

Utilization of Through-Space Effect to Design Donor-Acceptor Systems of Pyrrole, Indole, Isoindole, Azulene and Aniline

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Table of contents		Page no.
Table S1	Benchmark study	S3
Figure S1	The direction of TSE and the variation in V_m values in each pyrrole ring in $C_3N_{1'}$ and $C_3C_{2'}$ connected polypyrroles.	S4
Figure S2	Schematic representation of electronic distributions observed in frontier molecular orbitals of selected set of systems	S5
Figure S3	The direction of PoED and the variation in V_m values in each pyrrole unit in ${}^5P_{C_3N_{1'}}$	S6
Figure S4	Illustration of the directional nature of TSE in $(P_{C_3N_{1'}})_n$ clusters	S7
Figure S5	Illustration of the directional nature of TSE in $(P_{C_3C_{2'}})_n$ clusters.	S8
Figure S6	Atomic polar tensor charges demonstrating the donor-acceptor feature of ${}^n P_{C_3N_{1'}}$ systems	S9
Figure S7	The MESP mapped on to 0.01 au electron density isosurface for phenyldipyrrole (PhDP) systems	S9
Figure S8	The MESP mapped on to 0.01 au electron density isosurface for intramolecularly coupled octapyrrolynaphthalene (OPN) systems	S10
Figure S9	The MESP mapped on to 0.01 au electron density isosurface for intramolecularly coupled decapyrrylcorannulene (DPC) systems	S11
Figure S10	Complementary electrostatic interactions in the dimers of ${}^n P_{C_3N_{1'}}$.	S12
Figure S11	Representative examples for complementary complexes.	S13
Figure S12	Numbering in indole, isoindole, azulene and aniline systems adopted in the study	S13
Figure S13	The direction of TSE and the variation in V_m values in 3,1'-polyindoles (${}^n I_{C_3N_{1'}}$)	S14
Figure S14	The direction of TSE and the variation in V_m values in 3,2'-polyindoles (${}^n I_{C_3C_{2'}}$)	S15
Figure S15	The direction of TSE and the variation in V_m values in 6,1'-polyindoles (${}^n I_{C_6N_{1'}}$)	S16
Figure S16	The direction of TSE and the variation in V_m values in polyisoindoles (${}^6 i I_{C_5N_{1'}}$)	S17

Figure S17	The direction of TSE and the variation in V_m values in polyazulenes ($^n\mathbf{Az}_{C_{1C6}'}$).	S18
Figure S18	The direction of TSE and the variation in V_m values in polyanilines ($^n\mathbf{An}_{C_{4C2}'}$)	S19
Figure S19	The direction of TSE in clusters of $I_{C_{3N1}'}$, $I_{C_{3C2}'}$, $I_{C_{6N1}'}$, $iI_{C_{5N1}'}$, $\mathbf{An}_{C_{4C2}'}$ and $\mathbf{Az}_{C_{1C6}'}$ systems	S20
Table S2	The SCF energy, dipole moment, HOMO energy, LUMO energy and HOMO-LUMO gap (HLG) of all the systems	S21
Figure S20	NMR analysis	S23
Figure S21	Simulated absorption spectra of the molecules	S29
Figure S22	The difference in total density computed for the ground and excited states of 1- <i>PhP</i> and <i>HPB</i> _{N1} systems plotted at iso-contour value 0.001 au	S37
Table S3	Cartesian coordinates of all the geometries	S37

Table S1. Comparison V_m values corresponding to each ring in pyrrole and its C₃-N_{1'} connected polyrrroles using different DFT methods.

method	system	V_m in kcal/mol					
		ring1	ring2	ring3	ring4	ring5	ring6
B3LYP/6-311+g(d,p)	P	-25.5					
	² P _{C₃N_{1'}}	-17.7	-28.2				
	³ P _{C₃N_{1'}}	-14.1	-20.9	-30.1			
	⁴ P _{C₃N_{1'}}	-12.0	-17.4	-22.8	-31.3		
	⁵ P _{C₃N_{1'}}	-10.6	-15.4	-19.4	-24.0	-32.2	
	⁶ P _{C₃N_{1'}}	-9.8	-14.1	-17.5	-20.5	-24.9	-32.9
M06-L/6-311+g(d,p)	P	-25.9					
	² P _{C₃N_{1'}}	-18.5	-27.9				
	³ P _{C₃N_{1'}}	-15.0	-20.9	-29.4			
	⁴ P _{C₃N_{1'}}	-13.0	-17.7	-22.4	-30.5		
	⁵ P _{C₃N_{1'}}	-11.7	-15.7	-19.4	-23.8	-31.2	
	⁶ P _{C₃N_{1'}}	-10.8	-14.5	-17.6	-20.6	-24.4	-31.9
wB97XD/6-311+g(d,p)	P	-27.5					
	² P _{C₃N_{1'}}	-19.4	-30.4				
	³ P _{C₃N_{1'}}	-15.6	-22.6	-32.3			
	⁴ P _{C₃N_{1'}}	-13.3	-19.0	-24.7	-33.7		
	⁵ P _{C₃N_{1'}}	-12.0	-17.0	-21.1	-25.8	-34.6	
	⁶ P _{C₃N_{1'}}	-11.1	-15.6	-19.1	-22.1	-26.9	-35.2

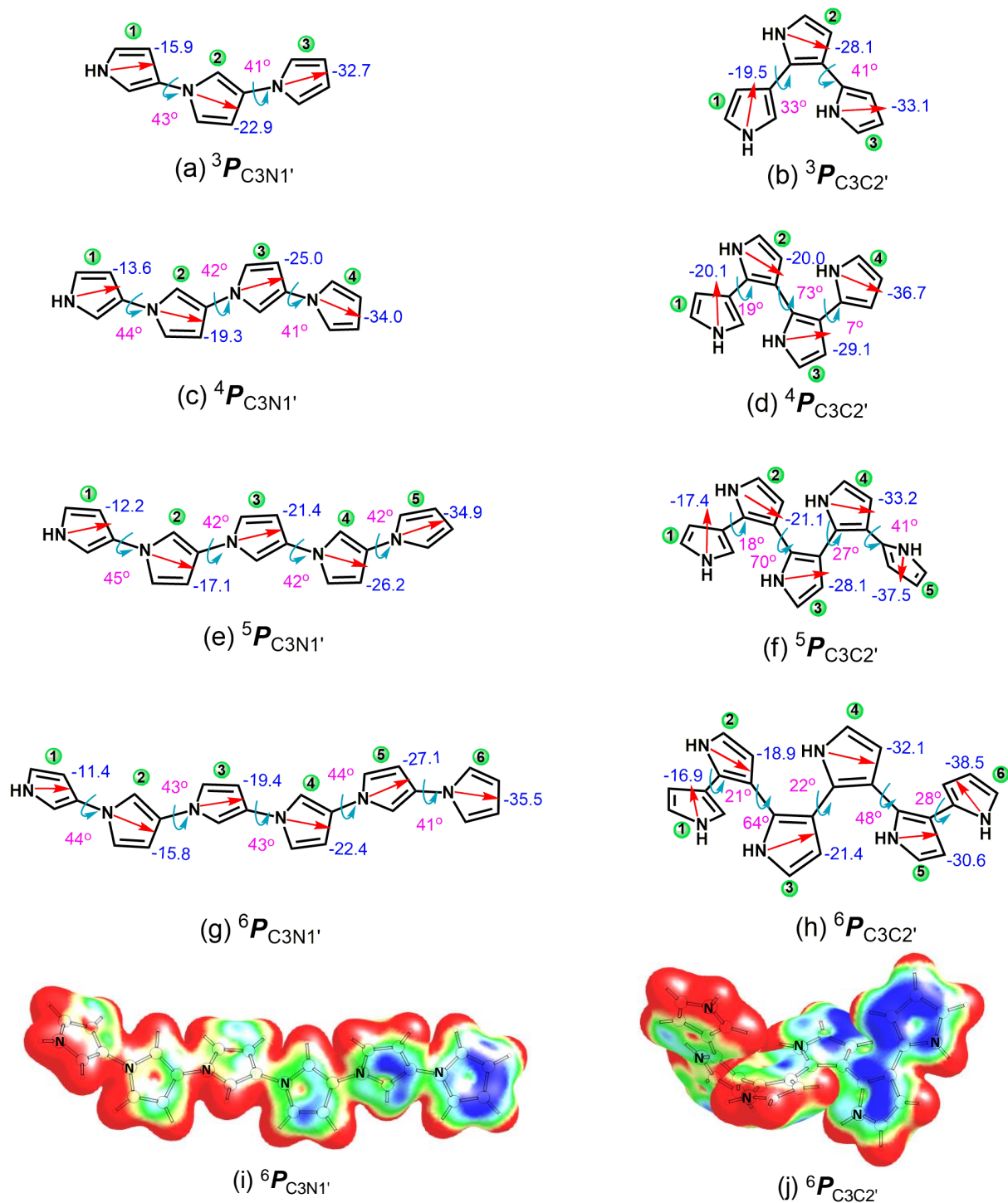
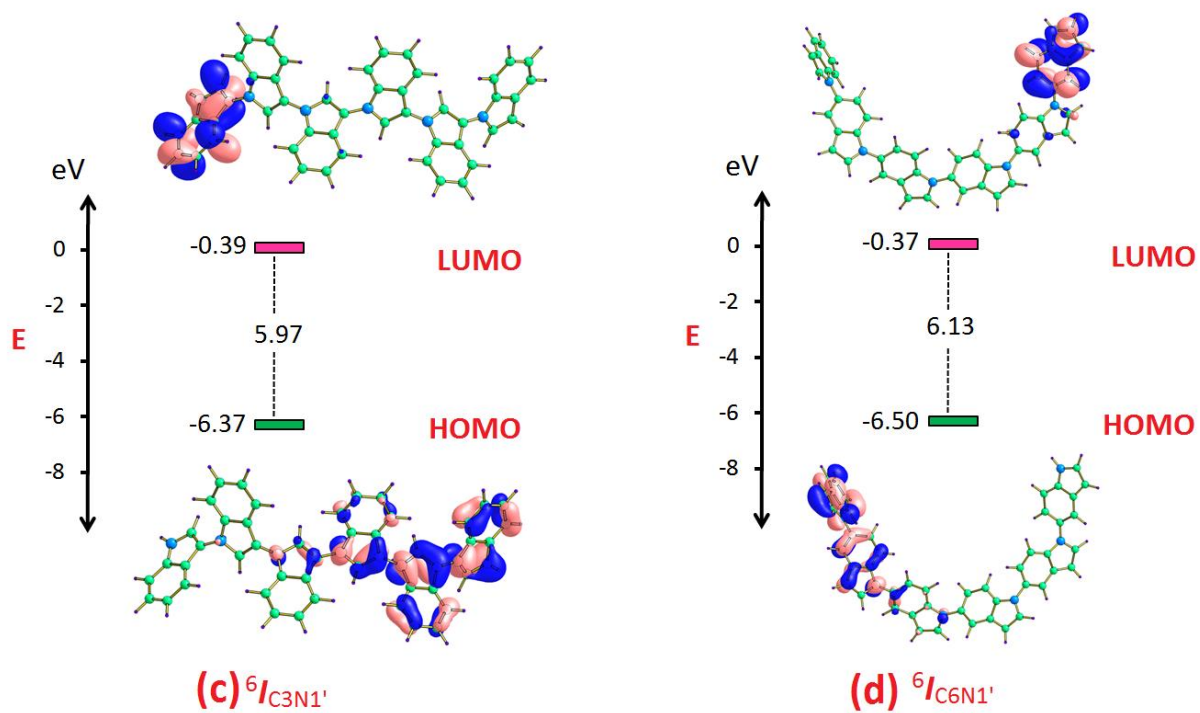
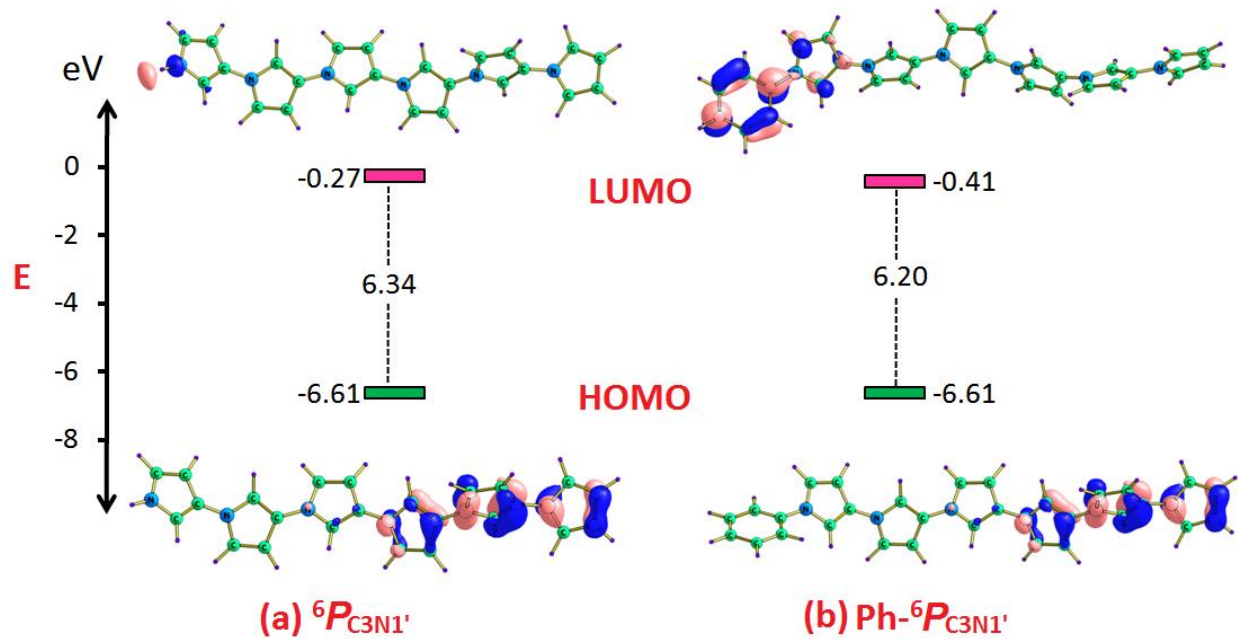


Figure S1. The direction of TSE and the variation in V_m values in each pyrrole ring in (a) C_3N_1' and (b) C_3C_2' connected polypyrroles. The V_m values are given in kcal/mol (blue font) and pyrrole rings from left to right are numbered from 1 to 6, respectively. The dihedral angle at the C_3N_1' and C_3C_2' junctions between the adjacent rings in ${}^n P_{C_3N_1'}$ and ${}^n P_{C_3C_2'}$ are given in pink font. The is MESP mapped on to 0.01 au electron density isosurface of (c) ${}^6 P_{C_3N_1'}$ and (d) ${}^6 P_{C_3C_2'}$ polypyrroles, where coding from blue to red indicates MESP values in the range -0.03 to 0.03 au.



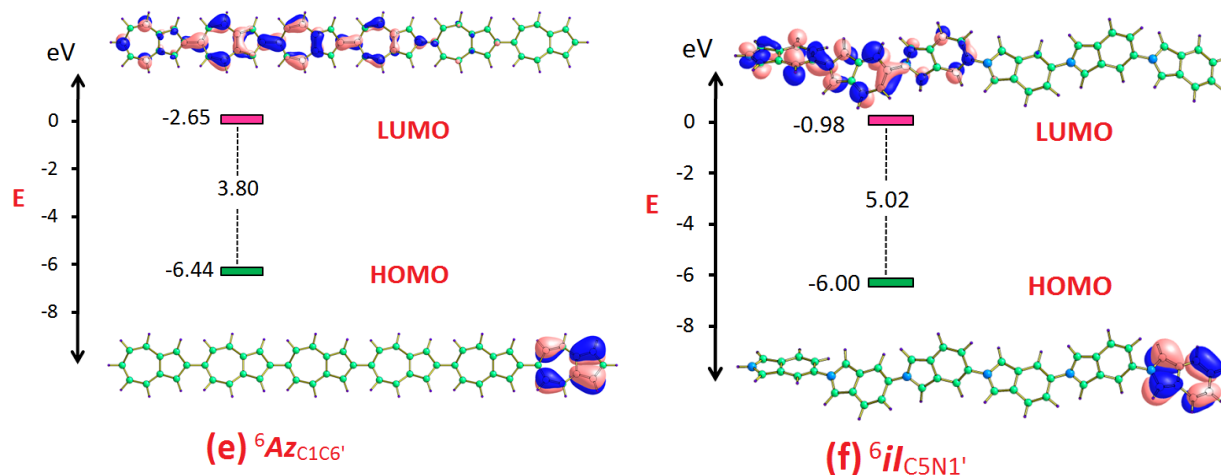


Figure S2. Schematic representation of electronic distributions observed in frontier molecular orbitals of representative set of systems. The MO energy and band gap values in eV are also depicted.

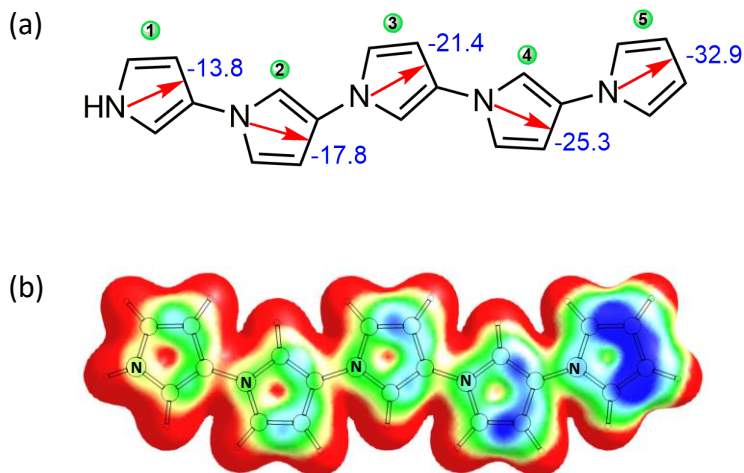


Figure S3. (a) The direction of PoED and the variation in V_m values in each pyrrole unit in ${}^5P_{C3N1'}$ (b) The MESP mapped on to 0.01 au electron density isosurface of ${}^5P_{C3N1'}$, where coding from blue to red indicates MESP values in the range -0.03 to 0.03 au.

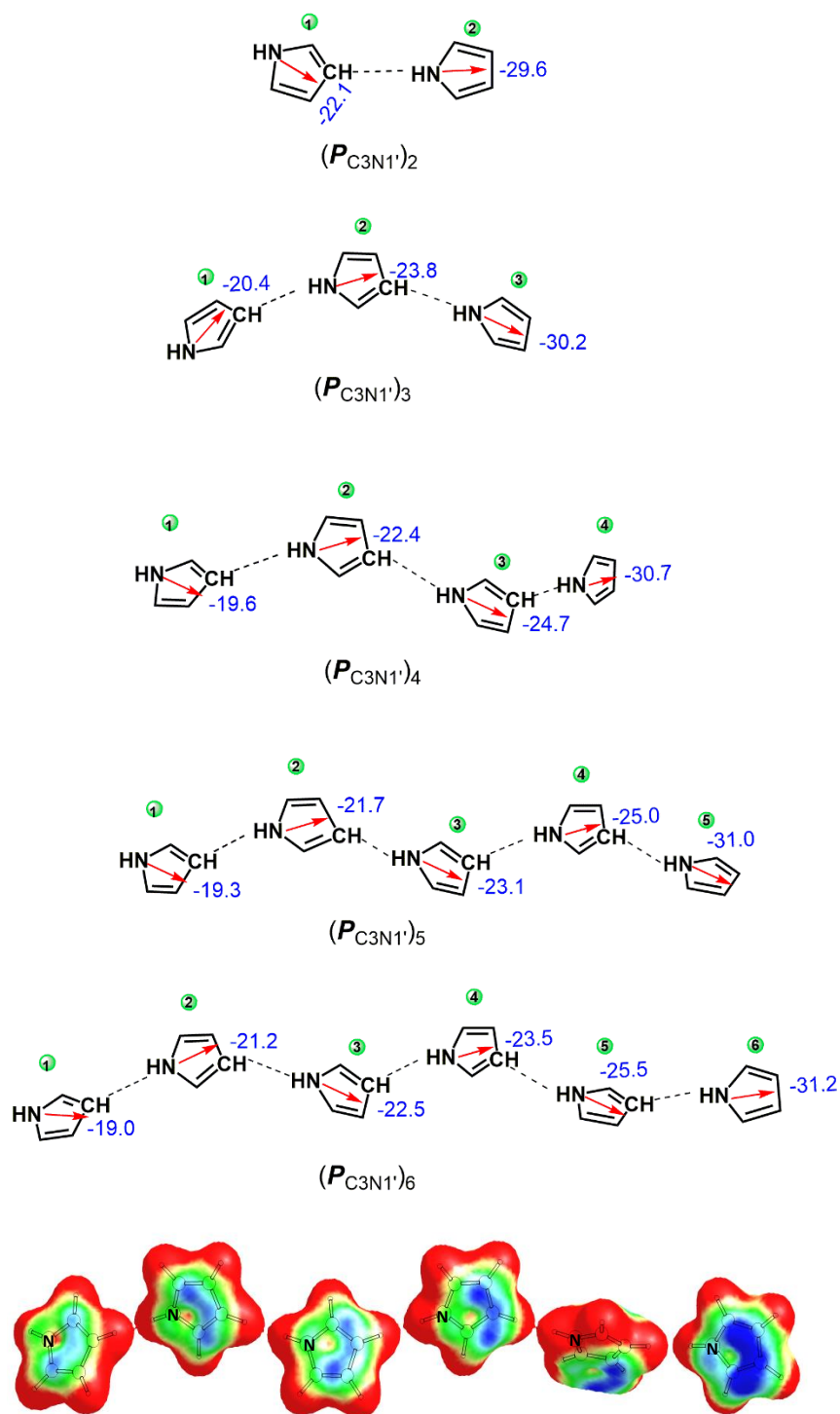


Figure S4. Illustration of the directional nature (red arrows) of TSE in $(P_{C3N1'})_n$ clusters. Pyrroles are numbered from 1 to 6 and V_m values of each ring is given in kcal/mol. The MESP of $(P_{C3N1'})_n$ clusters is mapped on to 0.01 au electron density isosurface, where coding from blue to red indicates MESP values in the range -0.03 to 0.03 au.

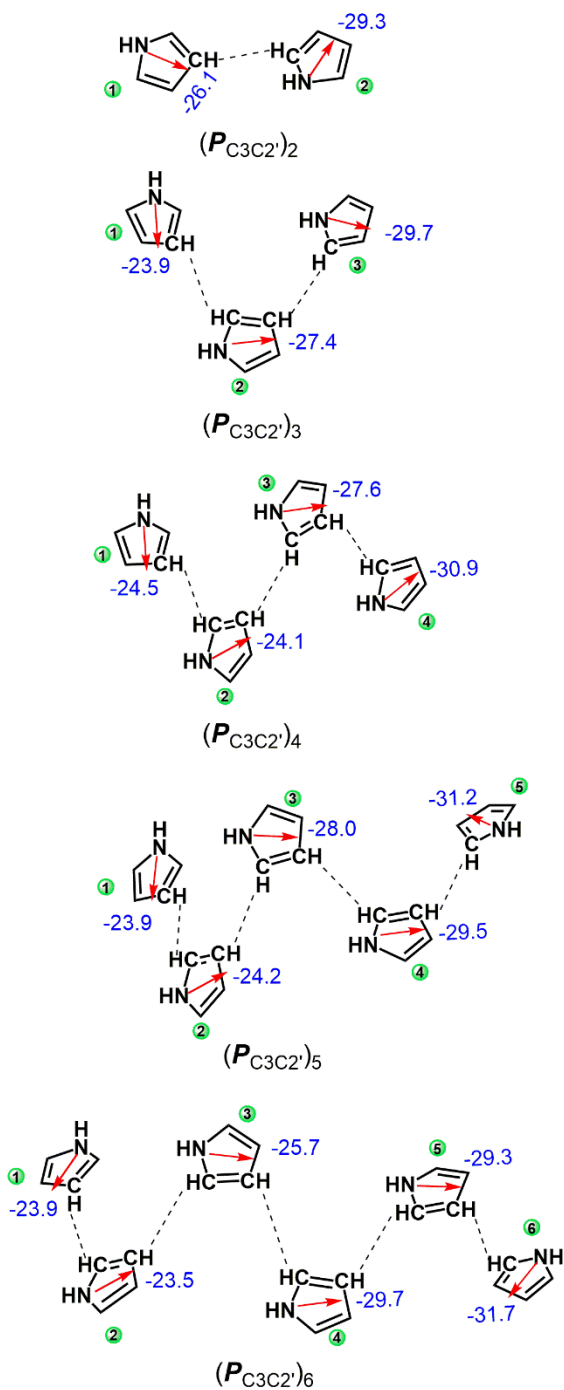


Figure S5. Illustration of the directional nature (red arrows) of TSE in $(P_{C_3C_2'})_n$ clusters. Pyrroles are numbered from 1 to 6 and V_m values of each ring is given in kcal/mol. The MESP of $(P_{C_3C_2'})_n$ clusters is mapped on to 0.01 au electron density isosurface, where coding from blue to red indicates MESP values in the range -0.03 to 0.03 au.

Atomic Polar Tensor Charges

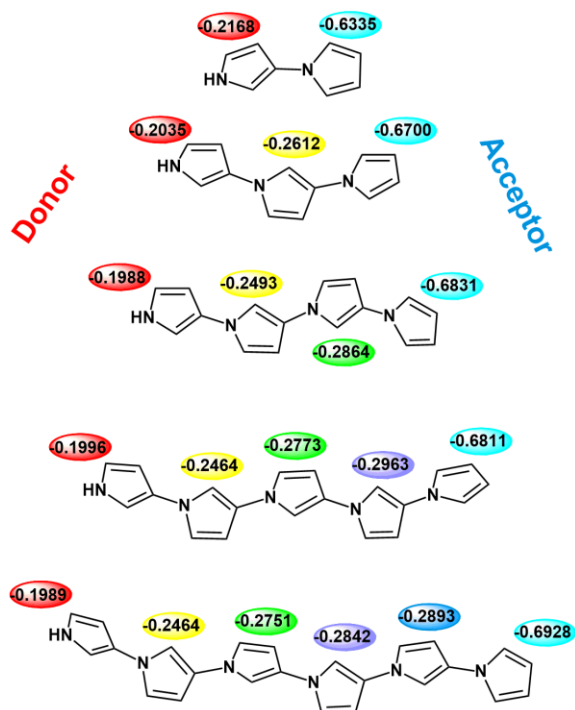


Figure S6. Atomic polar tensor (au) charges demonstrating the donor-acceptor feature of ${}^n\mathbf{P}_{\text{C}_3\text{N}_1}$ systems.

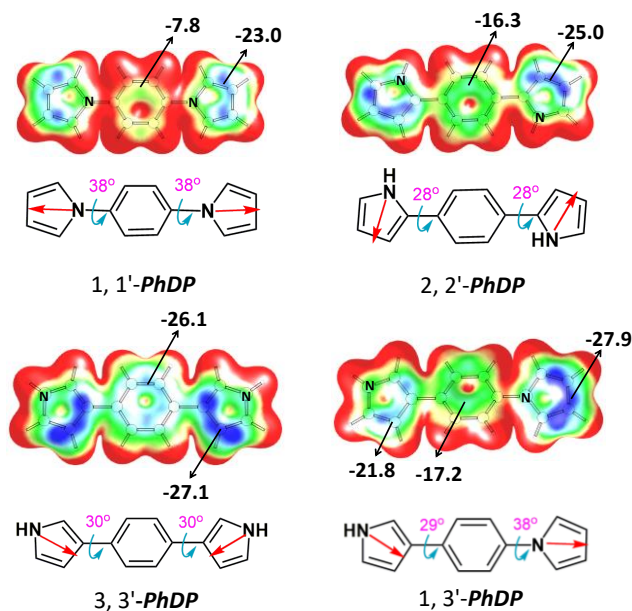


Figure S7. The MESP mapped on to 0.01 au electron density isosurface for phenyldipyrrole (*PhDP*) systems. Colour coding from blue to red indicates MESP values in the range -0.03 to 0.03 au and the V_m of each ring are given in kcal/mol. The red arrows represent the direction of TSE.

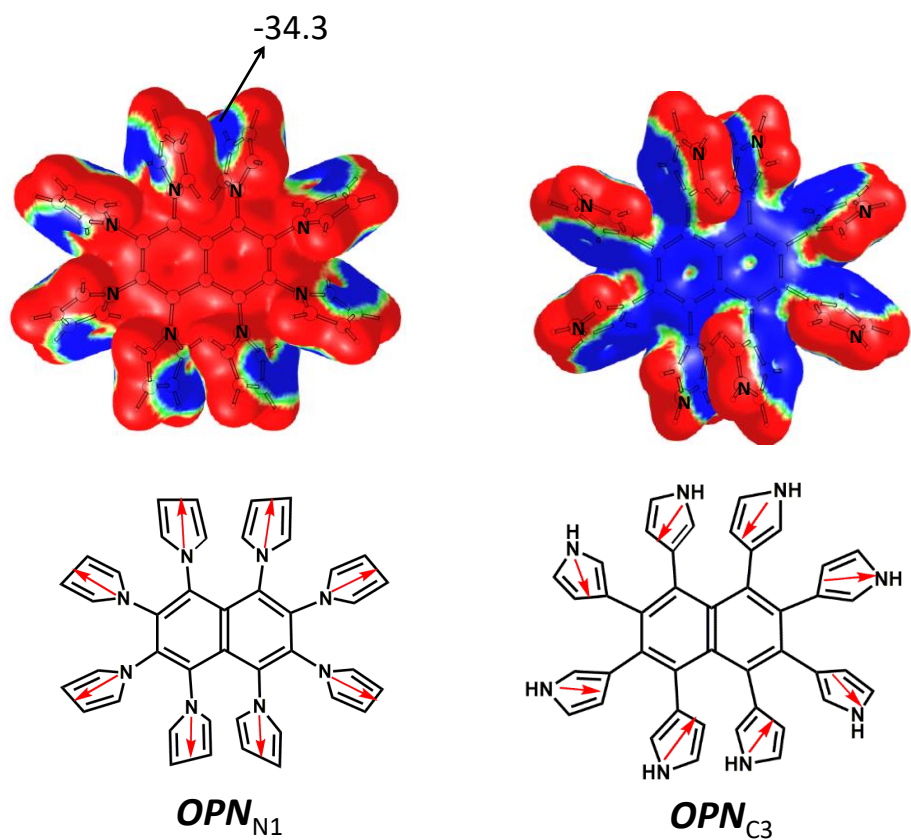


Figure S8. The MESP mapped on to 0.01 au electron density isosurface for intra-molecularly coupled octapyrrolynaphthalene (**OPN**) systems. Colour coding from blue to red indicates MESP values in the range -0.01 to 0.01 au and the V_m of each ring are given in kcal/mol. The direction of electron flow is denoted using red arrow.

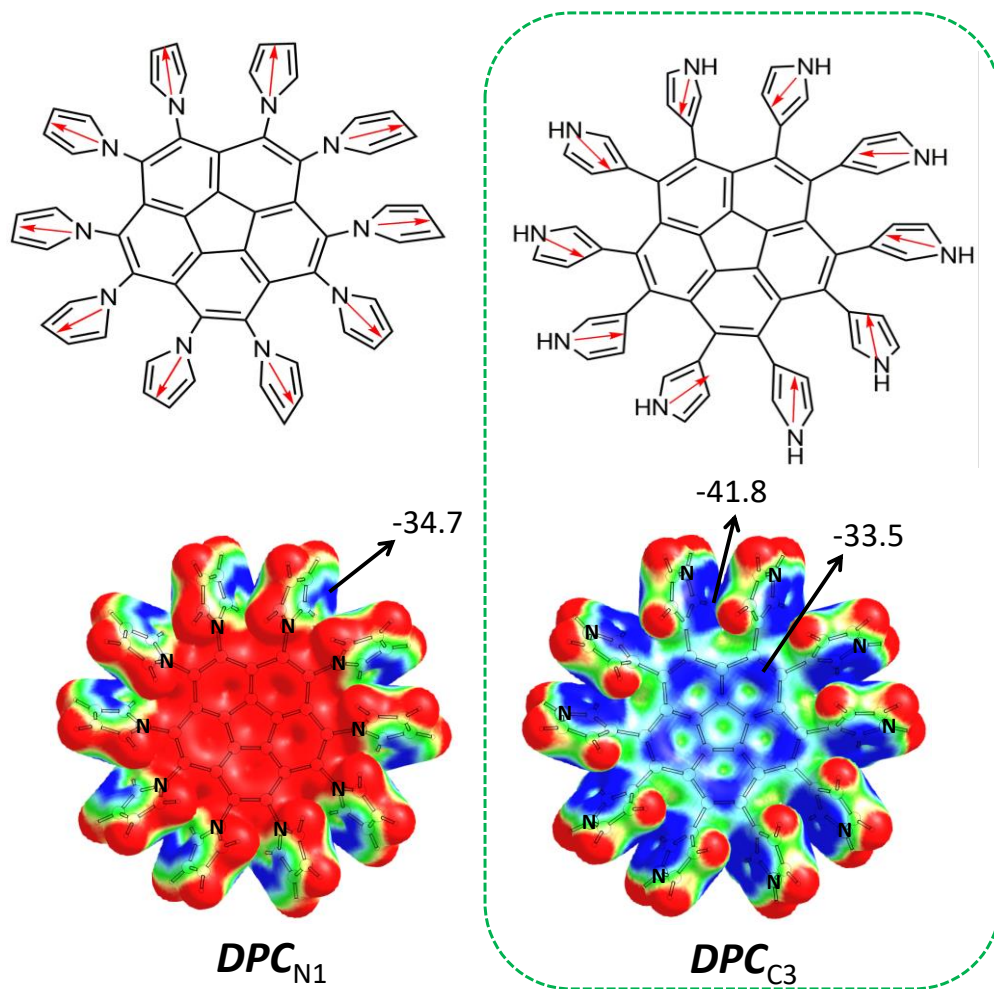


Figure S9. The MESP mapped on to 0.01 au electron density isosurface for intra-molecularly coupled decapyrrolylcorannulene (**DPC**) systems. Color coding from blue to red indicates MESP values in the range -0.03 to 0.03 au and the V_m of each ring are given in kcal/mol.

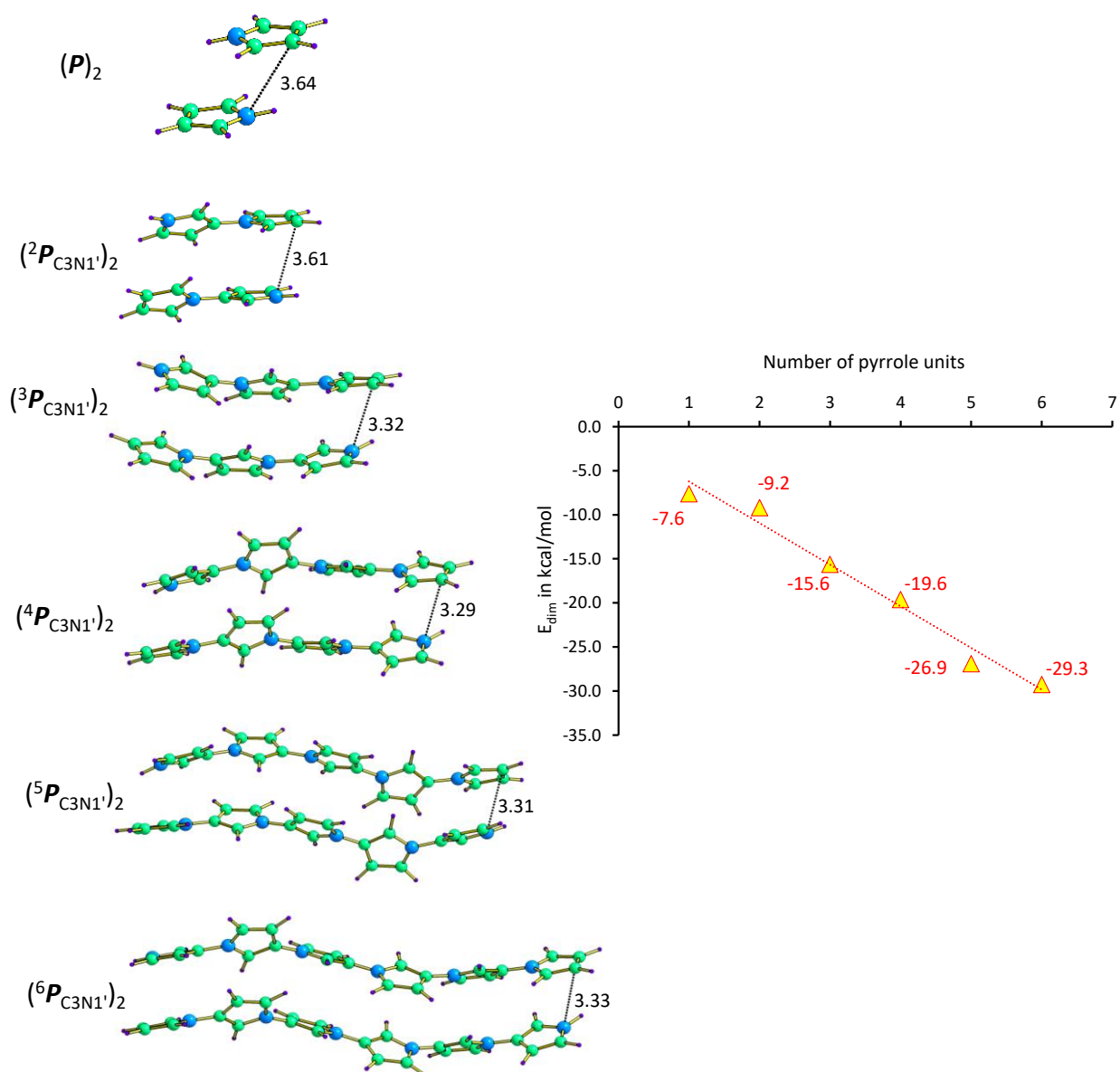


Figure S10. Complementary electrostatic interactions in the dimers of $nP_{C3N1'}$. The intermolecular distances are given in Å.

