Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Structure and optoelectronic properties of helical pyridine-furan, pyridine-pyrrole and pyridine-thiophene oligomers

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LIST OF FIGURES

LIST OF TABLES

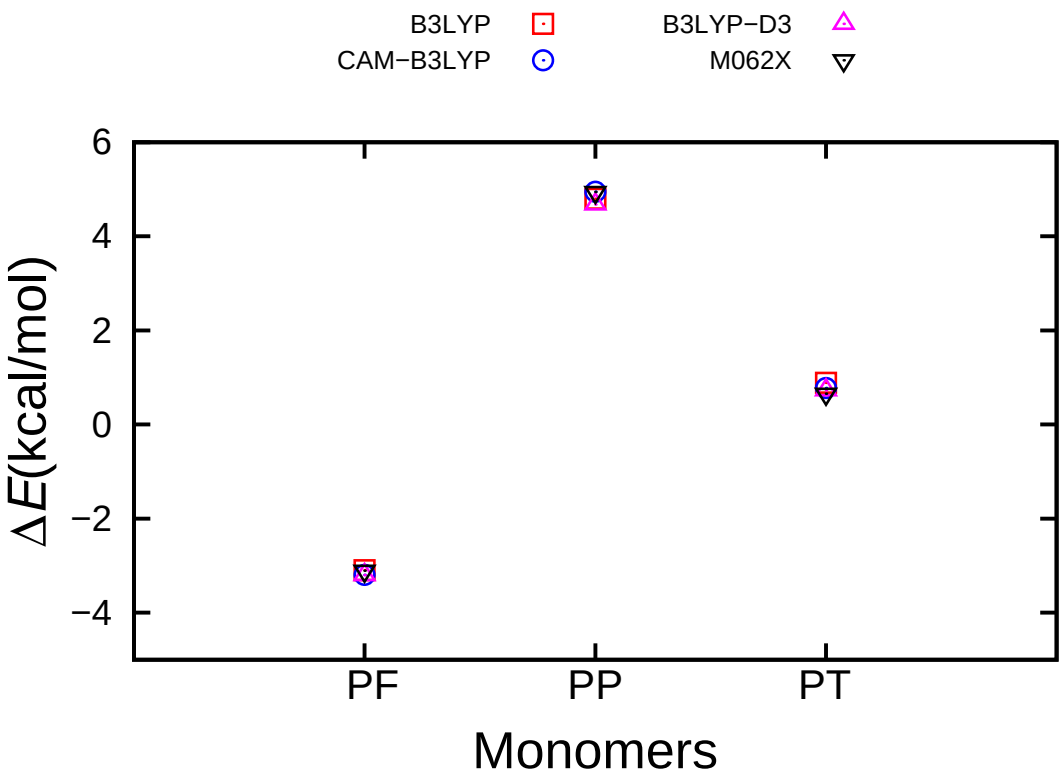

FIG. S1. Differences in energies (ΔE) between the two possible conformations (i.e., $E_{\boldsymbol{i}} - E_{\boldsymbol{ii}}$) of monomers calculated using B3LYP, CAM-B3LYP, B3LYP-D3 and M06-2X functionals in combination with 6-31G(d) basis set. Structures of conformations $\boldsymbol{i}$ and $\boldsymbol{ii}$ for $(PF)_1$ are shown in Fig. 2.

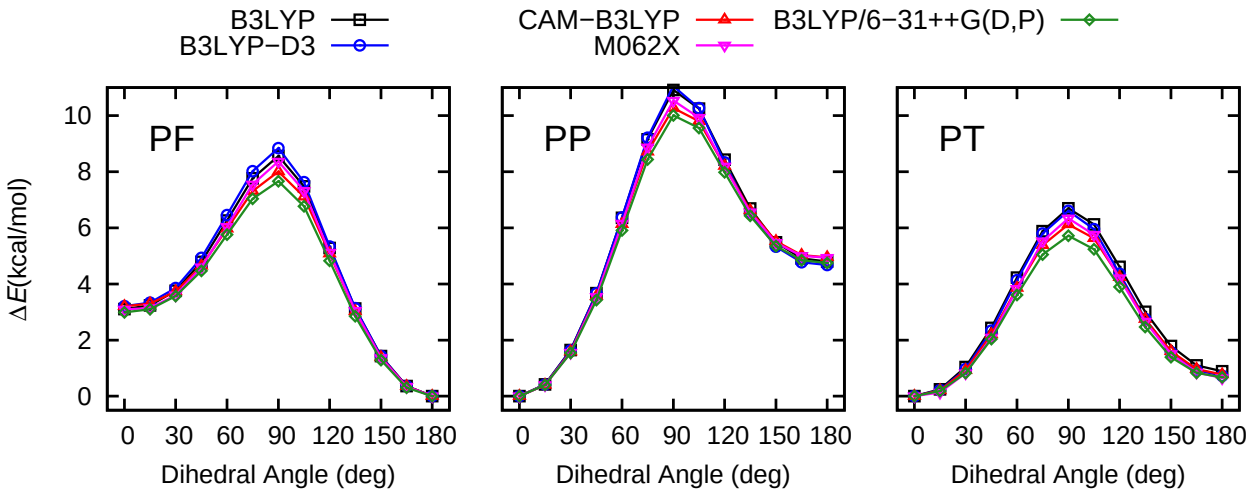

FIG. S2. Relaxed potential energy curves along ∠1-2-3-4, for $(PF)_1$ (a), $(PP)_1$ (b) and $(PT)_1$ (c). Energies are relative to the energy of the most stable structure in each case.

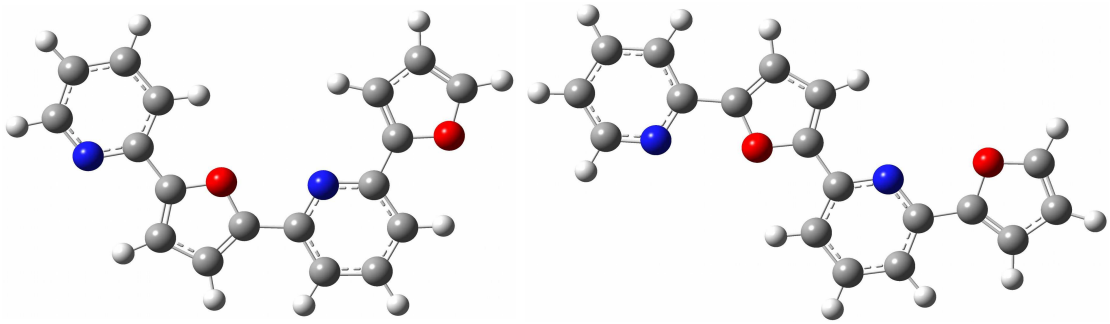

FIG. S3. Optimized structures of conformers **C** and **D** of $(PF)_2$ calculated at B3LYP-D3/6-31G(d) level.

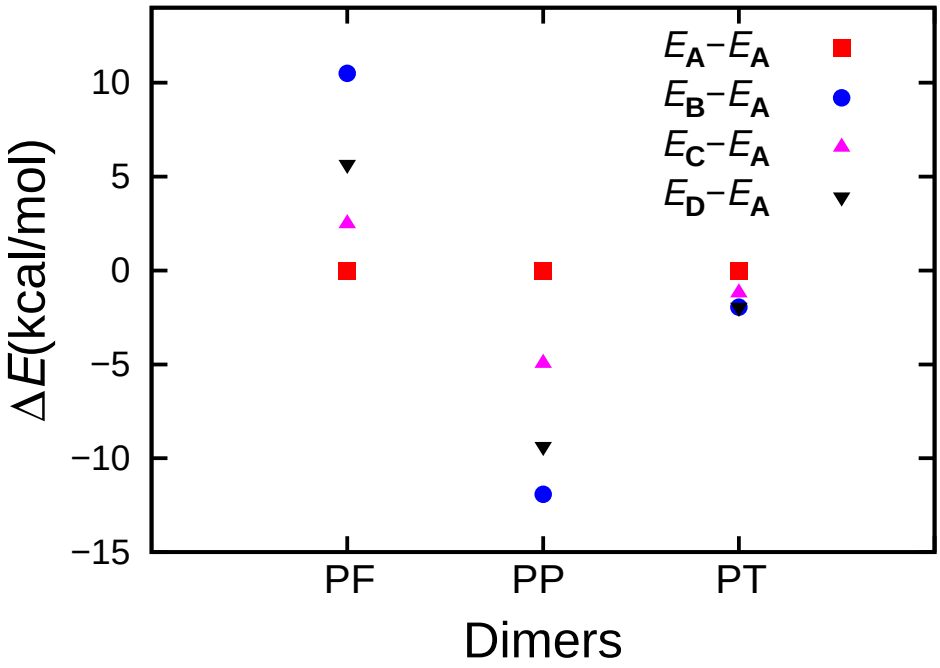

FIG. S4. Energies of different conformations of $(PF)_2$, $(PP)_2$ and $(PT)_2$ with respect to that of **A** calculated at B3LYP-D3/6-31G(d) level.

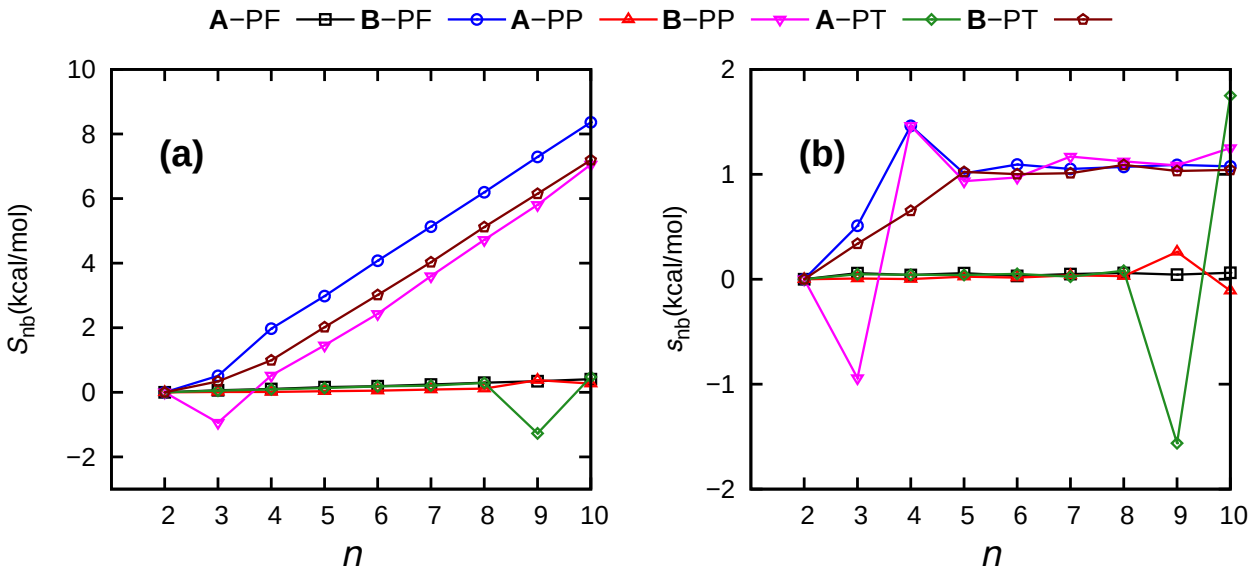

FIG. S5. Stabilization energies of the studied compounds at the B3LYP/6-31G(d) level. $S_{\mathrm{nb}} = [E_n - n \times E_1] - [(n-1)(E_2 - 2 \times E_1)]$ (a) and $s_{\mathrm{nb}} = (E_n - E_{n-1}) - (E_2 - E_1)$ (b) are plotted versus $n > 1$. Here, n and E_n are the number of repeating units and ground state energy of an oligomer having n number of repeating units, respectively.

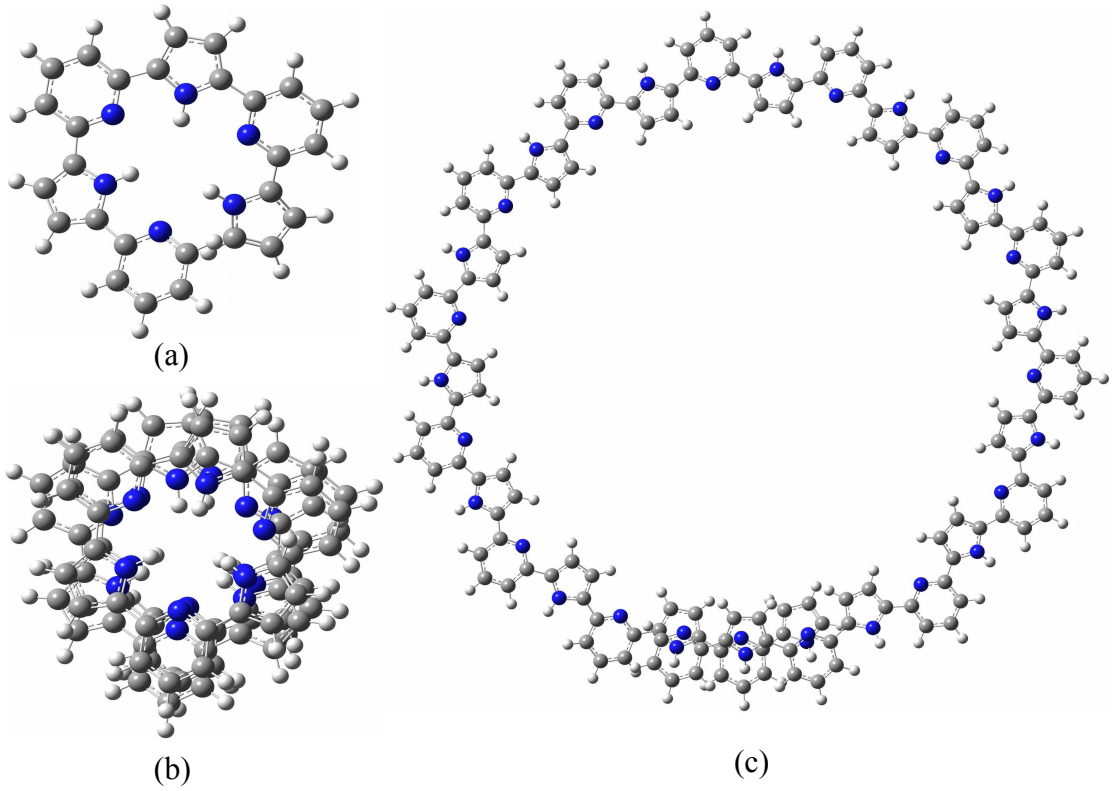

FIG. S6. Optimized structures of **B**-$(PP)_3$ (a), **B**-$(PP)_{10}$ (b) and **A**-$(PP)_{16}$ (c) obtained at B3LYP-D3/6-31G(d) level.

