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Supporting Information

Pressure- and temperature-driven transitions and conformational conversions of *n*-hexyl substituted perylene diimide (PDI-C₆) crystals

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1. PDI-C₆ at room conditions

1.1. UV-Vis absorption spectroscopy

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



Figure S1. Absorption spectra of PDI-C₆ at room conditions.





Figure S2. Arrangements of PDI-C₆ molecules in the unit-cell along direction: (a) [100]; (b) [010]; and (c) [001], at room conditions (296 K/0.1 MPa, phase I).

2. Effect of temperature on PDI-C₆

2.1. Thermal gravimetric analysis

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



Figure S3. TGA curve of PDI-C₆, a single degradation step is observed above 400 °C.



2.2. Variable-temperature X-ray diffraction

Figure S4. PXRD patterns of PDI-C₆ phase I at 298 K (a), phase II and III at 475 K (c), and phase III at 538 K (e), collected using an X-ray beam (λ = 0.41235 Å). The calculated diffractograms,

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

The PXRD pattern collected at 475 K is characterized by the presence of two distinct reflections at low 20 angles (Figure S4c). Upon increasing the temperature from 475 K, the reflections associated with phase II gradually diminish, and at 538 K, the PXRD pattern consists only phase III. Unfortunately, solving the crystal structure of phase III was not possible, we were only able to determine the unit-cell parameters. As a speculative hypothesis, we propose that phase III may exhibit an alternating criss-cross π -stacking arrangement. The unit-cell volume corresponds to two molecules in the unit cell, that could be rotated relative to each other, allowing for a shorter stacking vector corresponding to half of the *a* axis in phase III. The long *c* axis would likely correspond to the length of the molecule, while the *b* axis would be related to the distance between adjacent columns.



Figure S5. PXRD patterns of PDI-C₆ at different temperatures during heating, focusing on the low-angle region. At 456 K, the main reflection corresponds to phase I, while the reflection at 1.1° is ascribable to phase III; at 469 K, all three phases are present; at 479 K, phase I is no longer visible.



Figure S6. PXRD patterns of PDI-C₆ collected at different temperatures during cooling from 606 K to 364 K.



Figure S7. PXRD of PDI-C₆ at different temperatures during cooling from 362 K to room temperature. At 362 K, phase III is present, and the transition to phase II begins. As the temperature decreases, phase II becomes more prominent. At 344 K, phase I appears. By the end of the cooling process, at 308 K, both phases II and I are present.



Figure S8. PXRD of PDI-C₆ (phase I at 298 K) measured with Mo K α . The bottom pattern (purple) shows the calculated diffractogram from the single-crystal X-ray diffraction (XRD) measurement performed at 298 K/0.1 MPa. The top pattern (orange) represents the PXRD pattern of the sample after heating the crystal to 640 K and then cooling it back down to 298 K.



Figure S9. Temperature-resolved powder X-ray diffractograms of PDI-C₆ upon cooling. The dashed lines indicate the transition temperatures identified in the DSC measurement: $T_{III \rightarrow II} = 484$ K and $T_{II \rightarrow I} = 403$ K.

2.3. Pitch and roll angles

Table S2. Pitch and roll angles and $\pi-\pi$ distances for PDI-C₆ crystal structure at different temperatures. The data at 173 K were previously reported by Madhu et al.^[1]

<i>т</i> (К)	P (°)	R (°)	α _P (°)	β _R (°)	X (°)	Ψ (°)	<i>d</i> _{л-л} (Å)	Stacking Vector (Å)
440	42.31(4)	21.11(5)	47.69(4)	68.89(5)	49.49	74.08	3.4397(13)	4.8395
298	42.36(5)	20.82(6)	47.64(5)	69.18(6)	49.23	74.39	3.3809(15)	4.757
173	42.80(4)	20.58(5)	47.20(4)	69.42(5)	49.07	74.91	3.3458(14)	4.730
100	42.88(6)	20.49(7)	47.12(6)	69.51(7)	48.80	74.70	3.321(2)	4.706

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

 $P = 90^{\circ} - \alpha_P$

 $R = 90^\circ - \beta_R$

2.4. Thermal expansion coefficient of PDI-C₆ phase I

Table S3. Unit-cell parameters of PDI-C₆ phase I at different temperatures obtained by Rietveld refinement.

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

Table S4. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C₆ phase I in the range of temperature between 100 and 354 K.^[2]

				Direction	
Axes	α (ΜΚ-1)	σα(ΜΚ-1)	а	b	c
X1	-16.3096	1.6702	0.8168	-0.5675	-0.1039
X ₂	114.9742	5.4128	0.9023	-0.071	0.4253
X ₃	61.3	4.1265	0.8535	0.4905	-0.1757
v	161.749	1.7703			



Figure S10. Fits to variable-temperature lattice parameter data of PDI-C₆ phase I in the range 100-354 K.



Figure S11. Expansivity indicatrix of PDI-C₆ phase I determined in the range 100–354 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.

Table S5. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C₆ phase I in the range of temperature between 361 and 413 K.^[2]

				Direction	
Axes	α (MK ⁻¹)	σα(MK ⁻¹)	а	b	с
X ₁	-213.2833	11.3908	0.7294	-0.6664	-0.1547
X ₂	183.9475	7.64	0.9633	0.2672	-0.0237
X ₃	432.0147	17.4431	0.4776	-0.6164	0.626
v	398.2338	13.4492			



Figure S12. Fits to variable-temperature lattice parameter data of PDI-C₆ phase I in the range 361-413 K.



Figure S13. Expansivity indicatrix of PDI-C₆ phase I determined in the range 361–453 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.





Figure S14. Pawley refinement of PDI-C₆ at 447 K. Experimental pattern in blue, calculated pattern in red and difference plot in grey. The blue lines at 5.67 and 6.68 of 20 correspond to the two reflections used to describe the glass capillary contribution. R_{wp} =3.74; R_p =2.57, R_{exp} = 0.98. The intensity is reported in square root for the sake of clarity.



Figure S15. Pawley refinement of PDI-C₆ at 537 K. Experimental pattern in blue, calculated pattern in red and difference plot in grey. The blue lines at 5.67 and 6.68 of 20 correspond to the two reflections used to describe the glass capillary contribution. R_{wp} =4.38; R_p =3.06, Rexp= 0.96. The intensity is reported in square root for the sake of clarity.

2.6. Thermal expansion coefficient of PDI-C₆ phase III

Table S6. Unit-cell parameters of PDI-C₆ phase III at different temperatures obtained by Rietveld refinement.

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

Table S7. Linear thermal expansion coefficients along the corresponding principal axes and volumetric thermal expansion coefficient calculated using PASCal for PDI-C₆ phase III in the temperature range between 537 and 447 K.^[2]

				Direction	
Axes	α (MK ⁻¹)	σα(MK ⁻¹)	а	b	c
X1	325.7737	10.1782	0.2474	-0.6622	0.7073
X ₂	125.2688	1.4656	0.9934	0.0976	-0.0604
X ₃	-36.5578	5.0416	-0.0993	0.9802	0.1716
v	410.431	7.143			



Figure S16. Fits to variable-temperature lattice parameter data of PDI-C₆ phase III in the range of 537-447 K.



Figure S17. Expansivity indicatrix of PDI-C₆ phase III determined in the range 537–447 K using the PASCal program, showing the spatial orientation of positive (red) and negative (blue) thermal expansion.

2.7. Hot Stage Microscopy

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



Figure S18. HSM PDI-C₆ crystals at various stages of heating and cooling. The red scale bar corresponds to 100 μ m.



Figure S19. HSM PDI-C₆ crystals at various stages of heating and cooling.

3. Effect of pressure on PDI-C₆

3.1. Single crystal X-ray diffraction



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



Figure S21. Pressure dependence of angles α , β and γ for the PDI-C₆ crystal. The estimated standard deviations (ESDs) are smaller than the symbols. Data at 1.22, 1.33, 1.47, and 1.52 GPa are derived from quick-experiments, where only the unit-cell parameters were determined. The angles for phases IV and V have been calculated relative to the lattice corresponding to phase I, as specified in the inset formulas and illustrated in Figure 6.



Figure S22. Comparison of the PDI-C₆ crystal structures between ambient phase I (blue, 1.05 GPa) and high-pressure phase V (red, 1.52 GPa), highlighting differences in alkyl chain conformation. View perpendicular to the perylene plane of the two overlapped molecules (a), and along the perylene x-axis (b).



Figure S23. Graphical representations of the compressibility tensors for the PDI-C₆ crystal, calculated using PASCal program,^[3] are shown for pressure ranges of 0.1 MPa – 1.05 GPa (a), and 1.74 - 4.61 GPa (b).

Table S8. Compressibility related to crystallographic axes calculated for PDI-C₆ phase I in the range of 0.1 MPa – 1.05 GPa with Birch-Murnaghan Coefficients.

Avoc	K/TDa-1)			Direction			Empirical parameters					
Axes	K(IPd)	UN(IPA)	a	b	с	ε_{o}	Empirical parameters ε_0 λ P_c 0.2153 -40.2524 -0.5325 27.478 -27.5086 -0.2884 0.0 0.0073 0.0001 B' $\sigma B'$ 4.0 p/a	v				
X1	57.2089	nan	0.9146	-0.1288	0.3833	40.2153	-40.2524	-0.5325	0.0015			
X2	31.336	nan	0.9394	0.2892	-0.184	27.478	-27.5086	-0.2884	0.0009			
Х3	-6.1818	nan	-0.6128	0.7847	0.0932	0.0	0.0073	0.0001	0.6719			
v	88.433	8.6522										
Birch-N	Birch-Murnaghan Coefficients											
	B ₀ (0	GPa) σ	B₀(GPa)	<i>V</i> ₀ (ų)	σV₀ ((ų)	B'	σΒ'	P _c (GPa)			
2nd	8.8	668	1.1523	704.0333	5.6	11	4.0	n/a	0.0			

9.7046

23.2288

27.6322

706.8975

3rd

4.5489

3.8672

0.0

Δχρς		σK(TPa⁻¹)	Direction				Empirical parameters			
Axes	K(TPa-)		а	b	с	ε	λ	Pc	V	
X1	24.1068	3.0782	0.9804	0.0374	0.1934	53.9492	-53.9131	-0.0424	0.0011	
X2	10.6683	0.7894	0.9122	-0.1482	-0.3821	15.3673	-15.2803	-2.8848	0.0037	
Х3	0.0042	1.8947	0.316	0.9455	-0.0787	0.0008	-0.0	1.7399	6.3035	
v	29.3208	1.3911								

Table S9. Compressibility related to crystallographic axes calculated for PDI-C₆ phase V in the range of 1.74 GPa - 4.61 GPa with Birch-Murnaghan Coefficients.

