Supporting Information

Periodic B- and N-doped Phenalenyl π-Aggregates: Unexpected Nonlinear Optical Properties by Tuning Pancake π - π Bonding

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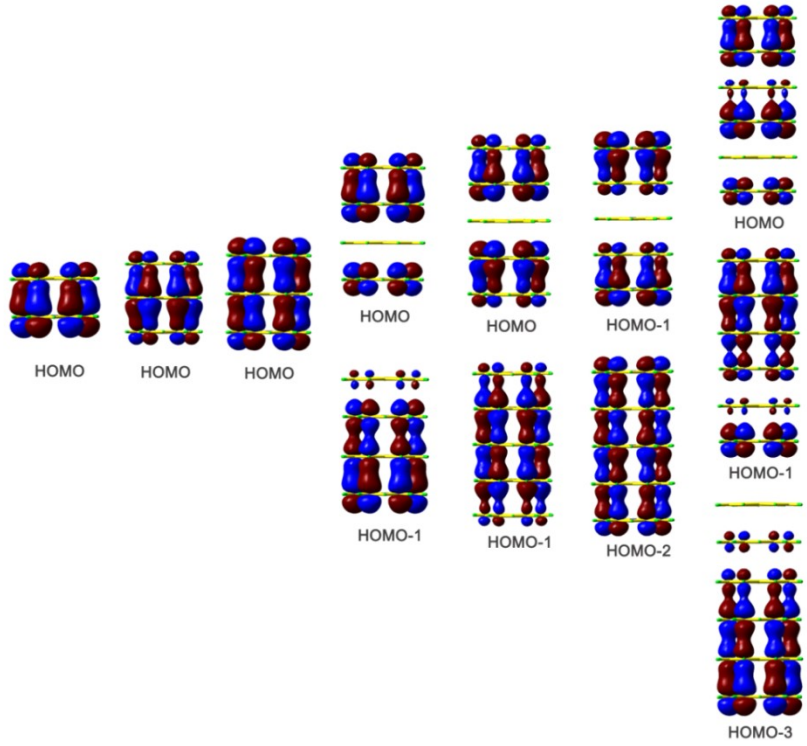
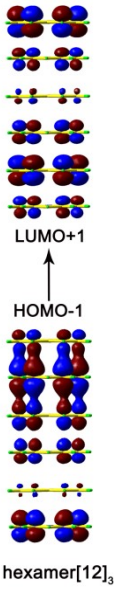
Figure S1. The qualitative frontier orbital visualizations of the studied π-aggregates.



dimer[12] trimer[12-1] trimer[12-2] tetramer[12]$_2$ pentamer[12]$_2$-1 pentamer[12]$_2$-2 hexamer[12]$_3$

Figure S1 shows the qualitative frontier orbital visualizations of the studied π-aggregates. For PLY-B and PLY-N dimer[12], the bonding character of dimer corresponds to the bonding combination of monomer orbitals, which can be attributed to the overlap of the highest-occupied molecular orbital (HOMO) of the N-PLY and the lowest-occupied molecular orbital (LUMO) of the B-PLY monomer [ref. Chem. Eur. J. 2011, 17, 11773 – 11779]. Figure S1 shows the qualitative frontier orbital visualizations of π-aggregates. Note that the HOMO exhibits effective orbitals overlap of the N-PLY and the B-PLY monomer in π-aggregates.

Figure S2. Frontier molecular orbital of the crucial excited state for hexamer $[12]_3$.



The crucial transitions of hexamer$[12]_3$ are mainly dominated from HOMO-1 to LUMO+1, which exhibits intermolecular charge transfer transitions though pancake π-π bonding. The above results further confirms that hexamer$[12]_3$ has the largest β_{tot} values compared to dimer[12] and tetramer$[12]_2$.

Table S1. The first hyperpolarizabilities (β_{tot}, a.u.) of the studied π-aggregates with even layers at the M05-2X/6-31+G** level.

		dimer[12]	tetramer$[12]_2$	hexamer$[12]_3$
6-31G**	β_x	1.93	-10.03	-4.65×10^2
	β_y	-1.43	12.05	-1.74×10^2
	β_z	2.67×10^3	-9.16×10^3	-5.68×10^4
	β_{tot}	2.67×10^3	9.16×10^3	5.68×10^4
6-31+G*	β_x	1.14	-13.37	-4.84×10^2
	β_y	-1.35	11.57	-1.76×10^2
	β_z	2.47×10^3	-8.97×10^3	-5.71×10^4
	β_{tot}	2.47×10^3	8.97×10^3	5.71×10^4
6-31+G**	β_x	1.45	-11.28	-4.78×10^2
	β_y	-0.97	11.64	-1.76×10^2
	β_z	2.55×10^3	-8.95×10^3	-5.71×10^4
	β_{tot}	2.55×10^3	8.95×10^3	5.72×10^4

Table S2. The first hyperpolarizabilities (β_{tot}, a.u.) of the studied π-aggregates with odd layers at the M05-2X/6-31+G**level.

