Supporting Information

Pressure- and temperature-driven transitions and conformational conversions of *n*-hexyl substituted perylene diimide (PDI-C_6) crystals

Paulina Ratajczyk, Szymon Sobczak, Michał Andrzejewski, Francesco Marin, Marianna Marchini, Lucia Maini, Andrzej Katrusiak**

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1. PDI-C_6 at room conditions

1.1. UV-Vis absorption spectroscopy

The UV-Vis-IR absorption spectra of the solid-state sample was recorded using a Jasco V-770 spectrophotometer. The absorbance was measured at a scan speed of 200 nm min^{-1} in the 350-1200 nm range.

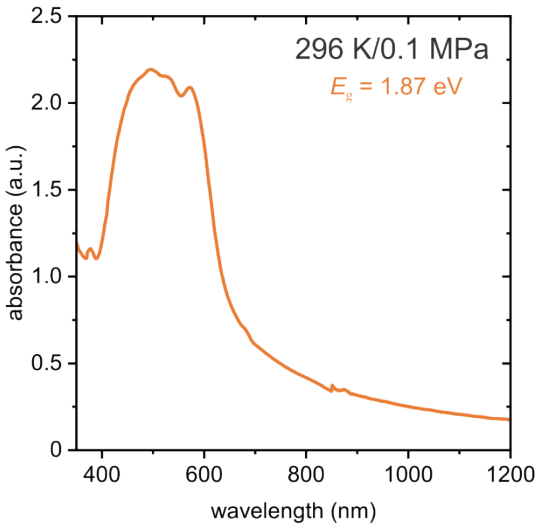

Figure S1. Absorption spectra of PDI-C_6 at room conditions.

1.2. Single-crystal X-ray diffraction

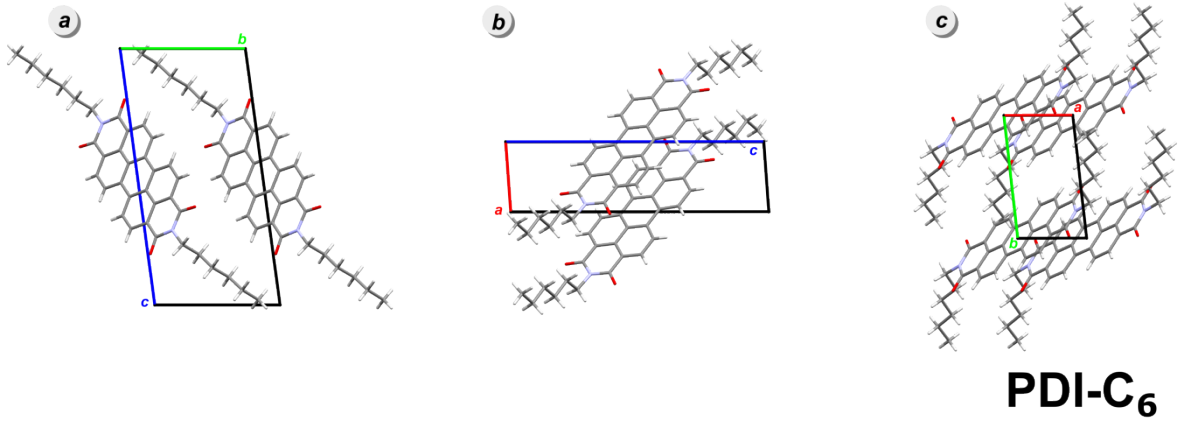

Figure S2. Arrangements of PDI-C_6 molecules in the unit-cell along direction: (a) [100]; (b) [010]; and (c) [001], at room conditions (296 K/0.1 MPa, phase I).

2. Effect of temperature on PDI-C_6

2.1. Thermal gravimetric analysis

TGA measurements were performed using a Perkin Elmer TGA7 in the temperature range 308-823 K under N_2 gas flow and heating was carried out at 20 K min^{-1}.

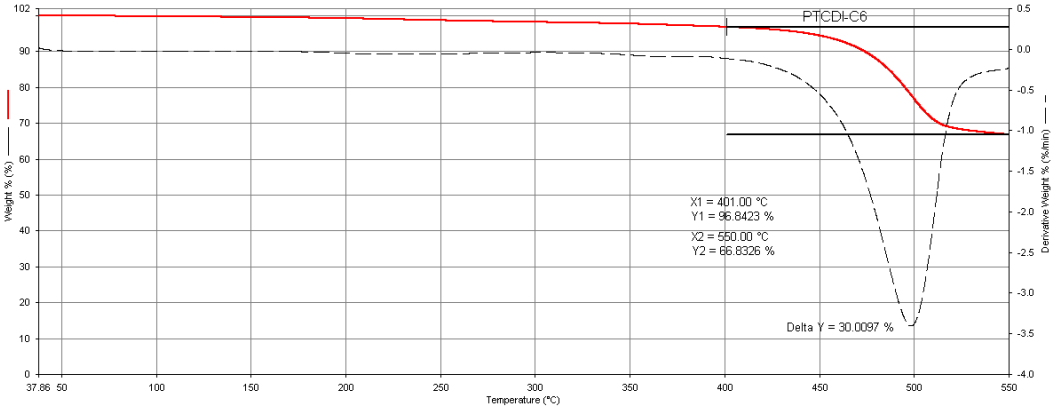

Figure S3. TGA curve of PDI-C_6, a single degradation step is observed above 400 °C.

2.2. Variable-temperature X-ray diffraction

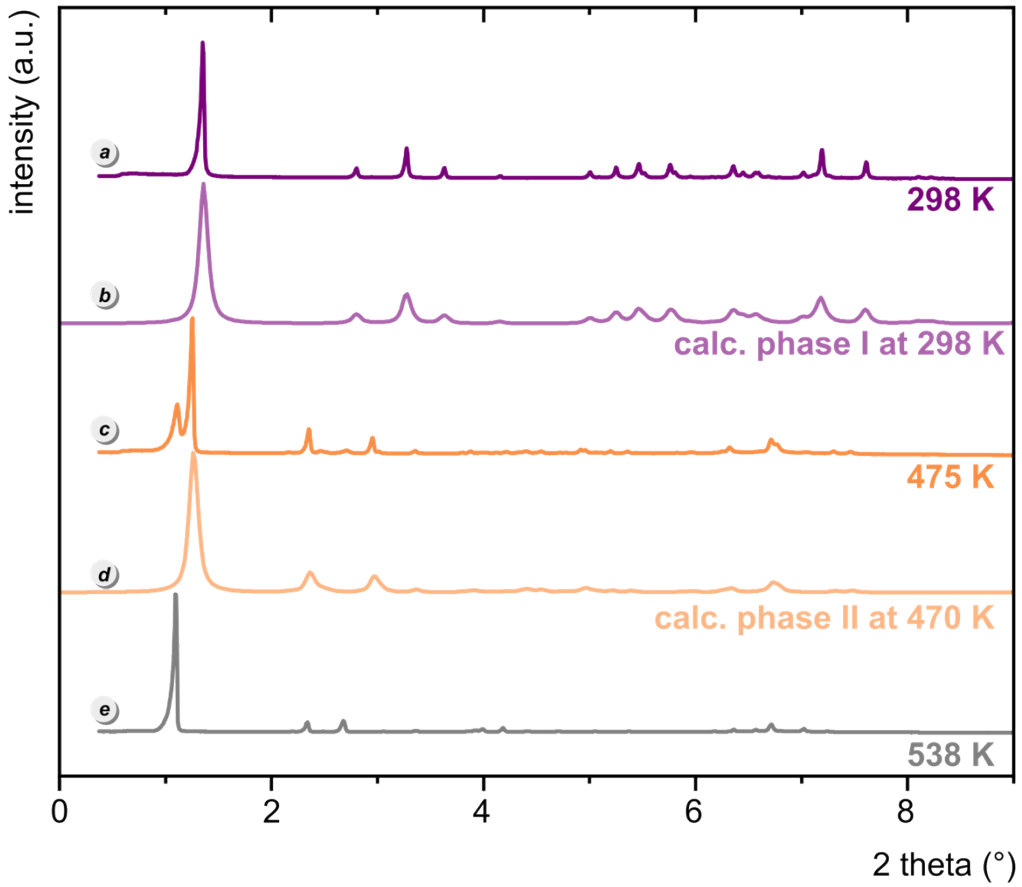

Figure S4. PXRD patterns of PDI-C_6 phase I at 298 K (a), phase II and III at 475 K (c), and phase III at 538 K (e), collected using an X-ray beam (λ= 0.41235 Å). The calculated diffractograms,

derived from single-crystal data collected at 298 K (phase I, b) and 470 K (phase II, d), are included for comparison.

The PXRD pattern collected at 475 K is characterized by the presence of two distinct reflections at low 2θ angles (Figure S4c). Upon increasing the temperature from 475 K, the reflections associated with phase II gradually diminish, and at 538 K, the PXRD pattern consists only phase III. Unfortunately, solving the crystal structure of phase III was not possible, we were only able to determine the unit-cell parameters. As a speculative hypothesis, we propose that phase III may exhibit an alternating criss-cross π-stacking arrangement. The unit-cell volume corresponds to two molecules in the unit cell, that could be rotated relative to each other, allowing for a shorter stacking vector corresponding to half of the *a* axis in phase III. The long *c* axis would likely correspond to the length of the molecule, while the *b* axis would be related to the distance between adjacent columns.

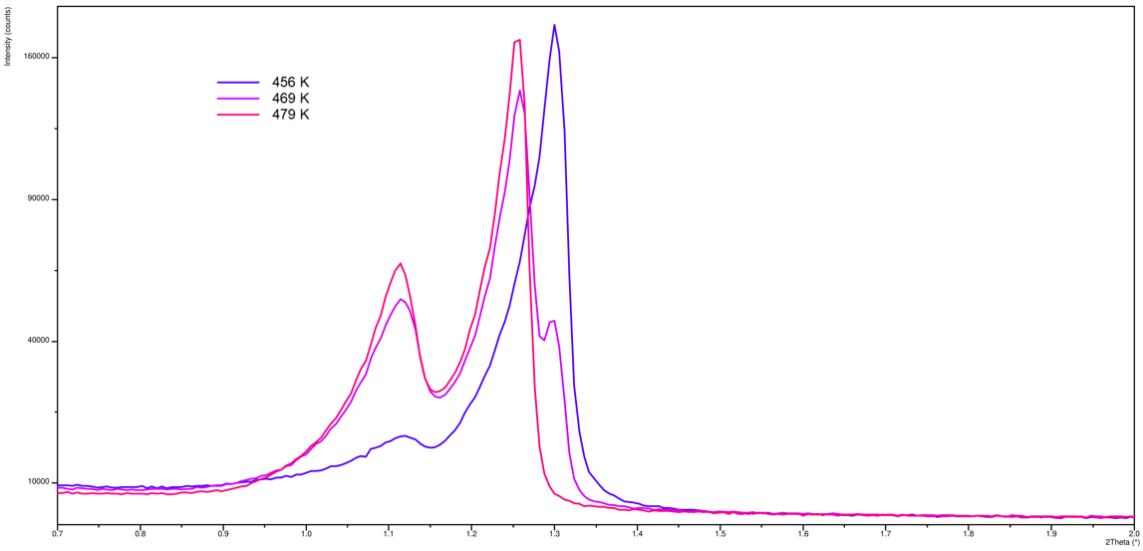

Figure S5. PXRD patterns of PDI-C_6 at different temperatures during heating, focusing on the low-angle region. At 456 K, the main reflection corresponds to phase I, while the reflection at 1.1° is ascribable to phase III; at 469 K, all three phases are present; at 479 K, phase I is no longer visible.

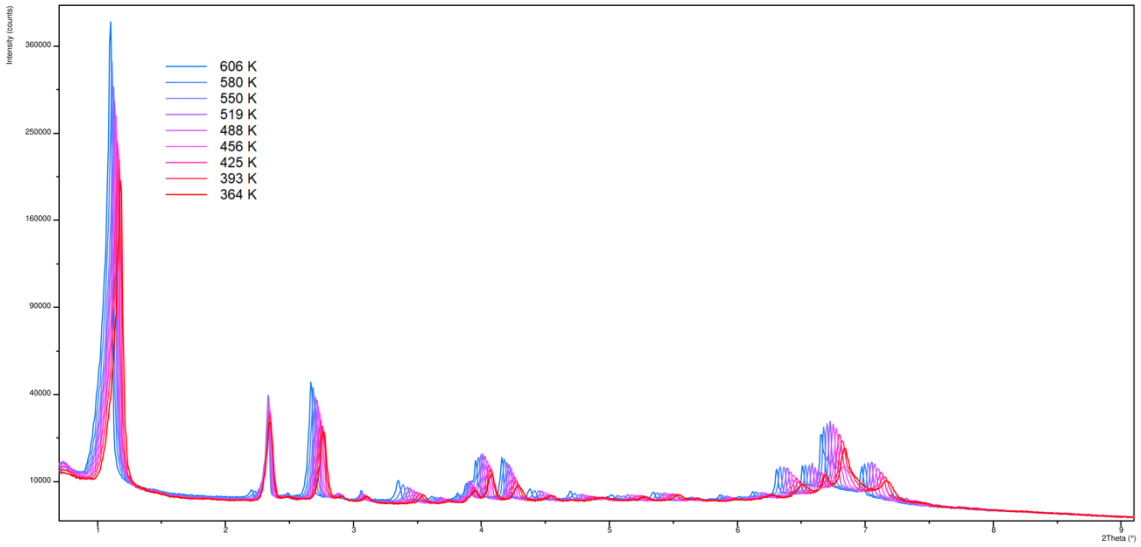

Figure S6. PXRD patterns of PDI-C_6 collected at different temperatures during cooling from 606 K to 364 K.

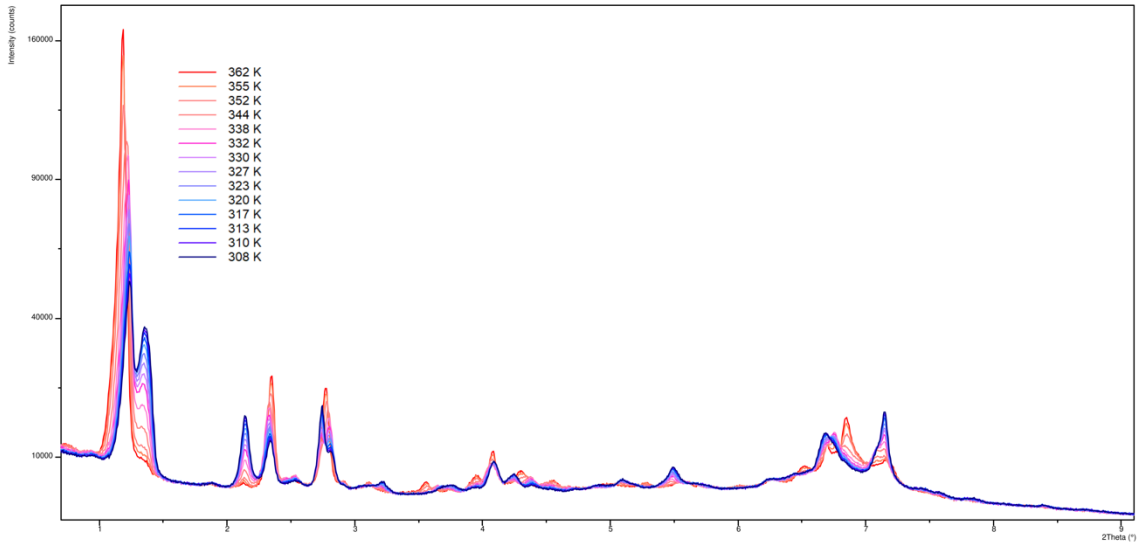

Figure S7. PXRD of PDI-C_6 at different temperatures during cooling from 362 K to room temperature. At 362 K, phase III is present, and the transition to phase II begins. As the temperature decreases, phase II becomes more prominent. At 344 K, phase I appears. By the end of the cooling process, at 308 K, both phases II and I are present.

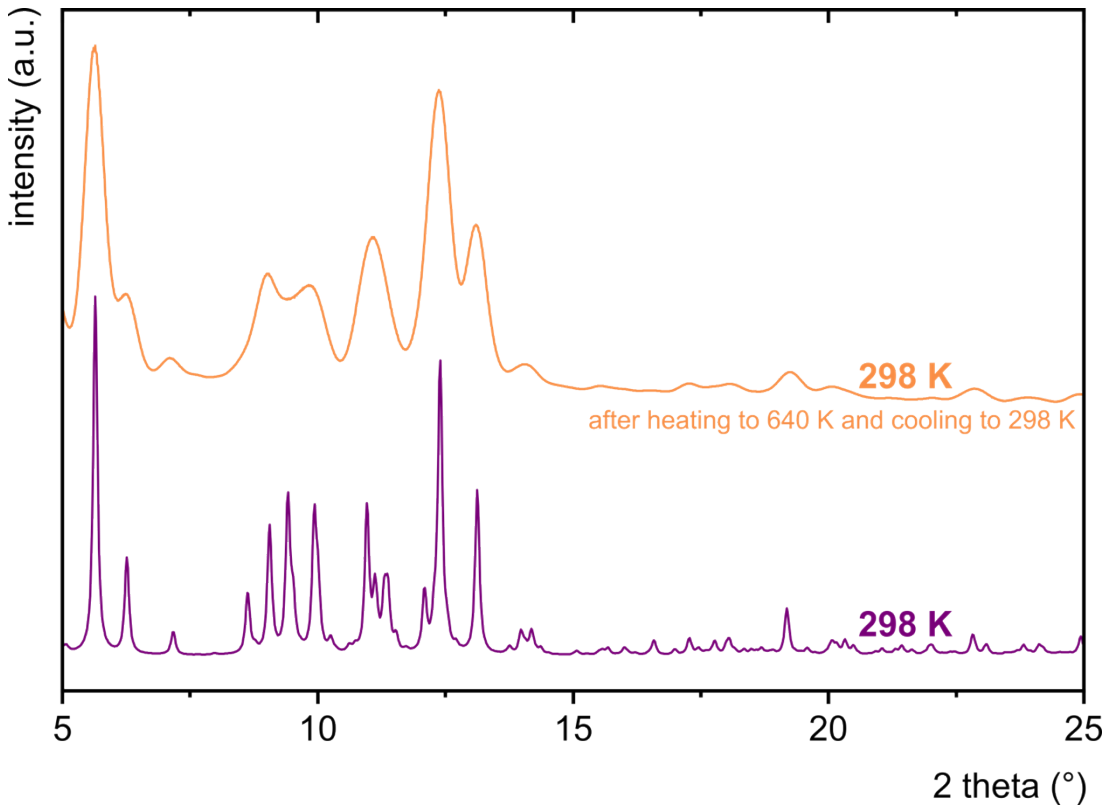

Figure S8. PXRD of PDI-C_6 (phase I at 298 K) measured with Mo Kα. The bottom pattern (purple) shows the calculated diffractogram from the single-crystal X-ray diffraction (XRD) measurement performed at 298 K/0.1 MPa. The top pattern (orange) represents the PXRD pattern of the sample after heating the crystal to 640 K and then cooling it back down to 298 K.