Birch-Murnaghan Coefficients

	B₀ (GPa)	σB₀(GPa)	<i>V</i> ₀ (ų)	<i>σV₀</i> (ų)	B'	σΒ'	P _c (GPa)
2nd	20.9551	1.0675	652.1741	3.0233	4.0	n/a	0.0
3rd	0.0755	907.392	733.9035	10472.1651	835.6777	9945915.5087	0.0

3.2. Pitch and roll angles

Table SIU. Pitch and roll angles and distances for PDI- C_{e} .	Table S10.	Pitch and	roll angles	and distance	s for PDI-C ₆ . ^[4]
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Pressure (GPa)	P (°)	R (°)	α _P (°)	β _R (°)	<i>d</i> _{π-π} (Å)	<i>d</i> ⊦ (Å)	d _R (Å)	d _{tot} (Å)	z (Å)
0.0001		42.53(2)	20.75(4)	47.47(2)	69.25(4)	3.3882(4)	3.11	1.28	3.36	4.77
0.50		42.36(4)	19.79(3)	47.64 (4)	70.21(3)	3.3209(4)	3.03	1.19	3.26	4.65
0.73		42.49(16)	19.2(3)	47.51(16)	70.8(3)	3.295(6)	3.02	1.15	3.23	4.62
1.05		42.2(2)	19.0(3)	47.8(2)	71.0(3)	3.278(6)	2.97	1.13	3.18	4.57
1 /1	1	41.49(3)	20.49(6)	48.51(3)	69.51(6)	3.2643(6)	2.89	1.22	3.14	4.53
1.41	2	43.22(3)	19.56(5)	46.78(3)	70.44(5)	3.2044(5)	3.01	1.14	3.22	4.54
1.74		43.05(19)	16.6(3)	46.95(19)	73.4(3)	3.207(6)	3.00	0.96	3.15	4.50
1.95		42.80(3)	15.96(4)	47.2(3)	74.04(4)	3.2049(6)	2.97	0.92	3.11	4.47
2.05		42.83(2)	16.04(3)	47.17(2)	73.96(3)	3.1977(5)	2.96	0.92	3.10	4.45
2.41		43.1(3)	15.4(5)	46.9(3)	74.6(5)	3.171(6)	2.97	0.87	3.09	4.43
2.74		42.73(3)	15.15(4)	47.27(3)	74.85(4)	3.1560(6)	2.92	0.85	3.04	4.38
3.43		43.01(3)	14.37(4)	46.99(3)	75.63(4)	3.1234(6)	2.91	0.80	3.02	4.34
4.61		43.27(3)	13.65(6)	46.73(3)	76.35(6)	3.0801(9)	2.90	0.75	3.00	4.30

 $P = 90^{\circ} - \alpha_P$

$$R = 90^\circ - \beta_R$$

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

The slip distance along the short molecular axis is: $d_R = d_{\pi - \pi} \operatorname{tg} R$

$$d_P = d_{\pi - \pi} \operatorname{ctg} \alpha_P$$

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

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

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

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



Figure S24. Packing of PDI-C₆ molecules under pressure (a): orange symbols represent the $\alpha_{\rm P}$ (b) and purple $\beta_{\rm R}$ (c) angles. and grey squares mark the distance between π -stacked molecules ($d_{\pi-\pi}$).^[4] In (b) and (c), the alkyl substituents and H-atoms are skipped for clarity.

4. Theoretical calculations

4.1. Geometry optimization, thermodynamic and optical properties in Orca

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

4.2. Interaction energies in Crystal Explorer

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

The analysis of intermolecular interactions present in the $PDI-C_6$ crystal revealed the dominant strengthen of the $\pi \cdots \pi$ interaction occurring between sandwich stacking PDI-C₆ molecules. Those noncovalent attractive interactions remain stable (E_{total}, Figure S29a) up to the highest achieved pressure, as both electrostatic and dispersion forces compensate the repulsion. As a result, the structure is the hardest in the [010] direction, what reflects in the compressibility of a crystal. Similarly, although three times weaker, interactions between neighboring PDI-C₆ molecules bond them by weak CH···O and aryl CH···CH contacts. The driving force of the transitions is the softness of the alkyl chains and their ability to change conformations. Two alkyl chains, interacting with each other side-to-side, are involved mainly into the structural transformations. However, the repulsion between them in phase IV increases significantly (molecules A, B at 1.41 GPa), in phase V it lowers back as the electrostatic and dispersion forces decrease as well (Figure 28c). This keeps the total energy of the interaction higher than for phase I, but another side alkyl interaction compensates lowering the total energy by the rise of dispersion and electrostatic interactions prevailing the repulsion (Figure S29d). On the other hand, the apical interactions, involving two CH₃ groups pushing against each other, destabilize the structure lowering its total energy as no other term can compensate the repulsion (Figure S29e).

Table S11. Gibbs free energies of single PDI-C₆ conformers, calculated in Orca at the B3LYPgCP-D3/6-31G* theory level. Two independent molecules in phase IV-were described as A and B. For comparison, energies of theoretical high-symmetry conformation (HSC) with C_{2v} molecular symmetry are listed in the bottom row.

(kJ/m	(el) (kJ/mol)	ol)	G-E(el) (kcal/mo	essure [GPa]
0	1478.25		353.31	0.0001
1.0878	1477.16		353.05	0.5
1.9246	1476.32		352.85	1.41 A
2.59408	1480.84		353.93	1.41 B
3.26352	1481.51		354.09	1.57
3.4308	1481.68		354.13	1.95
3.3053	1481.55		354.1	2.05
3.7237	1481.97		354.2	2.74
3.59824	1481.85		354.17	3.43
3.38904	1481.64		354.12	4.61
0.33472	1478.58		353.39	HSC



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



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

<i>p</i> [GPa]	CC	СН	CO	CN	NN	NO	NH	00	ОН	НН
0.0001	11	11.6	2	1.5	0	0	0.4	0	17	56.5
0.5	11.6	11.3	2.1	1.6	0	0	0.5	0	17	55.9
1.41 (mol A)	12.1	11	2	1.6	0	0	0.4	0	17.2	55.7
1.41 (mol B)	12.4	10.9	2.7	1.7	0	0	0.3	0	15.1	56.9
1.57	12.8	10.1	2.6	1.6	0	0	0.3	0	15.6	57
1.95	13.1	10	2.6	1.6	0	0	0.3	0	15.5	56.9
2.05	13.1	9.9	2.6	1.7	0	0	0.4	0	15.4	56.9
2.74	13.6	9.7	2.6	1.7	0	0	0.4	0	15.4	56.6
3.43	13.8	9.5	2.7	1.8	0	0	0.4	0	15.1	56.7
4.61	14.1	9.6	2.6	1.7	0	0	0.5	0	15.2	56.3

 $\label{eq:table_state} \textbf{Table S12}. \ Percentage \ of \ intermolecular \ interactions \ in \ PDI-C_6 \ calculated \ in \ Crystal Explorer.$

Table S13. Interaction energies (kJ/mol) between molecules in PDI-C₆.

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



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

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

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

Phase I



Phase IV mol A





Figure S28. Intermolecular interactions between PDI-C₆ molecules calculated in Crystal Explorer.



Figure S29. The evolution of selected interaction energies between PDI-C₆ molecules. (a) stacking π ··· π interactions (red molecule in Figure S27), (b) mainly CH···O interactions (blue

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



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

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



Figure S31. Fingerprints representing types of interactions present in all PDI-C₆ phases at 0.0001, 1.41 and 4.61 GPa, respectively.

Table S15. Coordinates of atoms of PDI-C₆ molecules – models taken from crystallographic data and optimized in Orca at the B3LYP-gCP-D3/6-31G* theory level.

0.0	0001 GPa		
0	5.98036540467279	5.63728838723651	6.54399564273697
0	4.80266860919056	8.70768934446812	3.35878195352622
Ν	5.43762181859984	7.19778397003556	4.95950420297917
С	3.68098358559165	8.45224453107502	6.81945386165904
С	2.22725476065085	10.70996323401918	6.03779352791769
Н	1.68129574870088	11.58393758526956	5.69547898909711
С	2.06691794458995	10.24426950407887	7.34575996004281
С	2.69126150818513	8.55094682365645	9.07833026347696
С	6.49733117825416	4.48732327541903	2.41891227494432
н	7.28749012789382	4.06722663587836	3.06498950622460
Н	7.01040255769945	5.10511244618193	1.66194200295232
С	4.42621509807529	7.30950531181688	7.20115993981614
С	5.33783862380753	6.63688406124100	6.24249281117603
С	3.08302543073055	10.07897648486867	5.12619442972611
Н	3.18933083306779	10.45656674040708	4.11210700094358
С	2.80583906318198	9.08787540721948	7.75568506736796
С	3.80891507636680	8.96023308500737	5.50253979982990
С	5.74794759733416	3.33825283811159	1.72226047711706
н	5.21778733554369	2.73683844142778	2.48166684953986
Н	4.96507931978703	3.75733726626633	1.06664700103192
С	3.44411042937749	7.42031957361874	9.40810281871623
Н	3.37906381354075	6.98766755320508	10.40188514725691
С	4.30012445639266	6.80578166288217	8.48581984793415
Н	4.87601235772827	5.92626267085259	8.76343795553828
С	5.56633631887268	5.36721695065569	3.26848103528216
Н	5.06823012107473	4.73979837337329	4.02187292414945