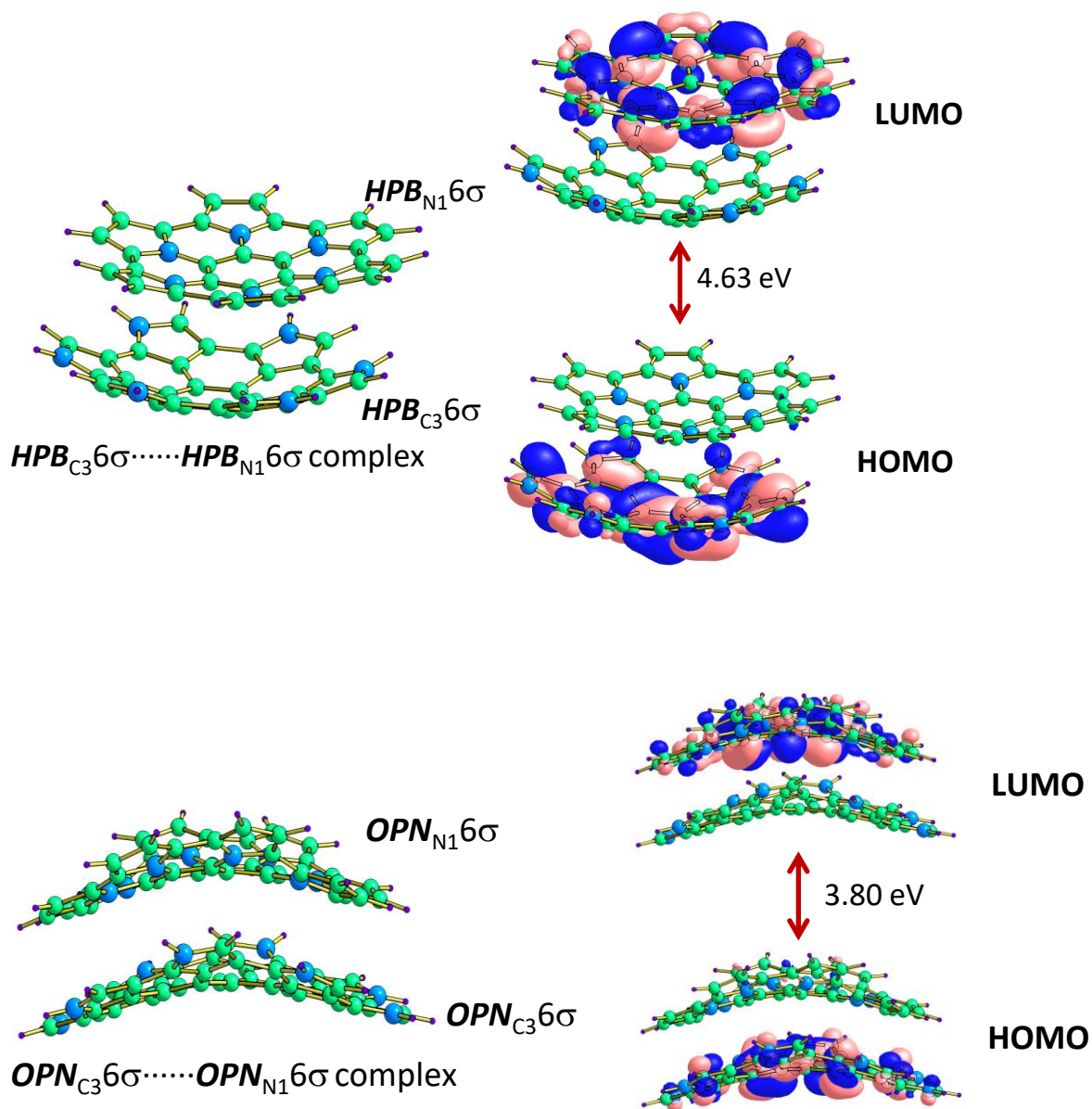


Figure S11. Representative examples for complementary complexes.

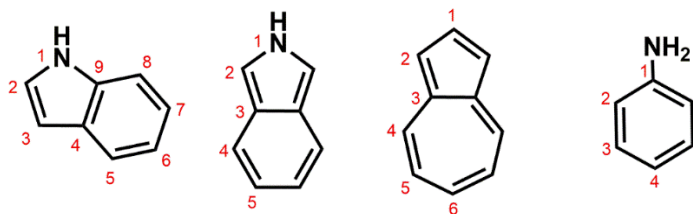


Figure S12. Numbering in indole, isoindole, azulene and aniline systems adopted in the study.

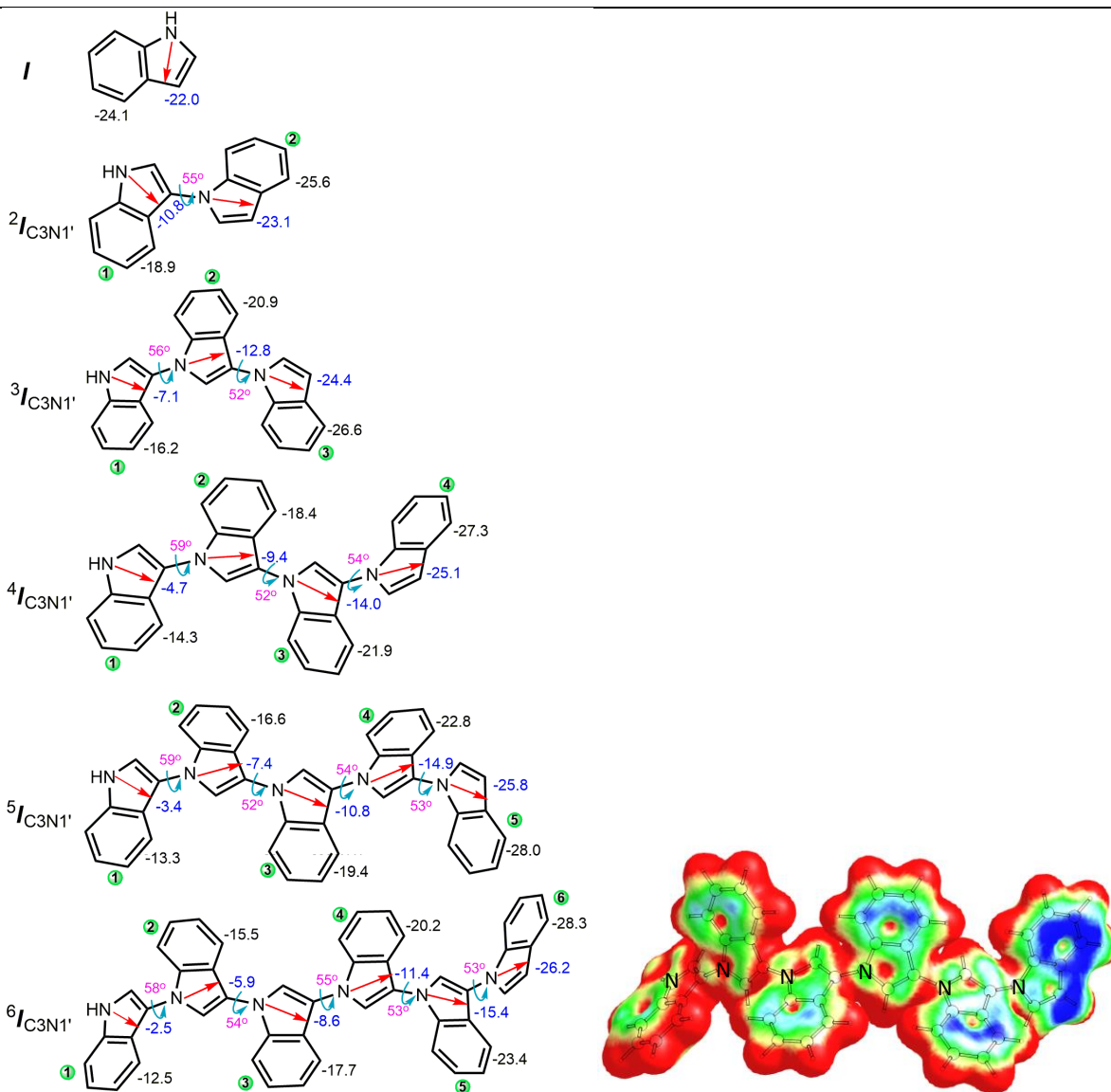


Figure S13. The direction of TSE and the variation in V_m values in 3, 1'-polyindoles (I to $6I_{C3N1'}$). The V_m values of five- and six-membered rings are given in kcal/mol are represented in blue and black font respectively. The dihedral angle at the CCCC junctions between the adjacent rings are given in pink font. The MESP mapped on to 0.01 au electron density isosurface of $6I_{C3N1'}$, where coding from blue to red indicates MESP values in the range -0.02 to 0.02 au.

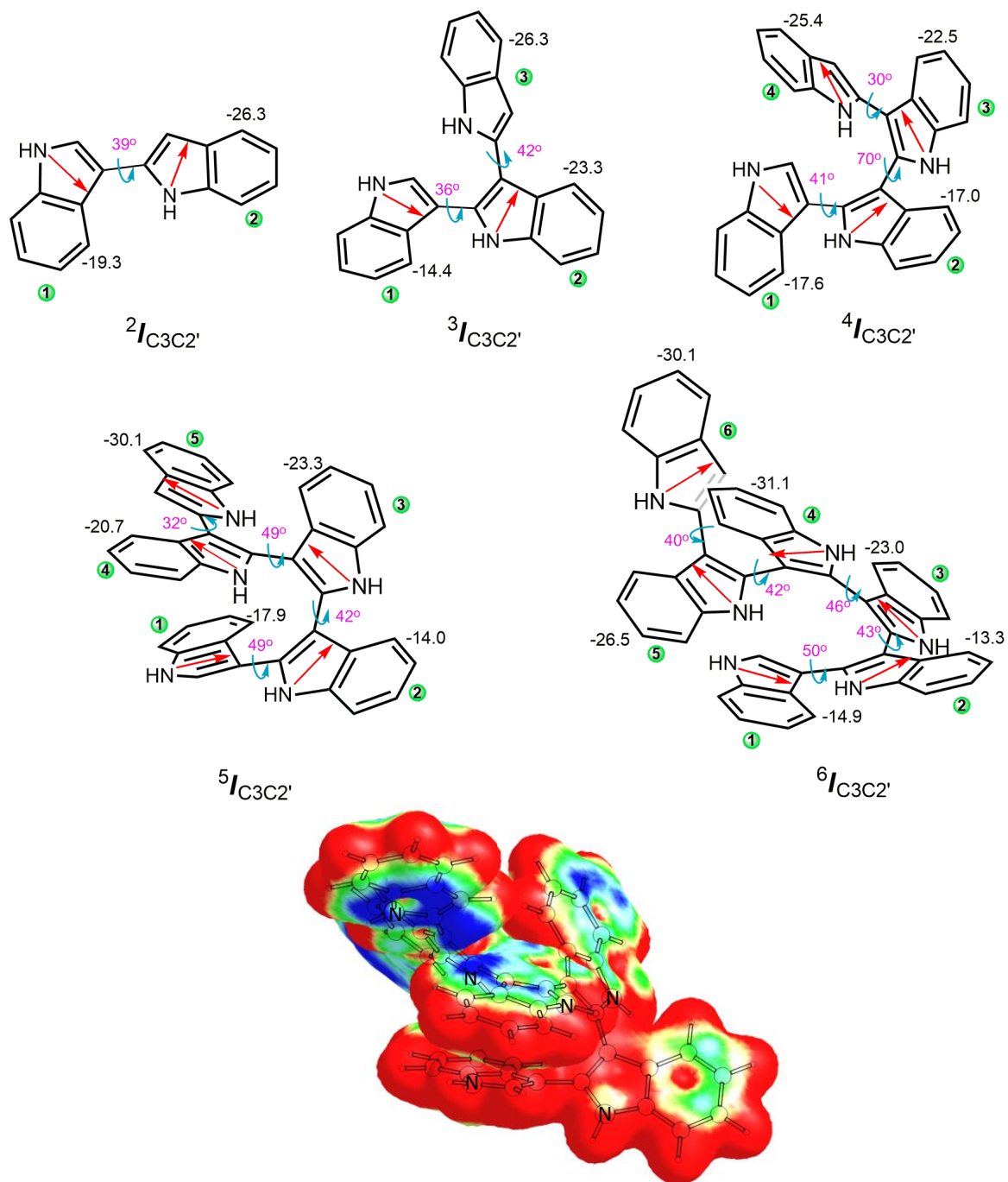


Figure S14. The direction of TSE and the variation in V_m values in 3,2'-polyindoles (2I_{C3C2'} to 6I_{C3C2'}). The V_m values of six-membered rings are given in kcal/mol are represented in black font respectively. The dihedral angle at the CCCC junctions between the adjacent rings are given in pink font. The MESP mapped on to 0.01 au electron density isosurface of 6I_{C3C2'}, where coding from blue to red indicates MESP values in the range -0.02 to 0.02 au.

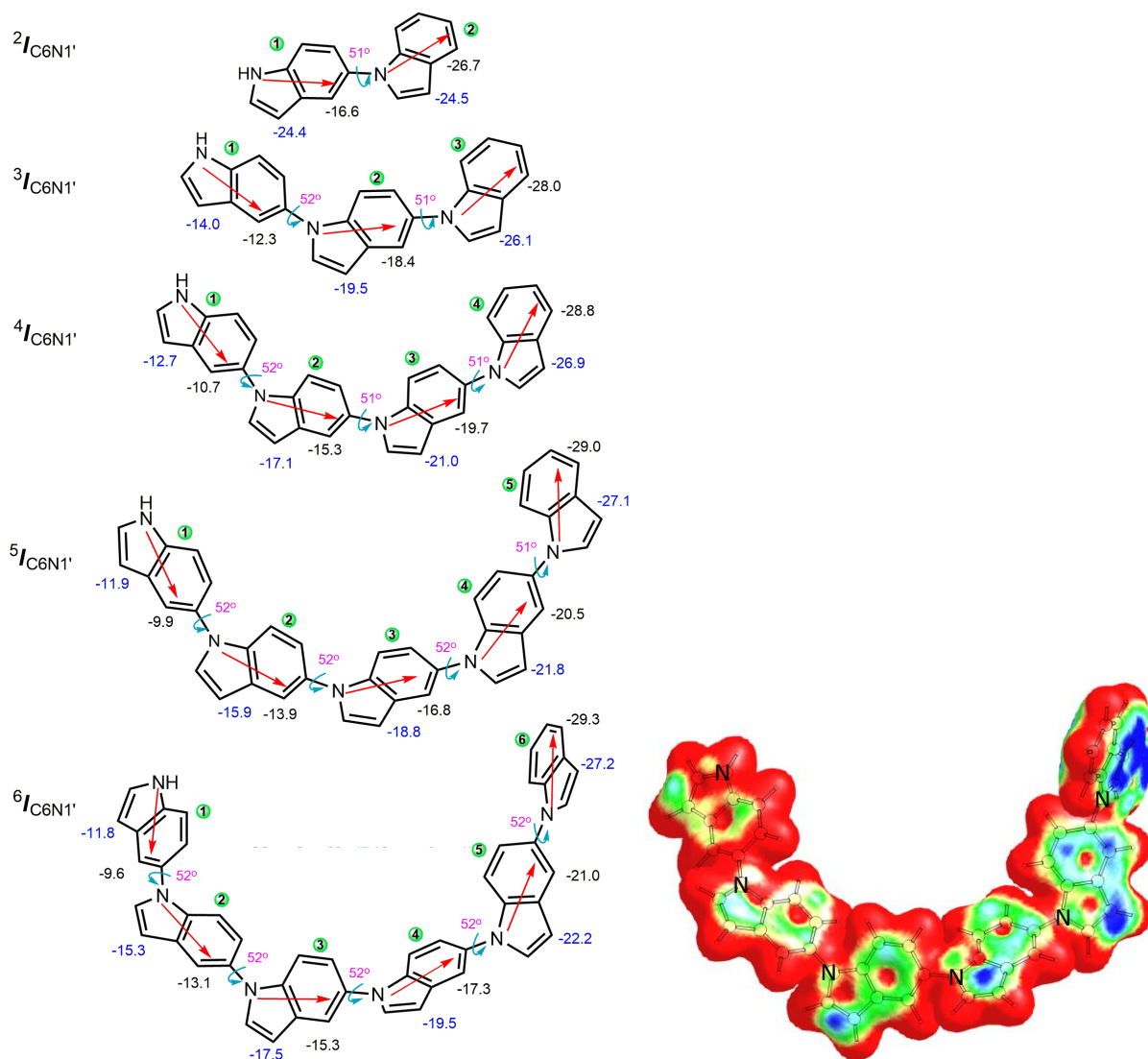


Figure S15. The direction of electron flow and the variation in V_m values in 6, 1'-polyindoles (${}^2I_{C6N1'}$ to ${}^6I_{C6N1'}$). The V_m values of five- and six-membered rings are given in kcal/mol are represented in blue and black font respectively. The dihedral angle at the CCCC junctions between the adjacent rings are given in pink font. The MESP mapped on to 0.01 au electron density isosurface of ${}^6I_{C3N1'}$, where coding from blue to red indicates MESP values in the range -0.02 to 0.02 au.

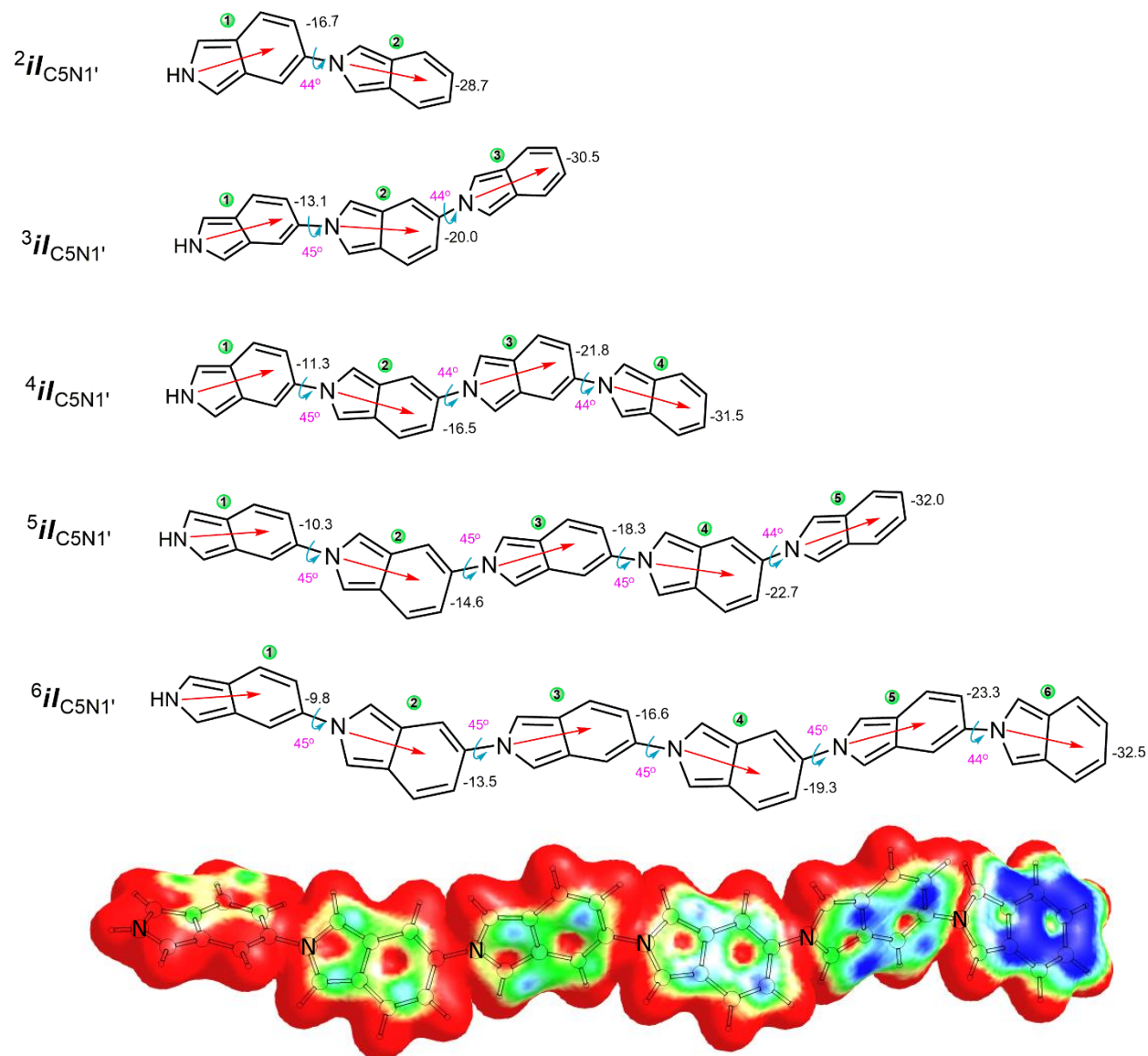


Figure S16. The direction of TSE and the variation in V_m values in polyisindoles (${}^2il_{C5N1'}$ to ${}^6il_{C5N1'}$). The V_m values are given in kcal/mol (black font) and the dihedral angle at the CCCC junctions between the adjacent rings are given in pink font. The MESP mapped on to 0.01 au electron density isosurface of ${}^6il_{C5N1'}$, where coding from blue to red indicates MESP values in the range -0.02 to 0.02 au.

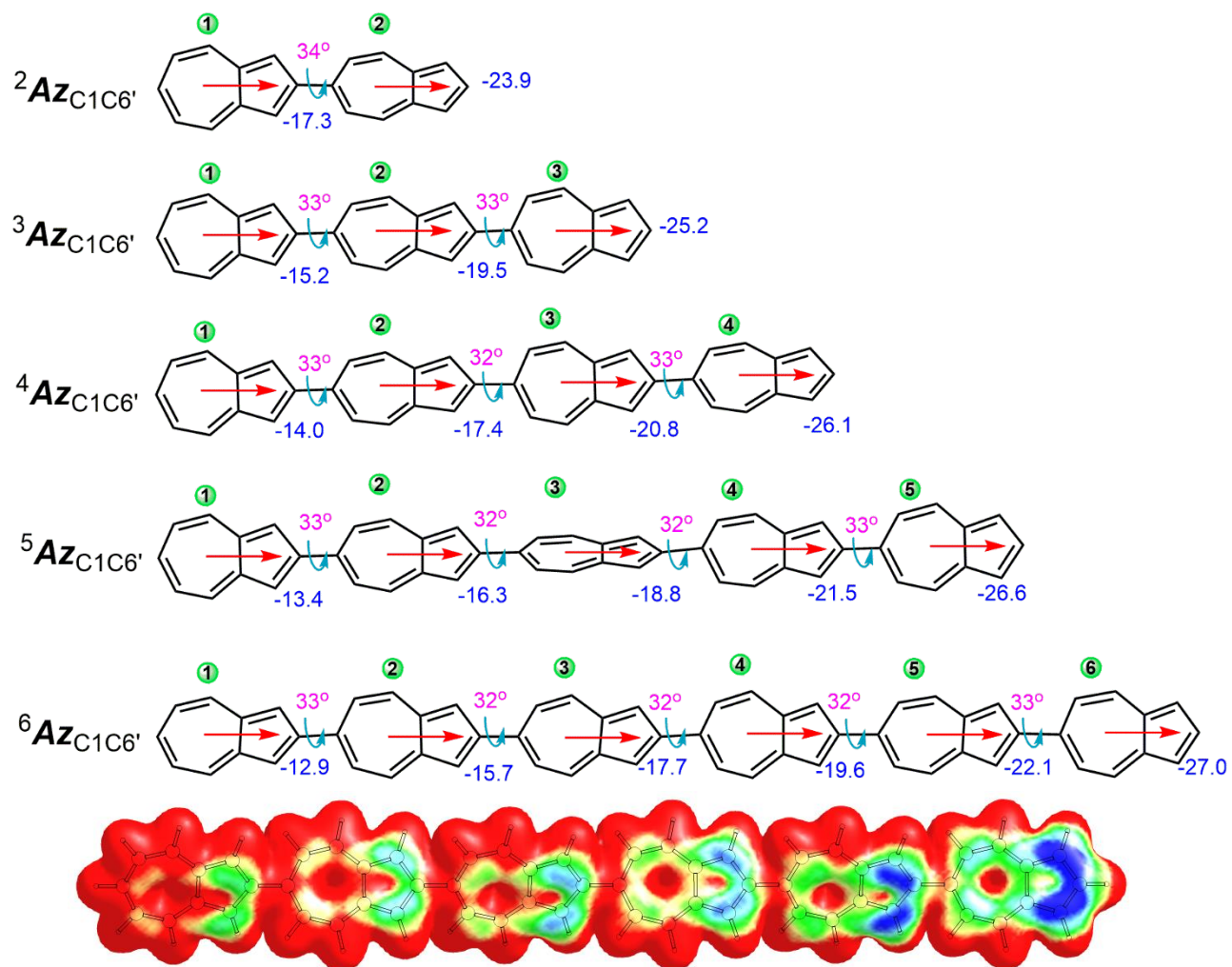


Figure S17. The direction of TSE and the variation in V_m values in polyazulenes ($^2\text{Az}_{\text{C1C6}'}$ to $^6\text{Az}_{\text{C1C6}'}$). The V_m values are given in kcal/mol (blue font) and azulene units from left to right are numbered from 1 to 6 respectively. The dihedral angle at the CCCC junctions between the adjacent units are given in pink font. The MESP mapped on to 0.01 au electron density isosurface of $^6\text{Az}_{\text{C1C6}'}$, where coding from blue to red indicates MESP values in the range -0.02 to 0.02 au.

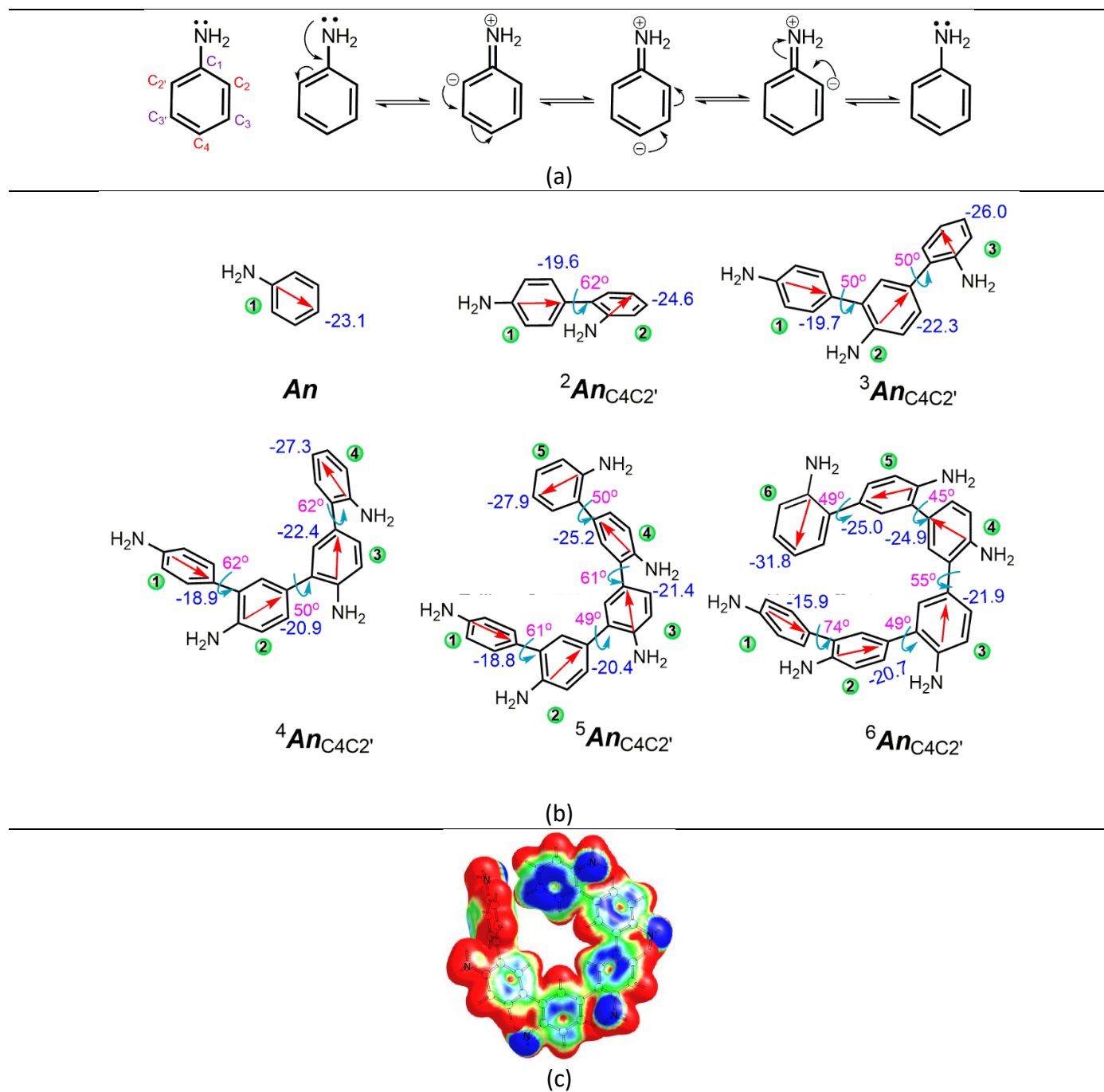


Figure S18. (a) Resonance contributors of aniline (b) The direction of TSE and the variation in V_m values in polyanilines (An to ${}^6An_{C4C2'}$). The V_m values are given in kcal/mol (blue font) and aniline rings from left to right are numbered from 1 to 6 respectively. The dihedral angle at the CCCC junctions between the adjacent rings are given in pink font. (b) The MESP mapped on to 0.01 au electron density isosurface of ${}^6An_{C4C2'}$, where coding from blue to red indicates MESP values in the range -0.03 to 0.03 au.

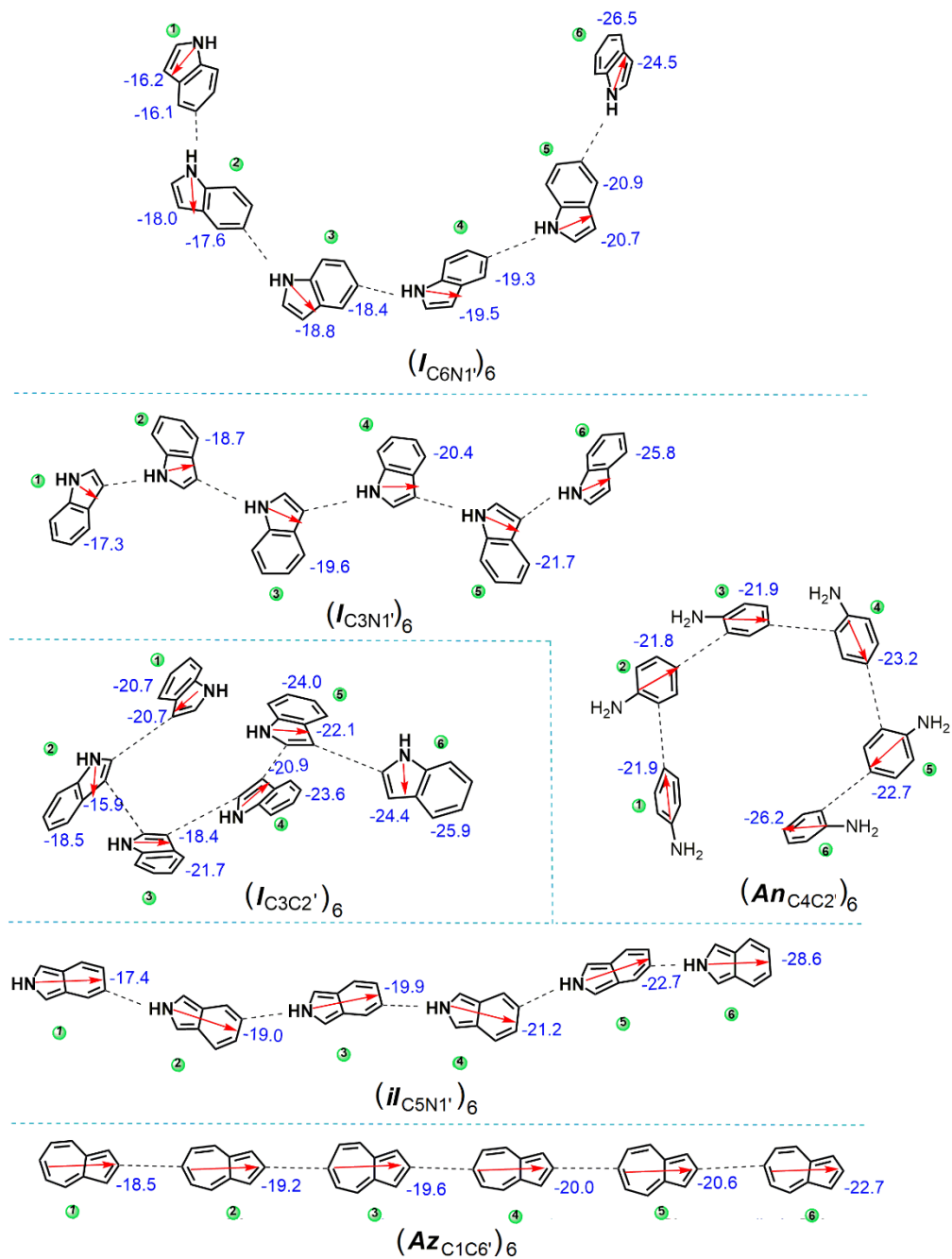


Figure S19. The direction of TSE in clusters of $I_{C3N1'}$, $I_{C3C2'}$, $I_{C6N1'}$, $il_{C5N1'}$, $An_{C4C2'}$ and $Az_{C1C6'}$ systems and the V_m values are given in kcal/mol (Dotted lines represent H...H distances $\cong 0$).

Table S2. The SCF energy, dipole moment, HOMO energy, LUMO energy and HOMO-LUMO gap (HLG) of all the systems at M06-2X/6-311+G(d, p) level of theory

System	SCF energy (au)	Dipole moment (D)	HOMO (eV)	LUMO (eV)	HLG (eV)
pyrrole	-210.135113	1.91	-7.28	0.22	7.50
² P _{C2C2'}	-419.092585	0.93	-6.46	0.10	6.56
² P _{C3C3'}	-419.087658	0.47	-6.45	0.23	6.68
² P _{N1N1'}	-419.037167	0.00	-7.53	0.38	7.91
² P _{C2N1'}	-419.078019	1.81	-7.17	0.10	7.27
² P _{C3N1'}	-419.077622	3.81	-7.12	-0.01	7.12
² P _{C3C2'}	-419.090301	2.86	-6.42	0.09	6.51
³ P _{C3N1'}	-628.020696	6.03	-6.86	-0.12	6.74
⁴ P _{C3N1'}	-836.963995	8.28	-6.72	-0.19	6.53
⁵ P _{C3N1'}	-1045.907306	10.57	-6.68	-0.24	6.44
⁶ P _{C3N1'}	-1254.850791	13.21	-6.61	-0.27	6.34
³ P _{C3C2'}	-628.048771	4.22	-6.15	-0.03	6.11
⁴ P _{C3C2'}	-837.008796	5.39	-5.99	-0.10	5.90
⁵ P _{C3C2'}	-1045.964679	6.35	-5.85	-0.14	5.70
⁶ P _{C3C2'}	-1254.923696	6.28	-5.75	-0.17	5.58
1-PhP	-441.140786	2.28	-7.24	0.10	7.34
2-PhP	-441.149684	1.85	-7.19	0.18	7.37
3-PhP	-441.148589	2.12	-7.32	0.18	7.50
1, 1'-PhDP	-650.089131	0.00	-7.38	-0.28	7.10
2, 2'-PhDP	-650.110482	0.00	-6.47	-0.33	6.14
3, 3'-PhDP	-650.106479	6.34	-6.47	0.15	6.62
1, 3'-PhDP	-650.098642	4.24	-6.91	-0.01	6.90
HPB_{N1}	-1478.755814	0.00	-7.34	-0.85	6.48
HPB_{C2}	-1478.711554	0.02	-6.56	-0.42	6.13
HPB_{C3}	-1478.787673	4.48	-6.07	0.13	6.20
HPB_{N1}6σ	-1485.854932	0.87	-5.82	-0.82	5.00
HPB_{C2}6σ	-1485.929707	3.88	-5.98	-0.70	5.28
HPB_{C3}6σ	-1485.902467	6.88	-5.33	-0.05	5.29
OPN_{N1}	-2057.335592	0.04	-7.09	-1.86	5.23
OPN_{N1}6σ	-2047.870308	0.00	-5.50	-1.51	3.99

OPN _{C36σ}	-2047.966596	0.03	-4.88	-0.26	4.61
DPC _{N1}	-2857.433340	0.29	-6.88	-2.03	4.85
DPC _{C3}	-2857.505526	4.60	-5.42	0.04	5.46
Indole	-363.756824	2.11	-7.06	0.11	7.17
² I _{C3N1'}	-726.335890	3.63	-6.73	-0.13	6.60
³ I _{C3N1'}	-1088.887740	5.52	-6.54	-0.23	6.31
⁴ I _{C3N1'}	-1451.453493	7.48	-6.45	-0.30	6.15
⁵ I _{C3N1'}	-1814.019290	9.49	-6.40	-0.36	6.05
⁶ I _{C3N1'}	-2176.585098	11.22	-6.37	-0.39	5.97
² I _{C3C2'}	-726.335890	3.63	-6.53	-0.12	6.41
³ I _{C3C2'}	-1088.918578	4.49	-6.54	-0.23	6.31
⁴ I _{C3C2'}	-1451.503285	3.30	-6.38	-0.32	6.06
⁵ I _{C3C2'}	-1814.101744	5.66	-6.09	-0.45	5.64
⁶ I _{C3C2'}	-2176.683402	7.09	-6.04	-0.51	5.52
² I _{C6N1'}	-726.324788	4.57	-6.71	-0.10	6.61
³ I _{C6N1'}	-1088.893201	6.91	-6.59	-0.25	6.34
⁴ I _{C6N1'}	-1451.461808	8.64	-6.53	-0.32	6.21
⁵ I _{C6N1'}	-1814.030487	9.50	-6.51	-0.36	6.15
⁶ I _{C6N1'}	-2176.599293	9.98	-6.50	-0.37	6.13
isoindole	-363.741162	2.69	-6.38	0.07	6.45
² il	-726.294333	6.06	-6.20	-0.49	5.71
³ il	-1088.847838	9.97	-6.11	-0.73	5.37
⁴ il	-1451.401615	13.97	-6.05	-0.86	5.19
⁵ il	-1813.955571	18.27	-6.02	-0.94	5.08
⁶ il	-2176.509521	22.31	-6.00	-0.98	5.02
Azulene	-385.754624	1.26	-6.68	-1.49	5.20
² Az	-770.329854	3.34	-6.59	-2.08	4.52
³ Az	-1154.905556	5.94	-6.53	-2.35	4.18
⁴ Az	-1539.481290	8.86	-6.49	-2.50	3.99
⁵ Az	-1924.057144	11.92	-6.46	-2.59	3.88
⁶ Az	-2308.632953	15.14	-6.44	-2.65	3.80
Aniline	-287.553474	1.52	-7.10	0.31	7.42
² An	-573.924979	2.82	-6.73	0.13	6.86

³ An	-860.299622	4.44	-6.52	0.13	6.65
⁴ An	-1146.669773	3.62	-6.43	0.05	6.49
⁵ An	-1433.042957	3.67	-6.33	0.02	6.35
⁶ An	-1719.417556	2.35	-6.25	0.04	6.29
<i>HAzB</i> _{C1}	-2539.639777	0.01	-6.31	-1.59	4.72
<i>HAzB</i> _{C6}	-2539.619065	0.00	-6.66	-1.93	4.72

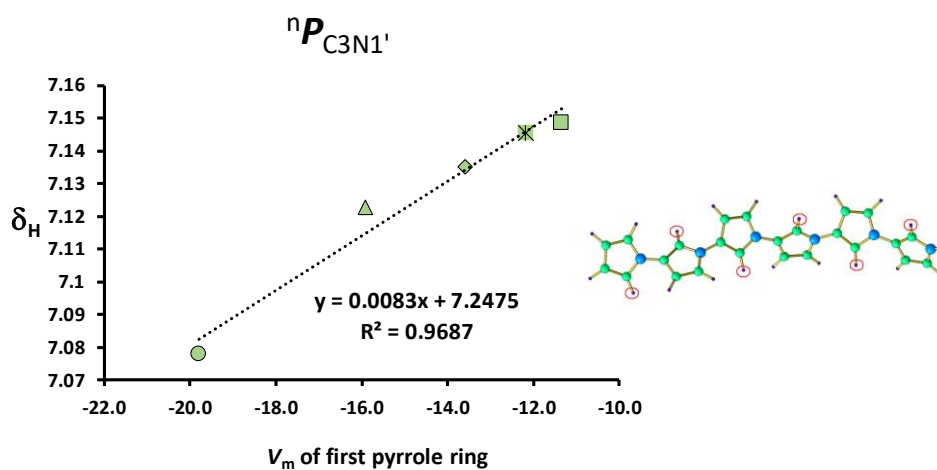


Figure S20a. Relation between chemical shift at the H center (in ppm) and MESP at the last pyrrole ring (in kcal/mol) in ${}^n\mathbf{P}_{\text{C3N1}'}$ systems (${}^2\mathbf{P}_{\text{C3N1}'}$ to ${}^6\mathbf{P}_{\text{C3N1}'}$).