		trimer[12-1]	trimer[12-2]	pentamer$[12]_2$-1	pentamer$[12]_2$-2
6-31G**	β_x	33.72	24.61	50.03	79.70
	β_y	3.67	3.36	-3.39	3.70
	β_z	-43.78	-38.42	-7.06×10^2	-6.41×10^2
	β_{tot}	55.38	45.75	7.07×10^2	6.46×10^2
6-31+G*	β_x	29.70	21.28	34.96	65.66
	β_y	3.88	3.24	-4.00	2.83
	β_z	-45.85	-38.22	-7.18×10^2	-6.36×10^2
	β_{tot}	54.77	43.87	7.19×10^2	6.40×10^2
6-31+G**	β_x	29.74	23.58	37.58	71.95
	β_y	4.02	3.30	-3.74	3.05
	β_z	-46.21	-38.51	-7.21×10^2	-6.41×10^2
	β_{tot}	55.10	45.28	7.22×10^2	6.41×10^2

Table S1 and S2 results show that the β_{tot} of π-aggregates with even layers (dimer[12], tetramer$[12]_2$ and hexamer$[12]_3$) are larger than those of π-aggregates with odd layers (trimer[12-1], [12-2] and pentamer$[12]_2$-1, pentamer$[12]_2$-2). Significantly, the β_{tot} values of these π-aggregates are found to increase with increasing of even layers thickness, which presents in the order of hexamer$[12]_3$>tetramer$[12]_2$>dimer[12].

Table S3. The transition energies (ΔE, eV), the oscillator strength (f_0), the difference of dipole moments ($\Delta\mu$, Debye) between the ground and excited states of the studied π-aggregates with odd-numbered layers.

	trimer[12-1]	trimer[12-2]	pentamer$[12]_2$-1	pentamer$[12]_2$-2
$\boldsymbol{\Delta E}$	1.8173	2.0215	1.5467	1.6184
$\boldsymbol{f_0}$	0.4431	0.4720	0.9627	0.9813
$\boldsymbol{\mu_g}$	0.0064	0.0073	0.0462	0.0464
$\boldsymbol{\mu_e}$	0.0075	0.0110	0.0336	0.0249
$\boldsymbol{\Delta\mu}$	0.0011	0.0037	0.0126	0.0215
$\boldsymbol{\Delta\mu \cdot f_0 / \Delta E}$	0.64	1.67	25.97	39.43

Table S4.The frequency-dependent $\beta(-\omega, \omega, 0)$ and $\beta(-2\omega, \omega, \omega)$ values of the studied π-aggregates with odd layers calculated at the M05-2X level at ω = 0.000, 0.0100 and 0.0239 a.u..

	ω (a.u.)	trimer [12-1]	trimer [12-2]	pentamer $[12]_2$-1	pentamer $[12]_2$-2
$\boldsymbol{\beta_{tot}}$	ω= 0	55	45	722	645
$\beta(-\omega, \omega, 0)$	ω= 0.0100	60	44	770	684
	ω= 0.0239	73	53	1077	923
$\beta(-2\omega, \omega, \omega)$	ω= 0.0100	65	48	882	772
	ω= 0.0239	138	89	3842	2683

Cartesian coordinates of the optimized structures of dimer[12], trimer[12-1], trimer[12-2], tetramer$[12]_2$, pentamer$[12]_2$-1, $[12]_2$-2, and hexamer$[12]_3$.

All the calculations were implemented in Gaussian09 package. The geometries of dimer[12], trimer[12-1], trimer[12-2], tetramer$[12]_2$, pentamer$[12]_2$-1, $[12]_2$-2, and hexamer$[12]_3$ were optimized with a well-tested density functional theory (DFT) method. The M05-2X functional with the 6-31G** basis set was used for all atoms. All the optimized structures with all real frequencies were obtained.

(1) **dimer [12]**

dimer [12]	Thetotal energy = -1004.9018 a.u.		
Atom	X	Y	Z
C	1.41045600	-2.45767500	1.52595300
C	-0.75704600	-1.30315700	1.57141700
C	1.50268900	-0.00367600	1.57417700
C	2.14269800	-1.26160200	1.52562900
C	-2.16657700	-1.22773200	1.52029800
C	-0.75197500	1.30469700	1.57455200
C	-2.16176800	1.23498400	1.52358900
C	-2.83517000	0.00489700	1.52105600
C	1.42007600	2.45078000	1.53126100
C	2.14755800	1.25180800	1.52809500
H	3.23514000	1.31319300	1.50940500
H	1.96419300	3.38811800	1.50872400
H	-2.76804300	-2.13573700	1.49822700
H	1.95084500	-3.39711500	1.50133800
H	-0.48162700	-3.46187200	1.50077400
H	3.23002300	-1.32724200	1.50704600
H	-3.91900000	0.00706000	1.49412400
H	-0.46798300	3.46254000	1.50952000
H	-2.75970700	2.14538200	1.50446800
C	2.80006100	-0.00454900	-1.51656000
C	2.10819200	1.18939900	-1.48535600
C	0.70175600	1.20811700	-1.48987800
C	0.69723800	-1.20947000	-1.49214300
C	2.10370300	-1.19594200	-1.48691200
C	-0.01282300	2.41952100	-1.48728200
C	-1.39458700	0.00318200	-1.49046000
C	-2.08090800	1.23071200	-1.48613400
C	-1.39290500	2.42703800	-1.51869900
C	-1.40197200	-2.42060900	-1.52407800
H	0.55234300	-3.33258700	-1.50138100
H	-1.94488200	-3.35700600	-1.53896700