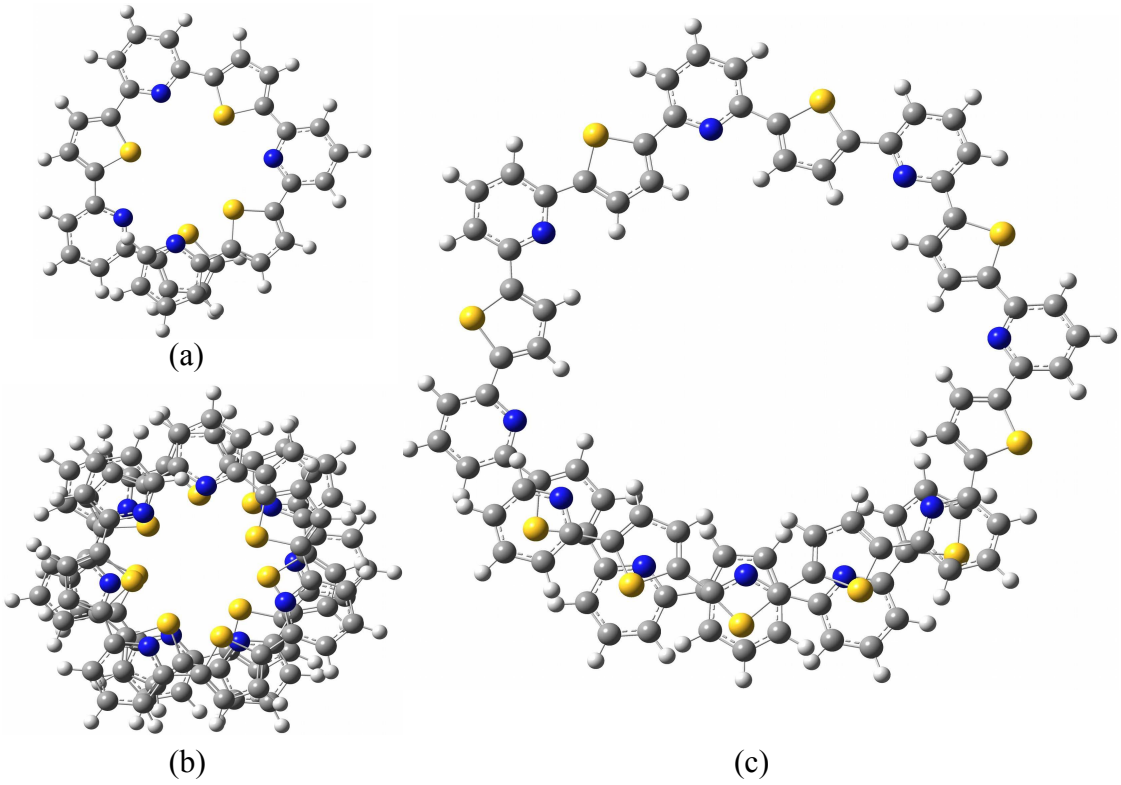

FIG. S7. Optimized structures of **B**-$(PT)_4$ (a), **B**-$(PT)_{10}$ (b) and **A**-$(PT)_{10}$ (c) obtained at B3LYP-D3/6-31G(d) level.

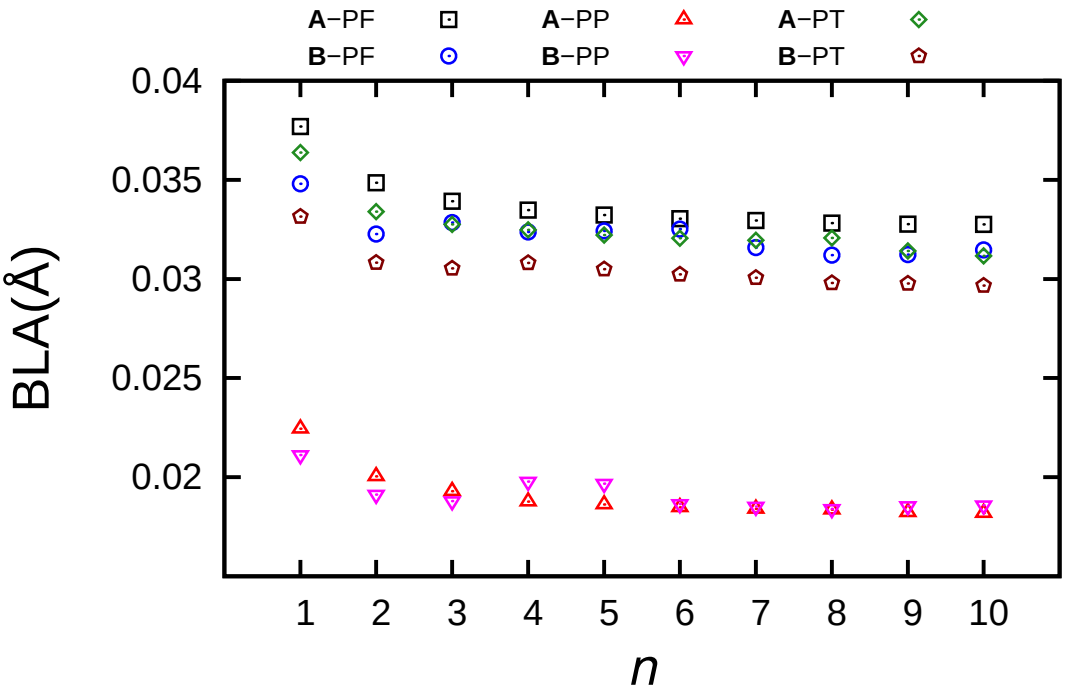

FIG. S8. Bond length alternation (Δr) values calculated as $(\frac{r_a+r_c+r_e}{3} - \frac{r_b+r_d}{2})/n$. Here, r_x is bond length of the x bond in each repeating unit of an oligomer. These bonds are shown in Fig 1.

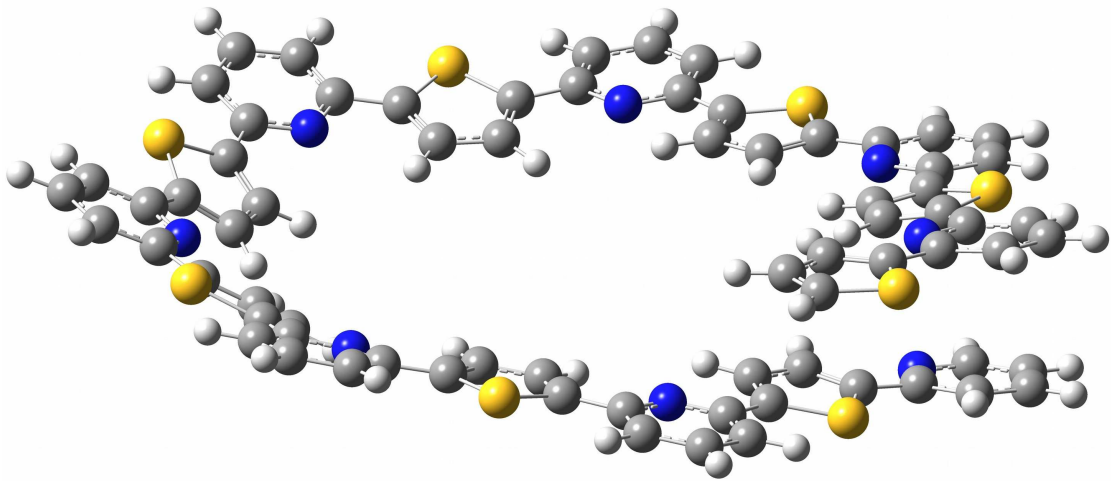

FIG. S9. Optimized structures of **A**-$(PT)_8$ obtained at B3LYP-D3/6-31G(d) level.

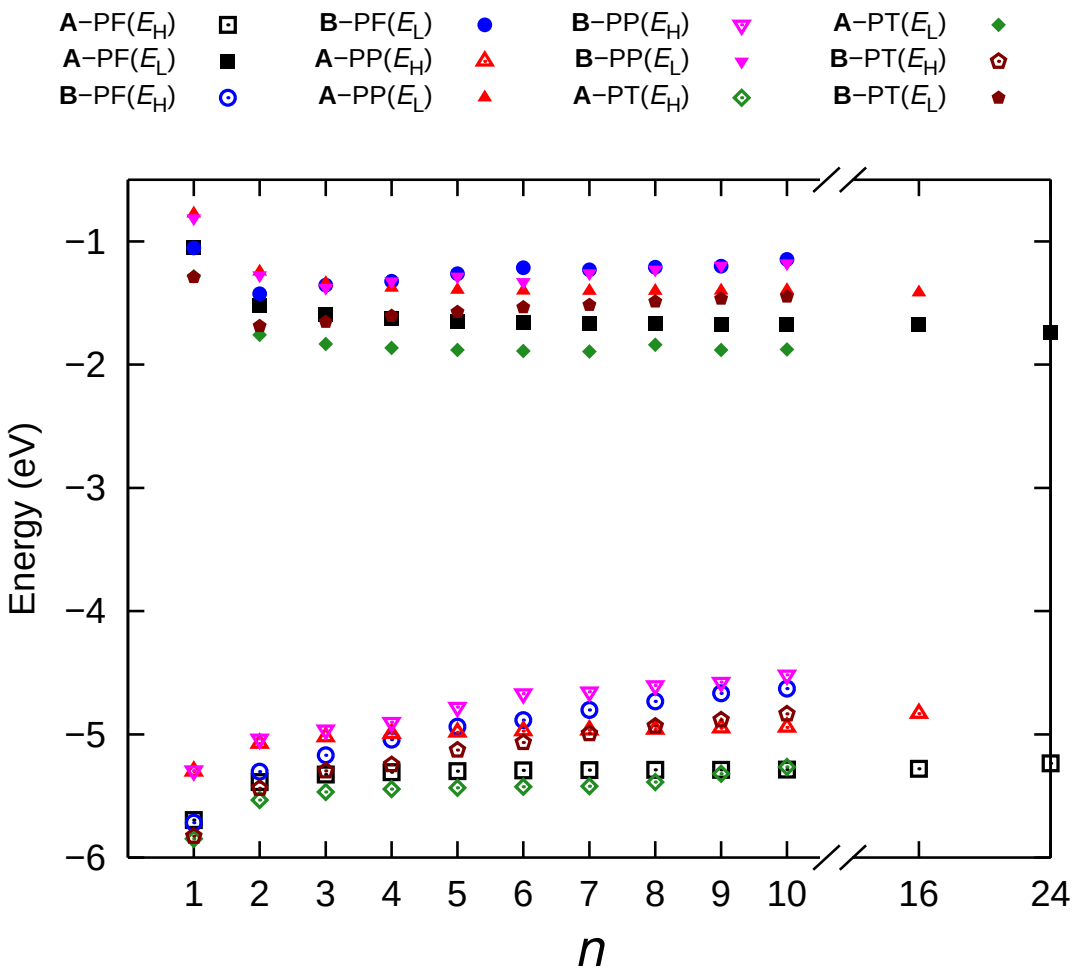

FIG. S10. Energies of HOMO and LUMO for all the studied compounds calculated at B3LYP-D3/6-31G(d) level. E_H and E_L represent energies of HOMO and LUMO, respectively. n stands for the number of repeating units. u values of **A**-PF, **B**-PF, **A**-PP, **B**-PP, **A**-PT and **B**-PT oligomers are 23, 3, 15, 3, 8 and 4, respectively.

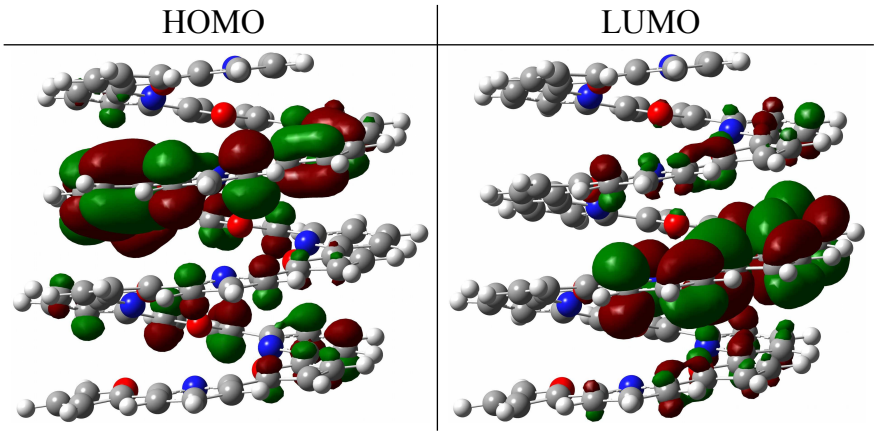

FIG. S11. HOMO and LUMO of **B**-$(PF)_{10}$at an isosurface value of 0.02.

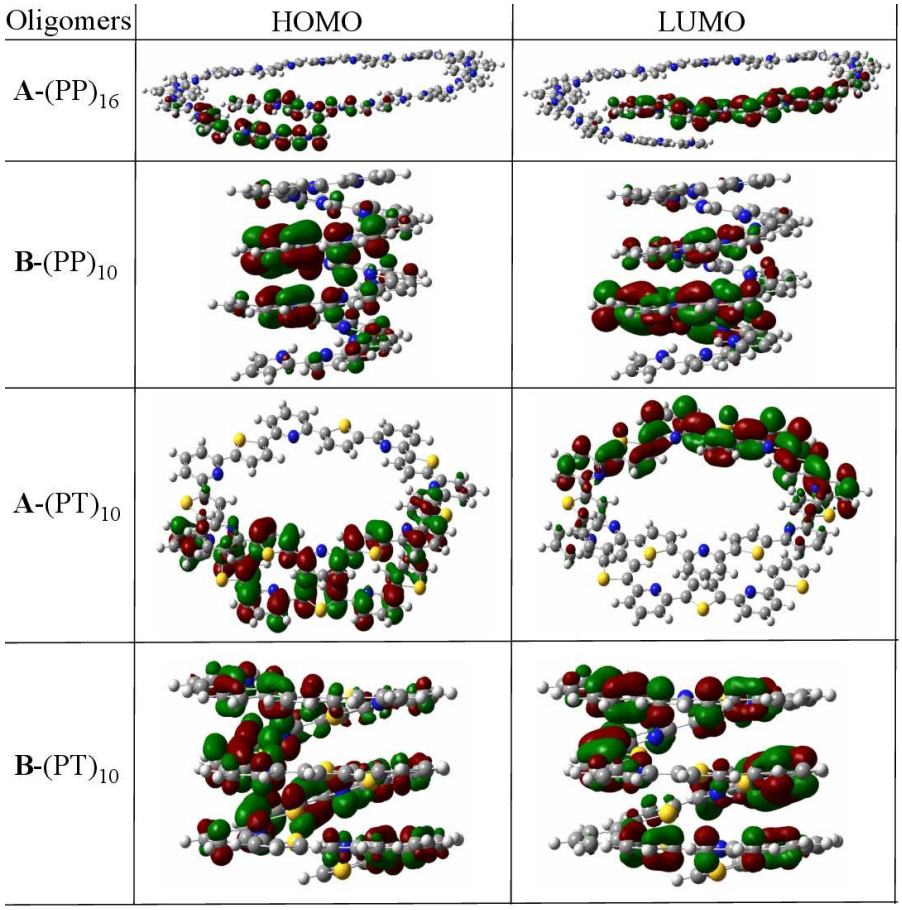

FIG. S12. Frontier molecular orbitals of **A**-$(PP)_{16}$, **B**-$(PP)_{10}$, **A**-$(PT)_{10}$ and **B**-$(PT)_{10}$ at an isosurface value of 0.02.