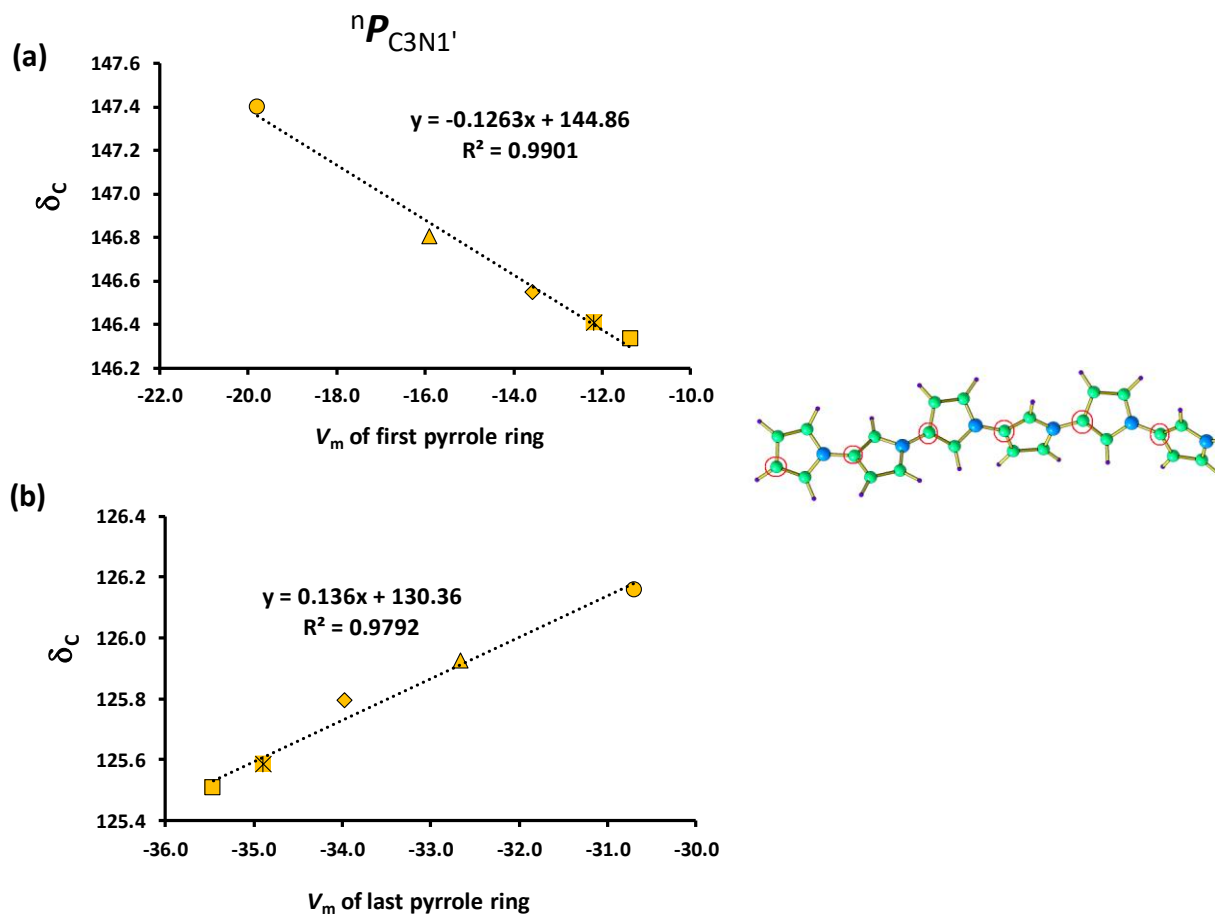


Figure S20b. Relation between chemical shift at the C center (in ppm) and MESP (in kcal/mol) at the (a) first pyrrole ring and (b) last pyrrole ring in ${}^n\text{P}_{\text{C3N1}'}$ systems (${}^2\text{P}_{\text{C3N1}'}$ to ${}^6\text{P}_{\text{C3N1}'}$).

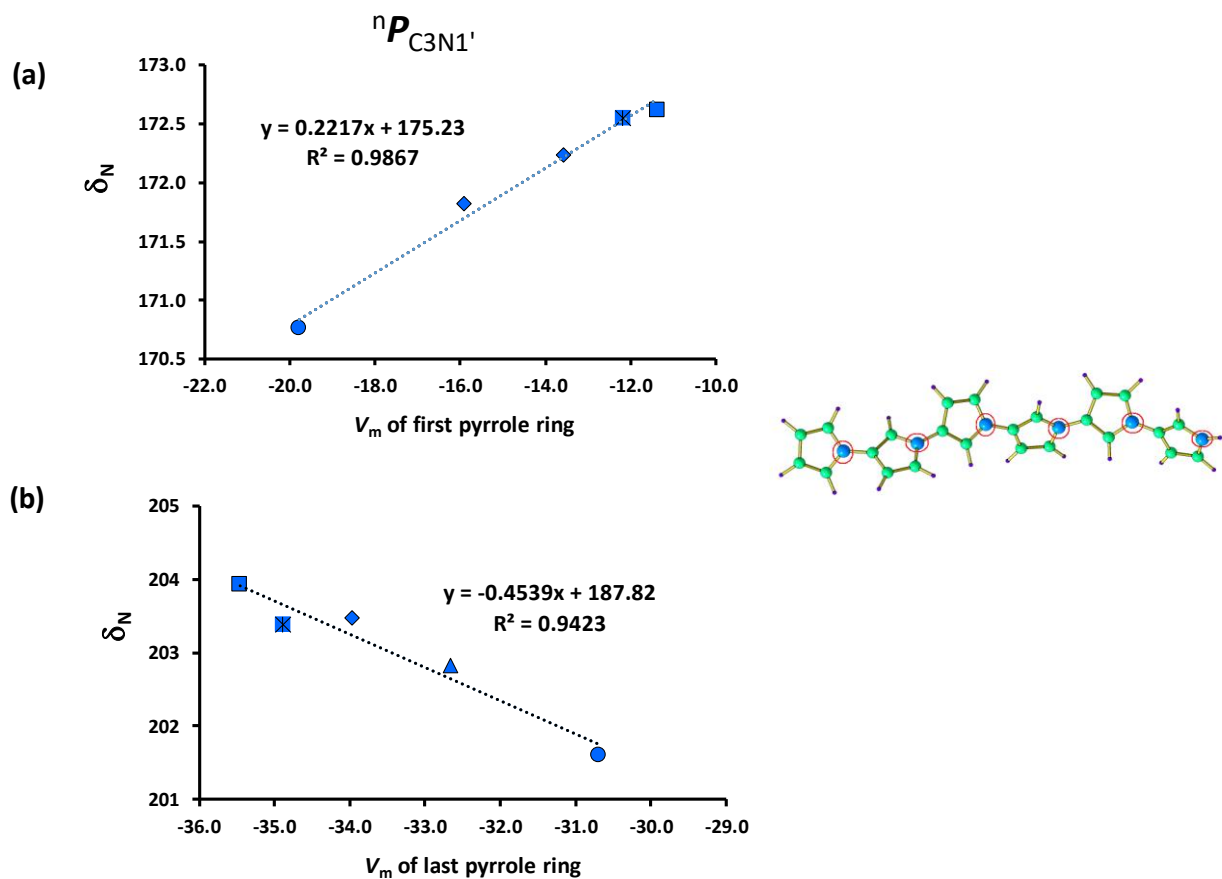


Figure S20c. Relation between chemical shift at the N center (in ppm) and MESP at the (a) first pyrrole ring and (b) last pyrrole ring (in kcal/mol) in ${}^n\text{P}_{\text{C3N1}'}$ systems (${}^2\text{P}_{\text{C3N1}'}$ to ${}^6\text{P}_{\text{C3N1}'}$).

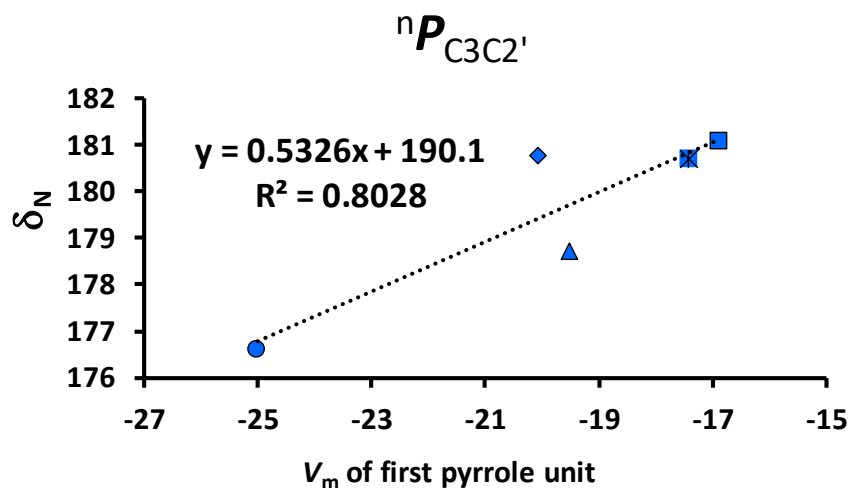


Figure S20d. Relation between chemical shift at the N center (in ppm) and MESP at the first pyrrole ring (in kcal/mol) in ${}^n\text{P}_{\text{C3C2}'}$ systems (${}^2\text{P}_{\text{C3C2}'}$ to ${}^6\text{P}_{\text{C3C2}'}$).

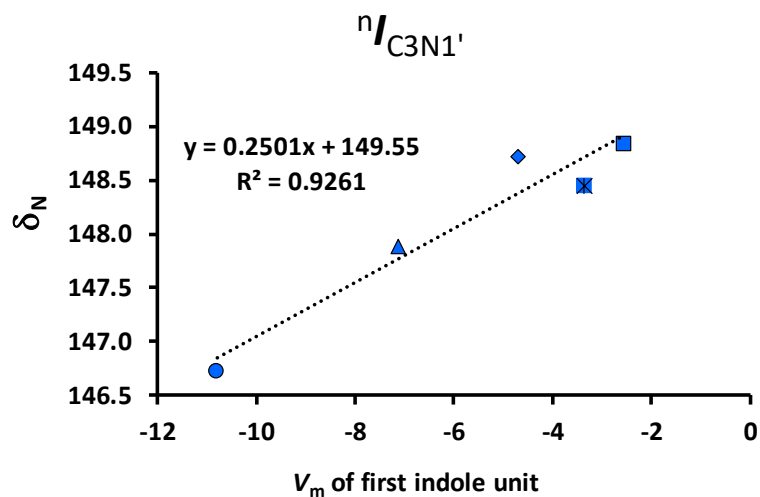


Figure S20e. Relation between chemical shift at the N center (in ppm) and MESP at the first indole unit (in kcal/mol) in ${}^nI_{C3N1'}$ systems (${}^2I_{C3N1'}$ to ${}^6I_{C3N1'}$).

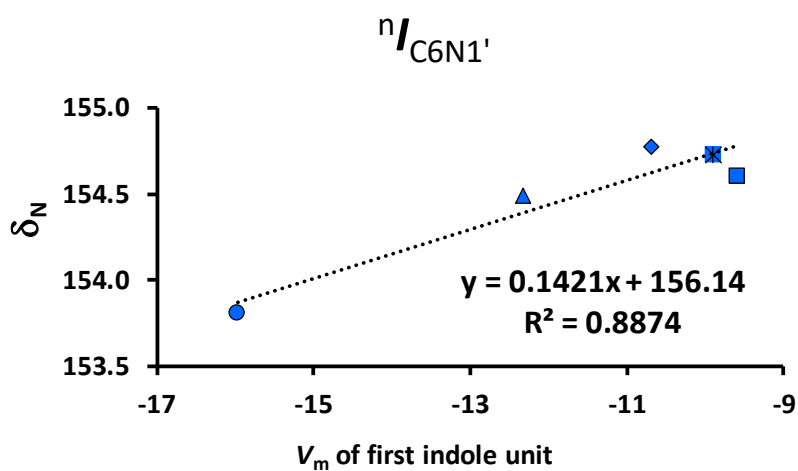


Figure S20f. Relation between chemical shift at the N center (in ppm) and MESP at the first indole unit (in kcal/mol) in ${}^nI_{C6N1'}$ systems (${}^2I_{C6N1'}$ to ${}^6I_{C6N1'}$).

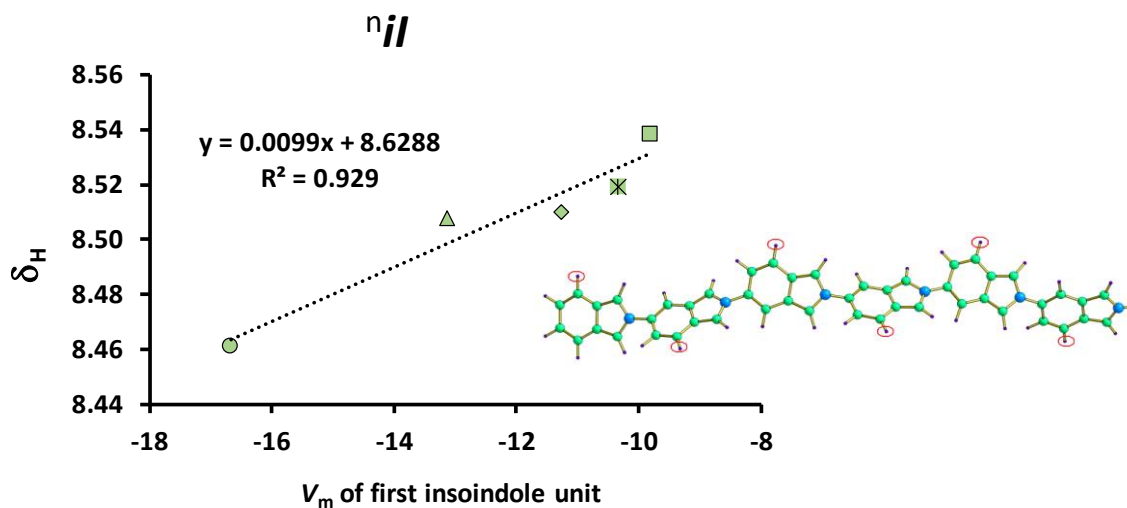


Figure S20g. Relation between chemical shift at the H center (in ppm) and MESP at the first isoindole unit (in kcal/mol) in nli systems (2li to 6li).

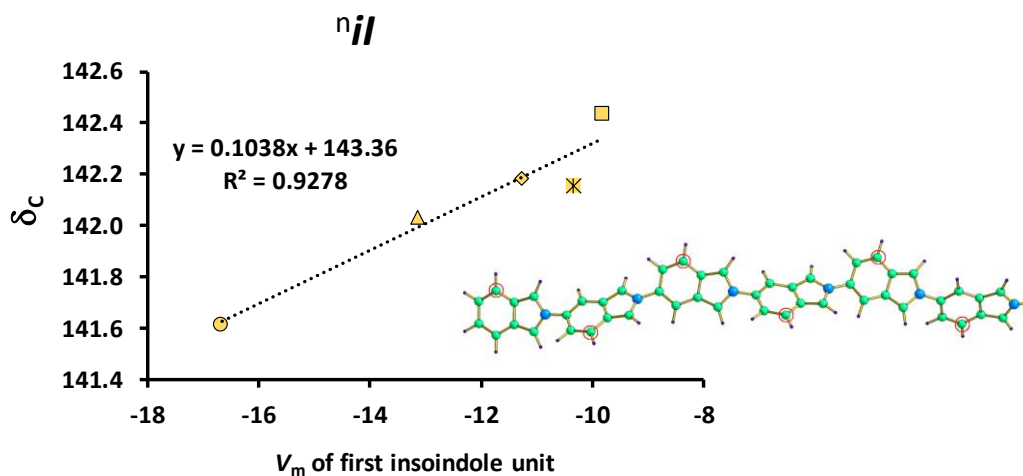


Figure S20h. Relation between chemical shift at the C center (in ppm) and MESP at the first isoindole unit (in kcal/mol) in nli systems (2li to 6li).

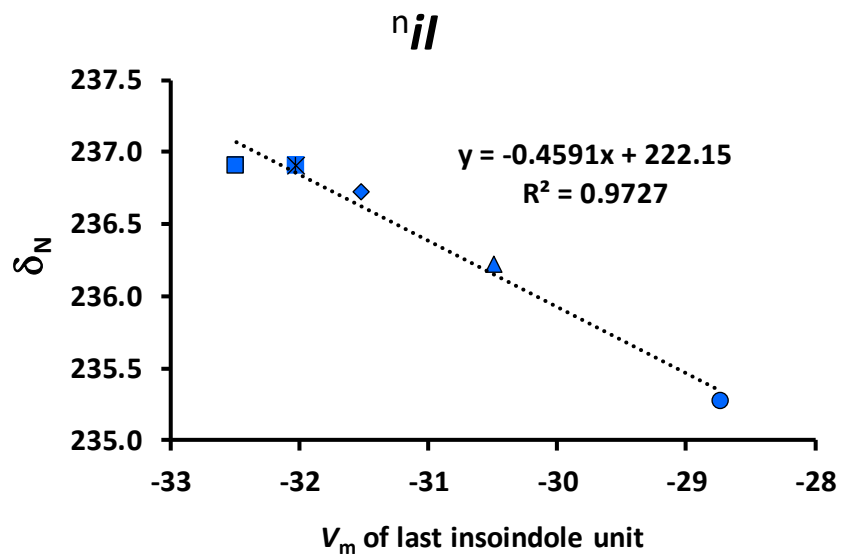


Figure S20i. Relation between chemical shift at the N center (in ppm) and MESP at the first isoindole unit (in kcal/mol) in ⁿII systems (²II to ⁶II).

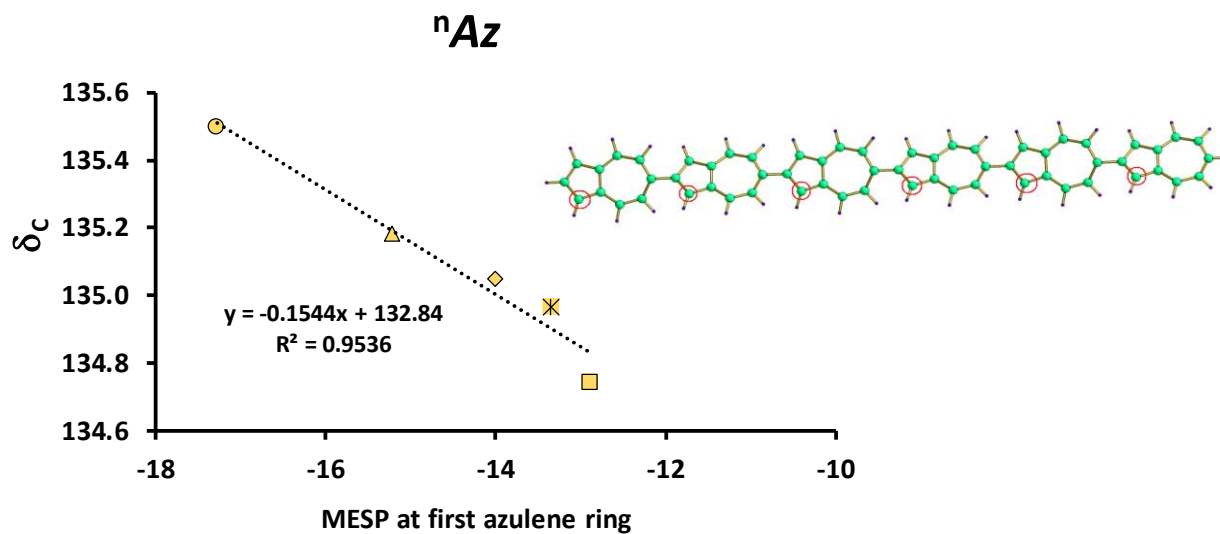


Figure S20j. Relation between chemical shift at the C center (in ppm) and MESP at the first azulene unit (in kcal/mol) in ⁿAz systems (²Az to ⁶Az).

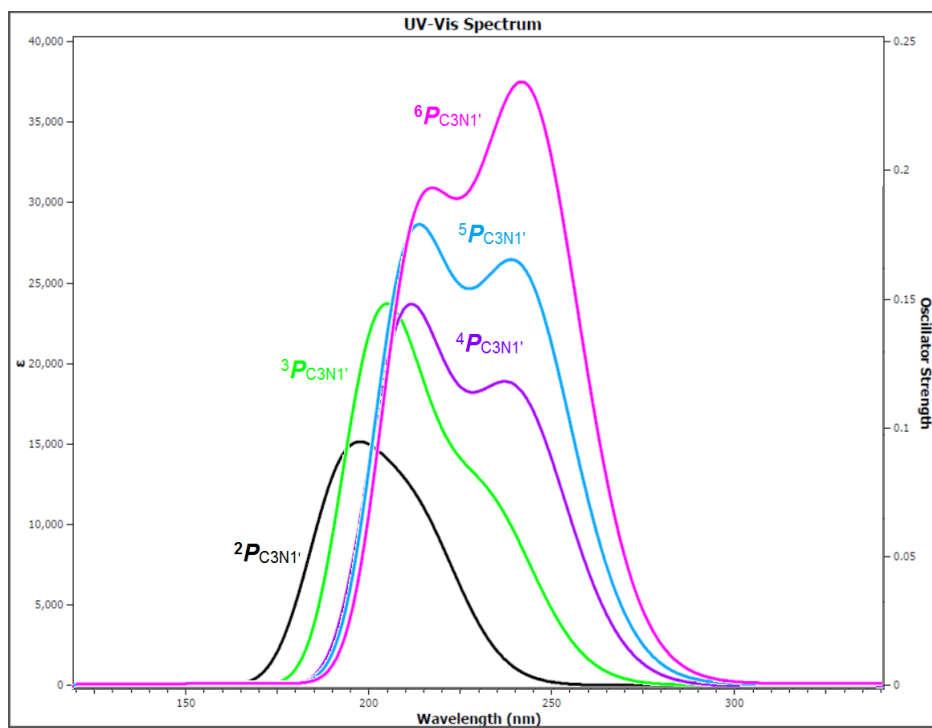


Figure S21a. Simulated absorption spectra of $^nP_{C3N1'}$ where $n = 2$ to 6 .

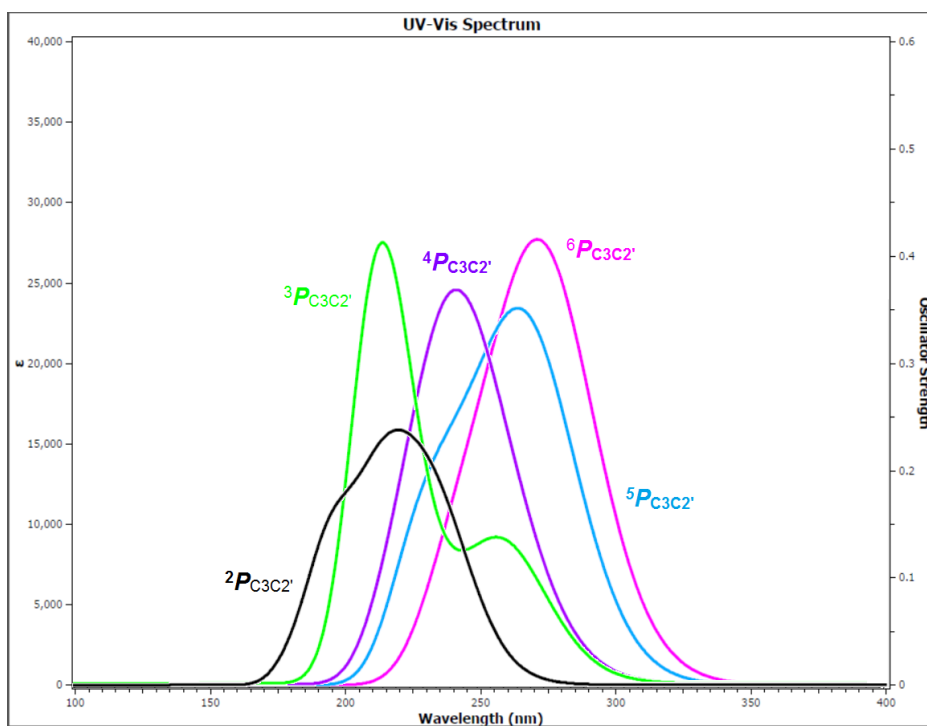


Figure S21b. Simulated absorption spectra of $^nP_{C3C2'}$ where $n = 2$ to 6 .

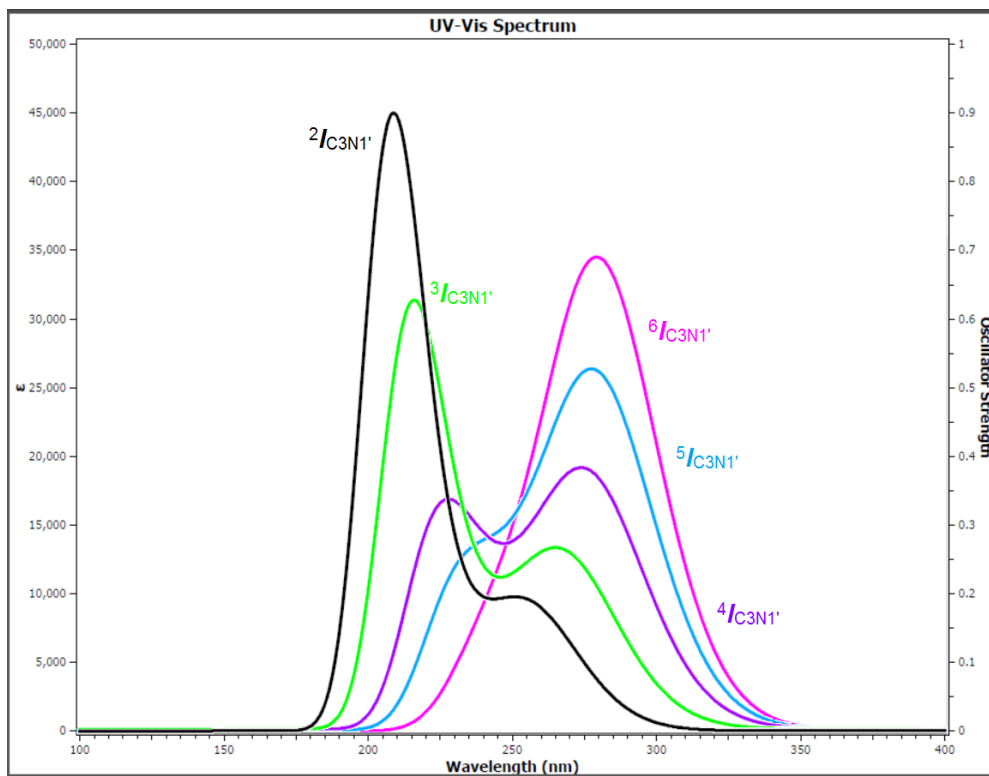


Figure S21c. Simulated absorption spectra of $nI_{C3N1'}$ where $n = 2$ to 6 .

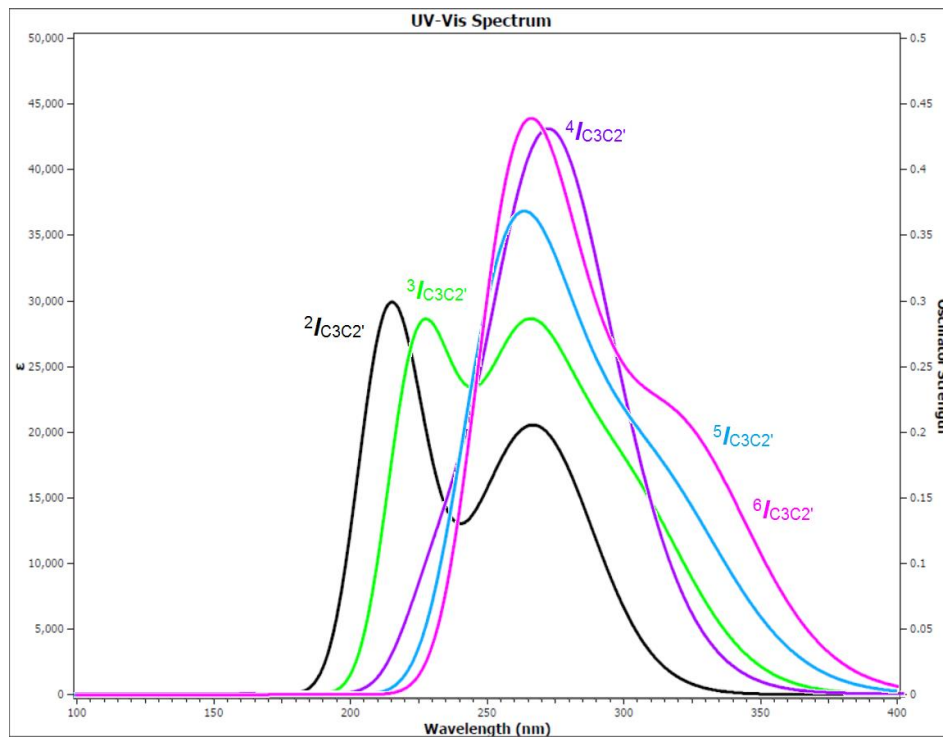


Figure S21d. Simulated absorption spectra of $nI_{C3C2'}$ where $n = 2$ to 6 .

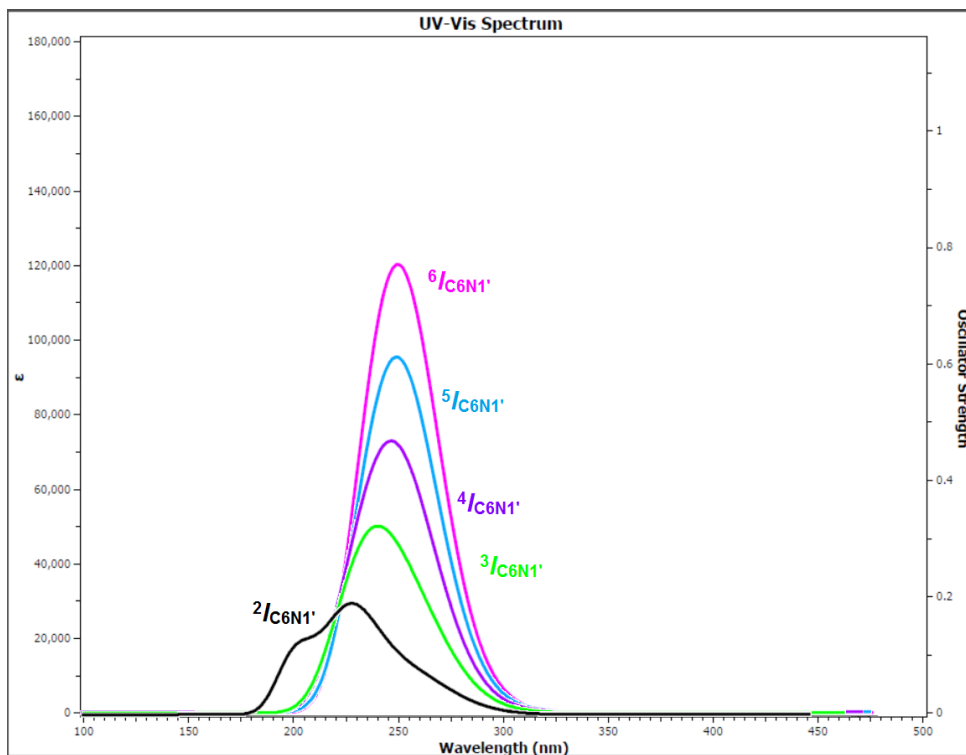


Figure S21e. Simulated absorption spectra of ${}^nI_{C6N1'}$ where n = 2 to 6.

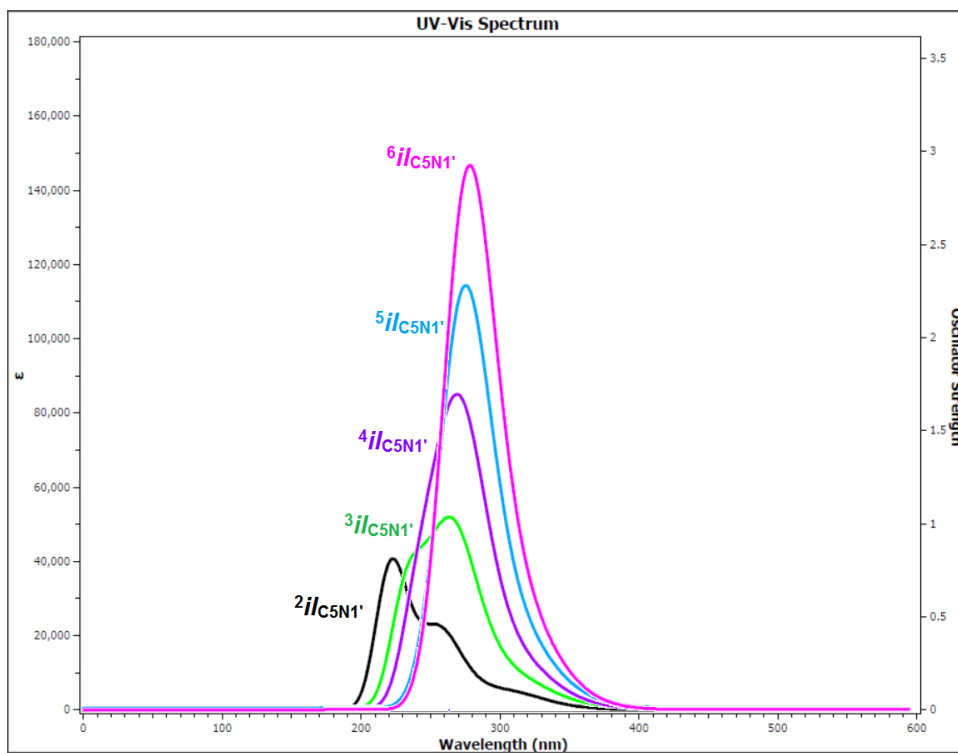


Figure S21f. Simulated absorption spectra of ${}^niI_{C5N1'}$ where n = 2 to 6.

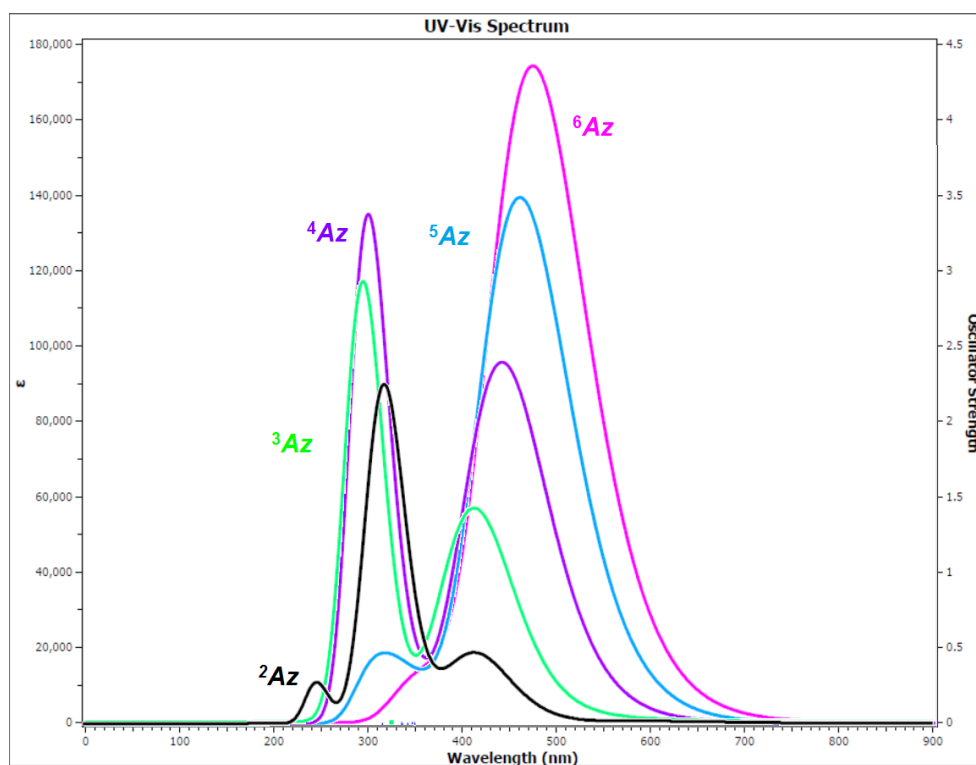


Figure S21g. Simulated absorption spectra of nAz , where $n = 2$ to 6 .

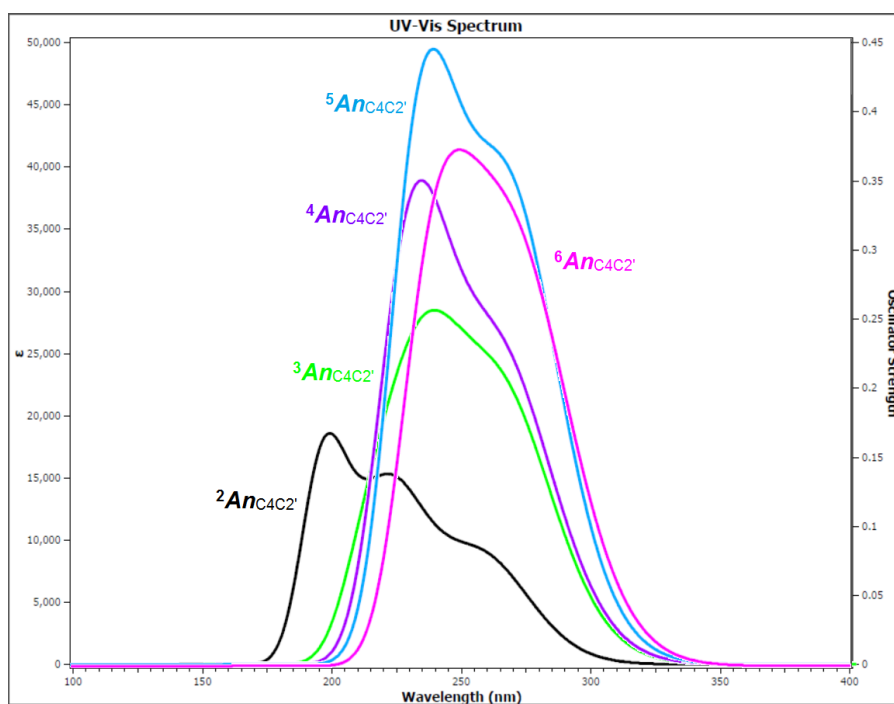


Figure S21h. Simulated absorption spectra of $^nAn_{C4C2'}$, where $n = 2$ to 6 .

