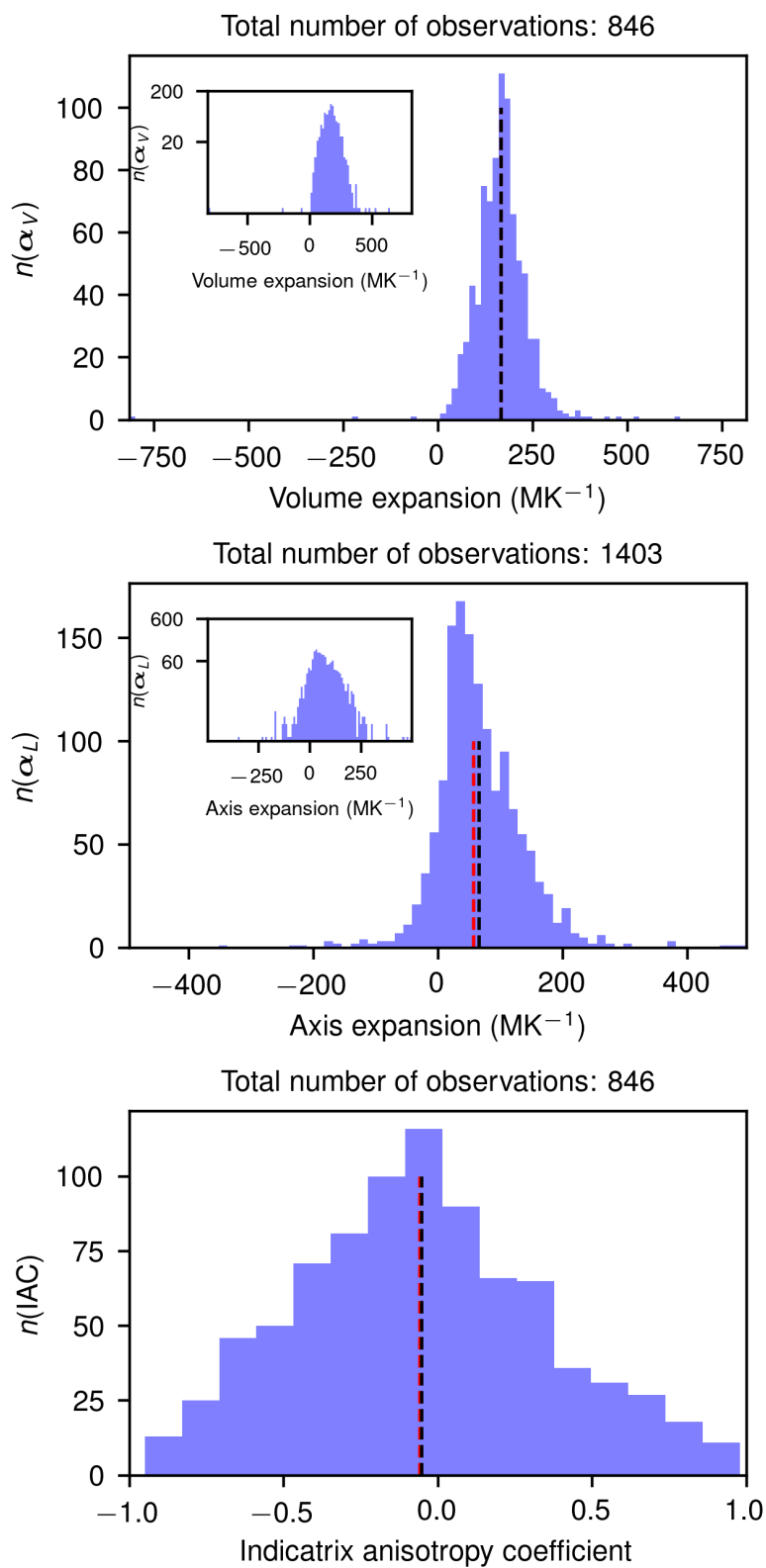


Figure S3 Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in the CSD (version 5.41). Only observations with $R^2 > 0.75$ were used and for each data point at least 3 temperature points

