Supporting Information

The odd-even alkyl chain effect on the structure and optoelectronic properties of alkyl-substituted perylene diimide (PDI) derivatives at highly strained environments

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1. Experimental methods

1.1. Crystallization

PDI-C_n (n = 5-8) were purchased from Aldrich and used without additional purification. Single crystals of PDI-C_n were obtained using a solvothermal reactor. The process involved preparing a supersaturated solution which was heated overnight and then gradually cooled to room temperature. Toluene, p-xylene, $CHCl_3$, and CH_2Cl_2 were used as solvents. The solutions were heated up to 453 K in the case of toluene and p-xylene, while $CHCl_3$ and CH_2Cl_2 were heated up to 373 K.

1.2. High-pressure single-crystal X-ray diffraction

All high-pressure experiments were conducted using a modified Merrill-Bassett diamond anvil cell (DAC) with diamond anvils supported on steel discs. The diamond culets were 0.8 mm in diameter. The gasket was made of 0.3 mm thick tungsten foil with sparked-eroded holes ranging from 0.4 to 0.5 mm in diameter. To calibrate the pressure, the ruby fluorescence method was used.[1,2] Daphne Oil 7575 was used as the pressure-transmitting medium.[3,4] Single-crystal X-ray diffraction measurements were conducted on a 4-circle diffractometer equipped with a CCD detector and MoKα X-ray source (λ = 0.71073 Å). The DAC chamber was centered using the gasket-shadowing method.[5] Data was collected and processed using CrysAlisPro software (version 1.171.40.79a). The crystal structures were initially solved using direct methods through SHELXS or intrinsic phasing methods through SHELXT and subsequently refined using SHELXL within the Olex2 suite.[6,7] All crystal structures were analyzed and compared using the software Mercury.[8]

Table S1. Selected crystallographic data of PDI-C_5, -C_6, -C_7, and -C_8 (cf. Tables S27-S30 for details).

PDI	Phase	*P* [GPa]	*a* (Å)	*b* (Å)	*c* (Å)	*α* (°)	*β* (°)	*γ* (°)	V (Å^3)	Z/Z'
PDI-C_5	I	0.0001	4.727(3)	8.493(3)	16.308(9)	86.78(8)	83.27(10)	84.12(4)	646.1(6)	1/0.5
PDI-C_5	IV	2.17	3.7606(6)	8.5729(5)	18.044(6)	87.221(17)	74.48(3)	101.631(8)	545.8(2)	1/0.5
PDI-C_6	I	0. 0001	4.7723(1)	8.5756(1)	17.6181(2)	81.734(1)	84.881(1)	83.010(1)	706.342(19)	1/0.5
PDI-C_6	IV	1.41	4.5308(1)	16.9532(3)	17.887(1)	66.484(3)	95.489(2)	96.287(1)	1250.21(8)	2/1
PDI-C_6	V	1.95	4.4643(1)	8.6151(1)	15.8664(8)	90.750(3)	92.236(3)	97.490(1)	604.46(3)	1/0.5
PDI-C_7	I	0.0001	4.8301(2)	8.3661(4)	19.3233(7)	79.542(4)	88.704(3)	81.683(4)	759.79(6)	1/0.5
PDI-C_7	IV	0.95	4.64199(18)	8.2981(3)	18.553(3)	78.624(7)	87.207(6)	83.704(3)	696.12(12)	1/0.5
PDI-C_8	I	0.0001	4.7686(3)	8.5193(4)	20.2896(10)	85.291(4)	89.680(4)	82.293(4)	814.05(8)	1/0.5
PDI-C_8	III	1.16	4.4866(3)	8.4612(5)	19.429(2)	80.771(10)	87.690(10)	84.078(5)	723.92(10)	1/0.5
PDI-C_8	IV	1.50	4.51620(10)	16.9424(5)	19.020(2)	76.517(5)	89.121(5)	83.351(2)	1405.59(16)	2/1

1.3. Synchrotron X-ray diffraction measurements

X-ray diffraction measurements were performed at the Materials Science beamline of the Swiss Light Source[9] using synchrotron radiation of approximately 0.4920 Å, focused and collimated to 150 μm (exact wavelengths were placed in Tables S26-29). Diffraction data were collected for single crystals of the PDI-C_n systems placed in a DAC in a steel gasket (thickness ~90 μm and a hole diameter 250 μm). A ruby fluorescent method was used to determine pressure inside a DAC. Daphne Oil 7575 was used as a pressure-transmitting medium.

1.4. Single-crystal X-ray diffraction at various temperatures

Single-crystal X-ray diffraction measurements for PDI-C_7 were performed using a Bruker D8 QUEST diffractometers equipped with CuKα (λ = 1.54178 Å) and MoKα (λ = 0.71073 Å) X-ray sources. Data were collected over a temperature range of 100 to 375 K. Data collection and processing were carried out using the APEX5 software (version 2023.9-2). The crystal structures were initially solved using intrinsic phasing methods through SHELXT and subsequently refined using SHELXL within the Olex2 suite.

1.5. High-pressure UV-Vis spectroscopy

UV-Vis absorption spectra measurements were carried out using a DAC equipped with low-fluorescence synthetic AII diamond anvils. The gasket was made of 0.2 mm thick tungsten foil with a sparked-eroded hole 0.4-0.5 mm in diameter. To minimize light diffusion from the sample, a thin film of the investigated sample was prepared directly on the diamond culet by pressing a small amount of the sample with a thick glass plate until a uniform layer was formed. The UV-vis absorption spectra were recorded on the Jasco V-770 spectrophotometer adapted for using the DAC. The absorbance was measured at a scan speed of 200 nm min^{-1} in the 1200 - 350 nm range.

1.6. High-pressure PL spectroscopy

Photoluminescence emission spectra measurements were carried out using DAC with synthetic diamond (IIas). The gasket was made of 0.2 mm thick steel foil with a sparked-eroded pressure chamber (hole) 0.12 mm in diameter. Materials were ground and loaded with a needle into the pressure chamber. Daphne Oil 7575 was used as a pressure-transmitting medium. Emission spectra were recorded using an Andor spectrometer with an iDus CCD camera as a detector and a 450 nm diode as an excitation source.

2. Previous crystallographic investigations of PDI-C_n

The structure of PDI-C_5 was originally characterized at room temperature by Hädicke and Graser,[10] later its thermal expansion behavior and high-temperature polymorphs were investigated by Maini et al.[11] Madhu et al. determined the crystal structures of PDI-C_6 and PDI-C_8, together with their absorption and fluorescence properties over the 353-523 K range.[12] The high-pressure and variable-temperature phase transition of PDI-C_6 was subsequently investigated by us.[13] The crystal structure of PDI-C_8 was first described by Xia et al. at 130 K,[14] followed by Okamoto et al. at 298 K.[15] Troshin et al. conducted a systematic study on the PDI-Cn series (n = 4-12), focusing on the influence of side-chain length and thermal annealing on the electrical performance of organic field-effect transistors (OFETs) which highlighted the presence of polymorphic phases at high temperature for the compounds.[16]

3. High-pressure single-crystal X-ray diffraction

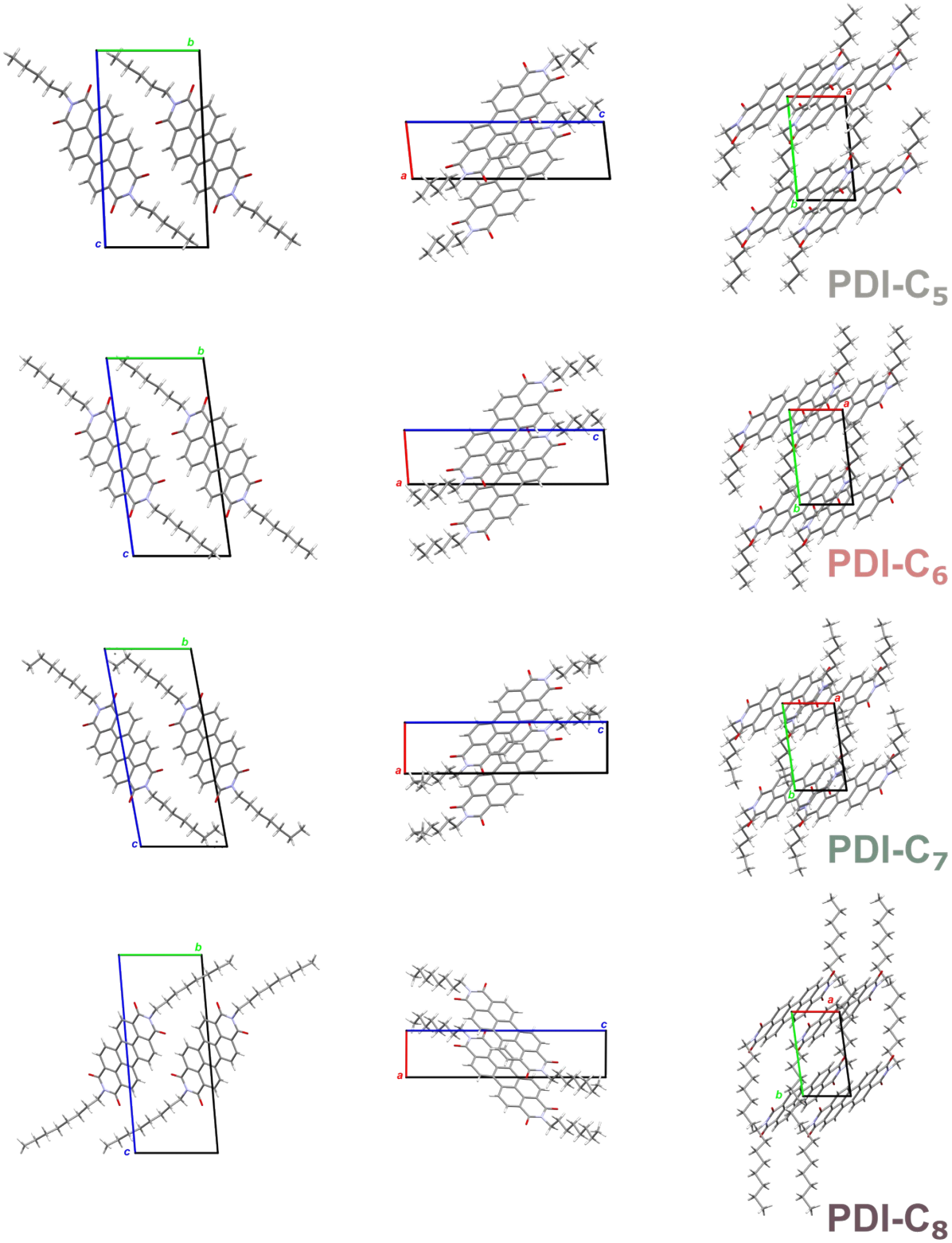
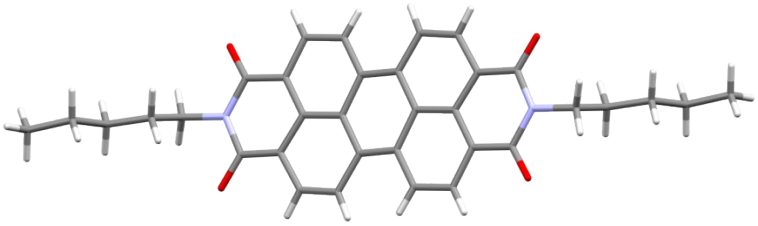


Figure S1. Arrangements of PDI-C_5, -C_6, -C_7, and -C_8 molecules in the unit-cell along directions [100], [010], [001], at 0.1 MPa. For PDI-C_7, the dominant conformation, with an occupancy of 0.596(14), is shown.

PDI-C_5 - phase I (0.1 MPa)



PDI-C_5 - phase IV (2.17 GPa)

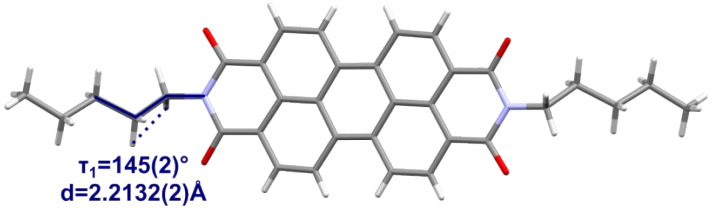
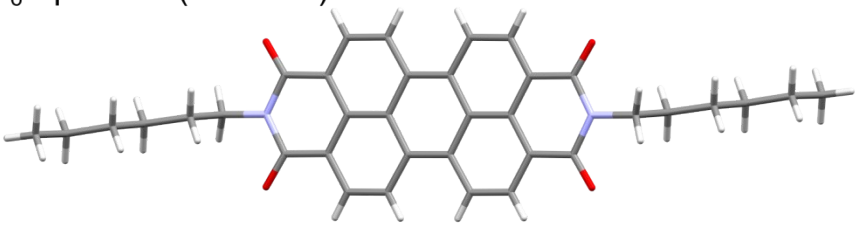
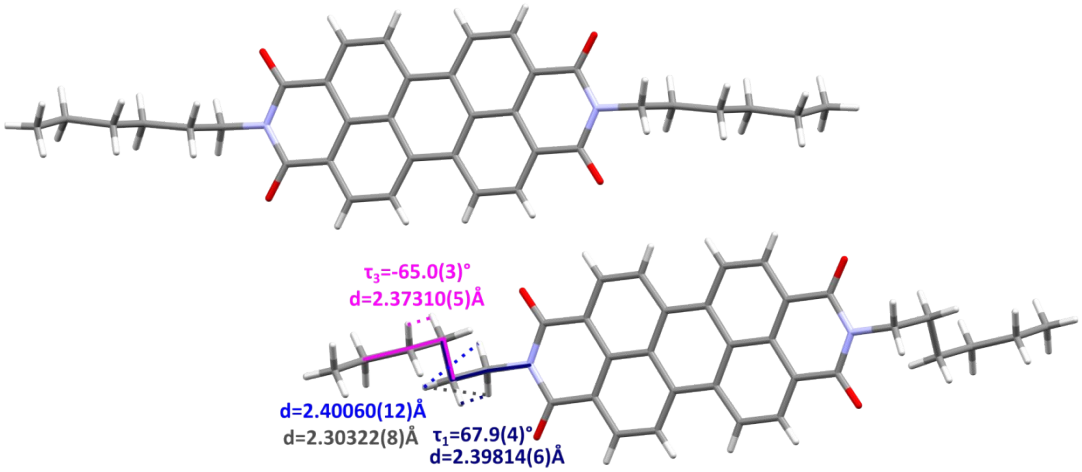


Figure S2. Conformational changes of alkyl chains in PDI-C_5 structure between phases I and IV.

PDI-C_6 - phase I (0.1 MPa)



PDI-C_6 - phase IV (1.41 GPa)



PDI-C_6 - phase V (1.74 GPa)

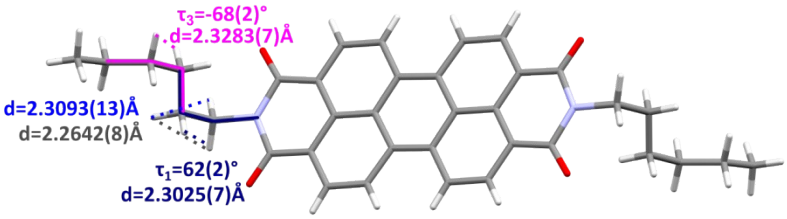


Figure S3. Conformational changes of alkyl chains in PDI-C_6 structure between phases I, IV and V.

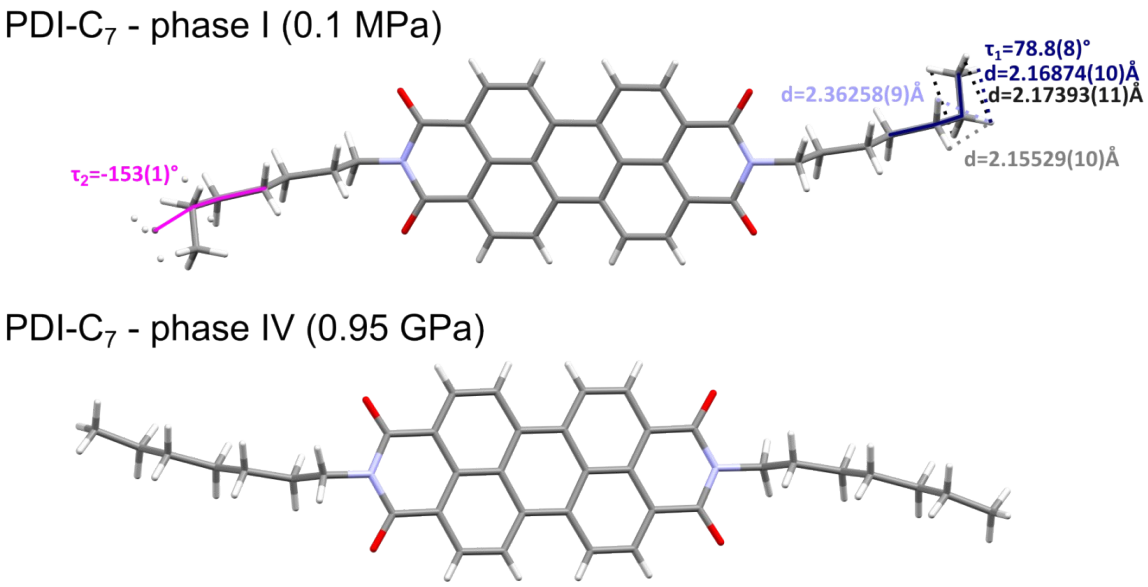


Figure S4. Conformational changes of alkyl chains in PDI-C_7 structure between phases I and IV. In phase I, the dominant conformation, with an occupancy of 0.596(14), is shown.

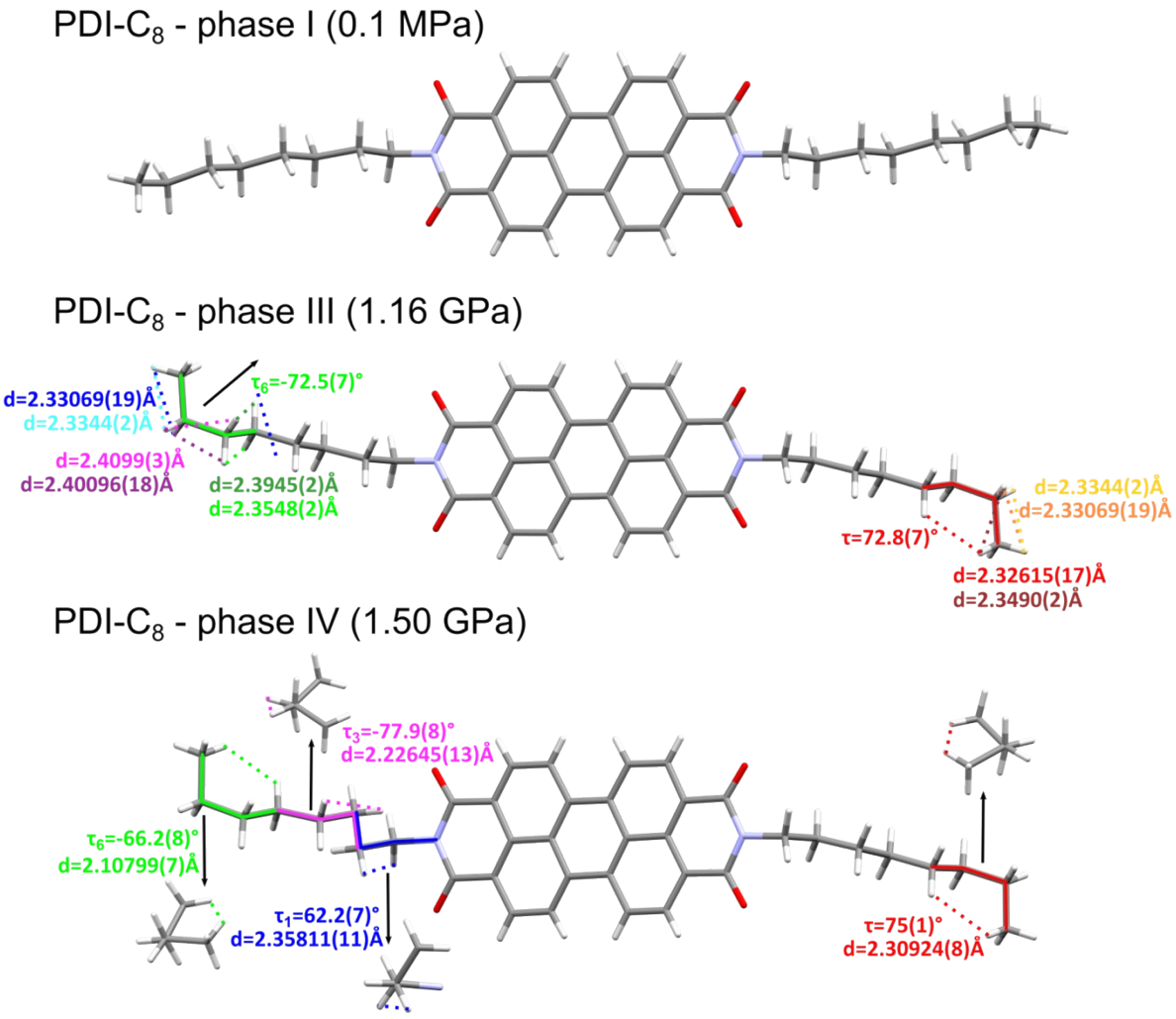


Figure S5. Conformational changes of alkyl chains in PDI-C_8 structure between phases I, III and IV.

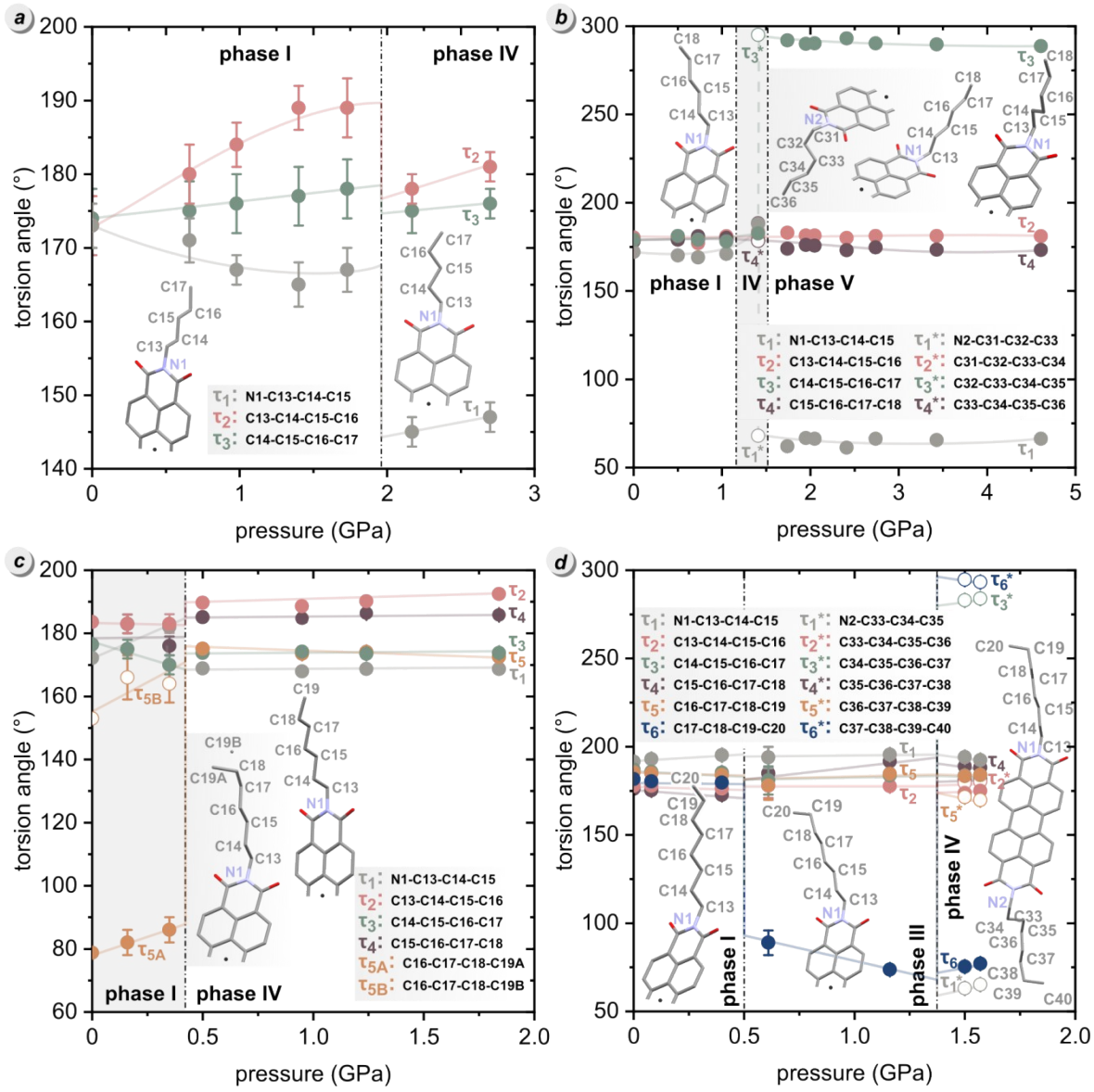


Figure S6. Torsion angles in alkyl substituents as a function of pressure for PDI-C_5 (a), PDI-C_6 (b), PDI-C_7 (c), and PDI-C_8 (d). Insets show the asymmetric parts of molecules with labeled alkyl atoms. Legends indicate the color code of torsion angles. Asterisks mark the corresponding torsion angles in independent molecules of PDI-C_6 phase IV and molecular fragments of PDI-C_8 phase IV, plotted with unfilled symbols. Hydrogen atoms are omitted for clarity.