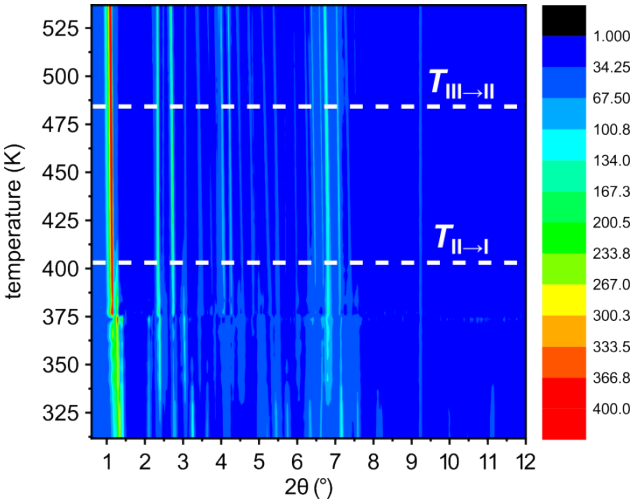

Figure S9. Temperature-resolved powder X-ray diffractograms of PDI-C_6 upon cooling. The dashed lines indicate the transition temperatures identified in the DSC measurement: $T_{III\rightarrow II}$ = 484 K and $T_{II\rightarrow I}$ = 403 K.

2.3. Pitch and roll angles

Table S2. Pitch and roll angles and π–π distances for PDI-C_6 crystal structure at different temperatures. The data at 173 K were previously reported by Madhu et al.[1]

T (K)	*P* (°)	*R* (°)	α_P (°)	β_R (°)	X (°)	Ψ (°)	$d_{\pi-\pi}$ (Å)	Stacking Vector (Å)
440	42.31(4)	21.11(5)	47.69(4)	68.89(5)	49.49	74.08	3.4397(13)	4.8395
298	42.36(5)	20.82(6)	47.64(5)	69.18(6)	49.23	74.39	3.3809(15)	4.757
173	42.80(4)	20.58(5)	47.20(4)	69.42(5)	49.07	74.91	3.3458(14)	4.730
100	42.88(6)	20.49(7)	47.12(6)	69.51(7)	48.80	74.70	3.321(2)	4.706

The α_P is defined as the angle between the plane formed by atoms of the perylene core and the plane generated by the C1 and C2 carbon atoms of two stacked molecules. The β_R angle is determined between the same plane of the perylene core and the plane formed by the carbon atoms (C6, C7, C11 and C12) of two stacked molecules.

$P = 90° - \alpha_P$

$R = 90° - \beta_R$

2.4. Thermal expansion coefficient of PDI-C_6 phase I

Table S3. Unit-cell parameters of PDI-C_6 phase I at different temperatures obtained by Rietveld refinement.

T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
100(10)	4.706	8.514	17.281	81.340	85.640	83.890
298(10)	4.757	8.549	17.576	81.678	84.850	83.169
320(10)	4.764	8.553	17.608	81.718	84.811	83.020
330(10)	4.768	8.554	17.629	81.775	84.756	82.978
338(10)	4.770	8.555	17.646	81.819	84.713	82.931
346(10)	4.773	8.553	17.670	81.891	84.645	82.877
354(10)	4.776	8.552	17.695	81.979	84.577	82.823
361(10)	4.780	8.551	17.724	82.071	84.507	82.760
368(10)	4.784	8.551	17.751	82.167	84.439	82.706
375(10)	4.788	8.548	17.783	82.290	84.373	82.628
382(10)	4.792	8.546	17.813	82.425	84.303	82.549
388(10)	4.796	8.543	17.843	82.577	84.233	82.473
394(10)	4.800	8.541	17.879	82.757	84.146	82.386
401(10)	4.805	8.540	17.911	82.928	84.067	82.314
403(10)	4.810	8.538	17.945	83.126	83.989	82.217
413(10)	4.815	8.537	17.975	83.321	83.912	82.109
417(10)	4.821	8.535	18.001	83.536	83.854	82.017
423(10)	4.829	8.533	18.047	83.840	83.705	81.894
430(10)	4.833	8.531	18.068	83.990	83.631	81.823
436(10)	4.837	8.531	18.092	84.170	83.546	81.733
443(10)	4.844	8.533	18.136	84.377	83.479	81.623
449(10)	4.850	8.533	18.167	84.568	83.396	81.524
456(10)	4.856	8.534	18.200	84.746	83.320	81.427
461(10)	4.862	8.533	18.235	84.938	83.239	81.310
468(10)	4.866	8.533	18.274	85.112	83.172	81.200

Table S4. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C_6 phase I in the range of temperature between 100 and 354 K.[2]

			Direction		
Axes	**α (MK-1)**	**σα(MK-1)**	***a***	***b***	***c***
X_1	-16.3096	1.6702	0.8168	-0.5675	-0.1039
X_2	114.9742	5.4128	0.9023	-0.071	0.4253
X_3	61.3	4.1265	0.8535	0.4905	-0.1757
V	161.749	1.7703			

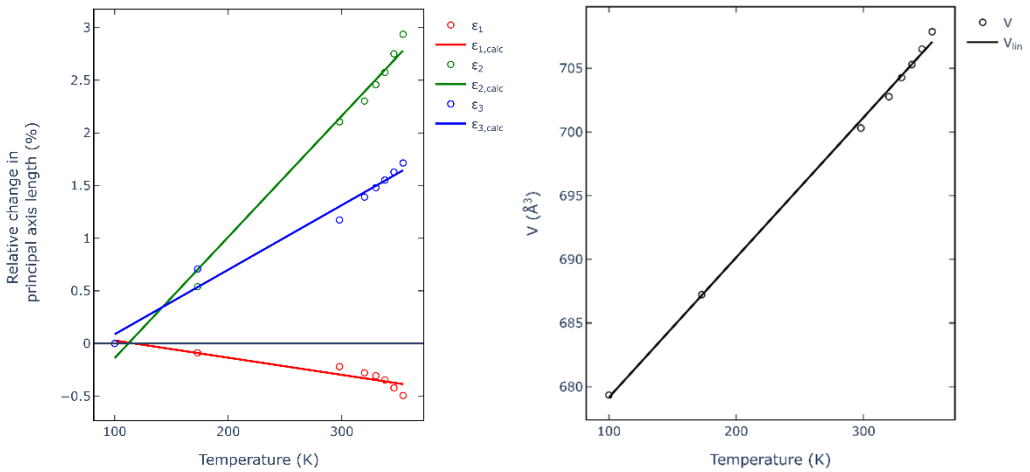

Figure S10. Fits to variable-temperature lattice parameter data of PDI-C_6 phase I in the range 100–354 K.

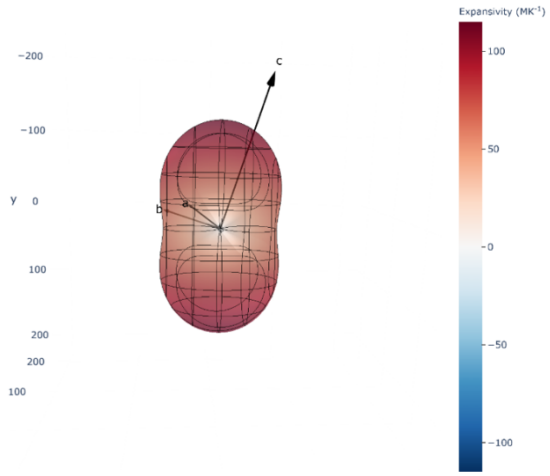

Figure S11. Expansivity indicatrix of PDI-C_6 phase I determined in the range 100–354 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.

Table S5. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C_6 phase I in the range of temperature between 361 and 413 K.[2]

			Direction		
Axes	**α (MK^{-1})**	**σα(MK^{-1})**	***a***	***b***	***c***
X_1	-213.2833	11.3908	0.7294	-0.6664	-0.1547
X_2	183.9475	7.64	0.9633	0.2672	-0.0237
X_3	432.0147	17.4431	0.4776	-0.6164	0.626
V	398.2338	13.4492			

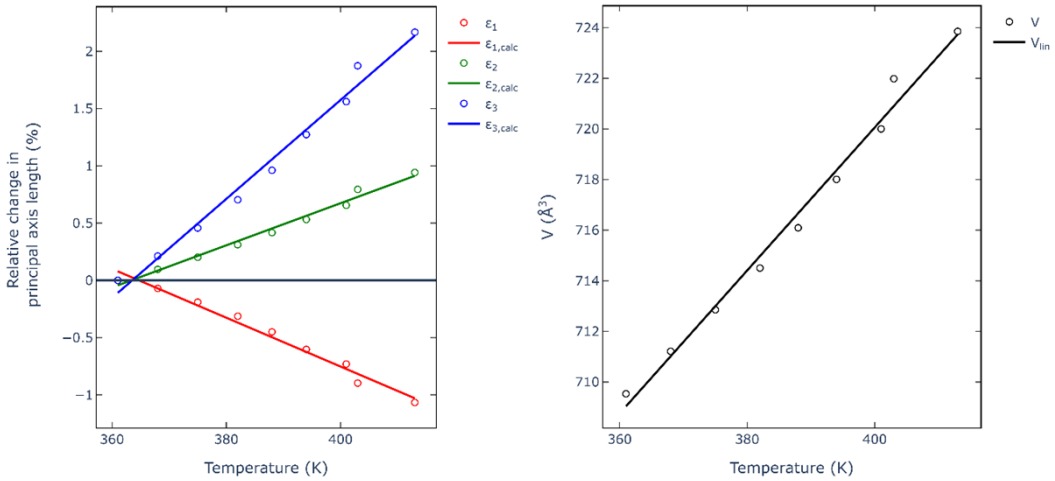

Figure S12. Fits to variable-temperature lattice parameter data of PDI-C_6 phase I in the range 361–413 K.

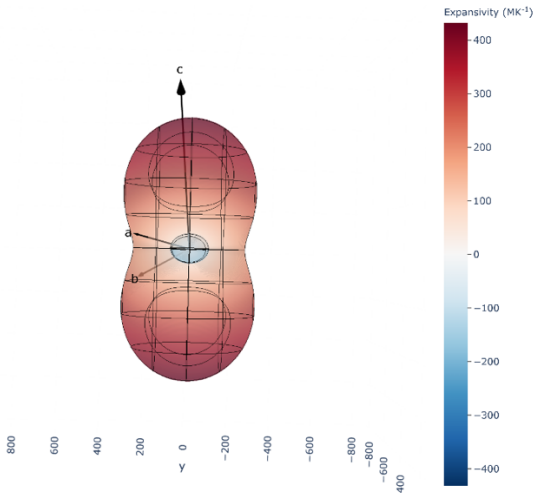

Figure S13. Expansivity indicatrix of PDI-C_6 phase I determined in the range 361–453 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.

2.5. Pawley refinement of PDI-C_6 phase III

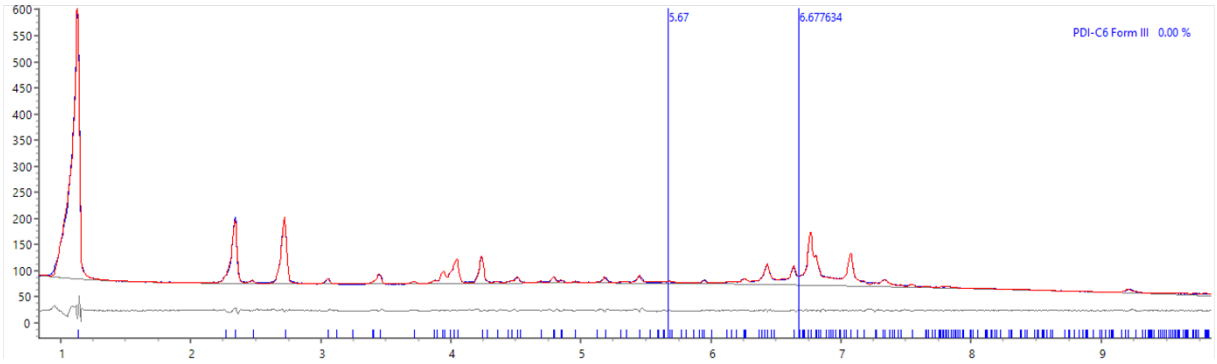

Figure S14. Pawley refinement of PDI-C_6 at 447 K. Experimental pattern in blue, calculated pattern in red and difference plot in grey. The blue lines at 5.67 and 6.68 of 2θ correspond to the two reflections used to describe the glass capillary contribution. R_{wp}=3.74; R_p=2.57, R_{exp}= 0.98. The intensity is reported in square root for the sake of clarity.

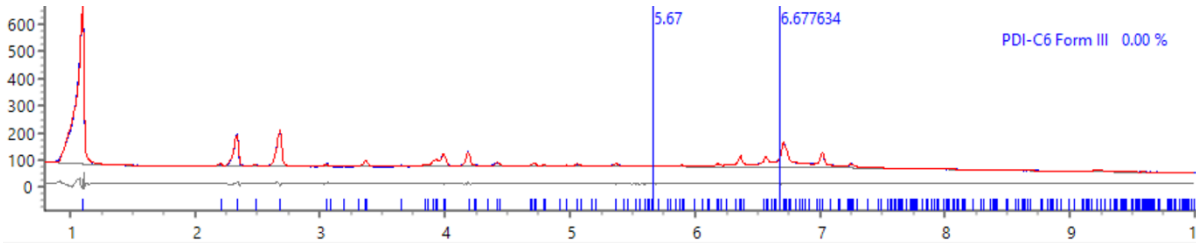

Figure S15. Pawley refinement of PDI-C_6 at 537 K. Experimental pattern in blue, calculated pattern in red and difference plot in grey. The blue lines at 5.67 and 6.68 of 2θ correspond to the two reflections used to describe the glass capillary contribution. R_{wp}=4.38; R_p=3.06, Rexp= 0.96. The intensity is reported in square root for the sake of clarity.

2.6. Thermal expansion coefficient of PDI-C_6 phase III

Table S6. Unit-cell parameters of PDI-C_6 phase III at different temperatures obtained by Rietveld refinement.

T (K)	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)
537	7.676	10.148	21.559	84.35	85.34	90.52
526	7.665	10.151	21.483	84.13	85.32	90.49
511	7.648	10.153	21.388	83.87	85.42	90.48
495	7.630	10.154	21.295	83.64	85.53	90.49
480	7.616	10.152	21.215	83.44	85.59	90.47
464	7.600	10.150	21.137	83.27	85.66	90.45
447	7.583	10.148	21.056	83.10	85.75	90.46

Table S7. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C_6 phase III in the temperature range between 537 and 447 K.[2]

			Direction		
Axes	**α (MK^{-1})**	**σα(MK^{-1})**	**a**	**b**	**c**
X_1	325.7737	10.1782	0.2474	-0.6622	0.7073
X_2	125.2688	1.4656	0.9934	0.0976	-0.0604
X_3	-36.5578	5.0416	-0.0993	0.9802	0.1716
V	410.431	7.143			

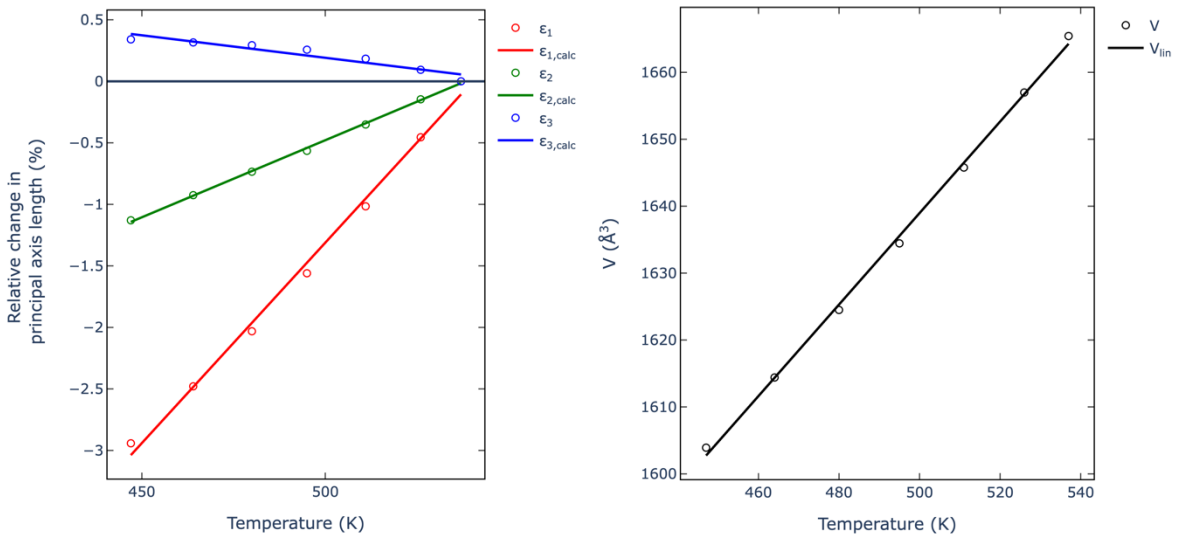

Figure S16. Fits to variable-temperature lattice parameter data of PDI-C_6 phase III in the range of 537–447 K.

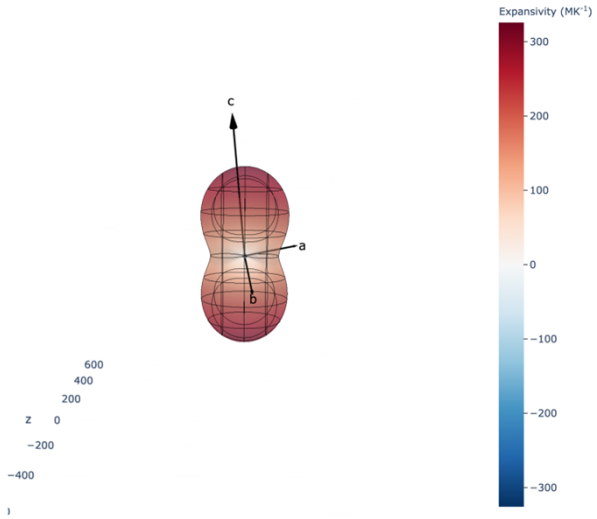

Figure S17. Expansivity indicatrix of PDI-C_6 phase III determined in the range 537–447 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.