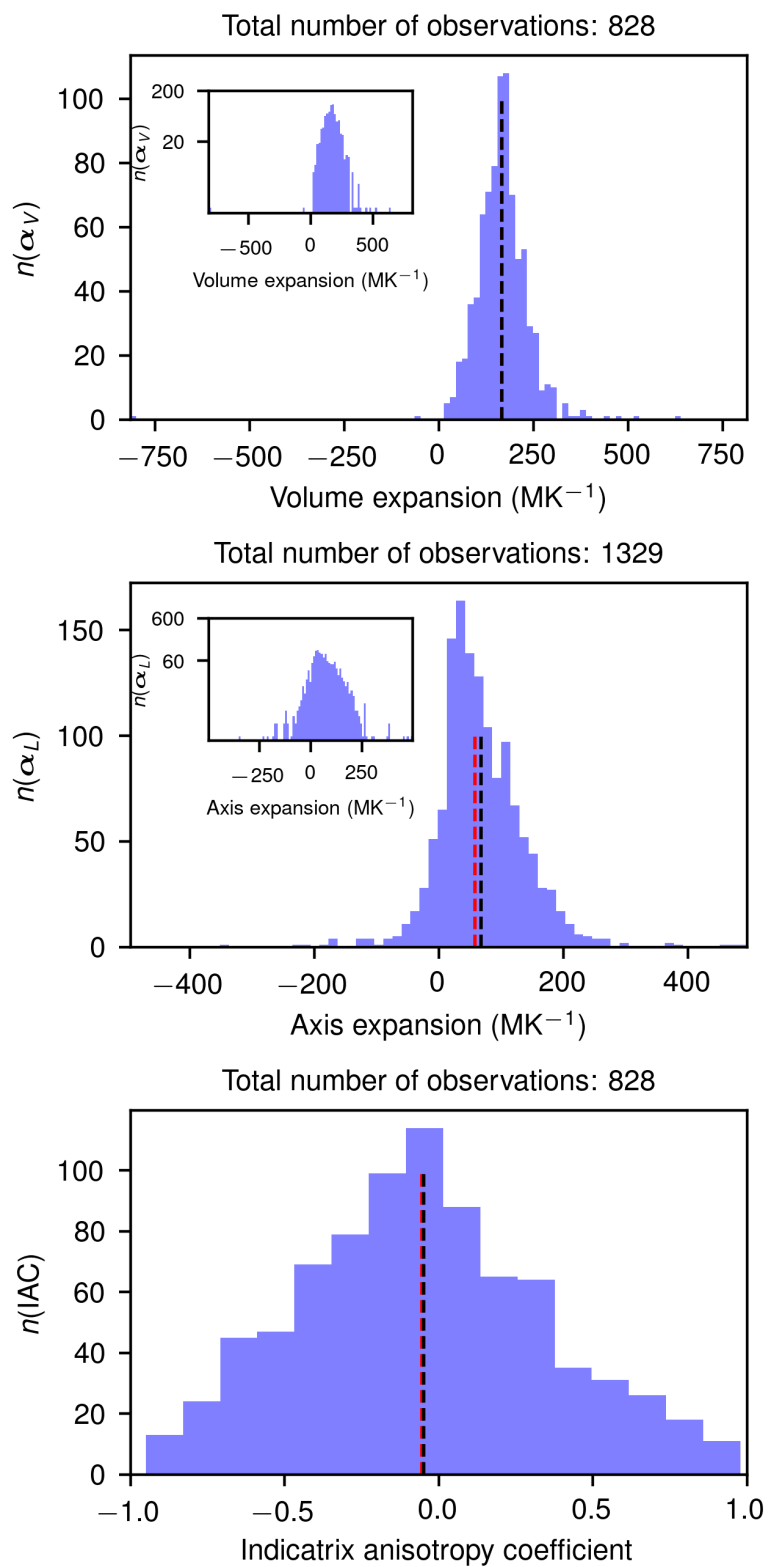


Figure S4 Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in the CSD (version 5.41). Only observations with $R^2 > 0.80$ were used and for each data point at least 3 temperature points