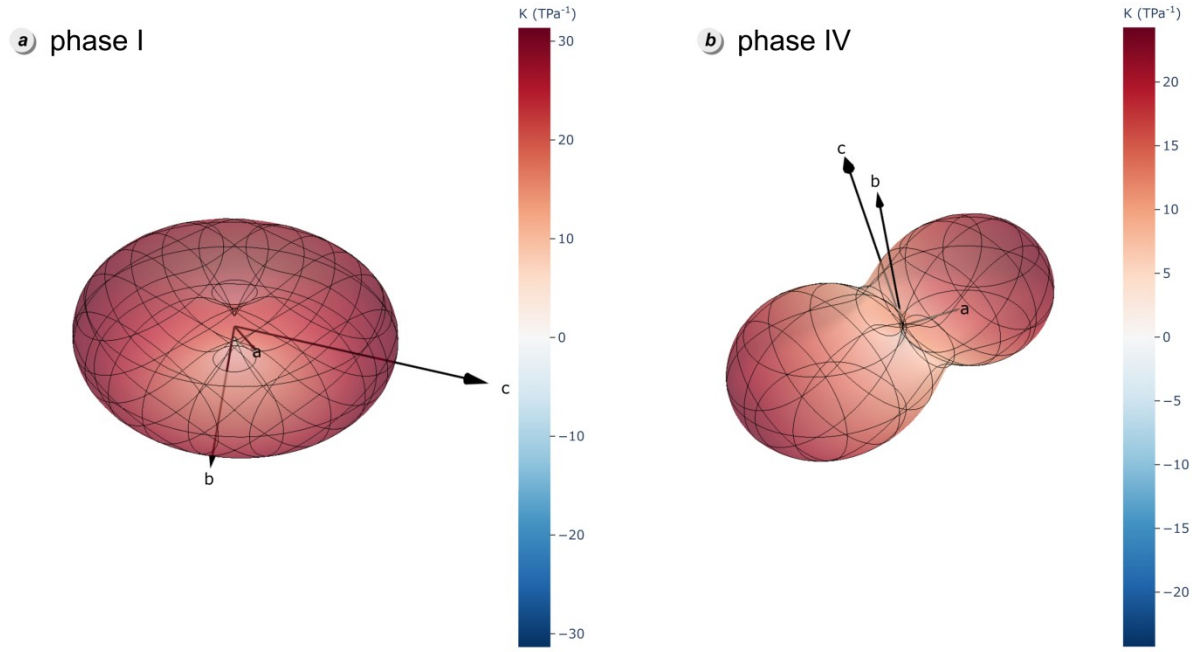


Figure S7. Graphical representations of the compressibility tensors for the PDI-C_5 crystal, calculated using PASCal program,[17] are shown for pressure ranges of 0.1 MPa – 1.73 GPa (a), and 2.17 – 3.84 GPa (b).

Table S2. Compressibility related to crystallographic axes calculated for PDI-C_5 phase I in the range of 0.1 MPa – 1.73 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	30.3775	6.2521	0.8509	0.3838	-0.3586	32.022	-32.0339	-0.8023	0.0017
X2	31.3459	9.9584	0.9724	0.0698	0.2226	16.3627	-16.0567	-5.0825	0.0116
X3	2.4844	2.6245	-0.6589	0.7436	0.1141	0.0002	-0.0014	0.0001	1.7891
V	66.7194	3.4072							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	*B'*	σ*B'*	P_c (GPa)
2nd	10.9546	0.802	645.9398	3.6023	4.0	n/a	0.0
3rd	9.845	3.0585	647.039	5.698	5.6375	4.5796	0.0

Table S3. Compressibility related to crystallographic axes calculated for PDI-C_5 phase IV in the range of 2.17 GPa – 3.84 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	24.2751	nan	0.9976	-0.0087	0.0684	0.0057	-0.0175	1.7198	1.4014
X2	8.7494	nan	0.9346	0.1035	-0.3403	0.003	-0.009	1.8529	0.9621
X3	-0.0158	nan	0.3619	0.9321	0.0145	-0.0005	0.0001	2.17	7.0196
V	32.9256	0.1524							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	B'	$\sigma B'$	P_c (GPa)
2nd	18.0059	1.1587	603.127	3.9884	4.0	n/a	0.0
3rd	33.8221	inf	582.809	inf	-0.2732	inf	0.0

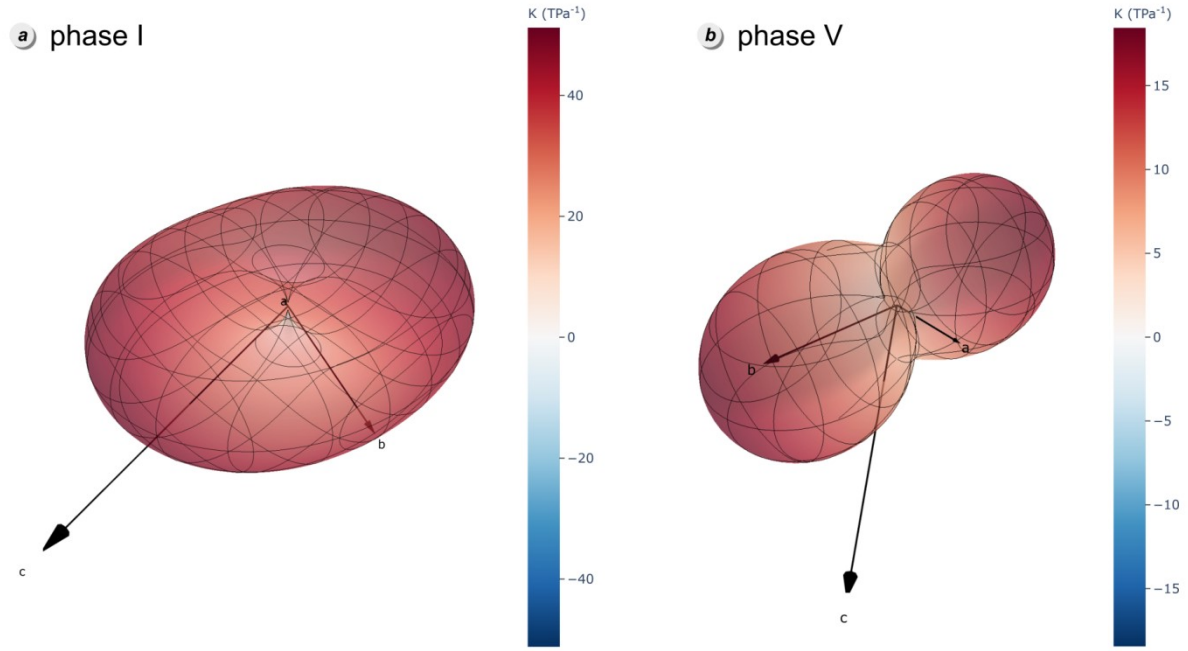


Figure S8. Graphical representations of the compressibility tensors for the PDI-C_7 crystal, calculated using PASCal program,[17] are shown for pressure ranges of 0.1 MPa – 0.35 GPa (a), and 0.5 – 1.84 GPa.

Table S4. Compressibility related to crystallographic axes calculated for PDI-C_7 phase I in the range of 0.1 MPa – 0.35 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	51.2043	nan	0.9318	-0.1624	0.3245	0.0007	-0.043	0.0001	0.3868
X2	43.1165	nan	0.6446	0.7517	-0.1398	0.0014	-0.0346	-0.0016	0.5038
X3	1.072	nan	0.8987	-0.4119	-0.1505	0.0871	-0.0907	0.0001	0.0019
V	133.8899	21.0553							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	B'	$\sigma B'$	P_c (GPa)
2nd	5.9038	2.3752	757.7948	10.0293	4.0	n/a	0.0
3rd	5.5415	inf	743.1666	inf	95.1813	inf	0.0

Table S5. Compressibility related to crystallographic axes calculated for PDI-C_7 phase IV in the range of 0.5 GPa – 1.84 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	18.4465	nan	-0.0336	0.9978	0.058	-0.0001	-0.0194	0.5	0.8306
X2	1.5543	nan	0.9978	-0.0641	0.0156	-0.0015	-0.0	-20.6877	111.5753
X3	6.0557	nan	-0.2751	-0.5482	0.7898	9.4535	-9.4594	0.3091	0.0004
V	43.3275	1.9607							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	*B'*	σ*B'*	P_c (GPa)
2nd	17.1253	2.6835	727.1499	6.4887	4.0	n/a	0.0
3rd	22.8565	21.8572	721.9266	17.5531	-0.2772	14.0714	0.0

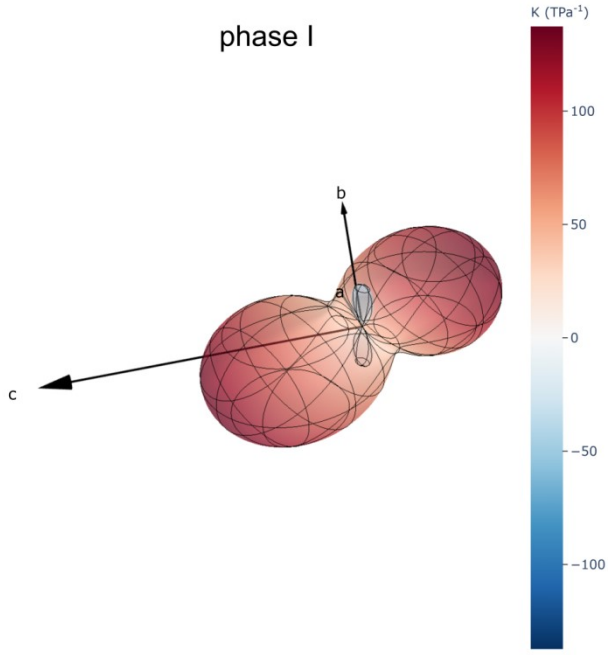


Figure S9. Graphical representation of the compressibility tensors for the PDI-C_8 crystal, calculated using PASCal program,[17] is shown for pressure range of 0.1 MPa – 0.40 GPa.

Table S6. Compressibility related to crystallographic axes calculated for PDI-C_8 phase I in the range of 0.1 MPa – 0.40 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	137.3201	nan	0.9069	0.024	-0.4206	0.0224	-0.1495	-0.2287	1.2863
X2	38.8085	nan	0.9923	0.0368	0.1183	0.0214	-0.0399	-0.5163	0.9453
X3	-37.5947	nan	-0.3271	0.9443	-0.0351	-0.0	0.0473	-0.0002	1.1445
V	145.6976	0.6478							

Birch-Murnaghan Coefficients

	B_0 (GPa)	σB_0 (GPa)	V_0 (Å^3)	σV_0 (Å^3)	*B'*	σ*B'*	P_c (GPa)
2nd	5.8346	0.2135	814.937	1.0813	4.0	n/a	0.0
3rd	7.3319	inf	814.0636	inf	-2.252	inf	0.0

Table S7. Pitch and roll angles and distances for PDI-C_5.[18]

Pressure (GPa)	$d_{\pi\text{-}\pi}$ (Å)	α_P (°)	β_R (°)	P (°)	R (°)	d_P (Å)	d_R (Å)	d_{tot} (Å)	z (Å)
0.0001	3.360(8)	48.0(3)	67.9(4)	42.0(3)	22.1(4)	3.03	1.36	3.32	4.72
0.66	3.282(8)	47.8(4)	68.4(4)	42.2(4)	21.6(4)	2.98	1.30	3.25	4.62
0.98	3.227(8)	47.2(3)	68.8(4)	42.8(3)	21.2(4)	2.99	1.25	3.24	4.57
1.40	3.202(8)	47.3(3)	69.4(4)	42.7(3)	20.6(4)	2.95	1.20	3.18	4.52
1.73	3.174(9)	47.6(4)	69.0(4)	42.4(4)	21.0(4)	2.90	1.22	3.15	4.47
2.17	3.217(8)	73.6(8)	62.0(3)	16.4(8)	28.0(3)	0.95	1.71	1.96	3.77
2.70	3.191(8)	73.0(7)	62.5(3)	17.0(7)	27.5(3)	0.98	1.66	1.93	3.73
3.84	3.128(13)	74.2(9)	62.0(6)	15.8(9)	28.0(6)	0.89	1.66	1.88	3.66

Table S8. Pitch and roll angles and distances for PDI-C_7.

Pressure (GPa)	$d_{\pi\text{-}\pi}$ (Å)	α_P (°)	β_R (°)	P (°)	R (°)	d_P (Å)	d_R (Å)	d_{tot} (Å)	z (Å)
0.0001	3.3704(9)	46.58(3)	68.59(4)	43.42(3)	21.41(4)	3.19	1.32	3.45	4.82
0.16	3.319(10)	45.8(4)	68.0(3)	44.2(4)	22.0(3)	3.23	1.34	3.50	4.82
0.35	3.297(8)	46.6(4)	68.8(3)	43.4(4)	21.2(3)	3.12	1.28	3.37	4.72
0.50	3.281(3)	46.71(13)	69.92(19)	43.29(13)	20.08(19)	3.09	1.20	3.31	4.66
0.95	3.2590(14)	46.86(7)	69.86(10)	43.24(7)	20.67(10)	3.06	1.23	3.30	4.64
1.24	3.2212(16)	46.26(7)	69.53(12)	43.74(7)	20.47(12)	3.08	1.20	3.31	4.62
1.84	3.1830(14)	46.34(7)	69.60(11)	43.66(7)	20.40(11)	3.04	1.18	3.26	4.56

Table S9. Pitch and roll angles and distances for PDI-C_8.

Pressure (GPa)	$d_{\pi\text{-}\pi}$ (Å)	α_P (°)	β_R (°)	P (°)	R (°)	d_P (Å)	d_R (Å)	d_{tot} (Å)	z (Å)
0.0001	3.3797(8)	47.30(3)	69.62(4)	42.70(3)	20.38(4)	3.12	1.26	3.36	4.77
0.08	3.3703(15)	47.44(8)	69.86(8)	42.56(8)	20.14(8)	3.09	1.24	3.33	4.74
0.40	3.3402(12)	47.99(6)	72.83(8)	42.01(6)	17.17(8)	3.01	1.03	3.18	4.61
0.61	3.293(12)	47.8(4)	70.0(7)	42.2(4)	20.0(7)	2.99	1.20	3.22	4.61
1.16	3.2395(10)	48.35(5)	71.38(7)	41.65(5)	18.62(7)	2.88	1.09	3.08	3.57
1.50	3.222(2)	47.00(13)	73.34(11)	43.00(13)	16.66(11)	3.00	0.96	3.15	4.51
1.57	3.2129(17)	46.83(9)	73.28(9)	43.17(9)	16.72(9)	3.01	0.97	3.16	4.51

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: $d_R = \mathrm{d}_{\pi-\pi}\,\mathrm{tg}\,R$

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:

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

$P = 90° - \alpha_P$

$R = 90° - \beta_R$

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

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

4. PDI-C_7 at various temperatures

4.1. Single-crystal X-ray diffraction

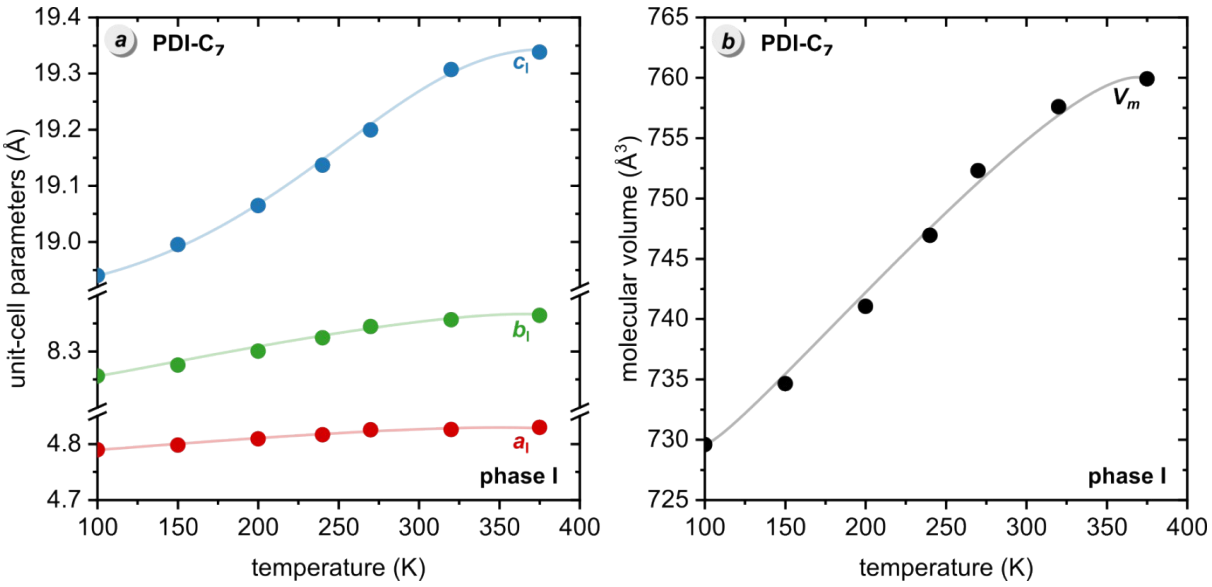


Figure S10. Temperature dependence of the unit-cell dimensions *a*, *b*, *c* (a) and its molecular volume (*b*) for PDI-C_7. The estimated standard deviations (ESDs) are smaller than the plotted symbols.

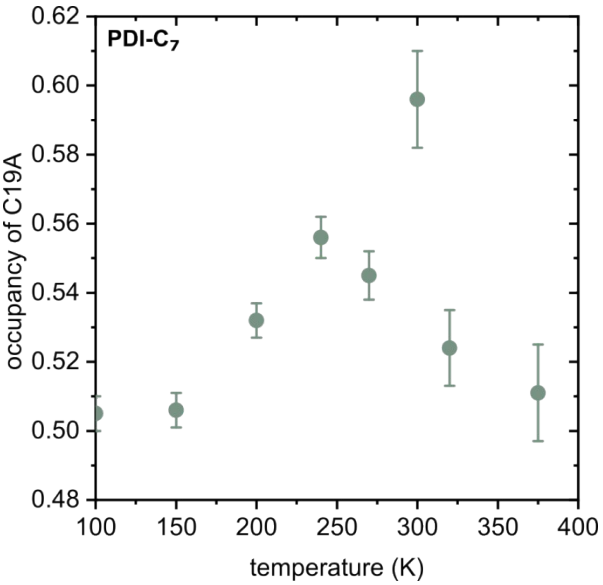


Figure S11. Temperature dependence of the occupancy of C19A atom for PDI-C_7.

4.2. Hot-stage microscopy (HSM)

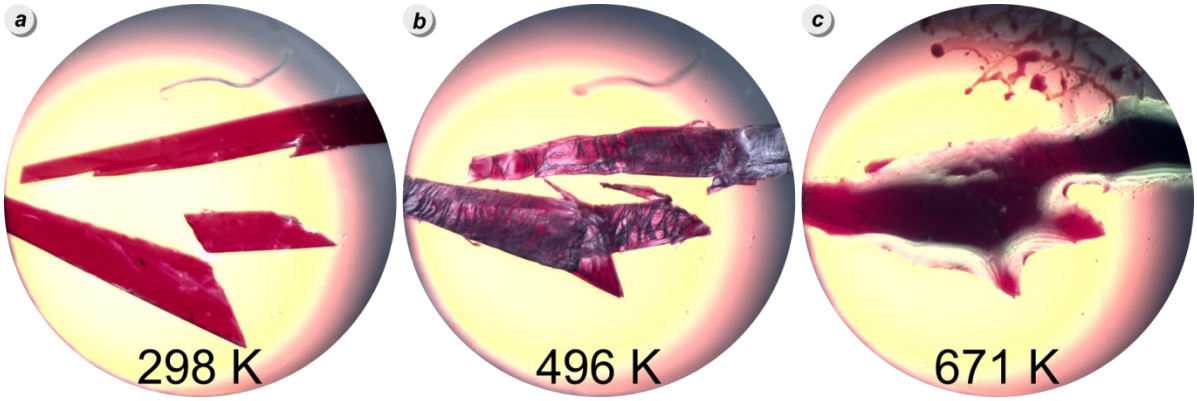


Figure S12. Hot stage microscopy images of PDI-C_7 crystals during the heating cycle: (a) phase I at 298 K, (b) after transition from phase I to phase II at 496 K, and (c) after melting at 671 K.

5. High-pressure optical absorption

In the solid state, the shape of UV-Vis absorption spectra is governed not only by intrinsic molecular electronic transitions but also by intermolecular interactions, excitonic coupling, polymorphism, and sample morphology, all of which can significantly affect band shape, bandwidth, and vibronic structure.[19] As demonstrated by our single-crystal X-ray diffraction data, the PDI-Cn derivatives adopt different crystal packings and undergo pressure-induced structural rearrangements and phase transitions. These structural differences directly modulate the relative π–π overlap, slip (*pitch* and *roll*) angles, and intermolecular distances, thereby altering the balance between H- and J-aggregate contributions and leading to variations in spectral shape and vibronic progression.[20–23] In addition, under high-pressure conditions the spectra may reflect contributions from multiple structural domains, particularly in the vicinity of phase transitions, resulting in broader or asymmetric absorption features. Experimental factors inherent to solid-state high-pressure UV-Vis measurements, such as scattering effects and variations in effective optical path length within the diamond anvil cell, may additionally influence the apparent spectral shape but do not affect the reproducible pressure-dependent trends of bathochromic shift discussed in the manuscript.