С	6.31015982926061	6.50563053581269	3.98641510070961
н	7.16815380379652	6.12051197874459	4.54702062696429
н	6.65669119071909	7.25834406685368	3.27215040231809
С	4.70214682863026	8.30626683080199	4.51248590675659
С	5.88675767836020	1.26224360238844	0.23258470031696
н	5 14607669658975	1 65775332514773	-0.48106806087714
	5.14007005050575	0.00773332314773	0.07722586274482
	5.54/9515/450141	0.05/2/4///19528	0.97733380274182
н	6.55952948444077	0.59245272108707	-0.32231491897212
С	6.65746533391756	2.41303671730426	0.89707924080922
Н	7.44748312707967	2.00202973655324	1.54542425185705
н	7.17644176678513	3.00304965610140	0.12308842512660
0	-2.15427334077883	13.78618401601648	10.83270002315935
0	-0 98819172777548	10 70486340463679	14 01099454087361
N	-1 62001/127053115	12 21703235330653	12 /1110820218066
2	0.16622124084122	10.00775627070215	10 56201417256500
C	0.10033124084133	10.96//502/6/9515	10.50501417550500
C	1.62419963799936	8./32941939/59/0	11.3458/245/65248
н	2.17135017041068	7.85983812112502	11.68842984785773
С	1.78826293467396	9.20212820973562	10.03965727316347
С	1.16648246219267	10.89759332092198	8.30824369930460
С	-2.92016956644253	14.83080847384852	14.93788889956791
н	-3.70292206374950	15.20684351918230	14.25606830142980
н	-3 42855702295366	14 16361491506603	15 65523104031847
с.	0 57076642414622	12 12096021561701	10 18107446204626
c	1 50627112122402	12.13080031301701	10.1013/440234030
C	-1.5005/112125495	12./9025/520565/2	11.154/905/801004
C	0.76064432290771	9.35/440/66/298/	12.25442836921362
н	0.64907969298795	8.97556839451494	13.26633750060613
С	1.04806172552960	10.35753156555908	9.62931662761832
С	0.03229332356986	10.47427208072497	11.87725140211432
С	-2.29890590213560	16.01640024279828	15.69473691115640
н	-1.77874057692875	16.67298475039693	14.97587919591688
н	-1.52285662928870	15.64459112910542	16.38598340473192
c	0.41672379828338	12.03082400531649	7,98026003587955
ы	0.48662326260410	12 46760071000407	6 988586/0010605
с П	0.44410609044245	12 64127046202220	0.00000045010000
L.	-0.44419698914211	12.0413/846292230	0.90082627338480
н	-1.01948289379803	13.52139435675910	8.62348586920375
С	-1.89210021578881	14.02889279570823	14.12316404857433
Н	-1.40023373217907	14.69583784998156	13.40020398253426
н	-1.10683138571373	13.63130002919718	14.78486001235588
С	-2.54699084272347	12.86463442665567	13.36317928906352
н	-3.40087034864354	13.22272752303946	12,77967252335424
н	-2.88578857874678	12.08951418896138	14.05691662924422
c	-0 87739452797089	11 11449233005731	12 86113839988173
ĉ	-2 70335501180032	18 03135561800874	17 22115680087450
	1.04740886530000	17.00155501050024	17.25115005007450
	-1.94/49880559909	17.09257149029297	17.95010729101547
н	-2.20661002491954	18./23//31/338035	16.53445894993039
н	-3 //63/1/6/163/1/1/50	18.60259815467149	1 / /84/1 /04051831
	-3.40307000314233		17.70421205051051
С	-3.32840392212015	16.84412677037222	16.48275718576291
C H	-3.32840392212015 -4.10265663111569	16.84412677037222 17.21432186661514	16.48275718576291 15.78954377361611
C H H	-3.32840392212015 -4.10265663111569 -3.84953671757934	16.84412677037222 17.21432186661514 16.18927371381773	16.48275718576291 15.78954377361611 17.20123193870022
С Н Н	-3.32840392212015 -4.10265663111569 -3.84953671757934	16.84412677037222 17.21432186661514 16.18927371381773	16.48275718576291 15.78954377361611 17.20123193870022
С Н Н	-3.32840392212015 -4.10265663111569 -3.84953671757934	16.84412677037222 17.21432186661514 16.18927371381773	16.48275718576291 15.78954377361611 17.20123193870022
С Н Н	-3.32840392212015 -4.10265663111569 -3.84953671757934 GPa	16.84412677037222 17.21432186661514 16.18927371381773	16.48275718576291 15.78954377361611 17.20123193870022
С Н Н 0.5 О	-3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651	16.48275718576291 15.78954377361611 17.20123193870022 6.54399564273697
С Н О.5 О	-3.32840392212015 -3.32840392212015 -3.849536711569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812	6.54399564273697 3.3587819532622
С Н О.5 О О N	-3.32840392212015 -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556	6.54399564273697 3.3587819532629 4.5595420297917
С Н О О О О С	-3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502	6.54399564273697 3.3587819532622 4.95950420297917 6.81945386165904
С Н Н 0.5 0 0 N С С	GPa 5.98036540467279 4.80266860919056 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918	6.54399564273697 3.5587819532622 4.595954273697 3.35878195352622 4.595950420297917 6.81945386165904 6.03779352791769
С Н Н 0.5 О О N С С Н	GPa 5.98036540467279 4.80265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956	6.54399564273697 3.587818576291 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.6654788909711
С Н Н 0.5 О О N С С Н С	-3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0660176445905	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.2442650400787	6.54399564273697 3.3587819532622 4.559504202977 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547838909711 7.2457596004291
С Н Н 0.5 О О N С С Н С С	GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 3.68129574870088	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.550640325554	6.54399564273697 3.3587819532622 4.959504273697 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.0783205247205
С Н Н 0.5 О О N С С Н С С С	GPa 5.98036540467279 4.80266860919056 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49729147975445	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.4872327540002	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.4189173746423
С H H 0.5 О O N C C H C C C :	GPa 5.98036540467279 4.80266860910056 5.98036540467279 4.80266860910056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.9733117825416	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.2442650407887 8.55094682365645 4.48732327541903	6.54399564273697 13.78954377361611 17.20123193870022 6.54399564273697 3.3587819535262 4.95950420397917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432
С H H 0.5 О O N C C H C C C H .	GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012783822	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41881227494432 3.06488950622460
С Н Н 0.5 О О N С С Н С С С Н Н	GPa 5.98036540467279 4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232
С Н Н 0.5 О О N С С Н С С С Н Н С	GPa 5.98036540467279 4.80266860910056 5.98036540467279 4.80266860910056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040257569945 4.42621509807529	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.2442650407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614
С Н Н 0.5 О О N С С Н С С С Н Н С С	GPa 5.98036540467279 4.80266860919056 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.2011599381614 6.24249281117603
С Н Н 0.5 О О N С С Н С С С Н Н С С С	GPa 5.98036540467279 4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.3378386280753 3.08302543073055	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.46732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.3587819535262 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611
С Н Н 0.5 О О N С С Н С С С Н Н С С С Н	GPa 5.98036540467279 4.80266860919056 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.2874901278382 7.01040257569945 4.42621509807529 5.33783862380753 3.08302543073055 3.189330833067795	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.1051124618193 7.30950531181688 6.63688406124100 10.0789764848687 10.45656674040708	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.9595042029717 6.8194538165904 6.03779352791769 5.695478989004281 9.07833026347696 2.41891227494432 3.06498550622460 1.661944200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358
С Н Н 0 0 О О О С С Н С С С Н Н С С С Н С	GPa 5.98036540467279 4.80266860919056 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.0833063306779 2.80583906318198	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839375852656 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.07897648488687 10.4565674040708 9.08787540721948	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796
СНН 0 00 N C C H C C C H H C C C H C C	GPa 5.98036540467279 4.80266860910056 5.4376218159984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.06691794458995 2.06691794458995 2.06691794458995 2.069126150818513 6.49733117825416 7.28749012789382 7.01040255769945 3.3783862380753 3.08302543073055 3.18933083306779 2.80583906318188 3.808915076366881	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.4555674040708 9.08787540721948 8.96023308500737	6.54399564273697 15.78954377365611 17.20123193870022 6.54399564273697 3.3587819535262 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.5568506736796 5.5025397982790
СНН 0 00NССНСССННСССНОСС	GPa 5.8036540467279 4.80266860919056 5.43762181859984 3.6809835559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.0104025769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.7479479733416	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.1051124618193 7.30950531181688 6.63688406124100 10.0789764848687 10.456556674040708 9.08787540721948 8.96023308500737	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.50253979982990 1.22226607711706
СНН 0 0 N C C H C C C H H C C C H C C C I C C C I C C C H C C C H C C C H C C C H C	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.0833063792 2.80583906318198 3.80891507636680 5.74794759733416 5.2177873252526	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.07897648488667 10.4565674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.736824414077	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993881614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.50253979982990 1.72226047711706 2.4816264292290
СНН 0.5 00 N С С Н С С С Н Н С С С И С С И С И С С И С И С И С И С И С С И И С И С И И С И И С И	GPa 5.98036540467279 4.826686911056 5.98036540467279 4.80266860910056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378556956 10.24426950407887 8.55094682365645 4.86732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.45656674040708 9.8787540721948 8.96023308500737 3.33825283811159 2.73683844142778	6.54399564273657 15.78954377365611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420397917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986
СНН 0.5 00 N С С Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С С С Н Н С	GPa 5.8036540467279 4.80266860919056 5.43762181859984 3.6809835859165 2.2272547605085 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.0830254307355 3.18933083306779 2.80583906318198 3.8091507636680 5.74794759733416 5.21778733554369 4.96507931978703	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.7076893444812 7.1977837003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.1051124618193 7.30950531181688 6.63688406124100 10.0789764846867 10.456556674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73638384142778 3.75733726626633	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.81945386165904 6.81945386165904 6.81945386165904 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.2429281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.5025397982990 1.72226047711706 2.48166684953986
СНН 0.5 ОО N С С Н Н С С С Н Н С С С Н Н С С С И Н С С С И Н С С С И Н С С С И Н С С И Н С С И Н С С И Н С С И Н С С И И И И	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.0789764848687 10.45656674040708 9.087540721948 8.96023308500737 3.33825283811159 2.73683844142778 3.757372626633 7.40031957361874	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.2011599388161 4.11210700094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623
СНН 0.5 ОО N С С Н Н С С С Н Н С С Н Н С Н Н С Н Н С С Н Н С С Н Н С С И Н С С И Н С И Н С И Н С И Н С И Н С И Н С И Н С И Н С И Н С И Н С И Н С И И И И	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910956 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040257569945 4.42621509807529 5.3783862380753 3.0830253763945 3.80891507636680 5.74794759733416 5.21778733554369 4.965079319703 3.44411042937749 3.37906381354075	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758525956 10.24426950407887 8.55094682365645 4.86732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.7573372662633 7.42031957361874 6.98766755320508	6.54399564273657 15.78954377365611 17.20123193870022 6.54399564273657 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547838909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 5.12619442972611 5.1262942972611 5.1262942972611 5.1262942972611 5.1262942972611 5.1262942972611 5.1262942972611 1.22226047711706 2.48166684953986 1.02664700103192 9.40810281871623 10.40188514725691
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	GPa 5.98036540467279 4.80266860910056 5.4376218159984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012783382 7.01040255769945 3.08302543073055 3.18933083306779 2.80883906318188 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.37001245639266 4.87601235772827 5.56633631887268 5.06823012107473 4.77610840978633	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73683844142778 3.7573726262633 3.75733726262633 3.7521626267085259 5.36721695065569 4.73979837337329 5.80181730767551	6.54399564273697 15.78954377365611 17.20123193870022 6.54399564273697 3.3587819535262 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.2424928117603 5.12619442972611 4.1121070094358 7.75568506736796 5.5025397982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 10.4018814725691 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258
СНН 0 00200H000HH000H000HH0H0H0HHc	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910956 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.069126150818513 6.49733117825416 7.28749012789382 7.01040257569945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306773 3.08302543073055 3.18933083306773 3.083055753945 5.74794759733416 5.7479475973417 5.7572827 5.75178735577827 5.75178735577827 5.75178735577827 5.75178735577827 5.7517877827 5.751787787787 5.751787787 5.751787787 5.751787787 5.751787787 5.7517	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648486867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.98766755320508 6.80578166288217 5.92626267085259 5.3672169505559 4.73979837337329 5.80181730767521	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.408102814725691 8.46543795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641519077061
СНН 5 00 Z U U U U U U U U U U U U U U U U U U	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.8091507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.30012445639266 4.87601235772827 5.56633631887268 5.06823012107473 4.77610840978630 6.31015982926061 7168159927665	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977837003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181668 6.63684406124100 10.0789764846867 10.45656674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73638384142778 3.75733726626633 7.42031957361874 6.89766755320508 6.80578166288217 5.92626207085259 5.36721695065569 4.73979837337329 5.80181730767521 6.5056305381829	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.81945386165904 6.81945386165904 6.8194538206347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094388 7.75568506736796 5.5025397982990 1.72226047711706 2.4816684953986 1.06664700103192 9.40810281871623 10.40188514725691 8.48581984793415 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062662490
Снн 5 00 хооноооннооонооннонононнон:	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.06691794458995 2.06691794458995 2.069126150818513 6.49733117825416 7.28749012789382 7.01040255769945 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.3001244563266 4.37061235772827 5.56633631887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 5.6556611073006	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.4555674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.89578166288217 5.92626267085259 5.36721695065569 4.73979837337329 5.80181730767521	6.54399564273697 15.78954377365611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420397917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.025397982990 1.72226047711706 2.4816688495386 1.06664700103192 9.40810281871623 1.040188514725691 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062696429 3.7721640321607
	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.0691274458995 2.0691274870088 2.0691794458995 2.0691274870088 2.0691794458995 2.0691274870088 2.069274870088 2.069274870088 3.08302543073055 3.189330833067739 3.08302543073055 3.189330833067739 3.08302543073055 3.189330833067739 3.08302543073055 3.189330833067739 3.08302543073055 3.18933083306774 3.08302543073055 3.189330833067749 3.37906381354079 3.37906381354079 3.37906381354077 3.3012445639266 4.87601235772827 5.56633631887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.65569119071909 4.720420220061	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.53684406124100 10.07897648486867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.98766755320508 6.80578166288217 5.92626267085259 5.3672169505559 4.73979837337329 5.80181730767521 6.5056305381269 6.12051197874459 7.25834406685368	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094338 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 1.040188514725691 0.40188514725691 8.4654103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062696429 3.27215040231809 4.113670477477