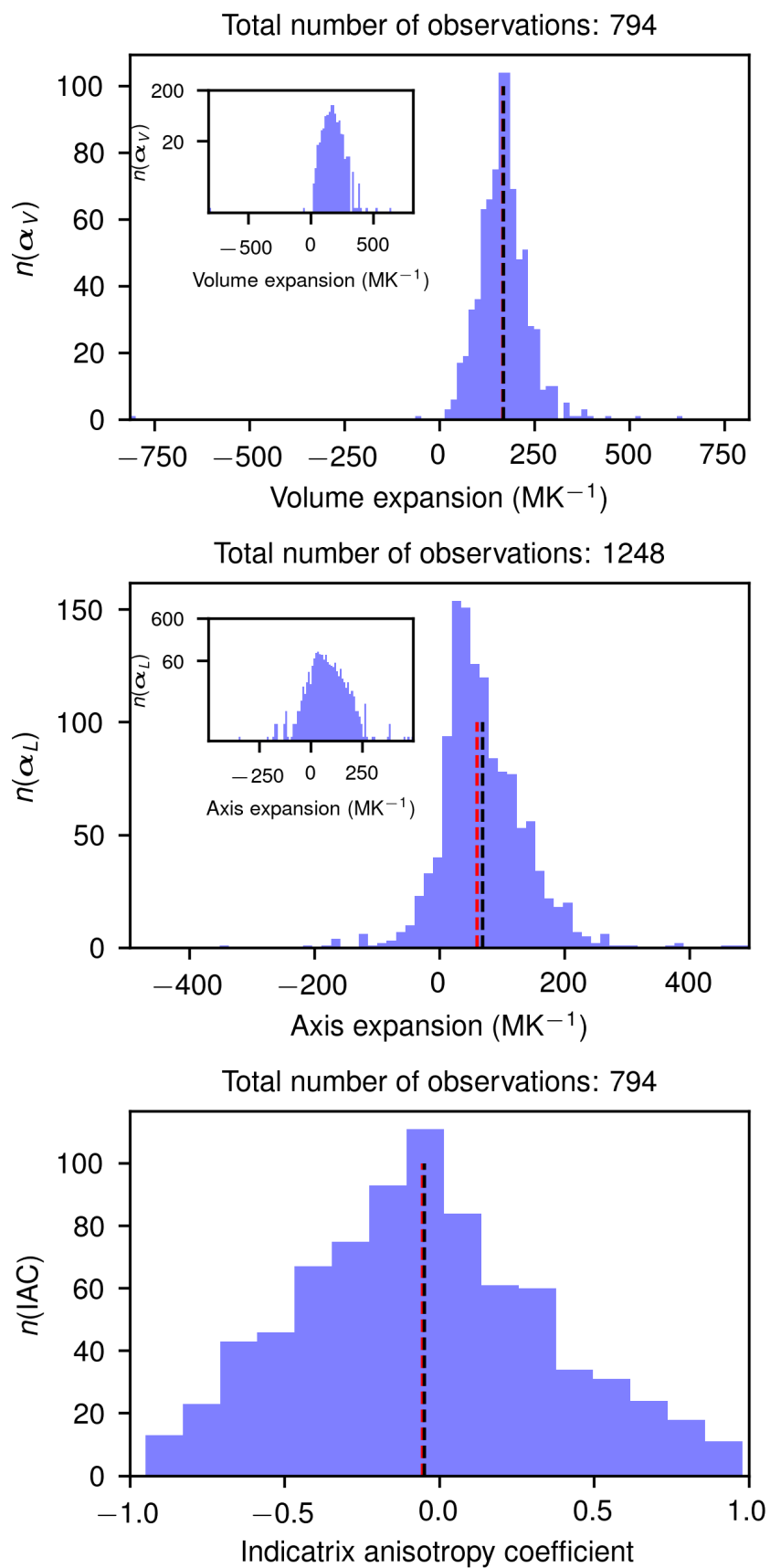


Figure S5 Histograms of the volume and axis expansions and the indicatrix anisotropy coefficient of organic compounds in the CSD (version 5.41). Only observations with $R^2 > 0.85$ were used and for each data point at least 3 temperature points