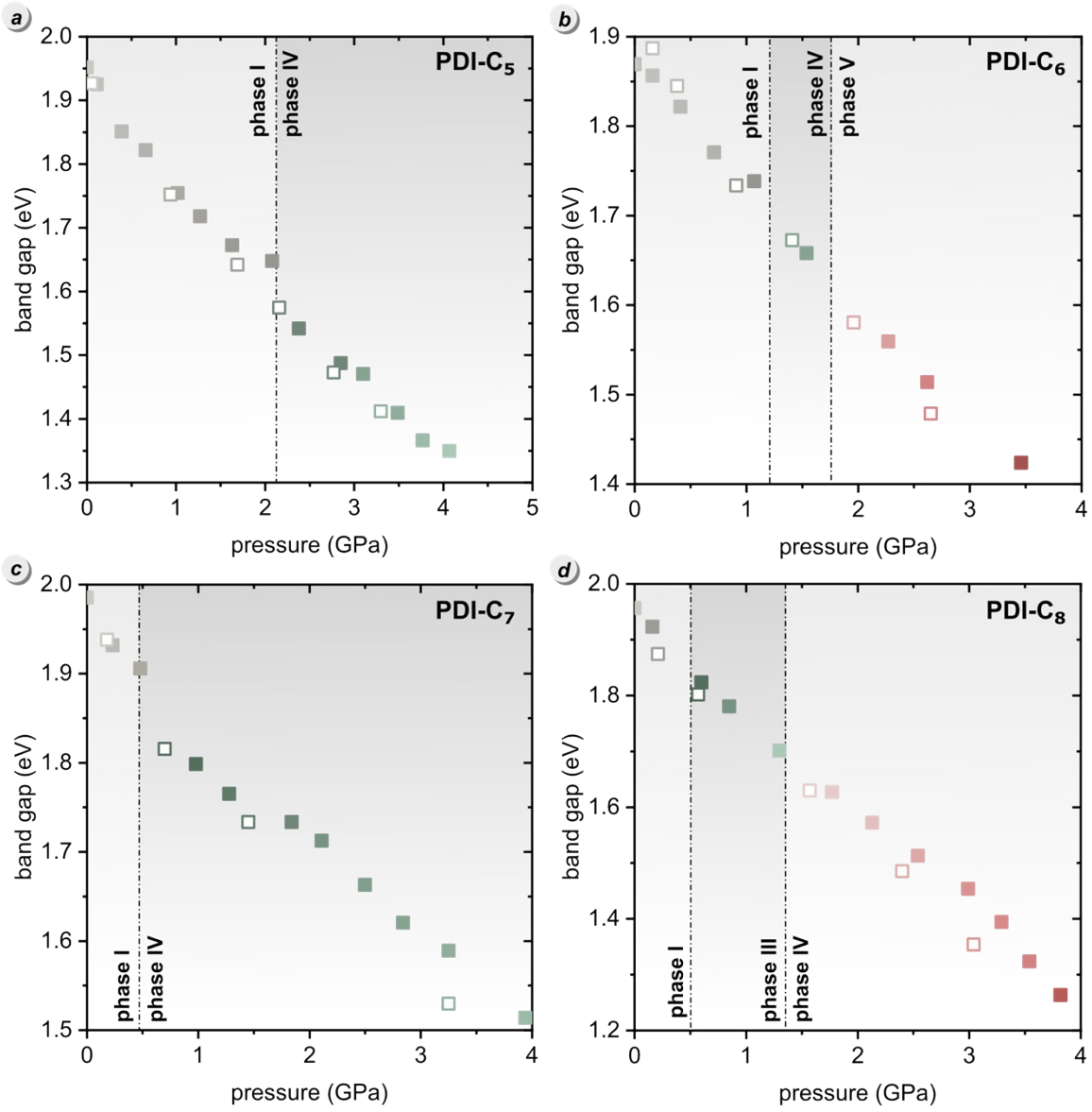


Figure S13. Pressure dependence of band-gap energy E_g for PDI-C_5 (a), -C_6 (b), -C_7 (c), and -C_8 (d).

Table S10. Variation of the absorption edge of PDI-C_5 with increasing and releasing pressure.

INCREASING PRESSURE			RELEASING PRESSURE		
Pressure (GPa)	Absorption edge (nm)	Band gap (eV)	Pressure (GPa)	Absorption edge (nm)	Band gap (eV)
0.0001	636	1.95	4.07	919	1.35
0.11	644	1.93	3.3	879	1.41
0.39	670	1.85	2.77	842	1.47
0.66	681	1.82	2.16	788	1.57
1.02	707	1.75	1.69	756	1.64
1.27	722	1.72	0.95	708	1.75
1.63	742	1.67	0.05	644	1.93
2.08	753	1.65			
2.38	805	1.54			
2.85	834	1.49			
3.1	844	1.47			
3.49	880	1.41			
3.77	908	1.37			
4.07	919	1.35			

Table S11. Variation of the absorption edge of PDI-C_6 with increasing and releasing pressure.

INCREASING PRESSURE			RELEASING PRESSURE		
Pressure (GPa)	Absorption edge (nm)	Band gap (eV)	Pressure (GPa)	Absorption edge (nm)	Band gap (eV)
0.0001	664	1.87	3.46	871	1.42
0.16	668	1.86	2.65	839	1.48
0.41	681	1.82	1.96	785	1.58
0.71	701	1.77	1.41	742	1.67
1.07	714	1.74	0.91	716	1.73
1.54	748	1.66	0.38	673	1.84
2.27	796	1.56	0.16	657	1.89
2.62	819	1.51			
3.46	871	1.42			

Table S12. Variation of the absorption edge of PDI-C_7 with increasing and releasing pressure.

INCREASING PRESSURE			RELEASING PRESSURE		
Pressure (GPa)	Absorption edge (nm)	Band gap (eV)	Pressure (GPa)	Absorption edge (nm)	Band gap (eV)
0.0001	625	1.99	3.94	819	1.51
0.23	642	1.93	3.25	811	1.53
0.48	651	1.91	1.45	716	1.73
0.98	690	1.80	0.7	683	1.82
1.28	703	1.77	0.18	640	1.94
1.84	716	1.73			
2.11	724	1.71			
2.5	746	1.66			
2.84	766	1.62			
3.25	781	1.59			
3.94	819	1.51			

Table S13. Variation of the absorption edge of PDI-C_8 with increasing and releasing pressure.

INCREASING PRESSURE			RELEASING PRESSURE		
Pressure (GPa)	Absorption edge (nm)	Band gap (eV)	Pressure (GPa)	Absorption edge (nm)	Band gap (eV)
0.0001	634	1.96	3.82	982	1.26
0.16	645	1.92	3.04	916	1.35
0.6	680	1.82	2.4	835	1.48
0.85	697	1.78	1.57	761	1.63
1.3	729	1.70	0.57	688	1.80
1.77	762	1.63	0.21	662	1.87
2.13	789	1.57			
2.54	820	1.51			
2.99	854	1.45			
3.29	890	1.39			
3.54	937	1.32			
3.82	982	1.26			

6. High-pressure photoluminescence

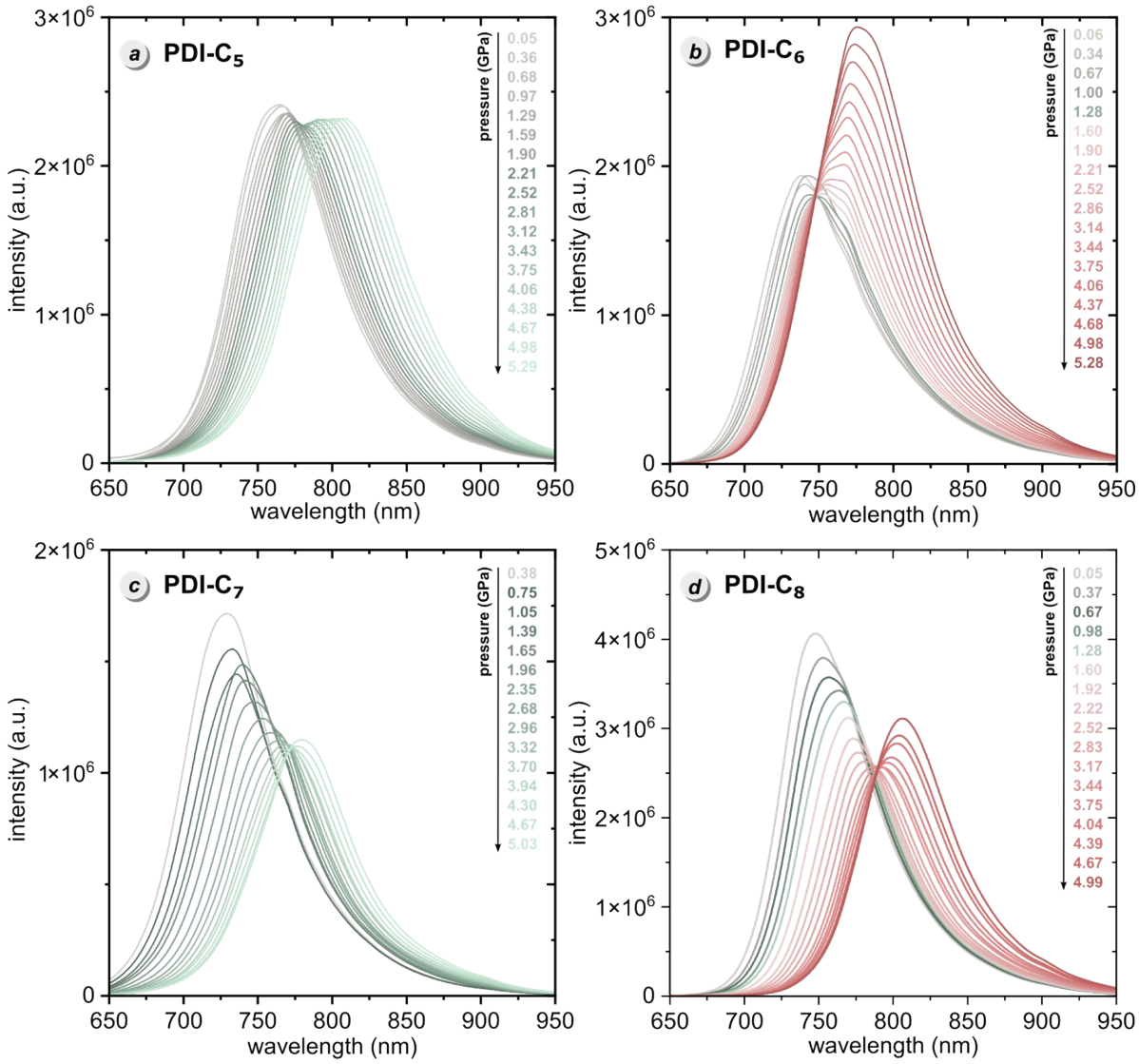


Figure S14. Emission spectra of PDI-C_5 (a), -C_6 (b), -C_7 (c), and -C_8 (d) in the compression cycles.

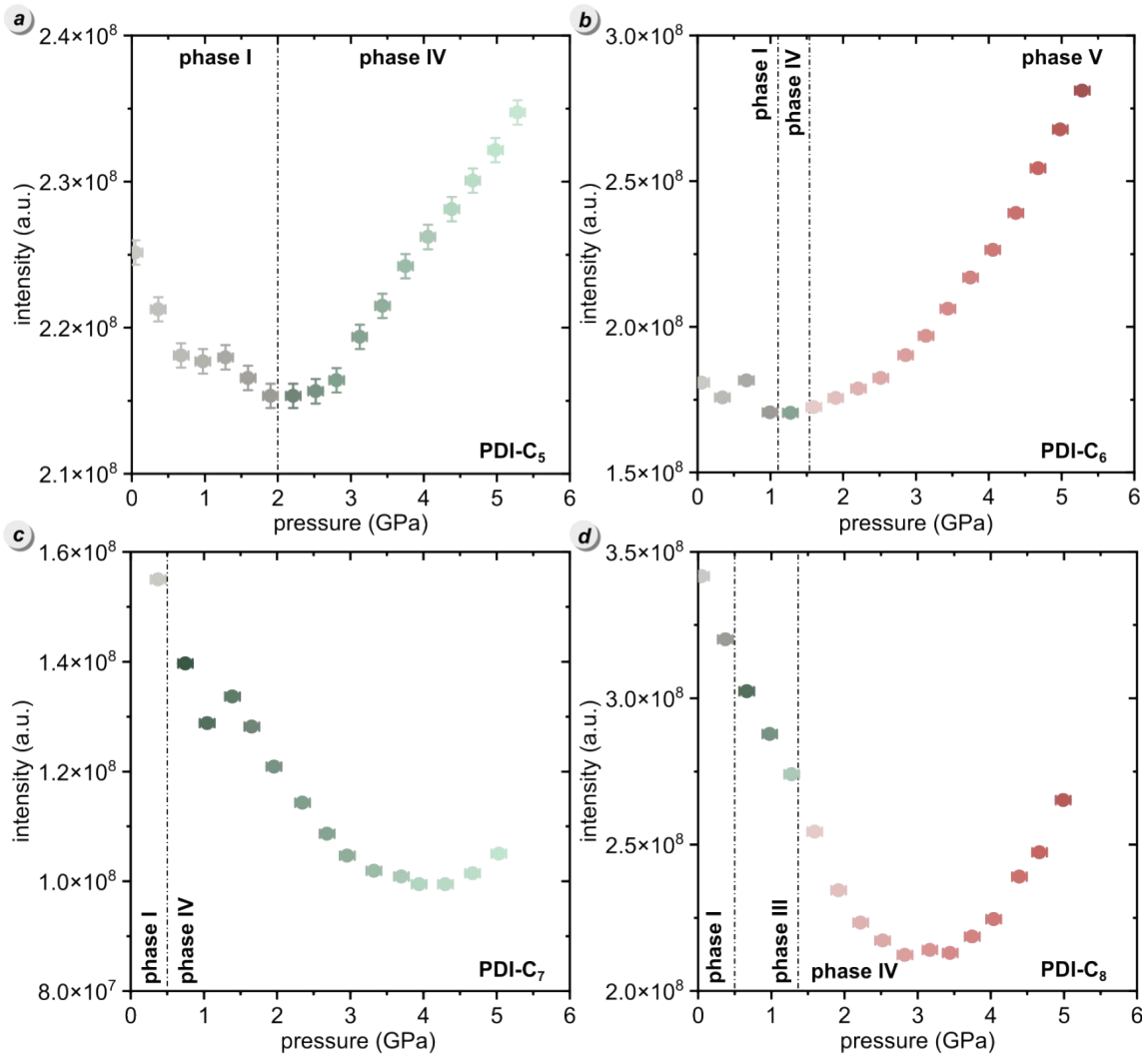


Figure S15. Changes of the PL intensity of the PDI-C_5 (a), -C_6 (b), -C_7 (c), and -C_8 (d) under high-pressure conditions.

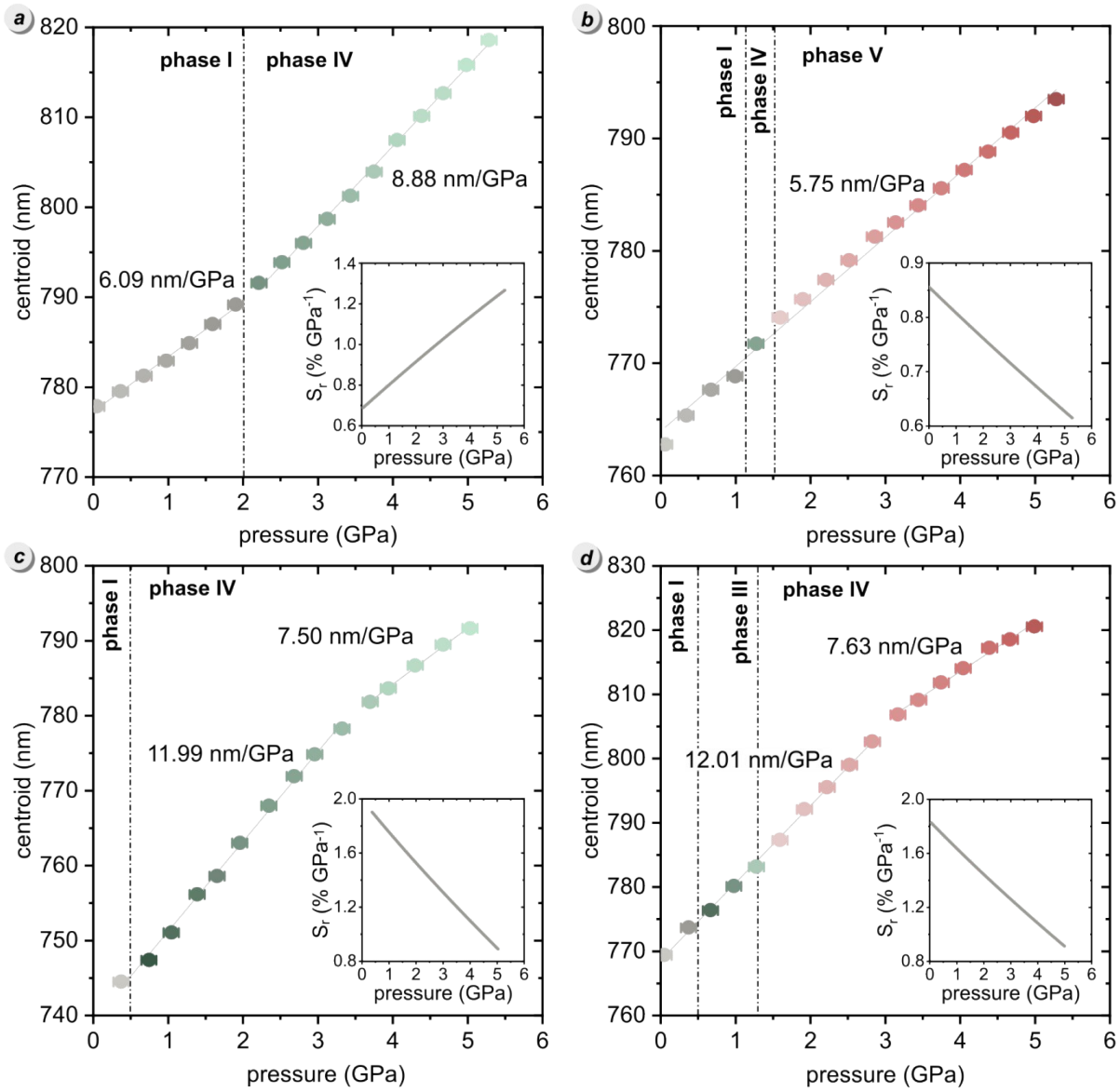


Figure S16. Emission band centroids shift of PDI-C_5 (a), -C_6 (b), -C_7 (c), and -C_8 (d) under high-pressure conditions.

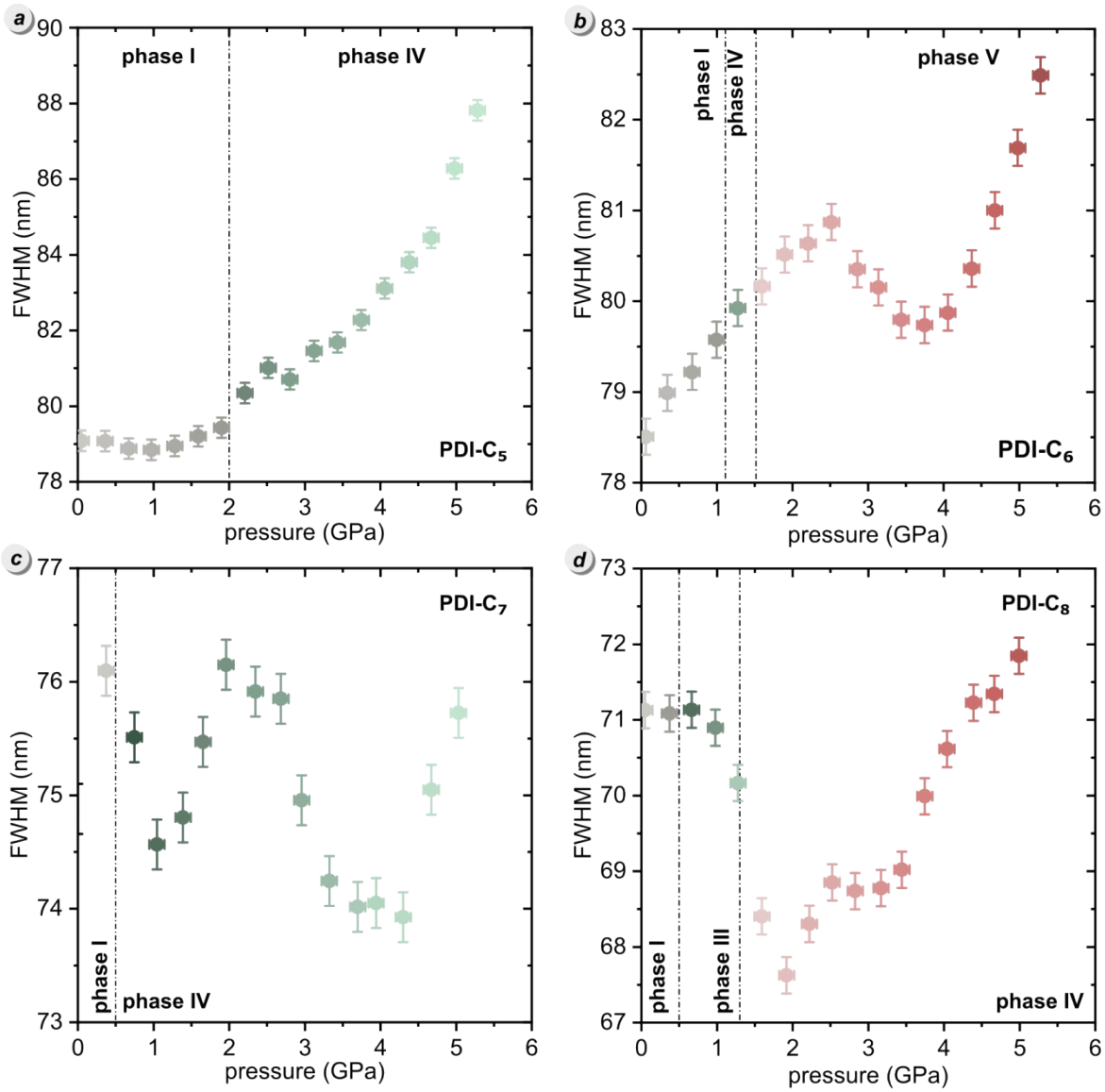


Figure S17. Changes in the full-width at half maximum (FWHM) of the PDI-C_5 (a), -C_6 (b), -C_7 (c), and -C_8 (d) emission band with increasing pressure.

Visible changes in intensity and FWHM trends (Figure S15 and S17) due to phase transitions occur at higher pressures than the corresponding phase transition identified in structural studies. This discrepancy is attributed to the faster compression rates employed during luminescence measurements.