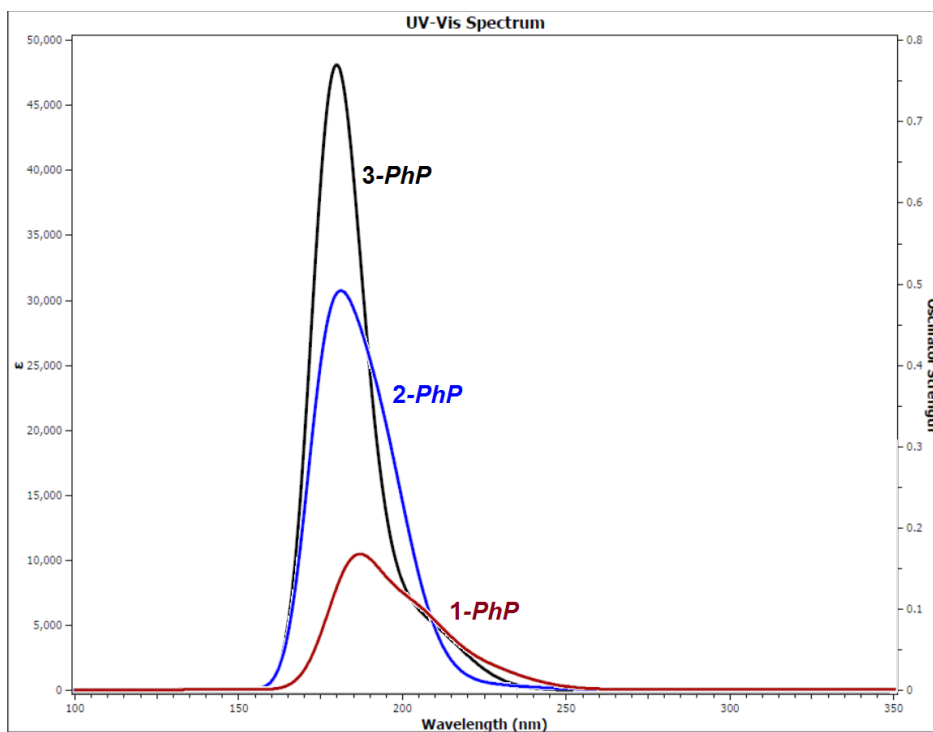


Figure S21i. Simulated absorption spectra of 1-*PhP*, 2-*PhP* and 3-*PhP*.

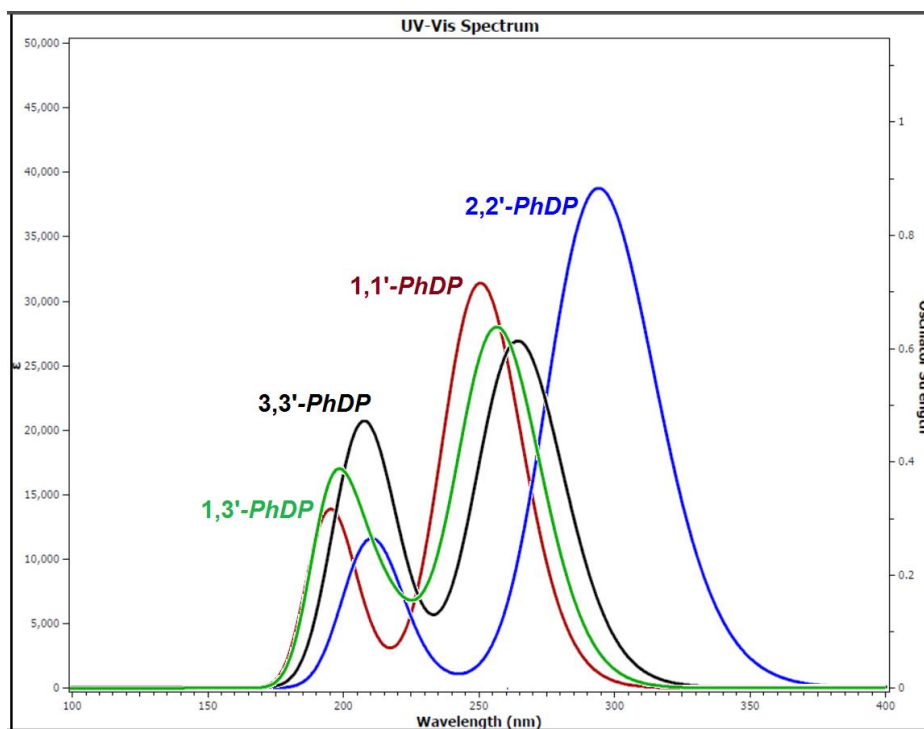


Figure S21j. Simulated absorption spectra of *PhDPs*.

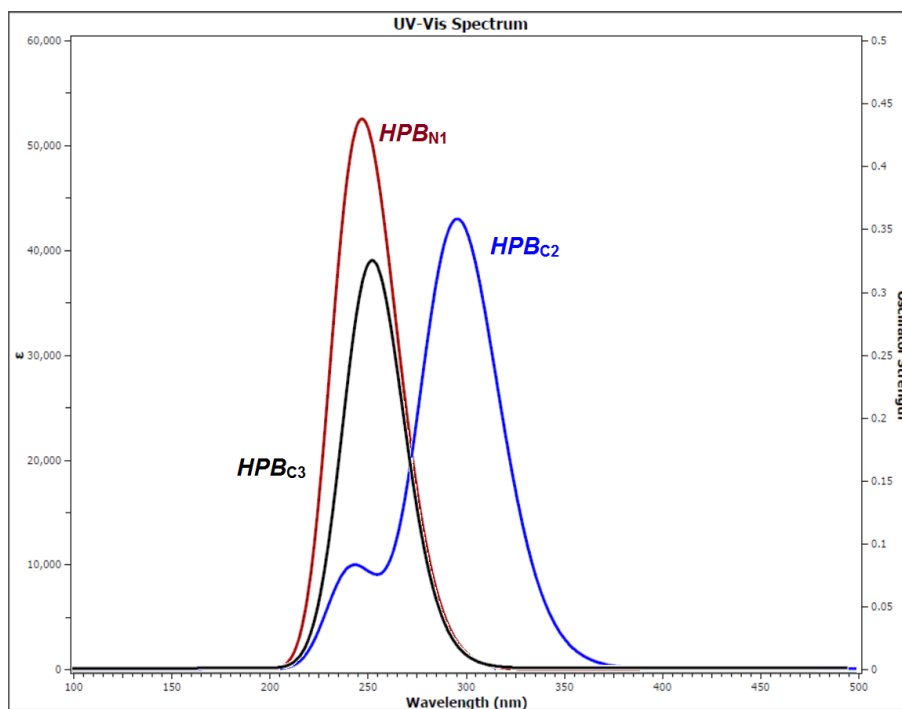


Figure S21k. Simulated absorption spectra of *HPBs*.

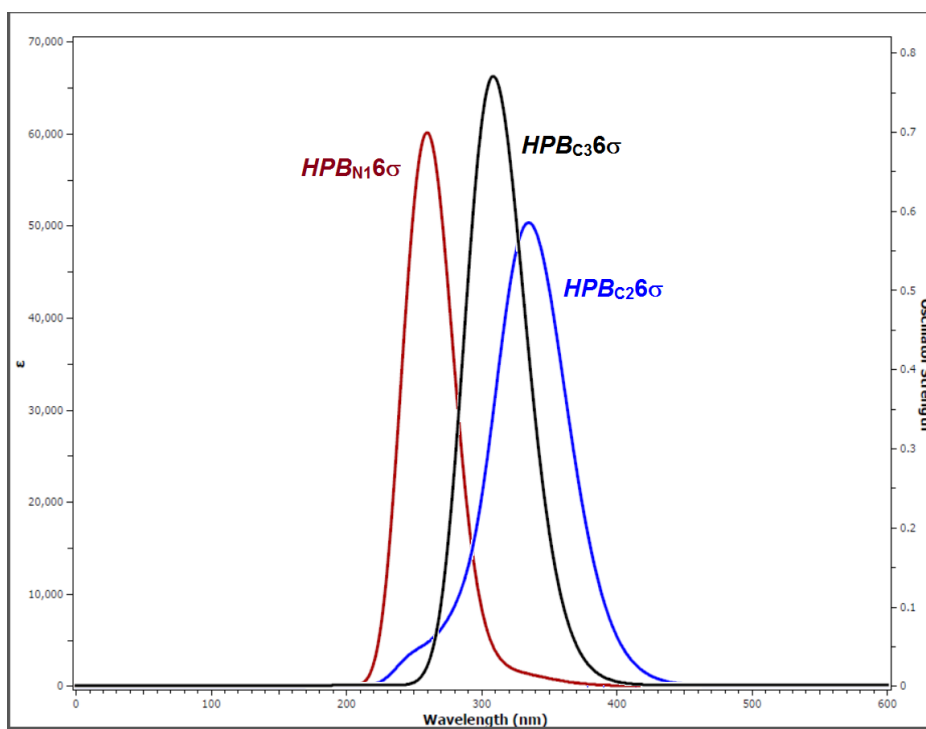


Figure S21l. Simulated absorption spectra of *HPB-6 σ* .

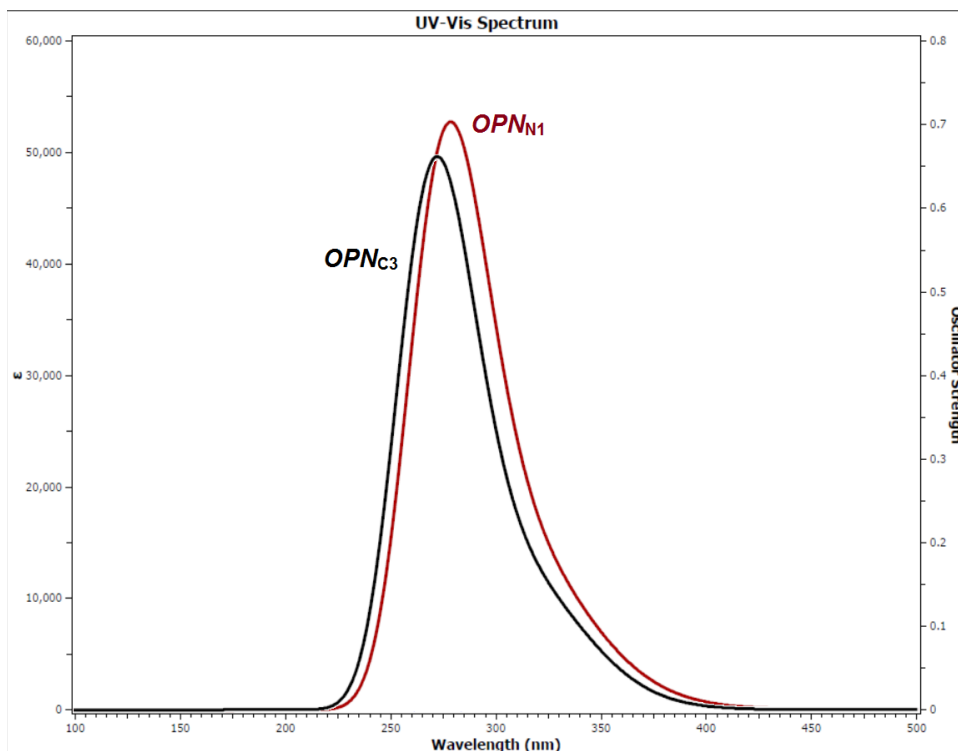


Figure S21m. Simulated absorption spectra of *OPN*.

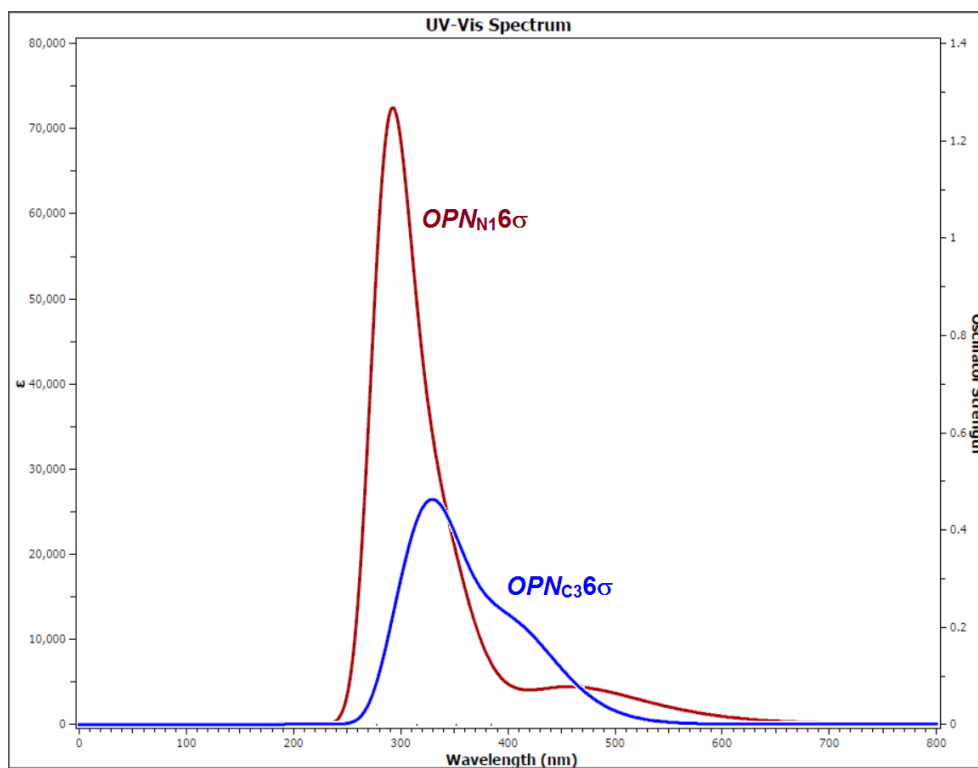


Figure S21n. Simulated absorption spectra of *OPN-6 σ* .

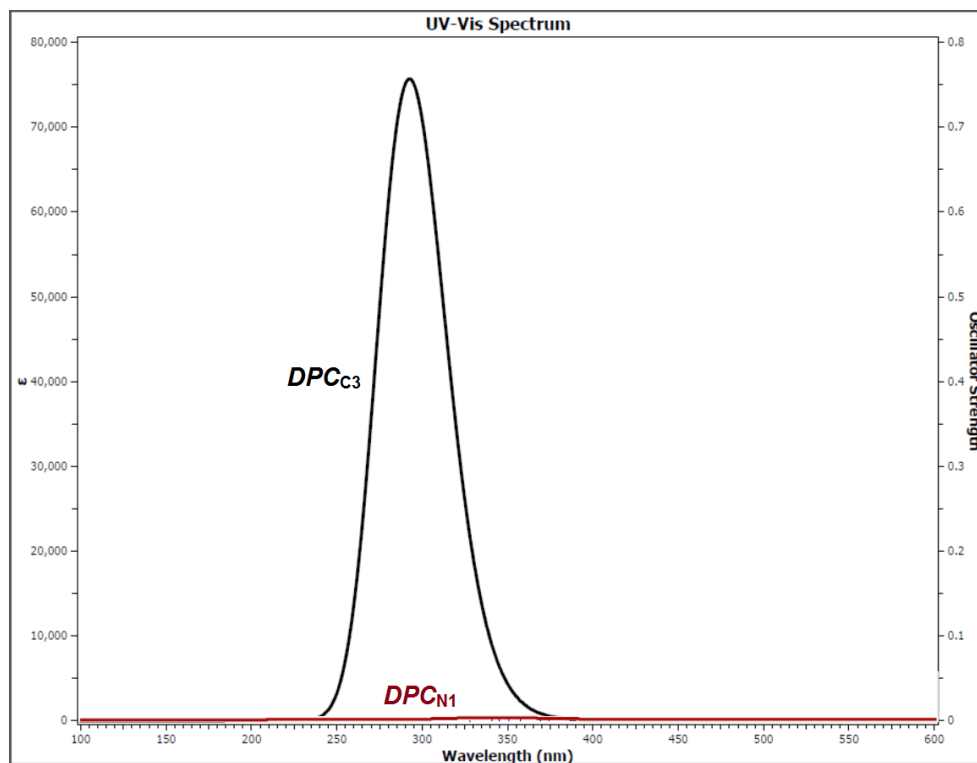


Figure S21o. Simulated absorption spectra of *DPC*.

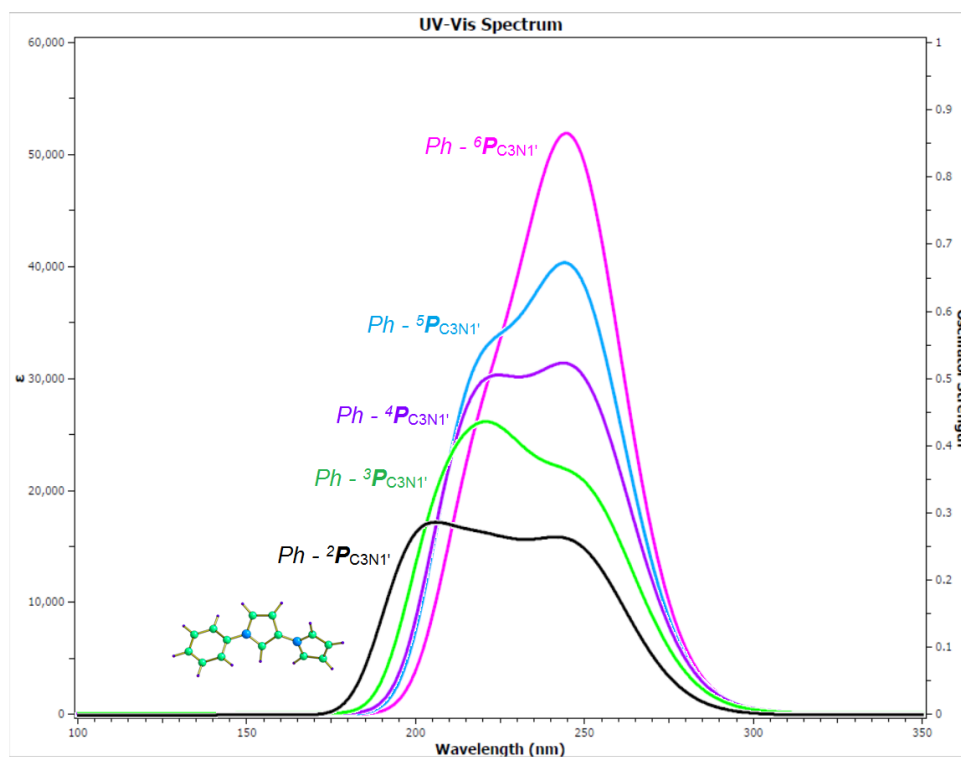


Figure S21p. Simulated absorption spectra of $Ph - ^n P_{C3N1'}$ systems.

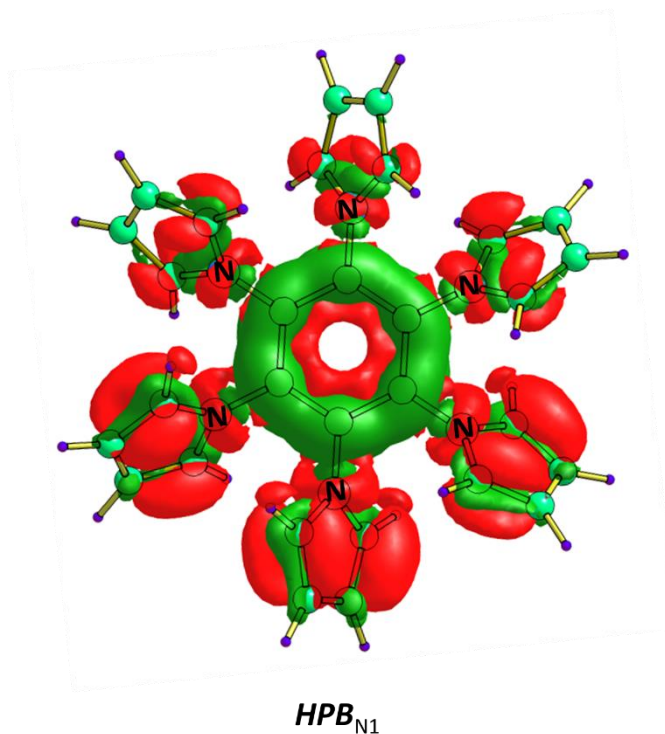
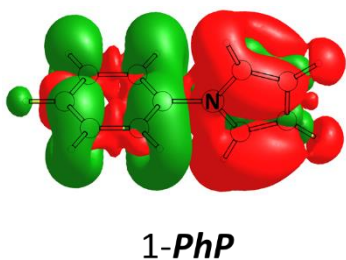


Figure S22. The difference in total density computed for the ground and excited states of 1-PhP and HPB_{N1} systems plotted at iso-contour value 0.001 au.

Table S3. Cartesian coordinates for all the systems (Given in the order Atomic number, x, y, z coordinates, respectively)

Pyrrole (<i>P</i>)							
6	0.000000	0.711553	-0.979918	1	0.000000	1.359481	-1.841490
6	0.000000	1.120834	0.330464	1	0.000000	2.107068	0.764107
7	0.000000	0.000000	1.117812	1	0.000000	-2.107068	0.764107
6	0.000000	-1.120834	0.330464	1	0.000000	-1.359481	-1.841490
6	0.000000	-0.711553	-0.979918	1	0.000000	0.000000	2.123534
<hr/>							
² P _{C2C2'}							
6	-1.560366	1.115201	-0.317518	6	2.897720	-0.657353	-0.165784
6	-0.724089	0.053881	-0.036671	6	2.839266	0.665182	0.197849
7	-1.518329	-1.020118	0.271879	7	1.518325	1.020142	0.271784
6	-2.839272	-0.665217	0.197713	6	0.724091	-0.053889	-0.036670
6	-2.897715	0.657387	-0.165677	6	1.560371	-1.115221	-0.317460
1	-1.244307	2.094948	-0.640663	1	3.798666	-1.229116	-0.318748
1	-3.620583	-1.375589	0.410780	1	3.620572	1.375534	0.411004
1	-3.798656	1.229179	-0.318556	1	1.244314	-2.094981	-0.640566

	1	-1.164118	-1.911692	0.578272	1	1.164104	1.911724	0.578142
${}^2P_{C3C3'}$	6	-1.582953	-1.127445	0.243552	6	2.880701	0.694673	0.144251
	6	-0.730923	-0.005785	0.005989	7	2.853657	-0.643665	-0.141161
	6	-1.554733	1.072219	-0.229679	6	1.554731	-1.072205	-0.229779
	7	-2.853659	0.643657	-0.141146	6	0.730923	0.005784	0.005966
	6	-2.880699	-0.694695	0.144202	6	1.582955	1.127465	0.243421
	1	-1.268137	-2.130779	0.484295	1	3.812673	1.222105	0.263124
	1	-3.663682	1.224326	-0.273743	1	3.663679	-1.224343	-0.273725
	1	-3.812669	-1.222149	0.262984	1	1.268139	2.130811	0.484113
	1	-1.315798	2.095536	-0.469152	1	1.315794	-2.095515	-0.469281
${}^2P_{N1N1'}$	6	-1.469213	0.798905	0.797783	6	2.774449	-0.504698	0.503758
	7	-0.685090	0.000027	-0.000072	6	2.774477	0.504667	-0.503712
	6	-1.469248	-0.798937	-0.797763	6	1.469250	0.798950	-0.797748
	6	-2.774476	-0.504670	-0.503714	7	0.685090	-0.000026	-0.000071
	6	-2.774450	0.504686	0.503766	6	1.469212	-0.798903	0.797787
	1	-1.012307	1.489278	1.487538	1	3.637835	-0.961394	0.959654
	1	-3.637871	-0.961274	-0.959627	1	3.637873	0.961266	-0.959629
	1	-3.637837	0.961371	0.959671	1	1.012305	-1.489273	1.487545
	1	-1.012446	-1.489354	-1.487552	1	1.012448	1.489374	-1.487529
${}^2P_{C2N1'}$	7	-1.423192	-0.945411	-0.451284	6	2.836654	0.615978	-0.324590
	6	-0.683782	0.089989	0.052952	6	2.809267	-0.662587	0.301406
	6	-1.540788	1.057095	0.511103	6	1.493915	-0.989304	0.508040
	6	-2.861067	0.583220	0.264273	7	0.717181	0.041393	0.024968
	6	-2.757596	-0.652093	-0.322787	6	1.536918	1.022407	-0.483157
	1	-1.029927	-1.752253	-0.908901	1	3.710188	1.169054	-0.629780
	1	-3.781538	1.088542	0.507220	1	3.658115	-1.266428	0.579194
	1	-3.513323	-1.344475	-0.653591	1	1.108181	1.906515	-0.925782
	1	-1.245446	1.978492	0.986184	1	1.034690	-1.839557	0.986230
${}^2P_{C3N1'}$	6	1.467041	-1.034203	-0.388756	6	-2.853394	0.662038	-0.254742
	6	0.663040	0.008823	0.002083	6	-2.851917	-0.671241	0.242115

6	1.498392	1.087269	0.401646	6	-1.540633	-1.046438	0.396961
6	2.793864	0.662355	0.240669	7	-0.744661	0.004342	0.010363
7	2.763709	-0.621505	-0.227379	6	-1.543035	1.048547	-0.387767
1	1.215521	-2.007715	-0.774472	1	-3.714848	1.265123	-0.492404
1	3.726529	1.165919	0.432654	1	-3.712046	-1.278812	0.473316
1	3.573664	-1.180470	-0.434802	1	-1.101262	1.961031	-0.753818
1	1.175984	2.044412	0.778320	1	-1.097022	-1.952246	0.777063

${}^2P_{C3C2'}$

6	-1.523795	-1.090192	0.338480	6	2.944882	0.626702	0.177394
6	-0.704851	0.035785	0.015452	6	2.847386	-0.685571	-0.213441
6	-1.556117	1.066862	-0.313427	7	1.514857	-0.997447	-0.293115
7	-2.840178	0.608857	-0.191018	6	0.751308	0.096500	0.031003
6	-2.832407	-0.702584	0.199091	6	1.620919	1.121844	0.335612
1	-1.186031	-2.059017	0.672547	1	3.863108	1.166575	0.344262
1	-3.665979	1.151890	-0.377689	1	3.606574	-1.416362	-0.437547
1	-3.749886	-1.244723	0.357093	1	1.328544	2.105655	0.667399
1	-1.339777	2.071382	-0.637835	1	1.136740	-1.871338	-0.620273

${}^3P_{C3N1'}$

6	-0.658251	1.637827	0.586447	1	-5.455996	0.265328	-0.811961
7	-1.065287	0.400803	0.159597	1	-2.396987	-2.093302	0.831995
6	0.037195	-0.368694	-0.123396	1	-3.411277	1.734992	-0.945157
6	1.149277	0.392501	0.143796	6	3.506683	0.745041	-0.503738
6	0.714534	1.668326	0.592280	7	2.486393	-0.023990	-0.000501
1	-1.384385	2.373813	0.890410	6	2.977604	-1.265907	0.320358
1	-0.060776	-1.362724	-0.527169	6	4.316653	-1.289360	0.018485
6	-4.267529	-1.253277	0.049247	6	4.653576	-0.009543	-0.503988
7	-4.550960	-0.027325	-0.484706	1	3.313526	1.750784	-0.839745
6	-3.417759	0.740401	-0.532180	1	4.981480	-2.124650	0.169080
6	-2.401865	-0.014922	0.001002	1	5.622366	0.317710	-0.845581
6	-2.933174	-1.280098	0.370289	1	2.332018	-2.006228	0.764009
1	-5.032954	-2.001521	0.169193	1	1.340302	2.485606	0.912591

${}^4P_{C3N1'}$

6	2.375835	-1.602154	0.662714	7	-0.699950	0.259882	0.413109
7	2.810970	-0.396007	0.179376	6	-1.069373	1.526662	0.782025
6	1.736586	0.442572	0.012270	6	-2.429331	1.646787	0.632666
6	0.615580	-0.244291	0.411128	6	-2.894407	0.395420	0.147700
6	1.013145	-1.543987	0.821975	1	-1.735431	-1.444331	-0.369620
1	3.082537	-2.382987	0.891105	1	-3.031462	2.507913	0.873544

1	1.852281	1.425974	-0.412371	1	-0.334357	2.218397	1.159546
6	6.082798	1.042388	-0.300198	1	0.376025	-2.318260	1.217800
7	6.220254	-0.196196	-0.861854	6	-5.135505	0.889994	-0.765790
6	5.040940	-0.886676	-0.777648	7	-4.231751	0.064371	-0.143810
6	4.146040	-0.068708	-0.132019	6	-4.837478	-1.137341	0.130220
6	4.799041	1.155911	0.172379	6	-6.132878	-1.078438	-0.320994
1	6.905300	1.737144	-0.269987	6	-6.323023	0.211995	-0.889174
1	7.060299	-0.546275	-1.290575	1	-4.838945	1.875480	-1.086090
1	4.375199	1.999920	0.691971	1	-6.864474	-1.866165	-0.239438
1	4.920462	-1.876043	-1.185715	1	-7.223439	0.596257	-1.340816
6	-1.812023	-0.440211	0.013188	1	-4.296337	-1.910911	0.650243

${}^5P_{C3N1}$

6	4.256967	1.638287	0.328213	1	0.053055	1.419512	0.858788
7	4.556926	0.318131	0.116444	1	-1.336497	-1.092288	-2.399429
6	3.420585	-0.353005	-0.260974	1	1.388533	-0.998022	-2.317179
6	2.398418	0.564120	-0.300162	1	2.383344	2.763148	0.117326
6	2.920666	1.829494	0.076085	6	-3.496332	-0.377326	-0.246691
1	5.032883	2.334983	0.599904	7	-2.489814	0.555293	-0.298676
1	3.424879	-1.418096	-0.423465	6	-2.992950	1.785261	0.035142
6	7.658903	-1.513380	-0.050419	6	-4.328750	1.647802	0.323643
7	7.802155	-0.795618	1.104081	6	-4.642166	0.274455	0.141249
6	6.684141	-0.039228	1.332157	1	-3.312272	-1.414360	-0.473499
6	5.824792	-0.274485	0.286754	1	-5.006094	2.427023	0.633743
6	6.435330	-1.208544	-0.592646	1	-2.356297	2.654496	0.019770
1	8.436853	-2.171064	-0.400202	6	-6.129308	-1.541055	0.928238
1	8.605061	-0.829069	1.709350	7	-5.903136	-0.321896	0.337992
1	6.026556	-1.586509	-1.515693	6	-7.104940	0.219872	-0.045611
1	6.575222	0.582002	2.205161	6	-8.102475	-0.657598	0.301367
6	-0.041365	0.789284	-0.009959	6	-7.481587	-1.778931	0.918791
7	1.062154	0.290171	-0.655613	1	-5.306240	-2.111041	1.327540
6	0.659537	-0.535593	-1.672265	1	-9.156560	-0.513890	0.126246
6	-0.713366	-0.564502	-1.695600	1	-7.970207	-2.651360	1.321993
6	-1.150421	0.280416	-0.641655	1	-7.134288	1.169908	-0.553889

${}^6P_{C3N1}$

6	6.046587	1.622657	0.225416	6	-1.740348	-0.299226	-0.187014
7	6.322898	0.288298	0.081516	7	-0.722508	0.614898	-0.294047
6	5.172767	-0.382477	-0.251236	6	-1.206391	1.867960	-0.024235
6	4.165607	0.548516	-0.331053	6	-2.542261	1.765896	0.278455
6	4.711527	1.822999	-0.026304	6	-2.874028	0.389549	0.171641
1	6.836166	2.319521	0.453846	1	-1.572702	-1.349199	-0.361074
1	5.158137	-1.454507	-0.358076	1	-3.206944	2.570330	0.549084
6	9.389926	-1.606327	-0.007494	1	-0.557925	2.726037	-0.089698

7	9.559117	-0.823591	1.100238	6	-4.380246	-1.347194	1.083290
6	8.457526	-0.034392	1.294170	7	-4.142033	-0.179689	0.407470
6	7.582167	-0.316052	0.273808	6	-5.333384	0.342612	-0.032717
6	8.165766	-1.312086	-0.554288	6	-6.332818	-0.502577	0.385888
1	10.151929	-2.298042	-0.325262	6	-5.734145	-1.579252	1.092465
1	10.368498	-0.835123	1.697690	1	-3.565324	-1.889047	1.534553
1	7.740005	-1.737059	-1.448754	1	-6.245672	-2.396466	1.574789
1	8.369963	0.639973	2.129325	1	-5.366013	1.234878	-0.635641
6	1.731840	0.823695	-0.033194	6	-8.591887	-1.325630	-0.181294
7	2.822129	0.278365	-0.662851	7	-7.710982	-0.327288	0.153622
6	2.399387	-0.586666	-1.637756	6	-8.386661	0.866920	0.207424
6	1.026026	-0.595617	-1.650243	6	-9.704496	0.629398	-0.096554
6	0.610588	0.303386	-0.633321	6	-9.835421	-0.765785	-0.341912
1	1.842762	1.492355	0.804342	1	-8.243857	-2.338834	-0.299684
1	0.389712	-1.145064	-2.325123	1	-10.487397	1.370105	-0.125937
1	3.116457	-1.089121	-2.265858	1	-10.734780	-1.296100	-0.610843
1	4.190327	2.766649	-0.031099	1	-7.869459	1.769902	0.488122

${}^3P_{C3C2'}$

6	-2.848067	-0.174124	-0.529768	6	0.749681	1.118829	0.001392
6	-1.550160	-0.082848	0.064101	1	2.107732	2.896057	-0.016046
6	-1.335150	-1.266046	0.738734	1	-0.226664	4.291122	0.002016
7	-2.439893	-2.053387	0.566241	1	-2.076922	2.583779	0.066947
6	-3.368569	-1.399375	-0.197464	6	2.471589	-2.018768	-0.651446
1	-3.326549	0.565811	-1.152735	7	1.456904	-1.112917	-0.809717
1	-2.554765	-2.974114	0.955307	6	1.679887	-0.006533	-0.029132
1	-4.309594	-1.858876	-0.450159	6	2.873223	-0.211910	0.631904
1	-0.485512	-1.590360	1.318427	6	3.372349	-1.484291	0.237980
6	1.104737	2.500618	0.008223	1	2.475141	-2.953564	-1.187320
6	-0.057385	3.227236	0.006776	1	0.643799	-1.229603	-1.393701
7	-1.102576	2.341218	-0.007478	1	4.284997	-1.953954	0.568261
6	-0.634067	1.051084	0.004135	1	3.318887	0.476066	1.333074

${}^4P_{C3C2'}$

6	3.654832	-0.229626	0.833869	6	-0.570772	2.595293	-1.803843
6	2.290194	-0.080482	0.434580	7	0.186012	1.461749	-1.906998
6	1.857812	1.135798	0.924186	6	-0.376753	0.443748	-1.175356
7	2.902805	1.707861	1.592622	6	-1.530873	0.943480	-0.594144
6	3.998823	0.889647	1.547861	6	-1.645987	2.307975	-1.002156
1	4.316865	-1.050173	0.603355	1	-0.296299	3.501949	-2.317268
1	2.864004	2.599833	2.056679	1	1.057943	1.370976	-2.402935
1	4.928186	1.170416	2.014487	1	-2.433992	2.992389	-0.730877
1	0.894313	1.617110	0.851473	6	-2.443570	0.254703	0.308804
6	-0.078420	-2.118195	-1.551093	7	-2.209242	-1.010610	0.787582

6	0.868298	-3.027690	-1.154028	6	-4.129312	-0.363127	1.686757
7	1.814410	-2.353426	-0.422634	6	-3.637367	0.680448	0.857620
6	1.488365	-1.026586	-0.327701	1	-1.405841	-1.569270	0.541170
6	0.308858	-0.844368	-1.032575	1	-4.103195	1.635968	0.675009
1	-0.949360	-2.319993	-2.154879	1	-5.041162	-0.359094	2.262049
1	0.954523	-4.085652	-1.337787	6	-3.224722	-1.394879	1.621540
1	2.599076	-2.777573	0.044757	1	-3.219386	-2.362753	2.094831

${}^5P_{C3C2'}$

6	4.808544	-0.522838	-0.746158	6	-1.066138	-1.763497	0.706267
6	3.435375	-0.363781	-0.381286	1	-0.090565	-3.426128	1.826873
6	2.734243	-1.378898	-1.002363	1	1.767432	-1.747256	2.169299
7	3.630054	-2.125478	-1.714528	1	-2.004071	-2.171486	0.366170
6	4.891781	-1.616625	-1.569402	6	-1.239372	0.601845	-0.322254
1	5.643961	0.078882	-0.422594	7	-0.500507	1.569237	-0.958154
1	3.390095	-2.931834	-2.266556	6	-2.599472	1.944206	-1.541274
1	5.740211	-2.074032	-2.050295	6	-2.566632	0.816069	-0.665298
1	1.680357	-1.613249	-0.990016	1	0.499771	1.660234	-0.859601
6	1.557642	2.022478	1.738564	1	-3.481671	2.400359	-1.963456
6	2.725785	2.687054	1.469627	6	-1.310089	2.384726	-1.697220
7	3.511159	1.861686	0.702565	1	-0.908409	3.213057	-2.256799
6	2.864447	0.677943	0.461427	6	-3.737583	0.071573	-0.212122
6	1.639416	0.744262	1.108608	7	-4.772036	-0.199987	-1.075852
1	0.728542	2.389697	2.322231	6	-5.377251	-1.041791	0.879764
1	3.065918	3.666580	1.761711	6	-4.096620	-0.438749	1.017473
1	4.406574	2.107909	0.313452	1	-4.753493	0.021992	-2.057816
6	-0.112819	-2.420210	1.441266	1	-3.497646	-0.370830	1.912000
7	0.911604	-1.544365	1.678354	1	-5.950443	-1.529415	1.652107
6	0.642235	-0.329852	1.100081	6	-5.769805	-0.878449	-0.426540
6	-0.595848	-0.431768	0.483816	1	-6.665516	-1.184312	-0.941269

${}^6P_{C3C2'}$

6	5.412775	1.691305	-0.284219	6	-0.286792	-0.526660	0.665163
6	4.172248	0.984006	-0.217135	7	0.312991	-0.080257	1.815308
6	3.265099	1.688880	-0.983590	6	-1.861591	-0.113148	2.243677
7	3.913356	2.776030	-1.497132	6	-1.653031	-0.564497	0.906877
6	5.216221	2.791368	-1.079499	1	1.311068	0.019134	1.924594
1	6.348421	1.412821	0.175864	1	-2.815735	-0.016371	2.736598
1	3.486747	3.467110	-2.091425	6	-0.631420	0.173441	2.774836
1	5.894526	3.570029	-1.385917	1	-0.349901	0.529862	3.751811
1	2.222387	1.498112	-1.188484	6	-2.676566	-1.033242	-0.024221
6	3.024044	-2.120963	1.442045	7	-2.537892	-2.228129	-0.685043
6	4.135388	-1.767702	2.162475	6	-4.466731	-1.391235	-1.364586
7	4.656161	-0.629112	1.598161	6	-3.883202	-0.483749	-0.426741

6	3.892376	-0.233006	0.532219	1	-1.723678	-2.815939	-0.598420
6	2.865840	-1.156509	0.401381	1	-5.393448	-1.258479	-1.901781
1	2.387696	-2.973050	1.620942	6	-3.608045	-2.452874	-1.504202
1	4.600649	-2.229350	3.017359	1	-3.672007	-3.337902	-2.115120
1	5.443880	-0.111752	1.953028	6	-4.444772	0.793040	-0.003637
6	1.034023	-0.984151	-2.731794	7	-5.803688	0.998954	-0.008093
7	2.142222	-1.201893	-1.959653	6	-3.860388	1.968334	0.421639
6	1.826035	-1.092229	-0.629162	6	-6.094040	2.271041	0.412096
6	0.471545	-0.805670	-0.550138	6	-4.903279	2.898778	0.684269
6	-0.022556	-0.738854	-1.892025	1	-6.480263	0.284701	-0.220947
1	1.081871	-1.031572	-3.807183	1	-2.798762	2.129013	0.522837
1	3.077053	-1.371570	-2.294804	1	-7.111645	2.617784	0.482715
1	-1.037171	-0.520912	-2.188721	1	-4.792818	3.914946	1.027845