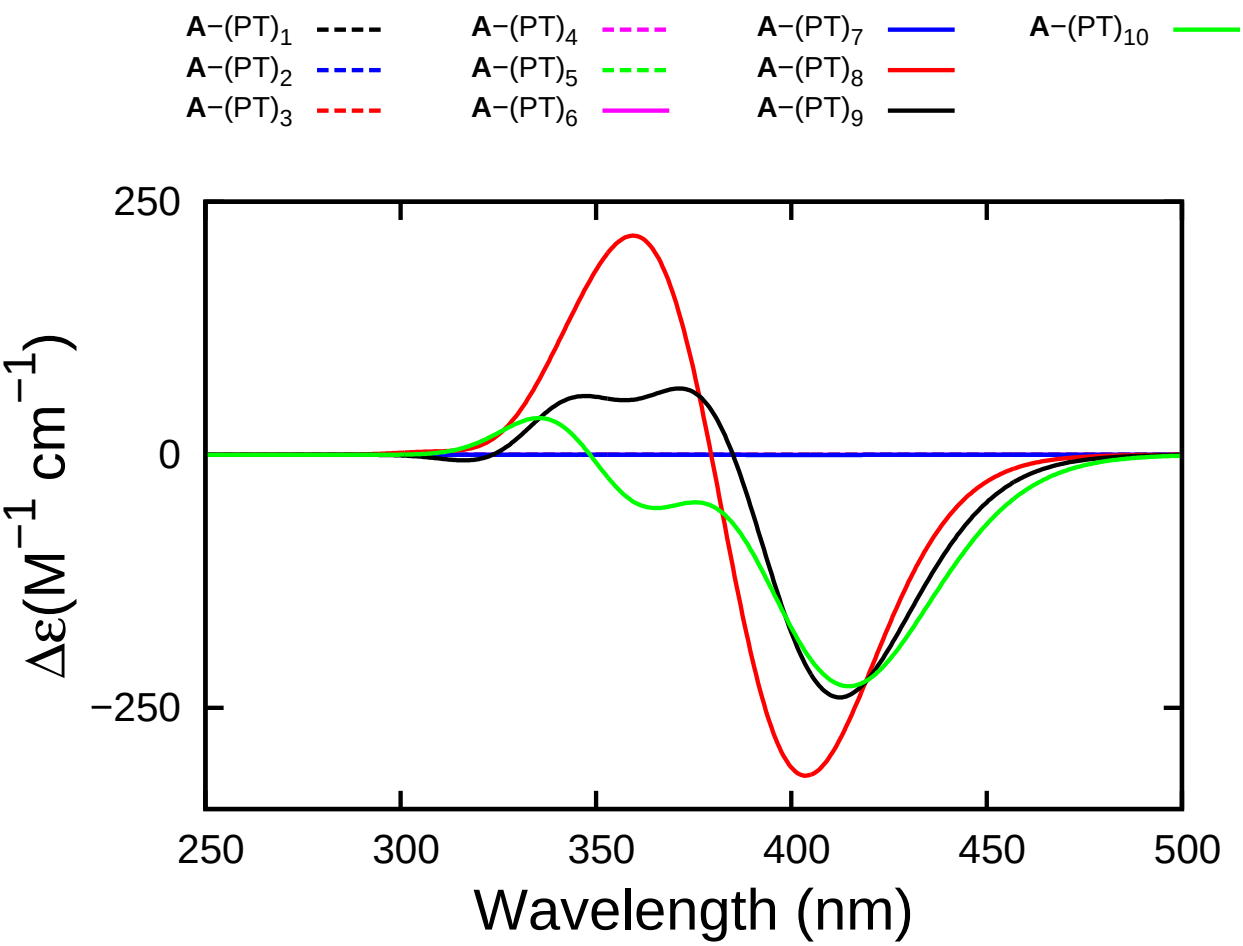

FIG. S13. CD spectra vs oligomer chain length of **A**-(PT).

TABLE S1. Differences in energies between the two possible conformations (i.e., $E_{\boldsymbol{i}} - E_{\boldsymbol{ii}}$) of monomers calculated using B3LYP, CAM-B3LYP, B3LYP-D3 and M06-2X functionals in combination with 6-31G(d) basis set. Values are in kcal/mol.

	B3LYP	CAM-B3LYP	B3LYP-D3	M06-2X
PF	-3.1	-3.2	-3.2	-3.1
PP	4.8	5.0	4.7	5.0
PT	0.9	0.8	0.7	0.7

TABLE S2. Energies of different conformations of $(PF)_2$, $(PP)_2$ and $(PT)_2$ with respect to that of **A** calculated at B3LYP-D3/6-31G(d) level. Values are in kcal/mol.

	$E_{\mathbf{B}}$-$E_{\mathbf{A}}$	$E_{\mathbf{C}}$-$E_{\mathbf{A}}$	$E_{\mathbf{D}}$-$E_{\mathbf{A}}$
PF	10.5	2.5	5.7
PP	-11.9	-5.0	-9.4
PT	-2.0	-1.2	-2.0

TABLE S3. The expectation values of the total spin, $<S^2>$, before annihilation (ba) and after annihilation (aa) of the studied molecules.

n	**A**-PF		**B**-PF		**A**-PP		**B**-PP		**A**-PT		**B**-PT	
	ba	aa	ba	aa	ba	aa	ba	aa	ba	aa	ba	aa
1	0.7652	0.7502	0.7647	0.7502	0.7661	0.7502	0.7652	0.7502	0.7665	0.7502	0.7658	0.7502
2	0.7661	0.7502	0.7663	0.7502	0.7678	0.7503	0.7684	0.7503	0.7669	0.7502	0.768	0.7503
3	0.7644	0.7502	0.7649	0.7502	0.7654	0.7502	0.7667	0.7502	0.7652	0.7502	0.7664	0.7502
4	0.7617	0.7501	0.7623	0.7501	0.7623	0.7501	0.7624	0.7501	0.7623	0.7501	0.7643	0.7502
5	0.7596	0.7501	0.7606	0.7501	0.7602	0.7501	0.7612	0.7501	0.7602	0.7501	0.761	0.7501
6	0.7583	0.7501	0.7597	0.7501	0.7587	0.7501	0.7598	0.7501	0.7588	0.7501	0.7595	0.7501
7	0.7573	0.7501	0.757	0.75	0.7577	0.7501	0.7576	0.7501	0.7578	0.7501	0.7585	0.7501
8	0.7565	0.75	0.7567	0.75	0.7568	0.75	0.7569	0.75	0.7568	0.75	0.7578	0.7501
9	0.7558	0.75	0.7571	0.7501	0.7562	0.75	0.757	0.7501	0.7564	0.75	0.7561	0.75
10	0.7553	0.75	0.7578	0.7501	0.7556	0.75	0.7561	0.75	0.7556	0.75	0.7582	0.7501
16	0.7534	0.75			0.7536	0.75						
24	0.7525	0.75										

TABLE S4. Electronic transition data obtained by TDDFT method for **A**-$(PP)_n$ and **B**-$(PP)_n$ at B3LYP-D3/6-31G(d) level. E_g, f_{osc}, H and L denote excitation energy, oscillator strength, HOMO and LUMO, respectively. Electronic transitions are from S_0 to S_m. E_gs are in eV.

n (**A**)	m	E_g	f_{osc}	Configuration/s
1	1	4.13	0.145	H → L (55%)
				H → L+1 (42%)
	2	4.49	0.427	H → L (44%)
				H → L+1 (54%)
2	1	3.49	0.416	H → L (63%)
	2	3.70	0.570	H-1 → L (38%)
				H → L (31%)
3	1	3.33	0.250	H → L+1 (74%)
	2	3.41	0.907	H → L (46%)
4	1	3.29	0.872	H → L+2 (54%)
5	1	3.26	2.407	H → L+3 (55%)
6	1	3.24	3.023	H → L+4 (43%)
7	1	3.22	3.340	H → L+5 (33%)
				H-1 → L-4 (22%)
8	1	3.20	3.399	H → L+6 (27%)
				H-1 → L+5 (20%)
9	1	3.19	3.209	H → L+7 (21%)
				H-1 → L+6 (19%)
10	1	3.18	2.885	H → L+8 (19%)
				H-1 → L+7 (17%)
	2	3.27	3.484	H → L+7 (14%)
				H → L+8 (12%)
16	1	2.98	0.069	H → L (47%)
	5	3.21	3.595	H → L+14 (12%)
	6	3.23	3.562	H → L (6%)
				H → L+4 (6%)

n (**B**)	m	E_g	f_{osc}	Configuration/s
1	1	4.12	0.165	H → L (62%)
	14	7.51	0.407	H-4 → L+1 (40%)
2	1	3.37	0.390	H → L (86%)
	2	3.79	0.344	H-1 → L (88%)
3	1	3.10	0.092	H → L (86%)
	8	3.97	0.595	H-2 → L+1 (34%)
4	1	3.01	0.025	H-1 → L (45%)
				H → L+1 (33%)
	14	3.98	0.373	H-3 → L (20%)
				H → L+4 (25%)
5	1	2.94	0.025	H → L+1 (64%)
	21	3.93	0.397	H-4 → L+3 (23%)
6	1	2.83	0.015	H → L (86%)
	37	4.06	0.617	H-5 → L+3 (18%)
7	1	2.84	0.015	H → L (46%)
8	1	2.84	0.012	H → L (46%)
9	1	2.84	0.022	H-1 → L+1 (32%)
10	1	2.80	0.003	H → L (75%)
	114	4.15	0.243	H-2 → L+13 (14%)
				H → L+18 (12%)
	117	4.18	0.310	H-9 → L+7 (13%)
				H-2 → L+15 (15%)

TABLE S5. Electronic transition data obtained by TDDFT method for **A**-$(PT)_n$ and **B**-$(PT)_n$ at B3LYP-D3/6-31G(d) level. E_g, f_{osc}, H and L denote excitation energy, oscillator strength, HOMO and LUMO, respectively. Electronic transitions are from S_0 to S_m. E_gs are in eV.

n (**A**)	m	E_g	f_{osc}	Configuration/s
1	1	4.30	0.422	H → L (90%)
	18	7.26	0.436	H-4 → L+1 (47%)
2	1	3.47	0.691	H → L (82%)
3	1	3.28	0.732	H → L+1 (94%)
4	1	3.23	1.277	H → L+2 (77%)
5	1	3.20	1.495	H → L+3 (63%)
6	1	3.17	1.406	H → L+4 (53%)
7	1	3.15	1.117	H → L+5 (45%)
	2	3.25	1.592	H → L+4 (42%)
8	1	3.13	0.016	H → L+4 (13%)
	2	3.23	0.651	H-1 → L+4 (21%)
				H → L+1 (30%)
9	1	3.07	0.065	H → L+5 (35%)
	6	3.21	0.635	H → L+7 (28%)
				H-1 → L+5 (17%)
10	1	3.02	0.252	H → L+3 (54%)
	8	3.21	0.502	H → L (30%)
	11	3.27	0.432	H-2 → L+2 (18%)
				H-2 → L+4 (12%)

n (**B**)	m	E_g	f_{osc}	Configuration/s
1	1	4.26	0.400	H → L (92%)
	16	7.23	0.511	H-4 → L+1 (39%)
2	1	3.40	0.555	H → L (85%)
3	1	3.16	0.307	H → L (82%)
	4	3.62	0.422	H-1 → L (61%)
4	1	3.07	0.049	H-1 → L (40%)
				H → L+1 (42%)
	5	3.43	0.459	H-1 → L+2 (72%)
5	1	2.98	0.015	H → L (56%)
	24	4.02	0.389	H-4 → L+3 (60%)
6	1	2.96	0.019	H → L+1 (56%)
	17	3.48	0.258	H-2 → L+3 (23%)
7	1	2.93	0.011	H-1 → L+1 (20%)
				H → L (23%)
	28	3.61	0.356	H-3 → L+5 (44%)
8	1	2.89	0.007	H → L (48%)
	35	3.56	0.301	H-5 → L (26%)
9	1	2.87	0.008	H-1 → L (26%)
				H → L+1 (31%)
	45	3.56	0.154	H-6 → L+1 (23%)
10	1	2.85	0.005	H → L (49%)
	52	3.52	0.163	H-5 → L+5 (21%)
	54	3.54	0.144	H-4 → L+8 (26%)
	108	4.08	0.157	H → L+10 (19%)

TABLE S6: xyz coordinates of the optimized structure of **A**-$(PF)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

162			
C	14.2790	-0.7472	0.0001
C	15.3586	-1.5959	0.0002
C	13.5549	-2.8675	0.0002
C	13.1184	-1.5654	0.0002
C	16.7934	-1.3554	0.0002
N	17.1647	-0.0644	0.0001
C	18.4776	0.2198	0.0001
C	19.4740	-0.7731	0.0002
C	19.0740	-2.1058	0.0003
C	17.7173	-2.4160	0.0002
H	20.5212	-0.4937	0.0002
H	19.8162	-2.8995	0.0003
H	17.3685	-3.4422	0.0003
H	14.3391	0.3307	0.0001
H	12.0830	-1.2597	0.0001
C	10.7970	-5.1954	0.0002
C	11.3974	-6.4675	0.0003
C	12.7872	-6.5382	0.0003
C	13.5350	-5.3646	0.0003
C	12.8463	-4.1381	0.0002
N	11.5057	-4.0543	0.0002
H	10.7823	-7.3599	0.0003
H	13.2855	-7.5038	0.0003
H	14.6187	-5.3807	0.0003
C	7.2694	-5.7697	0.0002
C	7.2034	-4.3980	0.0002
C	8.5428	-3.9263	0.0002