H	0.56478600	3.33177400	-1.49393700
H	3.88260400	-0.00660100	-1.52712000
H	2.61366900	2.14339400	-1.49201200
H	2.60564200	-2.15180000	-1.49482900
H	-1.93236900	3.36545900	-1.53108600
H	-3.16440700	-1.17875100	-1.49631700
H	-3.15993900	1.19176800	-1.49352100
C	-2.08553300	-1.22183100	-1.48864300
C	0.01814500	2.48780400	1.52860700
C	0.00837200	-2.48914500	1.52281500
C	-0.02185300	-2.41820500	-1.49260300
B	-0.00239900	-0.00075400	1.60698700
N	0.00148600	0.00064900	-1.49230000

(2) **trimer[12-1]**

trimer[12-1]	The total energy = -1492.4091 a.u.		
Atom	X	Y	Z
C	1.434838	-2.459864	1.572182
C	-0.731807	-1.303734	1.549912
C	1.524238	-0.005714	1.541574
C	2.165418	-1.262633	1.571247
C	-2.140829	-1.230049	1.589767
C	-0.727369	1.299920	1.552493
C	-2.136899	1.231068	1.592011
C	-2.811344	0.001740	1.594211
C	1.443414	2.448505	1.577666
C	2.169881	1.249092	1.574104
H	3.257364	1.310066	1.587136
H	1.986984	3.385642	1.593955
H	-2.741369	-2.138504	1.608592
H	1.975412	-3.398764	1.586330
H	-0.457272	-3.462657	1.596693
H	3.252683	-1.327493	1.583948
H	-3.894701	0.003437	1.616491
H	-0.445402	3.457618	1.603773
H	-2.734232	2.141599	1.612420
C	0.041366	2.483443	1.583728
C	0.032943	-2.490190	1.578524
B	0.021307	-0.003170	1.525241
C	1.467821	-2.469444	7.828336
C	-0.698168	-1.312646	7.875806
C	1.558376	-0.015500	7.864804

C	2.198851	-1.272658	7.825363
C	-2.107622	-1.238317	7.850508
C	-0.692654	1.291071	7.879859
C	-2.102401	1.222805	7.854349
C	-2.777470	-0.006350	7.856070
C	1.478175	2.438905	7.835734
C	2.204126	1.239024	7.828997
H	3.291458	1.299635	7.805166
H	2.022080	3.375793	7.816236
H	-2.708636	-2.146521	7.835404
H	2.007733	-3.408575	7.805988
H	-0.424938	-3.471396	7.819530
H	3.285916	-1.337867	7.801638
H	-3.860990	-0.004039	7.844827
H	-0.410270	3.448863	7.830579
H	-2.699546	2.133603	7.842177
C	2.834797	-0.014315	4.697027
C	2.140860	1.178380	4.702218
C	0.734474	1.195903	4.709280
C	0.729674	-1.216179	4.706079
C	2.136043	-1.204293	4.699071
C	0.021609	2.408095	4.714678
C	-1.357159	-0.006021	4.717764
C	-2.044288	1.220843	4.723114
C	-1.358580	2.418517	4.721392
C	-1.368295	-2.430605	4.714695
H	0.588446	-3.338779	4.703926
H	-1.911631	-3.367026	4.716158
H	0.601673	3.319072	4.713057
H	3.917522	-0.016503	4.691569
H	2.644555	2.133585	4.701159
H	2.635948	-2.161481	4.695546
H	-1.898188	3.357081	4.725480
H	-3.128237	-1.184804	4.725199
H	-3.123506	1.179825	4.728451
C	-2.049183	-1.230212	4.719665
C	0.076284	2.474464	7.843485
C	0.065759	-2.499130	7.835723
C	0.011935	-2.425561	4.708073
B	0.055646	-0.012414	7.896144
N	0.035803	-0.008723	4.711082

(3) trimer[12-2]