2.7. Hot Stage Microscopy

Decreasing the temperature, there is an overall thermal contraction of the unit-cell which increases the interdigitation of the alkyl chains also observed in phase II and probably avoid the rotation of the core center, the thermal contraction can induce strains and thus energy accumulation in the crystal, like loading a spring. This energy accumulated as strain, increases as the temperature is lowered and could act as a trigger for the transition that occurs in single crystals as observed in HSM.

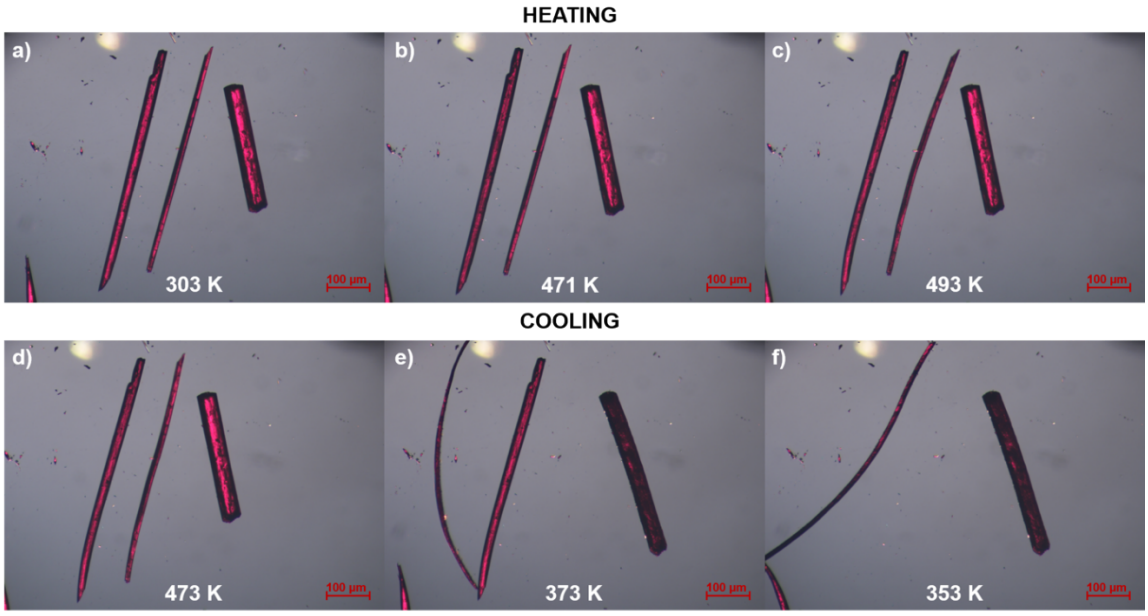

Figure S18. HSM PDI-C_6 crystals at various stages of heating and cooling. The red scale bar corresponds to 100 µm.

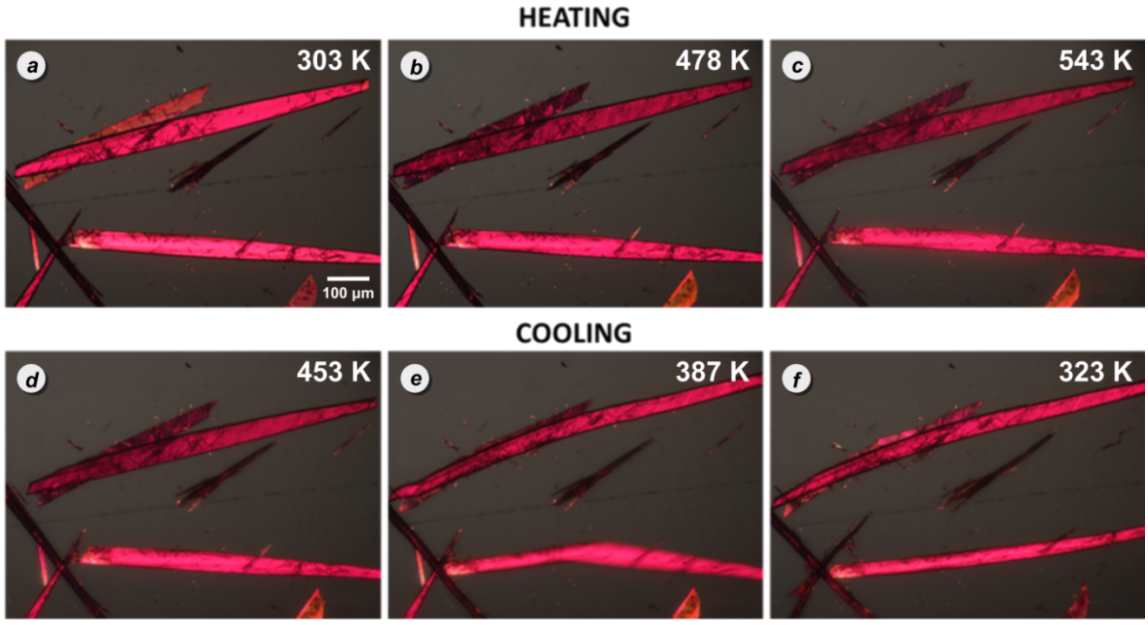

Figure S19. HSM PDI-C_6 crystals at various stages of heating and cooling.

3. Effect of pressure on PDI-C_6

3.1. Single crystal X-ray diffraction

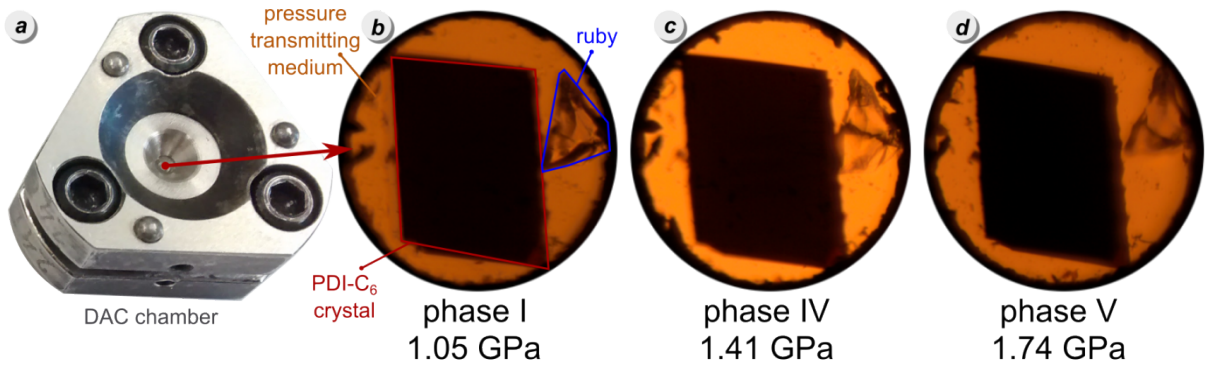

Figure S20. (a) Diamond anvil cell (DAC) chamber used for high-pressure generation. PDI-C_6 single crystals loaded in the DAC, showing phase I at 1.05 GPa (b), phase IV at 1.41 GPa and phase V at 1.74 GPa.

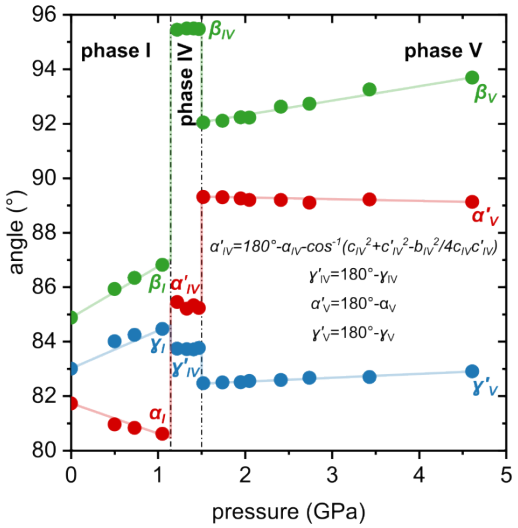

Figure S21. Pressure dependence of angles α, β and γ for the PDI-C_6 crystal. The estimated standard deviations (ESDs) are smaller than the symbols. Data at 1.22, 1.33, 1.47, and 1.52 GPa are derived from quick-experiments, where only the unit-cell parameters were determined. The angles for phases IV and V have been calculated relative to the lattice corresponding to phase I, as specified in the inset formulas and illustrated in Figure 6.

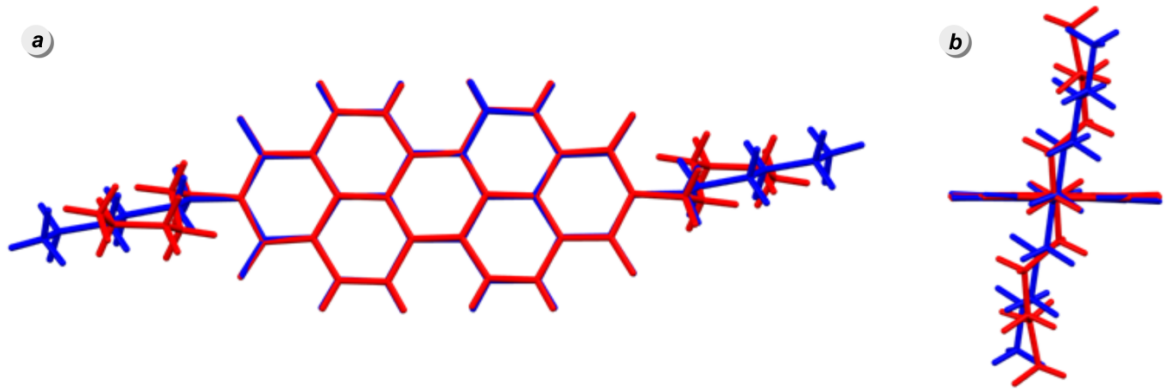

Figure S22. Comparison of the PDI-C_6 crystal structures between ambient phase I (blue, 1.05 GPa) and high-pressure phase V (red, 1.52 GPa), highlighting differences in alkyl chain conformation. View perpendicular to the perylene plane of the two overlapped molecules (a), and along the perylene x-axis (b).

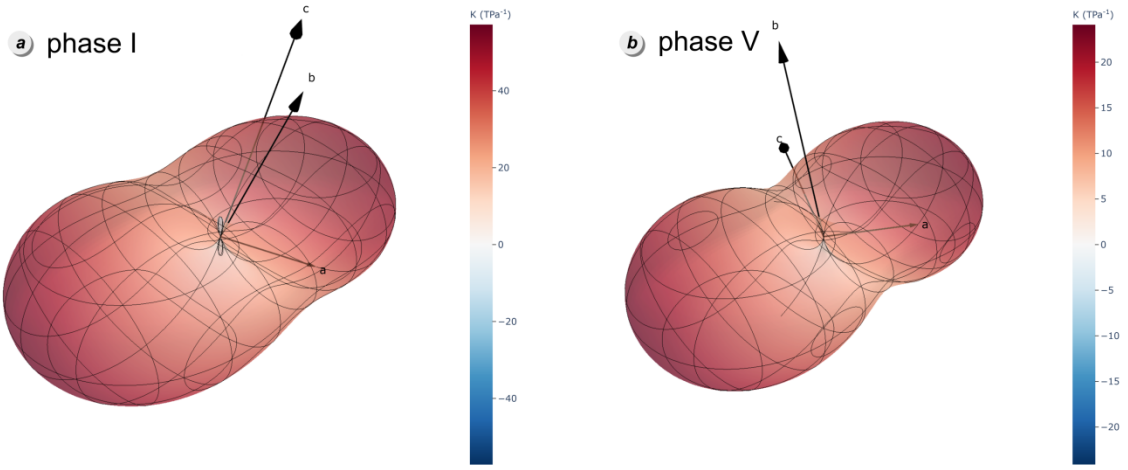

Figure S23. Graphical representations of the compressibility tensors for the PDI-C_6 crystal, calculated using PASCal program,[3] are shown for pressure ranges of 0.1 MPa – 1.05 GPa (a), and 1.74 – 4.61 GPa (b).

Table S8. Compressibility related to crystallographic axes calculated for PDI-C_6 phase I in the range of 0.1 MPa – 1.05 GPa with Birch-Murnaghan Coefficients.

Axes	K(TPa^{-1})	σK(TPa^{-1})	Direction			Empirical parameters			
			a	*b*	*c*	ε_0	λ	P_c	*v*
X1	57.2089	nan	0.9146	-0.1288	0.3833	40.2153	-40.2524	-0.5325	0.0015
X2	31.336	nan	0.9394	0.2892	-0.184	27.478	-27.5086	-0.2884	0.0009
X3	-6.1818	nan	-0.6128	0.7847	0.0932	0.0	0.0073	0.0001	0.6719
V	88.433	8.6522							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	*B'*	σ*B'*	P_c (GPa)
2nd	8.8668	1.1523	704.0333	5.611	4.0	n/a	0.0
3rd	4.5489	3.8672	706.8975	9.7046	23.2288	27.6322	0.0

Table S9. Compressibility related to crystallographic axes calculated for PDI-C_6 phase V in the range of 1.74 GPa – 4.61 GPa with Birch-Murnaghan Coefficients.

Axes	K(TPa^{-1})	σK(TPa^{-1})	Direction			Empirical parameters			
			a	*b*	*c*	ε_0	*λ*	P_c	*v*
X1	24.1068	3.0782	0.9804	0.0374	0.1934	53.9492	-53.9131	-0.0424	0.0011
X2	10.6683	0.7894	0.9122	-0.1482	-0.3821	15.3673	-15.2803	-2.8848	0.0037
X3	0.0042	1.8947	0.316	0.9455	-0.0787	0.0008	-0.0	1.7399	6.3035
V	29.3208	1.3911							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	*B′*	σ*B′*	P_c (GPa)
2nd	20.9551	1.0675	652.1741	3.0233	4.0	n/a	0.0
3rd	0.0755	907.392	733.9035	10472.1651	835.6777	9945915.5087	0.0

3.2. Pitch and roll angles

Table S10. Pitch and roll angles and distances for PDI-C_6.[4]

Pressure (GPa)		*P* (°)	*R* (°)	α_P (°)	β_R (°)	$d_{\pi\text{-}\pi}$ (Å)	d_P (Å)	d_R (Å)	d_{tot} (Å)	*z* (Å)
0.0001		42.53(2)	20.75(4)	47.47(2)	69.25(4)	3.3882(4)	3.11	1.28	3.36	4.77
0.50		42.36(4)	19.79(3)	47.64 (4)	70.21(3)	3.3209(4)	3.03	1.19	3.26	4.65
0.73		42.49(16)	19.2(3)	47.51(16)	70.8(3)	3.295(6)	3.02	1.15	3.23	4.62
1.05		42.2(2)	19.0(3)	47.8(2)	71.0(3)	3.278(6)	2.97	1.13	3.18	4.57
1.41	***1***	41.49(3)	20.49(6)	48.51(3)	69.51(6)	3.2643(6)	2.89	1.22	3.14	4.53
	2	43.22(3)	19.56(5)	46.78(3)	70.44(5)	3.2044(5)	3.01	1.14	3.22	4.54
1.74		43.05(19)	16.6(3)	46.95(19)	73.4(3)	3.207(6)	3.00	0.96	3.15	4.50
1.95		42.80(3)	15.96(4)	47.2(3)	74.04(4)	3.2049(6)	2.97	0.92	3.11	4.47
2.05		42.83(2)	16.04(3)	47.17(2)	73.96(3)	3.1977(5)	2.96	0.92	3.10	4.45
2.41		43.1(3)	15.4(5)	46.9(3)	74.6(5)	3.171(6)	2.97	0.87	3.09	4.43
2.74		42.73(3)	15.15(4)	47.27(3)	74.85(4)	3.1560(6)	2.92	0.85	3.04	4.38
3.43		43.01(3)	14.37(4)	46.99(3)	75.63(4)	3.1234(6)	2.91	0.80	3.02	4.34
4.61		43.27(3)	13.65(6)	46.73(3)	76.35(6)	3.0801(9)	2.90	0.75	3.00	4.30

$P = 90° - \alpha_P$

$R = 90° - \beta_R$

The slip distance along the long molecular axis d_P is: $d_P = d_{\pi-\pi}\mathrm{tg}\, P$

The slip distance along the short molecular axis is: $d_R = \mathrm{d}_{\pi-\pi}\,\mathrm{tg}\, R$

$d_P = d_{\pi-\pi}\mathrm{ctg}\,\alpha_P$

$d_R = \mathrm{d}_{\pi-\pi}\,\mathrm{ctg}\,\beta_R$

The total slip distance, d_{tot}, is: $d_{tot} = ({d_P}^2 + {d_R}^2)^{1/2}$

The crystallographic repeat distance, z, in the stack direction is:

$z = ({d_P}^2 + {d_R}^2 + {d_{\pi-\pi}}^2)^{1/2} = d(1 + tg^2P + tg^2R)^{1/2}$

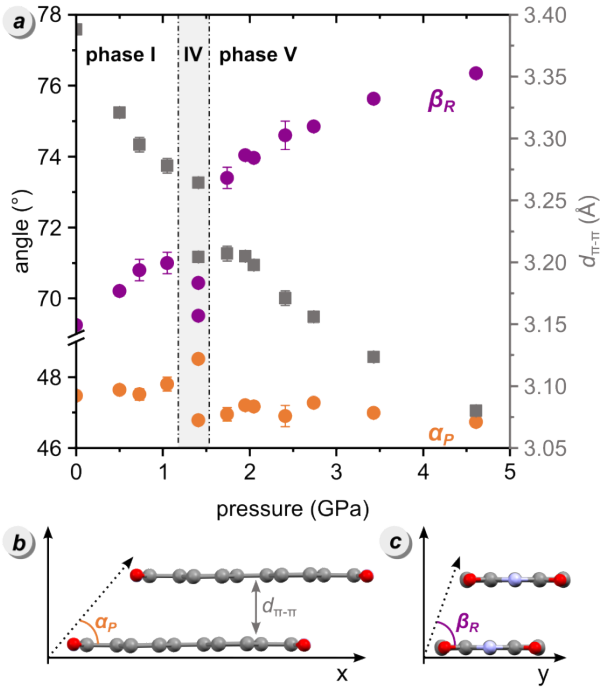

Figure S24. Packing of PDI-C_6 molecules under pressure (a): orange symbols represent the α_P (b) and purple β_R (c) angles. and grey squares mark the distance between π-stacked molecules ($d_{\pi-\pi}$).[4] In (b) and (c), the alkyl substituents and H-atoms are skipped for clarity.