7. Experimental and computational methods

7.1. Geometry optimization, thermodynamic and optical properties

Geometry optimization of the molecular structures as well as wavefunctions and energies calculations were performed in Orca[24] (version 5.0.3) using B3LYP-gCP-D3/6-31G*

method. Visualization of representations of wave functions were generated in IboView.[25,26] B3LYP/6-31G(d,p) basis set was used to calculate intermolecular energies and Hirschfeld Surfaces in Crystal Explorer.[27]

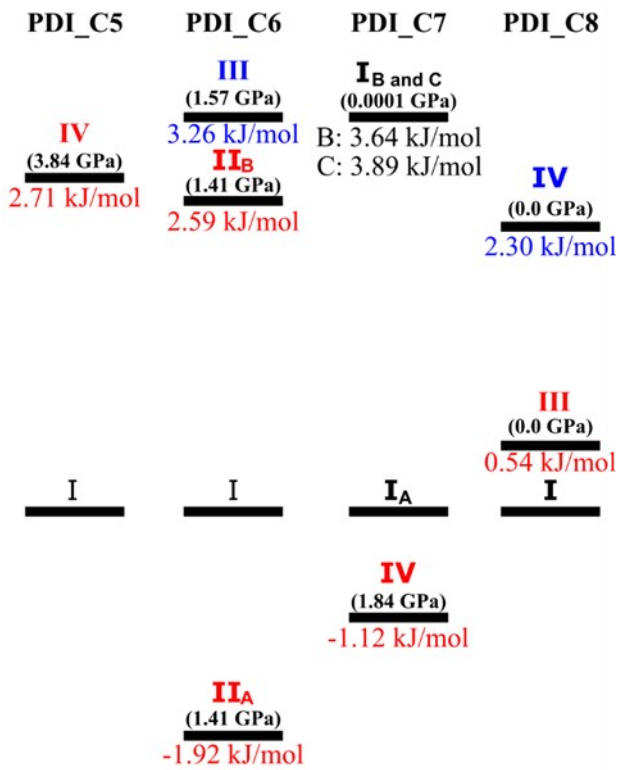


Figure S18. Gibbs free energies of PDI-C_n molecules at different conformations taken from crystallographic structures and optimized in Orca (B3LYP-gCP-D3/6-31G*). As a reference for each compound, energy of phase α was taken (0 kJ/mol). Energies of conformers are comparable within the same structure type only.

Optimization of all but five structures converged to the minimum of energy. Two PDI-C_5 molecules taken from crystallographic models at 2.17 and 2.7 GPa were optimized with a single negative vibrational frequency of ~-40 cm^{-1}, and one PDI-C_8 at 0.40 GPa thus their energies are not reliable. On the other hand, for PDI-C_7 disordered phase I, we calculated energy of three potential conformations: with straight chains on both sides (TTTTT/TTTTT, 0.0001 B in Table S14, 15) with bent chains on both sides ($TTTTG^+$/$TTTTG^-$, 0.001 A) and mixed straight-bent molecule (TTTTG/TTTTT, 0.0001 C). Only one of them converged to the minimum, but two contain a minor negative vibration of approximately ~7cm^{-1}. Out attempts to get the energy minimum failed as both tighter optimization and any distortion applied to restart calculation was not successful. For the reason of consistency of the method used we decided to keep these values.

Table S14. Energies of frontier orbitals and band gaps (in eV) for PDI-C_n molecules, calculated in Orca at the B3LYP-gCP-D3/6-31G* theory level. Two independent molecules in PDI-C_6 (phase IV) and two different conformations of disordered PDI-C_7 (phase I) were described as A and B.

PDI-C_5				PDI-C_6				PDI-C_7				PDI-C_8			
P [GPa]	HOMO	LUMO	Band Gap	P [GPa]	HOMO	LUMO	Band Gap	P [GPa]	HOMO	LUMO	Band Gap	P [GPa]	HOMO	LUMO	Band Gap
0.00001	-5.8647	-3.3377	2.5270	0.00001	-5.8612	-3.3341	2.5271	0.0001 A	-5.8598	-3.3317	2.5281	0.0001	-5.8595	-3.3318	2.5277
0.66	-5.8646	-3.3380	2.5266	0.5	-5.8621	-3.3348	2.5273	0.0001 B	-5.843	-3.385	2.458	0.08	-5.8824	-3.4041	2.4783
0.98	-5.8646	-3.3377	2.5269	1.41 A	-5.8614	-3.3342	2.5272	0.0001 C	-5.8397	-3.3817	2.458	0.4	-5.8905	-3.302	2.5885
1.40	-5.8648	-3.3379	2.5269	1.41 B	-5.8740	-3.3467	2.5273	0.95	-5.8603	-3.3326	2.5277	1.16	-5.8585	-3.3311	2.5274
1.73	-5.8648	-3.3379	2.5269	1.57	-5.8737	-3.3465	2.5272	1.24	-5.8576	-3.2183	2.6393	1.50	-5.8651	-3.3367	2.5284
2.17	-5.8982	-3.7358	2.1624	1.95	-5.8738	-3.3467	2.5271	1.84	-5.8598	-3.3327	2.5271	1.57	-5.879	-3.3238	2.5552
2.70	-5.9157	-3.6899	2.2258	2.05	-5.8737	-3.3465	2.5272								
3.84	-5.769	-3.8489	1.9201	2.74	-5.8739	-3.3467	2.5272								
				3.43	-5.8739	-3.3466	2.5273								
				4.61	-5.8734	-3.3468	2.5266								

Table S15. Gibbs free energies of single PDI-C_n conformers, calculated in Orca at the B3LYP-gCP-D3/6-31G* theory level. Two independent molecules in PDI-C_6 (phase IV) and two different conformations of disordered PDI-C_7 (phase I) were described as A and B. For comparison, energies of theoretical high-symmetry conformations (HSC) was listed in the bottom row.

PDI-C_5				PDI-C_6				PDI-C_7				PDI-C_8			
P [GPa]	G-E(el) (kcal/mol)	G-E(el) (kJ/mol)	ΔE (kJ/mol)	P [GPa]	G-E(el) (kcal/mol)	G-E(el) (kJ/mol)	ΔE (kJ/mol)	P [GPa]	G-E(el) (kcal/mol)	G-E(el) (kJ/mol)	ΔE (kJ/mol)	P [GPa]	G-E(el) (kcal/mol)	G-E(el) (kJ/mol)	ΔE (kJ/mol)
0.00001	319.61	1337.25	0	0.00001	353.31	1478.25	0	0.0001 A	387.23	1620.17	0	0.0001	420.75	1760.42	0
0.66	319.6	1337.21	-0.04184	0.50	353.05	1477.16	-1.08784	0.0001 B	388.10	1623.81	3.64008	0.08	420.76	1760.46	0.04184
0.98	319.59	1337.16	-0.08368	1.41 A	352.85	1476.32	-1.92464	0.0001 C	388.16	1624.06	3.89112	0.40	421.41	1763.18	2.76144
1.40	319.6	1337.21	-0.04184	1.41 B	353.93	1480.84	2.59408	0.95	386.98	1619.12	-1.046	1.16	420.88	1760.96	0.54392
1.73	319.63	1337.33	0.08368	1.57	354.09	1481.51	3.26352	1.24	386.91	1618.83	-1.33888	1.50	421.30	1762.72	2.3012
2.17	320.38	1340.47	3.22168	1.95	354.13	1481.68	3.43088	1.84	386.96	1619.04	-1.12968	1.57	421.30	1762.72	2.3012
2.70	320.59	1341.35	4.10032	2.05	354.1	1481.55	3.30536								
3.84	320.26	1339.97	2.7196	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	319.65	1337.42	0.16736	HSC	353.39	1478.58	0.33472	HSC	387.07	1619.50	141.25184	HSC			

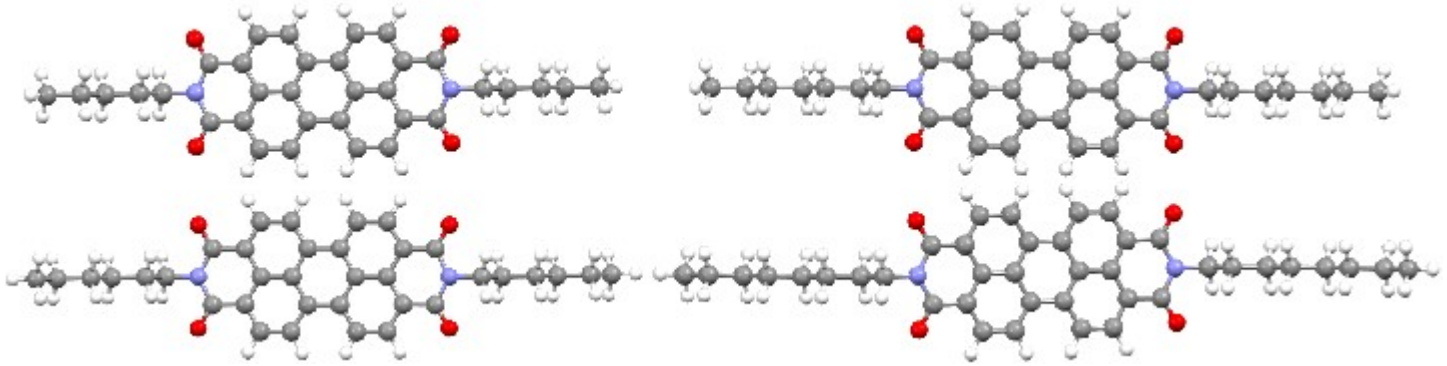


Figure S19. Theoretical high-symmetry conformations of PDI-C_n molecules, calculated in Orca at the B3LYP-gCP-D3/6-31G* theory level.

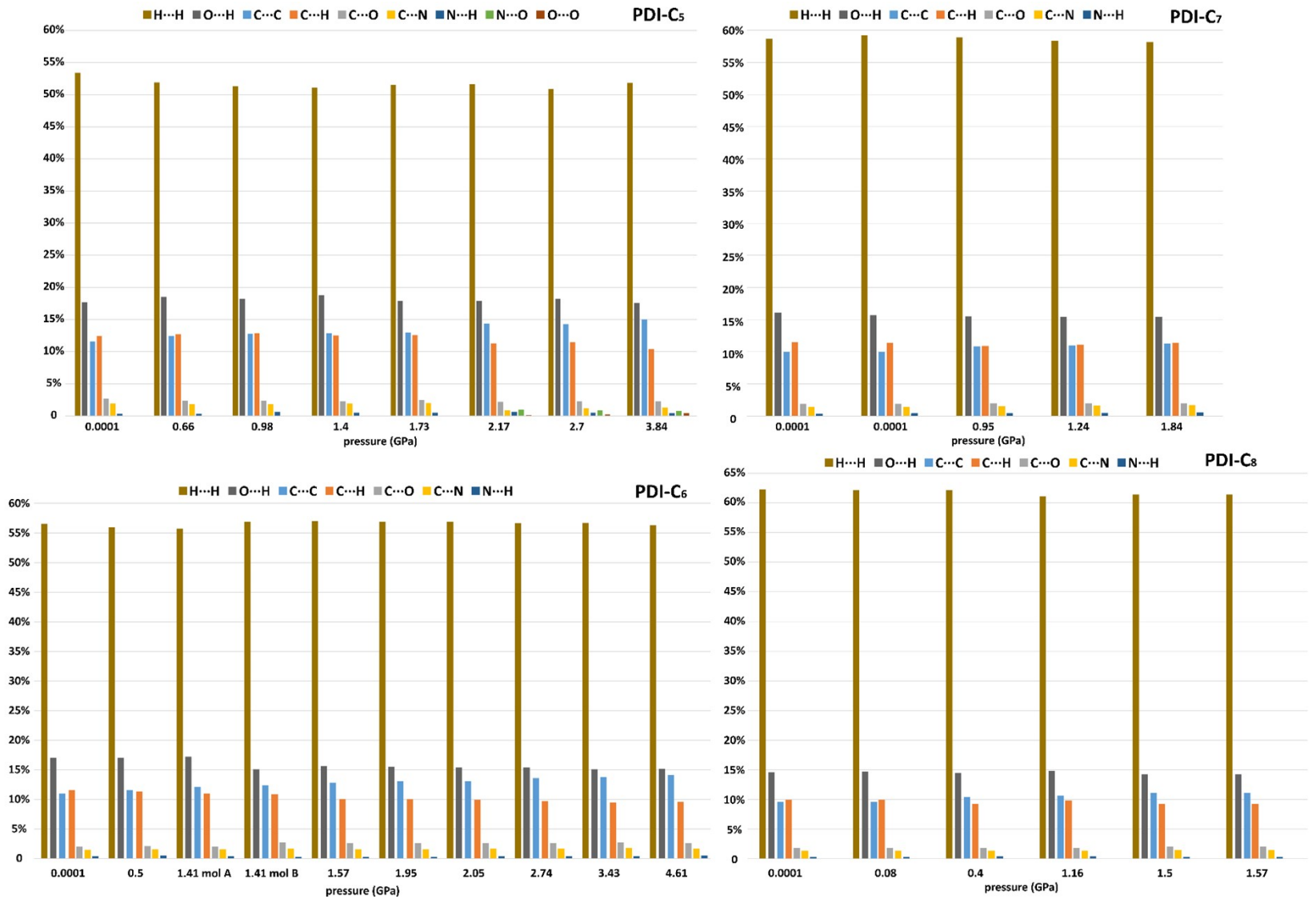


Figure S20. Percentage of intermolecular interaction present in PDI-C_n crystals calculated in Crystal Explorer (cf. Table S20, Figure S21 and S22).

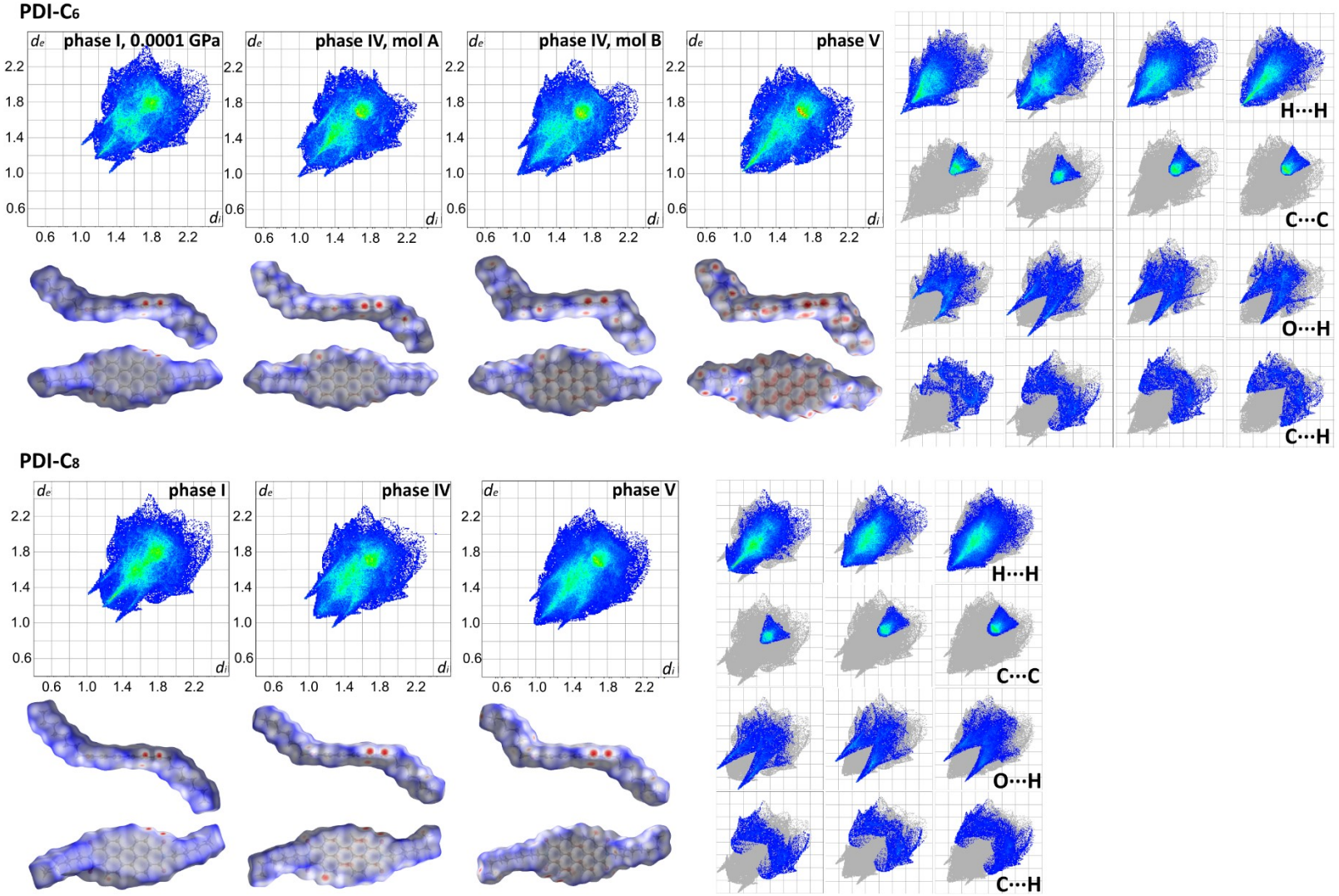


Figure S21. Hirschfeld surfaces and fingerprints showing strengthen and amount of interactions in PDI-C_6 and PDI-C_8 phases. Selected regions of the fingerprints showing four the most popular interactions. d_i and d_e are the distances from a point on the surface to the nearest atom inside and outside the surface, respectively (all in Å).

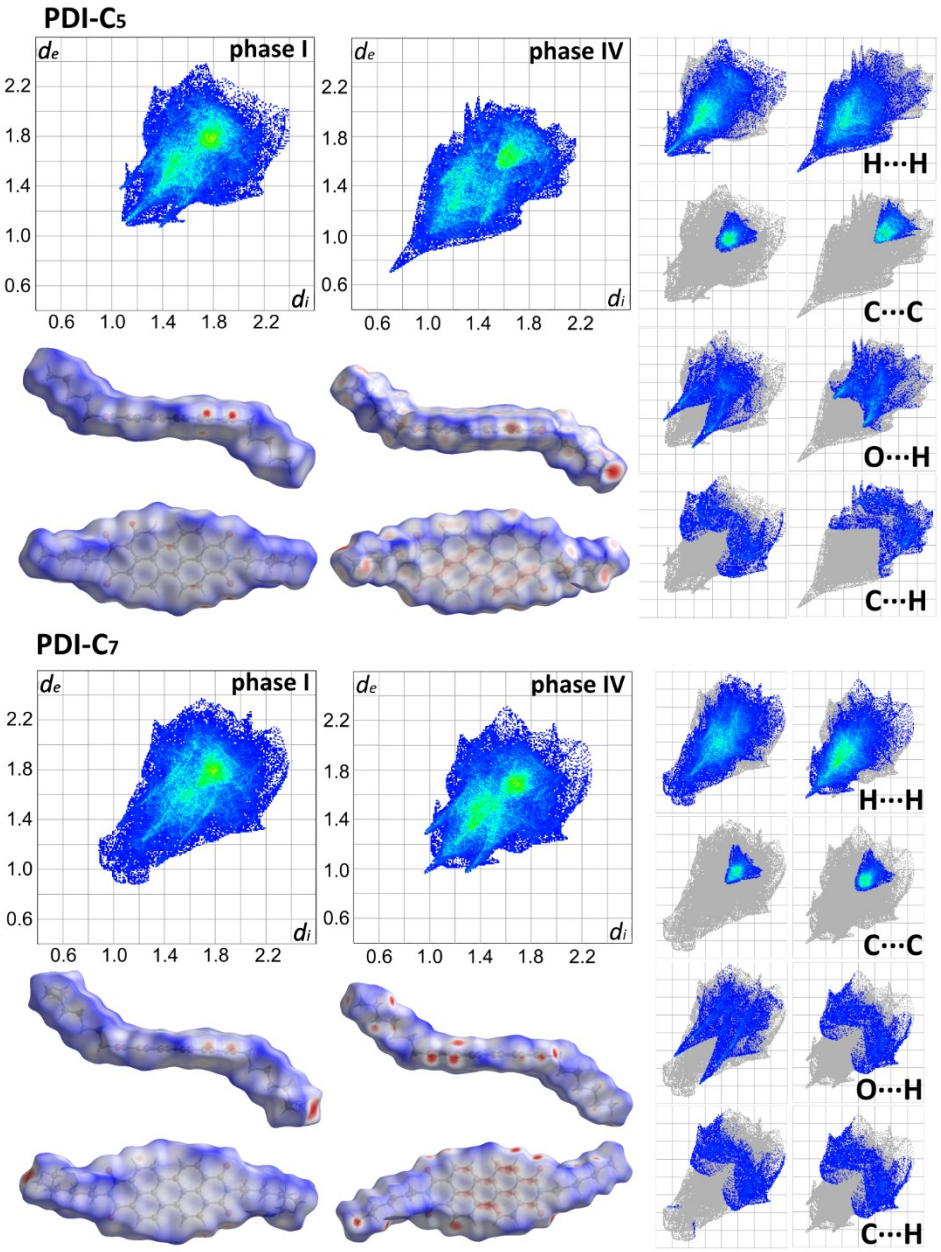


Figure S22. Hirschfeld surfaces and fingerprints showing strengthen and amount of interactions in PDI-C_5 and PDI-C_7 phases. Selected regions of the fingerprints showing four the most popular interactions. d_i and d_e are the distances from a point on the surface to the nearest atom inside and outside the surface, respectively (all in Å).

The number of H···H interactions systematically increases along the C5 to C8 alkyl chain series (from 53.4% to 62.3%), which is a natural consequence of the elongation of the alkyl substituent (Table S20). Interestingly, this trend is accompanied by a decrease in other intermolecular interactions, including C···C contacts, more specifically π···π* interactions, which are primarily responsible for the optical properties of perylene diimide (PDI) molecules, where the PDI core acts as the principal chromophore. This observation is consistent with literature reports that emphasize the dominant role of π···π* stacking in defining PDI's photophysical behaviour, and how modifications in peripheral substituents modulate these interactions without significantly perturbing the optical characteristics of the core chromophore. It's worth noted, that only the PDI-C_5 derivative exhibits additional N···O and O···O interactions, which appear upon compression above approximately 2 GPa. This occurs due to its short alkyl chain, which allows the PDI cores to approach each other more closely and mutually interact more efficiently.