trimer[12-2]	The total energy = -1522.3050 a.u.		
Atom	X	Y	Z
C	1.434228	-2.459811	1.582207
C	-0.734101	-1.306177	1.594337
C	1.526526	-0.005187	1.585103
C	2.166555	-1.263569	1.580545
C	-2.144132	-1.230902	1.601300
C	-0.729819	1.303156	1.597465
C	-2.140210	1.232584	1.604084
C	-2.812807	0.001961	1.606176
C	1.442429	2.449626	1.588457
C	2.170800	1.251117	1.583731
H	3.258785	1.312003	1.578803
H	1.986691	3.387771	1.586967
H	-2.744828	-2.139961	1.603100
H	1.975475	-3.399689	1.578293
H	-0.458764	-3.465089	1.589501
H	3.254330	-1.328106	1.575480
H	-3.897489	0.003668	1.611461
H	-0.447258	3.461091	1.597909
H	-2.737850	2.143650	1.607845
C	2.798872	-0.004211	-1.579618
C	2.110005	1.191192	-1.555471
B	0.703443	1.210718	-1.546966
C	0.698765	-1.211104	-1.549921
C	2.105386	-1.196991	-1.558203
C	-0.011772	2.421991	-1.544577
C	-1.396572	0.003837	-1.535456
C	-2.082333	1.231881	-1.531527
C	-1.391831	2.426478	-1.556001
C	-1.401215	-2.418752	-1.562258
C	0.552088	-3.334484	-1.555288
C	-1.944577	-3.355502	-1.568368
C	0.564990	3.334682	-1.547254
H	3.881835	-0.006301	-1.591785
H	2.616274	2.144665	-1.556459
H	2.607961	-2.152412	-1.561478
H	-1.931551	3.365343	-1.559726
H	-3.165907	-1.179282	-1.527457
H	-3.161298	1.193826	-1.523920
H	-2.087092	-1.221548	-1.534987
H	0.040309	2.486670	1.594768
H	0.032107	-2.492336	1.588628

C	-0.021154	-2.419595	-1.550689
C	0.020510	-0.002750	1.592166
C	0.001915	0.001174	-1.545888
C	2.833597	-0.014130	4.737450
C	2.144735	1.181449	4.723375
C	0.738125	1.201170	4.728811
C	0.733066	-1.220674	4.725417
C	2.139741	-1.206771	4.719873
C	0.023112	2.412497	4.736859
C	-1.362111	-0.005392	4.734410
H	-2.047675	1.222715	4.740713
H	-1.356764	2.417122	4.761518
H	-1.366910	-2.428017	4.755072
H	0.586117	-3.344001	4.726764
H	-1.910294	-3.364730	4.764113
H	0.600017	3.325100	4.736221
H	3.916632	-0.016414	4.738835
H	2.651172	2.134835	4.722096
H	2.642200	-2.162252	4.715952
C	-1.896239	3.356062	4.773060
C	-3.131636	-1.188277	4.740834
C	-3.126661	1.184848	4.743565
C	-2.052812	-1.230701	4.737628
B	0.013001	-2.429023	4.730172
N	0.036402	-0.008274	4.731432

(4) **tetramer [12]$_2$**

tetramer [12]$_2$	The total energy = -2009.8189 a.u.		
Atom	X	Y	Z
C	1.43475900	-2.46043900	1.51779600
C	-0.73328700	-1.30637600	1.55309100
C	1.52624700	-0.00579900	1.54232900
C	2.16653600	-1.26382500	1.51179100
C	-2.14334000	-1.23144800	1.53465900
C	-0.72903600	1.30203200	1.55710700
C	-2.13939700	1.23180400	1.53831000
C	-2.81237700	0.00128600	1.54188900
C	1.44279600	2.44914100	1.52532900
C	2.17066700	1.25022700	1.51551500
H	3.25853300	1.31104500	1.50295200
H	1.98689500	3.38705800	1.51228600
H	-2.74400500	-2.14042100	1.52966400
H	1.97582700	-3.40006500	1.50194100
H	-0.45830500	-3.46522700	1.51710800
H	3.25419300	-1.32821600	1.49907000

H	-3.89684000	0.00303300	1.53487200
H	-0.44700300	3.46003200	1.52775100
H	-2.73705100	2.14277300	1.53612100
C	2.80423400	-0.00395100	-1.57632700
C	2.11328600	1.19037900	-1.54407600
C	0.70671300	1.20909400	-1.53855200
C	0.70260000	-1.20994700	-1.54178200
C	2.10920300	-1.19602800	-1.54747200
C	-0.00825200	2.42037800	-1.53307500
C	-1.39061500	0.00312000	-1.52720600
C	-2.07705400	1.23073000	-1.52006100
C	-1.38852000	2.42661800	-1.55202300
C	-1.39681300	-2.42031000	-1.55847300
H	0.55737900	-3.33328400	-1.54971000
H	-1.93974600	-3.35690500	-1.56879400
H	0.56879400	3.33293100	-1.54097700
H	3.88683700	-0.00578500	-1.59291800
H	2.61891900	2.14424200	-1.55071000
H	2.61157700	-2.15158900	-1.55707100
H	-1.92823200	3.36509300	-1.55988400
H	-3.16012300	-1.17965500	-1.52132200
H	-3.15606800	1.19194000	-1.51833300
C	-2.08124300	-1.22217200	-1.52333000
C	0.04055000	2.48566800	1.52997700
C	0.03244600	-2.49248500	1.52231300
C	-0.01653900	-2.41879800	-1.53934000
B	0.02098300	-0.00342300	1.56694200
N	0.00625000	0.00077500	-1.53772200
C	1.46450400	-2.46967200	7.82629900
C	-0.70220000	-1.31478000	7.89047400
C	1.55743500	-0.01596700	7.87662300
C	2.19677400	-1.27375100	7.82184000
C	-2.11182200	-1.23912800	7.85039500
C	-0.69644600	1.29269900	7.89448700
C	-2.10634300	1.22334300	7.85396700
C	-2.78017000	-0.00645000	7.85605600
C	1.47529000	2.43829600	7.83391100
C	2.20226600	1.23910800	7.82567100
H	3.28964700	1.29980500	7.79464700
H	2.01937200	3.37546800	7.80375500
H	-2.71337800	-2.14716100	7.82932600
H	2.00438200	-3.40917200	7.79319500
H	-0.42815400	-3.47312500	7.81209500
H	3.28386700	-1.33920600	7.79058200