4. Theoretical calculations

4.1. Geometry optimization, thermodynamic and optical properties in Orca

Geometry optimization of the molecular structures taken from the crystal structures was performed in Orca (version 5.0.3) using B3LYP-gCP-D3/6-31G* method,[5] which balances well accuracy and computing time - providing decent corrections for the BSSE and dispersion effects.[6,7] The PDI core was freely optimized, whereas conformations of the alkyl chains were restrained according to the molecular geometry taken from the XRD experiments, allowing torsion angles to adjust within 5°. The energy minima were confirmed as no imaginary vibrational frequencies were calculated. Visualizations of Intrinsic Bond Orbitals (IBOs) and Virtual Valence Intrinsic Bond Orbitals (vvIBOs) showing localized representations of wave functions were generated in IboView, and Avogadro was used to examine calculated features.[8–10]

4.2. Interaction energies in Crystal Explorer

B3LYP/6-31G(d,p) basis set was used to calculate intermolecular energies and Hirschfeld Surfaces in Crystal Explorer.[11] These calculations helped us to quantify the interactions present in all investigated crystal forms.

The analysis of intermolecular interactions present in the PDI-C_6 crystal revealed the dominant strengthen of the π···π interaction occurring between sandwich stacking PDI-C_6 molecules. Those noncovalent attractive interactions remain stable (E_{total}, Figure S29a) up to the highest achieved pressure, as both electrostatic and dispersion forces compensate the repulsion. As a result, the structure is the hardest in the [010] direction, what reflects in the compressibility of a crystal. Similarly, although three times weaker, interactions between neighboring PDI-C_6 molecules bond them by weak CH···O and aryl CH···CH contacts. The driving force of the transitions is the softness of the alkyl chains and their ability to change conformations. Two alkyl chains, interacting with each other side-to-side, are involved mainly into the structural transformations. However, the repulsion between them in phase IV increases significantly (molecules A, B at 1.41 GPa), in phase V it lowers back as the electrostatic and dispersion forces decrease as well (Figure 28c). This keeps the total energy of the interaction higher than for phase I, but another side alkyl interaction compensates lowering the total energy by the rise of dispersion and electrostatic interactions prevailing the repulsion (Figure S29d). On the other hand, the apical interactions, involving two CH_3 groups pushing against each other, destabilize the structure lowering its total energy as no other term can compensate the repulsion (Figure S29e).

Table S11. Gibbs free energies of single PDI-C_6 conformers, calculated in Orca at the B3LYP-gCP-D3/6-31G* theory level. Two independent molecules in phase IV-were described as A and B. For comparison, energies of theoretical high-symmetry conformation (HSC) with C_{2v} molecular symmetry are listed in the bottom row.

Pressure [GPa]	G-E(el) (kcal/mol)	G-E(el) (kJ/mol)	ΔE (kJ/mol)
0.0001	353.31	1478.25	0
0.5	353.05	1477.16	-1.08784
1.41 A	352.85	1476.32	-1.92464
1.41 B	353.93	1480.84	2.59408
1.57	354.09	1481.51	3.26352
1.95	354.13	1481.68	3.43088
2.05	354.1	1481.55	3.30536
2.74	354.2	1481.97	3.72376
3.43	354.17	1481.85	3.59824
4.61	354.12	1481.64	3.38904
HSC	353.39	1478.58	0.33472

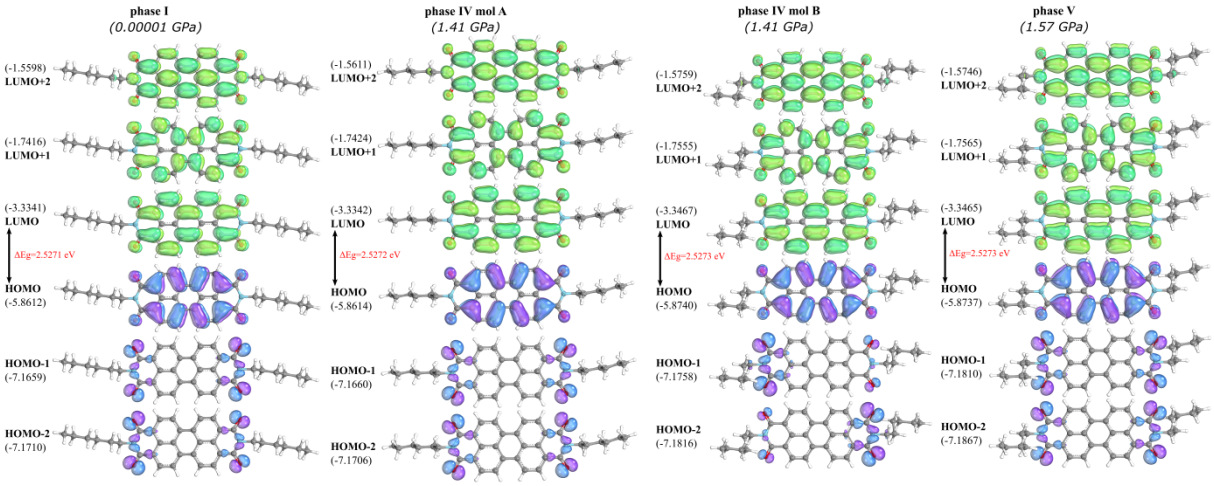

Figure S25. Frontier orbitals and their energies of all high-pressure phases I, IV and V, calculated in Orca,[5] and presented in IboView.[8,9] The band gap (ΔE_g energy difference between HOMO and LUMO orbitals) in red.

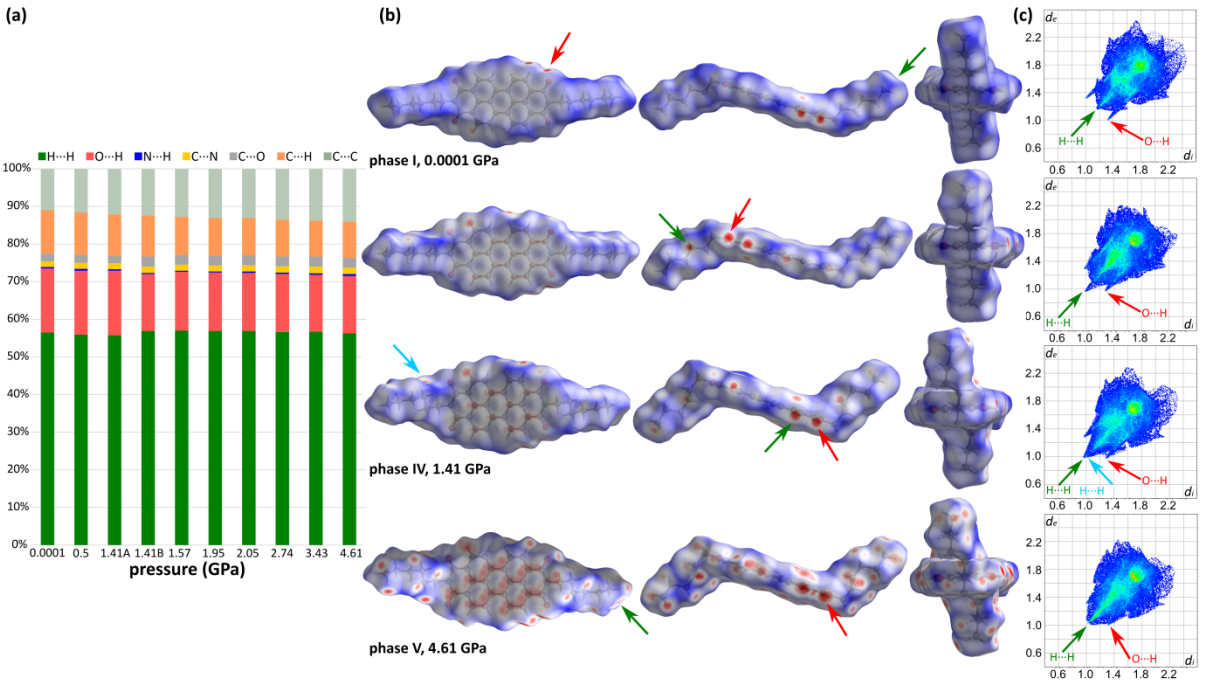

Figure S26. (a) Percentage of intermolecular interaction in PDI-C_6 calculated in Crystal Explorer (Table S12). (b) Hirschfeld surfaces and (c) fingerprints showing areas with the shortest intermolecular interactions (arrows) present in all high-pressure phases (Figure S31).

Table S12. Percentage of intermolecular interactions in PDI-C_6 calculated in CrystalExplorer.

p [GPa]	C…C	C…H	C…O	C…N	N…N	N…O	N…H	O…O	O…H	H…H
0.0001	11	11.6	2	1.5	0	0	0.4	0	17	56.5
0.5	11.6	11.3	2.1	1.6	0	0	0.5	0	17	55.9
1.41 (mol A)	12.1	11	2	1.6	0	0	0.4	0	17.2	55.7
1.41 (mol B)	12.4	10.9	2.7	1.7	0	0	0.3	0	15.1	56.9
1.57	12.8	10.1	2.6	1.6	0	0	0.3	0	15.6	57
1.95	13.1	10	2.6	1.6	0	0	0.3	0	15.5	56.9
2.05	13.1	9.9	2.6	1.7	0	0	0.4	0	15.4	56.9
2.74	13.6	9.7	2.6	1.7	0	0	0.4	0	15.4	56.6
3.43	13.8	9.5	2.7	1.8	0	0	0.4	0	15.1	56.7
4.61	14.1	9.6	2.6	1.7	0	0	0.5	0	15.2	56.3

Table S13. Interaction energies (kJ/mol) between molecules in PDI-C_6.

p [GPa]	R [Å]	E_ele	E_pol	E_dis	E_rep	E_tot	*p* [GPa]	R [Å]	E_ele	E_pol	E_dis	E_rep	E_tot
0.0001	4.77	-15.8	-2.1	-180.1	92.5	-118	**0.0001**	9.29	-12.5	-6.3	-62.5	34.5	-51
0.5	4.65	-22	-2.6	-201.8	125	-123.7	**0.5**	9.31	-18	-7.9	-73.3	52.3	-56.4
1.41	4.53	-30.4	-3	-222.5	161.7	-128.2	**1.41**	9.16	-21	-7.4	-75.2	65.6	-52.7
1.41	4.53	-41.8	-4	-248.2	204.9	-136.7	**1.41**	9.16	-21	-7.4	-75.2	65.6	-52.7
1.57	4.52	-37.9	-4	-244.6	195	-135.6	**1.57**	9.2	-23.9	-6.8	-73.6	69.9	-51.2
1.95	4.46	-44.4	-4.3	-258.7	224.4	-136.8	**1.95**	9.17	-26.3	-7.1	-77	78	-52
2.05	4.45	-45.8	-4.2	-261.4	229.9	-137.2	**2.05**	9.16	-26.7	-7	-77.5	78.6	-52.4
2.74	4.38	-56.4	-4.5	-280	276	-136.3	**2.74**	9.14	-30.9	-7.6	-83	93.8	-52.7
3.43	4.34	-64.8	-4.8	-293.2	310.4	-135.6	**3.43**	9.13	-34.7	-8	-87.1	106.9	-52.4
4.61	4.29	-77.3	-5.4	-310.9	363	-132.2	**4.61**	9.09	-41	-8.9	-92.4	128.6	-51
0.0001	12.03	-19.2	-4.9	-16.9	18.1	-27.5	**0.0001**	8.58	-2.6	-2	-19.3	4.6	-18.2
0.5	11.96	-21.7	-5.9	-18.4	23.9	-28.6	**0.5**	8.57	-2.8	-2.5	-22.9	8	-19.8
1.41	11.71	-24.2	-6.9	-20.6	28.3	-31.2	**1.41**	8.48	-7.2	-3.8	-30.7	19.6	-25
1.41	11.71	-24.2	-6.9	-20.6	28.3	-31.2	**1.41**	8.48	-7.2	-3.8	-30.7	19.6	-25
1.57	11.65	-22.4	-6.5	-20.9	24.3	-31.7	**1.57**	8.62	-6.1	-4.1	-31.3	19.5	-24.7
1.95	11.57	-24.1	-7	-22.4	29.1	-32.3	**1.95**	8.62	-7.2	-4.6	-33.2	23.3	-25.5
2.05	11.55	-23.8	-7.2	-22.6	29.4	-32.1	**2.05**	8.6	-7.7	-4.1	-33.9	24.6	-25.4
2.74	11.46	-26.3	-8	-24.6	36.5	-32.7	**2.74**	8.6	-9.5	-4.9	-36.3	31	-26.1
3.43	11.41	-27.6	-8.6	-25.9	40.5	-33.1	**3.43**	8.6	-10.2	-4.7	-38	35	-25.7
4.61	11.35	-32	-9.8	-27.5	51.8	-33	**4.61**	8.56	-14.3	-6.2	-41.1	47.4	-26.1

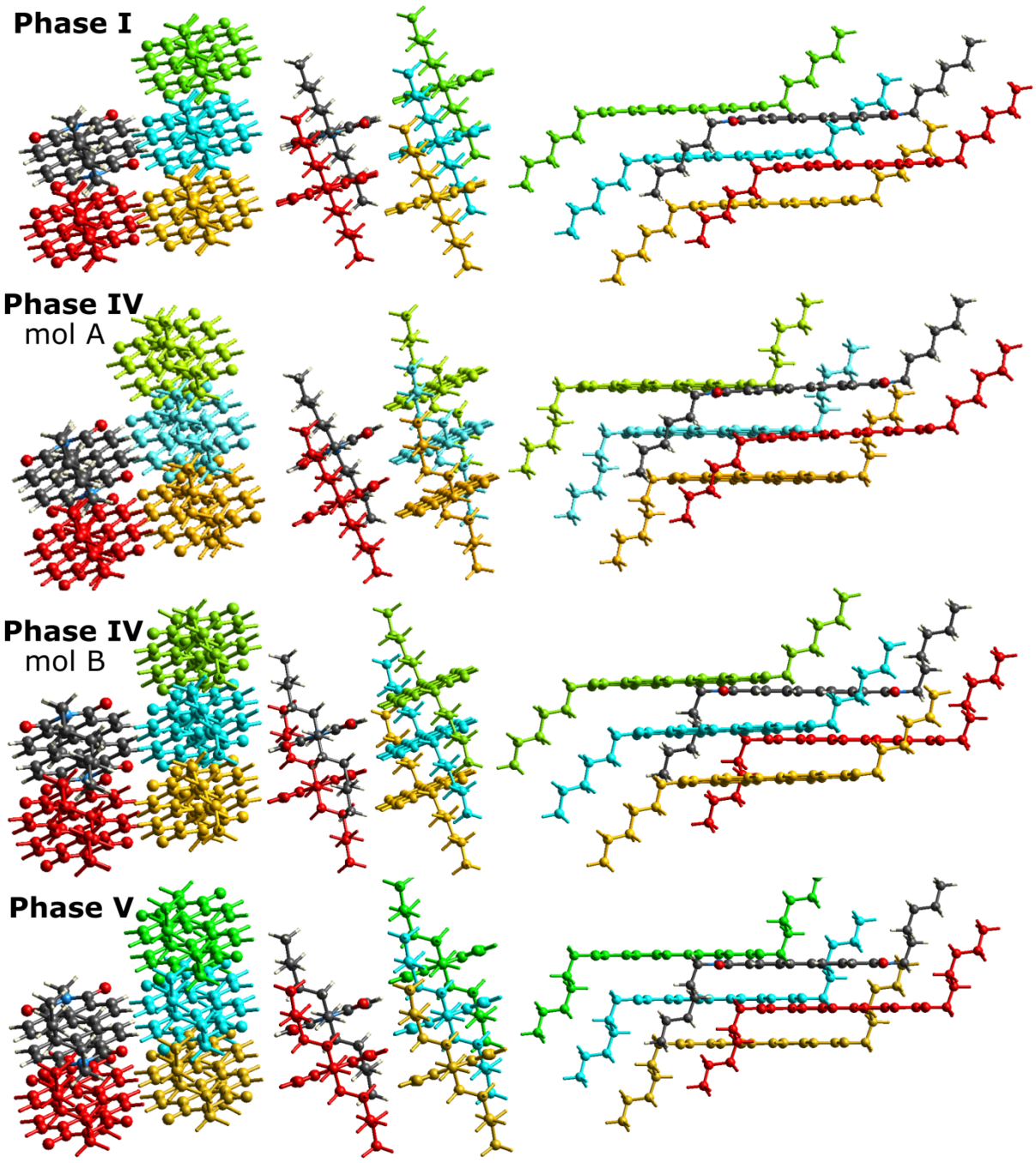

Figure S27. Intermolecular interactions between PDI-C_6 molecules calculated in Crystal Explorer.