1-PhP

6	0.000000	0.710936	3.110009	6	1.208709	0.000000	-1.112236
6	0.000000	1.119691	1.798704	6	-1.208709	0.000000	-1.112236
7	0.000000	0.000000	1.003743	6	1.205605	0.000000	-2.503086
6	0.000000	-1.119691	1.798704	6	-1.205605	0.000000	-2.503086
6	0.000000	-0.710936	3.110009	6	0.000000	0.000000	-3.197938
1	0.000000	1.360137	3.970765	1	2.134904	0.000000	-0.549806
1	0.000000	2.101963	1.354318	1	-2.134904	0.000000	-0.549806
1	0.000000	-2.101963	1.354318	1	2.144732	0.000000	-3.043078
1	0.000000	-1.360137	3.970765	1	-2.144732	0.000000	-3.043078
6	0.000000	0.000000	-0.423728	1	0.000000	0.000000	-4.281292

2-PhP

6	0.847011	3.075394	0.000000	6	-0.077704	-1.166240	1.203883
7	1.105985	1.729572	0.000000	6	-0.077704	-1.166240	-1.203883
6	-0.070796	1.022574	0.000000	6	-0.077704	-2.557185	1.204191
6	-1.097489	1.937478	0.000000	6	-0.077704	-2.557185	-1.204191
6	-0.515562	3.237207	0.000000	6	-0.076748	-3.254135	0.000000
1	1.646688	3.797431	0.000000	1	-0.085160	-0.616163	2.138077
1	2.019587	1.305779	0.000000	1	-0.085160	-0.616163	-2.138077
1	-2.147447	1.691035	0.000000	1	-0.081251	-3.096480	2.144058
1	-1.037530	4.180550	0.000000	1	-0.081251	-3.096480	-2.144058
6	-0.077571	-0.458129	0.000000	1	-0.078546	-4.337735	0.000000

3-PhP

7	0.664196	3.117571	0.000000	6	-0.002176	-1.193577	1.201926
6	1.099972	1.818767	0.000000	6	-0.002176	-1.193577	-1.201926
6	-0.004906	1.000521	0.000000	6	-0.002176	-2.584669	1.203012
6	-1.151236	1.849905	0.000000	6	-0.002176	-2.584669	-1.203012
6	-0.704134	3.147792	0.000000	6	-0.001947	-3.283479	0.000000
1	1.261076	3.927091	0.000000	1	-0.003416	-0.644727	2.136946

1	2.149467	1.573343	0.000000	1	-0.003416	-0.644727	-2.136946
1	-2.180964	1.529123	0.000000	1	-0.002326	-3.122977	2.143680
1	-1.242501	4.081109	0.000000	1	-0.002326	-3.122977	-2.143680
6	0.000448	-0.482206	0.000000	1	-0.001921	-4.367104	0.000000
1,1'-PhDP							
6	4.916996	-0.682587	0.202449	6	-1.393899	0.000003	-0.000009
6	3.608803	-1.074491	0.315902	1	1.238196	1.970895	0.834853
7	2.807682	0.000001	0.000008	1	1.238199	-1.970902	-0.834834
6	3.608799	1.074493	-0.315897	1	-1.238180	1.970897	0.834849
6	4.916994	0.682589	-0.202465	1	-1.238176	-1.970904	-0.834837
1	5.777705	-1.300782	0.400364	6	-4.917014	-0.682565	0.202498
1	3.172908	-2.007347	0.633900	6	-3.608805	-1.074469	0.315947
1	3.172897	2.007350	-0.633883	7	-2.807685	-0.000005	-0.000010
1	5.777699	1.300784	-0.400391	6	-3.608804	1.074473	-0.315942
6	1.393914	-0.000001	0.000003	6	-4.917012	0.682568	-0.202498
6	0.693570	1.117680	0.449436	1	-5.777727	-1.300755	0.400412
6	0.693573	-1.117683	-0.449427	1	-3.172896	-2.007299	0.633996
6	-0.693557	1.117684	0.449429	1	-3.172886	2.007292	-0.634007
6	-0.693556	-1.117685	-0.449426	1	-5.777730	1.300750	-0.400418
2,2'-PhDP							
6	-4.975664	-0.694861	-0.151348	6	1.413111	-0.037406	-0.004989
7	-3.648106	-1.021447	-0.216273	1	-1.181749	2.078307	-0.620822
6	-2.874840	0.091395	0.011559	1	-1.268984	-2.017195	0.644431
6	-3.738879	1.142840	0.241928	1	1.269032	2.017291	-0.644055
6	-5.064417	0.644542	0.140483	1	1.181712	-2.078204	0.621241
1	-5.740745	-1.434237	-0.320571	6	5.064295	-0.644693	-0.140796
1	-3.285961	-1.918163	-0.496613	6	3.738752	-1.142934	-0.241673
1	-3.443323	2.149227	0.493647	6	2.874839	-0.091315	-0.011463
1	-5.977962	1.200684	0.275333	7	3.648220	1.021470	0.215953
6	-1.413101	0.037459	0.005216	6	4.975765	0.694785	0.150747
6	-0.665243	1.170866	-0.330079	1	5.977770	-1.200714	-0.275938
6	-0.720335	-1.133880	0.335057	1	3.442861	-2.149244	-0.493310
6	0.720328	1.133984	-0.334764	1	3.286294	1.917764	0.497915
6	0.665263	-1.170768	0.330384	1	5.741007	1.434243	0.319403
3,3'-PhDP							
7	5.003150	-0.649984	0.165434	6	-1.415977	0.003055	-0.016193
6	3.704655	-1.073127	0.246986	1	1.229431	2.047288	0.616202
6	2.885627	0.006481	-0.005961	1	1.228378	-2.034857	-0.673454
6	3.743739	1.123656	-0.244758	1	-1.229412	2.047263	0.616237
6	5.038173	0.686068	-0.133739	1	-1.228334	-2.034854	-0.673488
1	5.809993	-1.229689	0.321767	7	-5.003203	-0.649939	0.165503
1	3.461730	-2.090950	0.505591	6	-3.704698	-1.073071	0.247158

1	3.436265	2.125612	-0.499675	6	-2.885621	0.006461	-0.005940
1	5.973433	1.207389	-0.253260	6	-3.743721	1.123643	-0.244720
6	1.416002	0.003070	-0.016201	6	-5.038175	0.686037	-0.133920
6	0.693944	1.151134	0.322818	1	-5.810071	-1.229736	0.321371
6	0.693499	-1.143107	-0.365059	1	-3.461823	-2.090931	0.505638
6	-0.693917	1.151131	0.322819	1	-3.436218	2.125642	-0.499415
6	-0.693459	-1.143114	-0.365059	1	-5.973417	1.207387	-0.253449

1,3'-PhDP

7	-4.946467	-0.653406	-0.129652	6	1.448898	0.000796	0.002162
6	-3.649819	-1.081332	-0.199337	1	-1.176232	2.015458	-0.715542
6	-2.829340	0.007178	0.007151	1	-1.172275	-2.005568	0.755102
6	-3.684588	1.134317	0.204409	1	1.291786	2.007874	-0.739588
6	-4.979465	0.693360	0.116403	1	1.294771	-2.003459	0.752814
1	-5.754638	-1.238209	-0.259275	6	4.973291	-0.674219	-0.243255
1	-3.409314	-2.108801	-0.419283	6	3.663264	-1.058117	-0.371786
1	-3.375958	2.145446	0.418428	7	2.864876	-0.000316	-0.001911
1	-5.913760	1.219813	0.219215	6	3.667481	1.055826	0.363492
6	-1.360270	0.002490	0.011782	6	4.975969	0.669321	0.227348
6	-0.640072	1.134624	-0.381411	1	5.832587	-1.283424	-0.473002
6	-0.638356	-1.128715	0.406554	1	3.224428	-1.974167	-0.731748
6	0.747459	1.137167	-0.394045	1	3.232598	1.972729	0.726049
6	0.748780	-1.134107	0.406463	1	5.837744	1.276839	0.452198

HPB_{N1}

6	-1.316450	-0.478093	-0.000861	6	1.253336	4.770404	0.588288
6	-1.072239	0.901221	-0.000912	6	0.458483	4.911071	-0.588045
6	0.244402	1.379262	-0.000914	6	-4.024139	2.852394	-0.586948
6	1.316766	0.477994	-0.000749	6	-3.504684	3.470180	0.589387
6	1.072573	-0.901335	-0.000616	6	-4.757818	-1.298979	0.589178
6	-0.244123	-1.379396	-0.000858	6	-4.482924	-2.057153	-0.587609
7	2.152577	-1.808530	0.000106	1	-0.243414	-5.823724	-1.120008
6	3.178163	-1.832965	-0.924361	1	-1.771138	-5.553157	1.118728
6	0.001426	-3.668324	-0.925608	1	3.924789	-4.308796	1.121715
7	-0.490144	-2.768309	-0.000738	1	4.923212	-3.121652	-1.117234
7	2.642477	0.959670	-0.000412	1	5.165157	2.701055	-1.119655
6	3.613198	0.631676	0.925504	1	5.694085	1.244656	1.120395
6	2.353214	-2.813582	0.925808	1	1.769233	5.553444	1.119969
7	0.490435	2.768139	-0.000882	1	0.241982	5.823778	-1.119153
6	-0.001285	3.668126	-0.925692	1	-4.923183	3.120951	-1.117613
6	3.176402	1.834652	-0.925788	1	-3.925038	4.308157	1.121457
7	-2.152184	1.808478	-0.000447	1	-5.693722	-1.243660	1.121178
6	-2.353073	2.813380	0.925351	1	-5.165549	-2.700485	-1.118777
6	1.260053	3.444865	0.924834	1	1.637000	-2.984252	1.714202

7	-2.642220	-0.959631	-0.000179	1	3.223300	-1.098522	-1.713152
6	-3.176550	-1.834537	-0.925393	1	0.660228	-3.339873	-1.714093
6	-3.177727	1.832809	-0.924963	1	-1.766664	-2.910011	1.712771
6	-1.260646	-3.444800	0.924364	1	-3.402213	0.073942	1.714541
6	-3.612728	-0.631219	0.925816	1	-2.563335	-2.240325	-1.714638
6	-0.459508	-4.911050	-0.588679	1	-3.222651	1.098480	-1.713872
6	-1.254583	-4.770267	0.587463	1	-1.636884	2.984134	1.713763
6	3.504649	-3.470643	0.589753	1	-0.659495	3.339476	-1.714604
6	4.024255	-2.852885	-0.586523	1	1.766008	2.910169	1.713340
6	4.482785	2.057635	-0.588265	1	2.562925	2.240206	-1.714954
6	4.758074	1.299660	0.588557	1	3.402963	-0.073325	1.714440

HPB_{C2}

6	1.157205	0.798957	-0.002280	6	0.245684	-5.077636	0.523283
6	1.271502	-0.600247	-0.001369	6	1.046926	-4.882982	-0.577372
6	0.112064	-1.402518	-0.003143	6	4.663947	-2.022286	-0.522496
6	-1.156538	-0.801795	-0.002014	6	4.201147	-2.695907	0.583550
6	-1.271578	0.603525	-0.002929	6	4.276164	2.747074	0.525878
6	-0.117092	1.402206	-0.001962	6	3.710603	3.341956	-0.577541
6	-2.612889	1.224216	0.024867	1	-0.935442	5.953292	-0.996424
7	-3.590199	0.886731	-0.877437	1	0.686897	5.765939	1.173207
6	-0.872619	3.714664	-0.909168	1	-5.234996	2.981028	0.999625
6	-0.224240	2.876502	-0.027374	1	-5.642195	1.392267	-1.164352
6	-2.379970	-1.631480	-0.027266	1	-4.691679	-3.781851	-0.997840
7	-3.392567	-1.460635	0.883041	1	-5.335182	-2.290875	1.177978
6	-3.164530	2.128134	0.907832	1	0.037364	-6.025399	0.992917
6	0.245176	-2.874629	0.022865	1	1.619157	-5.578403	-1.168852
7	1.027703	-3.550084	-0.879628	1	5.624158	-2.164033	-0.991711
6	-2.783718	-2.609220	-0.911227	1	4.652171	-3.471077	1.180693
6	2.602059	-1.243819	-0.026350	1	5.200710	3.040141	0.996557
7	2.960143	-2.207154	0.882927	1	4.029320	4.183418	-1.170186
6	-0.262702	-3.806210	0.903175	1	1.873005	2.956724	-1.554101
6	2.366431	1.648943	0.025459	1	3.580629	0.971804	1.712010
7	2.564569	2.661159	-0.879647	1	1.099138	3.318412	1.554458
6	3.652420	-1.101617	-0.907918	1	-1.513505	3.391169	-1.715048
7	0.435064	3.668719	0.878572	1	-3.501085	0.139117	-1.551008
6	3.426212	1.673980	0.907034	1	-2.632693	2.613959	1.711582
6	-0.578692	5.051187	-0.526122	1	-2.185347	-2.999323	-1.720280
6	0.238195	4.987586	0.578417	1	-3.420148	-0.712057	1.560775
6	-4.519456	2.326505	0.528686	1	1.631094	-3.097328	-1.551654
6	-4.753089	1.537765	-0.573361	1	-0.952008	-3.590657	1.705202
6	-4.087344	-3.023764	-0.526350	1	2.325355	-2.606376	1.559798
6	-4.437946	-2.288185	0.581391	1	3.692308	-0.386505	-1.715300

HPB_{C3}

6	-0.413934	-1.345150	-0.043579	7	-3.735755	3.371472	-0.51887
6	-1.371824	-0.314111	-0.043347	6	-3.184597	3.912388	0.61538
6	-0.957897	1.031039	-0.043422	6	-4.980592	-0.800509	0.615966
6	0.413944	1.345151	-0.043493	7	-4.788092	-1.548561	-0.5182
6	1.371833	0.314109	-0.04344	7	-1.052942	-4.920572	-0.52103
6	0.957912	-1.031047	-0.043533	6	-1.797085	-4.714109	0.613224
6	2.816964	0.648956	-0.02143	1	3.612864	-4.783156	1.083728
6	3.780338	0.224736	0.943816	1	4.571861	-3.698423	-0.97154
6	2.085738	-3.161200	0.943578	1	5.489787	2.108438	-0.97104
6	1.970680	-2.114971	-0.021765	1	5.948838	0.734976	1.084007
6	0.846559	2.764102	-0.022099	1	2.337455	5.520203	1.082024
6	0.469496	3.744243	-0.908804	1	0.918328	5.808081	-0.97317
6	3.477767	1.465822	-0.907577	1	-4.571697	3.698705	-0.97128
6	-1.970628	2.114983	-0.0216	1	-3.612610	4.783212	1.084022
6	-2.085566	3.161223	0.943743	1	-5.948722	-0.735129	1.084621
6	1.695504	3.386926	0.94285	1	-5.489733	-2.108788	-0.97035
6	-2.816951	-0.648996	-0.021153	1	-0.918843	-5.807869	-0.9741
6	-3.477838	-1.465729	-0.907329	1	-2.337625	-5.520246	1.081319
6	-3.008369	2.278449	-0.907839	1	-3.301075	1.676539	-1.75296
6	-0.846608	-2.764079	-0.022418	1	-1.413111	3.339700	1.768643
6	-1.695561	-3.387005	0.942457	1	-3.103239	-2.020286	-1.75252
6	-3.780228	-0.224821	0.94421	1	-3.598249	0.446866	1.768975
6	3.008241	-2.278483	-0.908175	1	-2.186298	-2.894169	1.767572
6	-0.469504	-3.744158	-0.909201	1	0.198195	-3.696452	-1.75425
6	3.184771	-3.912355	0.615089	1	3.300776	-1.676573	-1.75336
7	3.735721	-3.371449	-0.519276	1	1.413412	-3.339728	1.768571
7	4.788088	1.548550	-0.518595	1	3.598373	-0.446978	1.768563
6	4.980658	0.800403	0.615488	1	3.103125	2.020487	-1.75267
6	1.796959	4.714104	0.613786	1	-0.198178	3.696565	-1.75388
7	1.052833	4.920636	-0.520474	1	2.186299	2.894048	1.767905

HPB_{N16σ}

6	-1.322567	-0.370804	-0.339196	6	-0.489087	-4.798138	0.217221
6	-0.982462	0.959941	-0.339220	6	-1.873094	-4.444441	0.217108
6	0.340129	1.330769	-0.339144	6	3.910909	-2.822720	0.216752
6	1.322576	0.370807	-0.339315	6	2.912490	-3.844421	0.216908
6	0.982457	-0.959934	-0.339119	6	4.400025	1.975595	0.216244
6	-0.340130	-1.330776	-0.339213	6	4.785772	0.600180	0.216241
7	1.952305	-1.907517	-0.171331	6	0.489085	4.798129	0.217247
6	1.679551	-3.258591	-0.011328	6	1.873094	4.444433	0.217125
6	0.259530	-3.656748	-0.011263	6	-3.910906	2.822723	0.216764
7	-0.675878	-2.644443	-0.171311	6	-2.912490	3.844423	0.216905

7	2.628149	0.736889	-0.171627	6	-4.400030	-1.975596	0.216220
6	3.661999	-0.174788	-0.011889	6	-4.785777	-0.600179	0.216217
6	3.296787	-1.603655	-0.011662	1	-0.091722	-5.785795	0.386905
7	0.675879	2.644448	-0.171373	1	-2.695531	-5.120351	0.387030
6	1.982295	3.083813	-0.011396	1	4.964959	-2.972524	0.386182
6	3.037127	2.053173	-0.011663	1	3.086669	-4.894699	0.386385
7	-1.952305	1.907518	-0.171319	1	5.056662	2.813611	0.385630
6	-1.679552	3.258591	-0.011342	1	5.782466	0.226013	0.385743
6	-0.259531	3.656748	-0.011273	1	0.091720	5.785783	0.386948
7	-2.628145	-0.736888	-0.171603	1	2.695531	5.120340	0.387056
6	-3.661999	0.174792	-0.011878	1	-4.964953	2.972525	0.386215
6	-3.296785	1.603657	-0.011658	1	-3.086665	4.894701	0.386390
6	-1.982294	-3.083814	-0.011382	1	-5.056673	-2.813613	0.385576
6	-3.037126	-2.053174	-0.011643	1	-5.782477	-0.226013	0.385687

HPB_{C26σ}

6	0.133750	-1.387659	-0.970755	6	3.853998	-2.462267	0.594993
6	-1.134767	-0.809696	-0.970774	6	3.255149	3.236993	0.638110
6	-1.268550	0.577955	-0.970808	6	4.059442	2.106393	0.595039
6	-0.133749	1.387658	-0.970756	6	-1.175792	4.437630	0.637950
6	1.134766	0.809697	-0.970771	6	0.205531	4.568675	0.595205
6	1.268550	-0.577955	-0.970811	6	-4.431105	1.200496	0.637626
6	2.189541	1.616691	-0.491421	6	-3.853984	2.462272	0.595014
7	3.407692	1.101598	-0.079640	6	-3.255203	-3.237050	0.637968
6	3.549255	-0.314826	-0.032522	6	-4.059442	-2.106407	0.595025
6	2.494846	-1.087870	-0.491528	6	1.175769	-4.437550	0.638098
6	-0.305330	2.704591	-0.491410	6	-0.205543	-4.568668	0.595219
7	0.749825	3.501847	-0.079354	1	5.369482	-0.967402	1.114388
6	2.047254	2.916241	-0.032206	1	4.209411	-3.390393	1.010929
6	-2.494840	1.087865	-0.491504	1	3.522392	4.165988	1.115321
7	-2.657859	2.400284	-0.079453	1	5.040924	1.950014	1.010957
6	-1.501994	3.231134	-0.032242	1	-1.846689	5.133726	1.114959
6	-2.189549	-1.616695	-0.491444	1	0.831698	5.340469	1.011138
7	-3.407695	-1.101604	-0.079647	1	-5.369375	0.967374	1.114586
6	-3.549243	0.314820	-0.032488	1	-4.209407	3.390406	1.010920
6	0.305331	-2.704584	-0.491389	1	-3.522472	-4.166071	1.115115
7	-0.749828	-3.501841	-0.079347	1	-5.040908	-1.950022	1.010979
6	-2.047264	-2.916248	-0.032240	1	1.846656	-5.133610	1.115175
7	2.657865	-2.400283	-0.079461	1	-0.831713	-5.340479	1.011116
6	1.501993	-3.231121	-0.032208	6	4.431179	-1.200516	0.637487

HPB_{C36σ}

6	1.340930	-0.387631	0.824315	6	3.284359	1.568247	0.064612
6	1.006150	0.967441	0.824298	6	1.975585	-3.102444	0.032710

6	-0.334787	1.355073	0.824280	6	3.000386	-2.060156	0.064576
6	-1.340930	0.387631	0.824315	7	0.439154	-4.664599	-0.476072
6	-1.006150	-0.967441	0.824298	6	1.792983	-4.366379	-0.504079
6	0.334787	-1.355074	0.824281	7	-3.820553	-2.712807	-0.474928
6	-1.987051	-1.911057	0.427380	6	-2.885209	-3.736003	-0.503495
6	-1.699086	-3.262044	0.032664	7	-4.259733	1.952197	-0.474928
6	-0.283973	-3.628222	0.063971	6	-4.678299	0.630604	-0.503138
6	0.661537	-2.676336	0.427214	7	-0.439153	4.664596	-0.476080
6	-2.648668	0.765292	0.427484	6	-1.792982	4.366376	-0.504086
6	-3.674767	-0.159594	0.033085	7	3.820556	2.712810	-0.474919
6	-3.284358	-1.568246	0.064609	6	2.885212	3.736004	-0.503488
6	-0.661537	2.676334	0.427209	7	4.259729	-1.952196	-0.474937
6	-1.975585	3.102442	0.032705	6	4.678297	-0.630603	-0.503145
6	-3.000387	2.060156	0.064579	1	0.050696	-5.523437	-0.828575
6	1.987052	1.911058	0.427384	1	2.489961	-5.076354	-0.918043
6	1.699087	3.262045	0.032668	1	-4.758897	-2.806085	-0.826441
6	0.283973	3.628221	0.063967	1	-3.151755	-4.694653	-0.917199
6	2.648667	-0.765292	0.427480	1	-4.809567	2.718130	-0.826773
6	3.674766	0.159594	0.033080	1	-5.641864	0.382053	-0.916628
1	4.758901	2.806090	-0.826428	1	-0.050696	5.523434	-0.828584
1	3.151759	4.694656	-0.917189	1	-2.489960	5.076350	-0.918052
1	4.809563	-2.718129	-0.826782	1	5.641860	-0.382051	-0.916639

OPN_{N1}

7	-0.248053	1.405146	2.800191	6	-1.679205	-3.923076	-2.105517
7	-0.144355	3.705713	1.298307	6	-1.544722	-5.182556	-2.622566
7	0.516166	3.619058	-1.425355	6	-0.253425	-5.663262	-2.254993
7	0.732772	1.152201	-2.724543	6	0.355208	-4.685679	-1.516670
6	-0.070248	1.279146	1.404930	1	1.309317	-4.659271	-1.014075
6	0.535512	2.175047	3.638991	1	0.175641	-6.621943	-2.497542
6	-0.037294	2.170736	4.878030	1	-2.284991	-5.697905	-3.212896
6	-1.226527	1.385633	4.797963	1	-2.471747	-3.195811	-2.190304
6	-1.333854	0.935520	3.512251	6	0.000000	-2.451338	0.666991
6	0.000000	2.451338	0.666991	7	0.144355	-3.705713	1.298307
6	0.796948	4.716189	1.311822	6	-0.796948	-4.716189	1.311822
6	0.293642	5.749209	2.053425	6	-0.293642	-5.749209	2.053425
6	-1.002375	5.362323	2.506133	6	1.002375	-5.362323	2.506133
6	-1.243281	4.101500	2.034657	6	1.243281	-4.101500	2.034657
6	0.263280	2.417795	-0.729012	1	2.073514	-3.429253	2.183334
6	1.679205	3.923076	-2.105517	1	1.675742	-5.940978	3.117465
6	1.544722	5.182556	-2.622566	1	-0.793352	-6.685950	2.240264
6	0.253425	5.663262	-2.254993	1	-1.718803	-4.617534	0.759853
6	-0.355208	4.685679	-1.516670	6	0.070248	-1.279146	1.404930

6	0.286530	1.208322	-1.384198	7	0.248053	-1.405146	2.800191
6	1.940989	0.582766	-3.081171	6	-0.535512	-2.175047	3.638991
6	2.157140	0.848588	-4.406148	6	0.037294	-2.170736	4.878030
6	1.044479	1.605567	-4.875625	6	1.226527	-1.385633	4.797963
6	0.193381	1.786582	-3.819001	6	1.333854	-0.935520	3.512251
6	0.000000	0.000000	-0.679176	1	2.070388	-0.309723	3.034537
6	0.000000	0.000000	0.749590	1	1.916118	-1.167554	5.597362
1	1.420721	2.664886	3.266022	1	-0.351370	-2.672006	5.749521
1	0.351370	2.672006	5.749521	1	-1.420721	-2.664886	3.266022
1	-1.916118	1.167554	5.597362	1	-0.745274	2.310949	-3.739198
1	-2.070388	0.309723	3.034537	6	-0.286530	-1.208322	-1.384198
1	1.718803	4.617534	0.759853	7	-0.732772	-1.152201	-2.724543
1	0.793352	6.685950	2.240264	6	-1.940989	-0.582766	-3.081171
1	-1.675742	5.940978	3.117465	6	-2.157140	-0.848588	-4.406148
1	-2.073514	3.429253	2.183334	6	-1.044479	-1.605567	-4.875625
1	2.471747	3.195811	-2.190304	6	-0.193381	-1.786582	-3.819001
1	2.284991	5.697905	-3.212896	1	0.745274	-2.310949	-3.739198
1	-0.175641	6.621943	-2.497542	1	-0.885744	-1.971873	-5.876731
1	-1.309317	4.659271	-1.014075	1	-3.011383	-0.526762	-4.980029
1	2.524385	0.044257	-2.350787	1	-2.524385	-0.044257	-2.350787
1	3.011383	0.526762	-4.980029	6	-0.263280	-2.417795	-0.729012
1	0.885744	1.971873	-5.876731	7	-0.516166	-3.619058	-1.425355

OPN_{N16σ}

6	0.685693	-2.433486	0.152404	6	-4.964550	1.176635	0.975475
6	-0.685692	-2.433490	-0.152354	6	-4.599257	2.462088	1.420524
6	-1.423066	-1.266330	-0.181166	6	-3.278075	2.638839	1.098584
6	-0.735893	-0.000001	0.000005	6	-2.473776	3.814340	1.053158
6	0.735893	0.000001	0.000005	6	-2.653933	5.154396	1.318204
6	1.423066	-1.266327	0.181177	6	-1.502904	5.839341	0.847785
6	-1.423066	1.266327	0.181177	6	-0.645763	4.906883	0.308077
6	-0.685693	2.433486	0.152404	6	0.645765	4.906890	-0.307940
6	0.685692	2.433490	-0.152354	6	1.502890	5.839362	-0.847649
6	1.423066	1.266330	-0.181166	6	2.653904	5.154430	-1.318124
7	2.794368	1.464734	-0.495517	6	2.473779	3.814376	-1.053053
7	2.794374	-1.464727	0.495501	6	3.278058	2.638866	-1.098570
7	1.251636	-3.666070	0.440542	6	4.599200	2.462087	-1.420657
7	-1.251642	-3.666083	-0.440433	6	4.964483	1.176584	-0.975744
7	-2.794368	-1.464734	-0.495517	6	3.860787	0.600821	-0.387101
7	-2.794374	1.464727	0.495501	1	-1.317256	6.899978	0.897210
7	-1.251636	3.666070	0.440542	1	-3.525797	5.592967	1.775090
7	1.251642	3.666083	-0.440433	1	1.317229	6.899998	-0.897070
6	3.860813	-0.600865	0.386915	1	3.525743	5.593010	-1.775050

6	4.964550	-1.176635	0.975475	1	5.230340	3.207234	-1.876894
6	4.599257	-2.462088	1.420524	1	5.933139	0.708836	-1.044402
6	3.278075	-2.638839	1.098584	1	5.933230	-0.708917	1.044013
6	2.473776	-3.814340	1.053158	1	5.230420	-3.207226	1.876743
6	2.653933	-5.154396	1.318204	1	3.525797	-5.592967	1.775090
6	1.502904	-5.839341	0.847785	1	1.317256	-6.899978	0.897210
6	0.645763	-4.906883	0.308077	1	-1.317229	-6.899998	-0.897070
6	-0.645765	-4.906890	-0.307940	1	-3.525743	-5.593010	-1.775050
6	-1.502890	-5.839362	-0.847649	1	-5.230340	-3.207234	-1.876894
6	-2.653904	-5.154430	-1.318124	1	-5.933139	-0.708836	-1.044402
6	-2.473779	-3.814376	-1.053053	1	-5.933230	0.708917	1.044013
6	-3.278058	-2.638866	-1.098570	1	-5.230420	3.207226	1.876743
6	-4.599200	-2.462087	-1.420657	6	-3.860787	-0.600821	-0.387101
6	-4.964483	-1.176584	-0.975744	6	-3.860813	0.600865	0.386915

OPN_{C36σ}

6	-2.459728	0.702112	-0.100617	6	5.340178	2.860214	0.688459
6	-2.457751	-0.703641	0.091935	6	3.976409	2.666874	0.588434
6	-1.278060	-1.454052	0.117148	6	2.785685	3.437980	0.603944
6	0.000794	-0.739369	-0.001138	7	2.691822	4.791023	0.736132
6	-0.001023	0.739365	0.004898	6	1.402661	5.179543	0.489763
6	-1.280060	1.453419	-0.115780	6	0.677434	4.048477	0.206795
6	1.280352	-1.453735	-0.113037	1	7.057565	-1.629083	-0.481135
6	2.459614	-0.701663	-0.103872	1	5.737162	-3.722993	-0.895110
6	2.457664	0.703262	0.094583	1	6.928860	1.479765	0.428814
6	1.278304	1.454380	0.114522	1	5.935910	3.730230	0.906855
6	1.522915	2.902843	0.305257	1	3.465201	5.402412	0.932735
6	-1.522226	2.902033	-0.295539	1	1.107595	6.213965	0.555013
6	-3.753947	1.304886	-0.278656	1	-0.984678	6.052569	-0.508873
6	-3.750313	-1.309618	0.265603	1	-3.427238	5.607731	-0.937619
6	-1.522947	-2.902902	0.304157	1	-5.737043	3.722760	-0.896066
6	1.522208	-2.901984	-0.296678	1	-7.057494	1.628923	-0.481756
6	3.753983	-1.304857	-0.279115	1	-6.928768	-1.479501	0.430217
6	3.750355	1.309672	0.265373	1	-5.935820	-3.730309	0.906844
6	-0.689075	3.999594	-0.191470	1	-3.464483	-5.402417	0.934588
7	-1.393907	5.134632	-0.462952	1	-1.107820	-6.214222	0.551702
6	-2.703051	4.841434	-0.719849	1	0.984034	-6.052130	-0.513460
6	-2.823368	3.477750	-0.605435	1	3.427199	-5.607512	-0.939536
6	-3.954445	2.624813	-0.585444	6	-1.402754	-5.179699	0.487527
7	-5.299734	2.840186	-0.692962	6	-0.677460	-4.048494	0.205235
6	-5.981751	1.662168	-0.441634	6	0.689038	-3.999545	-0.193036
6	-5.044027	0.690027	-0.178035	7	1.393744	-5.134527	-0.465153
6	-4.989132	-0.696691	0.161375	6	2.702984	-4.841275	-0.721616

7	-5.935889	-1.642743	0.422310	6	2.823436	-3.477692	-0.606235
6	-5.340118	-2.860245	0.688527	6	3.954507	-2.624775	-0.585966
6	-3.976374	-2.666958	0.588032	7	5.299803	-2.840222	-0.692970
6	-2.785674	-3.438128	0.602944	6	5.981800	-1.662201	-0.441610
7	-2.692032	-4.791381	0.733297	6	5.044043	-0.689922	-0.178635
7	5.935948	1.642853	0.421585	6	4.989174	0.696776	0.160846

DPC_{N1}

7	4.018847	-2.399297	-0.048698	6	-1.870035	-5.186110	-0.958486
7	1.690657	-4.366275	0.002804	1	-2.177989	-4.672603	-1.855250
7	-1.039476	-4.563341	-0.045973	6	-5.410999	-0.898575	1.007691
7	-3.630202	-2.957278	0.002388	1	-4.942553	-1.434336	1.817226
7	-4.661567	-0.421473	-0.050069	6	-6.720934	-0.589927	0.769768
7	-3.934266	2.538605	0.001634	1	-7.546353	-0.825266	1.422010
7	-1.841043	4.302257	-0.045250	6	-6.783689	0.086935	-0.484289
7	1.198899	4.525486	0.003984	1	-7.663308	0.478849	-0.968832
7	3.523323	3.080692	-0.048374	6	-5.507985	0.176165	-0.964814
7	4.675242	0.258201	0.001455	1	-5.112339	0.627053	-1.860839
6	4.904932	-2.452384	1.009617	6	-4.677464	2.331017	1.144136
1	4.840154	-1.742785	1.818378	1	-4.339932	1.640721	1.900390
6	5.783883	-3.471817	0.773375	6	-5.812999	3.088831	1.053667
1	6.589625	-3.765485	1.426583	1	-6.603741	3.119697	1.785819
6	5.438003	-4.057678	-0.480378	6	-5.760434	3.791706	-0.184886
1	5.920015	-4.892070	-0.963649	1	-6.495396	4.477902	-0.573499
6	4.353357	-3.381091	-0.962305	6	-4.592052	3.442873	-0.805738
1	3.768561	-3.514837	-1.858321	1	-4.147217	3.771463	-1.731770
6	2.414287	-4.633046	1.145554	6	-2.526706	4.864877	1.013719
1	2.546137	-3.875141	1.900893	1	-2.891339	4.251779	1.821784
6	2.888866	-5.913125	1.056652	6	-2.638986	6.206466	0.778685
1	3.511172	-6.401223	1.789295	1	-3.118439	6.916970	1.432485
6	2.433477	-6.452956	-0.181118	6	-2.014730	6.478459	-0.474718
1	2.625712	-7.440434	-0.568388	1	-1.914483	7.437268	-0.957157
6	1.692032	-5.485623	-0.803040	6	-1.534921	5.294096	-0.957908
1	1.138586	-5.491806	-1.728808	1	-0.983311	5.059618	-1.854254
6	-0.816187	-5.420848	1.013719	6	0.773112	5.166559	1.147822
1	-0.160886	-5.138907	1.821757	1	0.222982	4.630875	1.904633
6	-1.514645	-6.571940	0.779433	6	1.141402	6.481110	1.058069
1	-1.544908	-7.428070	1.433856	1	0.926740	7.241739	1.791313
6	-2.178851	-6.425778	-0.474437	6	1.823949	6.650281	-0.181405
1	-2.823863	-7.142518	-0.956456	1	2.247806	7.562209	-0.569706
6	-0.454514	-3.295451	-0.255109	6	1.853527	5.431939	-0.803590
6	-1.320555	-2.141237	-0.469602	1	2.302363	5.111718	-1.730632
6	-2.739338	-1.884897	-0.245481	6	3.848474	3.906586	1.010071
6	-2.444302	0.594004	-0.469780	1	3.154573	4.063438	1.819829

6	-0.190104	2.507901	-0.468644	6	5.089056	4.428349	0.772546
6	2.326900	0.955654	-0.469967	1	5.617852	5.103714	1.425536
6	3.324110	-0.085741	-0.246097	6	5.537974	3.919556	-0.482123
6	2.993751	-1.450914	-0.256248	1	6.479651	4.121107	-0.966618
6	-3.662949	-3.726282	1.146197	6	4.559127	3.096975	-0.963410
1	-2.903003	-3.616551	1.903007	1	4.504716	2.500480	-1.860045
6	-4.733539	-4.573352	1.055954	6	5.153448	0.862910	1.144352
1	-5.007035	-5.315146	1.788897	1	4.474056	1.221449	1.900799
6	-5.385114	-4.308411	-0.183441	6	6.517432	0.919519	1.054088
1	-6.264253	-4.796514	-0.571926	1	7.174388	1.360138	1.786565
6	-4.692655	-3.305367	-0.805253	6	6.889151	0.320962	-0.184594
1	-4.867571	-2.782027	-1.732028	1	7.887365	0.199348	-0.572946
6	-3.274620	-0.586294	-0.256285	6	5.739575	-0.084948	-0.805906
6	-2.638964	2.022496	-0.245311	1	5.573737	-0.612202	-1.732133
6	-1.569152	2.932691	-0.254279	6	-0.628410	-1.019393	-0.838169
6	1.108352	3.134342	-0.244319	6	-1.163415	0.282512	-0.838065
6	2.304706	2.398483	-0.255385	6	-0.090574	1.193645	-0.837742
6	1.628232	-1.917757	-0.470067	6	1.107477	0.454882	-0.838175
6	0.945955	-3.187782	-0.245402	6	0.775081	-0.912831	-0.838331

DPC_{C3}

6	-2.154178	4.255564	-0.076015	1	-4.813093	-3.355545	-1.766872
6	0.916322	4.672699	0.017124	6	-5.477825	-1.202054	1.035348
6	3.381452	3.363914	-0.075321	1	-5.091965	-1.716863	1.900932
6	4.727541	0.572409	0.015854	6	-6.791463	-0.895723	0.795170
6	4.244280	-2.176485	-0.075704	1	-7.677230	-1.068282	1.384092
6	2.005255	-4.318985	0.017555	7	-6.859056	-0.275811	-0.427329
6	-0.758261	-4.709187	-0.075026	1	-7.691454	0.109085	-0.838716
6	-3.488229	-3.241625	0.017466	6	-5.603091	-0.171412	-0.958717
6	-4.713105	-0.733801	-0.075985	1	-5.428469	0.321080	-1.901377
6	-4.160757	2.315551	0.017512	6	-4.932863	2.084287	1.192991
6	-2.835877	4.837610	1.035563	1	-4.641285	1.482096	2.038657
1	-3.206468	4.311103	1.900783	6	-6.128934	2.736812	1.039914
6	-2.950323	6.181751	0.796139	1	-6.985179	2.804007	1.690919
1	-3.388108	6.970562	1.385467	7	-6.116022	3.350585	-0.187304
7	-2.381428	6.438250	-0.426129	1	-6.838013	3.953309	-0.542195
1	-2.272407	7.349081	-0.836959	6	-4.918328	3.108234	-0.808314
6	-1.894157	5.276236	-0.958158	1	-4.679142	3.540532	-1.766523
1	-1.371552	5.262854	-1.900688	6	1.077231	0.525654	-0.839124
6	0.457584	5.335600	1.192517	6	0.832859	-0.862158	-0.838783
1	-0.025238	4.872266	2.038099	6	-0.562539	-1.058647	-0.838688
6	0.708502	6.674783	1.039429	6	-1.180545	0.207779	-0.838979
1	0.507539	7.509894	1.690333	6	-0.167128	1.186897	-0.839220
7	1.296348	6.852155	-0.187749	6	-0.353270	2.494675	-0.477314