	GPa 5.98036540467279 4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 1.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.8091507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.30012445639266 4.87601235772827 5.56633631857288 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.65669119071909 4.70214682863026	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977837003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181668 6.63688406124100 10.0789764846867 10.45656674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.89766755320508 6.80578166288217 5.92626207085259 5.36721695065569 4.73979837337329 5.80181730767521 6.50563053581269 6.12051197874459 7.25834406683368 8.3062663308199	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.81945386165904 6.81945386165904 6.93779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094388 7.75568506736796 5.5025397982990 1.72226047711706 2.4816684953986 1.06664700103192 9.40810281871623 10.40188514725691 8.48581984793415 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062696429 3.27215040231809
	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.06691794458995 2.0691794458995 2.0691794458995 2.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.38012445639266 4.37012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.03012445639266 3.04710840978630 6.31015982926061 7.1684538037652 6.65669119071909 4.70214682883026 5.88675767836020	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.688406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.96023308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.98766755320508 6.80578166278227 5.36721695065569 4.73979837337329 5.80181730767521 6.5056303581269 6.12051197874459 7.2583440685368	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.9595042039917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993881614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.5025397982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 1.040188514725691 8.47635553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.51248590675659 0.23258470031696
СНН 0 002001000110001100011010101011011011001	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.4376218185994 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.0691794458995 2.0691794458995 2.0691794458995 2.0691794458995 2.0691794458995 2.0691794458995 2.069274870088 2.069274870088 2.069274870088 3.08302543073055 3.18933083306779 3.08302543073055 3.18933083306779 3.08302543073055 3.18933083306779 3.08302543073055 3.18933083306773 3.0802543073055 3.18933083306773 3.0802543073055 3.18933083306779 2.805839063181898 3.80891507636803 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.30012445639266 4.87601235772827 5.5663361387268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.5569119071909 4.70214682863026 5.88675767836020 5.14607669658975	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365407 4.06722663587836 5.10511244618193 7.30950531181688 6.53684406124100 10.07897648486867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.98766755320508 6.80578166288217 5.92626267085259 5.3672169505559 4.73979837337329 5.80181730767521 6.50563053581269 6.12051197874459 7.25834406685368 8.306268308199 1.26224360238844	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 1.040188514725691 8.46581984793415 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062696429 3.27215040231809 4.51248590675659 0.23258470031696 -0.23258470031696
СНН 0 00200100011000110001101010110110110011	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.0691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.30012445639266 4.87601235772827 5.56633613857065 4.87601235772827 5.56633613854075 4.30012445639266 4.87601235772827 5.56633613854075 4.30115982926061 7.16815380379652 6.65669119071909 4.70214682863026 5.84675767836020 5.1460766958975 5.44795157456141	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.0789764848687 10.45656674040708 9.0878540721948 8.96023308500737 3.3382528381159 2.73663844142778 3.7573726626633 7.42031957361874 6.805781628217 5.92626267085259 5.36721695065569 4.73979837337329 5.80181730767551 5.50563053581269 6.12051197874459 7.25834406685368 8.3062663080199 1.2622436023844 1.657753215477	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.81945386165904 6.81945386165904 6.93779352791769 5.69547888909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.5025397982990 1.72226047711706 2.4816684953986 1.06664700103192 9.40810281871623 10.40188514725631 8.48581984793415 8.76343795553828 3.26848103528216 4.02187292414945 2.63665159527258 3.9864151007961 4.54702062696429 3.27215040231809 4.51248590675659 0.23258470031696 -0.48106806687714 0.97733586274182
СНН 0 00200H000HH000H000HH0H0H0H0HH0HH00HHH	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910956 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.669126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.3783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.39012445639266 4.37012445639266 5.366331887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.65669119071909 4.70214682863026 5.84675767836020 5.34795157456141 6.55952948444077	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378556956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.688406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.96023308500737 1.42031957361874 6.98766755320508 6.80578166288217 5.9262627085259 5.36721695065569 4.73979837337329 5.80181730767521 6.50563053581269 6.12051197874459 7.2583440685368 8.3062663080199 1.26224360238844 1.65775332514773 0.65727477719328	6.54399564273697 15.78954377365611 17.20123193870022 6.54399564273697 3.3587819535262 4.95950420397917 6.81945386165904 6.03779352791769 5.69547838909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.5025397982590 1.72226047711706 2.4816684953986 1.06664700103192 9.40810281871623 1.040188514725691 8.458419827553828 3.26848103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.51248590675655 0.23258470031696 -0.8410680687714 0.97733586274182 -0.32231491897212
CHH 00 200 1000 11000 1000 110 1010 110 110	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860919056 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.0104025769945 4.42621509807529 5.33783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.8089150763681354075 4.30012445639266 4.8760123577287 5.5663361887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.5669119071909 4.70214682863026 5.88675767836020 5.14607669658975 5.34795157456141 6.55765330277	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.5509468236545 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.35684406124100 10.07897648486867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.98766755320508 6.8057816288217 5.9266267085259 5.36721695065569 4.73979837337329 5.80181730767521 6.50563053581269 6.12051197874459 7.25834406685368 8.306268308199 1.26224360238844 1.65775332514773 0.6572747719328 0.59245272108707	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195325622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547838909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.1121070094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 1.040188514725691 8.45851984793415 8.7654379553828 3.266448103528216 4.02187292414945 2.63665159527258 3.98641510070961 4.54702062696429 3.27215040231809 4.51248590675659 0.23258470031696 -0.48106806087714 0.97733586274182 -0.32231491897212
С Н Н 0.5 О О N С С Н С С С Н Н С С С Н Н С Н С Н Н С С Н Н С С Н Н С Н Н С Н Н С С Н Н С С Н Н С С Н Н Н С С Н Н Н С С Н	GPa 5.98036540467279 4.80266860910056 5.4376218159984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 3.08302543073055 3.1893083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.370012445639266 4.87601235772827 5.06836318187285 5.06823012107473 4.370012456392661 7.16815380379652 6.55669110971909 4.70214682863026 5.34795157456141 6.5595294844077 6.65767836020 5.1460766658975 5.34795157456141 6.5595294844077 6.6574653391756 7.44748312707967	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.1977839703556 8.45224453107502 10.70996323401918 11.58393758526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.63688406124100 10.07897648486867 10.45656674040708 9.0878540721948 8.96023308500737 3.33825283811159 2.73663844162778 3.7573372626633 7.42031957361874 6.80578166288217 5.9262667085259 5.36721695065569 4.73979837337329 5.80181730767521 6.50563053581269 6.12051197874459 7.25834406685368 8.30626683080199 1.2622436023844 1.65775332514773 0.65927477719328	6.54399564273697 15.78954377361611 17.20123193870022 6.54399564273697 3.35878195352622 4.95950420297917 6.81945386165904 6.03779352791769 5.69547898909711 7.34575996004281 9.07833026347696 2.41891227494432 3.0649850622460 1.66194200295232 7.20115993981614 6.2424928117603 5.12619442972611 4.11210700094358 7.75568506736796 5.5025397982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 10.40188514725691 8.48581984793415 8.76343795553828 3.2684810352816 4.02187292414945 2.63665159527258 3.98641510070961 4.51248590675659 0.23258470031696 -0.4810680687714 0.97733586274182 0.83707924080922 1.54542425185705
СНН 0.500 N С С Н С С С Н Н С С С Н Н С Н С С Н Н С С Н Н С С Н Н С Н Н С Н Н С С Н Н С Н Н С Н Н С С Н Н Н С С Н Н Н С И Н	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910956 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.69126150818513 6.49733117825416 7.28749012789382 7.01040255769945 4.42621509807529 5.3783862380753 3.08302543073055 3.18933083306779 2.80583906318198 3.80891507636680 5.74794759733416 5.21778733554369 4.96507931978703 3.44411042937749 3.37906381354075 4.387012445639266 4.87601235772827 5.56633631887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.65669119071909 4.7021462853026 5.88675767836020 5.1460769658975 5.34795157456141 6.55952948444077 6.55746533391756 7.44748312707677 7.1764176678513	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.5839378556956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75733726626633 7.42031957361874 6.89766755320508 6.80578166288217 5.9262627085259 6.30578166288217 5.9262627085259 6.30578166288217 5.9262627085259 6.12051197874459 7.2583440668388 8.3062663080199 1.26224360238844 1.65775332514773 0.65727477719328 0.592430217382	6.54399564273657 15.78954377361611 17.20123193870022 6.54399564273657 3.587819535262 4.95950420397917 6.81945386165904 6.03779352791769 5.69547838509711 7.3457596004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.50253979982990 1.72226047711706 2.4816684953986 1.06664700103192 9.40810281871623 1.040188514725691 8.4851984793415 8.7634379553828 1.2665159527258 3.98641510070961 4.5124850675659 0.23258470031696 -0.4810680687714 0.97733586274182 -0.3221491897212 0.89707924080922 1.54542425185705 0.12308842512660
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СНН 0.500 N С С Н С С С Н Н С С С Н Н С Н С Н Н С С Н Н С С Н Н С С С Н Н С Н С Н С Н Н С Н Н С С Н Н С С Н Н С С Н Н С С Н Н С И И И О О	GPa -3.32840392212015 -4.10265663111569 -3.84953671757934 GPa 5.98036540467279 4.80266860910956 5.43762181859984 3.68098358559165 2.22725476065085 1.68129574870088 2.06691794458995 2.06691794458995 2.0692174870088 2.0692174870088 2.0692174870088 2.0692174870088 2.0692174870088 2.069217487088 2.069217487088 2.069217487088 3.0830253769945 3.18933083306779 3.3783862380753 3.80891507636680 5.74794759733416 5.2177873354369 4.9650793197733 3.47411042937749 3.37906381354075 4.37012445639266 4.87601235772827 5.56633631887268 5.06823012107473 4.77610840978630 6.31015982926061 7.16815380379652 6.65669119071909 4.7021462863026 5.88675767836020 5.14607669658975 5.34795157456141 6.55952948444077 5.34795157456141 6.55952948444077 6.55952948444077 6.55952948444077 6.55952948444077 6.55952948444077 6.55952948444077 6.5595294844077 6.5595294844077 6.5595294844077 6.559529484407 6.55952948447 6.559529484407 6.559529484407 6.55952948447 6.5595294847 6.55952948447 6.55952948447 6.5595294847 6.559529487 6.559529487 6.	16.84412677037222 17.21432186661514 16.18927371381773 5.63728838723651 8.70768934446812 7.19778397003556 8.45224453107502 10.70996323401918 11.58393738526956 10.24426950407887 8.55094682365645 4.48732327541903 4.06722663587836 5.10511244618193 7.30950531181688 6.6368406124100 10.07897648485867 10.45656674040708 9.08787540721948 8.9602308500737 3.33825283811159 2.73683844142778 3.75773726626633 7.42031957361874 6.89766755320508 6.80578166288217 5.9262627085259 5.36771695065569 4.73979837337329 5.8018173076521 6.5055303581269 6.12051197874459 7.25834406683680199 1.2622436023884 1.65775332514773 0.65775372108707 2.41303671730426 2.0020273655324 3.00304965610140 13.78618401601648 10.70486340463679	6.54399564273657 15.78954377361611 17.20123193870022 6.54399564273657 3.587819535262 4.95950420397917 6.81945386165904 6.03779352791769 5.69547838909711 7.34575996004281 9.07833026347696 2.41891227494432 3.06498950622460 1.66194200295232 7.20115993981614 6.24249281117603 5.12619442972611 4.11210700094358 7.75568506736796 5.50253979982990 1.72226047711706 2.48166684953986 1.06664700103192 9.40810281871623 1.261944272691 8.48581984793415 8.7634379553828 3.2664810352816 4.0218729241945 2.63665159527258 3.98641510070961 4.54702062696429 3.7215040231809 4.51248590675659 0.23258470031696 -0.4810680687714 0.97733586274182 -0.32231491897212 0.89707924080922 1.54542425185705 0.1230842512660
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c	-0 87739452797089	11 11449233005731	12 86113839988173
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1.4	1 GPa – molecule A		
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Ν	2.08149672827976	10.85902641586197	4.63182141823924
С	3.89066498106743	12.09280615198707	6.45703336342035
ĉ	1 82187676067025	12 60/0057/803876	7 3623/022133100
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	2.10908330333090	9.03324120300703	2.93944337030471
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č	1 227607496622002	0 1770022055101	1 04765016976216
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H	8.94889552751923 7.31674042393774 7.22977703303414	15.55255860748382 15.99158526918400	7.50636471236554 6.51706392018571
H C	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915	15.55255860748382 15.99158526918400 12.76342880239674	7.50636471236554 6.51706392018571 9.60739518385649
H C C	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097
H C C H	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334
H C C H H	8.94889552751923 7.31674042393774 7.2297770303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419
H C C H H C	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002666913121	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041 19.66175764736724	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.01416864391174
H C C H H C U	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002696913121 8.76514121611041	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041 19.66175764736224 19.0010502542157	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.01416864391174 15.75523773210973
H C C H H C H H C H	8.94889552751923 7.31674042393774 7.2297770303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002696913121 8.76614121611941 9.79347520252	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041 19.66175764736224 19.20105025543169	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441686439419 15.01416864391174 15.75553272310872
H C C H H C H H C H H	8.9489552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002696913121 8.76614121611941 8.78315535384257	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041 19.66175764736224 19.20105025543169 20.10088803430178	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.0141684391174 15.75553272310872 14.24301986154469
Н С С Н Н С Н Н С Н Н С	8.94889552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002696913121 8.76614121611941 8.78315535384257 9.34100061361455	15.55255860748382 15.99158526918400 12.76342880239674 18.5636584234600 18.02684214140453 19.02882838320041 19.66175764736224 19.20105025543169 20.1008803430178 21.89012526407937	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.01416864391174 15.75553272310872 14.24301986154469 16.27417564844426
H C C H H C H H C H H C H H C H	8.94889552751923 7.31674042393774 7.2297770303414 5.92654310571915 10.30908533861747 10.86933026610539 11.06288578006943 9.44002696913121 8.76614121611941 8.78315535384257 9.34100061361455 8.66261512667255	15.55255860748382 15.99158526918400 12.7634280239674 18.56363584243460 18.02684214140453 19.0288283320041 19.66175764736224 19.20105025543169 20.10088803430178 21.89012526407937 21.48465701821732	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.01416864391174 15.75553272310872 14.24301986154469 16.27417564844426 17.04037971000677
Н С С Н Н С Н Н С Н Н С Н Н С Н Н С Н Н	8.9489552751923 7.31674042393774 7.22977703303414 5.92654310571915 10.30908533861747 10.86933026610539 11.0628578006943 9.44002696913121 8.76614121611941 8.78315535384257 9.34100061361455 9.34100061361455 9.93659041768919	15.55255860748382 15.99158526918400 12.76342880239674 18.56363584243460 18.02684214140453 19.02882838320041 19.66175764736224 19.20105025543169 20.10088803430178 21.89012526407937 21.48465701821732 22.68606799922206	7.50636471236554 6.51706392018571 9.60739518385649 14.37204435971097 15.15640485279334 13.71441684239419 15.01416864391174 15.75553272310872 14.24301986154469 16.27417564844426 17.04037971000677 16.74436066312059