Table S14. Interaction energies (kJ/mol) between molecules in PDI-C_6. *Attempts to calculate the energy in Crystal Explorer failed as E_rep is 0. The presented result is wrong and was listed just for consistency.

p [GPa]	R [Å]	E_ele	E_pol	E_dis	E_rep	E_tot	*p* [GPa]	R [Å]	E_ele	E_pol	E_dis	E_rep	E_tot
0.0001	26.7	-0.6	0	-5.3	3	-3.5	0.0001	21.65	-1.7	-0.6	-24.1	9.7	-17.2
0.5	26.61	-1.5	0	-7.4	6.8	-3.9	0.5	21.41	-3.9	-0.9	-32.9	18.5	-22
1.41	24.79	-1.5	0	-5.9	5.6	-3.3	1.41	19.61	1.0	-1.4	-18.7	0	-16.2
1.41	24.79	-1.5	0	-5.9	5.6	-3.3	1.41	19.61	-7.6	-0.4	-28.7	33.7	-12.5
1.57	23.74	-2.3	0	-6	8.1	-2.6	1.57	18.64	-1.7	-0.9	-21.6	16.3	-11.2
1.95	23.69	-2.6	0	-6.3	9.3	-2.5	1.95	18.57	-2.2	-1	-22.5	18.8	-11
2.05	23.67	-2.6	0	-6.3	9.3	-2.6	2.05	18.56	-2.4	-0.9	-22.5	19	-11.1
2.74	23.61	-3.1	0	-6.7	11.2	-2.3	2.74	18.47	-2.9	-1.1	-23.7	22.1	-10.8
3.43	23.49	-3.9	0	-7	14.1	-1.6	3.43	18.32	-3.7	-1.1	-25.4	26.1	-10.8
4.61	23.33	-4.6	-0.1	-7.5	16.6	-1.2	4.61	18.16	-4.7	-1.4	-27	31	-10.4
0.0001	28.14	-1	0	-4.9	3.4	-3.2	0.0001	23.61	-1.4	0	-10.8	5.7	-7.4
0.5	28.07	-0.8	0	-5.3	3	-3.6	0.5	23.38	-2.7	-0.1	-13.9	10.8	-8.3
1.41	25.81	-2.8	0	-11.7	11	-6.4	1.41	21.09	-3.3	-1.6	-47	0	-45.6
1.41	25.81	-2.8	0	-11.7	11	-6.4	1.41	21.09	-4.8	-0.3	-24.5	18.7	-15
1.57	24.68	-3.4	0	-13.5	13.2	-7.3	1.57	20.08	-10.2	-1.5	-38.5	34.1	-24.3
1.95	24.63	-3.9	0	-14.4	14.9	-7.5	1.95	20.01	-12.3	-1.7	-41.7	41.1	-25.1
2.05	24.61	-4.2	0	-14.6	15.5	-7.6	2.05	19.99	-12.7	-1.5	-42.4	42.8	-25.1
2.74	24.55	-5.2	0	-16.1	19.2	-7.7	2.74	19.89	-15.7	-1.9	-46.2	52.6	-25.8
3.43	24.43	-6.8	0	-17.8	24.7	-7.5	3.43	19.76	-19.5	-2	-50.6	66.1	-25.4
4.61	24.29	-6.7	0	-18.4	24.9	-7.8	4.61	19.61	-24.3	-2.7	-54.1	80.8	-24.9

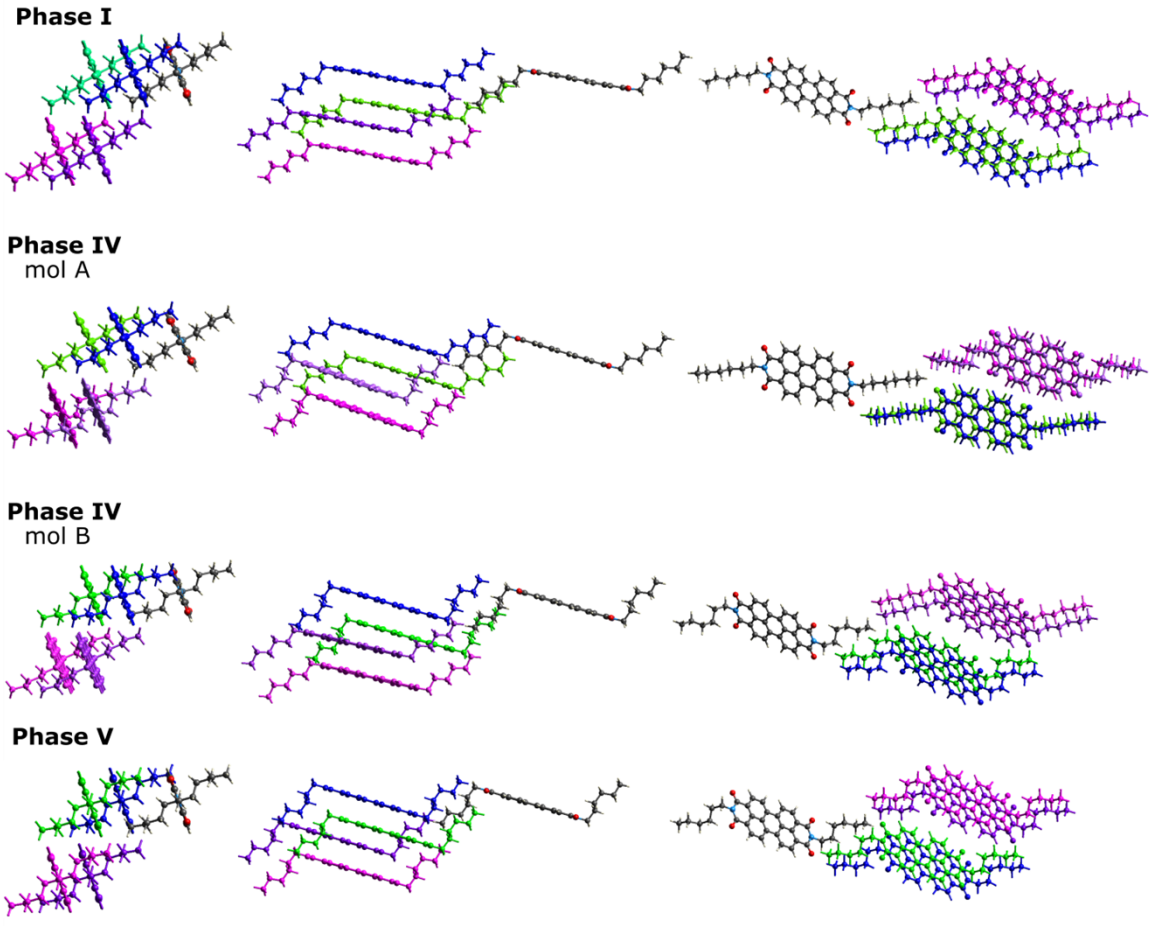

Figure S28. Intermolecular interactions between PDI-C_6 molecules calculated in Crystal Explorer.

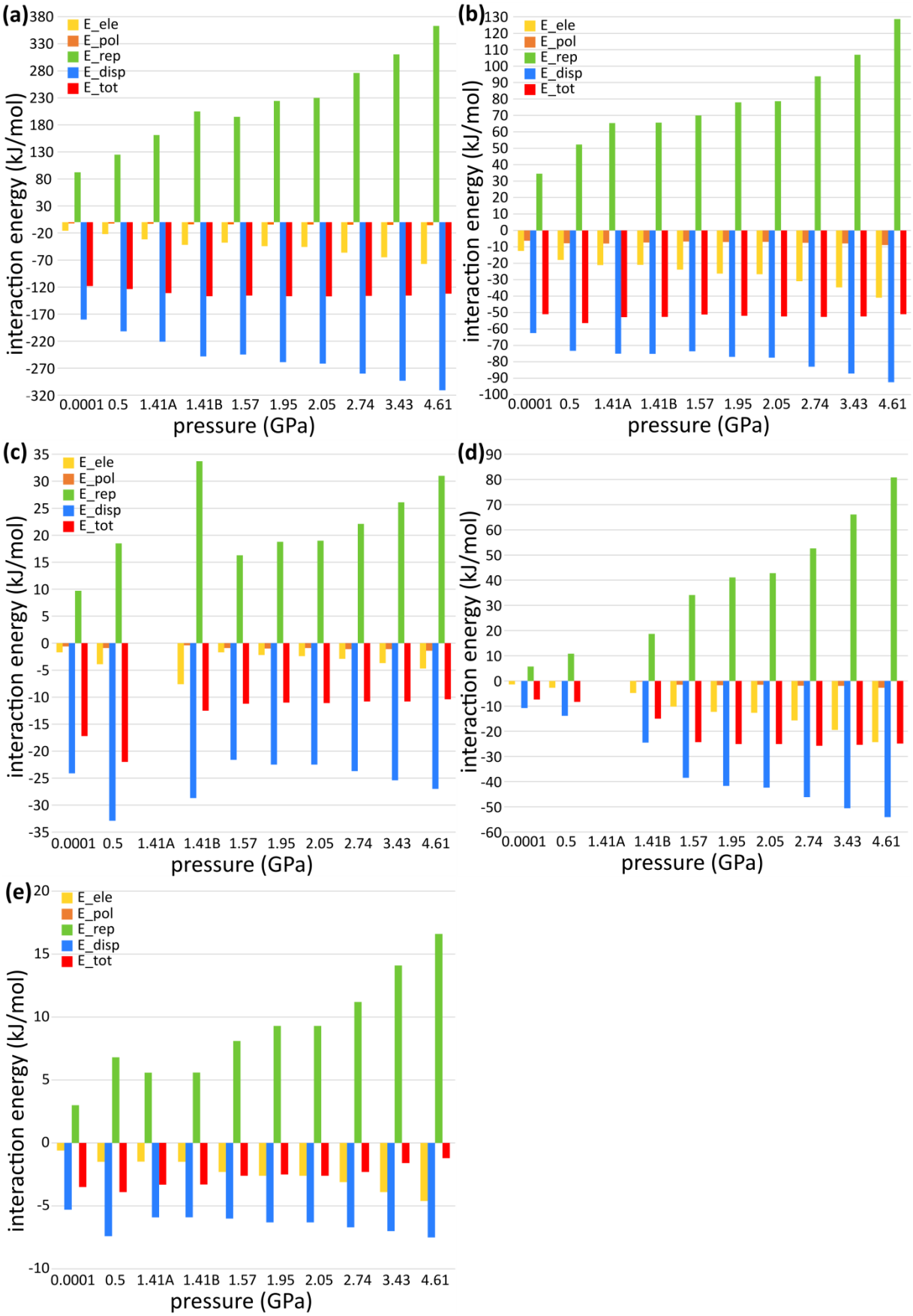

Figure S29. The evolution of selected interaction energies between PDI-C_6 molecules. (a) stacking π···π interactions (red molecule in Figure S27), (b) mainly CH···O interactions (blue

molecule in Figure S27), (c) side alkyl···alkyl interactions (green molecule in Figure S28), (d) side alkyl···alkyl interactions (blue molecule in Figure S28), (e) apical alkyl···alkyl interaction (pink molecule in Figure S28). For all the interactions see Figure S27, S28 and Table S13, S14. Missing values for molecule A at 1.41 GPa due to wrong calculations in Crystal Explorer (see Table S14).

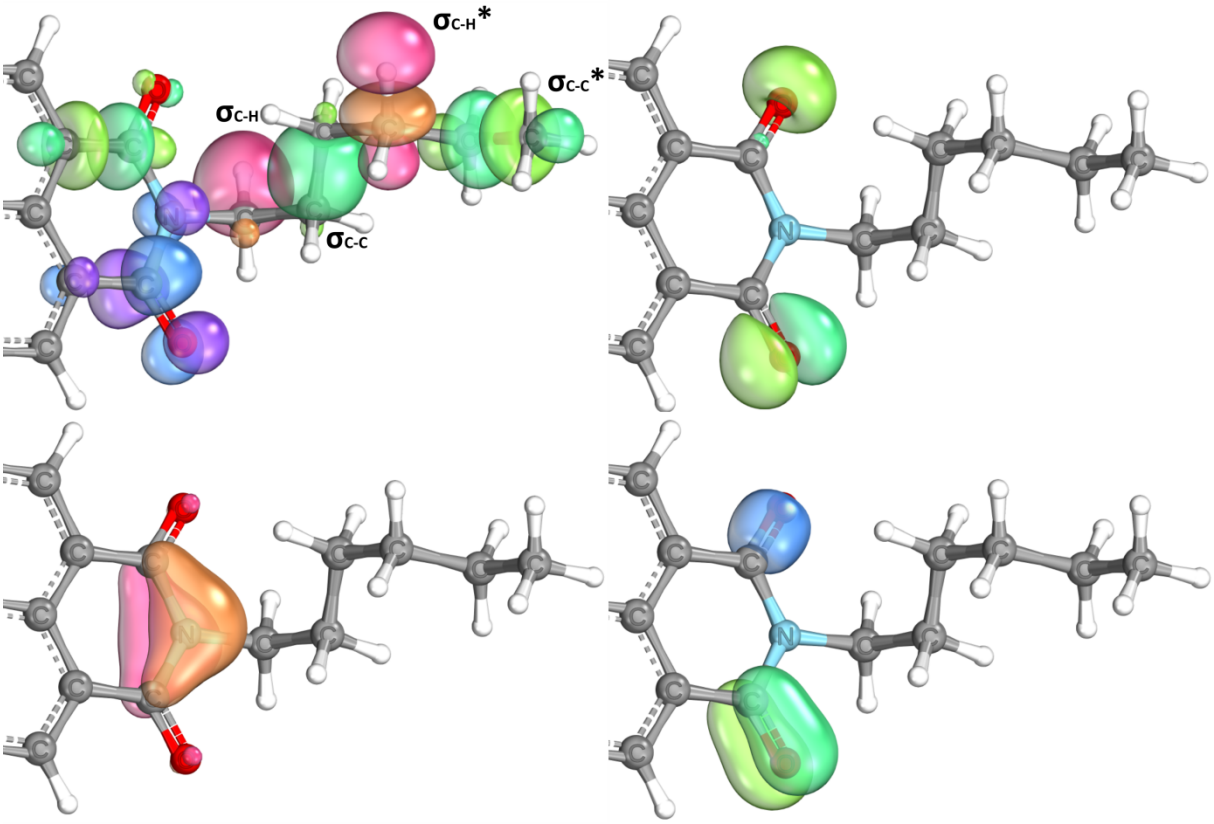

Figure S30. Visualizations of Intrinsic Bond Orbitals (IBOs) and Virtual Valence Intrinsic Bond Orbitals (vvIBOs). For clarity, IBOs and vvIBOs were presented independently, but they are present at each molecule simultaneously.

The polarity of the C=O bond results in its electron-withdrawing character. Hence, the lone electron pair of the nitrogen in PDI is diffused into the neighboring carbon atoms forming so called two-electron chemical bond over three centers (2e2c bond, Figure S30).

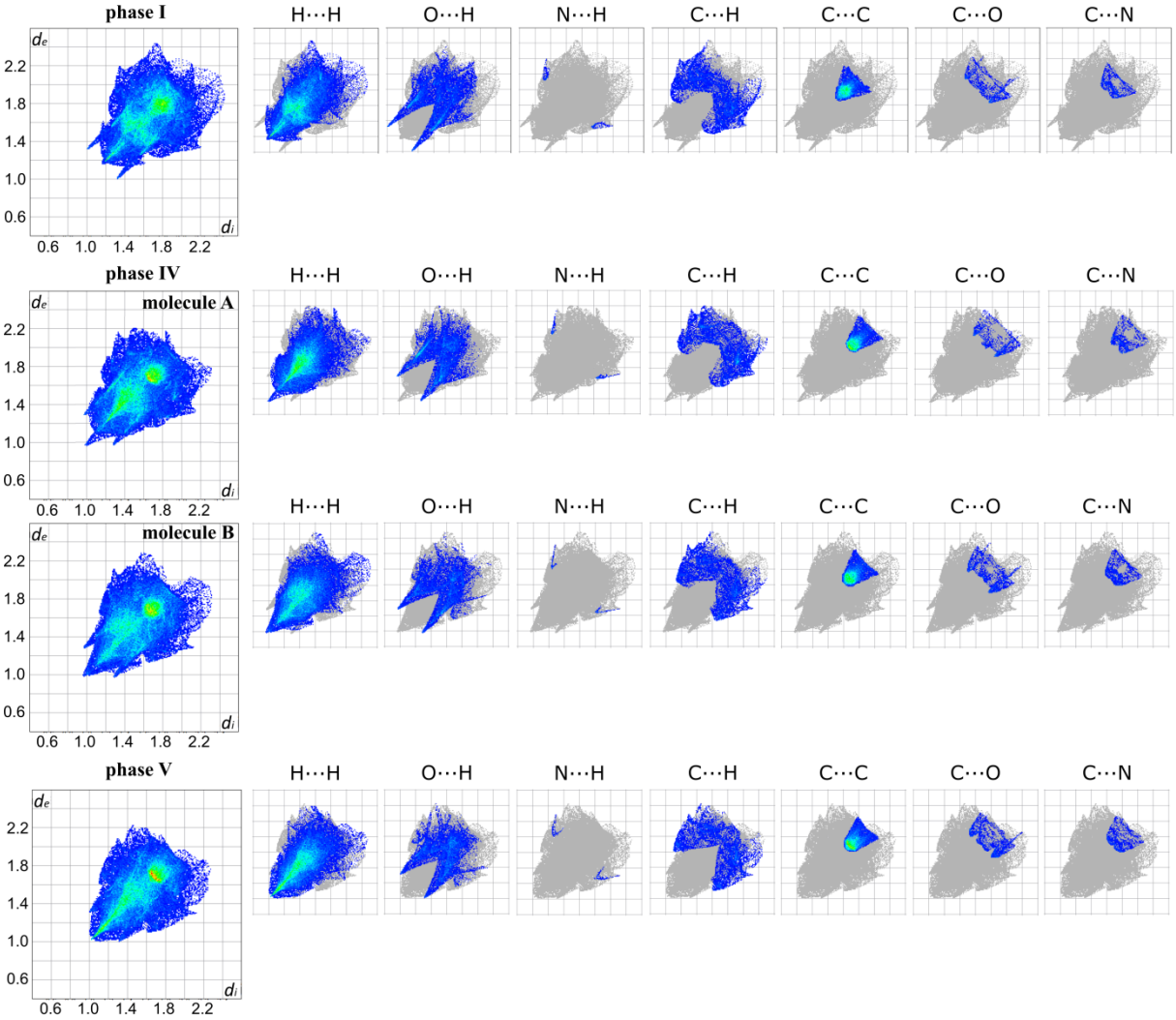

Figure S31. Fingerprints representing types of interactions present in all PDI-C_6 phases at 0.0001, 1.41 and 4.61 GPa, respectively.

Table S15. Coordinates of atoms of PDI-C_6 molecules – models taken from crystallographic data and optimized in Orca at the B3LYP-gCP-D3/6-31G* theory level.