C	9.3509	-5.0366	0.0002
H	6.2901	-3.8224	0.0002
H	8.8942	-2.9055	0.0002
O	14.9241	-2.8945	0.0002
O	8.5795	-6.1682	0.0002
C	18.8144	1.6350	0.0001
C	18.0416	2.7702	0.0000
O	20.1398	1.9799	0.0001
C	18.9373	3.8722	-0.0001
H	16.9621	2.7838	0.0000
C	20.2065	3.3477	0.0000
H	18.7035	4.9261	-0.0001
C	21.5229	3.9673	0.0000
C	22.6987	3.1954	0.0001
N	21.5316	5.3106	-0.0001
C	23.9212	3.8603	0.0001
H	22.6398	2.1131	0.0002
C	22.7190	5.9388	-0.0001
C	23.9465	5.2516	0.0000
H	24.8502	3.2966	0.0001
C	22.6613	7.3922	-0.0002
H	24.8793	5.8034	0.0000
C	21.6101	8.2759	-0.0003
O	23.8441	8.0828	-0.0002
C	22.1737	9.5792	-0.0003
H	20.5672	7.9966	-0.0003
C	23.5376	9.4178	-0.0003
H	21.6640	10.5309	-0.0004
C	24.6352	10.3715	-0.0003
N	24.2773	11.6724	-0.0004

C	25.9767	9.9520	-0.0003
C	25.2528	12.5818	-0.0005
C	26.9761	10.9194	-0.0003
H	26.2131	8.8937	-0.0002
C	26.6149	12.2672	-0.0004
H	24.9302	13.6220	-0.0006
H	28.0223	10.6253	-0.0003
H	27.3621	13.0547	-0.0004
C	6.2416	-6.7993	0.0002
N	4.9744	-6.3536	0.0002
C	6.5702	-8.1669	0.0002
C	3.9818	-7.2587	0.0001
C	5.5312	-9.0926	0.0002
H	7.6086	-8.4777	0.0002
C	2.6339	-6.7115	0.0001
C	4.2132	-8.6461	0.0001
H	5.7476	-10.1575	0.0002
O	1.5827	-7.5893	0.0001
C	2.1598	-5.4226	0.0001
H	3.3784	-9.3374	0.0001
C	0.4312	-6.8479	0.0001
C	0.7426	-5.5104	0.0001
H	2.7767	-4.5366	0.0002
H	0.0210	-4.7075	0.0001
C	-0.8387	-7.5577	0.0000
N	-1.9360	-6.7829	0.0000
C	-0.8957	-8.9631	0.0000
C	-3.1379	-7.3827	0.0000
C	-2.1481	-9.5700	-0.0001
H	0.0187	-9.5450	0.0000

C	-4.2854	-6.4883	0.0000
C	-3.2941	-8.7805	-0.0001
H	-2.2306	-10.6535	-0.0001
O	-5.5361	-7.0461	-0.0001
C	-4.3899	-5.1191	0.0001
H	-4.2860	-9.2175	-0.0001
C	-6.4418	-6.0188	-0.0001
C	-5.7774	-4.8169	0.0000
H	-3.5549	-4.4349	0.0001
C	-7.8571	-6.3554	-0.0001
H	-6.2521	-3.8473	0.0001
N	-8.7016	-5.3108	-0.0001
C	-8.2952	-7.6920	-0.0002
C	-10.0214	-5.5603	-0.0002
C	-9.6656	-7.9346	-0.0003
H	-7.5743	-8.5013	-0.0003
C	-10.8820	-4.3873	-0.0001
C	-10.5530	-6.8626	-0.0003
H	-10.0402	-8.9546	-0.0004
O	-12.2374	-4.5837	-0.0002
C	-10.6100	-3.0413	0.0000
H	-11.6264	-7.0125	-0.0003
C	-12.8293	-3.3487	-0.0002
C	-11.8630	-2.3730	0.0000
H	-9.6202	-2.6103	0.0001
C	-14.2828	-3.2870	-0.0003
H	-12.0563	-1.3109	0.0000
N	-14.8104	-2.0517	-0.0002
C	-15.0688	-4.4535	-0.0004
C	-16.1483	-1.9315	-0.0003

C	-16.4533	-4.3129	-0.0005
H	-14.5959	-5.4287	-0.0004
C	-16.6560	-0.5682	-0.0002
C	-17.0147	-3.0395	-0.0004
H	-17.0921	-5.1920	-0.0006
C	-16.0263	0.6522	0.0000
O	-18.0135	-0.3866	-0.0003
H	-18.0883	-2.8910	-0.0005
C	-17.0488	1.6375	0.0000
H	-14.9564	0.7963	0.0001
C	-18.2451	0.9632	-0.0002
H	-16.9445	2.7120	0.0001
C	-19.6264	1.4201	-0.0003
C	-20.7013	0.5131	-0.0005
N	-19.7960	2.7526	-0.0001
C	-21.9946	1.0270	-0.0005
H	-20.5131	-0.5543	-0.0006
C	-21.0500	3.2343	-0.0002
C	-22.1865	2.4052	-0.0004
H	-22.8494	0.3560	-0.0007
C	-21.1659	4.6843	0.0000
H	-23.1786	2.8415	-0.0005
C	-20.2274	5.6867	0.0002
O	-22.4224	5.2294	-0.0001
C	-20.9425	6.9136	0.0003
H	-19.1588	5.5336	0.0004
C	-22.2773	6.5911	0.0001
H	-20.5493	7.9190	0.0005
C	-23.4817	7.4076	0.0000
N	-23.2803	8.7361	0.0003

C	-24.7631	6.8288	-0.0003
C	-24.3542	9.5420	0.0002
C	-25.8665	7.6771	-0.0004
H	-24.8741	5.7506	-0.0005
C	-24.0705	10.9707	0.0005
C	-25.6738	9.0552	-0.0001
H	-26.8724	7.2659	-0.0006
O	-25.1349	11.8372	0.0004
C	-22.8988	11.6795	0.0009
H	-26.5083	9.7468	-0.0001
C	-24.6224	13.0986	0.0007
C	-23.2592	13.0618	0.0011
H	-21.9102	11.2459	0.0010
H	-25.3470	13.8990	0.0007
H	-22.5938	13.9138	0.0014

TABLE S7: xyz coordinates of the optimized structure of **A**-$(PF)_{24}$ obtained at B3LYP/3-21G level.

386

C	23.2564	-6.4990	-2.1206
C	21.9664	-6.1937	-1.6600
N	21.5167	-4.9252	-1.5415
C	22.3416	-3.9156	-1.8971
C	23.6449	-4.1379	-2.3720
C	24.1008	-5.4496	-2.4774
C	21.0351	-7.2431	-1.3018
C	19.7210	-7.2094	-0.9071
C	19.2946	-8.5622	-0.7313
C	20.3656	-9.3698	-1.0203
O	21.4643	-8.5749	-1.3753
C	20.5223	-10.8088	-1.0252
N	19.4142	-11.5354	-0.7640
C	19.5104	-12.8827	-0.7717
C	20.7187	-13.5513	-1.0268
C	21.8565	-12.7913	-1.2892
C	21.7669	-11.4009	-1.2945
C	18.2878	-13.6172	-0.5265
C	16.9978	-13.2042	-0.3060
C	16.1914	-14.3762	-0.1792
C	17.0203	-15.4602	-0.3247
O	18.3330	-15.0181	-0.5379
C	16.7617	-16.8841	-0.3081
N	15.4701	-17.2570	-0.1802
C	15.1767	-18.5753	-0.1750
C	16.1638	-19.5678	-0.2856
C	17.4935	-19.1715	-0.4120

C	17.8069	-17.8139	-0.4280
C	13.7756	-18.9210	-0.0682
C	12.6453	-18.1476	0.0171
C	11.5262	-19.0335	0.0645
C	12.0159	-20.3141	0.0074
O	13.4146	-20.2752	-0.0731
C	11.3555	-21.6017	0.0091
N	10.0058	-21.5825	0.0481
C	9.3435	-22.7593	0.0443
C	10.0054	-23.9969	0.0066
C	11.3981	-24.0047	-0.0314
C	12.0919	-22.7964	-0.0322
C	7.8987	-22.6831	0.0732
C	7.0380	-21.6147	0.0969
C	5.7095	-22.1388	0.1057
C	5.8098	-23.5072	0.0875
O	7.1619	-23.8753	0.0677
C	4.8061	-24.5496	0.0845
N	3.5186	-24.1421	0.0924
C	2.5457	-25.0786	0.0894
C	2.8238	-26.4548	0.0796
C	4.1558	-26.8635	0.0715
C	5.1679	-25.9061	0.0735
C	1.1835	-24.5903	0.0947
C	0.6648	-23.3200	0.0973
C	-0.7582	-23.4414	0.0991
C	-1.0541	-24.7813	0.0980
O	0.1360	-25.5213	0.0952
C	-2.3138	-25.4935	0.1003
N	-3.4317	-24.7358	0.0994

C	-4.6312	-25.3563	0.1023
C	-4.7569	-26.7547	0.1066
C	-3.5969	-27.5262	0.1073
C	-2.3539	-26.8969	0.1039
C	-5.7982	-24.5006	0.1001
C	-5.9352	-23.1354	0.0928
C	-7.3343	-22.8480	0.0931
C	-7.9982	-24.0488	0.1007
O	-7.0668	-25.0960	0.1051
C	-9.4078	-24.3755	0.1049
N	-10.2663	-23.3330	0.0985
C	-11.5921	-23.5898	0.1023
C	-12.1075	-24.8958	0.1129
C	-11.2125	-25.9634	0.1195
C	-9.8425	-25.7106	0.1154
C	-12.4712	-22.4403	0.0945
C	-12.2196	-21.0914	0.0827
C	-13.4820	-20.4231	0.0790
C	-14.4562	-21.3894	0.0887
O	-13.8558	-22.6557	0.0985
C	-15.9010	-21.3088	0.0902
N	-16.4344	-20.0682	0.0796
C	-17.7793	-19.9451	0.0801
C	-18.6384	-21.0557	0.0914
C	-18.0769	-22.3305	0.1022
C	-16.6908	-22.4697	0.1018
C	-18.3039	-18.5966	0.0682
C	-17.6879	-17.3705	0.0570
C	-18.7153	-16.3780	0.0485
C	-19.9193	-17.0361	0.0547

O	-19.6939	-18.4192	0.0670
C	-21.2853	-16.5587	0.0505
C	-22.3654	-17.4560	0.0578
C	-23.6589	-16.9392	0.0529
C	-23.8461	-15.5587	0.0410
C	-22.7135	-14.7289	0.0346
N	-21.4550	-15.2188	0.0393
C	-22.8449	-13.2878	0.0229
C	-21.9139	-12.2799	0.0166
C	-22.6268	-11.0421	0.0067
C	-23.9658	-11.3416	0.0071
O	-24.1317	-12.7331	0.0171
C	-25.1463	-10.5047	0.0001
C	-26.4327	-11.0678	0.0005
C	-27.5324	-10.2127	-0.0065
C	-27.3300	-8.8345	-0.0135
C	-26.0116	-8.3509	-0.0131
N	-24.9383	-9.1704	-0.0066
C	-25.7384	-6.9300	-0.0189
C	-24.5642	-6.2201	-0.0189
C	-24.9056	-4.8331	-0.0244
C	-26.2751	-4.7491	-0.0275
O	-26.8207	-6.0398	-0.0242
C	-27.1767	-3.6173	-0.0324
C	-28.5688	-3.8003	-0.0362
C	-29.3874	-2.6732	-0.0400
C	-28.8097	-1.4055	-0.0400
C	-27.4090	-1.3077	-0.0362
N	-26.6057	-2.3933	-0.0327
C	-26.7507	-0.0191	-0.0352

C	-25.4251	0.3352	-0.0321
C	-25.3662	1.7624	-0.0317
C	-26.6579	2.2249	-0.0344
O	-27.5420	1.1375	-0.0368
C	-27.2076	3.5635	-0.0343
C	-28.5954	3.7766	-0.0373
C	-29.0665	5.0879	-0.0365
C	-28.1575	6.1434	-0.0328
C	-26.7854	5.8461	-0.0300
N	-26.3175	4.5791	-0.0308
C	-25.7930	6.8992	-0.0258
C	-24.4211	6.8683	-0.0232
C	-23.9651	8.2220	-0.0192
C	-25.0759	9.0275	-0.0193
O	-26.2290	8.2310	-0.0235
H	-9.1120	-26.5068	0.1202
H	-11.5792	-26.9826	0.1278
H	-13.1777	-25.0442	0.1155
H	-7.8109	-21.8846	0.0883
H	-5.1173	-22.4379	0.0876
H	-1.4284	-27.4546	0.1044
H	-3.6610	-28.6075	0.1105
H	-5.7416	-27.1993	0.1088
H	-1.4889	-22.6531	0.1011
H	1.2509	-22.4189	0.0975
H	6.2139	-26.1766	0.0669
H	4.4027	-27.9183	0.0635
H	2.0065	-27.1616	0.0776
H	4.7837	-21.5928	0.1224
H	7.3417	-20.5837	0.1044

H	13.1712	-22.7544	-0.0634
H	11.9377	-24.9436	-0.0614
H	9.4262	-24.9092	0.0056
H	10.4840	-18.7787	0.1299
H	12.6385	-17.0729	0.0364
H	18.8231	-17.4609	-0.5295
H	18.2779	-19.9135	-0.5002
H	15.8737	-20.6086	-0.2758
H	15.1320	-14.4336	-0.0061
H	16.6836	-12.1775	-0.2531
H	22.6214	-10.7716	-1.4987
H	22.8032	-13.2780	-1.4913
H	20.7391	-14.6316	-1.0215
H	-11.2391	-20.6511	0.0773
H	-13.6691	-19.3647	0.0704
H	-19.7076	-20.8996	0.0912
H	-18.7133	-23.2069	0.1110
H	-16.2112	-23.4377	0.1099
H	-16.6237	-17.2194	0.0550
H	-18.6014	-15.3091	0.0387
H	-22.1719	-18.5190	0.0668
H	-24.5128	-17.6057	0.0581
H	-24.8303	-15.1133	0.0367
H	-22.2218	-10.0464	0.0003
H	-20.8494	-12.4290	0.0193
H	-26.5414	-12.1427	0.0060
H	-28.5375	-10.6166	-0.0066
H	-28.1522	-8.1337	-0.0188
H	-24.2400	-3.9889	-0.0259
H	-23.5829	-6.6589	-0.0152