Table S16. Percentage of intermolecular interactions in PDI-C_n calculated in CrystalExplorer. In PDI-C_6 mol A and B refer to symmetry-independent molecules in the unit cell. In PDI-C_7 mol A and B refer to straight and bent fragments of disordered molecules, respectively.

p [GPa]	C…C	C…H	C…O	C…N	N…N	N…O	N…H	O…O	O…H	H…H
PDI-C_5										
0.0001	11.6	12.4	2.7	1.9	0	0	0.3	0	17.7	53.4
0.66	12.4	12.7	2.4	1.8	0	0	0.3	0	18.5	51.9
0.98	12.8	12.9	2.4	1.8	0	0	0.6	0	18.2	51.3
1.40	12.9	12.5	2.3	1.9	0	0	0.5	0	18.8	51.1
1.73	13.0	12.6	2.5	2.0	0	0	0.5	0	17.9	51.5
2.17	14.4	11.3	2.2	0.9	0	1.0	0.6	0.1	17.9	51.6
2.70	14.3	11.5	2.3	1.2	0	0.9	0.5	0.2	18.2	50.9
3.84	15.0	10.4	2.3	1.3	0	0.8	0.4	0.4	17.6	51.8
PDI-C_6										
0.0001	11.0	11.6	2.0	1.5	0	0	0.4	0	17.0	56.5
0.50	11.6	11.3	2.1	1.6	0	0	0.5	0	17.0	55.9
1.41 (mol A)	12.1	11.0	2.0	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	57.0
1.95	13.1	10.0	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
PDI-C_7										
0.0001 (mol A)	10.0	11.5	1.9	1.4	0	0	0.4	0	16.1	58.7
0.0001 (mol B)	10.0	11.4	1.9	1.4	0	0	0.4	0	15.7	59.2
0.95	10.8	10.9	2.0	1.5	0	0	0.4	0	15.5	58.9
1.24	11.0	11.1	2.0	1.6	0	0	0.5	0	15.4	58.4
1.84	11.3	11.4	2.0	1.7	0	0	0.5	0	15.4	58.2
PDI-C_8										
0.0001	9.6	10.0	1.8	1.4	0	0	0.3	0	14.6	62.3
0.08	9.6	10.0	1.8	1.4	0	0	0.3	0	14.7	62.2
0.40	10.4	9.3	1.8	1.4	0	0	0.4	0	14.5	62.2
1.16	10.7	9.8	1.8	1.4	0	0	0.4	0	14.8	61.1
1.50	11.1	9.3	2.1	1.5	0	0	0.3	0	14.3	61.4
1.57	11.1	9.3	2.1	1.5	0	0	0.3	0	14.3	61.4

Table S17. Interaction energies (kJ/mol) between molecules in PDI-C_n. Color code refers to interactions with a molecule shown in that color in a figure below. *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
			PDI-C_5							PDI-C_6			
0.0001	4.73	-18.1	-3.1	-182.2	105.3	-115.0	0.0001	4.77	-15.8	-2.1	-180.1	92.5	-118.0
0.66	4.63	-24.9	-4.7	-199.8	139.3	-117.7	0.50	4.65	-22.0	-2.6	-201.8	125.0	-123.7
0.98	4.56	-31.9	-3.8	-214.7	171.2	-117.8	1.41	4.53	-30.4	-3.0	-222.5	161.7	-128.2
1.40	4.52	-35.6	-4.5	-226.4	188.1	-122.0	1.41	4.53	-41.8	-4.0	-248.2	204.9	-136.7
1.73	4.47	-43.2	-4.4	-237.0	216.5	-121.6	1.57	4.52	-37.9	-4.0	-244.6	195.0	-135.6
2.17	3.76	-55.7	-8.7	-287.4	265.2	-151.8	1.95	4.46	-44.4	-4.3	-258.7	224.4	-136.8
2.70	3.72	-61.6	-8.6	-299.8	290.3	-153.1	2.05	4.45	-45.8	-4.2	-261.4	229.9	-137.2
3.84	3.64	-89.7	-11.4	-332.3	390.5	-151.5	2.74	4.38	-56.4	-4.5	-280.0	276.0	-136.3
							3.43	4.34	-64.8	-4.8	-293.2	310.4	-135.6
							4.61	4.29	-77.3	-5.4	-310.9	363.0	-132.2
			PDI-C_7							PDI-C_8			
0.0001	4.83	-16.9	-2.6	-184.3	96.1	-120.9	0.0001	4.77	-18.1	-2.1	-194.6	102.0	-127.2
0.0001	4.83	-16.5	-2.5	-184.4	94.1	-121.8	0.08	4.75	-17.4	-2.8	-197.5	103.7	-128.5
0.50	4.66	-25.7	-3.0	-218.1	141.6	-131.8	0.40	4.62	-21.7	-2.7	-217.4	129.1	-134.6
0.95	4.67	-26.3	-2.6	-215.1	140.6	-130.2	1.16	4.49	-35.3	-3.3	-251.3	193.1	-139.3
1.24	4.60	-36.6	-2.8	-236.0	184.3	-132.4	1.50	4.52	-40.8	-3.5	-262.9	210.5	-144.6
1.84	4.56	-42.0	-3.0	-248.6	209.7	-133.6	1.57	4.50	-43.0	-3.8	-267.3	221.4	-144.3
			PDI-C_5							PDI-C_6			
0.0001	9.29	-17.6	-8.5	-69.2	49.4	-54.6	0.0001	9.29	-12.5	-6.3	-62.5	34.5	-51.0
0.66	9.27	-20.6	-10.2	-71.4	56.5	-56.6	0.50	9.31	-18.0	-7.9	-73.3	52.3	-56.4
0.98	9.24	-23.4	-10.3	-76.0	66.4	-57.5	1.41	9.16	-21.0	-7.4	-75.2	65.6	-52.7
1.40	9.23	-26.5	-11.2	-81.2	75.1	-60.6	1.41	9.16	-21.0	-7.4	-75.2	65.6	-52.7
1.73	9.20	-28.1	-11.1	-86.5	88.8	-58.5	1.57	9.20	-23.9	-6.8	-73.6	69.9	-51.2
2.17	8.64	-30.6	-10.6	-81.5	98.0	-50.7	1.95	9.17	-26.3	-7.1	-77.0	78.0	-52.0
2.70	8.63	-31.8	-11.1	-82.0	99.4	-51.9	2.05	9.16	-26.7	-7.0	-77.5	78.6	-52.4
3.84	8.61	-29.2	-10.5	-83.5	94.8	-52.8	2.74	9.14	-30.9	-7.6	-83.0	93.8	-52.7
							3.43	9.13	-34.7	-8.0	-87.1	106.9	-52.4
							4.61	9.09	-41.0	-8.9	-92.4	128.6	-51.0
			PDI-C_7							PDI-C_8			
0.0001	9.03	-12.7	-7.2	-65.3	36.3	-53.2	0.0001	9.19	-13.6	-7.2	-70.4	37.8	-57.7
0.0001	9.03	-15.7	-8.2	-71.0	42.1	-58.5	0.08	9.20	-15.5	-8.6	-72.4	40.7	-60.6
0.50	9.13	-23.6	-10.0	-82.9	63.3	-65.4	0.40	9.24	-21.0	-9.8	-81.0	54.8	-66.1
0.95	9.15	-23.6	-10.0	-83.3	63.9	-65.4	1.16	9.16	-31.7	-12.0	-95.2	86.5	-71.9
1.24	9.08	-27.1	-10.8	-92.6	80.7	-67.4	1.50	8.96	-37.3	-11.2	-103.3	103.0	-74.0
1.84	9.02	-33.5	-12.0	-98.0	98.2	-69.0	1.57	8.96	-36.7	-12.3	-104.3	102.2	-75.5
			PDI-C_5							PDI-C_6			
0.0001	12.04	-26.0	-4.6	-15.9	0	-44.8	0.0001	12.03	-19.2	-4.9	-16.9	18.1	-27.5
0.66	11.98	-21.4	-6.0	-16.7	18.9	-29.9	0.50	11.96	-21.7	-5.9	-18.4	23.9	-28.6
0.98	11.92	-26.7	-7.1	-17.8	30.5	-30.1	1.41	11.71	-24.2	-6.9	-20.6	28.3	-31.2
1.40	11.88	-27.8	-7.4	-18.3	30.4	-32.1	1.41	11.71	-24.2	-6.9	-20.6	28.3	-31.2
1.73	11.82	-28.7	-7.8	-19.2	35.8	-30.7	1.57	11.65	-22.4	-6.5	-20.9	24.3	-31.7
2.17	10.20	-22.5	-6.1	-27.0	29.6	-33.5	1.95	11.57	-24.1	-7.0	-22.4	29.1	-32.3
2.70	10.16	-25.4	-6.6	-27.5	35.1	-34.1	2.05	11.55	-23.8	-7.2	-22.6	29.4	-32.1
3.84	10.10	-23.9	-6.4	-28.7	33.6	-34.3	2.74	11.46	-26.3	-8.0	-24.6	36.5	-32.7
							3.43	11.41	-27.6	-8.6	-25.9	40.5	-33.1
							4.61	11.35	-32.0	-9.8	-27.5	51.8	-33.0
			PDI-C_7							PDI-C_8			
0.0001	11.83	-20.3	-5.4	-18.8	18.5	-30.4	0.0001	11.91	-19.3	-4.9	-18.6	18.5	-28.7

0.0001	11.83	-20.3	-5.4	-18.9	18.5	-30.5	**0.08**	11.90	-20.0	-5.3	-18.8	18.6	-30.0
0.50	11.83	-19.2	-5.6	-19.6	19.9	-29.2	**0.40**	11.76	-21.7	-6.0	-21.6	23.6	-31.6
0.95	11.86	-19.1	-5.4	-19.7	19.9	-29.0	**1.16**	11.68	-27.6	-7.5	-22.4	33.4	-33.6
1.24	11.76	-22.2	-6.4	-21.3	25.0	-31.3	**1.50**	11.45	-26.4	-7.5	-22.3	35.5	-31.0
1.84	11.69	-24.3	-7.0	-22.6	29.9	-32.0	**1.57**	11.44	-26.8	-7.3	-22.8	35.5	-31.7
			PDI-C_5							**PDI-C_6**			
0.0001	8.49	-1.2	-2.3	-18.5	4.5	-16.3	**0.0001**	8.58	-2.6	-2.0	-19.3	4.6	-18.2
0.66	8.44	-1.6	-2.9	-21.0	6.6	-18.0	**0.50**	8.57	-2.8	-2.5	-22.9	8.0	-19.8
0.98	8.39	-2.8	-3.1	-23.5	9.3	-20.1	**1.41**	8.48	-7.2	-3.8	-30.7	19.6	-25.0
1.40	8.37	-4.2	-3.9	-26.5	13.7	-22.0	**1.41**	8.48	-7.2	-3.8	-30.7	19.6	-25.0
1.73	8.35	-5.9	-4.4	-28.0	17.0	-23.3	**1.57**	8.62	-6.1	-4.1	-31.3	19.5	-24.7
2.17	8.57	-2.5	-3.2	-29.0	12.2	-22.8	**1.95**	8.62	-7.2	-4.6	-33.2	23.3	-25.5
2.70	8.56	-3.2	-3.6	-30.3	14.2	-23.7	**2.05**	8.60	-7.7	-4.1	-33.9	24.6	-25.4
3.84	8.54	-1.9	-3.5	-29.2	11.6	-22.9	**2.74**	8.60	-9.5	-4.9	-36.3	31.0	-26.1
							3.43	8.60	-10.2	-4.7	-38.0	35.0	-25.7
							4.61	8.56	-14.3	-6.2	-41.1	47.4	-26.1
			PDI-C_7							**PDI-C_8**			
0.0001	8.37	-0.4	-1.3	-19.4	12.1	-17.2	**0.0001**	8.52	-4.0	-2.8	-33.2	13.7	-26.8
0.0001	8.37	-3.3	-2.6	-31.3	13.5	-24.3	**0.08**	8.54	-4.3	-3.3	-33.3	12.5	-28.2
0.50	8.38	-6.5	-3.5	-32.7	21.0	-25.0	**0.40**	8.66	-7.0	-3.6	-39.0	22.5	-30.2
0.95	8.40	-6.9	-3.6	-33.1	21.4	-25.6	**1.16**	8.46	-11.7	-4.6	-52.1	38.3	-37.6
1.24	8.30	-10.6	-4.2	-39.3	35.0	-27.0	**1.50**	8.38	-12.4	-3.7	-49.8	39.2	-35.0
1.84	8.22	-12.7	-4.7	-42.1	41.1	-28.2	**1.57**	8.38	-12.8	-5.1	-50.1	40.6	-35.8
			PDI-C_5							**PDI-C_6**			
0.0001	24.62	-0.1	0	-2.4	0	-2.2	**0.0001**	26.70	-0.6	0	-5.3	3.0	-3.5
0.66	24.51	0	0	-7	0	-6.1	**0.50**	26.61	-1.5	0	-7.4	6.8	-3.9
0.98	24.37	0	0	-3.5	0	-3.1	**1.41**	24.79	-1.5	0	-5.9	5.6	-3.3
1.40	24.36	-0.2	0	-3.5	0	-3.2	**1.41**	24.79	-1.5	0	-5.9	5.6	-3.3
1.73	24.31	-0.2	0	-3.9	0	-3.6	**1.57**	23.74	-2.3	0	-6.0	8.1	-2.6
2.17	25.56	-2.3	-0.1	-5.7	0	-7.5	**1.95**	23.69	-2.6	0	-6.3	9.3	-2.5
2.70	25.49	-2.3	-0.2	-5.8	0	-7.6	**2.05**	23.67	-2.6	0	-6.3	9.3	-2.6
3.84	25.11	-0.9	0	-6.4	0	-6.5	**2.74**	23.61	-3.1	0	-6.7	11.2	-2.3
							3.43	23.49	-3.9	0	-7.0	14.1	-1.6
							4.61	23.33	-4.6	-0.1	-7.5	16.6	-1.2
			PDI-C_7							**PDI-C_8**			
0.0001	28.44	0.2	0	-6.4	0	-5.3	**0.0001**	31.76	-0.7	0	-5.9	3.7	-3.6
0.0001	28.44	0.3	0	-4.0	0	-3.1	**0.08**	31.72	-0.4	0	-5.0	2.5	-3.3
0.50	28.97	-2.1	-0.1	-6.3	8.7	-2.4	**0.40**	30.85	-0.2	0	-6.3	3.1	-4.2
0.95	29.02	-1.6	0	-6.0	5.9	-3.3	**1.16**	30.19	-1.4	0	-9.0	4.9	-6.3
1.24	28.86	-2.0	0	-6.9	7.0	-3.8	**1.50**	28.98	-2.9	0	-12.0	10.6	-7.0
1.84	28.82	-3.1	-0	-7.4	11.8	-2.5	**1.57**	28.94	-2.5	0	-11.7	8.9	-7.3
			PDI-C_5							**PDI-C_6**			
0.0001	19.76	8.1	-1.2	-17.2	0	-7.2	**0.0001**	21.65	-1.7	-0.6	-24.1	9.7	-17.2
0.66	19.52	3.4	-2.9	-30.4	0	-25.0	**0.50**	21.41	-3.9	-0.9	-32.9	18.5	-22.0
0.98	19.37	11.4	-2.8	-38.2	0	-23.2	**1.41***	19.61	1.0	-1.4	-18.7	0	-16.2
1.40	19.32	13.7	-2.3	-34.4	0	-17.1	**1.41**	19.61	-7.6	-0.4	-28.7	33.7	-12.5
1.73	19.26	15.1	-2.8	-40.1	0	-21.0	**1.57**	18.64	-1.7	-0.9	-21.6	16.3	-11.2
2.17	20.12	3.3	-2.7	-27.0	0	-22.1	**1.95**	18.57	-2.2	-1.0	-22.5	18.8	-11.0
2.70	20.04	3.7	-3.0	-28.0	0	-22.7	**2.05**	18.56	-2.4	-0.9	-22.5	19.0	-11.1
3.84	19.80	6.1	-1.2	-34.0	0	-24.0	**2.74**	18.47	-2.9	-1.1	-23.7	22.1	-10.8
							3.43	18.32	-3.7	-1.1	-25.4	26.1	-10.8
							4.61	18.16	-4.7	-1.4	-27.0	31.0	-10.4
			PDI-C_7							**PDI-C_8**			
0.0001	23.74	7.5	-0.2	-25.3	0	-14.3	**0.0001**	26.36	-1.5	-0.1	-19.0	6.6	-14.1
0.0001	23.74	1.1	-0.1	-18.4	0	-14.9	**0.08**	26.29	-2.3	-0.1	-21.5	9.6	-15.3
0.50	23.83	-6.5	-0.2	-36.0	26.0	-22.4	**0.40**	26.00	-4.2	-0.1	-29.6	16.3	-20.2

0.95	23.87	-5.8	-0.2	-34.5	23.7	-21.7	**1.16**	24.93	-5.6	-0.1	-29.8	20.9	-19.1
1.24	23.74	-7.6	-0.1	-39.6	29.3	-24.5	**1.50**	23.91	-6.0	-0.1	-34.3	23.6	-21.7
1.84	23.73	-10.7	-0.2	-44.6	40.8	-25.2	**1.57**	23.87	-5.6	-0.1	-32.9	21.8	-21.2
			PDI-C_5							**PDI-C_6**			
0.0001	26.14	0.2	0	-5.4	0	-4.5	**0.0001**	28.14	-1.0	0	-4.9	3.4	-3.2
0.66	26.00	-0.1	0	-2.5	0	-2.3	**0.5**	28.07	-0.8	0	-5.3	3.0	-3.6
0.98	25.89	0.3	0	-7.3	0	-6.2	**1.41**	25.81	-2.8	0	-11.7	11.0	-6.4
1.40	25.86	0.2	0	-6.7	0	-5.7	**1.41**	25.81	-2.8	0	-11.7	11.0	-6.4
1.73	25.81	-0.1	0	-7.5	0	-6.7	**1.57**	24.68	-3.4	0	-13.5	13.2	-7.3
2.17	25.49	0.7	0	-10.2	0	-8.2	**1.95**	24.63	-3.9	0	-14.4	14.9	-7.5
2.70	25.41	1.0	0	-11.7	0	-9.2	**2.05**	24.61	-4.2	0	-14.6	15.5	-7.6
3.84	24.97	3.5	-1.8	-13.3	0	-9.2	**2.74**	24.55	-5.2	0	-16.1	19.2	-7.7
							3.43	24.43	-6.8	0	-17.8	24.7	-7.5
							4.61	24.29	-6.7	0	-18.4	24.9	-7.8
			PDI-C_7							**PDI-C_8**			
0.0001	29.96	1.6	-0.3	-17.8	0	-14.0	**0.0001**	33.02	-0.2	0	-3.2	0.5	-2.6
0.0001	29.96	-0.1	0	-2.9	0.4	-2.4	**0.08**	32.99	-0.6	0	-3.8	1.9	-2.7
0.50	30.51	-2.2	-0.1	-8.9	10.1	-3.9	**0.40**	32.60	-0.9	0	-4.9	3.2	-3.7
0.95	30.56	-1.9	-0.1	-8.4	8.7	-3.9	**1.16**	31.55	-3.4	0	-11.8	11.6	-6.6
1.24	30.43	-2.6	-0.1	-9.5	11.9	-3.8	**1.50**	30.36	-6.0	0	-13.9	20.9	-5.6
1.84	30.38	-3.0	-0.1	-10.0	13.1	-3.8	**1.57**	30.31	-6.2	-0.1	-14.0	21.7	-5.4
			PDI-C_5							**PDI-C_6**			
0.0001	21.81	-0.3	-0.1	-9.0	0	-8.3	**0.0001**	23.61	-1.4	0	-10.8	5.7	-7.4
0.66	21.52	-2.7	-0.2	-17.2	0	-17.9	**0.50**	23.38	-2.7	-0.1	-13.9	10.8	-8.3
0.98	21.37	-1.8	-0.3	-21.2	0	-20.5	**1.41***	21.09	-3.3	-1.6	-47.0	0	-45.6
1.40	21.3	-0.7	-0.2	-19.0	0	-17.4	**1.41**	21.09	-4.8	-0.3	-24.5	18.7	-15.0
1.73	21.23	-0.7	-0.3	-21.1	0	-19.4	**1.57**	20.08	-10.2	-1.5	-38.5	34.1	-24.3
2.17	20.35	0.4	-0.6	-26.1	0	-22.8	**1.95**	20.01	-12.3	-1.7	-41.7	41.1	-25.1
2.70	20.25	-0.4	-0.8	-28.8	0	-26.1	**2.05**	19.99	-12.7	-1.5	-42.4	42.8	-25.1
3.84	19.67	-0.8	-4.2	-27.4	0	-27.7	**2.74**	19.89	-15.7	-1.9	-46.2	52.6	-25.8
							3.43	19.76	-19.5	-2.0	-50.6	66.1	-25.4
							4.61	19.61	-24.3	-2.7	-54.1	80.8	-24.9
			PDI-C_7							**PDI-C_8**			
0.0001	25.77	-0.1	0	-7.0	0	-6.2	**0.0001**	28.07	-0.7	0	-7.4	2.5	-5.7
0.0001	25.77	-0.4	0	-5.2	0.9	-4.4	**0.08**	28.01	-0.7	0	-7.5	2.5	-5.8
0.50	25.85	-0.6	0	-8.2	2.5	-6.2	**0.40**	27.74	-1.1	0	-8.6	4.0	-6.2
0.95	25.89	-0.6	0	-7.8	2.2	-6.1	**1.16**	26.71	-0.2	0	-5.4	0.5	-4.7
1.24	25.77	-0.8	0	-9.0	3.2	-6.7	**1.50**	25.53	-1.1	0	-12.3	4.9	-8.9
1.84	25.75	-1.0	0	-9.7	4.0	-7.1	**1.57**	25.47	-1.2	0	-12.6	5.3	-9.0

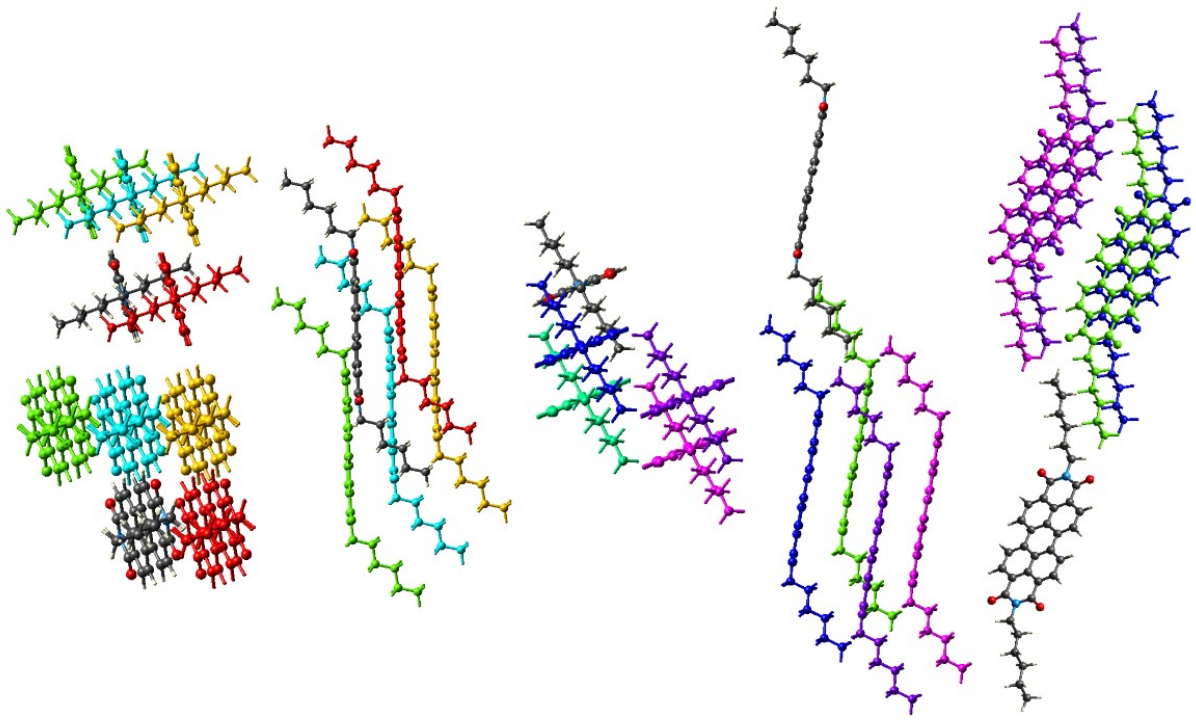


Figure S23. Intermolecular interactions between neighboring PDI-C_n molecules presented in the table S21 are consistent with the color code used here. Since all derivatives are isostructural, their molecular arrangements are comparable. Consequently, PDI-C_6 molecules were used to represent the mutual orientations, ensuring consistency with our earlier study on PDI-C_6.