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0 0.80032254641985	5.55372431697058	13.50782460402147
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H -7.15042678168027	0.96339345913674	1.76541895668145
C -5.09830539922196	-1.03675316179595	2.08016949112956
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H -6.43065440006858	-0.73989515262064	0.38380611925283
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н С	4.58092475665716	3.96660722418302 6.57380610819774	1.61420303096305
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С Н	4.39261667376401	2.69038915965216	3.30764350105205
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С	0.58985546503156	0.39722847144747	6.98048679175959
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н	2.26678110458764	7.07125909354543	-0.73673692694735
С	2.67299578440916	1.00358470891409	3.81749552687121
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N	-4.07767991759545	-0.82963315990782	11.55407474805850
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Н	-4.51217702393658	-5.93030897933070	15.70350446440233
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Н	-5.60245282249257	-2.27005078061341	12.95596455138252
Н	-5.69905300007904	-3.73709531064357	11.94683378152711
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C C	3.27054450276860 2.10397638348952	2.67958453554732 2.61960313702209	5.49386251319227 7.67809391862052
н	2.70400740472704	3.48022732675812	7.96416034115101
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H C	1.07598039359102	2.53194051975728 3.61330956090480	9.54616171798712 2.22577690808679
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Н	4.55778712692972	3.95968680042679	1.58182587217672
ι	3.47823331011005	0.30404815476585	0.90406301212562