H	-3.86413600	-0.00399200	7.83452300
H	-0.41283600	3.45012300	7.82268000
H	-2.70390100	2.13406600	7.83525400
C	2.83316300	-0.01347500	4.76124300
C	2.14010100	1.17934300	4.78323200
C	0.73386200	1.19718300	4.78335800
C	0.72876000	-1.21531700	4.77950400
C	2.13508500	-1.20338500	4.77916300
C	0.02101400	2.40925000	4.79738100
C	-1.35842900	-0.00468600	4.79669200
C	-2.04511700	1.22228900	4.81222200
C	-1.35893300	2.41924300	4.79129100
C	-1.36920100	-2.42855800	4.78375100
H	0.58721900	-3.33733800	4.77381100
H	-1.91270700	-3.36499400	4.78138300
H	0.60129900	3.31982500	4.78446300
H	3.91593400	-0.01574400	4.75067800
H	2.64343000	2.13450300	4.77163200
H	2.63434500	-2.16063200	4.76408600
H	-1.89845300	3.35797900	4.79185300
H	-3.12918600	-1.18299000	4.80741900
H	-3.12417600	1.18109600	4.81094900
C	-2.05030800	-1.22878700	4.80815800
C	0.07351800	2.47546100	7.84226900
C	0.06251200	-2.50069500	7.83462300
C	0.01078400	-2.42437900	4.78980900
B	0.05281200	-0.01274500	7.91948800
N	0.03478500	-0.00758400	4.78451100

(5) **pentamer[12]$_2$-1**

pentamer[12]$_2$-1 The total energy = -2497.3288 a.u.			
Atom	X	Y	Z
C	1.437551	-2.466197	1.569119
C	-0.729558	-1.310802	1.537837
C	1.528222	-0.012451	1.519373
C	2.168940	-1.269711	1.561217
C	-2.138626	-1.236100	1.587895
C	-0.724530	1.294576	1.528514
C	-2.133819	1.225636	1.579244
C	-2.808049	-0.003949	1.588445
C	1.446915	2.441956	1.551660
C	2.173686	1.242560	1.552491
H	3.261268	1.303491	1.566573

H	1.990959	3.379131	1.567484
H	-2.739441	-2.144295	1.615155
H	1.977928	-3.405355	1.591695
H	-0.454567	-3.469236	1.605750
H	3.256274	-1.334768	1.575686
H	-3.891507	-0.001712	1.617988
H	-0.441371	3.452428	1.580454
H	-2.731138	2.136297	1.600347
C	0.045101	2.477991	1.560376
C	0.035537	-2.496809	1.578366
B	0.024281	-0.009681	1.500873
C	1.489139	-2.444930	7.848914
C	-0.678202	-1.289629	7.864225
C	1.578914	0.009787	7.839996
C	2.219982	-1.247588	7.838641
C	-2.087743	-1.215772	7.875966
C	-0.674284	1.315998	7.855004
C	-2.084195	1.246507	7.867319
C	-2.757919	0.016448	7.878013
C	1.496671	2.464660	7.831325
C	2.223893	1.265307	7.829944
H	3.311679	1.325822	7.820820
H	2.040485	3.402374	7.822895
H	-2.687767	-2.125006	7.884120
H	2.030296	-3.384213	7.847178
H	-0.404042	-3.448505	7.868071
H	3.307574	-1.311537	7.829295
H	-3.841990	0.018048	7.887364
H	-0.393602	3.473889	7.842930
H	-2.681439	2.157605	7.869092
C	2.844367	-0.004551	4.644974
C	2.150569	1.188120	4.638312
C	0.744276	1.205540	4.652904
C	0.739877	-1.206899	4.661144
C	2.146214	-1.194701	4.646642
C	0.031087	2.417540	4.648780
C	-1.347487	0.003188	4.670471
C	-2.034749	1.229994	4.665697
C	-1.348922	2.427444	4.665020
C	-1.357822	-2.421032	4.682303
H	0.598813	-3.329339	4.668558
H	-1.901023	-3.357560	4.690114
H	0.611088	3.328464	4.645326
H	3.927134	-0.006566	4.638126