0.00001 GPa

O	5.98036540467279	5.63728838723651	6.54399564273697
O	4.80266860919056	8.70768934446812	3.35878195352622
N	5.43762181859984	7.19778397003556	4.95950420297917
C	3.68098358559165	8.45224453107502	6.81945386165904
C	2.22725476065085	10.70996323401918	6.03779352791769
H	1.68129574870088	11.58393758526956	5.69547898909711
C	2.06691794458995	10.24426950407887	7.34575996004281
C	2.69126150818513	8.55094682365645	9.07833026347696
C	6.49733117825416	4.48732327541903	2.41891227494432
H	7.28749012789382	4.06722663587836	3.06498950622460
H	7.01040255769945	5.10511244618193	1.66194200295232
C	4.42621509807529	7.30950531181688	7.20115993981614
C	5.33783862380753	6.63688406124100	6.24249281117603
C	3.08302543073055	10.07897648486867	5.12619442972611
H	3.18933083306779	10.45656674040708	4.11210700094358
C	2.80583906318198	9.08787540721948	7.75568506736796
C	3.80891507636680	8.96023308500737	5.50253979982990
C	5.74794759733416	3.33825283811159	1.72226047711706
H	5.21778733554369	2.73683844142778	2.48166684953986
H	4.96507931978703	3.75733726626633	1.06664700103192
C	3.44411042937749	7.42031957361874	9.40810281871623
H	3.37906381354075	6.98766755320508	10.40188514725691
C	4.30012445639266	6.80578166288217	8.48581984793415
H	4.87601235772827	5.92626267085259	8.76343795553828
C	5.56633631887268	5.36721695065569	3.26848103528216
H	5.06823012107473	4.73979837337329	4.02187292414945

H	4.77610840978630	5.80181730767521	2.63665159527258
C	6.31015982926061	6.50563053581269	3.98641510070961
H	7.16815380379652	6.12051197874459	4.54702062696429
H	6.65669119071909	7.25834406685368	3.27215040231809
C	4.70214682863026	8.30626683080199	4.51248590675659
C	5.88675767836020	1.26224360238844	0.23258470031696
H	5.14607669658975	1.65775332514773	-0.48106806087714
H	5.34795157456141	0.65727477719328	0.97733586274182
H	6.55952948444077	0.59245272108707	-0.32231491897212
C	6.65746533391756	2.41303671730426	0.89707924080922
H	7.44748312707967	2.00202973655324	1.54542425185705
H	7.17644176678513	3.00304965610140	0.12308842512660
O	-2.15427334077883	13.78618401601648	10.83270002315935
O	-0.98819172777548	10.70486340463679	14.01099454087361
N	-1.62001427953115	12.21703235330653	12.41110839218066
C	0.16633124084133	10.98775627879315	10.56301417356500
C	1.62419963799936	8.73294193975970	11.34587245765248
H	2.17135017041068	7.85983812112502	11.68842984785773
C	1.78826293467396	9.20212820973562	10.03965727316347
C	1.16648246219267	10.89759332092198	8.30824369930460
C	-2.92016956644253	14.83080847384852	14.93788889956791
H	-3.70292206374950	15.20684351918230	14.25606830142980
H	-3.42855702295366	14.16361491506603	15.65523104031847
C	-0.57876643414623	12.13086031561701	10.18197446294636
C	-1.50637112123493	12.79025732058372	11.13479637801604
C	0.76064432290771	9.35744076672987	12.25442836921362
H	0.64907969298795	8.97556839451494	13.26633750060613
C	1.04806172552960	10.35753156555908	9.62931662761832
C	0.03229332356986	10.47427208072497	11.87725140211432
C	-2.29890590213560	16.01640024279828	15.69473691115640
H	-1.77874057692875	16.67298475039693	14.97587919591688
H	-1.52285662928870	15.64459112910542	16.38598340473192
C	0.41672379828338	12.03082400531649	7.98026003587955
H	0.48663226360410	12.46760971098427	6.98858649010605
C	-0.44419698914211	12.64137846292230	8.90082627338480
H	-1.01948289379803	13.52139435675910	8.62348586920375
C	-1.89210021578881	14.02889279570823	14.12316404857433
H	-1.40023373217907	14.69583784998156	13.40020398253426
H	-1.10683138571373	13.63130002919718	14.78486001235588
C	-2.54699084272347	12.86463442665567	13.36317928906352
H	-3.40087034864354	13.22272752303946	12.77967252335424
H	-2.88578857874678	12.08951418896138	14.05691662924422
C	-0.87739452797089	11.11449233005731	12.86113839988173
C	-2.70335501189032	18.03135561890824	17.23115689087450
H	-1.94749886539909	17.69257149029297	17.95610729161547
H	-2.20661002491954	18.72377317338035	16.53445894993039
H	-3.46307606314259	18.60259815467149	17.78421209051831
C	-3.32840392212015	16.84412677037222	16.48275718576291
H	-4.10265663111569	17.21432186661514	15.78954377361611
H	-3.84953671757934	16.18927371381773	17.20123193870022

0.5 GPa

O	5.98036540467279	5.63728838723651	6.54399564273697
O	4.80266860919056	8.70768934446812	3.35878195352622
N	5.43762181859984	7.19778397003556	4.95950420297917
C	3.68098358559165	8.45224453107502	6.81945386165904
C	2.22725476065085	10.70996323401918	6.03779352791769
H	1.68129574870088	11.58393758526956	5.69547898909711
C	2.06691794458995	10.24426950407887	7.34575996004281
C	2.69126150818513	8.55094682365645	9.07833026347696
C	6.49733117825416	4.48732327541903	2.41891227494432
H	7.28749012789382	4.06722663587836	3.06498950622460
H	7.01040255769945	5.10511244618193	1.66194200295232
C	4.42621509807529	7.30950531181688	7.20115993981614
C	5.33783862380753	6.63688406124100	6.24249281117603
C	3.08302543073055	10.07897648486867	5.12619442972611
H	3.18933083306779	10.45656674040708	4.11210700094358
C	2.80583906318198	9.08787540721948	7.75568506736796
C	3.80891507636680	8.96023308500737	5.50253979982990
C	5.74794759733416	3.33825283811159	1.72226047711706
H	5.21778733554369	2.73683844142778	2.48166684953986
H	4.96507931978703	3.75733726626633	1.06664700103192
C	3.44411042937749	7.42031957361874	9.40810281871623
H	3.37906381354075	6.98766755320508	10.40188514725691
C	4.30012445639266	6.80578166288217	8.48581984793415
H	4.87601235772827	5.92626267085259	8.76343795553828
C	5.56633631887268	5.36721695065569	3.26848103528216
H	5.06823012107473	4.73979837337329	4.02187292414945
H	4.77610840978630	5.80181730767521	2.63665159527258
C	6.31015982926061	6.50563053581269	3.98641510070961
H	7.16815380379652	6.12051197874459	4.54702062696429
H	6.65669119071909	7.25834406685368	3.27215040231809
C	4.70214682863026	8.30626683080199	4.51248590675659
C	5.88675767836020	1.26224360238844	0.23258470031696
H	5.14607669658975	1.65775332514773	-0.48106806087714
H	5.34795157456141	0.65727477719328	0.97733586274182
H	6.55952948444077	0.59245272108707	-0.32231491897212
C	6.65746533391756	2.41303671730426	0.89707924080922
H	7.44748312707967	2.00202973655324	1.54542425185705
H	7.17644176678513	3.00304965610140	0.12308842512660
O	-2.15427334077883	13.78618401601648	10.83270002315935
O	-0.98819172777548	10.70486340463679	14.01099454087361
N	-1.62001427953115	12.21703235330653	12.41110839218066
C	0.16633124084133	10.98775627879315	10.56301417356500

C	1.62419963799936	8.73294193975970	11.34587245765248
H	2.17135017041068	7.85983812112502	11.68842984785773
C	1.78826293467396	9.20212820973562	10.03965727316347
C	1.16648246219267	10.89759332092198	8.30824369930460
C	-2.92016956644253	14.83080847384852	14.93788889956791
H	-3.70292206374950	15.20684351918230	14.25606830142980
H	-3.42855702295366	14.16361491506603	15.65523104031847
C	-0.57876643414623	12.13086031561701	10.18197446294636
C	-1.50637112123493	12.79025732058372	11.13479637801604
C	0.76064432290771	9.35744076672987	12.25442836921362
H	0.64907969298795	8.97556839451494	13.26633750060613
C	1.04806172552960	10.35753156555908	9.62931662761832
C	0.03229332356986	10.47427208072497	11.87725140211432
C	-2.29890590213560	16.01640024279828	15.69473691115640
H	-1.77874057692875	16.67298475039693	14.97587919591688
H	-1.52285662928870	15.64459112910542	16.38598340473192
C	0.41672379828338	12.03082400531649	7.98026003587955
H	0.48663226360410	12.46760971098427	6.98858649010605
C	-0.44419698914211	12.64137846292230	8.90082627338480
H	-1.01948289379803	13.52139435675910	8.62348586920375
C	-1.89210021578881	14.02889279570823	14.12316404857433
H	-1.40023373217907	14.69583784998156	13.40020398253426
H	-1.10683138571373	13.63130002919718	14.78486001235588
C	-2.54699084272347	12.86463442665567	13.36317928906352
H	-3.40087034864354	13.22272752303946	12.77967252335424
H	-2.88578857874678	12.08951418896138	14.05691662924422
C	-0.87739452797089	11.11449233005731	12.86113839988173
C	-2.70335501189032	18.03135561890824	17.23115689087450
H	-1.94749886539909	17.69257149029297	17.95610729161547
H	-2.20661002491954	18.72377317338035	16.53445894993039
H	-3.46307606314259	18.60259815467149	17.78421209051831
C	-3.32840392212015	16.84412677037222	16.48275718576291
H	-4.10265663111569	17.21432186661514	15.78954377361611
H	-3.84953671757934	16.18927371381773	17.20123193870022

1.41 GPa – molecule A

O	1.55960616056250	9.29984461589488	6.22559115310784
N	2.08149672827976	10.85902641586197	4.63182141823924
C	3.89066498106743	12.09280615198707	6.45703336342035
C	4.82187676967925	12.69400574893876	7.36234022133199
C	2.10908350355696	9.05324126300705	2.93944557636471
H	2.94154984960510	9.55216649114039	2.41899700126799
H	2.54511289128329	8.40795770887489	3.71516512010877
C	4.19695051456138	11.03446266974500	9.02732041259623
H	4.28563978411253	10.59380473941977	10.01577830728175
C	5.57885330213451	13.83075562033401	6.93125018023407
C	1.32760748663202	8.17790230573535	1.94765916876216
H	0.79374180028730	8.81239803281160	1.21979026379290
H	0.55351719226508	7.61077203870067	2.49207883314973
C	2.25183471265735	7.20230092859726	1.19408853186379
H	2.94036058294705	7.78124108002862	0.55458695978819
H	2.89273076036680	6.66880759309005	1.91775005538728
C	2.45046991760798	5.21554574328672	-0.41228607354994
H	3.11847332119071	5.76692414220754	-1.09153708589627
H	1.89149480497101	4.48497092407690	-1.01485783706562
H	3.08415417827340	4.65375810045760	0.29103342735850
C	3.73006192066481	12.61273425144006	5.14856146155317
C	1.26100368104757	10.12499573895143	3.64177075504752
H	0.87666921534207	10.85970728507110	2.92821226353194
H	0.42604550052178	9.67260083784671	4.18530532864233
C	4.97107689199413	12.14415644247229	8.67597322952110
C	4.47154072864800	13.71448918222660	4.75273891603096
H	4.34009086110669	14.10037092021974	3.74474472270387
C	2.19710299032883	10.29969713701363	5.91443072064740
C	1.50499724481085	6.17001927441544	0.33350335366837
H	0.86378834486255	6.69286934373029	-0.39419118106907
H	0.82464624397393	5.58640234728481	0.97609998851072
C	5.37981206456969	14.31306565765715	5.63476275507432
H	5.93866812028752	15.17264169713173	5.27749609176688
C	3.13408299843357	10.96332148835290	6.85584945525839
C	3.29280593385348	10.44835409623836	8.13252913169020
H	2.70822794499404	9.57913382505377	8.42413665539359
O	2.68053418170973	12.38222659289264	3.02978395331930
C	2.80453550469352	11.97371174456966	4.17883126170682
O	9.96964836027635	17.27343023955436	10.29700257029924
N	9.43722495577405	15.72678199365955	11.89914050896717
C	7.61902104601284	14.49654875501307	10.07952309306354
C	6.68528509425091	13.89836557954323	9.17510806568038
C	9.46413270082404	17.57826895548321	13.54829100808999
H	8.68802945414126	17.12162555517882	14.18207601672916
H	8.94889552751923	18.14022179011622	12.75741501227376
C	7.31674042393774	15.55255860748382	7.50636471236554
H	7.22977703303414	15.99158526918400	6.51706392018571
C	5.92654310571915	12.76342880239674	9.60739518385649
C	10.30908533861747	18.56363584243460	14.37204435971097
H	10.86933026610539	18.02684214140453	15.15640485279334
H	11.06288578006943	19.02882838320041	13.71441684239419
C	9.44002696913121	19.66175764736224	15.01416864391174
H	8.76614121611941	19.20105025543169	15.75553272310872
H	8.78315535384257	20.10088803430178	14.24301986154469
C	9.34100061361455	21.89012526407937	16.27417564844426
H	8.66261512667255	21.48465701821732	17.04037971000677
H	9.93659041768919	22.68606799922206	16.74436066312059
H	8.71913102679523	22.35481167400318	15.49374353760510

C	7.77624164901126	13.98207824622854	11.39072987941761
C	10.27649311790822	16.46014262239408	12.87402700711629
H	10.64206799492296	15.73233230431012	13.60400657682565
H	11.12281605901348	16.87552716161127	12.31846854405128
C	6.53795611876810	14.44739931321097	7.86064216628023
C	7.02959100859224	12.88458217043793	11.78875119615543
H	7.15690223762921	12.50168813811562	12.79844277823927
C	9.32431464859122	16.28019282445807	10.61371851448210
C	10.23875217614075	20.78966501137780	15.68740963098873
H	10.86765590925837	20.36938247191494	16.48814988349379
H	10.93176127066251	21.23327369280798	14.95305057621124
C	6.12220103551772	12.28498458761468	10.90601706349451
H	5.56149003559066	11.42719811677959	11.26475635831559
C	8.38109618877875	15.62092934532076	9.67670251737846
C	8.22477651110666	16.13471451616180	8.39932848941709
H	8.81463703021106	16.99974470716089	8.10601642028370
O	8.82315771370281	14.22008071457005	13.51116571104091
C	8.70430787056286	14.62156707148997	12.35929989211506

1.41 GPa – molecule B

O	2.11259734303578	8.62771751889581	10.37223697556179
C	1.39038412845563	7.68702628792767	10.68122137828540
N	1.46084632137925	7.10218042926815	11.95664815206242
C	0.21771717863732	7.71625871050126	8.49954766468317
H	0.81732072877732	8.58716760704535	8.24626161911157
C	-0.23712157689665	5.41494861475887	11.37551186891502
C	-0.70731607073400	7.19505494287267	7.58625723802469
H	-0.80685514216879	7.69552244480526	6.62774783185797
O	0.80032254641985	5.55372431697058	13.50782460402147
C	-0.38933649591525	5.99362576050726	10.09145247283842
C	-1.47963896863254	6.06735828289934	7.87863395010598
C	-0.99344019543466	4.30680804248315	11.72215212935967
H	-0.87145375391101	3.87698143531549	12.71345301203335
C	1.15092125133428	10.04008240871399	13.20480824816523
H	0.55768435758123	9.80120901372239	12.31137018473451
H	2.03041813245515	10.59545800397815	12.84005381237124
C	-2.09329259236768	4.29674982216159	9.53653323962232
C	2.33781276831302	7.73488909496568	12.96916750041240
H	3.13512675705811	8.23710232717687	12.41880710407042
H	2.76406059079147	6.92397251488196	13.56734687202318
C	0.69569820177451	6.00031431216304	12.37113005935538
C	-1.90270829953301	3.75514428970287	10.81082555134894
H	-2.46924522068214	2.88477104901063	11.12801920521289
C	1.60774286797217	8.73713550838724	13.88574846810122
H	0.74185262204217	8.24558894712275	14.35298842834978
H	2.30499020771250	8.97083291888031	14.70566718279932
C	0.29921575785344	10.94645803068157	14.11625774263145
H	-0.09340651740011	11.78291354846215	13.51222802630879
H	-0.58448389772773	10.38118738460214	14.46159099783448
C	-1.32770105097608	5.44714954750540	9.16035919564969
C	0.39155125807590	7.12192515258032	9.73916012712797
C	1.03741526894309	11.52196408560316	15.33819860631484
H	1.90814354412441	12.10517852401718	14.99383002792093
H	1.44168939035489	10.70407187574100	15.95555099896299
C	0.13740147731516	12.40728250040709	16.21407825189755
H	-0.26926609714383	13.25442700253168	15.64151189448451
H	0.68914899834262	12.81724059664934	17.07244153921807
H	-0.71649201131355	11.83515633627871	16.60808686017996
O	-6.62073846185540	1.14828386764736	6.06899196313704
C	-5.90207406451304	2.09240424044002	5.76216217208448
N	-5.98507865370762	2.68871847486479	4.49310378611390
C	-4.74689640422456	2.07881207778624	7.95346778632661
H	-5.34966350392005	1.21055069837662	8.20837453206942
C	-4.27958464195047	4.36982938919104	5.07159492377993
C	-3.82925384486999	2.60587704609740	8.87077211839697
H	-3.73916373586788	2.11304485737487	9.83415513118629
O	-5.35286582888905	4.26201025950210	2.95545535105484
C	-4.12753722637133	3.79083881857730	6.35541429704563
C	-3.05159606080408	3.72914679251634	8.57575220378181
C	-3.53367675796808	5.48670358262380	4.73029902389836
H	-3.66068355021456	5.92095397859217	3.74156613882426
C	-5.84317461825901	-0.15360005724422	3.10158048856717
H	-5.15648605399684	0.06434494796152	3.93170602772199
H	-6.68014306318181	-0.71723894902906	3.54504095861045
C	-2.43749902239900	5.49934865820338	6.91766579789208
C	-6.97074161699532	2.15066117345445	3.52752297269904
H	-7.75590472339477	1.67451787537645	4.12090436611671
H	-7.39340361048404	3.01170662604863	2.99967073333328
C	-5.22538678852151	3.79573879789466	4.08197195052751
C	-2.63172156057275	6.04417999074199	5.64533792975017
H	-2.07196944200943	6.92019210384267	5.33165017858997
C	-6.36431804536145	1.16815549124002	2.50927023163795
H	-5.55323846093529	1.67655812202268	1.96616969383245
H	-7.15042678168027	0.96339345913674	1.76541895668145
C	-5.09830539922196	-1.03675316179595	2.08016949112956
H	-4.64653569096692	-1.88988469763309	2.61533753888941
H	-4.25478175033406	-0.46329744956549	1.65681451280641
C	-3.19719238123725	4.34400008026538	7.29072020830975
C	-4.90594265174707	2.66021099649875	6.70582858173002
C	-5.96815671351404	-1.57654386328255	0.93096133914861
H	-6.80061986229435	-2.16516684173154	1.35251420369647
H	-6.43065440006858	-0.73989515262064	0.38380611925283
C	-5.17501049268667	-2.44180848937918	-0.06074620473388
H	-4.71155507492814	-3.30376568168794	0.44244159978212