н	4 4 3 4 3 0 4 6 5 0 0 0 6 7 7	F 0C7F0420CF4047	0 44 45 35 4 04 4 4 6 3 4
	4.13139465890677	5.86/5043865181/	0.41453519111634
н	4.13018053370004	7.09756713725411	1.67672148933916
С	1.50325024154914	0.95280541004901	6.02579392043821
С	0.39228117482886	0.96111077965007	8.22965383913581
С	1.67620148093248	0.40402511251820	4,73124910194057
ĉ	2 07800560117402	4 91772719199209	2 91460291672460
	2.57800505117455	4.01772710100350	2.01400201373430
п	3.03809211457977	5.37290749099028	5.49971389034265
н	2.14257378615074	4.44846365944542	3.43080008950360
С	0.00659608938505	-1.27247882679826	5.23239171713500
н	-0.55603041798131	-2.13427038152429	4.88549690574551
C	4 36784434764678	2 68161343877226	3 27371922029758
й	4 86564728700635	1 8/330151860230	2 77/221620220/7
		2,22207422,422,420	2.001 00 00 00 00 00
н	5.09821774512632	3.2230/122433428	3.88168495159948
C	2.41225414520803	5.//959/310/1451	1.75034560286943
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н	1.74289488006271	6.50084645855675	2.24909300245637
С	2.27479264957136	2.07546668628953	6.41510087913309
ĉ	0 558//2227/2068	0 37723745884058	6 0327/31/060873
č	0.55044225745500	0.57725745004550	6.55274514505075
C	-0.1948/81400980/	-0.70901000710824	0.52058477028104
C	0.92639761786051	-0.69626124539186	4.34713135314580
н	1.06700444386896	-1.10454826952923	3.34900986572090
С	2.87090862924368	7.56906620064371	-0.02740735083440
н	3.65238398547267	8.11964516976837	-0.57142945981136
н	2 24016692000238	8 30775212243590	0 49082116128895
	2.24010052000250	7 06062721724221	0.77206670662160
п	2.24017755701040	7.00002721734321	-0.77280079302138
C	2.64920940490842	0.99184506604866	3.77639540495160
0	-4.58943658821419	-4.15642420521084	9.93678157664344
0	-3.66059493645179	-0.87237850130033	12.99397619614655
Ν	-4.11671097267579	-2.53475589675225	11.48898298039451
C	-3 95861393878039	-3 14899663263823	10 23540719955409
ĉ	2 70702261196612	2 096252035005203025	0 0477010E204700
C	-2.79702201180012	-3.08023292301303	8.04770193304700
н	-3.35958372842036	-3.97789297878963	7.78101043377458
С	-1.88952832919602	-2.51749544531495	7.14510409060742
н	-1.77174176660810	-2.99782540732994	6.17813826741152
С	-4.36978889857381	-3.93368057703634	13.56734594461065
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C	-3.80941184492762	-6.68911367861958	15.21/26131636680
н	-4.58001750526375	-6.00496341556332	15.60430352119083
н	-4.35498016088827	-7.49174016183101	14.69290207050045
С	-2.26384043816075	-1.36282531280763	9.66395756769338
Ċ	-1 14803238842425	-1 37593146389852	7 46246166167291
ç	2 47197604161146	0.70421042554072	10.04000526272602
c	-2.4/18/004101140	-0.76431042334373	10.94000320373002
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н	-4.39832483942562	-5.88723127130816	12.62237530894508
н	-2.94310401868358	-4.95111674162887	12.29402593200671
С	-0.82874052134522	0.91356951091392	10.42541489617572
н	-0 29146816749919	1 79650523119720	10 75901887788139
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	-3.74124037408033		
С	-2.90570712371061	-5.95416922417392	14.21025790773035
С Н	-2.90570712371061 -2.26909925899531	-5.95416922417392 -5.23238211638720	14.21025790773035 14.75193756536815
С Н Н	-2.90570712371061 -2.26909925899531 -2.21574082336896	-5.95416922417392 -5.23238211638720 -6.68628098448065	14.21025790773035 14.75193756536815 13.75828815248879
С Н Н	-2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2 52113782487318	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266
C H H C	-2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266
C H C C	-2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124
C H C C C	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678
C H C C C C	-2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706
C H C C C C H	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953867 -0.58922524871118 -1.75851410214101 -1.93134828432325	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339
C H C C C C H C C C H C	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.346083682429830 0.78100799416816 -7.28099751252165	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080
С Н Н С С С С Н С Н	2.90570712371061 -2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28093751252165 -7.77684371257291	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359
СННССССНСНН	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.2881815520965	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.0732039753138	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.1197887208359
СННСССНСНН	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.9313482832325 -3.02751185285643 -3.69592875443142 -2.28818155520965 2.4932640007431	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 6.4046700262537	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.4004116213080 17.11978872036359 16.06181918184568
СННССССНСННН	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28093751252165 -7.77684371257291 -8.0232039753038 -6.49463029636277	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.66181918184568 16.94411086308106
С	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893
СННССССНСНННС	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.9313482832325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893
С Н Н С С С С Н С Н Н Н С	2.290570712371061 -2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893
Сннссснсннс 2.0	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893
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Сннсссснснннс 2.0 о о	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.0232039753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208
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С H H C C C C H C H H H C 2.0 O O N C	2.90570712371061 -2.290570712371061 -2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.73851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342	-5.95416922417392 -5.23238211638720 -6.86828098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.7768471257291 -8.02320399753038 -6.49463029636277 -1.37044235471981	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63666901497208 4.20809310932961 5.48343179323197
С Н Н С С С С Н С Н Н Н С 2.0 О О N С С	2.90570712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342 2.10059417173701	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -6.494630299753038 -0.5224845233190 2.09245286134966 2.67059566518313	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.4834317932961 5.483431793297
СННССССНСНННС 2.0 О О Х С С	5.7424577012371061 -2.290570712371061 -2.26909925899531 -2.21574082338896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.48135040907421 -3.44559533712063 5GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342 2.10059417173701 2.7010724450005	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.953261467707
С Н Н С С С С Н С Н Н Н С 2.0 О О N С С Н С	5.7412457742057 2.90570712371061 -2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.09592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.3445508823391 3.26835527122342 2.10059417173701 2.70107264689099	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.1197872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595
С Н Н С С С С Н С Н Н Н С 2.0 О О N С С Н С	2.90570712371061 -2.90570712371061 -2.26909925899531 -2.1574082336896 -2.99269829234707 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.4004116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63668901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159
СННССССНСНННС 20 00NССНСН	5.7412457740371061 -2.290570712371061 -2.290590712371061 -2.29059829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.3845560823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348 1.07129361970612	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.7768471257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008
Сннососноннно 2. 00 N сононо	5.042105712371061 -2.26909925899531 -2.21574082336896 -2.9925829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48133040907421 -3.44559533712063 5.GPa 3.96075664042752 2.80739122793221 3.3845508823391 3.26835527122342 2.10059417173701 2.70017264689909 1.6918586633348 1.07129361970612 3.73559015949628	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.3460856429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.5245489812151 3.6088868827127	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.1197872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895
Сннососноннно 2 00 N сононон	5.742457742857 2.90570712371061 -2.26909925899531 -2.21574082338896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 -3.8455608823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348 1.07129361970612 3.73559015949628 3.05925190368908	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 -3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.52455489812151 3.00264948095683	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63668901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895 1.57412704205381
СННОСОСНОНННО 2 00 N С С Н С Н С Н Н Н С Н С Н С Н С Н С Н	5.7412457740833 2.90570712371061 2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.09592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5.GPa 3.96075664042752 2.80739122793221 3.3445508823391 3.26835527122342 2.10059417173701 2.70107264689099 1.16918586633348 1.07129361970612 3.73559015949628 3.059251903689084 4.5600813481307	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.092452861384966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.52455489812151 3.608686868827127 3.02649480956983 3.9520134853007	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895 1.57412704205381 1.57412704205381
СННОСОСНОНННО 2.00 N С С Н С Н С Н Н Н С	5.99250712371061 -2.26909925899531 -2.21574082336896 -2.99269829234707 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5.GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348 1.07129361970612 3.73559015949628 3.05925190368908 4.56008134481397 3.400556204774	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.0232039753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.65143683161380 3.47156003166402 2.06197815364516 2.5245489812151 3.60868868827127 3.02649480956983 3.95290384853007 6.5532402920402	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895 1.57412704205381 1.57402291270533
СННССССНСНННС 2 00 N ССНСНСННС:	5.7412457740857 2.90570712371061 2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.5892252487118 -1.73851410214101 -1.73851410214101 -1.73851410214101 -2.28818155520965 -2.48135040907421 -3.44559533712063 5.6Pa 3.96075664042752 2.80739122793221 3.3845560823391 3.26835527122342 2.10059417173701 2.7010726468909 1.16918586633348 3.05925190368908 4.56008134481337 3.49055656924745	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.7768471257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 -3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.52455489812151 3.00868868827127 3.02649480956983 3.95220384853007 6.56324030830408	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.6366691497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895 1.57412704205381 1.57402291270533 0.96273765862846
СННСОСОНОНННО 2 00 N СОНОНОННОН	5.04205712371061 -2.290570712371061 -2.26909925899531 -2.1574082336896 -2.99269829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.09592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5.GPa 3.96075664042752 2.80739122793221 3.3845506882391 3.26835527122342 2.10059417173701 2.70107264689909 1.6918886633348 1.07129361970612 3.73559015949628 3.05925190368908 4.56008134481397 3.49055656924745	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34608368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.5245548812151 3.60868868827127 3.02649480956983 3.95290384853007 6.55324030830408 7.09290814548431	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.1197872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.4834317932916 5.4834317932916 5.4834317932916 5.4834317932916 5.4834317932917 5.65697104191024 7.95336216465595 8.55671518167159 9.534372215008 2.21810660730895 1.57412704205381 1.57402291270533 0.96273765862846 1.67603460695624
СННССССНСНННС 2 00 R ССНСНСННСНН	5.742457742857 2.90570712371061 2.26909925899531 -2.21574082338896 2.99269829234707 -0.5892252487118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.69592875443142 -2.28818155520965 -2.48135040907421 -3.44559533712063 5 GPa 3.96075664042752 2.80739122793221 3.38455608823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348 1.07129361970612 3.73559015949628 3.05925190368908 4.56008134481397 3.49055656924745 4.14483676864967 4.14081952233884	-5.95416922417392 -5.23238211638720 -6.6862809848065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 -3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.52455489812151 3.60268868827127 3.02649480956983 3.95290384853007 6.56324030830408 7.09290814548431	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63666901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.35433720215008 2.21810660730895 1.57412704205381 1.57402291270533 0.96273765862846 1.67603460695624
Сннососноннно 200 хоонононнонно	5.74245774265772371061 -2.290570712371061 -2.290590712371061 -2.29059829234707 -1.32590278953367 -0.58922524871118 -1.75851410214101 -1.93134828432325 -3.02751185285643 -3.02751185285643 -2.28818155520965 -2.48135040907421 -3.44559533712063 5.6GPa 3.96075664042752 2.80739122793221 3.3845508823391 3.26835527122342 2.10059417173701 2.70107264689909 1.16918586633348 1.07129361970612 3.73559015949628 3.05925190368084 4.56008134481397 3.49055656924745 4.1448367684967 4.14081952233884 1.49946872946168	-5.95416922417392 -5.23238211638720 -6.68628098448065 -2.52113782487318 -0.78204815680269 0.37786377233919 0.34008368429830 0.78100799416816 -7.28099751252165 -7.77684371257291 -8.02320399753038 -6.49463029636277 -1.37044235471981 -3.62591806281029 0.53248452303190 2.09245286134966 2.67059566518313 2.61143683161380 3.47156003166402 2.06197815364516 2.52455489812151 3.00868868827127 3.02649480956983 3.95290384853007 6.56324030830408 7.09290814584308 0.94521281327481	14.21025790773035 14.75193756536815 13.75828815248879 9.29781177483266 8.75329445264124 9.15689083013678 11.30559085122706 12.28723383447339 16.40041116213080 17.11978872036359 16.06181918184568 16.94411086308106 11.89459177880893 5.81503170349227 2.63686901497208 4.20809310932961 5.48343179323197 7.66697104191024 7.95336216465595 8.55671518167159 9.53433720215008 2.21810660730895 1.57412704205381 1.57402291270533 0.96273765862846 1.67603460695624 0.41164301402155
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2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547	5.78408560208160 2.57457568784066 4.16174171100316 5.44203330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.1866339189514 153886511338836
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501 H 4.51540196755656	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.0224902594180 2.47738068490547 3.61349535750435 3.03812757910537 3.9605784609296	5.78408560208160 2.57457568784066 4.16174171100316 5.44203330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514 1.53886511338836 1.5444956159092
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.4095246204322	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.5777092744605	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514 1.53886511338836 1.54449506158092 0.9525643145550
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.05020555050	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.1866339189514 1.53886511338836 1.54449506158092 0.95236412115659
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03826674103968 H 2.64170962213522 C 1.10014935744724 H 0.9995500942232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.10226506319164	5.78408560208160 2.57457568784066 4.1617417110316 5.44203330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.4811066390542 2.18663390549 1.54849506158092 0.95236412115659 1.66821836363535
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707225 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939 H 4.09827913727526	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.10226506319164 5.88268586953070	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514 1.53886511338836 1.54449506158092 0.95236412115659 1.6682183636333 0.39576895760691
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939 H 4.09827913727526 C 1.43888636984400	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.1026506319164 5.88268585953070 0.92407385669002	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.1866339189514 1.53886511338836 1.54449506158092 0.95236412115659 1.66821836363535 0.39576895760691 5.95075856254253
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.0382674103968 H 2.64170962213522 C 1.10014935744724 H 0.9995500942232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939 H 4.09827913727526 C 1.4388636984400 C 0.31556878556939	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.10226506319164 5.88268586953070 0.92047385669002 0.92067333038871	5.78408560208160 2.57457568784066 4.16174171100316 5.44203330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.4811066390542 2.1866399189514 1.5388651133836 1.54449506158092 0.95236412115659 1.66821836363535 0.39576895760591 5.95075856254253 8.14826969741524
2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.03862674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422232 C 3.69060930707295 H 3.01193443847501 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939 H 4.09827913727526 C 1.43888636984400 C 0.31556878556939 C 1.61526348224269	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.10226506319164 5.88268586953070 0.92063933038871 0.38552544287659	5.78408560208160 2.57457568784066 4.16174171100316 5.4420330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514 1.53886511338836 1.54449506158092 0.95236412115659 1.66821836363535 0.39576895760691 5.95075856254253 8.14826969741524 4.65235582256970
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2.74 GPa O 3.91114985828807 O 2.75710400339258 N 3.33506983632144 C 3.21712172413037 C 2.0382674103968 H 2.64170962213522 C 1.10014935744724 H 0.99955009422332 C 3.69060930707295 H 3.011934438475011 H 4.51549196750560 C 3.44955246004202 H 4.10532960669939 H 4.09827913727526 C 1.4388636984400 C 0.31556878556939 C 1.61526348224269 C 2.94372280993133 H 2.10755486226832	3.59699020427282 0.53623186677496 2.07982226687668 2.64658294972558 2.57476739034793 3.42976972589745 2.02249025594180 2.47738068490547 3.61349535750435 3.03812757910537 3.96057846088086 6.57778922744860 7.10226506319164 5.88268586953070 0.92063933038871 0.38552544287659 4.81736030015281 4.44788847334793	5.78408560208160 2.57457568784066 4.16174171100316 5.44203330447866 7.61950048795310 7.91598616345671 8.50003157557142 9.48110666390542 2.18663399189514 1.53886511338836 1.54449506158092 0.95236412115659 1.66821836363535 0.39576895760591 5.95075856254253 8.14826969741524 4.65235582256970 2.78828856390449 3.40339348679208
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H C	-4.5/3318/3864699	-3.3333/529419283 0.8765/3/75/6617	10 23402106044900
с µ	-0 484000751247	1 75998/205510/0	10.57920150544658
	2.10.000/0124/0/	T., 2220420201040	_0.0,02010001040/