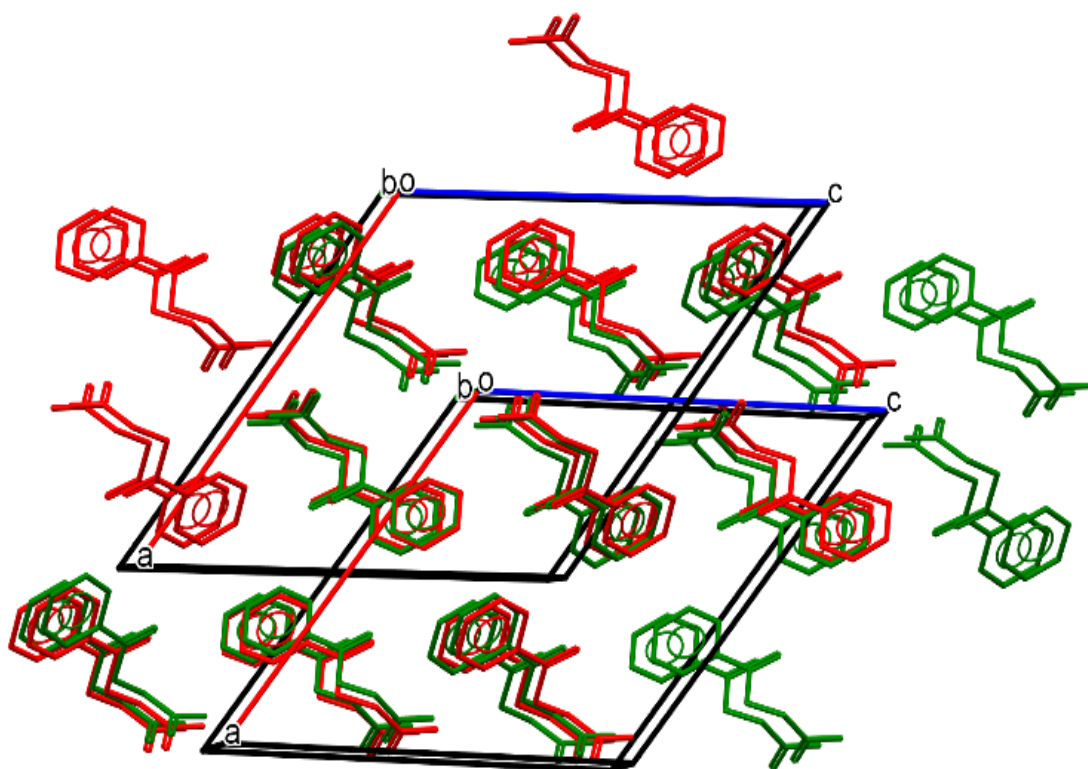


Figure S6 Best overlay of the structures with *refcodes* VERMAG (red) and VERMAG01 (green). The unit cell of the VERMAG01 structure has been transformed to its conventional setting in $P2_1/c$. The rms deviation between the two structures is 0.108 Å. The calculations and visualization have been performed with *MERCURY*. The two structure packings are strictly the same. The room temperature structure (*refcode* VERMAG) was determined from Weissenberg camera data¹, whereas the data for the 235 K structure were collected on a Syntex $P2_1$ diffractometer² (*refcode* VERMAG01). Interestingly, the densities of both structures were also determined using a standard flotation technique (1.31 and 1.17 gcm⁻³ both measured at room temperature for the 235 and 295 K structures, respectively) and found to be in close correspondence with the density calculated from the X-ray crystal structures (1.326 and 1.16 gcm⁻³ for the 235 K and 295 K structures, respectively). The difference in measured room temperature densities may seem suspicious or a sign of polymorphism. The latter can be ruled out by superposing the experimental structures, leaving the possibility that the room temperature density in the Selladurai study¹ was incorrectly assessed. Only a new temperature dependent X-ray study on the same crystal using the same diffractometer can validate or invalidate this result.

1. S. Selladurai, M. S. Kumar and K. Subramanian, *Proc. Indian Acad. Sci. (Chem. Sci.)*, 1990, **102**, 39-43
2. H. W. Thompson, P. A. Vanderhoff and R. A. Lalancette, *Acta Crystallographica Section C Crystal Structure Communications*, 1991, **47**, 1443-1445.

Table S1 Mean, median, and standard deviations of distributions of volumetric (α_v), uniaxial thermal expansion (α_l), and indicatrix anisotropy (IAC) coefficients as a function of R^2 .

	Global dataset	$R^2 > 0.75$	$R^2 > 0.80$	$R^2 > 0.85$	$R^2 > 0.90$
$n(\alpha_v)/n(\alpha_l)$	4719/14157	846/1403	828/1329	794/1248	745/1129
$\mu(\alpha_v)$	155.98	166.62	167.41	167.98	168.60
$\eta(\alpha_v)$	159.01	166.58	166.93	167.50	168.30
$\sigma(\alpha_v)$	90.85	73.87	73.05	72.55	72.51
$\mu(\alpha_l)$	51.64	66.20	67.80	69.34	71.43
$\eta(\alpha_l)$	42.57	56.98	58.23	59.74	62.57
$\sigma(\alpha_l)$	64.95	68.64	69.29	69.60	69.90
$\mu(\text{IAC})$	-0.06	-0.05	-0.05	-0.05	-0.05
$\eta(\text{IAC})$	-0.07	-0.06	-0.06	-0.05	-0.05
$\sigma(\text{IAC})$	0.40	0.40*	0.40*	0.40*	0.41*

Notes: $n(\alpha_v)/n(\alpha_l)$ are the numbers of observations for the volumetric (α_v) and axial (α_l) thermal expansion coefficients, respectively. μ is the mean value of the distribution, η the median value, and σ the standard deviation. The units of α_v and α_l are expressed in MK^{-1} . The data sets noted by an asterisk are normally distributed. The 'global dataset' includes all temperature data sets, even those measured only at 2 temperatures; the columns $R^2 > 0.75, 0.80, 0.85, 0.90$ include only data sets measured at at least 3 temperatures, and with goodness of fit values R^2 for a linear dependency of thermal expansion on temperature.