H	19.1430	-6.3123	-0.7786
H	18.3231	-8.9151	-0.4366
H	23.5652	-7.5321	-2.1892
H	24.2641	-3.2928	-2.6366
H	-29.4047	-0.5036	-0.0426
H	-30.4652	-2.7816	-0.0428
H	-28.9723	-4.8026	-0.0356
H	-24.6052	-0.3598	-0.0303
H	-24.4916	2.3874	-0.0293
H	-28.4769	7.1756	-0.0318
H	-30.1316	5.2849	-0.0386
H	-29.2630	2.9271	-0.0399
H	-23.8285	5.9717	-0.0243
H	-22.9506	8.5773	-0.0163
O	22.6352	-1.5003	-2.1437
C	21.8198	-2.5727	-1.7604
C	20.6213	-2.0900	-1.2966
H	19.8083	-2.6998	-0.9455
C	20.6770	-0.6637	-1.3775
H	19.9158	0.0436	-1.1006
C	21.9064	-0.3313	-1.8909
C	22.5299	0.9434	-2.1736
C	23.7795	1.0116	-2.8051
C	24.3429	2.2623	-3.0427
C	23.6485	3.4075	-2.6449
C	22.4103	3.2511	-2.0174
N	21.8500	2.0496	-1.7812
H	24.2799	0.0962	-3.0878
H	25.3095	2.3435	-3.5257
H	24.0572	4.3967	-2.8051

H	21.8550	4.1189	-1.6807
C	-25.2289	10.4665	-0.0155
C	-26.5013	11.0599	-0.0164
C	-26.5861	12.4504	-0.0121
C	-25.4178	13.2093	-0.0069
C	-24.1839	12.5392	-0.0063
N	-24.0899	11.1921	-0.0106
H	-27.3802	10.4314	-0.0204
H	-27.5535	12.9381	-0.0127
H	-25.4354	14.2896	-0.0032
O	-22.9816	14.6726	0.0053
C	-21.6517	15.1142	0.0104
C	-20.8110	14.0297	0.0074
H	-19.7376	14.0867	0.0103
C	-21.6280	12.8580	0.0004
H	-21.3102	11.8312	-0.0034
C	-22.9363	13.2720	-0.0007
C	-19.8116	18.2355	0.0313
C	-20.8084	19.2243	0.0341
C	-22.1425	18.8231	0.0284
C	-22.4506	17.4645	0.0203
C	-21.3953	16.5383	0.0181
N	-20.0986	16.9158	0.0234
H	-20.5226	20.2663	0.0406
H	-22.9345	19.5622	0.0303
H	-23.4704	17.1074	0.0159
O	-18.0598	19.9466	0.0465
C	-18.4086	18.5895	0.0369
C	-17.2687	17.8256	0.0346
H	-17.2514	16.7509	0.0276

C	-16.1563	18.7215	0.0430
H	-15.1098	18.4753	0.0438
C	-16.6594	19.9980	0.0501
C	-16.0144	21.2933	0.0604
C	-16.7681	22.4779	0.0674
C	-16.0919	23.6958	0.0773
C	-14.6989	23.7073	0.0799
C	-14.0188	22.4789	0.0724
N	-14.6639	21.2925	0.0629
H	-17.8470	22.4206	0.0652
H	-16.6452	24.6271	0.0830
H	-14.1326	24.6275	0.0875
O	-11.8582	23.6315	0.0855
C	-10.4993	23.2893	0.0847
C	-10.3731	21.9230	0.0736
H	-9.4374	21.3942	0.0705
C	-11.6919	21.3740	0.0672
H	-11.9758	20.3373	0.0582
C	-12.5727	22.4261	0.0745
C	-9.5182	24.3529	0.0944
C	-9.9115	25.7007	0.1062
C	-8.9225	26.6817	0.1148
C	-7.5816	26.3041	0.1111
C	-7.2712	24.9348	0.0989
N	-8.2215	23.9754	0.0911
H	-10.9637	25.9466	0.1083
H	-9.1940	27.7303	0.1240
H	-6.7811	27.0298	0.1170
O	-4.8757	25.4410	0.0969
C	-3.6652	24.7350	0.0851

C	-3.9235	23.3874	0.0746
H	-3.1715	22.6194	0.0640
C	-5.3429	23.2262	0.0795
H	-5.9035	22.3090	0.0735
C	-5.8969	24.4814	0.0926
C	-2.4279	25.4855	0.0820
C	-2.4339	26.8895	0.0961
C	-1.2126	27.5595	0.0890
C	-0.0282	26.8266	0.0674
C	-0.1077	25.4247	0.0545
N	-1.2860	24.7646	0.0626
H	-3.3772	27.4161	0.1115
H	-1.1840	28.6424	0.0996
H	0.9414	27.3032	0.0601
O	2.3335	25.2540	0.0082
C	1.0887	24.6110	0.0293
C	1.2776	23.2519	0.0176
H	0.4875	22.5232	0.0290
C	2.6868	23.0183	-0.0123
C	4.6989	24.6287	-0.0498
C	5.0738	25.9819	-0.0538
C	6.4305	26.2958	-0.0886
C	7.3712	25.2692	-0.1184
C	6.9148	23.9411	-0.1114
N	5.6023	23.6249	-0.0775
H	4.3088	26.7444	-0.0306
H	6.7514	27.3305	-0.0925
H	8.4334	25.4650	-0.1461
O	9.2186	23.1206	-0.1817
C	9.8836	21.8872	-0.1996

C	8.9610	20.8721	-0.1700
C	7.8474	22.8348	-0.1399
C	7.6659	21.4748	-0.1325
H	9.2015	19.8244	-0.1749
H	6.7100	20.9839	-0.1027
C	3.3042	24.2437	-0.0181
H	3.1994	22.0737	-0.0288
C	11.3303	21.8876	-0.2417
C	12.0487	23.0938	-0.2724
C	13.4398	23.0386	-0.3106
C	14.0764	21.7999	-0.3158
C	13.2863	20.6395	-0.2829
N	11.9367	20.6806	-0.2477
H	11.5116	24.0313	-0.2657
H	14.0220	23.9518	-0.3352
H	15.1526	21.7081	-0.3430
O	15.2955	19.2459	-0.3031
C	13.8969	19.3271	-0.2797
C	13.3682	18.0614	-0.2482
H	12.3173	17.8360	-0.2245
C	14.4627	17.1424	-0.2492
H	14.4228	16.0684	-0.2259
C	15.6177	17.8822	-0.2818
C	18.5869	15.8015	-0.2254
C	19.6487	16.7197	-0.2584
C	19.3516	18.0795	-0.3075
C	18.0207	18.4897	-0.3193
C	17.0162	17.5089	-0.2838
N	17.2922	16.1873	-0.2410
H	20.6656	16.3552	-0.2428

H	20.1489	18.8122	-0.3340
H	17.7424	19.5330	-0.3521
O	20.1729	13.9454	-0.0998
C	20.1364	12.5470	-0.0188
C	18.8311	12.1245	-0.0352
H	18.5180	11.0975	0.0188
C	18.0075	13.2891	-0.1253
H	16.9340	13.3373	-0.1559
C	18.8415	14.3781	-0.1605
C	21.3917	11.8351	0.0938
C	22.6119	12.5303	0.1045
C	23.7910	11.8024	0.2445
C	23.7295	10.4171	0.3732
C	22.4701	9.7960	0.3487
N	21.3204	10.4909	0.2063
H	22.6096	13.6064	0.0099
H	24.7477	12.3101	0.2568
H	24.6168	9.8121	0.4916
O	23.5173	7.6182	0.7217
C	22.3506	8.3602	0.4884
C	21.2725	7.5126	0.4534
H	20.2546	7.8205	0.2959
C	21.7643	6.1879	0.6728
H	21.2000	5.2742	0.7306
C	23.1243	6.2786	0.8366
C	24.1358	5.2879	1.1431
C	25.4635	5.6681	1.3930
C	26.3834	4.6785	1.7351
C	25.9654	3.3531	1.8174
C	24.6211	3.0521	1.5386

N	23.7217	4.0040	1.2046
H	25.7396	6.7108	1.3289
H	27.4147	4.9395	1.9399
H	26.6414	2.5533	2.0833
O	25.0198	0.6891	2.0344
C	24.1404	1.6894	1.5895
C	22.9377	1.1235	1.2489
H	22.1025	1.6525	0.8264
C	23.0504	-0.2817	1.4786
H	22.3059	-1.0366	1.3033
C	24.3147	-0.5196	1.9552
C	24.9777	-1.7408	2.3595
C	26.2897	-1.7272	2.8586
C	26.8655	-2.9365	3.2444
C	26.1328	-4.1153	3.1235
C	24.8280	-4.0451	2.6066
N	24.2602	-2.8791	2.2329
H	26.8191	-0.7882	2.9372
H	27.8761	-2.9598	3.6355
H	26.5373	-5.0753	3.4111
O	24.5548	-6.4582	2.8953
C	24.0265	-5.2411	2.4430
C	22.7889	-5.4499	1.8972
H	22.1673	-4.6959	1.4483
C	22.5100	-6.8568	2.0076
H	21.6208	-7.3588	1.6669
C	23.5888	-7.4343	2.6111
H	23.8378	-8.4379	2.9019
H	25.1040	-5.6520	-2.8339

TABLE S8: xyz coordinates of the optimized structure of **B**-$(PF)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

162

N	2.6632	-0.4103	-1.7257
C	2.7849	-1.5392	-2.4373
C	3.6153	-1.6364	-3.5732
C	4.3373	-0.5185	-3.9664
C	4.2220	0.6550	-3.2326
C	3.3684	0.6652	-2.1148
H	3.6882	-2.5626	-4.1322
H	4.9940	-0.5641	-4.8313
H	4.8001	1.5335	-3.4953
C	3.2401	1.8941	-1.3381
O	2.6088	1.8473	-0.1383
C	2.6589	3.0896	0.4122
C	3.3131	3.9479	-0.4419
C	3.6890	3.1776	-1.5715
H	4.2289	3.5226	-2.4419
H	3.5250	4.9921	-0.2631
C	2.1038	3.2576	1.7502
C	1.9538	4.5316	2.3316
C	1.4793	4.6041	3.6381
C	1.1593	3.4336	4.3240
C	1.3180	2.2104	3.6505
N	1.7841	2.1341	2.3963
H	2.2053	5.4286	1.7751
H	1.3578	5.5699	4.1219
H	0.7935	3.4620	5.3453
C	0.9942	-1.2666	4.2744
C	0.3193	-0.8770	5.4108

C	0.3266	0.5455	5.4125
C	0.9965	0.9309	4.2720
O	1.4023	-0.1694	3.5931
H	-0.1282	-1.5288	6.1474
H	-0.1291	1.2011	6.1411
C	1.3619	-2.5519	3.6864
N	2.2980	-2.5006	2.7309
C	0.7564	-3.7528	4.0916
C	2.6550	-3.6305	2.1123
C	1.1386	-4.9271	3.4489
H	-0.0180	-3.7529	4.8516
C	2.0962	-4.8795	2.4402
C	3.6709	-3.5003	1.0706
H	0.6743	-5.8720	3.7158
H	2.3979	-5.7799	1.9148
O	4.2393	-2.2767	0.9063
C	4.2164	-4.3848	0.1665
C	5.1454	-2.3625	-0.1014
C	5.1653	-3.6503	-0.5918
H	3.9494	-5.4245	0.0444
C	5.8844	-1.1537	-0.4522
H	5.7824	-4.0231	-1.3972
C	6.7498	-1.1415	-1.5611
N	5.6985	-0.0798	0.3303
C	7.4247	0.0382	-1.8567
H	6.8698	-2.0234	-2.1810
C	6.3542	1.0520	0.0401
C	7.2287	1.1600	-1.0578
H	8.0942	0.0859	-2.7118
C	6.1362	2.1895	0.9310

H	7.7400	2.0930	-1.2713
C	6.6677	3.4557	0.9829
O	5.2477	2.0313	1.9563
C	6.0680	4.1063	2.1037
H	7.4007	3.8724	0.3065
C	5.2168	3.1914	2.6543
H	6.2471	5.1139	2.4526
H	4.5348	3.2141	3.4903
C	2.0329	-2.7218	-2.0223
O	1.1641	-2.6571	-0.9737
C	2.0459	-4.0039	-2.5275
C	0.6209	-3.8959	-0.8038
C	1.1435	-4.7574	-1.7442
H	2.6433	-4.3667	-3.3511
C	-0.3648	-4.1377	0.2485
H	0.8974	-5.8017	-1.8698
N	-0.7770	-3.1094	1.0024
C	-0.8431	-5.4524	0.4293
C	-1.6890	-3.3492	1.9598
C	-1.7816	-5.6882	1.4238
H	-0.4846	-6.2657	-0.1915
C	-2.2227	-4.6271	2.2041
H	-2.1774	-6.6883	1.5803
H	-2.9834	-4.7728	2.9625
C	-2.1355	-2.2322	2.7869
O	-1.8432	-0.9675	2.3933
C	-2.8544	-2.1926	3.9638
C	-2.3744	-0.1083	3.3045
C	-3.0059	-0.8224	4.2971
H	-3.2234	-3.0423	4.5208

C	-2.1943	1.3200	3.0659
H	-3.5287	-0.4106	5.1485
N	-1.6937	1.6550	1.8755
C	-2.5247	2.2781	4.0438
C	-1.4934	2.9489	1.5908
C	-2.3106	3.6197	3.7432
H	-2.9192	1.9752	5.0085
C	-0.9443	3.2182	0.2681
C	-1.7876	3.9757	2.5025
H	-2.5496	4.3878	4.4745
O	-0.8328	2.1479	-0.5547
C	-0.4540	4.3383	-0.3679
H	-1.6176	5.0147	2.2423
C	-0.2618	2.5557	-1.7131
C	-0.0060	3.9082	-1.6467
H	-0.3990	5.3367	0.0429
C	-0.0530	1.5240	-2.7240
H	0.4406	4.5155	-2.4205
N	-0.6825	0.3633	-2.5097
C	0.7755	1.7424	-3.8382
C	-0.5015	-0.6407	-3.3731
C	0.9678	0.6893	-4.7270
H	1.2856	2.6908	-3.9708
C	-1.2370	-1.8723	-3.0955
C	0.3301	-0.5267	-4.5013
H	1.6221	0.8109	-5.5855
C	-1.2601	-3.1157	-3.6899
O	-2.1229	-1.8464	-2.0691
H	0.4615	-1.3607	-5.1822
C	-2.2152	-3.8861	-2.9737

H	-0.6537	-3.4399	-4.5231
C	-2.7188	-3.0636	-1.9886
H	-2.4936	-4.9145	-3.1576
C	-3.7103	-3.2485	-0.9329
C	-4.2625	-4.5126	-0.6548
N	-4.0545	-2.1508	-0.2486
C	-5.1885	-4.6126	0.3795
H	-3.9566	-5.3887	-1.2172
C	-4.9516	-2.2527	0.7395
C	-5.5461	-3.4753	1.0996
H	-5.6297	-5.5753	0.6250
C	-5.3014	-1.0011	1.4073
H	-6.2773	-3.5235	1.9006
O	-4.8820	0.1373	0.8005
C	-5.9960	-0.6804	2.5528
C	-5.3007	1.1944	1.5389
C	-5.9914	0.7390	2.6411
H	-6.4359	-1.3768	3.2528
C	-4.9781	2.5177	1.0123
H	-6.4481	1.3469	3.4098
N	-4.4832	2.5421	-0.2328
C	-5.1831	3.6839	1.7680
C	-4.1555	3.7181	-0.7790
C	-4.8414	4.9055	1.1926
H	-5.5705	3.6293	2.7800
C	-4.3143	4.9385	-0.0944
C	-3.6279	3.6739	-2.1396
H	-4.9773	5.8282	1.7507
H	-4.0398	5.8787	-0.5620
O	-3.5985	2.4634	-2.7583