H	2.653992	2.143380	4.635602
H	2.646162	-2.151781	4.650864
H	-1.888689	3.365985	4.665838
H	-3.118191	-1.175744	4.685034
H	-3.113846	1.188719	4.676145
C	-2.039251	-1.221097	4.674686
C	0.094481	2.499928	7.842869
C	0.087020	-2.476081	7.860847
C	0.022217	-2.416262	4.665642
B	0.075049	0.012025	7.852907
N	0.045690	0.000639	4.662689
C	1.569762	-2.419578	14.126784
C	-0.596279	-1.263549	14.191573
C	1.661481	0.034482	14.156895
C	2.301206	-1.223155	14.111837
C	-2.006006	-1.188840	14.168383
C	-0.590896	1.342009	14.181946
C	-2.000921	1.272936	14.159400
C	-2.675201	0.043457	14.172347
C	1.579918	2.488574	14.108190
C	2.306423	1.289042	14.102405
H	3.393568	1.349623	14.067226
H	2.123653	3.425489	14.074792
H	-2.607245	-2.097097	14.159065
H	2.109608	-3.358959	14.100534
H	-0.322762	-3.422462	14.133316
H	3.388075	-1.288549	14.076946
H	-3.759017	0.045688	14.163966
H	-0.308420	3.499286	14.107421
H	-2.598435	2.183568	14.143306
C	2.913672	0.018828	11.009857
C	2.220354	1.211756	11.021230
C	0.813983	1.229560	11.032895
C	0.808914	-1.182856	11.042197
C	2.215348	-1.171024	11.030674
C	0.101275	2.441742	11.041704
C	-1.278032	0.027838	11.062357
C	-1.964846	1.254886	11.071459
C	-1.278857	2.451988	11.050353
C	-1.289086	-2.396319	11.069056
H	0.667273	-3.305211	11.052700
H	-1.832477	-3.332721	11.078479
H	0.681377	3.352497	11.027585
H	3.996385	0.016487	10.996389

H	2.723954	2.166843	11.007892
H	2.714908	-2.128299	11.024834
H	-1.818294	3.390713	11.052612
H	-3.048945	-1.150589	11.091088
H	-3.043952	1.213940	11.081457
C	-1.970021	-1.196206	11.081093
C	0.178154	2.524857	14.125697
C	0.167830	-2.449955	14.144298
C	0.091086	-2.391906	11.060261
B	0.158084	0.037728	14.204199
N	0.115041	0.024866	11.044890

(6) **pentamer[12]$_2$-2**

pentamer[12]$_2$-2 The total energy = -2527.2229 a.u.			
Atom	X	Y	Z
C	1.43776400	-2.45819300	1.52993200
C	-0.73021000	-1.30430900	1.55496400
C	1.52985300	-0.00373200	1.53076100
C	2.16989500	-1.26193700	1.51949000
C	-2.14013600	-1.22919100	1.56041600
C	-0.72582000	1.30440700	1.55000900
C	-2.13609200	1.23407500	1.55610200
C	-2.80888200	0.00360900	1.56574600
C	1.44608900	2.45092900	1.52056600
C	2.17418500	1.25230700	1.51480800
H	3.26214600	1.31299300	1.50438000
H	1.99028800	3.38900900	1.51198000
H	-2.74074100	-2.13830000	1.56708800
H	1.97889400	-3.39807100	1.52484200
H	-0.45530800	-3.46315500	1.54812400
H	3.25763800	-1.32641000	1.50920900
H	-3.89349500	0.00540400	1.57411600
H	-0.44364600	3.46221900	1.53505400
H	-2.73359900	2.14523900	1.56008800
C	2.78517900	-0.01368600	-1.62654800
C	2.09601800	1.18155900	-1.60099500
C	0.68957900	1.20104700	-1.58637200
C	0.68477000	-1.21994900	-1.58149400
C	2.09126000	-1.20605900	-1.59590100
C	-0.02541600	2.41242600	-1.58335000
C	-1.40969300	-0.00525100	-1.56074700
C	-2.09543900	1.22272700	-1.55623900
C	-1.40551400	2.41753000	-1.58988600

C	-1.41515400	-2.42816100	-1.58027200
H	0.53830600	-3.34329800	-1.57878800
H	-1.95857100	-3.36479600	-1.58059900
H	0.55156100	3.32494500	-1.59231500
H	3.86797400	-0.01589600	-1.64416000
H	2.60214600	2.13508700	-1.60809300
H	2.59361500	-2.16160000	-1.59896500
H	-1.94519500	3.35631000	-1.59398100
H	-3.17909300	-1.18796400	-1.53914400
H	-3.17436300	1.18456800	-1.54357200
C	-2.10032300	-1.23050600	-1.55155200
C	0.04399200	2.48781900	1.53245600
C	0.03564400	-2.49044500	1.54193700
C	-0.03502800	-2.42846700	-1.57367500
B	0.02427000	-0.00122900	1.55022600
N	-0.01174000	-0.00803100	-1.57808000
C	1.50235900	-2.44546800	7.90836800
C	-0.66573000	-1.29156600	7.91492300
C	1.59444100	0.00895700	7.89812800
C	2.23457500	-1.24924900	7.90330400
C	-2.07560100	-1.21638500	7.93159900
C	-0.66128900	1.31712000	7.91050100
C	-2.07151700	1.24683700	7.92721900
C	-2.74436500	0.01640200	7.93359300
C	1.51079000	2.46362400	7.89999800
C	2.23891700	1.26501800	7.89919700
H	3.32691600	1.32571600	7.89246900
H	2.05504400	3.40170400	7.89593500
H	-2.67620800	-2.12549000	7.93738200
H	2.04349700	-3.38535700	7.90757800
H	-0.39079300	-3.45037900	7.92256500
H	3.32235200	-1.31376100	7.89646100
H	-3.82897100	0.01821500	7.94263000
H	-0.37897100	3.47494100	7.91027400
H	-2.66899200	2.15802200	7.92933600
C	2.85653300	-0.00024000	4.70341700
C	2.16501200	1.19339900	4.70705700
C	0.75874600	1.21157200	4.71892700
C	0.75398900	-1.20370200	4.72345600
C	2.16031600	-1.19111700	4.71168100
C	0.04514500	2.42347100	4.72277100
C	-1.33564400	0.00808800	4.73902500
C	-2.02223600	1.23530000	4.74286400
C	-1.33449300	2.43124800	4.73424700