Table S2 Possible organic compounds with negative volumetric thermal expansion.

refcode	α_v (MK^{-1})	ΔT (K)	N_m	χ_α	Ano	SS	Comments
EGIDUT	-623.12	230-296	2	-4.98			possibly x-ray-induced; polymerization reactions taking place; structure has the right metrics for photochemical SC-to-SC reactions, according to Schmid's rules; no heavy atoms
NEJQEY	-590.25	123-175	3	-3.07			data collection temperature at 175 K is not clear; hydrocarbon; $\pi \cdots \pi$ contacts but mostly H-H interactions and H-ring interactions
LATDAN	-460.18	120-173	2	-2.44			both are monohydrate, although one is reported as dehydrate, can be ok; H-bond backbone, π - π contacts but mostly H-H interactions and H-ring interactions

DOFSUM	-370.75	173-295		-4.52	s		void space present? Can be correct
RALQAW	-318.10	90-173	2	-2.64			can be ok; some H-bonds, $\pi\cdots\pi$ contacts but mostly H-H interactions and H-ring interactions
MIPQAG	-306.41	100-273	2	-5.30		o	porous structure, CO ₂ loss at RT?; no CO ₂ in structure, no H-bond backbone, H-ring interactions (first 3p element)
MEBVOH	-244.94	150-298	2	-3.63		o	can be ok; two 'isoforms' but why was one reported at 150 and the other at 298 K, structures seem to be the same; weak H-bonds, H-H dihydrogen contacts, 1 H- π interaction
MOTPUG	-215.59	160-295	2	-2.91			colorless at RT, orange at LT, weak H-bonds, H-H dihydrogen contacts, H- π interactions, some $\pi\cdots\pi$ contacts
ALAZAO	-211.50	173-291	2	-2.50			can be ok; flattest molecule so far, H-bond backbone, no dihydrogen contacts, π stacking and H- π contacts
UKOYUO	-194.64	168-273	2	-2.04	s		can be ok; weak H-bonds (N-H, S-H), H- π contacts and π stacking
WUVYIV	-173.06	150-294	2	-2.49			can be ok; heavy atom (Br), no amide H-bond, but others, such as CO- \cdots HC(benzene); π stacking results in this being the first relatively flat molecule in the series
VEPKEJ	-169.07	220-296	2	-1.28	s		color of LT crystal is colourless; that of RT crystal dark yellow; strange CH- $\cdots\pi$ interactions all over the aliphatic chain; no π stacking
XEQOH	-166.35	100-173	2	-1.21			can be correct; π -stacking, H-aromatic-Haliphatic interactions, weak H-bonds, CH- $\cdots\pi$ interactions
KIZQAO	-165.55	173-293	2	-1.99			can be correct; Sr salt, if you are really picky you could argue that it is organometallic; polymeric structure with strong H-bonds, some H-H interactions and H- π interactions
GEJVIB	-164.03	213-293	2	-1.31			can be correct; LT structure is really poor quality; no π stacking, many H-H contacts
SAJFIT	-156.67	215-296	2	-1.27			RT crystal colourless, LT structure bright yellow; H-bond backbone, π -stacking, many H- $\cdots\pi$ and some H-H contacts
JUMXAQ	-144.75	220-295	2	-1.09			can be correct; H-bonds provide the structure, some π -stacking; several CH- $\cdots\pi$ contacts (@ angle with respect to c axis)
MOXVIF	-142.37	85-173	2	-1.25		o	can be correct; H-bonds and π -stacking form the backbone, some CH- $\cdots\pi$ and H- \cdots H contacts present
CIWCIV	-135.56	223-296	2	-0.99	s		can be correct; very small difference between the R of the two structures (6.04% LT vs 6.07%) HT; H-bonds and π -stacking form the backbone, some CH- $\cdots\pi$ and H-H contacts present
KIKJEU	-135.13	125-294	2	-2.28			can be correct; some H-bonds, no π -stacking, many CH- π interactions in the bc plane (might be the mechanism)
VUTXUE	-134.68	103-273	2	-2.29			can be correct; however, should be rather classified as organometallic: Te covalent bond with C; S-S dipolar contacts, I-H H-bonds, some dihydrogen contacts
HOTNIO	-127.73	150-296	2	-1.86	s		can be correct; weak H-bonds, π -stacking
ATTAZ	-121.54	199-295	2	-1.17			can be correct; H-bonds, π -stacking, $\pi\cdots\pi$ interactions
LIYLAJ	-120.09	100-173	2	-0.88		o	photo-induced switching, Both temperatures 100, 173 should be probably 'room temperature'; CH- $\cdots\pi$ backbone in the ab plane (probably the cause of NTE), H-bond spiral between the diols along c, isolated from the rest of the interactions
NIZXEA	-106.37	150-293	2	-1.52			can be correct; Cl- $\cdots\pi$ interaction, some H-bonds, some dihydrogen contacts
MIYBAX	-102.58	123-293	2	-1.74	s		can be correct, H-bonds and dipole stacking in the bc