	-3.848381333333332	-2.38296148687403	12.61603034657633
н	-5.91968322346252	-3.8423/1/0480849	11.59395471230856
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н	-2.43281430332333	-5.28496054448722	14 46706649350591
С	-3.14776119979178	-2.56051065733565	9.05832496529164
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c	-0.75040618929445	0.34553172309901	8.96808608381632
С	-1.95601789077016	0.30343796243719	11.09637154763886
н	-2.14685071676599	0.73446934345711	12.07638238172604
С	-3.19823379758263	-7.33654782506201	16.14709931447467
н	-3.86681954122931	-7.79506024834433	16.89033976704621
н	-2.52843794911420	-8.12326200593680	15.76702793391837
н	-2.57509486952470	-6.59610593361344	16.67217009693379
С	-3.64433361531132	-1.42270205283903	11.65270967556853
4.6	1 GPa		
0	3.82090285076865	3.65143931122668	5.66406522790701
0	2.76643247139955	0.55221262767581	2.45726625786901
Ν	3.29429039869248	2.11516389777870	4.04275017982280
С	3.14596640009453	2.68925641927595	5.31663100290777
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н	2.52/10641999152	3.4/189092491565	7.78022385086513
L L	0.99283555888293	2.04940083048036	8.34605425449270
C I	3 66/0/67/780761	2.50552454505555	2 05720686620513
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С	3.38923149770015	6.58582022283977	0.79596514987888
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Н	-0.64998481144558	-2.13460398924857	4.60172243507232
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L L	2.31998/58019656	5.77578292040780 E 109EE442607201	1.551112/052395/
п Ц	1.71055105775455	5.19855442007201 6.49065666294010	0.82043303237204
Ċ	2 13647898429183	2 07361592327798	6 21506740817505
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č	-0.32787168611290	-0.77749074948473	6.25152347216695
C	0.84301832532944	-0.69243692687147	4.10486461043357
н	1.00748143393894	-1.09568102099831	3.10834323124533
С	2.78707747504930	7.56750143848265	-0.22173671770655
н	3.57017507871068	8.14039761008843	-0.73976099738524
н	2.11508009174328	8.28796652059969	0.26961509236223
н	2.20030399420539	7.03640494930546	-0.98699147933491
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	2 00674725422224	0.04699002252121	13 66319065946904
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N N	-3.90674725422234 -4.35241081459837 -4.17665615516439	-0.94688093352121 -2.58080530104706 -3.17880885201856	12.66218965846894 11.12332240159716 9.86425813847146
N C C	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997
N C C H	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598
N C C H C	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921
O N C C H C H C H	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.5878812792682	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034
O N C C H C H C H C	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390	12.66218965846894 11.12332240159716 9.86425813847146 7.69933136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150
O N C C H C H C H	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.9752892734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743
O N C C H C H C H H	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043
0 N C C H C H C H H C :	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035
О N C C H C H C H H C H ::	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.72359702944668 -4.0250702720007	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023114 -6.80992857222055 -7.57891664926314 -6.126070502575	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.4099355399598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035 14.19206290653099
О N C C H C H C H H C H H C	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.4423264488126 -4.17518441785539 -4.72359702944668 -4.933956027348995 -3.46047755241	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055 -7.57891664926314 -6.11660655864558 1.2002100540055	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035 14.19206290653099 15.15571195857194 0.2470692142555
ОNССНСНСННСННСС	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.72359702944668 -4.93596027348995 -2.46091277527412 -1.9042652764118	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055 -7.57891664926314 -6.11660655864558 -1.3959100644518055	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.720529036878035 14.19206290653099 15.15571195857194 9.34708830143556 7.1665590390107
ОNССНСНСННСННССС	-3.90674725422234 -4.35241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.72359702944668 -4.33596027348995 -2.46091277527412 -1.30436567464118 -2.6872140921880	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055 -7.57891664926314 -6.11660655864558 -1.39591906340955 -1.38820941451802 -0.9326669246630	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035 14.19206290653099 15.15571195857194 9.34708830143556 7.16665800399107 10.6273204431936
ОNССНСНСННСННСССС	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.72359702944668 -4.93596027348995 -2.46091277527412 -1.30436567464118 -2.86742420921880 -3.9400872588500	-0.94688093352121 -2.5808053014706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055 -7.57891664926314 -6.11660655864558 -1.38920941451802 -0.83366698546639 -5.28796811460433	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.4099355399598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035 14.19206290653099 15.15571195857194 9.3470883143556 7.16665800399107 10.62732044331934 12.6780067812637
ОNССНСНСННСННССССН	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.17518441785539 -2.46091277527412 -1.30436567464118 -2.68742420921880 -3.94008972580504 -4.66864189234152	-0.94688093352121 -2.58080530104706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.1056055864558 -1.39591906340955 -1.3820941451802 -0.8336698546639 -5.28796811460433 -5.28795811460433	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.40993553999598 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.89345725862043 14.76257936878035 14.19206290653099 15.15571195857194 9.34708830143556 7.16665800399107 10.62732044331934 12.67960767812637 12.17759977419266
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О И О О Н О Н О Н Н О Н Н О О О И Н О Н О	-3.90674725422234 -3.5241081459837 -4.17665615516439 -2.97528962734681 -3.53909414017007 -2.04719411486742 -1.91500144291488 -4.65302978716792 -3.94164771495003 -5.44232644888126 -4.17518441785539 -4.72359702944668 -4.93596027348995 -2.46091277527412 -1.30436567464118 -2.68742420921880 -3.94008972580504 -4.66864189234152 -3.1973485093119 -1.0290093703938 -0.49261361903896 -5.32434978938944 -5.89581979360418 -5.9959849373379 -3.22698235212212 -2.59632290669246 -2.53511066919800 -3.189750134405588 -1.50425833944861 -0.77197265832567 -1.9746473501119271 -3.44673501119271 -3.44673501119271 -3.44673501119271 -3.44673501119271 -3.44673501119271 -3.44673501119271 -3.4667350119271 -3.4667350119271 -3.4667350119271 -3.74667350119271 -3.7665289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -2.70655289356147 -3.7467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.4467350119271 -3.74673528356147 -3.76655283356147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.76655283556147 -3.767558558558 -3.767558558558 -3.767558558558558558 -3.76755858558558 -3.76755858558558558558 -3.767558585585585585585585585585585585585585	-0.94688093352121 -2.5808053014706 -3.17880885201856 -3.09468072529233 -3.97855298068089 -2.52067391357205 -2.98878812792682 -4.01544498530390 -3.37187141644916 -4.27838163023414 -6.80992857222055 -7.57891664926314 -6.11660655864558 -1.3891906340955 -1.38820941451802 -0.8336669356453 -5.28796811460433 -5.94593755794972 -5.013140563916062 1.73907293926397 -3.18675672785609 -2.36647519407376 -6.06492971163159 -5.36647519407376 -6.79665531658013 -2.54506852722616 -0.80819331231357 0.34507878933909 0.28793446355932 0.70960254213780 -7.47046722712828 -7.9904767772425	12.66218965846894 11.12332240159716 9.86425813847146 7.69893136126997 7.4999355399588 6.82097955219921 5.84992129208034 13.17139007112150 13.71025775832743 13.8934725862043 14.76257936878035 14.76257936878035 14.76257936878035 14.76257936878035 14.76257936878035 14.76257936878039 15.15571195857194 9.34708830143556 7.16665800399107 10.62732044331934 12.0760767812637 12.17759977419266 11.9145101955039 10.16263778573916 10.51718002429919 12.0662778247481 11.4606377515742 13.80587716736175 14.38368748231905 13.35610586400166 8.95288205532487 8.46060870809862 8.95044329608009 11.02013844699013 12.00508462990177 15.94286018018831 16.60769861408435
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C -5.26037713070462 -3.19981665861220 12.18435183587684