C	-1.34406500	-2.41507700	4.74363700
H	0.61173200	-3.32594600	4.72838700
H	-1.88758100	-3.35182400	4.74999500
H	0.62488000	3.33439700	4.71605300
H	3.93960200	-0.00239800	4.69445600
H	2.66873900	2.14835100	4.70131600
H	2.66027300	-2.14806000	4.70972200
H	-1.87429200	3.37015800	4.73692600
H	-3.10586400	-1.17120100	4.75713300
H	-3.10121300	1.19445300	4.75221600
C	-2.02705300	-1.21638900	4.74777700
C	0.10865200	2.50053100	7.90950400
C	0.10019200	-2.47767900	7.91817300
C	0.03559200	-2.41273700	4.73193900
B	0.08873700	0.01146800	7.90251800
N	0.05912500	0.00534400	4.72715900
C	2.90606600	0.01050900	11.03617800
C	2.21659700	1.20572700	11.01778900
C	0.81007200	1.22524100	11.02589600
C	0.80519500	-1.19581400	11.02982000
C	2.21177700	-1.18196700	11.02147100
C	0.09512100	2.43659700	11.03034200
C	-1.28935700	0.01894800	11.03763700
C	-1.97507800	1.24693600	11.03984800
C	-1.28470300	2.44176900	11.05833500
C	-1.29449300	-2.40381100	11.06660800
H	0.65872400	-3.31907100	11.03745000
H	-1.83777600	-3.34043800	11.07923100
H	0.67219400	3.34909600	11.02673400
H	3.98901300	0.00831300	11.03603100
H	2.72284100	2.15921100	11.01334800
H	2.71417500	-2.13749500	11.02011600
H	-1.82420400	3.38061500	11.06770000
H	-3.05886000	-1.16374400	11.04893800
H	-3.05405300	1.20882000	11.04431100
C	-1.98004500	-1.20628600	11.04436100
C	0.08535200	-2.40425000	11.03834200
N	0.10869500	0.01615300	11.03326900

(7) **hexamer [12]$_3$**

hexamer [12]$_3$ The total energy = -3014.7366 a.u.			
Atom	X	Y	Z
C	1.44024200	-2.45979600	1.49558300

C	-0.72774400	-1.30576400	1.53112500
C	1.53189500	-0.00513800	1.50781800
C	2.17208300	-1.26328200	1.48302900
C	-2.13784800	-1.23088600	1.52115000
C	-0.72354500	1.30277400	1.52575000
C	-2.13394100	1.23240700	1.51614500
C	-2.80680300	0.00186500	1.52630500
C	1.44821200	2.44969500	1.48521500
C	2.17618600	1.25086100	1.47789700
H	3.26402900	1.31166400	1.46211300
H	1.99226500	3.38762800	1.46834700
H	-2.73847700	-2.13992000	1.52250000
H	1.98131100	-3.39951200	1.48272000
H	-0.45277400	-3.46471500	1.50659300
H	3.25971400	-1.32771200	1.46714300
H	-3.89132800	0.00358100	1.52508900
H	-0.44159300	3.46067500	1.49165600
H	-2.73162000	2.14338100	1.51351400
C	2.79664900	-0.01401500	-1.62207700
C	2.10617800	1.18062400	-1.59233700
C	0.69966100	1.19955000	-1.58130700
C	0.69531900	-1.21989600	-1.57663800
C	2.10189500	-1.20602600	-1.58788800
C	-0.01526300	2.41089600	-1.57756400
C	-1.39806900	-0.00637700	-1.55867000
C	-2.08432500	1.22136200	-1.55369400
C	-1.39555300	2.41691000	-1.59071500
C	-1.40425400	-2.42978500	-1.58099800
H	0.54976900	-3.34326200	-1.57669400
H	-1.94734200	-3.36638600	-1.58557900
H	0.56174700	3.32341000	-1.58959100
H	3.87923500	-0.01600900	-1.64203800
H	2.61191000	2.13438500	-1.60304400
H	2.60421300	-2.16162100	-1.59513600
H	-1.93525300	3.35543900	-1.59912400
H	-3.16756900	-1.18907400	-1.54217700
H	-3.16332000	1.18274200	-1.54711900
C	-2.08871500	-1.23162400	-1.54861600
C	0.04601500	2.48632400	1.49502200
C	0.03798600	-2.49194900	1.50555000
C	-0.02394900	-2.42864300	-1.56801300
B	0.02657700	-0.00269300	1.53511600
N	-0.00101500	-0.00889300	-1.57399800
C	1.49215800	-2.44291000	7.83482100