1	1.646671	7.725031	-0.542524	6	0.907168	3.212997	-0.257458
6	1.436141	5.638155	-0.808668	6	2.152737	2.557160	-0.276451
1	1.921430	5.544281	-1.766759	6	2.263457	1.106885	-0.477186
6	3.724041	4.190916	1.037234	6	3.336137	0.130136	-0.257391
1	3.108711	4.379441	1.902658	6	1.752154	-1.810589	-0.476503
6	4.966928	4.715704	0.798508	6	-1.180666	-2.225971	-0.476355
1	5.581625	5.375285	1.388662	6	-2.481794	0.434915	-0.476902
7	5.386824	4.255523	-0.424299	6	-2.775372	1.855667	-0.257125
1	6.286839	4.433817	-0.834735	6	-1.766711	2.837571	-0.276443
6	4.432541	3.433351	-0.957341	6	5.217877	1.213138	1.190777
1	4.581476	2.933416	-1.900487	1	4.629175	1.529034	2.037206
6	5.137820	-2.246665	1.035948	6	6.568903	1.388054	1.035954
1	5.128078	-1.602933	1.901189	1	7.302032	1.836766	1.686078
6	6.020678	-3.266638	0.796448	7	6.917527	0.884086	-0.191816
1	6.838671	-3.647285	1.385671	1	7.855428	0.820776	-0.547962
7	5.711398	-3.808413	-0.425927	6	5.805238	0.376401	-0.811421
1	6.158907	-4.609105	-0.836906	1	5.864491	-0.113719	-1.769822
6	4.634060	-3.154921	-0.957920	6	3.097253	-1.257151	-0.276078
1	4.203593	-3.451194	-1.900562	6	1.154639	-3.132524	-0.256418
6	2.765925	-4.586614	1.192802	6	-0.238534	-3.334145	-0.275407
1	2.884152	-3.928663	2.038936	6	-2.622601	-2.066154	-0.256716
6	3.349942	-5.817482	1.038750	6	-3.244726	-0.803398	-0.276011
1	4.003108	-6.375715	1.689310	6	-1.246338	-6.735651	0.796735
7	2.978678	-6.305465	-0.188842	1	-1.355748	-7.631261	1.385884
1	3.208139	-7.217333	-0.544280	7	-1.857401	-6.608514	-0.425481
6	2.152129	-5.404933	-0.809077	1	-2.480957	-7.281230	-0.836458
1	1.704431	-5.613343	-1.767405	6	-1.568635	-5.381893	-0.957239
6	-0.548778	-5.581030	1.036353	1	-1.983593	-5.063634	-1.899662
1	0.060622	-5.373167	1.901553	6	-3.507370	-4.047578	1.192842
7	-5.077198	-4.780892	-0.187900	1	-2.844616	-3.956733	2.038610
1	-5.873760	-5.280824	-0.542936	6	-4.497898	-4.983079	1.039484
6	-4.476149	-3.716793	-0.808635	1	-4.826642	-5.776719	1.690288
Indole (I)							
6	0.247008	-0.667645	-0.000081	1	1.873352	-2.033154	-0.000891
6	0.248232	0.746120	0.000002	6	-2.127342	-0.716726	0.000143
6	1.623146	1.162937	-0.000279	6	-0.933942	-1.414208	-0.000207
6	2.381382	0.029526	0.000211	1	-3.062761	-1.263145	0.000076
7	1.560587	-1.077463	0.000236	1	-0.916149	-2.497933	-0.000504
6	-0.980210	1.424700	-0.000010	1	3.453619	-0.086045	0.000523
6	-2.151030	0.691463	0.000204	1	1.996710	2.174128	-0.000354
1	-3.105886	1.203135	-0.000205	1	-1.006455	2.508249	-0.000190
² J _{C3N1'}							
6	-2.774849	-0.820719	0.220395	6	2.834315	0.875683	0.233352

6	-1.804279	0.181202	0.005123	6	2.178927	1.973272	0.888019
6	-0.572948	-0.325995	0.543905	6	0.875297	1.612852	1.055891
6	-0.822917	-1.571516	1.046326	7	0.662310	0.345285	0.543799
7	-2.149581	-1.877077	0.843129	6	4.145706	0.642296	-0.206508
6	-2.168203	1.372078	-0.639936	6	4.440406	-0.554963	-0.831037
6	-3.480639	1.531099	-1.039650	6	3.446808	-1.531502	-1.034712
1	-2.590700	-2.740348	1.110729	6	2.145223	-1.332601	-0.610889
6	-4.438964	0.523919	-0.809660	1	3.706627	-2.455971	-1.536368
6	-4.103430	-0.661345	-0.182911	1	1.375551	-2.077101	-0.774675
1	-5.460287	0.681159	-1.134579	1	0.053996	2.141172	1.515713
1	-4.841315	-1.436437	-0.012325	1	2.623448	2.904972	1.198911
1	-0.150850	-2.260872	1.532234	1	4.913539	1.393217	-0.059662
1	-1.427858	2.142279	-0.824434	1	5.449409	-0.747815	-1.174899
1	-3.782529	2.441699	-1.542244	6	1.856524	-0.124328	0.027807

³I_{C3N1'}

6	4.315658	-0.878275	0.489953	1	-2.500754	3.102203	-0.804211
6	2.972550	-0.859164	0.057403	1	-1.175079	5.004633	-1.681643
6	2.403255	0.357480	0.565470	6	-3.050302	-0.864350	0.102355
6	3.378582	1.014957	1.260261	6	-4.412190	-0.864507	0.482086
7	4.537779	0.276390	1.206356	6	-4.659990	0.381923	1.150807
6	2.478803	-1.916912	-0.719748	6	-3.482392	1.068245	1.157791
6	3.329811	-2.958448	-1.032550	7	-2.496561	0.328946	0.528889
1	5.409755	0.538784	1.633558	6	-5.206102	-1.975139	0.160003
6	4.666213	-2.965539	-0.585744	6	-4.634993	-3.032689	-0.522358
6	5.178331	-1.931567	0.174889	6	-3.278977	-3.005325	-0.900019
1	5.306670	-3.799145	-0.846881	6	-2.469362	-1.926180	-0.594930
1	6.207807	-1.937815	0.512996	1	-2.862084	-3.845799	-1.441877
1	3.328946	1.954203	1.787902	1	-3.234461	2.032848	1.573774
1	1.452966	-1.906472	-1.070557	1	-5.591443	0.718367	1.576844
1	2.969879	-3.784429	-1.633367	1	-6.252595	-1.999282	0.441647
6	0.669675	1.984654	-0.183225	1	-5.237033	-3.896869	-0.775904
6	-0.741616	1.992318	-0.212995	1	-1.427710	-1.897793	-0.890742
6	-1.164654	0.744639	0.358214	6	0.735316	4.121294	-1.216268
6	-0.042636	0.047235	0.704200	6	1.425610	3.045892	-0.687933
7	1.077039	0.786513	0.374115	1	1.289839	4.960864	-1.617835
6	-1.417543	3.091939	-0.760372	1	2.508250	3.017681	-0.674137
6	-0.672735	4.146443	-1.252421	1	0.057393	-0.918462	1.175698

⁴I_{C3N1'}

6	-6.217814	0.036378	0.881752	6	1.844290	-0.099777	0.531373
6	-4.971586	0.297304	0.273769	7	0.645183	0.398564	0.060374
6	-4.076435	-0.725925	0.735604	6	2.709265	3.232248	-0.672879
6	-4.777707	-1.546023	1.573548	6	1.826105	4.127897	-1.244380
7	-6.073904	-1.094402	1.654673	6	0.464721	3.803669	-1.405087

6	-4.837191	1.391119	-0.593104	6	-0.040462	2.582775	-0.997388
6	-5.939209	2.191848	-0.819405	1	-0.200508	4.525564	-1.863305
1	-6.800363	-1.521316	2.204111	1	1.894786	-1.084945	0.969231
6	-7.174844	1.921664	-0.198093	1	3.760722	3.473243	-0.564309
6	-7.334225	0.845766	0.654450	1	2.183156	5.092794	-1.582848
1	-8.019135	2.570721	-0.395855	1	-1.084136	2.327653	-1.133088
1	-8.287130	0.638222	1.126725	6	5.034794	-0.313908	0.314533
1	-4.445959	-2.417452	2.115504	6	6.302219	-0.048402	0.882079
1	-3.888421	1.592038	-1.077979	6	6.180043	1.175441	1.623313
1	-5.859148	3.040527	-1.487330	6	4.889212	1.592357	1.489005
6	-2.131933	-1.938152	-0.246125	7	4.180825	0.702339	0.701953
6	-0.771978	-1.629329	-0.463785	6	7.356309	-0.940195	0.634388
6	-0.570263	-0.309354	0.063325	6	7.125640	-2.047432	-0.160078
6	-1.763969	0.123852	0.566124	6	5.857521	-2.284938	-0.723988
7	-2.720764	-0.853842	0.378250	6	4.797460	-1.426017	-0.496643
6	0.054834	-2.559661	-1.109394	1	5.710080	-3.156746	-1.350124
6	-0.492774	-3.762317	-1.511664	1	3.822558	-1.599689	-0.935799
6	-1.853133	-4.052539	-1.288396	1	4.382867	2.452649	1.899535
6	-2.690761	-3.150049	-0.659530	1	8.336986	-0.759059	1.059287
1	-2.252826	-5.002149	-1.623024	1	7.931186	-2.744142	-0.358215
1	-3.740327	-3.364510	-0.499730	1	6.951018	1.674677	2.187822
1	-2.016287	1.049874	1.059770	6	0.852857	1.681482	-0.412238
1	1.097747	-2.330310	-1.296973	6	2.220539	1.989750	-0.245577
1	0.128360	-4.493947	-2.013488	6	2.824372	0.835086	0.356713

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6	7.660084	-1.282100	1.287113	1	1.259732	-3.741810	-2.789677
6	6.480599	-1.145030	0.525124	1	0.069585	1.730256	0.749826
6	5.789353	-0.003823	1.055039	1	-2.517411	-1.989521	-1.723330
6	6.540263	0.500113	2.079058	1	-1.205671	-3.768377	-2.843560
7	7.675925	-0.263287	2.213764	1	2.491619	-1.942227	-1.610687
6	6.216486	-2.047228	-0.515121	6	-3.051064	1.821722	-0.341151
6	7.125405	-3.058063	-0.757224	6	-4.416555	1.776800	0.014904
1	8.400081	-0.104879	2.893802	6	-4.653257	0.462684	0.541775
6	8.294955	-3.185831	0.018477	6	-3.471784	-0.220826	0.493002
6	8.581082	-2.304784	1.044053	7	-2.493873	0.590663	-0.047845
1	8.986348	-3.991459	-0.196254	6	-5.228440	2.898227	-0.205636
1	9.483758	-2.403364	1.635296	6	-4.659056	4.025476	-0.765918
1	6.346671	1.346180	2.719246	6	-3.295280	4.052399	-1.118095
1	5.320975	-1.941904	-1.117281	6	-2.475065	2.957757	-0.915782
1	6.943292	-3.764879	-1.557225	1	-2.881382	4.949388	-1.562766
6	4.317747	1.765286	0.093999	1	-1.430011	2.971558	-1.199737
6	2.966833	1.825491	-0.310702	1	-3.236538	-1.224333	0.813232
6	2.406297	0.534116	-0.030864	1	-6.281761	2.869664	0.049693

6	3.392102	-0.237522	0.515370	1	-5.269058	4.901973	-0.946885
7	4.558153	0.497131	0.590478	6	-6.529478	-1.174882	0.608788
6	2.465344	3.006001	-0.877125	6	-7.733998	-1.275385	1.342252
6	3.317154	4.084107	-1.018705	6	-7.792284	-0.131297	2.208289
6	4.663771	4.004896	-0.612291	6	-6.660505	0.594255	1.982267
6	5.184094	2.850938	-0.056301	7	-5.883427	-0.023284	1.019073
1	5.307320	4.866115	-0.744835	6	-8.581651	-2.368162	1.107089
1	6.222721	2.782405	0.243136	6	-8.216660	-3.309399	0.163032
1	3.361345	-1.255327	0.873328	6	-7.017283	-3.181873	-0.563520
1	1.433939	3.061935	-1.206716	6	-6.159130	-2.117826	-0.352915
1	2.950347	5.004672	-1.455642	1	-6.762774	-3.931335	-1.303360
6	0.661434	-0.970367	-0.982975	1	-6.311319	1.509943	2.434614
6	-0.749972	-0.969038	-1.006824	1	-9.510048	-2.468392	1.657651
6	-1.163124	0.194857	-0.276051	1	-8.862149	-4.158367	-0.027163
6	-0.036748	0.836667	0.153933	1	-8.571573	0.113841	2.911803
7	1.076817	0.144019	-0.276933	1	-5.239545	-2.010859	-0.915344
6	-1.433815	-1.987199	-1.685904	6	0.711250	-2.957642	-2.282007
6	-0.697016	-2.973017	-2.312918	6	1.408968	-1.961763	-1.624028

⁶I_{C3N1'}

6	-9.168551	0.514621	2.261977	1	-1.295039	4.399145	-2.862472
6	-8.141031	0.624294	1.301085	1	-4.611172	2.088893	-1.380766
6	-7.276870	-0.503565	1.507524	6	1.337116	-1.239517	-1.396156
6	-7.785994	-1.235750	2.542584	6	2.730170	-1.122557	-1.200703
7	-8.934386	-0.629148	2.992439	6	2.936408	0.121292	-0.515367
6	-8.145098	1.699423	0.400710	6	1.712686	0.696658	-0.321802
6	-9.161418	2.630007	0.489875	7	0.735453	-0.116027	-0.859701
1	-9.507984	-0.966570	3.746831	6	3.584375	-2.126910	-1.677375
6	-10.176024	2.509080	1.460407	6	3.029244	-3.212688	-2.326103
6	-10.197594	1.455476	2.354328	6	1.636692	-3.312077	-2.515187
1	-10.957513	3.257740	1.504404	6	0.773792	-2.332825	-2.059330
1	-10.981522	1.362940	3.096610	1	1.233886	-4.173334	-3.034312
1	-7.412107	-2.143892	2.988320	1	-0.295757	-2.400480	-2.215592
1	-7.369159	1.787082	-0.351570	1	1.447982	1.619437	0.171502
1	-9.185659	3.466888	-0.197000	1	4.657332	-2.042084	-1.546237
6	-5.864042	-1.953814	0.053157	1	3.671293	-3.999204	-2.703087
6	-4.596770	-1.824069	-0.554173	6	4.694986	1.886578	-0.422035
6	-4.095951	-0.536676	-0.165330	6	5.982343	1.979671	0.150487
6	-5.034233	0.050852	0.634864	6	6.216277	0.732949	0.822509
7	-6.114605	-0.796926	0.768624	6	5.108105	-0.045678	0.645628
6	-4.106324	-2.859229	-1.362842	7	4.181411	0.640371	-0.114515
6	-4.885754	-3.986120	-1.537258	6	6.741769	3.143378	-0.035297
6	-6.150000	-4.097314	-0.925524	6	6.198147	4.175211	-0.775925
6	-6.658499	-3.088718	-0.128346	6	4.912898	4.064951	-1.342036

1	-6.739311	-4.991400	-1.088952	6	4.146498	2.925737	-1.178200
1	-7.636163	-3.165694	0.331312	1	4.518563	4.889535	-1.923580
1	-5.020701	1.005819	1.137787	1	4.890780	-1.037561	1.011432
1	-3.140726	-2.766720	-1.847312	1	7.737775	3.219950	0.386094
1	-4.526463	-4.796743	-2.159100	1	6.768901	5.082197	-0.933200
6	-2.636657	1.233269	-1.144740	1	3.164082	2.833483	-1.624697
6	-1.248725	1.371922	-1.362091	6	8.151565	-0.745394	1.347939
6	-0.641743	0.175652	-0.853160	6	9.222206	-0.689471	2.269755
6	-1.637721	-0.618896	-0.360726	6	9.068112	0.528231	3.015202
7	-2.853245	0.008475	-0.539984	6	7.947900	1.143620	2.540905
6	-0.756192	2.524851	-1.989365	7	7.379301	0.386549	1.532752
6	-1.654019	3.501136	-2.374982	6	10.160365	-1.732348	2.282969
6	-3.036529	3.345401	-2.152828	6	10.012681	-2.779009	1.392458
6	-3.547616	2.215902	-1.540943	6	8.944333	-2.807153	0.475762
1	-3.714571	4.127019	-2.473408	6	8.001737	-1.795747	0.439439
1	-1.583715	-1.583417	0.120732	1	8.860484	-3.636738	-0.216044
1	0.306233	2.636553	-2.175086	1	7.474210	2.066589	2.838814
1	9.704138	0.892843	3.805667	1	10.989326	-1.713162	2.981234
1	7.182965	-1.809004	-0.269622	1	10.729803	-3.591005	1.393567

$^2I_{C3C2'}$

6	3.234273	0.584835	-0.14017	1	1.142122	-2.01341	0.594998
6	2.018791	-0.1068	0.059736	1	3.331085	-3.14973	0.744329
6	0.955752	0.855487	-0.10692	6	-2.38894	-0.53752	-0.32047
6	1.554729	2.053062	-0.3911	6	-2.7088	0.673685	0.33724
7	2.920242	1.898813	-0.40444	6	-1.4762	1.382582	0.528621
6	2.058002	-1.46961	0.392778	6	-0.47591	0.613346	-0.00511
6	3.285266	-2.09885	0.486108	7	-1.02432	-0.55652	-0.50117
1	3.583538	2.626541	-0.60986	6	-4.04869	0.933228	0.661616
6	4.483247	-1.3942	0.262693	6	-5.01473	0.00525	0.318544
6	4.476441	-0.04641	-0.04565	6	-4.67374	-1.18833	-0.34426
1	5.428949	-1.91617	0.343515	6	-3.36002	-1.47704	-0.67014
1	5.399443	0.49926	-0.20299	1	-5.45344	-1.89481	-0.60217
1	1.098562	3.007101	-0.60395	1	-3.09582	-2.39825	-1.17643
1	-1.33497	2.324839	1.034168	1	-4.3205	1.850318	1.171534
1	-0.51432	-1.22441	-1.05666	1	-6.053	0.196297	0.561551

$^3I_{C3C2'}$

6	2.952502	-2.30479	0.541251	6	0.928708	3.04167	0.095027
6	2.792275	-0.99907	0.025736	6	-0.41071	2.604591	0.006313
6	1.515854	-0.51684	0.498313	6	-0.39394	1.167608	0.110957
6	0.972249	-1.52329	1.254792	6	0.923336	0.792158	0.265788
7	1.825774	-2.59642	1.277976	7	1.71852	1.920857	0.229884
6	3.791789	-0.46907	-0.80551	6	-1.42684	3.550901	-0.18404
6	4.913256	-1.23248	-1.071	6	-1.08525	4.889612	-0.25133

1	1.657516	-3.45644	1.772626	6	0.254129	5.305839	-0.14017
6	5.059681	-2.52409	-0.53114	6	1.278877	4.390599	0.026827
6	4.082684	-3.08001	0.273909	1	0.488594	6.362112	-0.19322
1	5.950683	-3.09655	-0.75821	1	2.31216	4.709265	0.099296
1	4.18897	-4.07957	0.678759	1	-2.45793	3.23177	-0.28173
1	0.02969	-1.54338	1.780946	1	-1.85913	5.633711	-0.39538
1	3.676633	0.512932	-1.25047	1	2.697311	1.919438	0.469232
1	5.69135	-0.83676	-1.71212	6	-2.72539	-1.5478	-0.5365
6	-3.15289	-2.77058	-1.05775	6	-3.56577	-0.72571	0.25275
1	-4.81281	-4.11053	-1.16363	6	-2.79841	0.432639	0.609278
1	-2.49699	-3.38351	-1.66521	6	-1.55378	0.287985	0.049478
1	-5.5357	-0.54882	1.127564	7	-1.51538	-0.9058	-0.64702
1	-6.30693	-2.71311	0.215239	6	-4.87223	-1.15832	0.524754
1	-3.10897	1.257968	1.230577	6	-5.29966	-2.36974	0.012504
1	-0.7129	-1.23079	-1.16228	6	-4.44779	-3.16817	-0.77321

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6	3.219152	-1.46586	-2.02377	1	-5.29474	2.674206	-3.71118
6	3.188597	-0.28528	-1.2489	1	-3.20632	3.739664	-2.90578
6	1.878356	-0.21956	-0.64073	1	-4.47331	-0.87428	-1.43629
6	1.191218	-1.32884	-1.06568	1	-5.92129	0.405282	-2.97263
7	1.989476	-2.07072	-1.89465	1	-0.95762	3.195371	-1.26444
6	4.315027	0.552551	-1.24755	6	-1.14032	-2.47789	1.819549
6	5.428278	0.179064	-1.97809	6	-1.88259	-3.20402	0.857614
1	1.71997	-2.94549	-2.31299	6	-2.31353	-2.26017	-0.13265
6	5.442944	-1.01343	-2.72426	6	-1.83953	-1.02479	0.24307
6	4.339633	-1.84625	-2.76415	7	-1.13552	-1.16153	1.423809
1	6.330465	-1.27836	-3.28575	6	-2.03708	-4.58875	1.026328
1	4.342932	-2.75684	-3.35163	6	-1.46153	-5.19909	2.125509
1	0.192944	-1.66157	-0.82607	6	-0.73003	-4.4555	3.070692
1	4.307211	1.490582	-0.70387	6	-0.55984	-3.08921	2.932433
1	6.302627	0.818329	-1.98599	1	-0.29328	-4.96233	3.92273
6	1.694837	2.303786	1.956204	1	0.001922	-2.51491	3.659791
6	0.366471	2.413211	1.492839	1	-2.60295	-5.16832	0.305829
6	0.208043	1.455572	0.425421	1	-1.57516	-6.26711	2.267246
6	1.42054	0.811784	0.276331	1	-2.86981	-2.47078	-1.03191
7	2.308466	1.33392	1.196507	1	-0.67972	-0.3977	1.899732
6	-0.49988	3.334831	2.098105	6	-2.65918	2.000844	-1.7348
6	-0.01936	4.113637	3.135466	6	-2.98111	0.68876	-1.32296
6	1.308894	3.989715	3.583337	6	-1.92525	0.255086	-0.44016
6	2.182967	3.085779	3.003984	6	-1.01957	1.292496	-0.35515
1	1.65388	4.612659	4.399553	7	-1.47703	2.343747	-1.12303
1	3.204994	2.989634	3.35119	6	-4.18016	0.113899	-1.76841
1	-1.52623	3.424198	1.758786	6	-4.99224	0.838026	-2.6221

	1	-0.67432	4.829611	3.61673	6	-4.63844	2.134236	-3.03944
	1	3.231571	0.958759	1.349201	6	-3.4739	2.735619	-2.5982
$^5I_{C3C2'}$								
	6	-0.76758	1.493626	2.331444	6	-0.91898	1.167588	-1.17051
	6	0.20762	0.487774	2.160821	6	0.239126	0.42213	-1.29327
	6	1.348455	1.113386	1.541041	7	1.257747	1.251254	-1.71528
	6	1.024793	2.435117	1.365348	6	-1.26579	3.746483	-1.44851
	7	-0.23456	2.669227	1.849847	6	-0.58719	4.91775	-1.74222
	6	-0.06773	-0.81812	2.592473	6	0.775563	4.901648	-2.09311
	6	-1.29601	-1.07713	3.176294	6	1.488124	3.715149	-2.13897
	1	-0.74888	3.521967	1.696756	1	1.275653	5.833133	-2.32962
	6	-2.25817	-0.05937	3.332801	1	2.540655	3.699264	-2.39794
	6	-2.01094	1.234088	2.913201	1	-2.31306	3.769886	-1.17137
	1	-3.21869	-0.29961	3.772012	1	-1.11289	5.864514	-1.70813
	1	-2.75814	2.011525	3.018655	1	2.208427	0.940978	-1.8435
	1	1.580989	3.22207	0.877548	6	-3.72746	-0.60625	0.294041
	1	0.671757	-1.60227	2.469131	6	-4.44909	0.362517	-0.44499
	1	-1.52634	-2.07929	3.51846	6	-3.47759	1.184515	-1.10387
	6	4.786206	0.08135	0.925363	6	-2.23426	0.70679	-0.75437
	6	4.125994	-0.94178	0.208499	7	-2.39349	-0.37311	0.085866
	6	2.710195	-0.69175	0.330449	6	-5.85207	0.335957	-0.4063
	6	2.564809	0.442473	1.103883	6	-6.48466	-0.62926	0.355479
	7	3.814877	0.912065	1.440579	6	-5.74581	-1.58188	1.083754
	6	4.891576	-1.90255	-0.46895	6	-4.36214	-1.58499	1.06205
	6	6.270748	-1.83693	-0.384	1	-6.27157	-2.32874	1.666756
	6	6.906906	-0.82446	0.356823	1	-3.78732	-2.32096	1.612334
	6	6.176822	0.150703	1.013887	1	-6.42956	1.062476	-0.96683
	1	7.988626	-0.80275	0.406864	1	-7.5671	-0.65941	0.392729
	1	6.667058	0.939637	1.572085	1	-3.66806	1.988404	-1.79693
	1	4.410075	-2.67473	-1.05887	1	-1.63532	-0.8489	0.555309
	1	6.874861	-2.57299	-0.90019	6	-1.13823	-4.73349	-1.86906
	1	3.965403	1.663263	2.095001	6	0.043336	-4.57634	-1.16717
	6	0.488095	-3.27111	-0.94768	1	-1.51749	-5.73129	-2.05382
	6	-0.22295	-2.14409	-1.41185	1	0.601192	-5.43108	-0.8029
	6	0.525019	-0.97962	-1.00666	1	-1.9747	-1.47846	-2.49393
	6	1.635798	-1.43197	-0.31966	1	-2.77904	-3.78464	-2.8944
	7	1.616926	-2.81038	-0.30319	1	2.272609	-3.37311	0.215285
	6	-1.41226	-2.33223	-2.13195	6	0.802809	2.539827	-1.82549
	6	-1.85732	-3.62242	-2.34941	6	-0.57238	2.528153	-1.49553
$^6I_{C3C2'}$								
	6	-0.72829	0.267245	3.106643	6	1.949795	-2.52521	0.878221
	6	-1.87166	0.543224	2.325063	6	1.907822	-3.88972	1.106303
	6	-2.3905	-0.72545	1.881561	6	0.836039	-4.67526	0.640397

6	-1.56107	-1.68975	2.395656	6	-0.21986	-4.10669	-0.051
7	-0.57379	-1.10093	3.139958	1	0.841128	-5.74343	0.821479
6	-2.27631	1.873792	2.142082	1	-1.04887	-4.70635	-0.40939
6	-1.53518	2.879202	2.739614	1	2.788833	-1.93214	1.224041
1	0.236896	-1.58855	3.487017	1	2.722761	-4.36808	1.636021
6	-0.39491	2.583166	3.513134	1	-2.00344	-2.16587	-1.21073
6	0.023905	1.279907	3.706741	6	1.719009	2.772655	0.706299
1	0.173405	3.393754	3.952771	6	2.973281	2.202718	0.388276
1	0.906754	1.054779	4.293011	6	2.724304	0.835371	0.008877
1	-1.56953	-2.759	2.244112	6	1.36028	0.629631	0.119427
1	-3.15169	2.101647	1.543363	7	0.77024	1.799534	0.53438
1	-1.83398	3.913025	2.611811	6	4.12082	3.009491	0.438071
6	-5.50118	-1.78541	0.313278	6	3.991813	4.331261	0.825336
6	-5.06022	-0.88334	-0.68059	6	2.735047	4.874172	1.152977
6	-3.79716	-0.34959	-0.2313	6	1.584174	4.108303	1.091063
6	-3.52675	-0.9273	0.992667	1	2.666775	5.915222	1.445273
7	-4.5434	-1.80287	1.303877	1	0.610743	4.526605	1.317577
6	-5.83169	-0.71548	-1.84023	1	5.088677	2.610511	0.154606
6	-7.0194	-1.41476	-1.9572	1	4.868808	4.966053	0.865289
6	-7.45238	-2.28877	-0.94345	1	-0.21662	1.899072	0.732292
6	-6.69887	-2.49217	0.19942	6	5.684269	-1.22465	-0.39945
1	-8.38908	-2.81906	-1.06373	6	4.916267	-1.74947	-1.46709
1	-7.02464	-3.17701	0.973461	6	3.679517	-1.02483	-1.48954
1	-5.4954	-0.05939	-2.63555	6	3.717101	-0.11743	-0.46415
1	-7.62667	-1.29448	-2.84595	7	4.935581	-0.23104	0.18817
1	-4.62635	-2.25873	2.198625	6	5.456015	-2.78878	-2.2395
6	-2.40111	2.388304	-2.17567	6	6.71651	-3.26911	-1.93435
6	-1.20794	1.666163	-1.96101	6	7.461237	-2.73162	-0.86822
6	-1.55881	0.494805	-1.19606	6	6.958271	-1.70338	-0.08946
6	-2.92131	0.552016	-0.97079	1	8.446205	-3.12862	-0.65372
7	-3.42435	1.682834	-1.57772	1	7.53261	-1.28685	0.730135
6	-0.00553	2.157208	-2.49214	1	4.888899	-3.20816	-3.06253
6	-0.02881	3.346342	-3.19584	1	7.142123	-4.07248	-2.52363
6	-1.22869	4.056674	-3.38978	1	2.850416	-1.16165	-2.16624
6	-2.42993	3.588258	-2.88885	1	5.18375	0.290855	1.013019
1	-1.21087	4.987492	-3.94369	6	-0.18016	-2.72658	-0.26208
1	-3.35559	4.130202	-3.0436	6	0.892743	-1.92152	0.18064
1	0.92415	1.61897	-2.34091	6	0.563233	-0.55896	-0.15707
1	0.89296	3.743563	-3.60261	6	-0.68536	-0.58558	-0.75249
1	-4.3799	1.989424	-1.4869	7	-1.1048	-1.89412	-0.84314

²I_{C6N1'}

6	3.066402	-0.64657	0.335033	6	-2.00346	-0.07184	-0.0205
6	2.74458	0.512521	-0.4076	6	-3.13748	0.764431	0.102286

6	3.963899	0.979348	-1.00405	6	-2.65875	2.0653	0.475938
6	4.948696	0.118806	-0.61503	6	-1.30129	1.975705	0.564366
7	4.416847	-0.8627	0.190932	7	-0.887	0.689606	0.272568
6	1.412772	0.949646	-0.44505	6	-4.40831	0.229247	-0.15551
6	0.461787	0.244401	0.268451	6	-4.51417	-1.09622	-0.53166
1	4.9353	-1.61618	0.609157	6	-3.36987	-1.90505	-0.6679
6	0.803581	-0.90195	1.016101	6	-2.10316	-1.4084	-0.41902
6	2.103709	-1.36424	1.049189	1	-3.48283	-2.93674	-0.97885
1	0.026896	-1.40662	1.57775	1	-1.2218	-2.02667	-0.53808
1	2.364981	-2.24487	1.623917	1	-0.56729	2.717336	0.839558
1	6.001595	0.12245	-0.84817	1	-5.29182	0.850759	-0.06504
1	1.119536	1.814664	-1.02865	1	-5.48988	-1.52152	-0.73342
1	4.091074	1.840684	-1.63929	1	-3.2483	2.947568	0.666286

³I_{C6N1'}

6	-5.24791	-1.31341	-0.03539	6	-0.59817	0.796628	-0.25359
6	-5.26663	0.004006	0.478235	6	0.219735	1.891604	-0.61764
6	-6.54147	0.18885	1.110693	6	-0.64484	2.893571	-1.16984
6	-7.2289	-0.9802	0.962461	6	-1.91136	2.388631	-1.12317
7	-6.45725	-1.8894	0.274084	7	-1.90154	1.120581	-0.57684
6	-4.13518	0.81522	0.312835	6	1.602221	1.813545	-0.39921
6	-3.04758	0.30474	-0.37031	6	2.117005	0.678586	0.199252
1	-6.73598	-2.8258	0.035119	6	1.282704	-0.38991	0.587504
6	-3.05112	-1.00683	-0.88859	6	-0.07864	-0.34685	0.360098
6	-4.14501	-1.83136	-0.71855	1	1.728453	-1.24138	1.087332
1	-2.18332	-1.35155	-1.43776	1	-0.72214	-1.16092	0.670117
1	-4.1482	-2.83886	-1.11715	1	-2.84549	2.812925	-1.45757
1	-8.21956	-1.24639	1.295119	1	2.265603	2.617598	-0.69658
1	-4.09727	1.819492	0.718876	1	-0.36041	3.856302	-1.56245
1	-6.89864	1.074364	1.610585	6	4.350274	-0.44602	0.098674
6	5.135749	-2.47838	-0.85	6	5.651827	-0.12225	0.548649
1	3.773627	2.436154	1.491073	6	5.564848	1.15837	1.190945
1	7.706096	-0.79212	0.634121	6	4.26146	1.551018	1.112896
1	7.236867	-2.88605	-0.59502	7	3.511088	0.591524	0.460154
1	6.364559	1.707903	1.660801	6	6.701227	-1.01825	0.296118
6	4.079113	-1.6172	-0.61525	6	6.435132	-2.18586	-0.39348
1	3.082104	-1.83528	-0.978	1	4.960646	-3.39501	-1.40047

⁴I_{C6N1'}

6	6.84277	2.355591	-0.12456	6	-1.97431	-1.50045	0.297107
6	7.299722	1.104843	0.351858	6	-3.09402	-2.21899	0.777712
6	8.594202	1.324595	0.930757	6	-2.5907	-3.40726	1.402646
6	8.869374	2.653294	0.789242	6	-1.23199	-3.36813	1.283221
7	7.820292	3.280581	0.155383	7	-0.84183	-2.22105	0.621966
6	6.476857	-0.02084	0.206675	6	-4.37856	-1.69267	0.582061

6	5.254836	0.128396	-0.42148	6	-4.51032	-0.50171	-0.10745
1	7.777916	4.260471	-0.06773	6	-3.38569	0.184632	-0.60995
6	4.820682	1.380224	-0.90406	1	-0.47957	-4.05639	1.636236
6	5.604017	2.506648	-0.75224	1	-5.25804	-2.1965	0.966387
1	3.865629	1.439914	-1.41184	1	-3.16246	-4.18075	1.889177
1	5.271025	3.46861	-1.12324	6	-2.10884	-0.30095	-0.40822
1	9.738741	3.21507	1.09182	1	-1.2449	0.218266	-0.80427
1	6.776573	-0.9909	0.586198	1	-3.54322	1.094616	-1.17625
1	9.234773	0.590939	1.392267	6	-6.22552	1.320003	-0.06138
6	3.093163	-1.11413	-0.23073	6	-7.58078	1.425273	-0.45371
6	2.647043	-2.40637	-0.59514	6	-7.96304	0.146276	-0.98095
6	3.759152	-3.0765	-1.20305	6	-6.86633	-0.6595	-0.89467
6	4.802841	-2.19799	-1.18715	7	-5.80502	0.034198	-0.34557
7	4.41703	-1.00583	-0.60753	6	-8.25207	2.641872	-0.26101
6	1.320049	-2.77067	-0.32839	6	-7.57329	3.698609	0.315427
6	0.50031	-1.86301	0.315669	6	-6.23026	3.56535	0.716884
6	0.970415	-0.59195	0.703997	1	-6.7252	-1.68423	-1.20204
6	2.266198	-0.20107	0.429868	1	-9.2898	2.746092	-0.55669
1	0.300471	0.06878	1.240889	1	-8.08024	4.643542	0.469723
1	2.633688	0.769766	0.738575	1	-8.9237	-0.13238	-1.38319
1	5.808415	-2.30107	-1.56485	6	-5.53949	2.380424	0.538575
1	0.931294	-3.73841	-0.62404	1	-4.51052	2.273052	0.859353
1	3.776068	-4.07412	-1.61083	1	-5.72879	4.407268	1.179082

⁵I_{C6N1'}

6	7.697973	3.665366	-0.05277	1	-3.83355	-4.5368	-1.31946
6	8.521892	2.622703	0.431367	1	-7.69781	-1.14938	-0.73776
6	9.668297	3.240239	1.034099	1	-6.4146	-3.77934	-1.52563
6	9.507394	4.588149	0.898389	6	-4.04788	-0.3194	0.441193
7	8.324154	4.851957	0.245642	1	-3.04596	-0.09143	0.783297
6	8.103607	1.294347	0.27041	1	-4.90822	1.525652	1.112892
6	6.908747	1.050261	-0.37977	6	-7.40539	2.551328	0.011961
1	7.975324	5.768485	0.021805	6	-8.63333	3.130865	0.409591
6	6.106225	2.101074	-0.86962	6	-9.39688	2.095159	1.045295
6	6.486659	3.417529	-0.70281	6	-8.63271	0.966107	1.013605
1	5.190754	1.856112	-1.39445	7	-7.42352	1.223955	0.397003
1	5.870779	4.225516	-1.07927	6	-8.87075	4.483678	0.12423
1	10.14654	5.395998	1.217486	6	-7.9028	5.208136	-0.54515
1	8.690477	0.468097	0.654842	6	-6.69589	4.605779	-0.94907
1	10.5014	2.746409	1.506979	1	-8.82695	-0.02145	1.402821
6	5.257528	-0.82052	-0.21709	1	-9.80336	4.949442	0.421696
6	5.254361	-2.18672	-0.58564	1	-8.07408	6.253666	-0.77154
6	6.528531	-2.4617	-1.18209	1	-10.3795	2.18292	1.480133
6	7.23399	-1.29416	-1.15549	6	-6.43023	3.27509	-0.68122

7	6.479649	-0.29124	-0.58025	1	-5.96175	5.195595	-1.48488
6	4.112989	-2.9593	-0.33081	1	-5.50783	2.807485	-1.00327
6	3.039445	-2.36498	0.305367	6	-1.285	-1.69477	-0.68741
6	3.071018	-1.01115	0.696794	1	2.805288	-4.75018	1.63647
6	4.174627	-0.22346	0.434565	1	-2.30798	-4.54705	0.888887
1	2.219078	-0.60241	1.226746	1	0.305007	-5.73907	1.857366
1	4.207474	0.813378	0.745593	6	0.077078	-1.73889	-0.4646
1	8.223187	-1.06734	-1.52227	1	0.732383	-0.9695	-0.85374
1	4.05895	-4.00015	-0.62876	1	-1.72041	-0.88815	-1.26489
1	6.869653	-3.3996	-1.58925	6	-4.34568	-1.54197	-0.16774
6	0.582129	-2.8264	0.253798	6	-5.65796	-1.87872	-0.57513
6	-0.25087	-3.86757	0.727757	6	-5.60068	-3.20763	-1.11021
6	0.601435	-4.82417	1.370641	6	-4.30178	-3.61438	-1.01224
6	1.875309	-4.34572	1.267643	7	-3.52891	-2.6191	-0.44933
7	1.881417	-3.13787	0.600012	6	-6.68694	-0.94171	-0.40597
6	-1.63342	-3.78736	0.510835	6	-6.38978	0.270988	0.187449
6	-2.13236	-2.70675	-0.19192	6	-5.08289	0.577153	0.619506

⁶I_{C6N1'}

6	-7.81558	5.085932	-0.42185	6	1.913879	-3.67397	0.145885
6	-8.96302	4.315502	-0.72244	6	3.082233	-4.35598	0.561314
6	-9.89374	5.188604	-1.37853	6	2.653088	-5.50693	1.300178
6	-9.3011	6.415415	-1.44928	6	1.288547	-5.4819	1.306724
7	-8.05046	6.361653	-0.87607	7	0.825686	-4.37928	0.618202
6	-8.98025	2.956968	-0.37677	6	4.336245	-3.83403	0.215065
6	-7.88113	2.424127	0.269674	6	4.387017	-2.68574	-0.55266
1	-7.41168	7.135077	-0.80078	6	3.213358	-2.03701	-0.98757
6	-6.75083	3.209744	0.575093	1	0.579964	-6.15192	1.768759
6	-6.70208	4.544012	0.224445	1	5.254124	-4.30794	0.54376
1	-5.92516	2.750884	1.105435	1	3.276364	-6.24678	1.775538
1	-5.83416	5.14852	0.459258	6	1.966935	-2.51804	-0.63832
1	-9.67066	7.338452	-1.86686	1	1.063038	-2.02929	-0.98018
1	-9.82727	2.324737	-0.61711	1	3.306161	-1.16161	-1.6191
1	-10.8737	4.936214	-1.74936	6	6.080571	-0.85597	-0.75262
6	-6.93032	0.112764	0.34548	6	7.390148	-0.75784	-1.27919
6	-7.33389	-1.11678	0.918145	6	7.734856	-2.05451	-1.78477
6	-8.5806	-0.87832	1.584344	6	6.658622	-2.86245	-1.5585
6	-8.87782	0.440408	1.399305	7	5.648868	-2.15403	-0.93967
7	-7.88945	1.055078	0.657007	6	8.071765	0.463913	-1.19122
6	-6.51945	-2.2456	0.75401	6	7.432881	1.540233	-0.60415
6	-5.36325	-2.12454	0.00643	6	6.129208	1.424264	-0.07958
6	-4.99241	-0.90072	-0.58661	1	6.500219	-3.90081	-1.80593
6	-5.76579	0.230905	-0.41864	1	9.086719	0.570406	-1.55676
1	-4.09667	-0.86738	-1.19513	1	8.656204	-2.34427	-2.26334