H	-5.82035987275331	-2.82957331143256	-0.86236164628437
H	-4.36724999521215	-1.86221694105342	-0.53332147934591

1.57 GPa

O	3.99209202347683	3.65151863583844	5.85668742726159
O	2.83316665346327	0.54749720633049	2.69089053704496
N	3.41362533369784	2.11217940899468	4.25617237374820
C	3.30044273834593	2.69390773449840	5.53015104993177
C	2.13835828328626	2.64045074026783	7.71688183654800
H	2.73973317073503	3.50119531959974	7.99950143836616
C	1.20910094021455	2.09347698993876	8.61040152948474
H	1.11379884071583	2.55858907249356	9.58707609388179
C	3.75809706620314	3.62240780716068	2.26040861047915
H	3.08188924614554	3.03722515640647	1.61902137399756
H	4.58092475665716	3.96660722418302	1.61420303096305
C	3.50647949717021	6.57380610819774	0.99874714387248
H	4.15785549570167	5.87584278485786	0.44900422677891
H	4.16007758736306	7.10675081675240	1.71021748795796
C	1.53288439858668	0.96998771626282	6.06994008604139
C	0.42633058036765	0.98493819453941	8.27596395050825
C	1.70234708969704	0.41816011850543	4.77623909758461
C	3.00596082026046	4.82877223153748	2.85027050041866
H	3.66939517999845	5.38266615771995	3.53371437713699
H	2.17116135446095	4.46164540403815	3.46847693004335
C	0.03320586952204	-1.25638712221961	5.28547807015097
H	-0.53078236943843	-2.11856008248867	4.94193734610578
C	4.39261667376401	2.69038915965216	3.30764350105205
H	4.88753177508728	1.85063497688763	2.80793279886923
H	5.12545882918175	3.23111001417808	3.91321183679840
C	2.44017685603285	5.79172758080911	1.78699840066281
H	1.80320095502093	5.22928442420247	1.08177541749360
H	1.77353257726218	6.51451067208470	2.28704292996932
C	2.30607376044416	2.09301529038296	6.45491525747066
C	0.58985546503156	0.39722847144747	6.98048679175959
C	-0.16471338830626	-0.74988783400082	6.57302912245266
C	0.95094169303788	-0.68255221858916	4.39646791056902
H	1.08849641554737	-1.09290471832063	3.39884257416173
C	2.89959931052934	7.57911543015680	0.00726713565334
H	3.68129640067589	8.12762775863408	-0.53841066299122
H	2.27112172055668	8.31949575082463	0.52571127674594
H	2.26678110458764	7.07125909354543	-0.73673692694735
C	2.67299578440916	1.00358470891409	3.81749552687121
O	-4.55062714936414	-4.12817150248485	10.00932143537649
O	-3.62227147802667	-0.82963315990782	13.05098897199264
N	-4.07767991759545	-2.49946552009620	11.55407474805850
C	-3.92055699924557	-3.11879208293904	10.30290003754578
C	-2.76209457068030	-3.06377799613431	8.11326161852449
H	-3.32437309949433	-3.95679688013461	7.85087962738515
C	-1.85642310837647	-2.49779025860637	7.20706554539034
H	-1.73973349312268	-2.98166945605372	6.24181066449413
C	-4.32607648025408	-3.88803716658046	13.63999389454432
H	-3.60942161429616	-3.22410882940749	14.14571350603104
H	-5.09750783380238	-4.13839382211729	14.38536529906576
C	-3.75333601350288	-6.62353570608076	15.30964623199912
H	-4.51217702393658	-5.93030897933070	15.70350446440233
H	-4.31286129702907	-7.42216683796162	14.79399762757085
C	-2.22783882178513	-1.33373866067390	9.72211259061031
C	-1.11531954918426	-1.35447790964752	7.51901163225257
C	-2.43484956237756	-0.75008902144698	10.99596475332642
C	-3.61284797677301	-5.16691810125401	13.16547802439674
H	-4.34861418925054	-5.84652027403877	12.70486080907950
H	-2.89745001791430	-4.90679213396459	12.36986756354365
C	-0.79285549925069	0.94625170434600	10.47289981844483
H	-0.25589768324613	1.83090769986108	10.80223072344701
C	-5.02691545106694	-3.09513218667734	12.52314482974021
H	-5.60245282249257	-2.27005078061341	12.95596455138252
H	-5.69905300007904	-3.73709531064357	11.94683378152711
C	-2.85368952364075	-5.90059417296180	14.29046191532936
H	-2.21134308549843	-5.17638143831797	14.82191460177678
H	-2.16911924418527	-6.63892116614252	13.84047288358327
C	-2.95647742309468	-2.49390674715713	9.36141025328172
C	-1.29138296494818	-0.75608256015099	8.80797162926991
C	-0.55432082747028	0.40537257618877	9.20640241825633
C	-1.72157965769248	0.38203638164757	11.35630539958211
H	-1.89369440687047	0.82092021809291	12.33623632176238
C	-2.96375858989377	-7.22002316713996	16.48535926907340
H	-3.62878696272663	-7.70758541467966	17.21338921998649
H	-2.23584980342751	-7.97034451151546	16.14015875964887
H	-2.40357688476914	-6.43795044224248	17.02080970440327
C	-3.40743746312903	-1.33264856725710	11.95382446501665

1.95 GPa

O	3.96000600233071	3.63759090179668	5.82378476896286
O	2.81217384313933	0.53849220275613	2.64908332327510
N	3.38757394321697	2.10038512554111	4.21904646228896
C	3.27054450276860	2.67958453554732	5.49386251319227
C	2.10397638348953	2.61960313702209	7.67809391862053
H	2.70400740472704	3.48022732675812	7.96416034115101
C	1.17348952487677	2.06944899249551	8.56838341097327
H	1.07598039359102	2.53194051975728	9.54616171798712
C	3.73404505007216	3.61330956090480	2.22577690808679
H	3.06054288112108	3.02719178083255	1.58235658327125
H	4.55778712692972	3.95968680042679	1.58182587217672
C	3.47825331011005	6.56404815476585	0.96408301212562

H	4.13139465890677	5.86750438651817	0.41453519111634
H	4.13018053370004	7.09756713725411	1.67672148933916
C	1.50325024154914	0.95280541004901	6.02579392043821
C	0.39228117482886	0.96111077965007	8.22965383913581
C	1.67620148093248	0.40402511251820	4.73124910194057
C	2.97800569117493	4.81772718188398	2.81460281573450
H	3.63869211457977	5.37290749099028	3.49971389034263
H	2.14257378615074	4.44846365944542	3.43080008950360
C	0.00659608938505	-1.27247882679826	5.23239171713500
H	-0.55603041798131	-2.13427038152429	4.88549690574551
C	4.36784434764678	2.68161343877226	3.27371922029758
H	4.86564728700635	1.84330151860239	2.77432162932947
H	5.09821774512632	3.22307122433428	3.88168495159948
C	2.41225414520803	5.77959731071451	1.75034560286943
H	1.77795683152249	5.21567100002478	1.04380809095943
H	1.74289488006271	6.50084645855675	2.24909300245637
C	2.27479264957136	2.07546668628953	6.41510087913309
C	0.55844223743968	0.37723745884958	6.93274314969873
C	-0.19487814009807	-0.76901606710824	6.52058477028164
C	0.92639761786051	-0.69626124539186	4.34713135314580
H	1.06700444386896	-1.10454826952923	3.34900986572090
C	2.87090862924368	7.56906620064371	-0.02740735083440
H	3.65238398547267	8.11964516976837	-0.57142945981136
H	2.24016692000238	8.30775212243590	0.49082116128895
H	2.24017735701646	7.06062721734321	-0.77286679562158
C	2.64920940490842	0.99184506604866	3.77639540495160
O	-4.58943658821419	-4.15642420521084	9.93678157664344
O	-3.66059493645179	-0.87237850130033	12.99397619614655
N	-4.11671097267579	-2.53475589675225	11.48898298039451
C	-3.95861393878039	-3.14899663263823	10.23540719955409
C	-2.79702261186612	-3.08625292501363	8.04770195304700
H	-3.35958372842036	-3.97789297878963	7.78101043377458
C	-1.88952832919602	-2.51749544531495	7.14510409060742
H	-1.77174176660810	-2.99782540732994	6.17813826741152
C	-4.36978889857381	-3.93368057703634	13.56734594461065
H	-3.65095565014874	-3.27420662438041	14.07592549246414
H	-5.14196285040473	-4.18490561398200	14.31176035511762
C	-3.80941184492762	-6.68911367861958	15.21726131636680
H	-4.58001750526375	-6.00496341556332	15.60430352119083
H	-4.35498016088827	-7.49174016183101	14.69290207050045
C	-2.26384043816075	-1.36282531280763	9.66395756769338
C	-1.14803238842425	-1.37593146389852	7.46246166167291
C	-2.47187604161146	-0.78431042554973	10.94000526373602
C	-3.66055846256572	-5.21274478116197	13.08734412233118
H	-4.39832483942562	-5.88723127130816	12.62237530894508
H	-2.94310401868358	-4.95111674162887	12.29402593200671
C	-0.82874052134522	0.91356951091392	10.42541489617572
H	-0.29146816749919	1.79650523119720	10.75901887788139
C	-5.06800813068082	-3.13347613063683	12.45416203170683
H	-5.64204546413151	-2.30929491750684	12.89082089855336
H	-5.74124097468699	-3.77079818317606	11.87389469833085
C	-2.90570712371061	-5.95416922417392	14.21025790773035
H	-2.26909925899531	-5.23238211638720	14.75193756536815
H	-2.21574082336896	-6.68628098448065	13.75828815248879
C	-2.99269829234707	-2.52113782487318	9.29781177483266
C	-1.32590278953367	-0.78204815680269	8.75329445264124
C	-0.58922524871118	0.37786377233919	9.15689083013678
C	-1.75851410214101	0.34608368429830	11.30559085122706
H	-1.93134828432325	0.78100799416816	12.28723383447339
C	-3.02751185285643	-7.28099751252165	16.40041116213080
H	-3.69592875443142	-7.77684371257291	17.11978872036359
H	-2.28818155520965	-8.02320399753038	16.06181918184568
H	-2.48135040907421	-6.49463029636277	16.94411086308106
C	-3.44559533712063	-1.37044235471981	11.89459177880893

2.05 GPa

O	3.96075664042752	3.62591806281029	5.81503170349227
O	2.80739122793221	0.53248452303190	2.63686901497208
N	3.38455608823391	2.09245286134966	4.20809310932961
C	3.26835527122342	2.67059566518313	5.48343179323197
C	2.10059417173701	2.61143683161380	7.66697104191024
H	2.70107264689909	3.47156003166402	7.95336216465595
C	1.16918586633348	2.06197815364516	8.55671518167159
H	1.07129361970612	2.52455489812151	9.53433720215008
C	3.73559015949628	3.60868868827127	2.21810660730895
H	3.05925190368908	3.02649480956983	1.57412704205381
H	4.56008134481397	3.95290384853007	1.57402291270533
C	3.49055656924745	6.56324030830408	0.96273765862846
H	4.14483676864967	7.09290814548431	1.67603460695624
H	4.14081952233884	5.86530315884089	0.41164301402155
C	1.49946872946168	0.94521281327481	6.01415669160466
C	0.38774202183005	0.95393675560969	8.21758594272681
C	1.67184851469042	0.39711945112655	4.71924984590604
C	2.98497654729816	4.81505490441511	2.80989135213792
H	2.14892700565035	4.44809875887339	3.42649959947232
H	3.64870142258758	5.36622861401555	3.49524658094681
C	0.00241392035235	-1.27963797427809	5.22031573185838
H	-0.56044676723137	-2.14113125121782	4.87322880601558
C	4.36656066301004	2.67264114143825	3.26388208874668
H	4.86171448452286	1.83391919666658	2.76270773371215
H	5.09854536789223	3.21060730312214	3.87294581733871
C	2.42203941778392	5.78134741296384	1.74814041416974
H	1.78488600643435	5.22150067276354	1.04100504217586
H	1.75604233070777	6.50418455196893	2.24895519520865

C	2.27154919718335	2.06732825509411	6.40399478908163
C	0.55463345442594	0.36960136571999	6.92101592714570
C	-0.19816879938508	-0.77704035093073	6.50898314409661
C	0.92161181509923	-0.70276961217031	4.33477729138904
H	1.06129791574701	-1.11010997747727	3.33621666006139
C	2.88657204392145	7.57245505564857	-0.02649743621381
H	3.66984525340240	8.12157439648683	-0.56930335620167
H	2.25839982935760	8.31213087177095	0.49332895405595
H	2.25411694543887	7.06789179890290	-0.77304787252940
C	2.64444558368587	0.98552109858543	3.76431006363803
O	-4.57808417671648	-4.17589360743021	9.93277549894585
O	-3.66747839476426	-0.87790649494197	12.98026726834646
N	-4.11335581139554	-2.54799384910100	11.48075874954722
C	-3.95225181286652	-3.16455083679368	10.22879963248152
C	-2.79298219239942	-3.10014127351986	8.03978997260225
H	-3.35235628610199	-3.99419008646022	7.77471011661389
C	-1.88773730162743	-2.52960770610839	7.13599680230571
H	-1.76873400352902	-3.01082350061574	6.16968960224366
C	-4.35420425144073	-3.93932764710951	13.56512165922678
H	-3.62614995339293	-3.27590862765017	14.05699607593036
H	-5.11997132531125	-4.17549191093790	14.32070616869513
C	-3.80968116526037	-6.64294482135778	15.26338030481680
H	-4.42903420859031	-7.40342881678429	14.75792329541832
H	-4.51087798305503	-5.90708394899287	15.68828718999468
C	-2.26542028742013	-1.37231623468989	9.65318506321302
C	-1.14944532403827	-1.38552504532478	7.45178741371919
C	-2.47632597192225	-0.79155308835711	10.92771117836430
C	-3.65826772522905	-5.22983349372133	13.09542303189298
H	-2.94626734932924	-4.98467566875431	12.29395423426768
H	-4.39970697078406	-5.90692712360776	12.63979407946782
C	-0.83704336434846	0.90940669072298	10.41126567677419
H	-0.30240462517328	1.79438438446899	10.74349196429890
C	-5.05976847395839	-3.14973529126410	12.44884236927519
H	-5.64034374249030	-2.32874276562247	12.88275746581142
H	-5.72839748665544	-3.79490016147000	11.87199388601107
C	-2.90231863283378	-5.96596653424982	14.22053248817084
H	-2.22869099341498	-5.25426315326348	14.72935671052381
H	-2.24971749295667	-6.73331571245216	13.77137427761449
C	-2.99023211804608	-2.53381577269122	9.28911471939763
C	-1.32870472504926	-0.79060091911440	8.74191374153083
C	-0.59457476749325	0.37132222998314	9.14432022064178
C	-1.76661485732467	0.34169786848641	11.29152557536387
H	-1.94199063046133	0.77847997258139	12.27181123065479
C	-3.02376382126652	-7.30111541194617	16.40764928571021
H	-3.69846664631570	-7.77151498074595	17.13808014405166
H	-2.34311252142248	-8.07959081771429	16.02992507399328
H	-2.41310893539734	-6.56047067356597	16.94677643767243
C	-3.44907237481291	-1.37850440867697	11.88269133477771

2.74 GPa

O	3.91114985828807	3.59699020427282	5.78408560208160
O	2.75710400339258	0.53623186677496	2.57457568784066
N	3.33506983632144	2.07982226687668	4.16174171100316
C	3.21712172413037	2.64658294972558	5.44203330447866
C	2.03862674103968	2.57476739034793	7.61950048795310
H	2.64170962213522	3.42976972589745	7.91598616345671
C	1.10014935744724	2.02249025594180	8.50003157557142
H	0.99955009422232	2.47738068490547	9.48110666390542
C	3.69060930707295	3.61349535750435	2.18663399189514
H	3.01193443847501	3.03812757910537	1.53886511338836
H	4.51549196750560	3.96057846088086	1.54449506158092
C	3.44955246004202	6.57778922744860	0.95236412115659
H	4.10532960669939	7.10226506319164	1.66821836363535
H	4.09827913727526	5.88268586953070	0.39576895760691
C	1.43888636984400	0.92407385669002	5.95075856254253
C	0.31556878556939	0.92063933038871	8.14826969741524
C	1.61526348224269	0.38552544287659	4.65235582256970
C	2.94372280993133	4.81736030015281	2.78828856390449
H	2.10755486226832	4.44788847334793	3.40339348679208
H	3.60975645569663	5.36230154147089	3.47645720862702
C	-0.06135402417702	-1.29007004092592	5.13304515365146
H	-0.62559863298688	-2.14704402275846	4.77681101588259
C	4.31938483185394	2.66705121000401	3.22443967172125
H	4.81333731037703	1.83204949194195	2.71578086473564
H	5.05195831202065	3.19796757203078	3.83908079548295
C	2.38110521460413	5.79188417932235	1.73381417501168
H	1.71627358488199	6.51206483670104	2.24013707047703
H	1.74264722539439	5.23739149401924	1.02350059043335
C	2.21342826164087	2.04009575683018	6.35297598389047
C	0.48752847153245	0.34492893611781	6.84846818050235
C	-0.26608840285865	-0.79686668239567	6.42470002872564
C	0.86331906450229	-0.70898283743761	4.25605902194620
H	1.00622102661447	-1.10903382199904	3.25488887575991
C	2.84519323191557	7.59411133497517	-0.02940200490868
H	3.62834406589213	8.14594382497727	-0.56980605685138
H	2.21864730713742	8.33104851632273	0.49642254955237
H	2.21095118463555	7.09508944948253	-0.77829235331175
C	2.59330990306612	0.97874766886309	3.70607241523251
O	-4.66648464376878	-4.21252464480671	9.80521426119018
O	-3.77373062234009	-0.92994083039761	12.87458389755718
N	-4.20996167157517	-2.59299379149019	11.36453789967803
C	-4.04241990753521	-3.20267659600672	10.10998547201594
C	-2.87008280846452	-3.12745193212351	7.92834343646332
H	-3.42828645879847	-4.01994245354549	7.65522718445661

C	-1.95934265849527	-2.55254572870075	7.03290826527935
H	-1.83463043508046	-3.02890382392398	6.06478739255880
C	-4.46216990604629	-3.99436329100515	13.44073436666259
H	-3.74274579138481	-3.33106280064097	13.94559627761127
H	-5.23405536123507	-4.24080140825181	14.18677193762272
C	-3.87318757206319	-6.66508912986543	15.15529921644413
H	-4.51332029126154	-7.42350326095259	14.67159235459410
H	-4.55598081165796	-5.91835396695395	15.59111225362486
C	-2.35120768160813	-1.40836393917921	9.55380732283671
C	-1.22250931218895	-1.41039018567628	7.35889930102117
C	-2.56931762877778	-0.83415656245226	10.83014560914656
C	-3.75460467436381	-5.27722243699014	12.96765890073935
H	-3.04862811864488	-5.02508880190431	12.16294778371250
H	-4.49113065903872	-5.96242400931266	12.51596081986287
C	-0.92558035849971	0.86820734816187	10.33254584622724
H	-0.39225416578628	1.75120310225214	10.67244300199173
C	-5.16154133497852	-3.20012031361413	12.32400676014612
H	-5.74571301337092	-2.38172683293795	12.75834598576859
H	-5.82595308625002	-3.84319487245020	11.73986246247897
C	-2.98313314770732	-6.00398214717383	14.08768881556529
H	-2.33977930403813	-6.77744770850138	13.63512613619038
H	-2.29858104415048	-5.28863985161322	14.57700354015833
C	-3.07446166418274	-2.56756206560721	9.17945284257781
C	-1.40837984505895	-0.82268448907399	8.65144583194828
C	-0.67497970028170	0.33585038560132	9.06473951191297
C	-1.86155928479274	0.29713450838662	11.20376592726047
H	-2.04314768203304	0.72941230529159	12.18503852315496
C	-3.06495374994909	-7.32017091101843	16.28579420388188
H	-3.72481485970457	-7.76568182046020	17.04464656728381
H	-2.41023879201593	-8.11690380716182	15.90020987508897
H	-2.42478627308996	-6.58220028767344	16.79368830651999
C	-3.54751653542672	-1.42596766163063	11.77652378342699