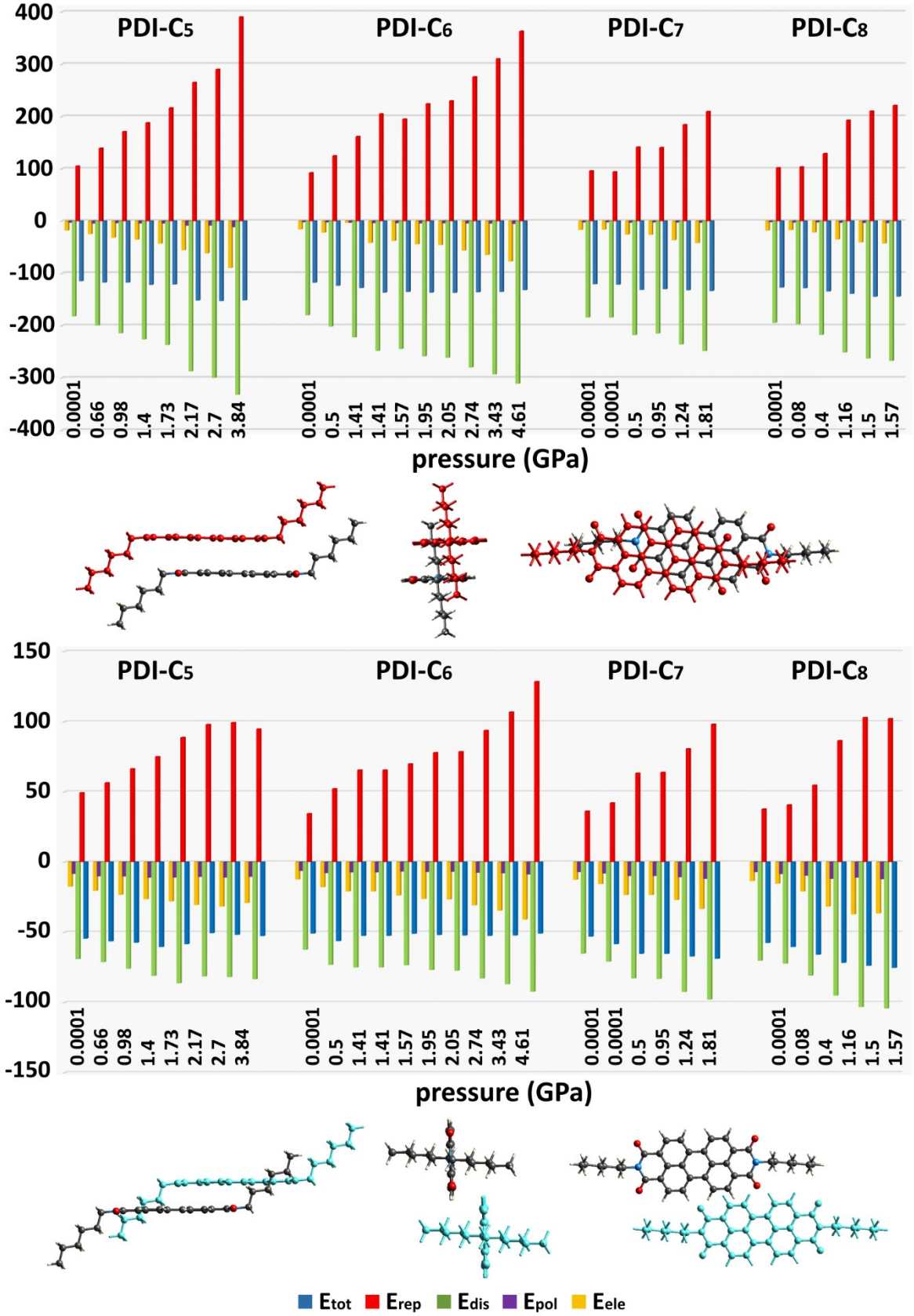


Figure S24. The evolution of selected interaction energies (in kJ/mol) between PDI-C_n molecules. Top: stacking π···π interactions (red molecule in Figure S23). Bottom: mainly CH···O interactions (cyan molecule in Figure S23). For all the interactions see Figure S23 and Table S17. E_{tot}, E_{rep}, E_{dis}, E_{pol} and E_{ele} are total, repulsive, dispersive, polarization and

electrostatic energy, respectively. $E_{tot}=k_{ele}E_{ele}+k_{pol}E_{pol}+k_{dis}E_{dis}+k_{rep}E_{rep}$ where k_{ele}, k_{pol}, k_{dis}, k_{rep} are equal to 1.057, 0.740, 0.871, 0.618 as B3LYP/6-31G(d,p) level was used.

Table S18. Coordinates of atoms of PDI-C_5 molecules – models taken from crystallographic data and optimized in Orca at the B3LYP-gCP-D3/6-31G* theory level.

0.00001 GPa

O	-4.07201806254148	4.00511182981839	2.16987755478169
O	-2.78218078510269	1.01245531368285	5.38915237503854
N	-3.43445176053149	2.51879268213709	3.78748307909764
C	-0.73291193228723	1.13935318685836	-0.35326470408375
C	-0.82439268163688	0.61685134135178	0.97722959283005
C	-0.06182549734930	-0.52165760329968	1.39373677069212
C	-0.19978688354856	-0.97260979063492	2.70940336001014
H	0.36470552845240	-1.83269765402914	3.05701484005136
C	-1.05597969941899	-0.34443871701167	3.62243520719150
H	-1.14368662831946	-0.71003044259046	4.64272988197302
C	-1.80531347677555	0.75670492491726	3.23985773500059
C	-1.70091628390420	1.24841672773928	1.91497530330979
C	-2.47133570957261	2.37191187468483	1.52606640517137
C	-2.36878325552891	2.86072462416412	0.23363746529022
H	-2.96550078367547	3.72461379551255	-0.04928942347733
C	-1.50995601251244	2.25141216544489	-0.68949583367020
H	-1.46351360982314	2.67200919678129	-1.68956143942611
C	-3.38618974346442	3.03895072134034	2.48522340661232
C	-2.69565721017615	1.40995321961552	4.23328330692462
C	-4.31526794161090	3.20920926071856	4.75378257827729
H	-5.25020640395493	3.43925204335775	4.23510596808460
H	-4.52072228556981	2.49603568382394	5.55660769580340
C	-3.69145332425966	4.49645119967121	5.31518911169402
H	-3.34599126937486	5.12706409645809	4.48217582882621
H	-2.80899821892558	4.23441456248158	5.92073027260734
C	-4.70324147121020	5.28873002417532	6.16057965921274
H	-5.52534502208432	5.62896256031383	5.50600247707747
H	-5.16172506845110	4.62578836327977	6.91503561711151
C	-4.08089644641002	6.50299035294442	6.87025484242472
H	-3.56403737964008	7.13375274341269	6.12839260271351
H	-3.30194306969530	6.15429682643624	7.56881015365178
C	-5.11275971372045	7.34881221890216	7.63204434204881
H	-5.87555718127581	7.75461271229281	6.94971198571163
H	-4.63650670869914	8.19824052293225	8.14295555847870
H	-5.63382277580875	6.75018038236507	8.39483435403005
O	4.12131075401799	-4.08434829292550	-2.11196286740046
O	2.87037517733525	-1.06779066721124	-5.32051516679872
N	3.53980059600088	-2.55143359608099	-3.71021760744056
C	0.83619313453738	-1.17479402088239	0.42897514109822
C	0.92775130578920	-0.65227155815899	-0.90158888729534
C	0.16682447685055	0.48764297829637	-1.31747904434946
C	0.30517747745747	0.93895286586883	-2.63301487153538
H	-0.25721195242026	1.80080922510069	-2.97966450294542
C	1.15817329747367	0.30824788369429	-3.54742188299403
H	1.24537108751515	0.67343550944932	-4.56794596012019
C	1.90433811778459	-0.79534083598645	-3.16604668792752
C	1.80041961734667	-1.28688410868175	-1.84088134379181
C	2.56398598121617	-2.41595425938564	-1.45436629780946
C	2.46036167289018	-2.90546738835360	-0.16222730789680
H	3.05032607256279	-3.77477706105019	0.11820309781945
C	1.60836767727747	-2.29069405722502	0.76348905814896
H	1.56143147867894	-2.71165258066325	1.76337769701821
C	3.46679284503809	-3.09359587439782	-2.41735192599398
C	2.78978076834997	-1.45392660355967	-4.16018235497127
C	4.39444976059451	-3.25391959214107	-4.68878473796684
H	5.23639290053164	-3.67425939927922	-4.13849910093393
H	4.74238834213844	-2.51755892450861	-5.41779440316519
C	3.65709927689650	-4.42380718105333	-5.36728691775719
H	3.22158890897210	-5.06422672570349	-4.58159864687616
H	2.83065848461855	-4.03522843465528	-5.98228122618133
C	4.61220557859920	-5.27581355427096	-6.22134018347201
H	5.35045202872804	-5.75810662263067	-5.55489615131578
H	5.18644226473398	-4.62638688260803	-6.90489290049597
C	3.88706297989319	-6.35465918725653	-7.04372793910500

H	3.26373939707194	-6.96754074436559	-6.37169273439517
H	3.18999859350378	-5.86626589278917	-7.74485642988409
C	4.84816871547781	-7.26499261223346	-7.82342423844042
H	5.52731564748274	-7.80072705820813	-7.14258958417742
H	4.30132737534709	-8.01743542817065	-8.41007367894144
H	5.46930892811581	-6.68385026802123	-8.52214734277788

0.66 GPa

O	-3.95143168224585	4.12615681979065	2.10773336903864
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N	-3.41981958840775	2.57045221551896	3.69876434344470
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C	-0.75460763165138	0.68404927880602	0.93150924604274
C	-0.01984498306919	-0.47219024841340	1.34886573583736
C	-0.20384502514894	-0.94647035800480	2.65064671473434
H	0.33526970145645	-1.82340353704519	2.99656225985958
C	-1.07854027809722	-0.32363303077533	3.54960364806910
H	-1.20509852709856	-0.70947768932000	4.55834576352960
C	-1.79765112675715	0.79763941692354	3.16748755601691
C	-1.64450579380168	1.31485473089238	1.85702523324741
C	-2.37893651787028	2.46306879616390	1.47038906630065
C	-2.22948883287877	2.97518585666490	0.19159831471675
H	-2.79675925247526	3.85954480304595	-0.08896399862637
C	-1.36367324319404	2.36158386749484	-0.72212300812550
H	-1.28178904002986	2.79978083578755	-1.71236199610718
C	-3.30653752341684	3.13032515082510	2.41707177506769
C	-2.71310542254562	1.44100662916362	4.14406793491533
C	-4.33552540681171	3.23998011472007	4.64633554622958
H	-4.61795196660031	2.49323211145389	5.39309225687662
H	-5.22244118963365	3.53962216421026	4.07724784566204
C	-3.70401595965545	4.46351102017490	5.32864319327362
H	-3.32199111268921	5.15006835091433	4.55898258180057
H	-2.84333925332755	4.13644320662203	5.93351049675869
C	-4.72824556401910	5.19373792458940	6.21344194262261
H	-5.10439523031192	4.50267806780837	6.98802975289419
H	-5.60182880511279	5.47110236130716	5.59830814979292
C	-4.17017015470629	6.45863225154768	6.88669609356203
H	-3.30894531238465	6.18911800895579	7.51957939454436
H	-3.77991365271632	7.13927049305835	6.11171540738954
C	-5.21808467957614	7.19586571841570	7.73464277505950
H	-6.07099953948536	7.51953675796762	7.11856263987873
H	-4.79154534921673	8.09104556749967	8.21020594305459
H	-5.61181527643306	6.54877293499520	8.53336671122154
O	4.19001587487065	-4.05187415806683	-2.11100417071724
O	2.97028528260474	-1.03676302503586	-5.33374183006349
N	3.61985890273203	-2.52575741974172	-3.71748167604302
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C	1.01689385097533	-0.58956070115734	-0.92614608096529
C	0.27719414500188	0.56284315352594	-1.34566944556760
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H	-0.11444218780491	1.88460373145305	-3.00900655047614
C	1.28664153987654	0.37446710943224	-3.56630671686494
H	1.38554816036015	0.73793213555090	-4.58639991847714
C	2.01517654374750	-0.73914809014679	-3.17972783512803
C	1.89448207817343	-1.23072311586139	-1.85626730366158
C	2.64437332427239	-2.36695090314557	-1.46329530240163
C	2.52369772330660	-2.85566281985209	-0.17240761910477
H	3.10521270098127	-3.72865370528254	0.11454214344683
C	1.66166919084288	-2.23847927616843	0.74247881839892
H	1.60003527566369	-2.66000174623661	1.74134598706550
C	3.54451080399303	-3.05679696545127	-2.42068631078152
C	2.88933738089162	-1.41578721758019	-4.17088177926481
C	4.42862939757599	-3.27139030822575	-4.70443185120414
H	4.69879121473428	-2.56755532367310	-5.49475031340685
H	5.32091435970219	-3.64371223153840	-4.19326516729625
C	3.61758391019913	-4.41866749907143	-5.34089140277060
H	3.14523567532548	-5.02731306794570	-4.55607928958767
H	2.79844936600530	-3.97806489504730	-5.93119501006430
C	4.48961487996286	-5.30764859525784	-6.24161757749087
H	4.89803846224722	-4.70185606691029	-7.06970108199222
H	5.35727739606195	-5.67008327197110	-5.66378106470773
C	3.73317226561702	-6.51573086127991	-6.82053708727638
H	2.88184870601418	-6.16102361406218	-7.42452478333214
H	3.29892569054931	-7.10021648979499	-5.99217023796649

C	4.62548330451487	-7.42810516957119	-7.67551640517875
H	5.46052068399439	-7.83161628222184	-7.08245716477756
H	4.05875408976748	-8.28037058659962	-8.07780287086173
H	5.05619405605649	-6.88061650383167	-8.52772755485495

0.98 GPa

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N	-3.47116140430754	2.49715899606739	3.74911760370379
C	-0.69814736689585	1.17742758166064	-0.36308418017554
C	-0.82475537984592	0.62632051682450	0.95301171822610
C	-0.08561810880581	-0.53101587803131	1.35960101149292
C	-0.26265260881862	-1.01384925286319	2.65921318256752
H	0.28099780284474	-1.89073257989330	2.99779946792861
C	-1.13339526299880	-0.39776093485489	3.56678944659005
H	-1.25218714271938	-0.78878019149298	4.57440518378721
C	-1.85664607795603	0.72441151434510	3.19536247756118
C	-1.71317747786614	1.24787670194401	1.88619848781217
C	-2.45499071715296	2.39420419294649	1.50874584991297
C	-2.31606583835106	2.91276067461015	0.23136106405872
H	-2.89054862264231	3.79447603619880	-0.04222295330484
C	-1.44916324745792	2.31025788198998	-0.68860308507347
H	-1.37401385757539	2.75417462028988	-1.67675847125462
C	-3.37645246919836	3.05551921973649	2.46509153349366
C	-2.76116071714385	1.36601264288207	4.18380258861599
C	-4.36053734302683	3.18143849103338	4.71208793732952
H	-4.62935699676477	2.44389093237517	5.47309095321604
H	-5.25857119705072	3.48086134952519	4.16074015975190
C	-3.69707683959708	4.40988651349051	5.35593082301368
H	-2.87207381963539	4.07655880465844	6.00661964694218
H	-3.26057100943648	5.03664397108497	4.56463120216451
C	-4.70443219441213	5.24566821811563	6.16260947427387
H	-5.13696691074625	4.63281933335621	6.97211214359376
H	-5.54585282340242	5.52615963596320	5.50578599407755
C	-4.08920647559849	6.52228875067302	6.75975764219935
H	-3.25793975217336	6.25012622684738	7.43062676273411
H	-3.64312235079438	7.12105238650594	5.94809718120305
C	-5.10934948817934	7.37961564761398	7.52392174392656
H	-5.92462298755763	7.70885361212757	6.86149026296973
H	-4.63993086556449	8.27928840750958	7.94757972170619
H	-5.56207919087317	6.81648926430823	8.35424537286114
O	4.16043048767206	-4.04284101984079	-2.12431284758985
O	2.94372752458030	-0.99310301450706	-5.31513457252607
N	3.59342087374352	-2.49730094425679	-3.71354320486461
C	0.83155714402634	-1.16830104528450	0.40234025051929
C	0.95334134432923	-0.62133860666432	-0.91571477887194
C	0.21004760635905	0.53278786362465	-1.32413976783690
C	0.37349297418711	1.00462266560546	-2.62955580437094
H	-0.17654035783097	1.87635953962928	-2.97110872482259
C	1.23469534544924	0.38063335739561	-3.54081720895805
H	1.33928313049380	0.75990153947533	-4.55449249117461
C	1.96639456839528	-0.73465430291564	-3.16532943440736
C	1.83928264032207	-1.24536202306061	-1.84960634715443
C	2.59216477571105	-2.38319345151286	-1.46763375109665
C	2.46389716248022	-2.89270292212279	-0.18552880443627
H	3.04695582672226	-3.76750456742228	0.09211694892057
C	1.59436917448181	-2.29180388135939	0.73305009841911
H	1.52716026903595	-2.72908178312813	1.72471158709773
C	3.50799299015733	-3.04976414959673	-2.42622468750613
C	2.85514105187786	-1.38950598535235	-4.15870423558790
C	4.43484256156848	-3.21223531733103	-4.69640821331588
H	4.71873360089344	-2.48927625828988	-5.46362982474591
H	5.32107492764294	-3.57575055590459	-4.16791926945883
C	3.66531433759271	-4.36928226321564	-5.35989646198684
H	2.86413312099168	-3.93951654044990	-5.98780234872104
H	3.18561403978778	-4.97859203667753	-4.57929022423564
C	4.58475532432560	-5.26516025921846	-6.20535944859797
H	5.04959118430646	-4.67181222024920	-7.01149532932407
H	5.41363967722597	-5.62702326447153	-5.57272319486907
C	3.85556363285249	-6.47474465551566	-6.81460519189756
H	3.03805462063754	-6.12184671816110	-7.46456515497681
H	3.37539819486751	-7.05011061479295	-6.00539242172207
C	4.78728740165918	-7.39868076898130	-7.61308246541838
H	5.58474688000502	-7.80497886941812	-6.97212998250691
H	4.23768440597472	-8.24905322121113	-8.04207563659762

H	5.26961499321267	-6.85974917800700	-8.44279768998417

1.4 GPa

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N	-3.48872083514800	2.49174295366302	3.74584816770173
C	-0.70968920294376	1.15663174209094	-0.35728128976335
C	-0.84141256612002	0.60767711652811	0.95925867702691
C	-0.10391652815559	-0.54903490466455	1.37065305106257
C	-0.28567812470587	-1.02900228992014	2.67069823927170
H	0.25728060081836	-1.90493058805824	3.01317270049145
C	-1.15880435905094	-0.41041743248942	3.57431730613600
H	-1.28039194299370	-0.79886364001445	4.58266995974758
C	-1.88014915466780	0.71151525572489	3.19840081860394
C	-1.73301457904196	1.23122100825735	1.88808804121209
C	-2.47378985012465	2.37644122964210	1.50537739938196
C	-2.33220749905374	2.89094649690893	0.22667803943593
H	-2.90698879963425	3.77123582081746	-0.05118893173053
C	-1.46132766960204	2.28730371343906	-0.68868202251952
H	-1.38292974895661	2.72894338943367	-1.67764173479180
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C	-2.78476598322700	1.35803043171685	4.18382336425957
C	-4.37042213211497	3.18850141322549	4.70704392805245
H	-4.63705476368986	2.46027740367865	5.47741803249697
H	-5.27087827474369	3.48477969939091	4.15797631522409
C	-3.69844425351047	4.42357972667475	5.33030380613701
H	-2.87734956915330	4.09632850374246	5.98987665222621
H	-3.25604533954642	5.03068844221814	4.52695215824942
C	-4.69860200185606	5.28643492710438	6.11842351748928
H	-5.08135930092552	4.72058453265659	6.98488434000638
H	-5.57281181016553	5.50032128047915	5.47952340526582
C	-4.09656846974539	6.61816197300086	6.59763076539859
H	-3.20365304138877	6.41887406787921	7.21219304473583
H	-3.74165650050094	7.18645886216352	5.72167492836440
C	-5.09071763483772	7.47611446871807	7.39454834842562
H	-5.97452685107281	7.72527854187203	6.78729532458569
H	-4.63296463986888	8.42131313091467	7.72083259345525
H	-5.44317461342854	6.94749005143427	8.29341352873484
O	4.15791960185083	-4.06465470813444	-2.08968573975692
O	2.97870214949048	-1.00121714325849	-5.28110048345484
N	3.61278825842196	-2.50912310851393	-3.67740432071264
C	0.81731382263677	-1.18779294443022	0.41819541027130
C	0.94748567089154	-0.64032759536108	-0.89893450089873
C	0.20562438840734	0.51301436941172	-1.31220102932647
C	0.37802951647521	0.98577339765245	-2.61614802806561
H	-0.17116507489726	1.85672415600393	-2.96130543313486
C	1.24804953263633	0.36467549904682	-3.52090543721492
H	1.36074597489115	0.74552333294000	-4.53319141604235
C	1.97852195763770	-0.74977614924922	-3.14066497876272
C	1.84082513751835	-1.26278265930154	-1.82682088356393
C	2.59010247888222	-2.40168828021598	-1.44093443055815
C	2.45191809868267	-2.91296303941195	-0.16057222981116
H	3.03210094123526	-3.78887551337458	0.11997778809821
C	1.57672995932728	-2.31240287604451	0.75284373983793
H	1.50199337713704	-2.75107215474522	1.74340797070257
C	3.51238047833769	-3.06772859539795	-2.39366770544757
C	2.87810665877430	-1.40079742909496	-4.12668570220289
C	4.46056833838728	-3.22261091341198	-4.65574962360728
H	4.77373102477616	-2.49340861846578	-5.40519118170426
H	5.32888568080527	-3.60994124440003	-4.11491857628357
C	3.68300042870132	-4.35693740539830	-5.34913493384869
H	2.90841693299657	-3.90454880237763	-5.99515812967328
H	3.17003842161600	-4.95870024489834	-4.58355480446072
C	4.60159333517758	-5.27093392443202	-6.17691402719345
H	5.04178830099247	-4.70204531617566	-7.01376817757351
H	5.44747695602568	-5.59842924562572	-5.54789975741015
C	3.87926836242963	-6.51452380546471	-6.72274568759681
H	3.01529239634170	-6.20188214431398	-7.33127359674317
H	3.46370017932023	-7.08693317715747	-5.87654285830775
C	4.79454377644575	-7.42544368177886	-7.55428359920510
H	5.64700811316140	-7.78186740779483	-6.95575898413184
H	4.25323790041191	-8.30866708079568	-7.92348113049018
H	5.20089528037288	-6.89310391691301	-8.42780681340187