C	-3.1207	4.6343	-2.9864
C	-3.0720	2.6348	-3.9978
C	-2.7595	3.9644	-4.1842
H	-3.0076	5.6870	-2.7694
C	-2.9548	1.4590	-4.8551
H	-2.3342	4.4062	-5.0744
N	-3.5767	0.3366	-4.4484
C	-2.2177	1.5220	-6.0515
C	-3.4678	-0.7492	-5.2138
C	-2.1298	0.3827	-6.8429
H	-1.7068	2.4363	-6.3354
C	-2.7635	-0.7861	-6.4200
H	-3.9626	-1.6426	-4.8368
H	-1.5607	0.4028	-7.7689
H	-2.7094	-1.7031	-6.9990

TABLE S9: xyz coordinates of the optimized structure of **A**-$(PP)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

172

C	13.3387	0.5161	-0.6484
C	14.4477	-0.3176	-0.5309
C	15.1671	1.8225	-0.3796
C	13.7860	1.8475	-0.5535
C	14.5169	-1.7730	-0.5615
N	13.3333	-2.4102	-0.5670
C	13.3079	-3.7537	-0.5972
C	14.4886	-4.5230	-0.6240
C	15.7118	-3.8614	-0.6162
C	15.7410	-2.4713	-0.5862
H	14.4568	-5.6070	-0.6784
H	16.6394	-4.4270	-0.6467
H	16.6914	-1.9469	-0.6099
H	12.3293	0.1634	-0.7986
H	13.1997	2.7521	-0.6162
C	16.3381	5.2133	0.1120
C	17.7440	5.1100	0.1105
C	18.3174	3.8610	-0.1023
C	17.4987	2.7517	-0.2864
C	16.1018	2.9308	-0.2303
N	15.5445	4.1398	-0.0455
H	18.3736	5.9761	0.2909
H	19.3986	3.7524	-0.1247
H	17.9356	1.7785	-0.4892
C	15.3771	8.7232	0.4776
C	14.1290	8.1266	0.6327
C	14.2986	6.7334	0.5195

C	15.6499	6.4842	0.2961
H	13.2168	8.6724	0.8228
H	13.5466	5.9629	0.6034
C	15.7384	10.1353	0.5089
C	17.0781	10.5694	0.5463
C	17.3303	11.9374	0.5493
C	16.2663	12.8325	0.5332
C	14.9530	12.3195	0.5311
N	14.7076	10.9978	0.5103
H	17.9007	9.8624	0.5946
H	18.3532	12.3047	0.5664
H	16.4566	13.9013	0.5105
C	13.7756	13.1789	0.5417
C	12.4367	12.8418	0.3953
C	11.6754	14.0335	0.4698
C	12.5615	15.0769	0.6644
H	12.0791	11.8346	0.2415
H	10.6008	14.1239	0.3883
H	12.3944	16.1382	0.7811
N	15.5519	0.4976	-0.3870
H	16.4709	0.1731	-0.1317
N	16.2915	7.7063	0.2939
H	17.2437	7.8470	-0.0044
N	13.8274	14.5534	0.6981
H	14.6617	15.0860	0.8864
C	11.9815	-4.3579	-0.6034
C	10.7352	-3.7508	-0.7328
N	11.7596	-5.7151	-0.4895
C	9.7547	-4.7593	-0.6762
H	10.5894	-2.6891	-0.8651

C	10.4056	-5.9792	-0.5130
H	12.4645	-6.3878	-0.2332
H	8.6834	-4.6506	-0.7571
C	9.8444	-7.3192	-0.3986
C	10.6440	-8.4789	-0.4466
N	8.5095	-7.3792	-0.2532
C	10.0274	-9.7166	-0.2974
H	11.7150	-8.4200	-0.6159
C	7.9141	-8.5779	-0.1289
C	8.6487	-9.7808	-0.1256
H	10.6192	-10.6281	-0.3150
C	6.4640	-8.5487	0.0132
H	8.1618	-10.7394	0.0261
C	5.6174	-7.4615	0.2119
N	5.6719	-9.6785	-0.0151
C	4.2980	-7.9481	0.2818
H	5.9554	-6.4405	0.3079
C	4.3439	-9.3307	0.1268
H	5.9909	-10.5886	-0.3073
H	3.3899	-7.3866	0.4441
C	3.2548	-10.2990	0.1257
C	3.4819	-11.6885	0.1928
N	2.0161	-9.7805	0.0685
C	2.3846	-12.5424	0.1569
H	4.4852	-12.0916	0.2925
C	0.9568	-10.6078	0.0542
C	1.1023	-12.0096	0.0765
H	2.5282	-13.6192	0.1915
H	0.2408	-12.6673	0.0112
C	-0.3475	-9.9599	0.0012

C	-0.6614	-8.6242	-0.2340
N	-1.5406	-10.6328	0.1695
C	-2.0626	-8.4948	-0.1858
H	0.0710	-7.8561	-0.4333
C	-2.5991	-9.7517	0.0795
H	-1.6153	-11.5768	0.5141
H	-2.6536	-7.6042	-0.3392
C	-3.9932	-10.1484	0.2294
C	-4.3913	-11.4988	0.2975
N	-4.8802	-9.1401	0.2883
C	-5.7412	-11.7847	0.4716
H	-3.6714	-12.3055	0.1979
C	-6.1864	-9.4202	0.4362
C	-6.6590	-10.7429	0.5536
H	-6.0768	-12.8160	0.5433
C	-7.0769	-8.2674	0.4778
H	-7.7103	-10.9535	0.7250
C	-6.7668	-6.9135	0.5723
N	-8.4530	-8.3659	0.4434
C	-7.9761	-6.1922	0.5735
H	-5.7616	-6.5263	0.6477
C	-9.0201	-7.1083	0.4800
H	-8.9557	-9.2080	0.2115
H	-8.1128	-5.1238	0.6502
C	-10.4578	-6.8725	0.4443
C	-11.3965	-7.9161	0.5725
N	-10.8329	-5.5909	0.2918
C	-12.7497	-7.6036	0.4996
H	-11.0813	-8.9405	0.7466
C	-12.1418	-5.2895	0.2399

C	-13.1406	-6.2807	0.3220
H	-13.4973	-8.3883	0.5812
C	-12.4555	-3.8755	0.0788
H	-14.1935	-6.0316	0.2302
C	-11.6059	-2.8092	-0.2043
N	-13.7325	-3.3615	0.1690
C	-12.3869	-1.6403	-0.2698
H	-10.5413	-2.9073	-0.3564
C	-13.7109	-1.9956	-0.0246
H	-14.5324	-3.8802	0.4945
H	-12.0598	-0.6332	-0.4812
C	-14.8997	-1.1536	0.0179
N	-14.6778	0.1677	-0.0929
C	-16.1982	-1.6827	0.1613
C	-15.7201	1.0161	-0.0693
C	-17.2747	-0.8028	0.1866
H	-16.3704	-2.7528	0.2273
C	-17.0480	0.5642	0.0687
C	-15.3844	2.4282	-0.2015
H	-18.2883	-1.1821	0.2858
H	-17.8853	1.2553	0.0572
C	-14.1571	3.0204	-0.4878
N	-16.3042	3.4485	-0.0712
C	-14.3445	4.4154	-0.5102
H	-13.2463	2.4694	-0.6686
C	-15.6859	4.6706	-0.2386
H	-17.2416	3.3298	0.2785
H	-13.6114	5.1816	-0.7142
C	-16.3856	5.9460	-0.1525
C	-17.7905	6.0329	-0.0783

N	-15.6033	7.0391	-0.1605
C	-18.3728	7.2914	0.0290
H	-18.4145	5.1454	-0.1237
C	-16.1702	8.2549	-0.0766
C	-17.5647	8.4233	0.0410
H	-19.4527	7.3897	0.1032
C	-15.2480	9.3829	-0.1036
H	-18.0062	9.4081	0.1607
C	-13.8596	9.3923	-0.0023
N	-15.6540	10.6964	-0.2231
C	-13.4297	10.7306	-0.0805
H	-13.2561	8.5066	0.1299
C	-14.5572	11.5340	-0.2309
H	-16.5895	10.9798	-0.4677
H	-12.4201	11.1093	-0.0246
C	-14.6471	12.9818	-0.3618
C	-15.8754	13.6712	-0.3453
N	-13.4701	13.6322	-0.4955
C	-15.8795	15.0545	-0.4898
H	-16.8127	13.1409	-0.2015
C	-13.4955	14.9585	-0.6240
C	-14.6649	15.7240	-0.6365
H	-16.8184	15.6018	-0.4804
H	-12.5243	15.4412	-0.7256
H	-14.6198	16.8025	-0.7510

TABLE S10: xyz coordinates of the optimized structure of **A**-$(PP)_{16}$ obtained at B3LYP-D3/6-31G(d) level.

274

C	13.8300	-2.3220	0.9262
C	12.7507	-1.8845	0.1693
C	12.7151	-0.4713	0.2393
C	13.7685	-0.0732	1.0429
C	14.2933	-3.6772	1.1724
C	15.5275	-3.9542	1.8020
C	15.8871	-5.2829	2.0055
C	15.0324	-6.3016	1.5896
C	13.8221	-5.9426	0.9591
N	13.4731	-4.6604	0.7622
C	12.8692	-6.9339	0.4819
C	11.7015	-6.7511	-0.2527
C	11.1135	-8.0156	-0.4496
C	11.9299	-8.9623	0.1602
C	11.7728	-10.4060	0.2596
C	12.8554	-11.2521	0.5773
C	12.6143	-12.6151	0.7086
C	11.3288	-13.1082	0.5044
C	10.3102	-12.2035	0.1440
N	10.5360	-10.8815	0.0373
C	8.9419	-12.6271	-0.1228
C	7.1962	-14.0279	-0.4569
C	6.7217	-12.7211	-0.5531
C	7.8069	-11.8501	-0.3463
C	6.4727	-15.2850	-0.5982
N	5.1726	-15.1711	-0.9217
C	4.4304	-16.2815	-1.0706

C	4.9695	-17.5713	-0.8903
C	6.3158	-17.6869	-0.5620
C	7.0877	-16.5397	-0.4128
C	3.0339	-16.0645	-1.4264
C	0.9299	-16.5678	-2.0898
C	0.9924	-15.1941	-1.8735
C	2.3018	-14.8810	-1.4605
C	-0.1914	-17.3881	-2.5296
N	-1.2678	-16.7155	-2.9719
C	-2.3372	-17.4014	-3.4112
C	-2.3605	-18.8105	-3.4416
C	-1.2542	-19.5034	-2.9619
C	-0.1542	-18.7966	-2.4883
C	-3.4621	-16.5934	-3.8644
C	-5.5517	-16.1138	-4.5883
C	-4.8439	-14.9180	-4.5040
C	-3.5433	-15.2165	-4.0546
C	-6.9271	-16.3507	-5.0078
N	-7.6907	-15.2535	-5.1507
C	-8.9734	-15.3912	-5.5283
C	-9.5547	-16.6544	-5.7593
C	-8.7562	-17.7858	-5.6309
C	-7.4227	-17.6456	-5.2619
C	-9.7280	-14.1526	-5.6708
C	-11.4397	-12.7896	-6.2479
C	-10.4643	-12.0125	-5.6290
C	-9.3983	-12.8606	-5.2713
C	-12.7275	-12.3943	-6.8038
N	-12.9533	-11.0707	-6.8701
C	-14.1138	-10.6270	-7.3830

C	-15.0978	-11.5065	-7.8786
C	-14.8705	-12.8754	-7.7883
C	-13.6808	-13.3381	-7.2367
C	-14.2870	-9.1801	-7.4004
C	-15.3453	-7.1937	-7.6350
C	-14.0268	-6.9347	-7.2718
C	-13.3677	-8.1712	-7.1268
C	-16.4363	-6.2663	-7.9063
N	-16.2164	-4.9860	-7.5607
C	-17.1836	-4.0752	-7.7666
C	-18.4339	-4.4228	-8.3171
C	-18.6491	-5.7436	-8.6952
C	-17.6432	-6.6843	-8.5029
C	-16.8629	-2.7099	-7.3706
C	-17.1020	-0.4685	-7.1700
C	-15.9295	-0.8334	-6.5142
C	-15.7806	-2.2284	-6.6391
C	-17.7078	0.8474	-7.3287
N	-16.9503	1.8899	-6.9458
C	-17.4377	3.1364	-7.0706
C	-18.7133	3.3904	-7.6141
C	-19.5029	2.3087	-7.9886
C	-19.0109	1.0167	-7.8393
C	-16.5609	4.2088	-6.6178
C	-15.9315	6.3022	-6.0326
C	-14.8269	5.4676	-5.8869
C	-15.2187	4.1646	-6.2514
C	-16.0548	7.7334	-5.7871
N	-15.0192	8.3091	-5.1522
C	-15.0651	9.6244	-4.8786

C	-16.1780	10.4204	-5.2178
C	-17.2380	9.8264	-5.8942
C	-17.1840	8.4705	-6.1979
H	-3.2104	-19.3532	-3.8441
H	-1.2498	-20.5902	-2.9567
H	0.7001	-19.3265	-2.0780
H	-2.7232	-14.5333	-3.8915
H	-5.2516	-13.9529	-4.7660
H	-10.6066	-16.7535	-6.0093
H	-9.1714	-18.7728	-5.8175
H	-6.7804	-18.5185	-5.1952
H	-8.4833	-12.5991	-4.7606
H	-10.5551	-10.9503	-5.4569
H	-16.0075	-11.1338	-8.3397
H	-15.6174	-13.5790	-8.1468
H	-13.5084	-14.4049	-7.1310
H	-12.3340	-8.3469	-6.8688
H	-13.6145	-5.9438	-7.1516
H	-19.2254	-3.6878	-8.4285
H	-19.5968	-6.0384	-9.1383
H	-17.7848	-7.7101	-8.8293
H	-14.9952	-2.8516	-6.2377
H	-15.2845	-0.1399	-5.9952
H	-19.0725	4.4045	-7.7604
H	-20.4975	2.4720	-8.3953
H	-19.6326	0.1637	-8.0938
H	-14.6133	3.2706	-6.2745
H	-13.8521	5.8035	-5.5660
H	-16.2259	11.4701	-4.9448
H	-18.1026	10.4180	-6.1836