3.43 GPa

O	3.86053199302812	3.61560933157778	5.73131368170535
O	2.73712571987082	0.55803887020055	2.50794449378436
N	3.29896607910485	2.10089094297250	4.10162406930433
C	3.16996464227850	2.66537199515429	5.38181985235135
C	1.97435520093369	2.58813859918034	7.54976808554622
H	2.57430173058081	3.44299949991648	7.85278576217633
C	1.02904439512212	2.03361743773736	8.42154652310250
H	0.92006976693692	2.48643242724526	9.40263511245157
C	3.66639841003768	3.63839849758920	2.13194534707972
H	2.99353923826174	3.06261020972242	1.47859120039860
H	4.49508847620220	3.98816176453832	1.49626410571684
C	3.42517140349782	6.60274533897675	0.89750870873288
H	4.07467218616375	7.12922055322172	1.61752380541540
H	4.07953979547210	5.90975642510182	0.34499184063048
C	1.38972913733061	0.93989335318176	5.87325755364203
C	0.24793470969533	0.93206359126883	8.06121549923840
C	1.57748710590107	0.40349897162365	4.57557200416514
C	2.91267875256823	4.84004506351839	2.72965884461684
H	2.07361275404352	4.46833429811075	3.33936344354703
H	3.57309841111164	5.38633486703483	3.42207907477472
C	-0.10167695323497	-1.27426665889001	5.03947947517914
H	-0.66266435416224	-2.13076344332407	4.67715325427670
C	4.28937058273901	2.69158912967205	3.17295573405399
H	4.78881770332204	1.85848934416276	2.66662697347034
H	5.01630899664173	3.22277155774805	3.79395861823869
C	2.35411526539246	5.81341914336985	1.67190910929089
H	1.68374119557899	6.53136018484758	2.17397652506542
H	1.72214277332357	5.25707198190269	0.95730885044606
C	2.15979830463417	2.05603956813156	6.28368172957285
C	0.43142732489409	0.35846883790134	6.76206920632114
C	-0.31747863879788	-0.78338486227499	6.33022595492831
C	0.82993271925321	-0.69109787137421	4.17124601259131
H	0.98139230013373	-1.08922850618740	3.17062515194031
C	2.82380489601640	7.61740223672169	-0.08791982928808
H	3.60860018577068	8.17029869648277	-0.62473898914435
H	2.19334662432966	8.35340153894116	0.43441116207359
H	2.19426257812954	7.11670325488780	-0.83957796017955
C	2.56245711654612	0.99948618899945	3.63822644882071
O	-4.74437194567700	-4.20719804808484	9.66779948364842
O	-3.87992880605446	-0.92887645025236	12.74979180193432
N	-4.30217844348954	-2.58972864615201	11.23339266326071
C	-4.12336118870626	-3.19758580326095	9.97954977652538
C	-2.93177483259249	-3.11872093674805	7.80842457891304
H	-3.48666027843153	-4.01136920934932	7.52932603947432
C	-2.01364785122396	-2.54194051157227	6.92175336746464
H	-1.87972668355499	-3.01707188513482	5.95431187532519
C	-4.56850847820917	-3.99553340378787	13.30465755385414
H	-3.85648397129250	-3.33146520052691	13.81884799112022
H	-5.34634126104216	-4.24790803333736	14.04247777708998
C	-3.99295045804212	-6.68079919265772	15.00740690296137
H	-4.61661319917463	-7.44174476812516	14.50656627038289
H	-4.69099528607896	-5.94437806885840	15.43651131016888
C	-2.42896023747992	-1.40103927359676	9.44042121363944
C	-1.28104340521978	-1.39929497738917	7.25548685338215
C	-2.65894145904583	-0.82842487188504	10.71538622318795
C	-3.85092727403400	-5.27373147724425	12.83395575052911
H	-3.13607989474266	-5.01532124670947	12.03916487876216
H	-4.57931879864699	-5.95937529419283	12.37004073980944
C	-1.01309121659447	0.87654347546617	10.23402196944898
H	-0.48400075124757	1.75998430551048	10.57920159515497

C	-5.26037713070462	-3.19981665861220	12.18435183587684
H	-5.84858159359952	-2.38296148687403	12.61603034657633
H	-5.91968322346252	-3.84237170480849	11.59395471230856
C	-3.09105781537826	-6.00263069120282	13.96061185417114
H	-2.43281430992339	-6.76621385481074	13.51296525734815
H	-2.42164280028690	-5.28496054448722	14.46706649350591
C	-3.14776119979178	-2.56051065733565	9.05832496529164
C	-1.47883416533101	-0.81335320676869	8.54704968172297
C	-0.75040618929445	0.34553172309901	8.96808608381632
C	-1.95601789077016	0.30343796243719	11.09637154763886
H	-2.14685071676599	0.73446934345711	12.07638238172604
C	-3.19823379758263	-7.33654782506201	16.14709931447467
H	-3.86681954122931	-7.79506024834433	16.89033976704621
H	-2.52843794911420	-8.12326200593680	15.76702793391837
H	-2.57509486952470	-6.59610593361344	16.67217009693379
C	-3.64433361531132	-1.42270205283903	11.65270967556853

4.61 GPa

O	3.82090285076865	3.65143931122668	5.66406522790701
O	2.76643247139955	0.55221262767581	2.45726625786901
N	3.29429039869248	2.11516389777870	4.04275017982280
C	3.14596640009453	2.68925641927595	5.31663100290777
C	1.93771755526097	2.60961443093064	7.47746876354286
H	2.52710641999152	3.47189092491565	7.78022385086513
C	0.99283555888293	2.04940083048036	8.34605425449270
H	0.87336433223615	2.50592454963953	9.32419346348190
C	3.66494674789761	3.63148917922892	2.05730686629513
H	3.01470916695113	3.03611925959646	1.39874927858409
H	4.49777431103528	3.99042925805122	1.43216021128854
C	3.38923149770015	6.58582022283977	0.79596514987888
H	4.00119009125229	7.14181508940156	1.52652938742541
H	4.08009449987298	5.90528744866962	0.27309441048637
C	1.37814705558743	0.94962286742541	5.80415875411679
C	0.22352372367020	0.93959031399270	7.98548970118477
C	1.58100503066991	0.40795231192030	4.51094862717563
C	2.87766554634552	4.82430172346999	2.62899808146887
H	3.51443691395379	5.39030683077766	3.32779949200943
H	2.03497814429874	4.44236943419187	3.22735902906346
C	-0.09637320048110	-1.27401209968446	4.96564307815518
H	-0.64998481144558	-2.13460398924857	4.60172243507232
C	4.28796184047350	2.70820891325920	3.11912109455463
H	4.80732962111979	1.87623887584879	2.63110377769689
H	4.99813346905962	3.25881723831805	3.74261188811809
C	2.31998758019656	5.77578292040780	1.55111276523957
H	1.71895105775439	5.19855442607201	0.82645369257204
H	1.62065524645149	6.48065666284910	2.03171122989452
C	2.13647898429183	2.07361592327798	6.21506740817505
C	0.41604090237908	0.36607410457476	6.68756609328639
C	-0.32787168611290	-0.77749074948473	6.25152347216695
C	0.84301832532944	-0.69243692687147	4.10486461043357
H	1.00748143393894	-1.09568102099831	3.10834323124533
C	2.78707747504930	7.56750143848265	-0.22173671770655
H	3.57017507871068	8.14039761008843	-0.73976099738524
H	2.11508009174328	8.28796652059969	0.26961509236223
H	2.20030399420539	7.03640494930546	-0.98699147933491
C	2.57312939827264	1.00319781697734	3.58074407628657
O	-4.81009913944875	-4.17671901393950	9.54018226863766
O	-3.90674725422234	-0.94688093352121	12.66218965846894
N	-4.35241081459837	-2.58080530104706	11.12332240159716
C	-4.17665615516439	-3.17880885201856	9.86425813847146
C	-2.97528962734681	-3.09468072529233	7.69893136126997
H	-3.53909414017007	-3.97855298068089	7.40993553999598
C	-2.04719411486742	-2.52067391357205	6.82097955219921
H	-1.91500144291488	-2.98878812792682	5.84992129208034
C	-4.65302978716792	-4.01544498530390	13.17139007112150
H	-3.94164771495003	-3.37187141644916	13.71025775832743
H	-5.44232644888126	-4.27838163023414	13.89345725862043
C	-4.17518441785539	-6.80992857222055	14.76257936878035
H	-4.72359702944668	-7.57891664926314	14.19206290653099
H	-4.93596027348995	-6.11660655864558	15.15571195857194
C	-2.46091277527412	-1.39591906340955	9.34708830143556
C	-1.30436567464118	-1.38820941451802	7.16665800399107
C	-2.68742420921880	-0.83366698546639	10.62732044331934
C	-3.94008972580504	-5.28796811460433	12.67960767812637
H	-4.66864189234152	-5.94593755794972	12.17759977419266
H	-3.19734850993119	-5.01314056391091	11.91451019559039
C	-1.02900993703938	0.86381263916062	10.16263778573916
H	-0.49261361903896	1.73907293926397	10.51718002429919
C	-5.32434978938944	-3.18675672785609	12.06277884943991
H	-5.89581979360418	-2.36450096318151	12.50662778247481
H	-5.99598493773779	-3.80528425219108	11.46063577515742
C	-3.22698235212212	-6.06492971163159	13.80587716736175
H	-2.59632290669246	-5.36647519407376	14.38368748231905
H	-2.53511606919800	-6.79665531658013	13.35610586400166
C	-3.18975013440568	-2.54506852722616	8.95288205532487
C	-1.50425833942861	-0.80819331231357	8.46060870809862
C	-0.77197265832567	0.34507878933909	8.89044329608009
C	-1.97464512066366	0.28793446355932	11.02013844699113
H	-2.16100440935191	0.70960254213780	12.00508462990177
C	-3.44673501119271	-7.47046722712828	15.94286018018831
H	-4.15232858924814	-7.99047679772425	16.60769861408435
H	-2.70695289356147	-8.20821815551094	15.59556249146925
H	-2.91021094489709	-6.72196648665479	16.54621658104826
C	-3.67945886386475	-1.42798988667737	11.55772259399206

5. Detailed crystallographic data

Table S16. Detailed crystallographic data for PDI-C_6 at high pressure.

Pressure		0.1 MPa	0.50 GPa	0.73 GPa	1.05 GPa	1.41 GPa	1.74 GPa	1.95 GPa	2.05 GPa	2.41 GPa	2.74 GPa	3.43 GPa	4.61 GPa
Phase		I	I	I	I	IV	V	V	V	V	V	V	V
CCDC numbers		2412018	2412019	2412020	2412021	2412022	2412023	2412024	2412025	2412026	2412027	2412028	2412029
λ		0.49172	0.49173	0.71073	0.71073	0.49173	0.71073	0.49163	0.49173	0.71073	0.49173	0.49173	0.49172
Crystal system		triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group		*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
Unit cell dimensions	*a* (Å)	4.7723(1)	4.64520(10)	4.5971(3)	4.5494(4)	4.5308(1)	4.4771(8)	4.4643(1)	4.4549(1)	4.4179(4)	4.3785(1)	4.3382(2)	4.2926(1)
	b (Å)	8.5756(1)	8.5703(3)	8.5635(10)	8.5761(10)	16.9532(3)	8.5973(12)	8.6151(1)	8.6003(1)	8.5938(6)	8.5972(2)	8.5989(3)	8.5559(3)
	c (Å)	17.6181(2)	17.076(2)	16.880(6)	16.782(5)	17.887(1)	15.894(10)	15.8664(8)	15.8585(8)	15.738(6)	15.7128(8)	15.5271(14)	15.3181(19)
	α (°)	81.734(1)	80.961(6)	80.833(20)	80.612(16)	66.484(3)	90.70(4)	90.750(3)	90.799(2)	90.801(18)	90.904(4)	90.778(6)	90.875(6)
	β (°)	84.881(1)	85.933(4)	86.337(16)	86.817(15)	95.489(2)	92.11(4)	92.236(3)	92.222(2)	92.621(19)	92.733(4)	93.255(6)	93.694(4)
	γ (°)	83.010(1)	84.011(2)	84.247(7)	84.468(8)	96.287(1)	97.502(13)	97.490(1)	97.443(1)	97.410(7)	97.328(2)	97.299(3)	97.093(2)
Volume (Å^3)		706.342(19)	666.68(8)	651.9(3)	642.5(2)	1250.21(8)	606.0(4)	604.46(3)	601.91(3)	591.8(2)	585.83(4)	573.47(6)	556.97(7)
Z/Z'		1/0.5	1/0.5	1/0.5	1/0.5	2/1	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5
Calculated density (g/cm^3)		1.313	1.391	1.423	1.444	1.484	1.531	1.535	1.541	1.568	1.583	1.618	1.666
Absorption (mm^{-1})		0.045	0.047	0.093	0.094	0.051	0.100	0.052	0.052	0.102	0.054	0.055	0.057
F(000)		296.0	296.0	296.0	296.0	592.0	296.0	296.0	296.0	296.0	296.0	296.0	296.0
Crystal size (mm)		0.216 × 0.152 × 0.072	0.209 × 0.152 × 0.07	0.324 × 0.197 × 0.039	0.322 × 0.197 × 0.039	0.2 × 0.151 × 0.069	0.314 × 0.197 × 0.038	0.197 × 0.15 × 0.068	0.197 × 0.149 × 0.068	0.311 × 0.197 × 0.037	0.195 × 0.149 × 0.067	0.193 × 0.149 × 0.066	0.19 × 0.149 × 0.065
2θ-range for data collection (°)		3.24 to 50.542	6.11 to 50.946	8.922 to 52.466	9.01 to 52.938	6.27 to 50.598	9.19 to 52.812	3.298 to 48.87	3.724 to 48.732	9.316 to 51.252	3.726 to 48.974	3.738 to 48.796	6.632 to 48.148
Min/max indices: h, k, l		-4/7, -8/14, -26/25	-6/7, -12/12, -12/9	-5/5, -10/10, -6/6	-5/5, -10/10, -6/6	-7/6, -25/25, -11/14	-5/5, -10/10, -4/4	-6/6, -12/12, -8/8	-7/7, -14/14, -9/10	-5/5, -10/10, -4/4	-7/7, -14/14, -8/10	-7/7, -14/14, -9/10	-6/6, -11/12, -8/10
Reflect. Collected/unique		2943/2560	6772/1306	1850/410	5266/555	13675/2491	2964/526	3501/1202	6537/1204	4347/490	5996/1158	6044/1144	5719/1082
Data/restrains/parameters		2560/0/191	1306/0/191	410/374/179	555/531/191	2491/0/381	526/374/191	1202/0/192	1204/6/191	490/276/191	1158/0/191	1144/0/191	1082/0/191
Goodness-of-fit on F2		1.711	1.069	1.134	1.134	1.064	1.134	1.068	1.125	1.105	1.097	1.112	1.07
Final R1/wR2 (I>2σ1)		0.1202/0.3750	0.0577/0.1754	0.0569/0.0808	0.0735/0.1495	0.0610/0.1714	0.0799/0.1663	0.0493/0.1462	0.0398/0.1291	0.0730/0.1953	0.0444/0.1393	0.0397/0.1275	0.0578/0.1709
R1/wR2 (all data)		0.1246/0.3800	0.0607/0.1832	0.1640/0.1241	0.1384/0.1936	0.0651/0.1786	0.1663/0.2181	0.0535/0.1520	0.0417/0.1318	0.1337/0.2615	0.0480/0.1445	0.0448/0.1364	0.0676/0.1854
Largest diff. peak/hole (e.Å^{-3})		0.37/-0.28	0.17/-0.15	0.09/-0.09	0.12/-0.13	0.23/-0.26	0.16/-0.16	0.19/-0.20	0.11/-0.12	0.13/-0.15	0.12/-0.14	0.10/-0.09	0.18/-0.12

Table S17. Detailed crystallographic data for PDI-C_6 at various temperatures.

Temperature (K)		100	298	440	470
Phase		I	I	I	II
CCDC numbers		2421994	2422224	2412030	2421130
Method		SC-XRD	SC-XRD	SC-XRD	SC-XRD
λ		0.71073	0.71073	1.54184	1.54184
Crystal system		triclinic	triclinic	triclinic	triclinic
Space group		*P-1*	*P*-1	*P*-1	*P*-1
Unit cell dimensions	*a* (Å)	4.7056(19)	4.7568(10)	4.8395(10)	11.443(7)
	b (Å)	8.514(3)	8.5487(16)	8.5365(13)	11.988(8)
	c (Å)	17.281(5)	17.576(2)	18.158(3)	19.506(9)
	α (°)	81.34(3)	81.678(14)	84.478(12)	96.05(5)
	β (°)	85.64(3)	84.850(15)	83.426(15)	73.16(5)
	γ (°)	83.89(3)	83.169(16)	81.495(16)	114.90(6)
Volume (Å^3)		679.3(4)	700.3(2)	734.6(2)	2323(3)
Z/Z′		1/0.5	1/0.5	1/0.5	3/1.5
Calculated density (g/cm^3)		1.366	1.325	1.263	1.198
Absorption (mm^{-1})		0.089	0.086	0.656	0.623
F(000)		296.0	296.0	296.0	888.0
Crystal size (mm)		0.618x0.065x0.021	0.621 × 0.066 × 0.023	0.315x0.098x0.047	0.319x0.099x0.050
2θ-range for data collection (°)		7.17 to 58.72	7.048 to 59.036	9.838 to 146.182	8.132 to 76.258
Min/max indices: h, k, l		-6/ 6, -11/ 11, -22/23	-5/ 6, -10/11, -23/16	-5/5, -8/10, -22/19	-9/8, -9/8, -15/15
Reflect. Collected/unique		4984/3054	5401/3166	4371/2807	4375/2037
Data/restrains/parameters		3054/0/191	3166/0/191	2807/78/191	2037/1117/220
Goodness-of-fit on F2		0.970	0.914	0.952	1.059
Final R1/wR2 (I>2σ1)		0.0853/0.1549	0.0724/0.1256	0.0797/0.2516	0.1768/0.3850
R1/wR2 (all data)		0.2527/0.2334	0.2545/0.1986	0.1250/0.3256	0.4206/0.5407
Largest diff. peak/hole (e.Å^{-3})		0.37/-0.36	0.15/-0.23	0.17/-0.25	0.23/-0.26

6. Literature

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