1.73 GPa

O	-4.06585804122572	4.02970147301497	2.13016555480716
O	-2.91861524444301	0.94298532536811	5.31405928993468
N	-3.50720354995210	2.48885525248128	3.72672870584993
C	-0.71481137827960	1.15827582231870	-0.36900287826386
C	-0.84610628005950	0.61178455078975	0.94848388374563
C	-0.10397890339216	-0.54066543982093	1.36346750717774
C	-0.28602151921599	-1.01931935900258	2.66392690503522
H	0.25930194496291	-1.89295768999829	3.00858353540285
C	-1.16273099908303	-0.40227670459970	3.56509523058750
H	-1.28412354743633	-0.78909647345673	4.57412285392649
C	-1.88796173414431	0.71599738861030	3.18582074001250
C	-1.74137892862207	1.23383408345978	1.87481090738943
C	-2.48621581571922	2.37549165772424	1.48910027689551
C	-2.34427576340429	2.88822696157474	0.20970210946257
H	-2.92131528623133	3.76633939462946	-0.07055585255491
C	-1.47030766478755	2.28557438203071	-0.70343697768771
H	-1.39254803661654	2.72533954180582	-1.69333322372404
C	-3.41198279721039	3.03969440228058	2.43951377995662
C	-2.79612481620026	1.36104957248426	4.16862850464846
C	-4.39133145547154	3.18126218407351	4.68926502869034
H	-4.66698652688996	2.44442902441949	5.44753878189651
H	-5.28605362343060	3.49016689545580	4.13797833346229
C	-3.71163538535024	4.40367445331664	5.32776234641206
H	-2.87482831517424	4.06681379251638	5.96045119861145
H	-3.28892435103838	5.02832319575478	4.52704299431476
C	-4.68581449702740	5.25141547123190	6.16311276766515
H	-5.58397175933127	5.47603346878733	5.56336894001329
H	-5.03630152903640	4.67378499539898	7.03550501731777
C	-4.05773981210743	6.57472023041747	6.63398145558761
H	-3.65998967043528	7.10944456107383	5.75406155614166
H	-3.19011380338249	6.35892401694499	7.27989816303972
C	-5.04510242733903	7.48400069401093	7.38140944651571
H	-5.45474272052763	6.98648650086671	8.27353266525833
H	-5.89445771255902	7.76046767318200	6.73815253284538
H	-4.56052879727727	8.41432112140813	7.71188404686302
O	4.18406613393921	-4.04122694940880	-2.08134586590532
O	2.98414886034955	-0.99786941008938	-5.28445552149183
N	3.62833893170422	-2.49615092400214	-3.67523413084081
C	0.82232722618705	-1.17653948203797	0.41404653783713
C	0.95152891560971	-0.63202744424652	-0.90425560992757
C	0.20387100687752	0.51606406103579	-1.32164719396035
C	0.37452097953821	0.98560204249742	-2.62696034030342
H	-0.17899819108372	1.85259575843311	-2.97527111736164
C	1.24822360620386	0.36596104241801	-3.52916200027769
H	1.35899720385220	0.74368991813051	-4.54285200855143
C	1.98491767945765	-0.74289053563967	-3.14452057262677
C	1.84944127854823	-1.25235560839979	-1.82918764662496
C	2.60563477112148	-2.38527399105941	-1.43897884029221
C	2.46884406051045	-2.89326877664796	-0.15714278957591
H	3.05394574609587	-3.76478979257155	0.12701546700937
C	1.58869341197742	-2.29516557387277	0.75316623874389
H	1.51604557326629	-2.73059711938784	1.74535561939143
C	3.53258673456797	-3.04933649187546	-2.38901823746204
C	2.88749442643305	-1.39304957064889	-4.12818128367948
C	4.47464653621236	-3.21016398776081	-4.65512015680941
H	4.77105765568048	-2.48194200305213	-5.41104678324525
H	5.35126019699443	-3.58836957046409	-4.12131733857679
C	3.69493386480387	-4.35079076385812	-5.33521693125438
H	2.89449105829853	-3.90601453995484	-5.95333874205148
H	3.21483786034397	-4.96529445473862	-4.55861930795772
C	4.58915672407132	-5.24885393889272	-6.20618498603088
H	5.46794720811722	-5.57078911170138	-5.62247923012015
H	4.98373508814926	-4.67296900271888	-7.06073968872240
C	3.84738157283355	-6.49609434687068	-6.71818773430672
H	3.40760372321343	-7.02425644826423	-5.85431412493527
H	2.99969998568196	-6.18429804862555	-7.35117141820864
C	4.75014413821390	-7.46094707182410	-7.50177190977011
H	5.19832055100877	-6.97047329500365	-8.37915049969231
H	5.57459983320793	-7.83074746643451	-6.87312260614774
H	4.18633639545149	-8.33446952301564	-7.86041537350799

3.84 GPa

C	-0.26151495586034	-1.48174754219497	-3.58296073181406
C	-2.00985740419567	-4.16848057038335	-5.65355185703987
H	-1.79466425608589	-3.58932981089165	-6.55411541553047

H	-3.08923381529371	-4.33473974206316	-5.58524710863655
C	-1.23271514588374	-5.50776224697594	-5.65818182683737
H	-1.84099210151893	-6.27577730182652	-5.15783270378770
H	-0.32784466039170	-5.37981980031413	-5.04373311434798
N	-1.63004979337941	-3.30111002194602	-4.51702707985746
C	-0.78332214383853	-5.96145513251358	-7.06140768953198
H	-1.64204644122304	-6.20406546075730	-7.70556793677551
H	-0.26447933630517	-5.11298263016103	-7.53874064320113
C	-0.62553303475505	-2.34429009519103	-4.73541970142316
C	-2.23004657597789	-3.55724809442211	-3.27651675538217
C	0.17091289032196	-7.17346750653467	-7.02488598314209
H	-0.40691365173857	-8.09672111012640	-6.85521980723223
H	0.85211437722674	-7.07785048623018	-6.16282565963718
O	-0.08589128340181	-2.23052901286016	-5.83014924704131
O	-3.04936718699099	-4.46083616537207	-3.15229520980587
C	1.01181240411266	-7.30726419082465	-8.30453902749364
H	0.38157914213767	-7.31455252165485	-9.20494343068319
H	1.60705383010684	-8.23196448595908	-8.30255004587166
H	1.70762213115180	-6.46029056482255	-8.40264095001360
C	-0.86719876981766	-1.66266895858471	-2.31487098767675
C	-1.83487885395655	-2.68338841629211	-2.14395113355050
C	-2.42245165722741	-2.87133492516519	-0.90334875500586
H	-3.16274646286732	-3.65934751454377	-0.78745349434253
C	-2.06728747096554	-2.05820980248139	0.18012768321028
H	-2.55629429250434	-2.24318013457496	1.13182212544093
C	-1.11962932097197	-1.03791792752341	0.05932569443723
C	-0.50107815955355	-0.82518270339167	-1.21461355111543
C	-0.73873632930044	-0.18042629789233	1.19213246628527
C	-1.28904066316205	-0.33902520964075	2.46708517559542
H	-2.02054777835490	-1.11890436036710	2.65646589048931
C	-0.92823465597902	0.48859880166554	3.53756392102147
H	-1.37066730932431	0.34900153161214	4.52101433817778
C	0.00001539686294	1.50191230588200	3.36007602634486
C	1.69751429839576	4.22281233146348	5.41684051688334
H	1.67886786912693	3.60331714690457	6.32984413605161
H	2.72801695040989	4.54765809806260	5.24302766934409
C	0.77533371797893	5.46270985119585	5.55614771814152
H	1.02514710782849	6.16110475358698	4.74124186539658
H	-0.27341289963228	5.15746936177238	5.42276396364159
N	1.32829057882376	3.35788377296671	4.28000805019671
C	0.98169133207697	5.99965842093216	6.97784290208485
H	2.04086841637101	6.19503563553040	7.16727297536089
H	0.74923222718213	5.13719201963491	7.62996385546085
C	0.36153488949475	2.36672734841878	4.51090250710807
C	1.91621268144998	3.62752378235595	3.03406022166238
C	0.26849402441539	7.20280197640428	7.63212358161091
H	0.70030509424380	8.14970809155060	7.28088562798918
H	-0.79312844485040	7.23169416535269	7.32938010769118
O	-0.14802642652970	2.23108093821555	5.61734785946204
O	2.71001630743748	4.55142253361158	2.89744584739084
C	0.33814365233821	7.12378388622830	9.16447836587879
H	1.36748876362307	6.96532676679509	9.51617553588519
H	-0.04045911345889	8.04485490212440	9.63020056206050
H	-0.26547950379936	6.28381277004714	9.53987656335775
C	0.58774615967406	1.69966021411629	2.08598027257632
C	1.53226624685068	2.74083833989809	1.90708150156619
C	2.10486166020015	2.94092343483660	0.66122488243176
H	2.82464143346194	3.74662647504617	0.53803834934023
C	1.76129762658379	2.11761000770229	-0.41822197070863
H	2.23622343455831	2.31439578410538	-1.37467750909967
C	0.83804250263193	1.07628213120726	-0.28902880899782
C	0.22630930689721	0.85787730699181	0.98728390210731
C	0.47467058455611	0.20361678219640	-1.41591930352017
C	1.04878365409857	0.34093888847936	-2.68280794466570
H	1.79872431717227	1.10465616719941	-2.86607538599302
C	0.69041876844674	-0.48911363769237	-3.75238434461978
H	1.15151612084716	-0.36553234191802	-4.72934754730107

Table S19. 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	5.58589892483765	5.66363408524681	6.55381541365107
N	5.00931051704316	7.08073362106130	4.85063722021432
C	6.28271114782136	4.46330482287664	2.30780727730779
H	7.14506029987427	4.11800053059190	2.90377829840661
H	6.68508814842561	5.17925424310926	1.57051104700691
C	5.28632817723545	5.18582073381143	3.22953279416898
H	4.89990222746601	4.48441532448168	3.98490987039115
H	4.42634477409711	5.54552461135760	2.64396585506130
C	3.89237355451729	6.95994378420519	8.40177788026693
H	4.49087325339517	6.12147985962613	8.74993595360138
C	3.03322882394062	7.63699467597163	9.27614094532349
H	2.98855078141766	7.29450503953699	10.30558196221060
C	2.25246762873138	8.71760487742268	8.85626654541676
C	4.92013901253060	6.62000563450038	6.17329453999214
C	6.05331575189622	1.34108116591902	-0.08907393110327
H	6.79443245261681	0.84205960244970	-0.73040183628104
H	5.21571358632666	1.65614861125798	-0.73008106822981
H	5.66577189951432	0.59220160532706	0.61846317988465
C	2.33776867258833	9.13332791948449	7.48859970857005
C	3.21979241603206	8.43747900401939	6.60290059082553
C	1.56325703759836	10.22742680016229	6.98431917528216
C	3.32255757904688	8.82852119479463	5.24487838888691
C	3.99543669883117	7.35019897513835	7.07633508344303
C	5.94076497890127	6.37839736952867	3.94351558711159
H	6.78468545116036	6.04242482668150	4.55439862216454
H	6.29305289144682	7.11521149315465	3.21475276082142
C	1.69405863151228	10.57298989492586	5.63638609826269
H	1.11837144135251	11.39532081584952	5.22214616519658
C	6.66841556641060	2.53849840403661	0.65159865603942
H	7.07597288258111	3.25431578494824	-0.08208884979254
H	7.52720696344761	2.19641594109700	1.25335692730106
C	5.66717994352501	3.26484786796049	1.56601156253047
H	4.80755385340123	3.60891396092982	0.96531809766921
H	5.25965728430041	2.55002500109903	2.30166651497469
C	2.55949763173763	9.88584216756728	4.77606306674811
H	2.64645750144530	10.17254785304647	3.73076801746115
O	4.33191083573759	8.43140603212374	3.13046763723498
C	4.23820611375942	8.12303534184648	4.31310117386717
O	-2.65355430320039	14.01685149696215	10.20727285863972
N	-2.07531945174603	12.60022013435981	11.91037897353486
C	-3.25248263724489	15.16926258535912	14.55307654165142
H	-4.17024982209973	15.51012426134814	14.05553644905002
H	-3.57921468580225	14.41115515798423	15.28639127964268
C	-2.31025741535239	14.49035031577954	13.54033385396143
H	-1.95823882334353	15.20817578465037	12.78298085495784
H	-1.42031020860499	14.11576251340334	14.06926948897769
C	-0.97668311986929	12.70667704084348	8.35267529581533
H	-1.57475590023956	13.54556386451871	8.00476356558499
C	-0.12154924721639	12.02636019548024	7.47670040973391
H	-0.08030290890773	12.36628479385598	6.44624226191748
C	0.66069065683551	10.94677021925679	7.89651907635510
C	-1.99139250794630	13.05734973910572	10.58608105881973
C	-2.82097907680226	18.02349179610819	17.23217710446033
H	-3.50028079491069	18.43740113543318	17.99188295133610
H	-1.96880781183037	17.57157030880392	17.76255403068634
H	-2.43192120964002	18.86245250606308	16.63527629788798
C	0.57743602929891	10.53264409441804	9.26482280784828
C	-0.30081746351460	11.23144031653199	10.15194859603914
C	1.35124477235633	9.43792670629768	9.76875676660460
C	-0.40044294751889	10.84225314351895	11.51066005021677
C	-1.07514358848345	12.32020353460067	9.67962106076144
C	-2.99171884231854	13.31243773431005	12.82561814841573
H	-3.83406280361995	13.66118084200544	12.22030169717631
H	-3.34831746126198	12.57738955704405	13.55410207301264
C	1.22294288760629	9.09381771447972	11.11727160277785
H	1.79895293760544	8.27164477817110	11.53130209756911

C	-3.52937976131774	16.98698156543769	16.34596947482479
H	-3.97064344538755	16.20224552413871	16.98223662213516
H	-4.37552379310666	17.46186289427436	15.82168806775103
C	-2.59367505289815	16.33086606634647	15.31494317409986
H	-1.69561997337369	15.95057918130479	15.83224928320741
H	-2.23733706011008	17.09360551979626	14.60163516197635
C	0.36099624064116	9.78353031403480	11.97881827411863
H	0.27638967155026	9.49866941668306	13.02479667413529
O	-1.39960110179923	11.24579006519252	13.62822760213034
C	-1.30883831293009	11.55304770494898	12.44501548029761

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

Table S22. Coordinates of atoms of theoretical high-symmetry conformers of PDI-C_n molecules – models taken from crystallographic data and freely optimized in Orca at the B3LYP-gCP-D3/6-31G* theory level.

PDI-C_5

O	-4.08738922238615	4.14654947800171	1.96317188627697
O	-2.81959028631590	1.28602366080360	5.30430513813695
N	-3.50406300913364	2.68404421243747	3.62530874639860
C	-0.79472015321345	1.12965561904393	-0.44558476189686
C	-0.87211813700420	0.67925840543390	0.91158542655085
C	-0.09828658792672	-0.43029724960687	1.38213003118818
C	-0.21914193631152	-0.80852245082566	2.72211398330278
H	0.35723698647510	-1.64237907828941	3.11159655682438
C	-1.07438486208250	-0.13944251879874	3.60640406735608
H	-1.15324967448836	-0.45092773883711	4.64522630830593
C	-1.83641778262572	0.93254524767791	3.17039224381714
C	-1.74319306406403	1.35693487842419	1.82173338490655
C	-2.51656981417516	2.46026568044380	1.38278340608312
C	-2.42201778693293	2.88322935363160	0.06670303803055
H	-3.01815617758795	3.73390459270447	-0.25494268977653
C	-1.57337771084548	2.22438342887551	-0.83154747410648
H	-1.53424120069742	2.59351040925366	-1.85200864206139
C	-3.42611885395620	3.17548435080667	2.31293028083818
C	-2.73665246724493	1.62195436588818	4.12838715245423
C	-4.40759064764776	3.38072533026979	4.56466386086411
H	-5.25532934995468	3.74737714616724	3.97738454732615
H	-4.76078151102708	2.63300834659719	5.28173905909717
C	-3.71489876656699	4.54211735270041	5.29397834363927
H	-3.33101383958463	5.25478090241727	4.54769128645066
H	-2.84912061264529	4.15034972605249	5.84966583351555
C	-4.67219895564104	5.26171529983322	6.25810103588121
H	-5.54183562912518	5.64170192065422	5.69461885925437
H	-5.07193251403632	4.53673977152979	6.98819442332717
C	-4.00908729021282	6.42650623245698	7.01329011586569
H	-3.60847650897422	7.15064573234754	6.28435706374062
H	-3.14032249693173	6.04645305508295	7.57618019939843
C	-4.96984485390001	7.14328166269627	7.97424978436074

H	-5.83029363933643	7.56629479358841	7.43364861539650
H	-4.46889121556944	7.96768825193942	8.50223280455587
H	-5.36363148685425	6.45063473847379	8.73380197981689
O	4.08738439195168	-4.14655433834254	-1.96317165540918
O	2.81959435293860	-1.28602039222078	-5.30430092144410
N	3.50406275295302	-2.68404460620177	-3.62530600147244
C	0.79471001246302	-1.12966509869455	0.44558447404055
C	0.87211091149793	-0.67926508702718	-0.91158462754866
C	0.09827843101430	0.43028978778951	-1.38212974156189
C	0.21913547579997	0.80851661683135	-2.72211306610453
H	-0.35724467989867	1.64237249126440	-3.11159543644101
C	1.07438154016780	0.13943944054134	-3.60640198784972
H	1.15324788324237	0.45092663214110	-4.64522354698353
C	1.83641560396374	-0.93254749986840	-3.17038990710899
C	1.74318617853632	-1.35694118626786	-1.82173265482282
C	2.51656442636867	-2.46027099378473	-1.38278255404283
C	2.42200771521203	-2.88323882223815	-0.06670381260681
H	3.01814460900038	-3.73391526192059	0.25494155611883
C	1.57336607128590	-2.22439424592482	0.83154627729586
H	1.53422719405632	-2.59352297529757	1.85200664700875
C	3.42611534155619	-3.17548789690388	-2.31292898974443
C	2.73665312135119	-1.62195402764854	-4.12838403001338
C	4.40759355241520	-3.38072256546514	-4.56466051719254
H	5.25533198604690	-3.74737381321963	-3.97738045692141
H	4.76078404229601	-2.63300366558282	-5.28173388201434
C	3.71490447450660	-4.54211453606228	-5.29397766690839
H	3.33102113253315	-5.25478042772666	-4.54769207683550
H	2.84912544329434	-4.15034758387044	-5.84966432177126
C	4.67220590068592	-5.26170869771185	-6.25810188601235
H	5.54184299252833	-5.64169545640215	-5.69462046943950
H	5.07193856394808	-4.53673095624945	-6.98819355145293
C	4.00909569376920	-6.42649869952553	-7.01329362723602
H	3.60848521906600	-7.15063998262240	-6.28436218897751
H	3.14033079311820	-6.04644511932128	-7.57618327026149
C	4.96985432513508	-7.14327132392057	-7.97425429567729
H	5.83030347985541	-7.56628436902503	-7.43365365448563
H	4.46890181259629	-7.96767762176932	-8.50223884252168
H	5.36364031326957	-6.45062262762762	-8.73380520872147

PDI-C_6

O	5.86889376828612	5.51510519369606	6.69451002799370
O	4.65969117685918	8.43911699083092	3.38698697846551
N	5.31583408021109	7.00910010309788	5.05055865828331
C	3.56000002439010	8.33251799553727	6.86162454140711
C	2.07730900125069	10.53627476318024	5.98555049048150
H	1.51785757956579	11.38609776605979	5.60605825199832
C	1.94232575794939	10.14007010269389	7.31904717479884
C	2.60316635763487	8.54239142153434	9.12721427875871
C	6.53213567697224	4.45527156906227	2.41643838685360
H	7.39332238232792	4.08168438454636	2.99678268167223
H	6.94007884715854	5.18565402523409	1.69652380002362
C	4.31364166386792	7.21111270305096	7.28881596910725
C	5.22074879583804	6.49843314101842	6.35437606116725
C	2.92598884379468	9.86593564600666	5.09590022566067
H	3.01631963940165	10.19195079372996	4.06246213650281
C	2.69472844782665	9.01075604298283	7.77698121393347
C	3.66757082693492	8.77488697702192	5.51980575596453
C	5.89513651010864	3.28613104549423	1.64640338340418
H	5.48124577152003	2.55796030055964	2.36526798653885
H	5.03718969626941	3.65806612127431	1.06013248558226
C	3.36238988685394	7.43004283888033	9.50134276256599
H	3.31291809199990	7.04752099315537	10.51643154785411
C	4.20536171910364	6.77067951260433	8.59807769474759
H	4.78668461683089	5.90649496442908	8.91068459590466
C	5.55212572617305	5.16562277591961	3.36493828021927
H	5.15640802237158	4.44730288437939	4.09924072536392
H	4.69615102225569	5.55855029354362	2.79491914019537
C	6.22998464918454	6.32353793842446	4.11336750440609
H	7.07347285299534	5.95454767804106	4.70559671115158
H	6.58760374344533	7.07942410859820	3.40722065316975
C	4.56479578671872	8.08733833510085	4.55732504354964
C	6.24514546050794	1.39955318313098	-0.05886114003453
H	5.40576261247732	1.74095281304202	-0.68387802098501
H	5.85471358983503	0.63691614117640	0.63222064274573
H	6.97458535885508	0.90879170504215	-0.71967439516585

C	6.88073367766939	2.56990290493682	0.70733188980093
H	7.73849593126238	2.20157779130178	1.29492296931973
H	7.29363630589083	3.29844405611751	-0.01070606468649
O	-2.20962955057090	13.86783217627941	10.69397800712078
O	-1.00043999880573	10.94380930320376	14.00149521232429
N	-1.65657986920394	12.37382750138689	12.33792379903751
C	0.09928671104786	11.05043746955098	10.52686972536729
C	1.58198518779444	8.84668608727636	11.40294594345918
H	2.14143966758250	7.99686541334197	11.78243907531026
C	1.71697206184621	9.24289431412729	10.06945068564735
C	1.05613260862286	10.84057415065358	8.26128395582807
C	-2.87298518593301	14.92757031746105	14.97207972261315
H	-3.73416717986093	15.30115740947744	14.39172833778420
H	-3.28092887903701	14.19715693684478	15.69196265549209
C	-0.65435566415335	12.17184231105364	10.09967833188986
C	-1.56147774895868	12.88450942322621	11.03411347067197
C	0.73329602463670	9.51701751776971	12.29259292497258
H	0.64295863900829	9.19099689067610	13.32602871851695
C	0.96456755217497	10.37220707568127	9.61151609973779
C	-0.00829109726207	10.60806206190470	11.86868583771561
C	-2.23602848266104	16.09670013863613	15.74216582774673
H	-1.82214065341391	16.82490479572209	15.02333395059035
H	-1.37808473150705	15.72476558531112	16.32844157446217
C	0.29691060196003	11.95292421358509	7.88715635538178
H	0.34638646604290	12.33544914950933	6.87206900756656
C	-0.54606876091259	12.61228137750384	8.79041901477398
H	-1.12739223317864	13.47646541270866	8.47781166431486
C	-1.89294008910642	14.21726724177973	14.02357974084466
H	-1.49722030058285	14.93561599818839	13.28930663642430
H	-1.03697047669808	13.82433966223696	14.59360635913777
C	-2.57076258280291	13.05936087820281	13.27510444117112
H	-3.41423840361883	13.42835397740491	12.68285936049388
H	-2.92839310385468	12.30345558934403	13.98122530193870
C	-0.90553654623862	11.29559382150848	12.83115953064359
C	-2.58611809128848	17.98321243670736	17.44748701472190
H	-1.74674026444249	17.64181221349152	18.07251030219145
H	-2.19568986886744	18.74588189681491	16.75643894989276
H	-3.31558378839550	18.47393442721078	18.10830112390061
C	-3.22166199952694	16.81287305074946	16.68124152617176
H	-4.07942124491883	17.18119719767259	16.09364540832666
H	-3.63456162751438	16.08429757136026	17.39924637709489

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O	5.60240471243012	6.10245192497839	10.86412619444734
O	4.26156205427868	8.78867130841519	14.31993824567293
C	3.97377933857923	7.75670954382640	10.35715221399198
C	2.27051027067932	9.50035840854140	9.96243541171773
C	2.20095407964882	9.10088163864645	8.58902159943105
C	4.91049234211817	7.03566259337142	11.25519171755226
N	4.97754538376695	7.47600936235536	12.58610876895658
C	1.58287383808550	10.89791534190218	11.83112391565508
H	0.98421237697392	11.69914269293427	12.25414799352278
C	3.88765126508327	7.38343179017213	9.02559461440598
H	4.51003219594427	6.56642435080099	8.66835315361889
C	3.25475031752943	9.19134775512306	12.20565710582330
C	3.16766823110824	8.81639402672934	10.84205446958096
C	1.46519543672842	10.56629520458188	10.47850476313423
C	6.24753537497841	4.84754776956236	15.11870997203587
H	7.11521581660213	4.50381891945409	14.52971459593714
H	6.64298735981446	5.56251329023281	15.86069071067689
C	2.46310339867147	10.22236650939556	12.68545108887912
H	2.53866000434269	10.49699110645819	13.73490661019914
C	3.01389572137191	8.04920670039712	8.15706136423757
H	2.98321752408334	7.72091910903527	7.12244854071092
C	5.99914339105550	1.73389096555421	17.53281274502908
H	5.13782936717795	2.08477129517266	18.12590572999921
H	5.59329773625899	1.01353336112648	16.80265256496896
C	5.90961674354325	6.77452368544602	13.49343043706613
H	6.24837533653008	7.50800163305711	14.23198950843556
H	6.76175997141341	6.45262320307254	12.88658863644443
C	6.61666249827899	2.92546248749902	16.78100192427189
H	7.47960563845208	2.57438034969118	16.18870837584158
H	7.02304508438951	3.64503714192217	17.51309541713183
C	5.62519467155620	3.64849057464126	15.85422440874802
H	5.22695441812481	2.93311848669645	15.11413441695656