C	-0.67539900	-1.28843300	7.87371000
C	1.58376900	0.01165800	7.84767800
C	2.22387400	-1.24632800	7.82072500
C	-2.08530200	-1.21356500	7.86323400
C	-0.67092700	1.31953100	7.86734000
C	-2.08115100	1.24949100	7.85735700
C	-2.75432200	0.01914700	7.86915500
C	1.50066000	2.46638000	7.82236300
C	2.22824600	1.26732600	7.81454900
H	3.31606500	1.32772600	7.79491800
H	2.04472800	3.40417600	7.80131800
H	-2.68590900	-2.12264700	7.86235600
H	2.03306300	-3.38262300	7.81856700
H	-0.40112800	-3.44729400	7.84432200
H	3.31146500	-1.31063800	7.80104900
H	-3.83880000	0.02096300	7.86599300
H	-0.38920200	3.47722300	7.82653800
H	-2.67860100	2.16063900	7.85230800
C	2.85004700	0.00101200	4.70943900
C	2.15733000	1.19407200	4.72402700
C	0.75098200	1.21171100	4.73051500
C	0.74651400	-1.20179800	4.73613200
C	2.15292400	-1.18936300	4.72968800
C	0.03769500	2.42363700	4.73962500
C	-1.34176800	0.00887000	4.75405800
C	-2.02870800	1.23587500	4.76387100
C	-1.34224900	2.43252600	4.74162100
C	-1.35125500	-2.41478300	4.75338900
H	0.60508100	-3.32401900	4.73918500
H	-1.89454200	-3.35144300	4.75677200
H	0.61749100	3.33445400	4.72385000
H	3.93288000	-0.00103700	4.69604400
H	2.66059400	2.14921100	4.70935500
H	2.65266400	-2.14640700	4.71935600
H	-1.88204900	3.37120400	4.74040800
H	-3.11214400	-1.17017700	4.77452600
H	-3.10773900	1.19464500	4.76801400
C	-2.03327200	-1.21547300	4.77017200
C	0.09852500	2.50292000	7.83298900
C	0.08997300	-2.47467500	7.84560600
C	0.02869600	-2.41098900	4.75102200
B	0.07883500	0.01427000	7.87663800
N	0.05196700	0.00627400	4.73850500
C	1.56228600	-2.42377100	14.13613500

C	-0.60408300	-1.26880600	14.20866000
C	1.65542300	0.03016200	14.17525200
C	2.29444500	-1.22781400	14.12170000
C	-2.01388300	-1.19332200	14.17633300
C	-0.59853100	1.33889200	14.20101500
C	-2.00867000	1.26921900	14.16904300
C	-2.68223900	0.03939300	14.18077800
C	1.57280900	2.48415700	14.12155400
C	2.29986800	1.28505200	14.11432600
H	3.38704500	1.34563900	14.07602100
H	2.11660400	3.42123300	14.08300000
H	-2.61548400	-2.10147400	14.16222100
H	2.10209200	-3.36335500	14.10318300
H	-0.33030300	-3.42748400	14.13736300
H	3.38134100	-1.29334600	14.08366000
H	-3.76633200	0.04164200	14.16510100
H	-0.31540500	3.49591500	14.11631700
H	-2.60638800	2.17983800	14.14948200
C	2.91163900	0.01887900	11.05363000
C	2.21863800	1.21172000	11.07456100
C	0.81245000	1.22957100	11.08272600
C	0.80724500	-1.18257000	11.08939800
C	2.21352900	-1.17077000	11.08098400
C	0.09984400	2.44169000	11.09525900
C	-1.27948800	0.02807800	11.11279400
C	-1.96607900	1.25509700	11.12661800
C	-1.28012000	2.45189100	11.09670600
C	-1.29060400	-2.39572600	11.11070200
H	0.66570700	-3.30447400	11.09265900
H	-1.83412100	-3.33212100	11.11459300
H	0.68012900	3.35208900	11.07392300
H	3.99429200	0.01649100	11.03557500
H	2.72172800	2.16686200	11.05473200
H	2.71250900	-2.12815400	11.06611700
H	-1.81957600	3.39063400	11.09504200
H	-3.05024400	-1.14982100	11.13809500
H	-3.04511900	1.21384900	11.13050100
C	-1.97139400	-1.19580400	11.13384000
C	0.17108600	2.52134400	14.13800000
C	0.16042600	-2.45492700	14.15291900
C	0.08938200	-2.39147500	11.10904100
B	0.15097200	0.03349900	14.22744700
N	0.11343800	0.02503400	11.09325500