							plane
QOYJOD	-91.33	223-293	2	-0.64			α polymorph, probably correct, H-bonds and π stacking
YEDPAZ	-89.84	100-153	2	-0.48	s		can be correct, H-bond, π and dipole stacking, weak CH- π interaction
BEWKUM	-89.21	173-290	2	-1.04			can be correct, H-bond, π stacking, CH- π contact
TIFQOO	-89.21	225-293	2	-0.61			can be correct, π -stacking and H-bonds
TUKWOL	-86.87	125-177	2	-0.45			can be correct, H-bonds, dihydrogen contacts
FAGSUB	-86.83	173-293	2	-1.04			can be correct, weak H-bond, CH- π contacts
MUBJOJ	-86.72	130-296	3	-1.44		o	isosymmetric phase transition; no agreement between room temperature structure reported in Acta Cryst E and that in CrystEngComm, CH- π contacts, weak H-bond,
MATZEO	-86.12	173-293	2	-1.03	s		can be correct, weak CH \cdots O bond, Type II Cl-Cl halogen bond, weak CH \cdots Cl contacts
TYRAMH	-85.64	200-295	2	-0.81			can be correct, possible reorientation of the H-bond network
ROHBOF	-82.14	100-173	2	-0.60			can be correct, weak CH \cdots N H-bond, CH- π contacts
DADMED	-82.13	150-296	2	-1.20	s		can be correct, some H-bonds, π stacking
YUHHUE	-80.13	203-295	2	-0.74		o	can be correct, H-bond (OH \cdots OH), CH \cdots π contacts, π stacking
TIJDAR	-79.47	150-295	2	-1.15			can be correct
CEYYAG	-79.42	173-295	2	-0.97			can be correct, H-bond (OH \cdots OH), CH \cdots π contacts, π stacking
LUZXOU	-71.53	173-296	2	-0.88	s		LT crystal colourless, RT crystal yellow, H-bonds, π stacking, $\pi\cdots\pi$ contacts
ZUZBUT	-69.38	173-293	2	-0.83	s		can be correct, weak CH \cdots O bonds, dihydrogen contacts, CH \cdots π contacts
CAZKUK	-68.92	150-205	2	-0.38			can be correct, H-bonds, π stacking, CH \cdots O contacts
ADEREH	-66.98	173-292	2	-0.80			can be correct, π stacking, CH \cdots O contacts, CH \cdots π contacts
ELEPOB	-59.65	100-200	3	-0.60			can be correct, H-bonds, π stacking, $\pi\cdots\pi$ contacts
NOJJUU	-54.78	173-296	2	-0.67			can be correct, CH \cdots O contacts, CH \cdots π contacts, π stacking, $\pi\cdots\pi$ contacts
FIGKOY	-53.84	155-293	2	-0.74	s	o	can be correct, Cl atom half occupancy
KERNOM	-53.32	200-295	2	-0.51			can be correct, H-bonds, CH \cdots O contacts, $\pi\cdots\pi$ contacts
BEWYAE	-50.39	173-293	2	-0.60			can be correct, H-bonds, $\pi\cdots\pi$ contacts (unoccupied B orbitals)
AXUBUR	-49.30	90-293	2	-1.00			can be correct π stacking, CH \cdots π contacts, CH \cdots F bonds
FELCEH	-48.62	100-293	2	-0.94		o	can be correct, CH \cdots π contacts, π stacking (double bond – ring)
PESKII	-47.25	100-193	2	-0.44			can be correct, π stacking, CH \cdots O contacts, dihydrogen contacts
SOVBAG	-46.82	163-273	2	-0.51			can be correct, poorly solved, probably dihydrogen contacts
FOMZUD	-43.48	150-293	2	-0.62			can be correct, CH \cdots O contacts, π stacking
ASONOM	-43.06	133-296	2	-0.70			can be correct, dihydrogen contacts, CH \cdots π contacts
DOCKUE	-42.27	200-293	2	-0.39			can be correct, π stacking, dihydrogen contacts,
QEDHUE	-41.96	153-293	2	-0.59			LT crystal yellow, RT colourless, H-bonds, π stacking
CAPLAC	-40.34	123-295	2	-0.69			can be correct, H-bonds, dihydrogen contacts (along a axis)
TIGYUE	-39.32	150-293	2	-0.56			can be correct, H-bonds, CH \cdots π contacts
FOKZUB	-38.98	213-293	2	-0.31	s		can be correct, H-bonds, dihydrogen contacts
WONVEA	-38.47	100-295	2	-0.75			can be correct
KUQSAS	-37.53	173-293	2	-0.45			color RT ligh-green, color LT colorless, CH \cdots π contacts, π stacking, $\pi\cdots\pi$ contacts
DAPSUO	-37.17	295-373	7	-0.29			Isosymmetric phase transition, H-bonds, CH \cdots O/CH \cdots N weak H-bonds, CH \cdots π contacts
WEDMOI	-36.09	20-100	2	-0.29			can be correct, fluorine contacts, odd one out