H	4.75834145608109	3.99299126430123	16.44402175885922
C	5.25772900069381	5.57084639057195	14.19086106420116
H	4.88342047686104	4.87278280620173	13.42620032998766
H	4.38938513788679	5.92032901240852	14.77030795842507
C	6.99916482667424	1.02011729023954	18.45543369702749
H	7.85462407138137	0.62648174939811	17.88535116560579
H	6.53025234584830	0.17501854815988	18.98037669850091
H	7.39763670720461	1.70713691009025	19.21775373517116
C	4.18157959727224	8.49458324098556	13.13264001006018
O	-2.85636537071330	14.27018763708942	7.29821451747913
O	-1.51551309332386	11.58397720867522	3.84239969176740
C	-1.22772808485232	12.61594051778679	7.80518483122594
C	0.47554758853372	10.87229749037084	8.19990025635291
C	0.54510526384412	11.27177645837765	9.57331338534248
C	-2.16444907798974	13.33698032568433	6.90714797357020
N	-2.23150307161477	12.89663247587821	5.57623142123356
C	1.16318697929217	9.47474358465420	6.33121020941855
H	1.76185059779145	8.67351810588760	5.90818562918246
C	-1.14159783639506	12.98922085511784	9.13674149761055
H	-1.76398158933104	13.80622575657206	9.49398379203763
C	-0.50869548566046	11.18130584341975	5.95667925255880
C	-0.42161271026788	11.55625965548954	7.32028180221541
C	1.28086505646727	9.80636348349067	7.68382947590850
C	-3.50154951404421	15.52507651887769	3.04364066773065
H	-4.36922960085982	15.86879166572003	3.63264464981485
H	-3.89699765010611	14.81010477242970	2.30166385831239
C	0.28295538040856	10.15029078941563	5.47688382024289
H	0.20739851547513	9.87566610951807	4.42742832788506
C	-0.26783812114912	12.32345017393493	10.00527368162390
H	-0.23715864641570	12.65173889829378	11.03988596510955
C	-3.25323773563434	18.63873660676210	0.62953441653867
H	-2.39192588534032	18.28787058105413	0.03642978371136
H	-2.84739425420500	19.35910108225633	1.35968900554922
C	-3.16358844037218	13.59810582410811	4.66891480038901
H	-3.50234105066240	12.86462319491648	3.93035762003868
H	-4.01573272666279	13.91999403807197	5.27576177065504
C	-3.87072716984398	17.44715505419849	1.38135356595618
H	-4.73366894120134	17.79822305457208	1.97365754995479
H	-4.27710676560468	16.72757321651611	0.64926546877040
C	-2.87923624230040	16.72414371747215	2.30811951616688
H	-2.48099935434572	17.43952235953064	3.04820497060985
H	-2.01238420176216	16.37965710101049	1.71831219598621
C	-2.51172332199060	14.80179277919314	3.97148012483616
H	-2.13741877610680	15.49986135928221	4.73613826653387
H	-1.64337929942223	14.45232327827619	3.39202553024998
C	-4.25328347081973	19.35249370154977	-0.29307307373188
H	-5.10874125148447	19.74611562163542	0.27702107683133
H	-3.78439191198760	20.19759986302621	-0.81802280531216
H	-4.65175473788643	18.66546738006645	-1.05538739836372
C	-1.43553151095901	11.87806411666736	5.02969827508724

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O	5.37784171884881	5.14759363322839	11.92049349403592
O	4.07923030920345	7.94104843670909	15.30656601551860
C	3.79063586635175	6.82647781961291	11.36618465777844
N	4.77287824965986	6.57159573567193	13.60788703383994
C	2.13017437977877	8.59852687165405	10.92148705702565
C	3.00829268463953	7.91632609761409	11.82134605026054
C	2.05427697196599	8.16514507133203	9.55854629843315
C	3.10010526633925	8.32333339108519	13.17549120124094
C	1.34967416886881	9.69644497385930	11.40690771975300
C	2.33485604116397	9.38728284522504	13.62479971003360
H	2.41509097678248	9.68786010313179	14.66679963762160
C	3.70009639426510	6.42178018474564	10.04406564039479
H	4.30414316102399	5.58155734817683	9.70998520830410
C	1.47454282623354	10.06227591544699	12.75006611312378
H	0.89711890314743	10.89030370730333	13.14984891058097
C	5.67016230586706	5.85557508523522	14.53954170120587
H	6.00915288205658	6.58559912264454	15.28130679539630
H	6.52785357824520	5.51014419816605	13.95359999781455
C	4.70531940419503	6.10505985178448	12.28590316345288
C	4.00121324208014	7.62339961162623	14.12539513450714
C	5.24836747289208	2.71136396488663	16.85519485141848
H	4.38362208233332	3.06894783729293	17.44052026390538
H	4.83830894231329	2.03133989554627	16.08869270567496

C	2.84411267916554	7.08477337328196	9.15616159837105
H	2.80855658607274	6.73080051488102	8.12995281411964
C	5.92187085784757	3.90723776565774	16.16160666922947
H	6.31828898940000	4.59718498588999	16.92632037008016
H	6.79377972182836	3.55076164495589	15.58638465120809
C	4.97242338650376	4.67089696049251	15.22400389114654
H	4.10627285652395	5.04468385146649	15.79161563755529
H	4.58830655481992	3.98892816700483	14.44989241053450
C	5.52610964849802	0.72711508916345	18.46617295193504
H	5.11063611990927	0.05024048235553	17.69926070818877
H	4.66395392632598	1.08131377322932	19.05810973717287
C	6.19729571651064	1.92586218426530	17.77573403381051
H	6.60835406531697	2.60552105551116	18.54233220799310
H	7.06200668967382	1.57083845677365	17.18836838654990
C	6.47636689840636	-0.06507989291741	19.38012937224865
H	7.33833320405002	-0.41842963625918	18.78926642904910
H	6.89011681907127	0.61052415665714	20.14758868808359
C	5.79932295386405	-1.26250137596170	20.06428832099066
H	5.40904099607219	-1.97595279096834	19.32232636950826
H	4.95297511697028	-0.93854476503545	20.68943625642905
H	6.50285048208087	-1.80646465994148	20.71185702744362
O	-2.87626118381959	13.41578187298421	8.11951263356290
O	-1.57765142099775	10.62232576864812	4.73344060409764
C	-1.28905671241436	11.73689656711049	8.67382186998691
N	-2.27129857315556	11.99177910056374	6.43211935302235
C	0.37140376430688	9.96484666807492	9.11851982072253
C	-0.50671422309826	10.64704769594086	8.21866070431980
C	0.44730124288851	10.39822854454849	10.48146055732476
C	-0.59852695804900	10.24004026093442	6.86451559613955
C	1.15190374320980	8.86692837477265	8.63309922084396
C	0.16672175991499	9.17609036271990	6.41520724931243
H	0.08648664231210	8.87551292447785	5.37320739008814
C	-1.19851707017656	12.14159435656942	9.99594083459021
H	-1.80256315016284	12.98181777721124	10.33002103619338
C	1.02703483135004	8.50109719011597	7.28994090953196
H	1.60445850480815	7.67306916284694	6.89015824231787
C	-3.16858162964622	12.70780055403290	5.50046436510529
H	-3.50757305803691	11.97777672926301	4.75869944011675
H	-4.02627250357848	13.05323271761546	6.08640589380863
C	-2.20373938194608	12.45831524972850	7.75410309600528
C	-1.49963454359456	10.93997438090178	5.91461155022318
C	-2.74678222145407	15.85201021366424	3.18481010101789
H	-1.88203721692370	15.49442490206291	2.59948499517064
H	-2.33672287511953	16.53203402364921	3.95131204482700
C	-0.34253386443807	11.47860075275468	10.88384506262320
H	-0.30697748641120	11.83257383273593	11.91005376643604
C	-3.42028737392836	14.65613764991558	3.87839868314675
H	-3.81670633881814	13.96619065839077	3.11368520124310
H	-4.29219583846671	15.01261520974991	4.45362041476515
C	-2.47084108575877	13.89247756012997	4.81600192554378
H	-1.60469090527025	13.51868939871478	4.24839048222600
H	-2.08672354720607	14.57444610605591	5.59011327663610
C	-3.02452125318014	17.83625872937370	1.57383105831405
H	-2.60904687564236	18.51313306903316	2.34074308121409
H	-2.16236592934613	17.48205852835024	0.98189459204492
C	-3.69570918207911	16.63751293389079	2.26427039655756
H	-4.10676839264967	15.95785431345180	1.49767245637742
H	-4.56041974558954	16.99253817077031	2.85163574060462
C	-3.97477719556511	18.62845465988840	0.65987410905452
H	-4.83674305191004	18.98180598175791	1.25073676425613
H	-4.38852803125119	17.95285083177910	-0.10758491661983
C	-3.29773137912093	19.82587478399280	-0.02428535035074
H	-2.90744852333298	20.53932602753415	0.71767629134990
H	-2.45138388411681	19.50191661350425	-0.64943294665318
H	-4.00125797970257	20.36983874730661	-0.67185449006783

8. Detailed crystallographic data

Table S27. Detailed crystallographic data for PDI-C_5 at high pressure.

Pressure		0.1 MPa	0.66 GPa	0.98 GPa	1.40 GPa	1.73 GPa	2.17 GPa	2.70 GPa	3.84 GPa
Phase		I	I	I	I	I	IV	IV	IV
CCDC numbers		2493894	2493895	2493896	2493897	2493898	2493899	2493900	2493901
λ		0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Crystal system		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
Unit cell dimensions	*a* (Å)	4.727(3)	4.6276(7)	4.5635(9)	4.5189(16)	4.4671(8)	3.7606(6)	3.7203(3)	3.639(3)
	b (Å)	8.493(3)	8.4373(8)	8.3918(9)	8.3710(17)	8.3465(11)	8.5729(5)	8.5616(7)	8.536(7)
	c (Å)	16.308(9)	15.934(8)	15.696(8)	15.611(8)	15.502(7)	18.044(6)	17.928(7)	17.49(3)
	α (°)	86.78(8)	85.82(2)	85.64(3)	85.46(5)	85.32(3)	87.221(17)	87.10(2)	87.48(16)
	β (°)	83.27(10)	82.97(3)	83.32(3)	83.42(6)	83.75(3)	74.48(3)	74.75(2)	76.36(15)
	γ (°)	84.12(4)	85.077(10)	85.608(13)	85.97(2)	86.216(13)	101.631(8)	101.539(7)	101.09(7)
Volume (Å^3)		646.1(6)	613.9(3)	593.9(3)	583.7(4)	571.7(3)	545.8(2)	536.6(2)	515.8(11)
Z/Z'		1/0.5	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)		1.364	1.435	1.484	1.509	1.541	1.614	1.642	1.708
Absorption (mm^{-1})		0.090	0.094	0.097	0.099	0.101	0.106	0.108	0.112
F(000)		280.0	280.0	280.0	280.0	280.0	280.0	280	280
Crystal size (mm)		0.252 × 0.115 × 0.043	0.247 × 0.114 × 0.042	0.245 × 0.114 × 0.042	0.244 × 0.114 × 0.042	0.243 × 0.114 × 0.042	0.243 × 0.114 × 0.041	0.28 × 0.15 × 0.04	0.237 × 0.114 × 0.04
2θ-range for data collection (°)		8.804 to 53.756	8.902 to 52.944	9.104 to 53.574	9.19 to 54.05	9.302 to 53.694	9.768 to 53.834	9.78 to 54.5	9.778 to 51.324
Min/max indices: h, k, l		-5/5, -10/10, -5/5	-5/5, -10/10, -5/6	-5/5, -10/10, -5/6	-5/5, -10/10, -5/6	-5/5, -10/10, -5/5	-4/ 4, -10/10, -6/6	-4/4, -10/10, -6/6	-4/4, -10/10, -7/7
Reflect. Collected/unique		4469/530	2905/500	3430/523	2888/509	1738/425	2859/460	2487/452	1824/377
Data/restrains/parameters		530/539/183	500/361/182	523/291/182	509/460/183	425/357/182	460/352/182	452/318/182	377/291/170
Goodness-of-fit on F2		1.085	1.125	1.063	1.096	1.091	1.160	1.135	1.153
Final R1/wR2 (I>2σ1)		0.1066/0.2300	0.0999/ 0.1503	0.1037/0.1790	0.1020/0.1734	0.0967/0.1601	0.0898/0.2091	0.0790/0.2115	0.1383/0.2056
R1/wR2 (all data)		0.2291/0.3155	0.2017/ 0.2048	0.1956/0.2416	0.2009/0.2288	0.1860/0.2119	0.1491/0.2502	0.1542/0.2788	0.3610/0.3363
Largest diff. peak/hole (e.Å^{-3})		0.16/-0.16	0.15/-0.17	0.19/-0.21	0.23/-0.20	0.16/-0.19	0.20/-0.17	0.18/-0.19	0.14/-0.12

Table S28. Detailed crystallographic data for PDI-C_7 at high pressure.

Pressure		0.1 MPa	0.16 GPa	0.35 GPa	0.50 GPa	0.95 GPa	1.24 GPa	1.84 GPa
Phase		I	I	I	IV	IV	IV	IV
CCDC numbers		2493902	2493903	2493904	2493905	2493906	2493907	2493908
λ		0.4919	0.71073	0.71073	0.71073	0.4919	0.4919	0.4919
Crystal system		triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group		*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
Unit cell dimensions	*a* (Å)	4.8301(2)	4.7703(5)	4.744(2)	4.6610(6)	4.64199(18)	4.6043(3)	4.5578(2)
	b (Å)	8.3661(4)	8.2802(12)	8.250(4)	8.3844(14)	8.2981(3)	8.2991(5)	8.2194(4)
	c (Å)	19.3233(7)	19.028(10)	19.015(16)	18.520(7)	18.553(3)	18.274(5)	18.170(4)
	α (°)	79.542(4)	79.32(3)	78.90(9)	78.29(3)	78.624(7)	78.666(12)	79.124(9)
	β (°)	88.704(3)	89.42(3)	89.92(11)	87.11(3)	87.207(6)	86.695(11)	86.465(8)
	γ (°)	81.683(4)	82.010(11)	82.32(4)	83.681(14)	83.704(3)	84.238(5)	84.599(4)
Volume (Å^3)		759.79(6)	731.3(4)	723.5(8)	704.1(3)	696.12(11)	680.7(2)	664.82(14)
Z/Z'		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)		1.282	1.332	1.347	1.384	1.400	1.431	1.465
Absorption (mm^{-1})		0.044	0.086	0.087	0.089	0.048	0.049	0.050
F(000)		312.0	312.0	312.0	312	312.0	312.0	312.0
Crystal size (mm)		0.099 × 0.035 × 0.019	0.345 × 0.143 × 0.024	0.284 × 0.156 × 0.054	0.37 × 0.23 × 0.2	0.096 × 0.035 × 0.018	0.095 × 0.035 × 0.018	0.094 × 0.035 × 0.018
2θ-range for data collection (°)		10.536 to 46.056	5.056 to 60.766	5.124 to 52.746	4.988 to 56.462	6.114 to 45.866	10.546 to 46.656	10.574 to 46.708
Min/max indices: h, k, l		-5/7, -4/11, -27/30	-6/6, -10/10, -7/7	-5/5, -9/10, -6/6	-6/6, -10/11, -8/8	-7/7, -12/12, -9/13	-7/7, -12/12, -8/12	-7/7, -11/12, -9/12
Reflect. Collected/unique		1468/1395	1413/550	2080/641	4109/759	3290/1193	3008/1114	3177/1102
Data/restrains/parameters		1395/0/199	550/506/210	641/550/199	759/261/200	1193/126/200	1114/132/200	1102/132/200
Goodness-of-fit on F2		1.096	1.122	1.010	0.991	1.070	1.034	1.115
Final R1/wR2 (I>2σ1)		0.0684/0.2292	0.0852/ 0.2083	0.1019/ 0.1865	0.0694/0.1487	0.0829/ 0.2345	0.0855/0.2339	0.0859/0.2378
R1/wR2 (all data)		0.0733/0.2371	0.1579/ 0.2874	0.2604/0.2600	0.1287/0.1826	0.1058/ 0.2612	0.1172/0.2650	0.1129/0.2730
Largest diff. peak/hole (e.Å^{-3})		0.15/-0.12	0.19/-0.16	0.12/-0.13	0.17/-0.18	0.23/-0.21	0.21/-0.19	0.24/-0.24

Table S29. Detailed crystallographic data for PDI-C_7 at various temperatures.

Temperature (K)	100	150	200	240	270	320	375
Phase	I	I	I	I	I	I	I
CCDC numbers	2493915	2493914	2493913	2493912	2493911	2493910	2493909
λ	1.54178	1.54178	1.54178	1.54178	1.54178	0.71073	0.71073
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group	*P*-1	P-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
Unit cell dimensions: *a* (Å)	4.78950(10)	4.79800(10)	4.8090(3)	4.8161(3)	4.8251(4)	4.8258(9)	4.8295(13)
Unit cell dimensions: *b* (Å)	8.2562(2)	8.2755(2)	8.3005(5)	8.3243(6)	8.3440(7)	8.3561(13)	8.364(2)
Unit cell dimensions: *c* (Å)	18.9401(4)	18.9953(6)	19.0649(11)	19.1367(13)	19.1997(17)	19.307(4)	19.338(5)
Unit cell dimensions: *α* (°)	79.3950(10)	79.460(2)	79.525(3)	79.565(4)	79.494(5)	79.577(10)	79.563(15)
Unit cell dimensions: *β* (°)	90.1040(10)	89.925(2)	89.687(3)	89.387(4)	89.114(5)	88.648(11)	88.468(17)
Unit cell dimensions: *γ* (°)	82.5010(10)	82.325(2)	82.082(3)	81.920(4)	81.836(5)	81.636(10)	81.572(15)
Volume (Å^3)	729.60(3)	734.65(3)	741.05(8)	746.94(9)	752.29(11)	757.6(2)	759.9(3)
Z/Z'	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)	1.335	1.326	1.315	1.304	1.295	1.286	1.282
Absorption (mm^{-1})	0.686	0.681	0.675	0.670	0.665	0.083	0.083
F(000)	312	312	312	312	312	312	312
Crystal size (mm)	0.345 × 0.098 × 0.034	0.345 × 0.098 × 0.034	0.345 × 0.098 × 0.034	0.345 × 0.098 × 0.034	0.345 × 0.098 × 0.034	0.294 × 0.055 × 0.025	0.294 × 0.055 × 0.025
2θ-range for data collection (°)	9.504 to 145.174	9.474 to 125.418	9.436 to 129.988	9.4 to 161.61	9.37 to 145.428	4.29 to 42.514	4.284 to 39.174
Min/max indices: h, k, l	-5/5, -10/10, -23/23	-5/5, -9/9, -21/ 21	-5/5, -9/9, -22/22	-6/5, -10/10, -23/24	-5/5, -10/9, -23/23	-4/4, -8/8, -19/19	-4/4, -7/7, -18/18
Reflect. Collected/unique	25548/2862	21646/2352	22978/2467	18928/3095	21576/2920	22724/1654	18169/1321
Data/restrains/parameters	2862/0/209	2352/1/209	2467/1/209	3095/7/209	2920/1/209	1654/7/209	1321/7/209
Goodness-of-fit on F2	1.072	1.048	1.046	1.023	1.044	1.028	1.048
Final R1/wR2 (I>2σ1)	0.0472/0.1316	0.0434/0.1184	0.0461/0.1260	0.0607/0.1667	0.0559/0.1501	0.0528/0.1335	0.0531/0.1368
R1/wR2 (all data)	0.0555/0.1390	0.0506/0.1252	0.0594/0.1371	0.0855/0.1848	0.0814/0.1682	0.0881/0.1652	0.0840/0.1694
Largest diff. peak/hole (e.Å^{-3})	0.34/-0.34	0.21/-0.30	0.21/-0.28	0.36/-0.25	0.21/-0.24	0.17/-0.13	0.14/-0.15

Table S30. Detailed crystallographic data for PDI-C_8 at high pressure.

Pressure		0.1 MPa	0.08 GPa	0.40 GPa	0.61 GPa	1.16 GPa	1.50 GPa	1.57 GPa
Phase		I	I	I	IIII	III	IV	IV
CCDC numbers		2493916	2493917	2493918	2493919	2493920	2493921	2493922
λ		0.4919	0.4919	0.4919	0.71073	0.4919	0.4917	0.4919
Crystal system		triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group		*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1	*P*-1
Unit cell dimensions	*a* (Å)	4.7686(3)	4.74670(10)	4.62072(16)	4.5642(19)	4.4866(3)	4.51620(10)	4.50300(10)
	b (Å)	8.5193(4)	8.5395(3)	8.6608(3)	8.442(4)	8.4612(5)	16.9424(5)	16.9388(6)
	c (Å)	20.2896(10)	20.108(4)	19.439(4)	19.398(12)	19.429(2)	19.020(2)	18.982(3)
	α (°)	85.291(4)	85.287(7)	84.805(7)	83.02(8)	80.771(10)	76.517(5)	76.548(6)
	β (°)	89.680(4)	89.336(7)	87.168(7)	88.30(9)	87.690(10)	89.121(5)	89.101(6)
	γ (°)	82.293(4)	82.367(2)	82.076(3)	82.94(3)	84.078(5)	83.351(2)	83.403(3)
Volume (Å^3)		814.05(8)	805.12(16)	766.82(15)	736.2(6)	723.92(11)	1405.60(19)	1398.7(2)
Z/Z'		1/0.5	1/0.5	1/0.5	1/0.5	1/0.5	2/1	2/1
Calculated density (g/cm^3)		1.254	1.268	1.331	1.387	1.410	1.453	1.460
Absorption (mm^{-1})		0.042	0.043	0.045	0.089	0.048	0.049	0.049
F(000)		328.0	328.0	328.0	328.0	328.0	656.0	656.0
Crystal size (mm)		0.067 × 0.039 × 0.012	0.066 × 0.039 × 0.012	0.065 × 0.039 × 0.012	0.2 × 0.13 × 0.04	0.065 × 0.039 × 0.013	0.064 × 0.039 × 0.013	0.064 × 0.039 × 0.013
2θ-range for data collection (°)		10.67 to 46.19	10.568 to 45.98	10.902 to 45.498	9 to 51.32	10.938 to 46.782	10.802 to 35.954	10.726 to 46.356
Min/max indices: h, k, l		-5/7, -13/11, -30/21	-7/7, -13/13, -9/10	-7/7, -13/13, -9/10	-5/5, -10/10, -5/5	-7/6, -12/12, -10/11	-5/5, -21/21, -10/12	-7/7, -25/26, -10/14
Reflect. Collected/unique		2702/2287	7240/1315	3297/1229	2951/569	5857/1152	3480/1213	6206/2247
Data/restrains/parameters		2287/0/230	1315/138/209	1229/0/209	569/418/209	1152/138/209	1213/240/417	2247/241/417
Goodness-of-fit on F2		1.028	1.174	1.065	1.043	1.271	1.292	1.182
Final R1/wR2 (I>2σ1)		0.0751/0.2205	0.0882/0.2620	0.0748/0.2013	0.1632/0.3449	0.0845/0.2542	0.0835/0.2255	0.0952/0.2582
R1/wR2 (all data)		0.1055/0.2543	0.1166/0.2993	0.0972/0.2290	0.4366/0.5347	0.0911/0.2657	0.0959/0.2509	0.1269/0.2950
Largest diff. peak/hole (e.Å^{-3})		0.24/-0.21	0.19/-0.17	0.16/-0.17	0.20/-0.21	0.25/-0.21	0.17/-0.22	0.26/-0.28

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