H	-17.9890	8.0040	-6.7577
H	0.1558	-14.5225	-1.9957
H	2.7009	-13.9136	-1.1941
H	8.1361	-16.6241	-0.1432
H	6.7600	-18.6676	-0.4126
H	4.3507	-18.4595	-0.9744
H	5.6912	-12.4643	-0.7490
H	7.8030	-10.7701	-0.3427
H	11.1268	-14.1677	0.6321
H	13.4247	-13.2926	0.9651
H	13.8564	-10.8510	0.6977
H	11.3478	-5.7919	-0.5999
H	10.2073	-8.2494	-0.9886
H	15.3133	-7.3410	1.7195
H	16.8389	-5.5253	2.4725
H	16.1969	-3.1539	2.0979
H	14.0638	0.9070	1.3865
H	12.0035	0.1865	-0.2405
H	12.0858	-2.5391	-0.3745
N	-16.9699	5.5214	-6.4977
H	-17.9318	5.8202	-6.5311
N	-17.6642	-1.6264	-7.6673
H	-18.4275	-1.6489	-8.3247
N	-15.4776	-8.5640	-7.7283
H	-16.3612	-9.0427	-7.8034
N	-10.9813	-14.0912	-6.2449
H	-11.3998	-14.8419	-6.7711
N	-4.6882	-17.1223	-4.2126
H	-4.9713	-18.0715	-4.0278
N	2.1756	-17.0815	-1.7922

H	2.4697	-18.0188	-2.0170
N	8.5461	-13.9465	-0.1853
H	9.1713	-14.7346	-0.1377
N	13.0114	-8.2911	0.6953
H	13.5781	-8.6795	1.4354
N	14.4534	-1.1927	1.4325
H	15.1336	-1.1981	2.1786
C	-12.5082	11.7317	-3.3305
C	-11.9477	10.4796	-3.0909
C	-12.8115	9.5082	-3.6315
C	-13.8972	10.1701	-4.1989
N	-13.7013	11.5196	-3.9901
H	-14.2548	12.2462	-4.4151
H	-11.0170	10.3230	-2.5664
H	-12.6979	8.4345	-3.6153
C	-12.0112	13.0541	-2.9723
C	-12.7762	14.2230	-3.1598
C	-12.2259	15.4442	-2.7867
C	-10.9479	15.4829	-2.2403
C	-10.2450	14.2707	-2.0862
N	-10.7743	13.0888	-2.4466
H	-13.7849	14.1820	-3.5596
H	-12.7966	16.3611	-2.9086
H	-10.5238	16.4283	-1.9160
C	-8.9021	14.2166	-1.5223
C	-8.1400	13.1123	-1.1499
N	-8.1510	15.3386	-1.2394
C	-6.9106	13.5836	-0.6516
H	-8.4751	12.0891	-1.2323
C	-6.9250	14.9743	-0.7225

H	-8.3928	16.2728	-1.5284
H	-6.0850	13.0053	-0.2644
C	-5.8994	15.9335	-0.3322
C	-6.1276	17.3245	-0.3357
N	-4.7185	15.4061	0.0352
C	-5.0935	18.1684	0.0542
H	-7.0929	17.7398	-0.6088
C	-3.7209	16.2243	0.4127
C	-3.8719	17.6255	0.4372
H	-5.2433	19.2446	0.0721
C	-2.4780	15.5690	0.7998
H	-3.0699	18.2753	0.7739
C	-2.2106	14.2153	0.9865
N	-1.3120	16.2527	1.0777
C	-0.8599	14.0891	1.3637
H	-2.9432	13.4310	0.8671
C	-0.3072	15.3663	1.4066
H	-1.1644	17.2299	0.8815
H	-0.3178	13.1862	1.6025
C	1.0484	15.7802	1.7453
C	1.3946	17.1323	1.9439
N	1.9473	14.7884	1.8688
C	2.7186	17.4428	2.2347
H	0.6486	17.9197	1.8930
C	3.2217	15.0903	2.1714
C	3.6554	16.4206	2.3420
H	3.0193	18.4776	2.3768
C	4.1265	13.9553	2.3020
H	4.6987	16.6538	2.5324
C	3.9243	12.6176	1.9739

N	5.4120	14.0620	2.7921
C	5.1008	11.9121	2.2920
H	3.0153	12.2316	1.5367
C	6.0168	12.8217	2.8135
H	5.7741	14.8780	3.2596
H	5.3025	10.8601	2.1551
C	7.3741	12.5989	3.2950
N	7.7436	11.3126	3.4208
C	8.2483	13.6614	3.6009
C	8.9766	11.0236	3.8714
C	9.5159	13.3590	4.0868
H	7.9562	14.6954	3.4449
C	9.8935	12.0291	4.2386
C	9.2972	9.6050	3.9647
H	10.2070	14.1568	4.3459
H	10.8680	11.7825	4.6493
C	8.4649	8.4983	3.8214
N	10.5610	9.1272	4.2460
C	9.2485	7.3419	3.9990
H	7.4045	8.5592	3.6258
C	10.5562	7.7469	4.2514
H	11.3959	9.6914	4.2370
H	8.9280	6.3110	3.9720
C	11.7428	6.9408	4.5062
N	11.6112	5.6226	4.2774
C	12.9483	7.5019	4.9745
C	12.6641	4.8122	4.4797
C	14.0417	6.6634	5.1630
H	13.0250	8.5599	5.2067
C	13.9149	5.3022	4.9064

C	12.4320	3.3982	4.2144
H	14.9891	7.0692	5.5084
H	14.7713	4.6433	5.0141
C	11.3508	2.7795	3.5932
N	13.3326	2.4045	4.5455
C	11.5964	1.3924	3.5761
H	10.5014	3.3089	3.1877
C	12.8258	1.1703	4.1875
H	14.1085	2.5330	5.1764
H	10.9909	0.6122	3.1396
C	13.5435	-0.0808	4.3900
N	12.8211	-1.2007	4.2251
C	14.9198	-0.1127	4.6997
C	13.4177	-2.3977	4.3617
C	15.5276	-1.3536	4.8806
H	15.5004	0.8015	4.7788
C	14.7795	-2.5150	4.7179
C	12.5724	-3.5579	4.1337
H	16.5813	-1.4139	5.1424
H	15.2349	-3.4866	4.8739
C	11.1938	-3.6188	3.9515
N	13.0487	-4.8556	4.1115
C	10.8400	-4.9711	3.7910
H	10.5426	-2.7573	3.9599
C	12.0048	-5.7287	3.8781
H	14.0133	-5.0878	3.9204
H	9.8546	-5.3888	3.6471
C	12.1652	-7.1734	3.8139
N	11.0761	-7.8689	3.4203
C	13.3706	-7.8176	4.1598

C	11.1643	-9.1958	3.3503
C	13.4410	-9.2067	4.0852
H	14.2253	-7.2447	4.5050
C	12.3180	-9.9222	3.6678
H	14.3585	-9.7223	4.3588
H	12.3285	-11.0031	3.5799
H	10.2714	-9.7132	3.0048

TABLE S11: xyz coordinates of the optimized structure of **B**-$(PP)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

172

N	-4.1940	1.2354	1.4087
C	-4.5709	2.5178	1.2558
C	-5.1480	3.2514	2.3062
C	-5.3543	2.6086	3.5240
C	-4.9837	1.2750	3.6795
C	-4.3917	0.6188	2.5889
H	-5.4406	4.2854	2.1570
H	-5.8020	3.1484	4.3545
H	-5.1151	0.7591	4.6243
C	-3.9322	-0.7625	2.6488
C	-2.8293	-2.5578	1.8464
C	-3.4232	-2.9337	3.0536
C	-4.1095	-1.8076	3.5603
H	-4.6763	-1.7548	4.4800
H	-3.3463	-3.9067	3.5183
N	-3.1584	-1.2512	1.6354
H	-2.8790	-0.7209	0.8241
C	-2.0316	-3.2582	0.8485
N	-1.5581	-2.4901	-0.1502
C	-1.8030	-4.6408	0.8958
C	-0.8565	-3.0586	-1.1479
C	-1.0770	-5.2247	-0.1390
H	-2.2019	-5.2346	1.7105
C	-0.5996	-4.4386	-1.1828
C	-0.3739	-2.1424	-2.1712
H	-0.8838	-6.2939	-0.1317
H	-0.0214	-4.8672	-1.9937

C	0.2609	-2.3108	-3.4037
N	-0.5325	-0.7979	-1.9898
C	0.4613	-1.0286	-3.9596
H	0.5442	-3.2555	-3.8448
C	-0.0405	-0.0932	-3.0527
H	-0.9907	-0.3812	-1.1938
H	0.9528	-0.8000	-4.8947
C	-0.0973	1.3601	-3.0172
N	-0.4564	1.8786	-1.8280
C	0.1799	2.1723	-4.1256
C	-0.5648	3.2105	-1.6865
C	0.0601	3.5523	-3.9765
H	0.4633	1.7291	-5.0730
C	-0.3232	4.0921	-2.7523
C	-0.9213	3.6494	-0.3460
H	0.2667	4.2074	-4.8185
H	-0.4047	5.1632	-2.6049
C	-1.2806	4.8738	0.2201
N	-0.9527	2.7248	0.6592
C	-1.5400	4.6498	1.5895
H	-1.3630	5.8122	-0.3095
C	-1.3226	3.2919	1.8421
H	-0.7361	1.7465	0.5415
H	-1.8424	5.3883	2.3192
C	-1.4024	2.4616	3.0325
N	-0.9394	1.2011	2.8966
C	-1.9389	2.9389	4.2376
C	-0.9903	0.3702	3.9519
C	-1.9961	2.0721	5.3240
H	-2.3206	3.9516	4.3022

C	-1.5169	0.7741	5.1941
C	-0.4607	-0.9721	3.7651
H	-2.4129	2.4082	6.2701
H	-1.5380	0.0840	6.0301
C	-0.5277	-2.0976	4.5872
N	0.2468	-1.3335	2.6478
C	0.1564	-3.1399	3.9397
H	-1.0461	-2.1569	5.5336
C	0.6437	-2.6409	2.7283
H	0.4794	-0.7114	1.8878
H	0.2888	-4.1467	4.3099
C	1.4356	-3.2927	1.6945
N	1.8628	-2.5478	0.6542
C	1.7295	-4.6642	1.8089
C	2.5980	-3.1482	-0.3051
C	2.4816	-5.2736	0.8145
H	1.3606	-5.2339	2.6537
C	2.9243	-4.5156	-0.2606
C	3.0739	-2.3322	-1.4134
H	2.7219	-6.3318	0.8773
H	3.5255	-4.9609	-1.0444
C	3.8029	-2.6878	-2.5511
N	2.8642	-0.9809	-1.4793
C	4.0112	-1.5219	-3.3084
H	4.1556	-3.6801	-2.7938
C	3.4139	-0.4637	-2.6246
H	2.3184	-0.4593	-0.8093
H	4.5811	-1.4371	-4.2226
C	3.3784	0.9555	-2.9353
N	3.0702	1.7942	-1.9289

C	3.6882	1.4232	-4.2264
C	3.0586	3.1252	-2.1622
C	3.7044	2.7945	-4.4516
H	3.9146	0.7205	-5.0204
C	3.3889	3.6677	-3.4139
C	2.7031	3.9576	-1.0237
H	3.9551	3.1835	-5.4351
H	3.3920	4.7425	-3.5599
C	2.4926	5.3288	-0.8468
N	2.5050	3.3698	0.1909
C	2.1567	5.5366	0.5099
H	2.5691	6.0856	-1.6157
C	2.1760	4.2919	1.1422
H	2.5599	2.3770	0.3636
H	1.9353	6.4827	0.9843
C	1.9685	3.8217	2.5067
N	2.3462	2.5480	2.7054
C	1.4111	4.5988	3.5327
C	2.1936	1.9821	3.9154
C	1.2396	4.0059	4.7826
H	1.0929	5.6173	3.3395
C	1.6319	2.6856	4.9925
C	2.6923	0.6179	4.0059
H	0.7947	4.5732	5.5955
H	1.5104	2.2077	5.9583
C	2.5989	-0.3973	4.9593
N	3.4314	0.1198	2.9672
C	3.3023	-1.5150	4.4601
H	2.0452	-0.3447	5.8860
C	3.8258	-1.1629	3.2130

H	3.7018	0.6481	2.1512
H	3.4095	-2.4754	4.9440
C	4.6796	-1.8458	2.2495
N	5.1026	-1.0948	1.2115
C	5.0531	-3.1882	2.4062
C	5.9322	-1.6394	0.3022
C	5.8913	-3.7539	1.4489
H	4.6769	-3.7688	3.2410
C	6.3458	-2.9823	0.3860
C	6.3914	-0.7673	-0.7698
H	6.1856	-4.7970	1.5307
H	6.9953	-3.4022	-0.3743
C	7.3523	-0.9383	-1.7615
N	5.8741	0.4986	-0.9297
C	7.3926	0.2499	-2.5328
H	7.9682	-1.8167	-1.8982
C	6.4558	1.1179	-1.9970
H	5.0793	0.8392	-0.4085
H	8.0371	0.4540	-3.3773
H	6.1476	2.1078	-2.3003
C	-4.3793	3.0612	-0.0823
N	-3.9849	2.2228	-1.0857
C	-4.5360	4.3271	-0.6519
C	-3.8814	2.8861	-2.2734
H	-3.8035	1.2372	-0.9665
C	-4.2170	4.2196	-2.0231
H	-4.8260	5.2255	-0.1248
C	-3.5146	2.1409	-3.4704
H	-4.2397	5.0146	-2.7560
N	-3.4794	0.8029	-3.3201

C	-3.2161	2.7608	-4.6931
C	-3.1507	0.0263	-4.3674
C	-2.8558	1.9541	-5.7697
H	-3.2395	3.8415	-4.7805
C	-3.2173	-1.4087	-4.1285
C	-2.8145	0.5714	-5.6190
H	-2.6052	2.4046	-6.7267
N	-3.7309	-1.8788	-2.9523
C	-2.8885	-2.5241	-4.9028
H	-2.5505	-0.0779	-6.4469
C	-3.7550	-3.2440	-2.9386
H	-4.0699	-1.3028	-2.1946
C	-3.2208	-3.6736	-4.1567
H	-2.4408	-2.4996	-5.8866
C	-4.3115	-3.9402	-1.7881
H	-3.0936	-4.7023	-4.4654
N	-4.8257	-3.1480	-0.8216
C	-4.3177	-5.3419	-1.6873
C	-5.3500	-3.7283	0.2593
C	-4.8738	-5.9282	-0.5567
H	-3.8860	-5.9472	-2.4779
C	-5.4027	-5.1113	0.4450
H	-5.7305	-3.0528	1.0223
H	-4.8885	-7.0103	-0.4538
H	-5.8388	-5.5282	1.3474

TABLE S12: xyz coordinates of the optimized structure of **A**-$(PT)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