5. Detailed crystallographic data

Pre	essure	0.1 MPa	0.50 GPa	0.73 GPa	1.05 GPa	1.41 GPa	1.74 GPa	1.95 GPa	2.05 GPa	2.41 GPa	2.74 GPa	3.43 GPa	4.61 GPa
Phase		I	I	I	I	IV	V	V	v	V	V	V	V
CCDC numbers		2412018	2412019	2412020	2412021	2412022	2412023	2412024	2412025	2412026	2412027	2412028	2412029
	λ	0.49172	0.49173	0.71073	0.71073	0.49173	0.71073	0.49163	0.49173	0.71073	0.49173	0.49173	0.49172
Crystal system		triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic
Space group		<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1
Linit cell	a (Â)	4.7723(1)	4.64520(10)	4.5971(3)	4.5494(4)	4.5308(1)	4.4771(8)	4.4643(1)	4.4549(1)	4.4179(4)	4.3785(1)	4.3382(2)	4.2926(1)
	<i>b</i> (Å)	8.5756(1)	8.5703(3)	8.5635(10)	8.5761(10)	16.9532(3)	8.5973(12)	8.6151(1)	8.6003(1)	8.5938(6)	8.5972(2)	8.5989(3)	8.5559(3)
	<i>c</i> (Å)	17.6181(2)	17.076(2)	16.880(6)	16.782(5)	17.887(1)	15.894(10)	15.8664(8)	15.8585(8)	15.738(6)	15.7128(8)	15.5271(14)	15.3181(19)
dimensions	α (°)	81.734(1)	80.961(6)	80.833(20)	80.612(16)	66.484(3)	90.70(4)	90.750(3)	90.799(2)	90.801(18)	90.904(4)	90.778(6)	90.875(6)
	β (°)	84.881(1)	85.933(4)	86.337(16)	86.817(15)	95.489(2)	92.11(4)	92.236(3)	92.222(2)	92.621(19)	92.733(4)	93.255(6)	93.694(4)
	γ (°)	83.010(1)	84.011(2)	84.247(7)	84.468(8)	96.287(1)	97.502(13)	97.490(1)	97.443(1)	97.410(7)	97.328(2)	97.299(3)	97.093(2)
Volu	me (ų)	706.342(19)	666.68(8)	651.9(3)	642.5(2)	1250.21(8)	606.0(4)	604.46(3)	601.91(3)	591.8(2)	585.83(4)	573.47(6)	556.97(7)
ž	Z/Z'	1/0.5	1/0.5	1/0.5	1/0.5	2/1	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5	1/0.5
Calculated c	density (g/cm ³)	1.313	1.391	1.423	1.444	1.484	1.531	1.535	1.541	1.568	1.583	1.618	1.666
Absorpt	ion (mm ⁻¹)	0.045	0.047	0.093	0.094	0.051	0.100	0.052	0.052	0.102	0.054	0.055	0.057
F(000)	296.0	296.0	296.0	296.0	592.0	296.0	296.0	296.0	296.0	296.0	296.0	296.0
Crystal	size (mm)	0.216 × 0.152 × 0.072	0.209 × 0.152 × 0.07	0.324 × 0.197 × 0.039	0.322 × 0.197 × 0.039	0.2 × 0.151 × 0.069	0.314 × 0.197 × 0.038	0.197 × 0.15 × 0.068	0.197 × 0.149 × 0.068	0.311 × 0.197 × 0.037	0.195 × 0.149 × 0.067	0.193 × 0.149 × 0.066	0.19 × 0.149 × 0.065
2θ-range for d	lata collection (°)	3.24 to 50.542	6.11 to 50.946	8.922 to 52.466	9.01 to 52.938	6.27 to 50.598	9.19 to 52.812	3.298 to 48.87	3.724 to 48.732	9.316 to 51.252	3.726 to 48.974	3.738 to 48.796	6.632 to 48.148
Min/max indices: h, k, l		-4/7, -8/14, -26/25	-6/7, -12/12, -12/9	-5/5, -10/10, -6/6	-5/5, -10/10, -6/6	-7/6, -25/25, -11/14	-5/5, -10/10, -4/4	-6/6, -12/12, -8/8	-7/7, -14/14, -9/10	-5/5, -10/10, -4/4	-7/7, -14/14, -8/10	-7/7, -14/14, -9/10	-6/6, -11/12, -8/10
Reflect. Collected/unique		2943/2560	6772/1306	1850/410	5266/555	13675/2491	2964/526	3501/1202	6537/1204	4347/490	5996/1158	6044/1144	5719/1082
Data/restrains/parameters		2560/0/191	1306/0/191	410/374/179	555/531/191	2491/0/381	526/374/191	1202/0/192	1204/6/191	490/276/191	1158/0/191	1144/0/191	1082/0/191
Goodness-of-fit on F2		1.711	1.069	1.134	1.134	1.064	1.134	1.068	1.125	1.105	1.097	1.112	1.07
Final R1/wR2 (I>2o1)		0.1202/0.3750	0.0577/0.1754	0.0569/0.0808	0.0735/0.1495	0.0610/0.1714	0.0799/0.1663	0.0493/0.1462	0.0398/0.1291	0.0730/0.1953	0.0444/0.1393	0.0397/0.1275	0.0578/0.1709
R1/wR2	2 (all data)	0.1246/0.3800	0.0607/0.1832	0.1640/0.1241	0.1384/0.1936	0.0651/0.1786	0.1663/0.2181	0.0535/0.1520	0.0417/0.1318	0.1337/0.2615	0.0480/0.1445	0.0448/0.1364	0.0676/0.1854
Largest diff. p	eak/hole (e.Å ⁻³)	0.37/-0.28	0.17/-0.15	0.09/-0.09	0.12/-0.13	0.23/-0.26	0.16/-0.16	0.19/-0.20	0.11/-0.12	0.13/-0.15	0.12/-0.14	0.10/-0.09	0.18/-0.12

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

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Table S17. Detailed crystallographic da	ta for PDI-C ₆ at various temperatures.
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Temperature (K)		100	298	440	470	
Phase		I	I I		II	
CCDC numbers		2421994	2422224	2412030	2421130	
Method		SC-XRD	SC-XRD	SC-XRD	SC-XRD	
λ		0.71073	0.71073	1.54184	1.54184	
Crystal system		triclinic	triclinic	triclinic	triclinic	
Space group		P-1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	
	a (Å)	4.7056(19)	4.7568(10)	4.8395(10)	11.443(7)	
	b (Å)	8.514(3)	8.5487(16) 8.5365(13)		11.988(8)	
Unit call dimensions	<i>c</i> (Å)	17.281(5)	17.576(2)	18.158(3)	19.506(9)	
Unit cell dimensions	α (°)	81.34(3)	81.678(14)	84.478(12)	96.05(5)	
	в (°)	85.64(3)	84.850(15)	83.426(15)	73.16(5)	
	γ (°)	83.89(3)	83.169(16)	81.495(16)	114.90(6)	
Volume (ų)		679.3(4)	700.3(2)	734.6(2)	2323(3)	
Z/Z'		1/0.5	1/0.5	1/0.5	3/1.5	
Calculated density (g/cm ³)		1.366	1.325	1.263	1.198	
Absorption (mm ⁻	¹)	0.089	0.086	0.656	0.623	
F(000)		296.0	296.0	296.0	888.0	
Crystal size (mm)		0.618x0.065x0.021	0.621 × 0.066 × 0.023	0.315x0.098x0.047	0.319x0.099x0.050	
2θ-range for data collection (°)		7.17 to 58.72	7.048 to 59.036	9.838 to 146.182	8.132 to 76.258	
Min/max indices: h, k, l		-6/ 6, -11/ 11, -22/23	-5/ 6, -10/11, -23/16	-5/5, -8/10, -22/19	-9/8, -9/8, -15/15	
Reflect. Collected/ur	nique	4984/3054	5401/3166	4371/2807	4375/2037	
Data/restrains/parameters		3054/0/191	3166/0/191	2807/78/191	2037/1117/220	
Goodness-of-fit on F2		0.970	0.914	0.952	1.059	
Final R1/wR2 (I>20	51)	0.0853/0.1549	0.0724/0.1256	0.0797/0.2516	0.1768/0.3850	
R1/wR2 (all data	ı)	0.2527/0.2334	0.2545/0.1986	0.1250/0.3256	0.4206/0.5407	
Largest diff. peak/hole (e.Å-3)		0.37/-0.36	0.15/-0.23	0.17/-0.25	0.23/-0.26	

6. Literature

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