FORBAQ	-34.60	110-296	2	-0.64			can be correct, π stacking, $\pi\cdots\pi$ contacts, dipolar contacts
MAZMAE	-34.18	100-153	2	-0.18			can be correct, H-bonds, dihydrogen contacts
NOTLAL	-33.38	113-293	2	-0.60			RT crystal grey, LT crystal yellow, π stacking, $\pi\cdots\pi$ contacts, CH \cdots O bonds
WIMVIZ	-33.37	173-293	2	-0.40	s		can be correct, π stacking, π - π contacts, CH \cdots I bonds
SARCAC	-32.95	129-295	5	-0.55		o	can be correct, CH \cdots O contacts, dihydrogen contacts
ACUFIO	-32.82	150-297	2	-0.48			can be correct, H-bonds, π stacking,
KAKCEH	-32.23	150-295	2	-0.47		o	can be correct void space 20-30%, π stacking, CH $\cdots\pi$ contacts
HELHUD	-28.17	200-293	2	-0.26			can be correct, H-bonds, CH $\cdots\pi$ contacts
REZSIZ	-28.08	100-293	2	-0.54			can be correct, H-bonds, π stacking, F contacts
RAKYOR	-28.06	293-546	2	-0.71	s		can be correct, H-bonds, CH $\cdots\pi$ contacts
MEHBOR	-27.11	173-273	2	-0.27			can be correct, H-bonds, CH $\cdots\pi$ contacts
BATLOZ	-26.58	173-296	2	-0.33	s		can be correct, π stacking, dihydrogen contacts, CH \cdots F contacts
RETNEM	-26.41	93-180	2	-0.23			can be correct, H-bonds, CH $\cdots\pi$ contacts, π stacking
VIZGIX	-25.46	113-295	2	-0.46		o	can be correct, π stacking, dihydrogen contacts, CH \cdots O contacts
NUZQOO	-25.30	130-295	2	-0.42			can be correct, H-bonds
ANULEN	-25.29	100-295	3	-0.49			can be correct, CH $\cdots\pi$ contacts, π stacking, possible phase transition due to changing occupancies
TEZZUU	-16.69	173-295	2	-0.20			can be correct, H-bonds, π stacking, weak CH \cdots O contacts
RURQAX	-16.64	100-200	2	-0.17			can be correct, π stacking, weak CH \cdots O contacts, O \cdots Br contacts, dihydrogen contacts
KIYFED	-15.35	123-295	2	-0.26			can be correct, H-bonds, dihydrogen contacts
FAHDOI	-14.60	150-295	2	-0.21			can be correct, first 3d polymer structure, π stacking, H-bonds, dihydrogen contacts
QOCXAJ	-14.30	150-296	2	-0.21	s		can be correct, CH $\cdots\pi$ contacts, weak CH \cdots O contacts, dihydrogen contacts
BOGCAC	-13.96	90-150	2	-0.08			can be correct, H-bonds, CH $\cdots\pi$ contacts, π stacking
NOBFEP	-13.46	173-293	2	-0.16			can be correct, π stacking CH $\cdots\pi$ contacts, dihydrogen contacts
HAPLAN	-13.44	100-293	2	-0.26	s		can be correct, CH $\cdots\pi$ contacts, weak CH \cdots O contacts
BOWMIK	-13.35	100-298	2	-0.26		o	False hit, synchrotron powder data, however no carbon present, but only boron; see text
AMASOY	-12.75	90-296	3	-0.26			Color red or orange, π stacking CH $\cdots\pi$ contacts, dihydrogen contacts, possible phase transition (disorder in HT)
ZETFIQ	-12.63	150-296	2	-0.18			can be correct, CH $\cdots\pi$ contacts, weak CH \cdots O contacts
SECHUG	-12.09	150-293	2	-0.17			can be correct, H-bonds, weak CH \cdots O contacts, π stacking
MORPHM	-12.01	25-295	2	-0.32			can be correct, H-bonds, weak CH \cdots O contacts, π stacking
TEJNAX	-10.71	85-150	2	-0.07			can be correct, H-bonds, π stacking (carboxylates)
TARDOF	-10.29	173-295	2	-0.13			can be correct, H-bonds, π stacking, dihydrogen contacts
OMERUT	-9.58	110-293	2	-0.18		o	CSD notes that there is doubt about the reported temperature of one of the structures, a methylene bridge between to N changes in a strange manner, I would not include it
PEVNUC	-8.86	280-400	4	-0.11		o	correct, same crystal same machine; longest single C-C bond ever reported (makes sense from a chemical point of view: high steric hinderance), π stacking CH $\cdots\pi$ contacts, dihydrogen contacts
XOTGIY	-8.59	173-296	2	-0.11			can be correct, π stacking, CH $\cdots\pi$ contacts, weak CH \cdots O contacts
JEJSUP	-8.57	110-293	2	-0.16			can be correct, CH $\cdots\pi$ contacts, weak CH \cdots O contacts