1	-5.49077	1.16959	-0.8835	6	5.445332	0.225847	-0.13587
1	-9.71254	1.024846	1.754489	1	5.666758	2.299157	0.361158
1	-6.77661	-3.19668	1.206132	1	4.448805	0.131176	0.277393
1	-9.1704	-1.58982	2.139031	6	8.272127	3.57125	0.594339
6	-3.18197	-3.34475	0.065626	6	8.976344	4.736787	0.210475
6	-2.75594	-4.65187	-0.27034	6	9.220418	4.631253	-1.19995
6	-3.91034	-5.35877	-0.74184	6	8.673996	3.449955	-1.60713
6	-4.95739	-4.48576	-0.67798	7	8.09216	2.797859	-0.53715
7	-4.53425	-3.26364	-0.19676	6	9.296027	5.69105	1.187842
6	-1.40646	-4.99295	-0.10434	6	8.922387	5.460343	2.498131
6	-0.54366	-4.04715	0.416543	6	8.239581	4.283568	2.861199
6	-0.99076	-2.7604	0.779258	1	8.620322	3.005268	-2.58891
1	-5.99152	-4.61368	-0.95856	1	9.833282	6.592583	0.916184
1	-1.03433	-5.97216	-0.38326	1	9.163687	6.189125	3.262584
1	-3.95348	-6.37633	-1.09471	1	9.725407	5.346085	-1.8295
6	-2.30989	-2.39279	0.601398	6	7.907892	3.324352	1.921601
1	-2.66009	-1.40929	0.889337	1	7.972815	4.12358	3.89905
1	-0.28299	-2.06816	1.219268	1	7.395435	2.412384	2.202559
Isoindole (II)							
6	-0.2516	0.720765	-0.00012	1	-2.02422	2.110268	0.000602
6	-0.25157	-0.72064	-7.4E-05	6	2.147119	0.716248	-3.7E-05
6	-1.57871	-1.12982	-0.00016	6	0.984054	1.428395	-7.5E-05
7	-2.34213	-0.00006	0.000064	1	3.097436	1.236904	-7.5E-05
6	-1.57882	1.129839	0.000151	1	0.994286	2.512376	-0.00018
6	0.984013	-1.42838	0.000193	1	-3.3496	-6.9E-05	-0.00046
6	2.147108	-0.71631	0.000096	1	-2.02399	-2.11035	-2.8E-05
1	3.097442	-1.23694	-0.00025	1	0.994013	-2.51236	0.000048
²II							
6	3.523806	0.598992	0.190813	6	-2.70907	-0.69559	0.290052
6	2.947051	-0.65435	-0.22514	6	-2.80318	0.614821	-0.30183
6	3.998756	-1.51049	-0.52137	6	-1.5083	1.099795	-0.42397
7	5.150043	-0.81545	-0.29383	7	-0.66122	0.140139	0.060864
6	4.903446	0.453883	0.134425	6	-1.36073	-0.95194	0.49763
6	1.5345	-0.80456	-0.28196	6	-4.07845	1.149096	-0.63905
6	0.758156	0.254841	0.085743	6	-5.19142	0.404174	-0.37778
1	5.703251	1.138302	0.361233	1	-0.85081	-1.78201	0.957146
6	1.323584	1.501351	0.51233	6	-5.09883	-0.89222	0.223657
6	2.673135	1.677828	0.56047	6	-3.89334	-1.43913	0.554716
1	0.649652	2.291815	0.818845	1	-6.01153	-1.44398	0.415588
1	3.09258	2.620909	0.890566	1	-3.83335	-2.42182	1.008533
1	6.073496	-1.19647	-0.42667	1	-1.12285	2.010584	-0.85105
1	4.014496	-2.53014	-0.86694	1	-4.15859	2.130229	-1.09313
1	1.078456	-1.72383	-0.62962	1	-6.17133	0.794533	-0.62614

3//

6	6.345194	-0.95954	0.02093	6	-1.90914	1.821867	-0.80293
6	5.917196	0.34802	0.449978	6	-0.60812	2.185595	-0.98336
6	7.044527	1.020001	0.901975	1	-2.71554	2.487419	-1.08532
7	8.098412	0.167886	0.751629	1	-0.3617	3.156718	-1.39643
6	7.716513	-1.02912	0.226008	1	1.459499	-1.68198	0.530436
6	4.544567	0.708753	0.371947	1	-1.5772	-1.32927	0.510507
6	3.667268	-0.20431	-0.1345	6	-5.77425	0.413353	0.443939
1	8.426785	-1.81724	0.04187	6	-5.54184	-0.90392	-0.09178
6	4.084994	-1.50269	-0.57456	6	-4.19357	-0.97921	-0.41423
6	5.391439	-1.87958	-0.49633	7	-3.6257	0.22457	-0.09763
1	3.33978	-2.16775	-0.99332	6	-4.558	1.08234	0.419782
1	5.701774	-2.86033	-0.83691	6	-6.62318	-1.82174	-0.20679
1	9.04767	0.39696	1.001164	6	-7.86229	-1.43159	0.211241
1	7.172423	2.00932	1.30721	1	-4.2735	2.062544	0.764357
1	4.192878	1.670633	0.725692	6	-8.09041	-0.12727	0.756392
6	0.419549	1.266116	-0.63746	6	-7.07943	0.781668	0.874998
6	0.071178	-0.03285	-0.12115	1	-9.09135	0.135345	1.078121
6	1.259633	-0.71107	0.109038	1	-3.60954	-1.75538	-0.87971
7	2.284365	0.12448	-0.24495	1	-6.45983	-2.81191	-0.61689
6	1.805094	1.321231	-0.69859	1	-8.69771	-2.11746	0.133625
6	-1.29276	-0.37741	0.077955	1	-7.26219	1.767379	1.287634
6	-2.24564	0.537622	-0.26417	1	2.477071	2.078831	-1.06548

4//

6	-9.27309	0.750036	0.486614	6	2.871044	-0.08337	-0.32794
6	-8.74953	-0.55255	0.812921	6	2.534977	1.24015	-0.78691
6	-9.79635	-1.29342	1.344002	6	1.160471	1.266558	-0.97984
7	-10.8946	-0.48556	1.336571	7	0.676173	0.030395	-0.65702
6	-10.6184	0.747797	0.829296	6	1.686514	-0.80346	-0.26153
6	-7.37794	-0.84602	0.583598	6	3.562784	2.205559	-0.96665
6	-6.59569	0.126554	0.034165	6	4.851012	1.860984	-0.68415
1	-11.3763	1.508803	0.751369	1	1.475979	-1.80591	0.071545
6	-7.10923	1.42093	-0.30419	6	5.172452	0.550387	-0.20349
6	-8.41603	1.733283	-0.08085	6	4.219106	-0.40881	-0.01972
1	-6.43842	2.136038	-0.76425	1	0.504046	2.03211	-1.35814
1	-8.80006	2.711451	-0.34514	1	3.327996	3.197397	-1.33492
1	-11.8035	-0.76796	1.668435	1	5.660427	2.563619	-0.83966
1	-9.8409	-2.30282	1.716078	1	4.489442	-1.38193	0.372804
1	-6.95219	-1.80406	0.857421	6	8.616265	0.456754	0.845792
6	-3.35587	-1.16938	-0.85431	6	8.479327	-0.82123	0.194253
6	-3.01214	0.119983	-0.31097	6	7.17248	-0.90366	-0.26745
6	-4.19899	0.73172	0.067138	7	6.538939	0.258625	0.077414
7	-5.21764	-0.1333	-0.22633	6	7.387927	1.0965	0.747687

6	-4.73723	-1.28502	-0.78296	6	9.594906	-1.70163	0.122578
6	-1.65088	0.517207	-0.22862	6	10.7737	-1.31522	0.691551
6	-0.70092	-0.33827	-0.7061	1	7.03999	2.040777	1.132092
1	-5.41067	-2.05555	-1.11889	6	10.90563	-0.05133	1.351417
6	-1.03427	-1.6112	-1.27143	6	9.859923	0.821805	1.43298
6	-2.33109	-2.02486	-1.34265	1	11.86078	0.209465	1.79194
1	-0.23309	-2.22636	-1.66219	1	6.661277	-1.65606	-0.84431
1	-2.57733	-2.98686	-1.7765	1	9.504263	-2.66121	-0.37376
1	-4.39638	1.672601	0.552933	1	11.63371	-1.9732	0.648904
1	-1.36412	1.460612	0.220751	1	9.96987	1.777191	1.933463

5//

6	6.333116	1.311812	-0.43556	6	-11.4609	-0.54153	-1.10972
6	5.895807	0.020426	0.030107	6	-11.3085	-1.20336	0.161138
6	7.014029	-0.80098	0.061272	6	-10.0332	-0.90638	0.623171
7	8.082351	-0.05455	-0.35479	7	-9.43283	-0.10503	-0.30884
6	7.699635	1.220808	-0.66099	6	-10.273	0.131301	-1.36245
6	4.527647	-0.19687	0.343136	6	-12.3842	-1.96758	0.693696
6	3.660648	0.846651	0.196133	6	-13.5391	-2.06646	-0.02677
1	8.410949	1.929634	-1.0504	1	-9.94449	0.70985	-2.20969
6	4.084508	2.1332	-0.26822	6	-13.6856	-1.41952	-1.29567
6	5.390046	2.364677	-0.58464	6	-12.6783	-0.6728	-1.83446
1	3.347952	2.924213	-0.33762	1	-14.6207	-1.52995	-1.83222
1	5.706633	3.34257	-0.92782	1	-9.52757	-1.15233	1.541863
1	7.144162	-1.8214	0.380643	1	-12.2823	-2.46229	1.652992
1	4.169362	-1.16744	0.66536	1	-14.3684	-2.64586	0.361791
6	0.430121	0.047292	1.572969	1	-12.799	-0.18529	-2.79526
6	0.065099	0.750816	0.369815	6	11.77067	-0.28737	-0.08724
6	1.245844	1.122649	-0.25795	6	11.99172	-1.58944	-0.66431
7	2.280642	0.673237	0.515477	6	13.35962	-1.82433	-0.63195
6	1.817265	0.023345	1.624098	7	13.93518	-0.72777	-0.06549
6	-1.30405	0.917387	0.031192	6	13.01228	0.215848	0.275942
6	-2.24394	0.424658	0.8894	6	10.8854	-2.35114	-1.13247
1	2.501123	-0.35317	2.366149	6	9.631419	-1.83053	-1.02355
6	-1.89182	-0.25464	2.099681	1	13.29963	1.144883	0.738144
6	-0.5848	-0.44586	2.437026	6	9.421331	-0.53978	-0.43781
1	-2.68854	-0.59144	2.751501	6	10.44993	0.224592	0.028336
1	-0.32434	-0.95581	3.357072	1	10.25498	1.183255	0.494245
1	1.43272	1.620355	-1.19471	1	14.92671	-0.62552	0.084323
1	-1.60288	1.400601	-0.89156	1	13.94771	-2.66421	-0.96097
6	-5.78938	0.135018	0.32754	1	11.03891	-3.3247	-1.58272
6	-5.54806	1.503091	-0.05396	1	8.771573	-2.37111	-1.3997
6	-4.19277	1.742635	0.128221	6	-7.09629	-0.41228	0.224786
7	-3.63021	0.588171	0.5942	1	-3.60026	2.634674	0.013035

6	-4.57053	-0.3971	0.724579	1	-6.46732	3.350461	-0.76198
6	-6.62975	2.312593	-0.4956	1	-8.7282	2.368148	-0.86699
6	-7.87811	1.769292	-0.56412	1	-7.2932	-1.45175	0.45909
1	-4.29056	-1.38834	1.039579	6	-8.1039	0.400411	-0.20783

6//

6	-9.19399	-0.51595	-1.25223	6	2.869894	-1.16016	0.456114
6	-8.73543	0.126281	-0.04673	6	2.597687	-1.93199	-0.72974
6	-9.81228	0.829477	0.474623	6	1.222826	-2.1165	-0.78692
7	-10.8771	0.625829	-0.35959	7	0.678852	-1.49287	0.299741
6	-10.5317	-0.17991	-1.40757	6	1.649005	-0.90875	1.066697
6	-7.38824	-0.03057	0.374443	6	3.672153	-2.35282	-1.55923
6	-6.56217	-0.80408	-0.38803	6	4.945678	-2.00181	-1.22203
1	-11.2416	-0.40406	-2.18594	1	1.39022	-0.33616	1.941534
6	-7.00718	-1.44529	-1.58853	6	5.203138	-1.2133	-0.05499
6	-8.29262	-1.30284	-2.01929	6	4.203891	-0.79002	0.772724
1	-6.30537	-2.06611	-2.13176	1	0.601188	-2.66838	-1.47179
1	-8.626	-1.79671	-2.9244	1	3.483885	-2.95445	-2.44071
1	-9.91936	1.410795	1.375046	1	5.788615	-2.33227	-1.81645
1	-7.01169	0.467948	1.259842	1	4.428912	-0.16947	1.632118
6	-3.41651	-1.36585	1.273882	6	8.656513	-0.19192	-0.02274
6	-2.99103	-1.15381	-0.08631	6	8.439529	-0.51712	1.36388
6	-4.13465	-0.92846	-0.83978	6	7.121971	-0.93909	1.480732
7	-5.20493	-0.99785	0.008845	7	6.558409	-0.87629	0.237927
6	-4.80081	-1.26093	1.28686	6	7.461649	-0.4299	-0.68763
6	-1.60887	-1.17957	-0.41101	6	9.506048	-0.38355	2.293919
6	-0.7179	-1.44133	0.589127	6	10.71514	0.067194	1.854318
1	-5.52287	-1.39517	2.074679	1	7.170769	-0.27912	-1.7137
6	-1.13173	-1.67782	1.939168	6	10.91405	0.412947	0.47864
6	-2.4511	-1.63785	2.280648	6	9.920166	0.296924	-0.44958
1	-0.37416	-1.91278	2.676712	1	6.561348	-1.3167	2.319291
1	-2.75918	-1.82307	3.302964	1	9.364443	-0.64799	3.335335
1	-4.27021	-0.68524	-1.88027	1	11.55612	0.150724	2.53169
1	-1.26103	-0.97566	-1.41685	1	10.09287	0.593986	-1.47724
6	14.06528	1.183917	-1.08749	6	-14.5596	0.965988	-0.12621
6	14.11429	2.017736	0.086724	6	-14.6684	2.346553	0.273084
6	12.93778	1.797933	0.790447	6	-16.0213	2.628995	0.404453
7	12.20168	0.883409	0.087917	7	-16.6946	1.484031	0.103959
6	12.85912	0.497199	-1.04773	6	-15.8502	0.463279	-0.2183
6	15.24271	2.854159	0.313916	6	-13.4912	3.12555	0.448437
6	16.2662	2.835211	-0.58877	6	-12.2774	2.545785	0.234664
1	12.44088	-0.25665	-1.69347	1	-16.2198	-0.51353	-0.4801
6	16.22391	1.996075	-1.74819	6	-12.1797	1.169326	-0.15133
6	15.15555	1.185482	-2.00172	6	-13.2794	0.382341	-0.32722

1	17.06272	2.012039	-2.43415	1	-13.1708	-0.66348	-0.58911
1	12.54912	2.242048	1.691662	1	-17.699	1.40058	0.118352
1	15.28438	3.491576	1.18988	1	-16.5385	3.532302	0.680153
1	17.1344	3.464561	-0.43209	1	-13.5593	4.168827	0.733145
1	15.13218	0.554582	-2.88308	1	-11.364	3.120232	0.327918
Azulene (Az)							
6	0.000000	0.000000	-2.491976	1	0.000000	2.101480	-2.591336
6	0.000000	1.262799	-1.903399	1	0.000000	2.653356	-0.318494
6	0.000000	1.590576	-0.549931	1	0.000000	-2.101480	-2.591336
6	0.000000	-1.262799	-1.903399	1	0.000000	-2.653356	-0.318494
6	0.000000	0.746254	0.551515	6	0.000000	1.147020	1.894282
6	0.000000	-1.590576	-0.549931	1	0.000000	2.171667	2.237453
6	0.000000	-0.746254	0.551515	6	0.000000	0.000000	2.697615
1	0.000000	0.000000	-3.578188	1	0.000000	0.000000	3.779496
1	0.000000	-2.171667	2.237453	6	0.000000	-1.147020	1.894282
²Az							
6	-0.831208	-0.000038	-0.000052	6	-6.061109	0.000029	0.000060
6	-1.454674	1.199567	-0.377488	1	-7.142977	0.000046	0.000087
6	-2.806225	1.507063	-0.472231	6	-5.256991	-1.095023	0.342826
6	-1.454687	-1.199624	0.377399	1	-5.598990	-2.073286	0.649056
6	-3.915376	0.709667	-0.221231	6	5.845833	0.000035	0.000061
6	-2.806245	-1.507088	0.472191	6	5.257013	1.202353	0.387333
6	-3.915384	-0.709661	0.221251	6	3.904900	1.517665	0.479534
1	-0.778692	1.999012	-0.660115	6	5.257053	-1.202309	-0.387240
1	-3.032314	2.520139	-0.797681	6	2.802719	0.713214	0.214612
1	-0.778717	-1.999084	0.660012	6	3.904966	-1.517653	-0.479506
1	-3.032347	-2.520164	0.797631	6	2.802742	-0.713225	-0.214631
6	-5.256976	1.095063	-0.342742	1	6.931944	0.000046	0.000082
1	-5.598968	2.073335	-0.648954	1	5.945491	1.999648	0.646003
6	1.464170	1.100432	0.321627	1	3.672692	2.531330	0.797662
1	1.123514	2.073152	0.647520	1	5.945568	-1.999581	-0.645881
6	0.646494	-0.000028	-0.000038	1	3.672792	-2.531319	-0.797653
6	1.464217	-1.100459	-0.321746	1	1.123599	-2.073172	-0.647697
³Az							
6	-4.190631	0.000033	-0.000050	6	-1.894977	1.061596	0.434439
6	-4.815356	1.235260	-0.235021	1	-2.234453	1.995367	0.860221
6	-6.166759	1.551381	-0.292619	6	-2.713853	0.000164	-0.000097
6	-4.815163	-1.235266	0.234983	6	-1.894859	-1.061278	-0.434762
6	-7.276253	0.730282	-0.136427	1	-2.234365	-1.995051	-0.860507
6	-6.166524	-1.551555	0.292792	6	9.202525	-0.000372	0.000347
6	-7.276138	-0.730591	0.136807	6	8.613897	1.239572	-0.242017
1	-4.140010	2.062566	-0.422898	6	7.262094	1.563739	-0.296017
1	-6.392936	2.595536	-0.497583	6	8.613705	-1.240081	0.242617

1	-4.139695	-2.062487	0.422785	6	6.159795	0.733423	-0.128029
1	-6.392537	-2.595744	0.497760	6	7.261702	-1.564023	0.296431
6	-8.617903	1.127394	-0.211827	6	6.159655	-0.733579	0.128427
1	-8.959907	2.134876	-0.401061	1	10.288615	-0.000416	0.000389
6	-9.422090	-0.000292	0.000373	1	9.302561	2.061652	-0.404698
1	-10.503965	-0.000351	0.000468	1	7.029958	2.607901	-0.492044
6	-8.617736	-1.127870	0.212436	1	9.302097	-2.062374	0.405364
1	-8.959573	-2.135398	0.401730	1	7.029454	-2.608186	0.492341
6	2.527158	0.000290	-0.000207	6	4.821521	1.131187	-0.187917
6	1.902297	1.150169	0.509081	1	4.481756	2.135884	-0.396628
6	0.552405	1.448886	0.630040	6	4.003737	0.000002	0.000077
6	1.902354	-1.149451	-0.510184	6	4.821220	-1.131234	0.188099
6	-0.558046	0.684987	0.285523	1	4.481246	-2.135917	0.396529
6	0.552513	-1.448180	-0.631118	1	0.326123	2.421883	1.060261
6	-0.558032	-0.684516	-0.286094	1	2.577983	-1.911666	-0.882306
1	2.577916	1.912510	0.880970	1	0.326181	-2.421054	-1.061611

⁴Az

6	0.831067	0.000069	-0.000022	6	-12.560745	-0.000296	-0.000173
6	1.457598	1.202274	0.369161	6	-11.972287	1.202541	0.386438
6	2.807181	1.513329	0.451838	6	-10.620475	1.517988	0.478459
6	1.457520	-1.202167	-0.369420	6	-11.972066	-1.202993	-0.386696
6	3.918128	0.713857	0.200499	6	-9.518204	0.713004	0.213867
6	2.807043	-1.513273	-0.452190	6	-10.620148	-1.518232	-0.478583
6	3.918059	-0.713860	-0.200843	6	-9.518044	-0.713093	-0.213899
1	0.782511	2.003240	0.649120	1	-13.646820	-0.000393	-0.000233
1	3.033803	2.530837	0.762257	1	-12.660984	1.999763	0.644494
1	0.782379	-2.003058	-0.649447	1	-10.388258	2.531819	0.795888
1	3.033624	-2.530772	-0.762661	1	-12.660599	-2.000333	-0.644823
6	5.255075	1.106270	0.302233	1	-10.387759	-2.532031	-0.795998
1	5.594220	2.084762	0.612103	6	-8.179940	1.101258	0.320238
6	6.074126	-0.000074	-0.000150	1	-7.840564	2.074365	0.646241
6	5.254968	-1.106383	-0.302514	6	-7.362094	0.000108	0.000143
1	5.594089	-2.084881	-0.612399	6	-8.179702	-1.101107	-0.320231
6	-5.885672	0.000172	0.000245	1	-7.840167	-2.074152	-0.646243
6	-5.260551	1.204077	-0.364326	6	7.550749	-0.000110	-0.000128
6	-3.910964	1.515568	-0.446692	6	8.175951	1.198025	-0.381621
6	-5.260537	-1.203790	0.364882	6	9.527213	1.505002	-0.476242
6	-2.800417	0.714631	-0.198349	6	8.175926	-1.198142	0.381408
6	-3.911014	-1.515264	0.447196	6	10.637065	0.708663	-0.222716
6	-2.800438	-0.714352	0.198644	6	9.527267	-1.505105	0.476182
1	-5.936309	2.005933	-0.640244	6	10.637072	-0.708761	0.222839
1	-3.684295	2.534132	-0.753415	1	7.500504	1.996527	-0.667871
1	-5.936327	-2.005615	0.640804	1	9.753333	2.517189	-0.804546

1	-3.684304	-2.533807	0.753957	1	7.500507	-1.996679	0.667629
6	-1.463724	1.107563	-0.298999	1	9.753347	-2.517297	0.804504
1	-1.125620	2.087028	-0.606771	6	11.978699	1.094168	-0.345060
6	-0.644470	0.000121	-0.000002	1	12.320503	2.071823	-0.653583
6	-1.463781	-1.107363	0.298957	6	12.783036	-0.000048	0.000238
1	-1.125592	-2.086824	0.606654	6	11.978764	-1.094230	0.345432
1	13.864937	0.000039	0.000301	1	12.320453	-2.071903	0.654018

⁵Az

6	4.190498	-0.000136	0.000105	6	10.910396	0.000148	-0.000146
6	4.817193	-1.245090	-0.178500	6	11.535705	-1.128787	0.553400
6	6.166672	-1.564138	-0.218595	6	12.886971	-1.418626	0.691753
6	4.817058	1.244778	0.178682	6	11.535664	1.129051	-0.553716
6	7.277798	-0.735507	-0.093897	6	13.996830	-0.668218	0.324036
6	6.166618	1.563902	0.218632	6	12.886943	1.418987	-0.692036
6	7.277675	0.735366	0.093855	6	13.996830	0.668682	-0.324260
1	4.141786	-2.088356	-0.270216	1	10.860319	-1.876531	0.954050
1	6.393209	-2.619023	-0.356235	1	13.113048	-2.371695	1.165052
1	4.141649	2.088030	0.270496	1	10.860255	1.876741	-0.954433
1	6.393090	2.618802	0.356247	1	13.112957	2.372060	-1.165361
6	8.614701	-1.138918	-0.134691	6	15.338469	-1.031594	0.501677
1	8.953931	-2.152596	-0.295542	1	15.680190	-1.953598	0.949997
6	9.433755	0.000114	-0.000107	6	16.142854	0.000301	-0.000057
6	8.614651	1.138948	0.134615	6	15.338476	1.032134	-0.501838
1	8.953752	2.152670	0.295471	1	15.680099	1.954172	-0.950156
6	-2.527725	-0.000293	0.000168	1	17.224757	0.000288	-0.000015
6	-1.901188	0.929397	0.847406	6	-15.918816	0.000392	-0.000131
6	-0.551967	1.175532	1.054804	6	-15.330332	-1.134922	0.554040
6	-1.901201	-0.929974	-0.846946	6	-13.978452	-1.433777	0.690466
6	0.559228	0.559526	0.486113	6	-15.330114	1.135746	-0.554362
6	-0.551880	-1.176065	-1.054281	6	-12.876272	-0.674873	0.313662
6	0.559180	-0.559937	-0.485687	6	-13.978332	1.434390	-0.690771
1	-2.576341	1.534079	1.442531	6	-12.876159	0.675260	-0.313945
1	-0.325336	1.963260	1.769745	1	-17.004887	0.000486	-0.000142
1	-2.576285	-1.534740	-1.442061	1	-16.018935	-1.887281	0.923144
1	-0.325207	-1.963868	-1.769126	1	-13.746356	-2.391792	1.149692
6	1.895861	0.871622	0.745669	1	-16.018666	1.888163	-0.923443
1	2.233895	1.624143	1.444156	1	-13.746039	2.392359	-1.149987
6	2.715155	-0.000217	0.000130	6	-11.537966	-1.043928	0.474606
6	1.895916	-0.872009	-0.745327	1	-11.198800	-1.960483	0.936461
1	2.233910	-1.624533	-1.443832	6	-10.720318	-0.000014	-0.000051
6	-9.243956	-0.000053	-0.000029	6	-11.537910	1.044083	-0.474853
6	-8.618923	-1.243642	-0.189876	1	-11.198483	1.960542	-0.936709
6	-7.269418	-1.560972	-0.244590	1	-9.294740	2.076934	0.345844

6	-8.618845	1.243524	0.189897	1	-7.042717	2.610085	0.419003
6	-6.158827	-0.731195	-0.123691	6	-4.822179	-1.129436	-0.202172
6	-7.269340	1.560729	0.244668	1	-4.484097	-2.146624	-0.341541
6	-6.158804	0.730851	0.123777	6	-4.003064	-0.000250	0.000118
1	-9.294880	-2.077008	-0.345815	6	-4.822144	1.129020	0.202271
1	-7.042898	-2.610356	-0.418895	1	-4.483973	2.146179	0.341640

⁶Az

6	-7.550123	0.000302	0.000247	6	-14.270569	-0.000175	0.000037
6	-8.177273	1.203687	-0.364813	6	-14.896079	1.196284	0.386296
6	-9.526736	1.514892	-0.445912	6	-16.247384	1.502687	0.481976
6	-8.177127	-1.203151	0.365356	6	-14.895825	-1.196746	-0.386286
6	-10.637971	0.714565	-0.197540	6	-17.357235	0.707264	0.225390
6	-9.526552	-1.514507	0.446402	6	-16.247058	-1.503437	-0.482059
6	-10.637869	-0.714322	0.197937	6	-17.357098	-0.708264	-0.225501
1	-7.502341	2.005632	-0.642272	1	-14.220727	1.993710	0.675782
1	-9.753423	2.533582	-0.752512	1	-16.473625	2.513576	0.814261
1	-7.502107	-2.005004	0.642862	1	-14.220289	-1.994029	-0.675740
1	-9.753141	-2.533215	0.753019	1	-16.473059	-2.514365	-0.814391
6	-11.974982	1.107537	-0.297746	6	-18.698987	1.092195	0.349408
1	-12.314101	2.087226	-0.603845	1	-19.040754	2.068650	0.661736
6	-12.794026	-0.000048	0.000110	6	-19.503213	-0.000708	-0.000088
6	-11.974827	-1.107503	0.298046	6	-18.698765	-1.093453	-0.349567
1	-12.313830	-2.087237	0.604131	1	-19.040310	-2.069979	-0.661915
6	-0.831195	0.000379	-0.000089	1	-20.585109	-0.000803	-0.000103
6	-1.458152	1.204186	0.364383	6	12.603001	-0.000044	-0.000176
6	-2.807372	1.515226	0.446069	6	11.977899	1.204713	0.361995
6	-1.458196	-1.203493	-0.364525	6	10.628456	1.516325	0.443483
6	-3.918701	0.714419	0.198060	6	11.977806	-1.204777	-0.362482
6	-2.807363	-1.514534	-0.446049	6	9.517845	0.714752	0.196590
6	-3.918718	-0.713704	-0.197922	6	10.628404	-1.516302	-0.444098
1	-0.783004	2.006183	0.641107	6	9.517769	-0.714675	-0.197178
1	-3.034113	2.533891	0.752641	1	12.653694	2.007040	0.636396
1	-0.783044	-2.005461	-0.641312	1	10.401714	2.535506	0.748115
1	-3.034158	-2.533198	-0.752584	1	12.653593	-2.007124	-0.636849
6	-5.255403	1.107933	0.298522	1	10.401613	-2.535444	-0.748828
1	-5.593069	2.087581	0.606196	6	8.181195	1.108399	0.296058
6	-6.074885	0.000372	0.000200	1	7.843428	2.088553	0.601937
6	-5.255369	-1.107226	-0.298239	6	7.362022	0.000157	-0.000289
1	-5.593107	-2.086858	-0.605885	6	8.181149	-1.108198	-0.296650
6	5.886871	0.000188	-0.000284	1	7.843287	-2.088317	-0.602532
6	5.260167	1.202577	-0.369744	6	19.277735	-0.000559	0.000593
6	3.911000	1.513564	-0.452078	6	18.689353	1.201552	-0.388338
6	5.260114	-1.202176	0.369192	6	17.337580	1.516801	-0.481044

6	2.799754	0.713734	-0.200489	6	18.689079	-1.202577	0.389352
6	3.910933	-1.513054	0.451592	6	16.235270	0.712294	-0.214940
6	2.799737	-0.713124	0.200092	6	17.337215	-1.517597	0.481692
1	5.935301	2.003340	-0.650004	6	16.235129	-0.712890	0.215348
1	3.684275	2.531051	-0.762478	1	20.363813	-0.000629	0.000742
1	5.935206	-2.002986	0.649411	1	19.378081	1.998261	-0.647874
1	3.684135	-2.530528	0.761981	1	17.105401	2.530030	-0.800447
6	1.463138	1.107182	-0.301714	1	19.377608	-1.999403	0.649056
1	1.125404	2.085851	-0.612406	1	17.104775	-2.530798	0.800996
6	0.643812	0.000356	-0.000141	6	14.897027	1.100497	-0.322081
6	1.463108	-1.106510	0.301395	1	14.557745	2.073002	-0.649916
1	1.125330	-2.085157	0.612110	6	14.079305	-0.000152	-0.000040
1	14.557291	-2.073363	0.649946	6	14.896785	-1.100906	0.322188
Aniline (An)							
6	1.167497	-1.198476	0.003556	6	1.167539	1.198478	0.003614
6	-0.220872	-1.203763	-0.006305	1	1.700393	2.142340	0.007099
6	1.874615	0.000003	0.009223	6	-0.220817	1.203741	-0.006342
1	-0.762939	-2.143566	-0.017012	1	-0.762795	2.143585	-0.017233
1	2.957092	-0.000164	0.017499	1	1.700526	-2.142234	0.006901
6	-0.933284	-0.000014	-0.008859	7	-2.327919	0.000017	-0.073703
1	-2.772473	-0.836056	0.274743	1	-2.772445	0.836165	0.274601
²An							
6	-1.132617	-0.954554	0.838815	6	1.096244	-0.224394	-0.057298
6	-2.520104	-0.922347	0.843557	6	1.870682	0.908626	0.259647
6	-0.390038	-0.165342	-0.041559	6	1.743701	-1.416705	-0.381172
6	-3.214966	-0.087410	-0.036423	6	3.266721	0.811898	0.212737
6	-1.092741	0.659862	-0.924669	6	3.129615	-1.509979	-0.419508
6	-2.479673	0.703442	-0.925862	6	3.887686	-0.380517	-0.126715
1	-3.074343	-1.548167	1.535178	1	1.133240	-2.280026	-0.624365
1	-0.540305	1.263147	-1.638704	1	3.862258	1.682803	0.466419
1	-3.002276	1.339930	-1.632260	1	4.970117	-0.427278	-0.155451
7	-4.609872	-0.089511	-0.071362	7	1.274647	2.088971	0.694349
1	-5.031822	0.747539	-0.444522	1	0.292296	2.196526	0.494416
1	-5.059844	-0.392718	0.779302	1	1.810964	2.930737	0.554915
1	3.608873	-2.444623	-0.681654	1	-0.609644	-1.599565	1.536518
³An							
6	-2.442758	-0.849621	1.020555	6	2.765787	-0.303538	-0.223315
6	-3.655515	-1.515523	1.119800	6	2.829295	-1.377094	-1.113850
6	-2.203477	0.084415	0.008547	6	3.855980	-0.075565	0.639680
6	-4.680030	-1.265384	0.201657	6	3.936152	-2.213899	-1.177988
6	-3.233085	0.326829	-0.907185	6	4.971531	-0.916603	0.566758
6	-4.449063	-0.334152	-0.816678	6	5.013036	-1.972993	-0.330793
1	-3.814242	-2.237209	1.914197	1	1.988573	-1.539293	-1.779995

1	-3.070661	1.035830	-1.711802	1	3.960977	-3.034789	-1.883425
1	-5.225760	-0.140589	-1.549116	1	5.810486	-0.733718	1.230453
7	-5.881029	-1.970736	0.262890	1	5.889615	-2.609283	-0.365723
1	-6.669147	-1.521962	-0.178861	7	3.854092	0.992501	1.541689
1	-6.115411	-2.347700	1.168794	1	4.461590	0.861250	2.337031
6	-0.883511	0.756564	-0.106844	1	2.935001	1.314337	1.813615
6	-0.775608	2.157552	-0.202363	1	-1.663651	-1.051102	1.747973
6	0.283691	-0.007616	-0.096364	1	0.580820	3.809861	-0.391705
6	0.496446	2.731471	-0.303535	1	2.612936	2.420526	-0.388934
6	1.555662	0.557926	-0.189112	7	-1.908723	2.973171	-0.228315
6	1.640270	1.949911	-0.297122	1	-2.729134	2.575591	0.208567
1	0.191172	-1.086822	-0.021018	1	-1.742370	3.924433	0.065017

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6	3.843783	0.652082	1.247715	6	-1.102186	-1.569080	0.319398
6	4.715084	1.700403	1.507669	6	-1.792635	-0.396298	0.008133
6	3.519771	0.283738	-0.059389	6	-1.760485	-2.566226	1.065166
6	5.298681	2.416965	0.458481	6	-3.111506	-0.175137	0.400516
6	4.100288	1.010822	-1.102920	6	-3.086291	-2.352846	1.457935
6	4.975518	2.058379	-0.854797	6	-3.749231	-1.179667	1.133802
1	4.947785	1.970082	2.532458	1	-1.285920	0.360869	-0.581974
1	3.842789	0.763718	-2.128402	1	-3.591375	-3.115896	2.041472
1	5.399598	2.618738	-1.681394	1	-4.768982	-1.027693	1.473758
7	6.133106	3.504378	0.714652	7	-1.126121	-3.767064	1.392489
1	6.770565	3.744573	-0.029444	1	-1.507555	-4.228322	2.205264
1	6.585994	3.497670	1.616116	1	-0.116495	-3.718600	1.420095
6	2.566296	-0.825144	-0.331312	1	3.408015	0.101007	2.074001
6	2.977086	-1.982533	-1.020211	6	-3.807775	1.096003	0.065190
6	1.247519	-0.731701	0.108710	6	-3.327424	2.307610	0.561842
6	2.035239	-2.989042	-1.266681	6	-4.951539	1.101328	-0.757189
6	0.305628	-1.734977	-0.125022	6	-3.958638	3.514471	0.285571
6	0.726015	-2.866902	-0.831408	6	-5.588799	2.318685	-1.026801
1	0.946858	0.163551	0.644592	6	-5.101365	3.508805	-0.508301
1	2.345729	-3.881789	-1.799687	1	-2.445608	2.286984	1.193612
1	0.013867	-3.655544	-1.048340	1	-3.570389	4.441044	0.688995
7	4.305727	-2.173215	-1.382167	1	-6.464185	2.322361	-1.668072
1	4.890662	-1.352154	-1.399540	1	-5.614151	4.436803	-0.733338
1	4.469442	-2.806628	-2.148727	7	-5.404630	-0.064854	-1.366110
1	-5.072331	-0.934004	-0.977747	1	-6.379097	-0.079908	-1.622309

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6	4.050149	1.816436	1.161841	6	-2.710082	-1.639254	-0.288763
6	4.280990	3.178695	1.289934	6	-2.895707	-0.294938	0.028122
6	4.084840	1.187490	-0.084117	6	-3.647771	-2.281117	-1.120628
6	4.560829	3.961411	0.165597	6	-3.989624	0.441288	-0.430395

6	4.356495	1.978402	-1.204642	6	-4.752371	-1.551533	-1.577271
6	4.592396	3.340590	-1.087961	6	-4.922695	-0.219711	-1.236161
1	4.243783	3.644828	2.268885	1	-2.170487	0.184442	0.678671
1	4.360149	1.520038	-2.188976	1	-5.467381	-2.035841	-2.234370
1	4.783675	3.936246	-1.974358	1	-5.779549	0.325342	-1.616834
7	4.740796	5.338933	0.282095	7	-3.451655	-3.586416	-1.555670
1	5.263297	5.771780	-0.464413	1	-4.277359	-4.094055	-1.830530
1	5.037314	5.660605	1.191120	1	-2.780557	-4.138649	-1.044738
6	3.809072	-0.268039	-0.217073	6	-4.124753	1.882677	-0.097273
6	4.787139	-1.150990	-0.714187	6	-5.312488	2.404948	0.452226
6	2.569840	-0.777328	0.165354	6	-3.050087	2.748083	-0.312198
6	4.468141	-2.509060	-0.836735	6	-5.386073	3.770792	0.746034
6	2.248284	-2.131202	0.055378	6	-3.124546	4.102182	-0.011554
6	3.223807	-2.989229	-0.463281	6	-4.306519	4.610817	0.517133
1	1.828179	-0.086050	0.554172	1	-2.142393	2.338583	-0.742718
1	5.217169	-3.193035	-1.222242	1	-6.305237	4.168152	1.164519
1	2.998864	-4.043443	-0.582599	1	-2.276925	4.750321	-0.194995
7	6.074014	-0.713050	-1.003931	1	-4.390596	5.664822	0.754935
1	6.196925	0.280470	-1.123353	7	-6.425023	1.588880	0.678880
1	6.594882	-1.270848	-1.662049	1	-7.051997	1.936793	1.389374
6	0.895821	-2.618935	0.428734	1	-6.209216	0.609639	0.809082
6	-0.235139	-1.970865	-0.070315	1	-0.094500	-1.136383	-0.750117
6	0.721811	-3.717065	1.293715	1	-0.712597	-4.967375	2.287038
6	-1.531610	-2.371279	0.247731	1	-2.679794	-3.789967	1.386398
6	-0.577171	-4.128171	1.612353	7	1.815302	-4.413735	1.812210
6	-1.683132	-3.467726	1.101025	1	1.623931	-4.904828	2.673006
1	3.843545	1.223330	2.046073	1	2.673762	-3.881419	1.858187