162

C	-3.3720	-5.1948	-1.8445
C	-4.6566	-5.6620	-2.0077
S	-4.6450	-7.3961	-2.2615
C	-2.9177	-7.4538	-2.1456
C	-2.3836	-6.2135	-1.9197
C	-5.8896	-4.8678	-1.9663
N	-5.7169	-3.5390	-1.8932
C	-6.7893	-2.7313	-1.8514
C	-8.1029	-3.2332	-1.8807
C	-8.2815	-4.6109	-1.9586
C	-7.1719	-5.4486	-1.9984
C	-6.4842	-1.3001	-1.7673
S	-7.7009	-0.0461	-1.8654
C	-6.5050	1.2117	-1.6519
C	-5.2471	0.6630	-1.5161
C	-5.2351	-0.7465	-1.5840
C	-6.8241	2.6419	-1.6130
N	-5.7585	3.4480	-1.4991
C	-5.9267	4.7776	-1.4459
C	-7.2017	5.3681	-1.5114
C	-8.3085	4.5323	-1.6360
C	-8.1337	3.1522	-1.6841
C	-4.6836	5.5390	-1.2916
S	-4.5918	7.2858	-1.3075
C	-2.8703	7.2526	-0.9982
C	-2.4205	5.9521	-0.9073
C	-3.4378	4.9909	-1.0727

C	-2.0415	8.4476	-0.8161
N	-0.7246	8.2026	-0.7406
C	0.1384	9.2116	-0.5469
C	-0.2958	10.5432	-0.4226
C	-1.6633	10.7996	-0.4982
C	-2.5588	9.7510	-0.6936
C	1.5448	8.7946	-0.4839
S	2.8852	9.8692	-0.1313
C	4.0415	8.5558	-0.2521
C	3.3969	7.3740	-0.5483
C	1.9989	7.5077	-0.6788
C	5.4883	8.7018	-0.0502
N	6.1673	7.5446	-0.0697
C	7.4980	7.5427	0.1004
C	8.2197	8.7328	0.3024
C	7.5165	9.9350	0.3201
C	6.1350	9.9356	0.1424
C	8.1093	6.2080	0.0676
S	9.8344	5.9075	0.1602
C	9.5944	4.1734	0.0545
C	8.2514	3.8796	-0.0441
C	7.4196	5.0192	-0.0381
C	10.6810	3.1863	0.0691
N	10.2708	1.9089	0.0369
C	11.1717	0.9145	0.0399
C	12.5546	1.1683	0.0778
C	12.9812	2.4935	0.1108
C	12.0455	3.5249	0.1064
C	10.5891	-0.4329	0.0070
S	11.5294	-1.9110	-0.0661

C	10.0808	-2.8991	-0.0657
C	8.9567	-2.1033	-0.0107
C	9.2415	-0.7217	0.0288
C	10.0845	-4.3663	-0.1182
N	8.8688	-4.9291	-0.0371
C	8.7441	-6.2646	-0.0806
C	9.8614	-7.1091	-0.2091
C	11.1230	-6.5259	-0.2943
C	11.2516	-5.1401	-0.2503
C	7.3626	-6.7503	0.0243
S	6.9009	-8.4378	-0.0937
C	5.2063	-8.0482	0.1331
C	5.0429	-6.6884	0.2885
C	6.2506	-5.9611	0.2262
C	4.1264	-9.0428	0.1490
N	2.9098	-8.5373	0.4047
C	1.8402	-9.3473	0.4376
C	1.9518	-10.7311	0.2118
C	3.2136	-11.2559	-0.0558
C	4.3227	-10.4145	-0.0918
C	0.5729	-8.6675	0.7307
S	-1.0017	-9.4395	0.6587
C	-1.8125	-7.9545	1.1144
C	-0.8962	-6.9431	1.3010
C	0.4409	-7.3430	1.0881
C	-3.2699	-7.8045	1.2025
N	-3.6841	-6.5336	1.2995
C	-4.9955	-6.2584	1.3538
C	-5.9663	-7.2765	1.3213
C	-5.5354	-8.5977	1.2431

C	-4.1733	-8.8810	1.1815
H	-3.8200	-9.9059	1.1218
H	-6.2608	-9.4064	1.2231
H	-7.0250	-7.0388	1.3516
C	-5.3126	-4.8296	1.4234
H	-1.2083	-5.9443	1.5762
H	1.3031	-6.6968	1.1894
H	5.3112	-10.8095	-0.3047
H	3.3329	-12.3208	-0.2353
H	1.0796	-11.3762	0.2527
H	4.0649	-6.2505	0.4395
H	6.3309	-4.8865	0.3251
H	12.2284	-4.6717	-0.3208
H	12.0058	-7.1512	-0.3950
H	9.7467	-8.1883	-0.2371
H	7.9622	-2.5299	-0.0025
H	8.4964	0.0618	0.0736
H	12.3640	4.5625	0.1274
H	14.0429	2.7225	0.1399
H	13.2730	0.3545	0.0846
H	7.9003	2.8588	-0.1188
H	6.3399	4.9965	-0.1052
H	5.5751	10.8657	0.1471
H	8.0453	10.8718	0.4725
H	9.2955	8.7173	0.4466
H	3.9424	6.4469	-0.6650
H	1.3191	6.6984	-0.9105
H	-3.6281	9.9318	-0.7377
H	-2.0309	11.8177	-0.4023
H	0.4134	11.3518	-0.2748

H	-1.3826	5.7256	-0.7021
H	-3.2961	3.9202	-1.0131
H	-8.9876	2.4873	-1.7685
H	-9.3078	4.9561	-1.6859
H	-7.3209	6.4454	-1.4530
H	-4.3750	1.2844	-1.3621
H	-4.3532	-1.3662	-1.4901
H	-7.2939	-6.5259	-2.0480
H	-9.2834	-5.0312	-1.9793
H	-8.9562	-2.5642	-1.8339
H	-3.1712	-4.1472	-1.6613
H	-1.3216	-6.0420	-1.7871
H	-2.3991	-8.3999	-2.2238
S	-6.9375	-4.1946	1.5433
C	-6.3551	-2.5448	1.5231
C	-4.9798	-2.5191	1.4334
C	-4.3947	-3.8012	1.3740
H	-3.3348	-3.9958	1.2796
H	-4.4358	-1.5850	1.3924
C	-7.2322	-1.3712	1.5601
N	-6.5945	-0.1941	1.6587
C	-7.3013	0.9463	1.6776
C	-8.7069	0.9496	1.6009
C	-9.3677	-0.2712	1.5065
C	-8.6344	-1.4536	1.4804
C	-6.5008	2.1701	1.7811
H	-9.2639	1.8811	1.6115
H	-10.4521	-0.3004	1.4437
H	-9.1315	-2.4141	1.3892
S	-7.2015	3.7692	1.8810

C	-5.6233	4.5220	1.9437
C	-4.6307	3.5662	1.8925
C	-5.1238	2.2458	1.7989
H	-4.5095	1.3573	1.7345
H	-3.5842	3.8417	1.9062
C	-5.4278	5.9727	2.0042
N	-4.1466	6.3782	2.1295
C	-3.8989	7.6866	2.1685
C	-4.8893	8.6703	2.1004
C	-6.2136	8.2525	1.9748
C	-6.4911	6.8904	1.9194
H	-2.8505	7.9675	2.2505
H	-4.6236	9.7221	2.1388
H	-7.0215	8.9768	1.9132
H	-7.5133	6.5421	1.8055

TABLE S13: xyz coordinates of the optimized structure of **B**-$(PT)_{10}$ obtained at B3LYP-D3/6-31G(d) level.

162

N	-0.9717	3.5900	1.5549
C	-0.0873	4.2517	2.3166
C	-0.0714	5.6563	2.3757
C	-0.9997	6.3581	1.6093
C	-1.9085	5.6680	0.8126
C	-1.8649	4.2620	0.8143
H	0.6372	6.1769	3.0111
H	-1.0120	7.4449	1.6316
H	-2.6263	6.1981	0.1965
C	-2.7749	3.4336	0.0273
S	-2.4986	1.7178	-0.0388
C	-3.9045	1.4941	-1.0390
C	-4.5423	2.6924	-1.2970
C	-3.8964	3.7974	-0.6934
H	-4.2584	4.8167	-0.7670
H	-5.4349	2.7794	-1.9064
C	-4.2523	0.1375	-1.4554
C	-5.4412	-0.1834	-2.1333
C	-5.6864	-1.5204	-2.4362
C	-4.7613	-2.4975	-2.0787
C	-3.5853	-2.0921	-1.4222
N	-3.3590	-0.8055	-1.1229
H	-6.1574	0.5887	-2.3929
H	-6.6019	-1.8015	-2.9510
H	-4.9331	-3.5424	-2.3133
C	-0.3761	-3.9565	-0.2014
C	-1.2523	-4.9294	-0.6426

C	-2.4727	-4.3941	-1.1187
C	-2.5231	-3.0163	-1.0318
S	-1.0542	-2.3617	-0.3641
H	-1.0243	-5.9893	-0.6402
H	-3.2861	-5.0028	-1.4974
C	0.8357	3.4093	3.0764
C	1.9700	3.7586	3.7833
S	0.5568	1.6896	3.1194
C	2.6254	2.6422	4.3559
H	2.3423	4.7742	3.8559
C	1.9848	1.4470	4.0904
H	3.5414	2.7180	4.9320
C	2.3588	0.0832	4.4642
C	3.5685	-0.2364	5.1070
N	1.4739	-0.8661	4.1289
C	3.8357	-1.5740	5.3846
H	4.2821	0.5387	5.3640
C	1.7305	-2.1570	4.3894
C	2.9187	-2.5585	5.0235
H	4.7636	-1.8507	5.8787
C	0.6849	-3.0903	3.9736
H	3.1088	-3.6054	5.2345
S	-0.8122	-2.4330	3.3729
C	0.6786	-4.4714	3.9552
C	-1.4434	-4.0331	3.0946
C	-0.5314	-5.0077	3.4509
H	1.5223	-5.0801	4.2603
C	-2.7791	-4.1562	2.5133
H	-0.7168	-6.0715	3.3462
N	-3.4361	-2.9978	2.3588

C	-3.3464	-5.3802	2.1179
C	-4.6571	-2.9764	1.8057
C	-4.6165	-5.3636	1.5471
H	-2.8016	-6.3100	2.2406
C	-5.2904	-4.1564	1.3771
H	-5.0806	-6.2937	1.2291
H	-6.2808	-4.1261	0.9359
C	-5.2623	-1.6507	1.6965
C	-6.4313	-1.2577	1.0756
S	-4.4293	-0.2957	2.4114
C	-6.6608	0.1357	1.1703
H	-7.0863	-1.9377	0.5427
C	-5.6694	0.8009	1.8672
H	-7.5178	0.6297	0.7253
C	-5.5248	2.2293	2.1465
C	-6.4574	3.1846	1.7030
N	-4.4263	2.5817	2.8443
C	-6.2311	4.5269	1.9866
H	-7.3339	2.8790	1.1413
C	-4.2194	3.8723	3.1021
C	-5.0853	4.8898	2.6965
H	-6.9376	5.2818	1.6508
H	-4.8628	5.9269	2.9275
H	-3.3075	4.1046	3.6486
C	0.9641	-4.0945	0.3647
N	1.6086	-2.9425	0.6005
C	1.5468	-5.3383	0.6655
C	2.8334	-2.9506	1.1466
C	2.8138	-5.3508	1.2416
H	1.0122	-6.2618	0.4716

C	3.4456	-1.6366	1.3300
C	3.4742	-4.1523	1.4964
H	3.2875	-6.2966	1.4932
S	2.6303	-0.2356	0.6949
C	4.6353	-1.2970	1.9448
H	4.4666	-4.1441	1.9338
C	3.8997	0.8078	1.2700
C	4.8916	0.0942	1.9145
H	5.2959	-2.0170	2.4142
C	3.7895	2.2460	1.0358
H	5.7813	0.5486	2.3355
N	2.7693	2.6233	0.2527
C	4.6726	3.1867	1.5951
C	2.5629	3.9209	-0.0144
C	4.4544	4.5356	1.3302
H	5.4907	2.8674	2.2316
C	1.4413	4.1971	-0.9106
C	3.3893	4.9232	0.5213
H	5.1163	5.2870	1.7538
S	0.6105	2.8491	-1.6334
C	0.9047	5.4032	-1.3187
H	3.2129	5.9686	0.2924
C	-0.4675	3.9209	-2.4839
C	-0.1838	5.2461	-2.2114
H	1.2650	6.3668	-0.9761
C	-1.5161	3.3374	-3.3203
H	-0.7368	6.0785	-2.6338
N	-1.4352	2.0103	-3.4955
C	-2.5586	4.0912	-3.8882
C	-2.3660	1.3633	-4.2127

C	-3.5201	3.4247	-4.6429
H	-2.6207	5.1619	-3.7261
C	-2.1708	-0.0812	-4.3270
C	-3.4396	2.0446	-4.8122
H	-4.3376	3.9811	-5.0945
S	-0.6804	-0.7701	-3.7431
C	-3.0181	-1.0509	-4.8262
H	-4.1769	1.5089	-5.4003
C	-1.2092	-2.3730	-4.1792
C	-2.4727	-2.3542	-4.7378
H	-4.0106	-0.8415	-5.2089
C	-0.3316	-3.5062	-3.8896
H	-2.9995	-3.2450	-5.0626
N	0.8735	-3.1877	-3.3944
C	-0.7139	-4.8449	-4.0884
C	1.7444	-4.1517	-3.0599
C	0.1906	-5.8474	-3.7505
H	-1.6947	-5.0893	-4.4812
C	1.4356	-5.5134	-3.2237
C	3.0206	-3.6824	-2.5233
H	-0.0775	-6.8913	-3.8924
H	2.1534	-6.2814	-2.9568
S	3.3528	-1.9716	-2.5290
C	4.0575	-4.3987	-1.9584
C	4.8954	-2.2315	-1.7602
C	5.1213	-3.5735	-1.5217
H	4.0439	-5.4752	-1.8307
C	5.7263	-1.0732	-1.4335
H	6.0156	-3.9564	-1.0421
C	6.9114	-1.1700	-0.6830

N	5.2731	0.1068	-1.8829
C	7.6150	-0.0013	-0.4073
H	7.2592	-2.1294	-0.3161
C	5.9457	1.2357	-1.6132
C	7.1373	1.2231	-0.8666
H	8.5344	-0.0439	0.1711
C	5.3593	2.4633	-2.1481
H	7.6742	2.1433	-0.6633
C	5.7295	3.7770	-1.9581
S	3.9462	2.3535	-3.1707
C	4.8815	4.6984	-2.6328
H	6.5635	4.0766	-1.3333
C	3.8788	4.0729	-3.3292
H	5.0033	5.7754	-2.5889
H	3.0824	4.5320	-3.9002