QAVTUE	-8.39	193-296	2	-0.09			can be correct, H-bonds, π stacking, CH \cdots π contacts, weak CH \cdots O contacts
WUXNIM	-7.58	92-180	2	-0.07			can be correct, F \cdots π contacts, π stacking
QUWYAJ	-6.59	123-293	2	-0.11			can be correct, H-bonds, π stacking
ETDAMS	-6.54	100-295	2	-0.13			can be correct, H-bonds, dihydrogen contacts
NEZGAD	-6.04	105-295	2	-0.11		o	can be correct, H-bonds, π stacking, weak CH \cdots O/CH \cdots F contacts
SILTEP	-5.94	160-273	2	-0.07			can be correct, CH \cdots π contacts, dihydrogen contacts
HOQMIL	-5.76	173-293	3	-0.07			can be correct, porous structure with solvent inside (DMF)
JAGRIV	-5.75	150-298	2	-0.09	s		can be correct, H-bonds, π stacking, CH \cdots π contacts, weak CH \cdots O contacts
ROYHAQ	-5.65	100-294	2	-0.11			can be correct, H-bonds, π stacking, CH \cdots π contacts, weak CH \cdots O contacts, dihydrogen contacts
XUKKET	-3.83	170-593	3	-0.16		o	can be correct, second 3D polymeric structure, some π stacking (acetylenes)
KOZTOK	-3.35	90-293	2	-0.07			LT color yellow; RT light colorless, π stacking, CH \cdots π contacts, weak CH \cdots O contacts
BAXSIC	-3.19	80-295	2	-0.07			can be correct, H-bonds, weak CH \cdots O contacts
ITIRAE	-2.71	140-296	2	-0.04	s		can be correct H-bonds, weak CH \cdots O contacts, $\pi\cdots\pi$ contacts (B to Ph)
DOPLOL	-2.69	120-451	2	-0.09		o	can be correct, H-bonds, π stacking
CELLOB	-2.27	120-173	3	-0.01			can be correct, H-bonds, weak CH \cdots O contacts
JOYQUJ	-2.06	173-295	2	-0.03			can be correct, H-bonds, π stacking, CH \cdots Br contacts
ODAKOV	-2.04	173-293	2	-0.02	s		can be correct, H-bonds, dihydrogen contacts, possible rearrangement of the of the H-bond network inside the channel
IPABIL	-1.82	200-293	2	-0.02			can be correct, 3 rd 3D polymeric structure, π stacking
TOHIJ	-1.64	153-293	3	-0.02			can be correct, H-bonds, π stacking, weak CH \cdots O contacts
CEMCAZ	-1.54	153-295	2	-0.02			can be correct, π stacking, weak CH \cdots O contacts, dihydrogen contacts
GLUTAS	-1.29	100-295	3	-0.03			can be correct, H-bonds, weak CH \cdots O contacts
KIMSUU	-1.17	122-295	2	-0.02			can be correct, CH \cdots π contacts, dihydrogen contacts
DAYGUH	-1.04	100-296	2	-0.02	s		can be correct, 4 th polymeric structure, H-bonds, π stacking
HEKMEP	-0.59	121-295	2	-0.01			can be correct, , H-bonds, weak CH \cdots O contacts, dihydrogen contacts
WADQEY	-0.36	220-295	2	-0.00			can be correct, CH \cdots π contacts, weak CH \cdots O contacts
KOYRUN	-0.26	10-100	2	-0.00		o	can be correct, paper also gives powder data at 245 K which proves uniaxial thermal expansion along c, H-bonds
EZUWAX	-0.21	120-293	2	-0.00			can be correct, H-bonds, dihydrogen contacts
WEJZUH	-0.21	175-293	2	-0.00			can be correct, H-bonds, weak CH \cdots O contacts, CH \cdots π contacts
CLAHMB	-0.00	123-423	2	-0.00			probably not correct – identical cell parameters at 123 and 423 K

Notes: The thermal expansion coefficient, temperature range, Nm and the NTE capacity parameter $\chi\alpha$ are provided for each individual CSD entry. The column Ano indicates whether there is a $\langle U_{eq} \rangle$ anomaly, where higher temperatures correspond to lower values, and such entries are denoted with an 's'. Datasets collected in the same study are denoted with an 'o' in the SS column and other general remarks on the structure are included as well. The comments column describes some structural features and the possibility whether the negative volumetric expansion is correct or not.