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6	4.087665	1.444855	1.259704	6	-2.268435	-3.011696	-0.221535
6	4.115974	2.816377	1.475465	6	-2.564921	-1.701140	0.143817
6	3.886796	0.917485	-0.016639	6	-3.187793	-3.719918	-1.020067
6	3.942919	3.706002	0.411142	6	-3.740127	-1.053773	-0.241625
6	3.709883	1.813709	-1.074597	6	-4.379911	-3.085929	-1.393177
6	3.732903	3.185818	-0.869703	6	-4.652064	-1.780915	-1.013989
1	4.267776	3.204500	2.477453	1	-1.852051	-1.172541	0.768903
1	3.532073	1.425685	-2.072549	1	-5.081348	-3.619161	-2.026569
1	3.562382	3.862271	-1.700549	1	-5.568945	-1.308352	-1.348623
7	3.898052	5.084399	0.633587	7	-2.894221	-4.984964	-1.510846
1	4.138618	5.651901	-0.165916	1	-3.677771	-5.563856	-1.766281
1	4.368261	5.397896	1.470023	1	-2.133395	-5.481787	-1.075577
6	3.862292	-0.553815	-0.250746	6	-3.949233	0.371421	0.117746
6	4.950752	-1.192727	-0.873851	6	-5.160737	0.843977	0.657829
6	2.764044	-1.313218	0.141804	6	-2.898239	1.274212	-0.056523

6	4.888715	-2.574892	-1.088599	6	-5.272478	2.200285	0.983447
6	2.692601	-2.692002	-0.072342	6	-2.994517	2.621684	0.283001
6	3.780486	-3.309250	-0.698091	6	-4.210037	3.073058	0.804935
1	1.933337	-0.805710	0.622756	1	-1.972012	0.911080	-0.490193
1	5.724973	-3.072662	-1.568517	1	-6.203305	2.562694	1.408034
1	3.748194	-4.375232	-0.895613	1	-4.312987	4.111688	1.103718
7	6.098120	-0.481862	-1.207846	7	-6.253109	-0.007245	0.851793
1	5.990935	0.519046	-1.281854	1	-6.899243	0.311474	1.559129
1	6.663746	-0.881423	-1.940500	1	-6.007595	-0.980406	0.977319
6	1.466658	-3.445854	0.295513	6	-1.819065	3.520965	0.136227
6	0.222340	-2.966355	-0.112425	6	-1.856865	4.654981	-0.697061
6	1.518399	-4.626765	1.061599	6	-0.642305	3.231693	0.829432
6	-0.974989	-3.605648	0.206549	6	-0.723826	5.474151	-0.781015
6	0.321639	-5.278413	1.380307	6	0.481829	4.041954	0.737661
6	-0.902688	-4.776908	0.965082	6	0.428451	5.174613	-0.069075
1	0.190751	-2.067613	-0.720241	1	-0.628701	2.354220	1.467711
1	0.359193	-6.180297	1.982800	1	-0.753519	6.343003	-1.430931
1	-1.816049	-5.283683	1.261132	1	1.383194	3.801498	1.286664
7	2.736158	-5.165615	1.480950	1	1.295928	5.820683	-0.139788
1	2.670395	-5.755822	2.297113	7	-2.965369	4.925250	-1.497211
1	3.492300	-4.497949	1.551663	1	-3.099091	5.891812	-1.749539
1	4.230337	0.767775	2.094778	1	-3.820493	4.451400	-1.250137

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6	-1.405266	0.028952	0.001509	1	-0.526905	3.536038	-1.773910
6	-0.727391	-1.203279	0.001199	1	-2.702403	2.333334	1.781829
6	0.678716	-1.232304	0.001565	1	2.796040	2.221148	-1.778702
6	1.406784	-0.029047	0.001694	1	0.674540	3.510384	1.779414
6	0.728893	1.203214	0.002201	1	3.378357	1.171526	1.778383
6	-0.677191	1.232224	0.002511	1	3.321116	-1.310709	-1.779398
6	-1.392260	2.531111	0.003553	1	2.704557	-2.333650	1.780267
6	1.496641	2.471592	0.000825	1	0.527705	-3.535978	-1.774775
6	2.889105	-0.059817	0.000094	1	-0.674823	-3.510247	1.779052
6	1.393705	-2.531198	0.002290	1	-2.794820	-2.220109	-1.779610
6	-1.495740	-2.471323	-0.000153	1	-3.376609	-1.171464	1.778396
6	-2.887648	0.059444	-0.000291	1	-3.319792	1.309323	-1.780376
6	-1.218358	3.555333	-0.942456	1	4.353026	4.269207	-2.184423
6	-2.062773	4.618678	-0.611227	1	5.267281	6.375330	-1.728296
6	-2.798664	4.211808	0.622219	1	4.750508	7.843830	-0.006134
6	-2.350336	2.929788	0.951120	1	3.211477	7.625356	1.717921
6	2.469050	2.831062	-0.947509	1	1.768510	5.840416	2.179270
6	2.969659	4.093856	-0.618724	1	-1.524054	5.909054	-2.173456
6	2.252038	4.530013	0.615557	1	-2.892706	7.751358	-1.712540
6	1.365478	3.502060	0.947350	1	-4.423738	8.031899	0.009840

6	3.716034	0.568746	0.946261	1	-5.003057	6.584567	1.729916
6	5.049686	0.314782	0.614059	1	-4.175959	4.442453	2.186123
6	5.030262	-0.525021	-0.620009	1	-5.941522	-1.389197	2.177410
6	3.686495	-0.722851	-0.948305	1	-8.208474	-1.033131	1.714996
6	2.351877	-2.930013	0.949750	1	-8.153468	1.371543	-1.731741
6	2.799350	-4.212434	0.621309	1	-5.872026	1.633856	-2.186781
6	2.062977	-4.619374	-0.611821	1	-1.771663	-5.838940	2.180090
6	1.219182	-3.555634	-0.943357	1	-3.216528	-7.622103	1.719525
6	-1.365770	-3.501342	0.946996	1	-4.755886	-7.839704	-0.004557
6	-2.253406	-4.528551	0.615697	1	-5.271132	-6.371440	-1.727169
6	-2.970585	-4.092220	-0.618788	1	-4.354201	-4.266367	-2.184266
6	-2.468629	-2.830164	-0.948207	1	4.176645	-4.443794	2.185246
6	-3.714464	-0.568991	0.946118	1	5.001897	-6.586440	1.729730
6	-5.048118	-0.315471	0.613785	1	4.421557	-8.033982	0.009981
6	-5.028862	0.523807	-0.620657	1	2.890620	-7.753076	-1.712197
6	-3.685066	0.721668	-0.949091	1	1.522913	-5.909749	-2.173446
6	3.955300	4.783549	-1.312639	1	5.943214	1.388810	2.177373
6	4.499236	6.036544	-1.041125	1	8.210139	1.032057	1.715201
6	4.187631	6.914780	-0.005091	1	9.168528	-0.190932	-0.009681
6	3.265862	6.786274	1.032465	1	8.154761	-1.373449	-1.730951
6	2.407671	5.724654	1.307017	1	5.873270	-1.635702	-2.185819
6	-2.168398	5.818844	-1.302007	1	-9.167068	0.189286	-0.010194
6	-2.982621	6.914886	-1.027631	6	-4.191891	-6.911331	-0.003875
6	-3.899465	7.080521	0.008672	6	-4.502598	-6.033169	-1.040296
6	-4.248424	6.214926	1.043796	6	-3.957167	-4.781010	-1.312341
6	-3.756512	4.940863	1.315255	6	3.756640	-4.942001	1.314534
6	-6.160436	-0.778063	1.304865	6	4.247531	-6.216550	1.043444
6	-7.509087	-0.566271	1.029594	6	3.897962	-7.082231	0.008618
6	-8.081034	0.166984	-0.008328	6	2.981108	-6.916374	-1.027649
6	-7.475973	0.876254	-1.044311	6	2.167604	-5.819870	-1.302216
6	-6.119020	1.032240	-1.315113	6	6.162022	0.777337	1.305040
6	-2.410530	-5.722620	1.307699	6	7.510696	0.565158	1.029885
6	-3.270011	-6.783359	1.033580	6	8.082497	-0.168433	-0.007808
6	6.120388	-1.033827	-1.314366	6	7.477310	-0.877909	-1.043660

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6	-1.175869	-0.768133	0.000092	6	-6.409224	-3.569868	-1.035541
6	0.077211	-1.402472	0.000768	6	-0.107507	-7.338400	-1.020457
6	1.253039	-0.634308	0.000537	6	0.447542	-8.111581	0.007369
6	1.175868	0.768133	0.000037	6	0.914189	-7.279867	1.033523
6	-0.077211	1.402472	0.000767	6	6.301850	-3.759430	-1.025871
6	-1.253039	0.634307	0.000591	6	7.250498	-3.663883	0.000381
6	-2.594694	1.313145	0.000928	6	6.764278	-2.844055	1.027010
6	-2.435071	-1.589927	-0.001883	1	-1.449660	5.023313	2.378084

6	0.160117	-2.903851	0.001883	1	-1.076290	2.782196	1.892284
6	2.594694	-1.313146	0.000816	1	-4.020479	3.347882	-2.371367
6	2.435070	1.589927	-0.002000	1	-5.078051	1.253286	2.373847
6	-0.160116	2.903851	0.001882	1	-2.949277	0.457686	1.890392
6	0.355015	3.546326	-1.128564	1	-3.634619	-3.766342	2.369884
6	0.429344	4.905302	-1.416111	1	-4.904966	-1.804503	-2.379874
6	0.001493	5.988160	-0.661522	1	-2.877373	-0.779787	-1.892766
6	-0.660488	5.950283	0.671785	1	1.449766	-5.023305	2.378035
6	-0.966608	4.825252	1.423946	1	1.076371	-2.782190	1.892246
6	-0.743054	3.483412	1.133507	1	4.020377	-3.347883	-2.371540
6	-2.892240	2.081307	-1.129295	1	5.078151	-1.253290	2.373631
6	-4.032168	2.824426	-1.418053	1	2.949357	-0.457689	1.890266
6	-5.185272	2.993565	-0.665218	1	1.876932	2.324882	1.889133
6	-5.484883	2.400487	0.667366	1	3.634723	3.766359	2.369699
6	-4.663946	1.573339	1.420413	1	4.904856	1.804493	-2.380105
6	-3.389345	1.097116	1.131464	1	5.892036	4.997648	1.935988
6	-2.649104	-2.385166	1.128647	1	7.711273	5.027852	-0.010993
6	-3.701411	-3.248271	1.415901	1	6.944388	3.372742	-1.953646
6	-4.827415	-3.543481	0.660778	1	0.546235	7.706128	-1.936949
6	-5.187160	-2.988082	-0.673164	1	-0.507065	9.191779	0.008556
6	-4.460353	-2.076442	-1.425246	1	-1.390482	7.595322	1.950737
6	-3.246279	-1.463021	-1.134081	1	-6.400155	4.323548	-1.941993
6	-0.355063	-3.546330	-1.128539	1	-8.216290	4.151347	0.000542
6	-0.429401	-4.905306	-1.416080	1	-7.276783	2.588258	1.943557
6	-0.001515	-5.988162	-0.661507	1	-5.891954	-4.997629	1.936284
6	0.660523	-5.950281	0.671772	1	-7.711280	-5.027842	-0.010613
6	0.966673	-4.825247	1.423917	1	-6.944481	-3.372745	-1.953311
6	0.743104	-3.483409	1.133485	1	-0.546308	-7.706135	-1.936907
6	2.892192	-2.081307	-1.129420	1	0.507079	-9.191779	0.008557
6	4.032106	-2.824428	-1.418225	1	1.390575	-7.595316	1.950696
6	5.185241	-2.993570	-0.665439	1	6.400068	-4.323554	-1.942264
6	5.484909	-2.400492	0.667132	1	8.216285	-4.151357	0.000195
6	4.664005	-1.573343	1.420214	1	7.276862	-2.588266	1.943248
6	3.389392	-1.097119	1.131319	1	0.763204	2.887645	-1.888837
6	2.649154	2.385173	1.128515	1	0.887409	5.157425	-2.369821
6	3.701473	3.248282	1.415716	1	-2.116495	2.106734	-1.888291
6	4.827441	3.543490	0.660540	1	-1.876847	-2.324871	1.889228
6	5.187126	2.988083	-0.673415	1	-0.763285	-2.887652	-1.888796
6	4.460286	2.076437	-1.425458	1	-0.887507	-5.157433	-2.369769
6	3.246226	1.463016	-1.134234	1	2.116415	-2.106732	-1.888384
6	5.854042	4.426920	1.019204	1	2.877287	0.779776	-1.892898
6	6.804927	4.437156	-0.009501	6	-6.301897	3.759424	-1.025604
6	6.409172	3.569870	-1.035853	6	-7.250502	3.663874	0.000688

6	0.107473	7.338397	-1.020480	6	-6.764237	2.844047	1.027297
6	-0.447531	8.111581	0.007368	6	-5.854002	-4.426907	1.019496
6	-0.914135	7.279871	1.033544	6	-6.804933	-4.437147	-0.009166

$(P)_2$

6	1.568875	1.118319	-0.501676	6	-1.569072	-1.118385	0.501578
7	1.031710	-0.000160	-1.076453	7	-1.031956	-0.000034	1.076704
6	1.569117	-1.118415	-0.501437	6	-1.569068	1.118360	0.501660
6	2.483626	-0.712885	0.440799	6	-2.483362	0.713068	-0.440878
6	2.483534	0.713181	0.440596	6	-2.483370	-0.713014	-0.440924
1	1.256527	2.103317	-0.807202	1	-1.256839	-2.103460	0.806978
1	0.213869	-0.000326	-1.668772	1	-3.098328	1.361727	-1.044045
1	3.098493	1.361956	1.043643	1	-3.098523	-1.361633	-1.043943
1	1.257051	-2.103551	-0.806792	1	-1.256867	2.103420	0.807148
1	3.098715	-1.361402	1.044003	1	-0.214051	-0.000071	1.668924

$(^2P_{C3N1'})_2$

6	-2.469807	0.418071	-1.049212	6	3.730733	-0.029860	-0.663408
7	-1.875574	1.058303	0.007308	1	1.926170	-0.274401	-1.967476
6	-2.744238	1.073119	1.068731	1	4.776602	-0.300206	1.304097
6	-3.903020	0.441319	0.686261	1	4.445813	0.491961	-1.279853
6	-3.729837	0.027301	-0.663826	1	2.465130	-1.548879	1.996056
1	-1.923489	0.266546	-1.966371	6	-1.457405	-2.273783	0.660813
1	-4.778551	0.305939	1.300988	7	-1.269321	-2.621595	-0.644969
1	-4.443748	-0.497776	-1.278856	6	-0.026958	-2.224175	-1.066185
1	-2.468682	1.558831	1.990564	6	0.582972	-1.617811	0.006392
6	1.456450	2.275815	0.658609	6	-0.316643	-1.653513	1.105339
7	1.271572	2.616367	-0.649512	1	-2.395230	-2.452901	1.159210
6	0.029711	2.217872	-1.071179	1	-1.977024	-3.021671	-1.236832
6	-0.583278	1.618466	0.003541	1	-0.153524	-1.243316	2.088425
6	0.313986	1.659437	1.104234	1	0.334868	-2.422554	-2.060952
1	2.393342	2.456986	1.158011	6	2.471003	-0.421667	-1.048744
1	1.981602	3.010656	-1.242482	7	1.874973	-1.056847	0.009830
1	0.147708	1.256025	2.089611	6	2.742286	-1.067520	1.072419
1	-0.329526	2.410582	-2.067992	6	3.901874	-0.437975	0.688758

$(^3P_{C3N1'})_2$

6	-0.032411	2.272437	1.660161	7	-3.803501	-2.634413	-0.225763
7	0.386000	1.930540	0.402484	6	-2.686650	-2.640888	0.565296
6	-0.690635	1.513389	-0.336824	6	-1.715073	-1.945877	-0.114043
6	-1.805180	1.612565	0.461706	6	-2.260214	-1.509640	-1.350882
6	-1.393057	2.089855	1.734303	1	-4.331983	-1.794886	-2.115323

1	0.671445	2.653028	2.382084	1	-2.653959	-3.142431	1.517921
1	-0.569019	1.154146	-1.345244	6	0.737520	-1.811702	-0.390411
6	3.488089	2.207760	-1.417478	7	-0.409817	-1.696466	0.355595
7	3.907891	1.794254	-0.185799	6	-0.093587	-1.271701	1.615033
6	2.833655	1.622167	0.641191	6	1.268861	-1.115759	1.695662
6	1.713522	1.968137	-0.071947	6	1.789861	-1.452319	0.418783
6	2.121793	2.347553	-1.380590	1	0.709158	-2.176996	-1.403452
1	4.188206	2.372769	-2.219235	1	1.817617	-0.767210	2.555790
1	4.826447	1.427396	0.014694	1	-0.871891	-1.061523	2.330208
1	1.487744	2.702904	-2.176951	1	-1.765465	-0.920929	-2.106176
1	2.940348	1.233746	1.639466	6	4.212941	-1.519252	0.893361
6	-4.038726	0.617971	0.815011	7	3.146447	-1.401313	0.039066
7	-3.128988	1.322973	0.070627	6	3.612300	-1.189219	-1.232535
6	-3.720722	1.721486	-1.101499	6	4.986325	-1.184001	-1.195519
6	-5.018572	1.269525	-1.104508	6	5.370145	-1.386298	0.159696
6	-5.221844	0.569752	0.117017	1	4.055757	-1.731684	1.938326
1	-3.750066	0.196671	1.764790	1	5.638355	-1.042255	-2.042856
1	-5.742335	1.438670	-1.885914	1	6.373246	-1.462203	0.548783
1	-3.170582	2.320851	-1.808609	1	2.923273	-1.010714	-2.041976
1	-2.029481	2.306654	2.577268	1	-4.697141	-3.012278	0.038663
6	-3.559411	-1.949579	-1.381454	1	-6.129489	0.089074	0.447093

$({}^4P_{C_3N_1'})_2$

6	4.573847	1.438156	1.048581	7	1.335372	-1.796488	0.282630
7	5.730680	1.888375	0.478571	1	2.233955	-1.520554	-1.640443
6	5.446152	2.731791	-0.557059	1	1.128720	-2.042489	2.383583
6	4.081414	2.867524	-0.636766	1	3.820799	-1.670036	2.401986
6	3.535462	2.037913	0.381344	6	-0.407509	-2.720837	-1.281760
1	4.569548	0.705345	1.837345	6	0.000848	-2.021667	-0.115669
1	3.534876	3.500518	-1.317345	6	-1.126606	-1.632243	0.568268
1	6.229842	3.172433	-1.150163	7	-2.211121	-2.090011	-0.136069
6	1.189006	1.765929	-0.313935	6	-1.781611	-2.738365	-1.261303
7	2.163811	1.846299	0.648918	1	0.231133	-3.185769	-2.015485
6	1.594771	1.713990	1.884164	1	-2.489785	-3.194965	-1.932686
6	0.241241	1.530539	1.726704	1	-1.242059	-1.017642	1.446098
6	-0.008847	1.567594	0.328730	6	-4.652731	-1.793762	-0.676260
1	1.429837	1.843812	-1.361022	6	-3.561558	-1.911083	0.225344
1	-0.482662	1.393166	2.514228	6	-4.048871	-1.812042	1.506435
1	2.201718	1.773300	2.772440	7	-5.404449	-1.635053	1.401195
6	-1.478374	0.819993	-1.509329	6	-5.777420	-1.614477	0.089238
7	-1.260427	1.404199	-0.292499	1	-4.606843	-1.794708	-1.753019
6	-2.465236	1.757691	0.265444	1	-6.023434	-1.452649	2.172594

6	-3.452413	1.382396	-0.614686	1	-6.797207	-1.424017	-0.201027
6	-2.831166	0.794966	-1.747797	1	-3.549481	-1.878735	2.458183
1	-0.658064	0.406806	-2.073785	1	8.095946	-1.442669	-0.232613
1	-3.318546	0.362442	-2.606405	1	6.632125	1.468782	0.647181
1	-2.513485	2.286639	1.202449	6	5.990637	-1.684783	0.312910
6	-5.785937	1.609721	-1.394684	6	7.055633	-1.253180	-0.445350
7	-4.837166	1.529426	-0.407588	6	6.518904	-0.565162	-1.568804
6	-5.457160	1.592195	0.813610	6	5.150734	-0.593248	-1.446473
6	-6.809845	1.719481	0.606819	7	4.833492	-1.284692	-0.305442
6	-7.019416	1.727057	-0.800540	1	5.953660	-2.283070	1.208731
1	-5.495807	1.605755	-2.432509	1	4.375882	-0.133201	-2.038453
1	-7.561370	1.800968	1.376231	1	7.068908	-0.089119	-2.365015
1	-7.960409	1.825068	-1.317807	6	2.387764	-1.594197	-0.576791
1	-4.880084	1.508266	1.720293	6	3.531265	-1.513626	0.181131
6	1.804225	-1.857409	1.565019	6	3.166286	-1.677200	1.544869

$({}^5P_{C3N1'})_2$

6	3.892885	2.905200	0.961361	7	-0.684472	-1.846613	-0.455059
7	4.245605	2.159269	-0.130818	1	0.129158	-2.120108	1.509581
6	3.115631	1.723904	-0.771094	1	-0.806564	-1.416640	-2.534105
6	2.035983	2.221859	-0.081325	1	1.847969	-0.872959	-2.279600
6	2.521415	2.969819	1.023050	1	2.196905	-0.111477	2.142645
1	4.652217	3.358701	1.577068	6	-3.118100	-1.630797	-0.849159
1	3.173651	1.063340	-1.620033	6	-2.032283	-2.181389	-0.211375
6	7.378593	1.349493	-1.726172	6	-2.503801	-3.112453	0.748725
7	7.677203	1.211777	-0.400764	6	-3.876696	-3.096445	0.659195
6	6.571729	1.473774	0.357376	7	-4.240198	-2.208552	-0.315050
6	5.562445	1.819741	-0.505360	1	-3.189383	-0.828183	-1.565974
6	6.067804	1.748128	-1.832242	1	-4.625888	-3.675841	1.173363
1	8.116882	1.159129	-2.487052	1	-1.909294	-3.742802	1.390311
1	8.498737	0.748308	-0.041361	6	-6.066778	-1.643491	-1.967077
1	5.536812	1.987370	-2.739596	6	-5.562113	-1.852950	-0.654811
1	6.571616	1.351646	1.427307	6	-6.576465	-1.616175	0.238566
6	-0.283441	1.662300	0.511130	7	-7.684704	-1.288881	-0.489244
7	0.675493	2.019422	-0.401402	6	-7.383241	-1.277908	-1.821404
6	0.093301	2.198659	-1.625423	1	-5.529456	-1.772125	-2.892913
6	-1.253219	1.940835	-1.513413	1	-8.123816	-1.015876	-2.558390
6	-1.485372	1.605643	-0.152710	1	-6.579064	-1.613453	1.315602
1	-0.032835	1.487926	1.544329	1	-8.514946	-0.882654	-0.084246
1	-1.982537	1.985819	-2.306540	1	-9.353969	1.691963	1.835864
1	0.687687	2.506226	-2.469943	7	2.734951	-1.287160	0.455400
1	1.930624	3.514247	1.742285	6	2.994564	-0.600643	1.607957

6	-3.942736	1.763579	0.000997	1	4.862838	-0.138718	2.652200
7	-2.728111	1.286405	0.429913	1	3.921842	-2.356268	-0.965910
6	-2.919315	0.457512	1.499700	6	8.253672	-2.048631	-0.401698
6	-4.264943	0.390076	1.769729	6	8.468204	-1.900362	0.997341
6	-4.909275	1.217997	0.812966	6	7.245309	-1.629955	1.568450
1	-4.010441	2.488551	-0.792702	7	6.302159	-1.602310	0.573127
1	-4.728956	-0.212568	2.533927	6	6.912554	-1.850441	-0.628874
1	-2.087705	-0.067835	1.940755	1	8.993974	-2.268995	-1.154487
6	-6.965237	1.797792	-0.434416	1	9.399201	-2.013994	1.529905
7	-6.296428	1.448214	0.709839	1	6.345635	-1.817746	-1.544988
6	-7.193621	1.357554	1.743247	1	6.957554	-1.499349	2.598918
6	-8.446057	1.652877	1.254922	6	0.314946	-1.844475	0.484503
6	-8.298283	1.941203	-0.130986	6	1.468901	-1.442373	-0.146687
1	-6.439152	1.867561	-1.372548	6	1.165126	-1.196767	-1.510674
1	-9.076169	2.215934	-0.825804	6	-0.173300	-1.460920	-1.663744
1	-6.855890	1.133952	2.742124	6	4.928576	-1.343169	0.758570
6	4.350363	-0.617261	1.833105	6	3.914322	-1.747020	-0.077508

$({}^6P_{C3N1'})_2$

6	-5.876954	-2.097329	1.955719	7	4.298027	-1.235871	-0.450679
7	-6.189433	-1.868255	0.642549	6	5.472670	-1.701372	0.086969
6	-5.043690	-1.894221	-0.107440	6	6.489088	-1.336654	-0.765067
6	-3.998393	-2.164241	0.742958	6	5.917449	-0.630628	-1.855742
6	-4.518498	-2.287717	2.058114	1	3.769505	-0.105289	-2.172530
1	-6.655509	-2.141290	2.699576	1	6.439875	-0.182045	-2.685364
1	-5.061248	-1.687725	-1.165100	1	5.477612	-2.297311	0.984659
6	-9.242911	-1.685381	-1.268101	6	8.740499	-1.920169	-1.596750
7	-9.540945	-0.927671	-0.172047	7	7.853304	-1.639793	-0.589151
6	-8.466306	-0.877758	0.670044	6	8.499322	-1.734119	0.615955
6	-7.478039	-1.648123	0.110662	6	9.807098	-2.083919	0.378429
6	-7.966651	-2.170576	-1.119046	6	9.961728	-2.198533	-1.030878
1	-9.956537	-1.821410	-2.063304	1	8.412767	-1.929266	-2.623501
1	-10.328906	-0.301121	-0.104061	1	#####	-2.235320	1.129853
1	-7.447455	-2.838235	-1.787761	1	#####	-2.468389	-1.567610
1	-8.471208	-0.278043	1.563604	1	7.974416	-1.508383	1.530404
6	-1.556917	-1.781105	0.932682	6	-6.258777	1.473968	1.382126
7	-2.657854	-2.344353	0.339531	6	-6.569157	1.688929	0.013994
6	-2.264434	-3.085252	-0.740381	6	-5.401188	1.603034	-0.707985
6	-0.895633	-3.015595	-0.846663	7	-4.390925	1.329599	0.181187
6	-0.455381	-2.187200	0.216668	6	-4.905679	1.248081	1.444198
1	-1.660679	-1.079016	1.744403	1	-6.944942	1.453782	2.213441
1	-0.284153	-3.528307	-1.571394	1	-5.197998	1.757614	-1.754606

1	-2.990790	-3.641084	-1.310091	6	-9.606687	1.921109	-1.887108
1	-3.964929	-2.525949	2.952180	6	-9.992647	2.530833	-0.660912
6	1.879519	-1.796312	-0.479056	6	-8.890595	2.516263	0.164000
7	0.880249	-1.807841	0.461705	7	-7.856238	1.920652	-0.511795
6	1.391273	-1.418291	1.669530	6	-8.289985	1.548542	-1.757928
6	2.726973	-1.140489	1.513723	1	#####	1.764290	-2.758505
6	3.030853	-1.385066	0.150454	1	#####	2.962981	-0.421285
1	1.699651	-2.080860	-1.502421	1	-7.636045	1.006915	-2.422017
1	3.405228	-0.792885	2.276541	1	-8.737664	2.917966	1.152525
1	0.761160	-1.376199	2.542316	6	-1.987211	1.671345	0.613022
6	4.562876	-0.587388	-1.625286	6	-3.027381	1.182490	-0.141586
7	6.170661	2.142325	-0.097337	6	-2.483024	0.510482	-1.265930
6	5.741712	2.904384	-1.150638	6	-1.116808	0.606342	-1.147488
1	3.733925	3.565343	-1.753276	7	-0.820827	1.303817	-0.007695
1	6.453993	3.339664	-1.832144	1	-1.989463	2.292815	1.492747
1	5.204114	1.049681	1.466500	1	-0.329819	0.180864	-1.748954
6	8.504061	1.507869	-0.803301	1	-3.023656	-0.021387	-2.032481
6	7.515916	1.815950	0.168757	1	-4.271507	0.984904	2.274667
6	8.097521	1.752345	1.412373	6	1.602856	1.707984	-0.327312
7	9.410757	1.414870	1.216726	6	0.469450	1.645611	0.446662
6	9.664565	1.258260	-0.115406	6	0.823302	2.000773	1.775440
1	8.363395	1.439243	-1.869785	6	2.171398	2.268845	1.760240
1	10.072465	1.229560	1.951034	7	2.639237	2.082683	0.489106
1	10.630296	0.939001	-0.468896	1	1.762095	1.520175	-1.375941
1	7.690775	1.948197	2.390206	1	2.838352	2.591055	2.542853
6	3.969362	2.266529	0.053277	1	0.174164	2.044748	2.635046
6	5.091672	1.733176	0.640539	6	4.372983	3.007555	-1.087570

HPB_{C36σ}..HPB_{N16σ}

6	-2.594734	-0.659075	-0.673086	6	1.329883	-1.320428	2.092837
6	-1.439846	-1.373804	-0.872612	6	2.618231	-1.034884	1.650917
6	-0.247782	-0.716548	-1.071176	6	3.029740	0.286539	1.512214
6	-0.215561	0.662431	-1.069341	6	2.150808	1.322223	1.813014
6	-1.377728	1.373506	-0.877215	6	0.862870	1.036803	2.256724
6	-2.562087	0.711221	-0.667302	6	0.451019	-0.285318	2.395248
7	-1.400334	2.725583	-1.095088	6	-0.115192	2.053728	2.211129
6	-2.558376	3.488429	-1.059678	6	-1.528853	1.823479	2.331875
6	-3.813509	2.785827	-0.750783	6	-1.916067	0.414945	2.487665
7	-3.733572	1.413486	-0.588989	6	-0.930924	-0.566614	2.485033
7	0.907727	1.317433	-1.499862	6	2.437271	2.619513	1.335647
6	0.928507	2.676283	-1.789340	6	1.487861	3.696568	1.299327
6	-0.298513	3.441910	-1.525551	6	0.143289	3.349816	1.775357

7	0.839870	-1.421534	-1.513943	6	4.180346	0.566909	0.742796
6	1.987734	-0.812729	-1.998656	6	4.532104	1.874202	0.262943
6	2.022300	0.656424	-1.995482	6	3.582625	2.937237	0.613998
7	-1.520134	-2.727001	-1.071639	6	3.368062	-2.053402	1.024173
6	-0.469142	-3.481968	-1.558037	6	4.563040	-1.826554	0.260470
6	0.793938	-2.776789	-1.814617	6	4.949967	-0.416675	0.130307
7	-3.798463	-1.305420	-0.613204	6	0.813426	-2.619169	1.892653
6	-3.930029	-2.679175	-0.693437	6	1.552516	-3.702455	1.304382
6	-2.708183	-3.440180	-1.002973	6	2.910990	-3.356931	0.864752
6	-4.975096	0.816221	-0.425932	6	-1.504484	-1.874767	2.312439
6	-5.005227	-0.656889	-0.410075	6	-0.536132	-2.937152	2.006905
6	-5.162002	3.083250	-0.638744	7	-3.101075	-0.281670	2.393271
6	-5.880224	1.865186	-0.437659	6	-2.873549	-1.648465	2.291691
6	-0.760264	4.734062	-1.716671	7	-1.093039	3.948957	1.712739
6	-2.161742	4.761633	-1.431892	6	-2.101914	3.050198	2.029128
6	2.809093	1.642088	-2.563003	7	3.384366	4.235751	0.205601
6	2.132526	2.890494	-2.435378	6	2.137412	4.701282	0.597693
6	1.992946	-3.048096	-2.448390	7	5.818157	0.279090	-0.681390
6	2.731845	-1.833797	-2.560804	6	5.586922	1.647769	-0.606927
6	-2.381077	-4.721791	-1.420313	7	3.862538	-3.962264	0.077919
6	-0.997514	-4.745564	-1.768115	6	4.851556	-3.062857	-0.297261
6	-5.947753	-1.670382	-0.337104	7	-0.623736	-4.238482	1.567615
6	-5.282418	-2.922139	-0.513914	6	0.610210	-4.705666	1.141125
1	-5.597873	4.066310	-0.716555	1	-4.022439	0.127872	2.361374
1	-6.950251	1.772186	-0.343570	1	-3.711662	-2.317858	2.172523
1	-0.169073	5.565956	-2.064931	1	-1.275503	4.856849	1.313212
1	-2.809878	5.618555	-1.526653	1	-3.132401	3.363998	1.978086
1	3.766107	1.481999	-3.032771	1	4.027243	4.774587	-0.350432
1	2.482989	3.842653	-2.800996	1	1.824353	5.694767	0.320714
1	2.302142	-4.013128	-2.817698	1	6.553984	-0.130183	-1.233021
1	3.699730	-1.720348	-3.021945	1	6.181902	2.321383	-1.202031
1	-3.070971	-5.545945	-1.510677	1	3.833451	-4.917159	-0.238384
1	-0.455144	-5.597831	-2.145327	1	5.652029	-3.389399	-0.940983
1	-7.008607	-1.533798	-0.201298	1	-1.483130	-4.743933	1.415513
1	-5.755649	-3.890759	-0.528930	1	0.683823	-5.693777	0.717742

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6	-2.446880	1.375504	-1.905848	6	-2.309475	-0.047791	1.647308
6	-2.763678	-0.000169	-1.790778	6	-1.989058	-1.404215	1.850991
6	-1.786085	-0.976317	-1.585872	6	-0.680075	-1.854774	1.849781
6	-0.387726	-0.557199	-1.638064	6	0.400504	-0.884869	1.687872
6	-0.070477	0.875715	-1.607882	6	0.063160	0.556248	1.766897

6	-1.151626	1.852790	-1.685509	6	-1.340558	0.944741	1.675458
6	0.688375	-1.527721	-1.817891	6	1.789075	-1.260318	1.444639
6	1.970271	-1.038740	-2.077751	6	2.756362	-0.264656	1.420549
6	2.295176	0.327401	-1.892035	6	2.457661	1.069503	1.758790
6	1.332107	1.290271	-1.588275	6	1.154471	1.513319	1.916143
6	1.901238	2.600999	-1.238348	7	1.059431	2.886691	2.300527
6	-1.071137	3.319537	-1.605038	7	-1.873055	2.262913	1.552965
6	-3.544291	2.255124	-2.180771	7	-3.656644	0.240581	1.460481
6	-4.157036	-0.330857	-1.838039	7	-3.065429	-2.257027	2.094900
6	-2.335326	-2.308024	-1.286396	7	-0.561329	-3.253839	2.115867
6	0.614582	-2.995216	-1.809041	7	2.299394	-2.562448	1.158633
6	3.045218	-1.895508	-2.480368	7	4.083742	-0.533177	1.098485
6	3.685939	0.656986	-1.985846	7	3.552087	1.911966	1.955347
6	-0.065594	4.156654	-1.148829	6	-1.302299	3.490216	1.797318
7	-0.512736	5.443300	-1.190600	6	-2.199318	4.486960	1.480421
6	-1.796874	5.501290	-1.660011	6	-3.389523	3.877242	1.058994
6	-2.179596	4.205956	-1.918604	6	-3.185963	2.525101	1.126147
6	-3.432638	3.621094	-2.250659	6	-4.128845	1.470587	1.082867
7	-4.682932	4.130354	-2.471918	6	-5.497413	1.390232	0.944591
6	-5.607382	3.098326	-2.534677	6	-5.872030	0.063092	1.261181
6	-4.927611	1.915220	-2.343948	6	-4.727377	-0.630936	1.579795
6	-5.207879	0.523377	-2.136704	6	-4.413425	-1.948792	2.009309
7	-6.354923	-0.209040	-2.032380	6	-5.124753	-3.042639	2.452762
6	-6.071162	-1.507378	-1.651300	6	-4.188634	-4.040730	2.830730
6	-4.699169	-1.598351	-1.517014	6	-2.930965	-3.523570	2.605167
6	-3.709099	-2.553462	-1.151551	6	-1.607147	-4.024178	2.650888
7	-3.895359	-3.829043	-0.697817	6	-1.150286	-5.284811	2.935070
6	-2.677949	-4.442388	-0.560015	6	0.198123	-5.325608	2.541672
6	-1.709547	-3.555372	-0.962523	6	0.522129	-4.091935	2.015490
6	-0.357242	-3.857263	-1.327821	6	1.732043	-3.807073	1.324342
7	0.086922	-5.139338	-1.469235	6	2.600100	-4.772554	0.864545
6	1.329653	-5.167361	-2.036935	6	3.773562	-4.132354	0.437987
6	1.696644	-3.859099	-2.250191	6	3.584647	-2.790991	0.638982
6	2.923418	-3.253636	-2.637741	6	4.527163	-1.736746	0.617182
7	4.150631	-3.742645	-2.988257	6	5.880206	-1.642328	0.374786
6	5.073461	-2.708262	-3.037573	6	6.274202	-0.328199	0.722017
6	4.414514	-1.542380	-2.715300	6	5.156572	0.341364	1.164450
6	4.712994	-0.170325	-2.417423	6	4.881307	1.633900	1.686557
7	5.862003	0.563593	-2.352382	6	5.629166	2.719123	2.088596
6	5.608384	1.825197	-1.852054	6	4.736420	3.678966	2.632505
6	4.249172	1.900445	-1.612518	6	3.466870	3.149064	2.539549
6	3.281573	2.832285	-1.140351	6	2.155274	3.627189	2.772165

7	3.493039	4.082940	-0.633070	6	1.730736	4.854650	3.209182
6	2.284489	4.698629	-0.429150	6	0.347674	4.911286	2.972668
6	1.296998	3.836780	-0.843214	6	-0.030049	3.720209	2.387730
1	6.101001	-2.902290	-3.296764	1	7.264495	0.094696	0.662561
1	4.362653	-4.707113	-3.179392	1	6.503689	-2.437459	-0.000244
1	6.781603	0.211565	-2.560340	1	6.703230	2.789663	2.025441
1	6.404927	2.537268	-1.716354	1	4.985428	4.643953	3.043472
1	4.378416	4.395668	-0.266133	1	2.370218	5.621085	3.616637
1	2.226264	5.694044	-0.018707	1	-0.324367	5.725763	3.187030
1	0.062859	6.240704	-0.976448	1	-1.987582	5.541608	1.539904
1	-2.330177	6.433577	-1.738599	1	-4.312439	4.345405	0.755214
1	-4.904323	5.103406	-2.598469	1	-6.143035	2.203404	0.654594
1	-6.649646	3.305973	-2.711266	1	-6.865941	-0.354418	1.251405
1	-7.283213	0.145770	-2.190578	1	-6.199383	-3.094789	2.525397
1	-6.859119	-2.230290	-1.523103	1	-4.402802	-5.022344	3.221301
1	-4.761276	-4.165210	-0.307471	1	-1.748664	-6.080845	3.348167
1	-2.599481	-5.454484	-0.195374	1	0.880332	-6.156101	2.617673
1	-0.465833	-5.949998	-1.244675	1	2.386674	-5.828571	0.855107
1	1.862252	-6.090900	-2.189540	1	4.678726	-4.574069	0.053406