

## Supplementary Material

# Theoretical design of a dual-motor nanorotator composed of all-carboatomic cyclo[18]carbon and figure-of-eight carbon hoop

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## Section S1. Computational details

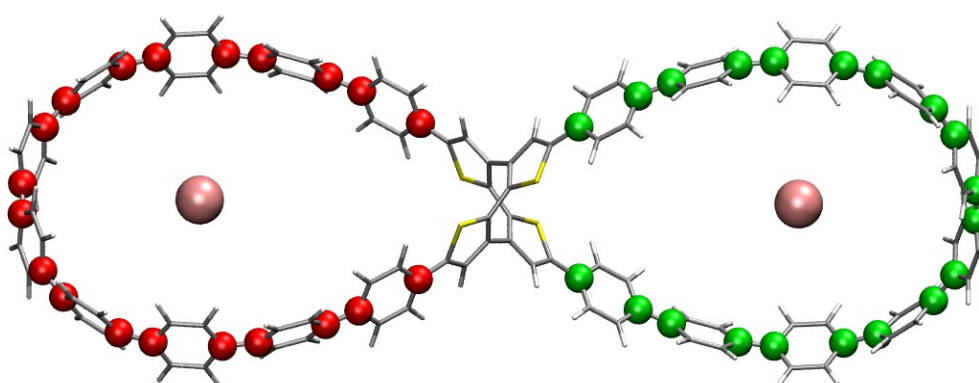
Many theoretical studies have demonstrated that hybrid density functional containing more than 25% global Hartree-Fock (HF) exchange, such as M06-2X,<sup>S1</sup> or containing very high HF exchange at long-range region, such as  $\omega$ B97XD,<sup>S2</sup> combined with at least 6-311G(d) basis set,<sup>S3</sup> can replicate the ground-state polyynic structure of C<sub>18</sub> with alternating long and short bonds.<sup>S4-S6</sup> In contrast, the geometry of organic conjugated macrocycles with normal coordinated carbon atoms is relatively insensitive to the level of basis set. Therefore, we adopted the  $\omega$ B97XD method combined with 6-311G(d) for C<sub>18</sub> ring and 6-31G(d)<sup>S7</sup> for OPP to optimize all molecules and complexes studied. The vibrational frequencies were used to characterize the stationary point as local minimum or transition state. The PES scanning is also carried out at the same calculation level. Gaussian 16 (A.03)<sup>S8</sup> was used to conduct optimizations for minima and transition states, frequency analyses and potential surface scanning.

Intermolecular interaction between C<sub>18</sub> and OPP as well as C<sub>18</sub>@OPP was calculated using  $\omega$ B97X-V<sup>S9</sup> functional in combination with def2-TZVP basis set<sup>S10</sup> with counterpoise correction, because this level is able to accurately estimate  $E_{\text{int}}$  for a wide variety of weakly interacting complexes.<sup>S11</sup> The binding free energy of C<sub>18</sub>@OPP and 2C<sub>18</sub>@OPP was evaluated as  $G_{\text{bind}} = E_{\text{bind}} + \Delta G_{\text{b}}^{\text{corr}}$ , where  $\Delta G_{\text{b}}^{\text{corr}}$  is the variation of thermal correction to free energy during binding.  $\Delta G_{\text{b}}^{\text{corr}}$  and entropy were obtained based on harmonic frequencies by Shermo code.<sup>S12</sup> ORCA 5.0.3 program<sup>S13</sup> was used for calculations of electronic energies. The symmetry-adapted perturbation theory analysis was performed by PSI4 1.5 program.<sup>S14</sup>

MD simulation was realized by GROMACS 2018.8 program<sup>S15</sup> basically based on general amber force field (GAFF).<sup>S16</sup> Specifically, for representing C<sub>18</sub>, c1 atom type (suitable for *sp*-hybridized carbon) was assigned for the carbons, and c1-c1-c1 angle parameter was employed. Parameters of long and short C-C bonds in C<sub>18</sub> were respectively generated by modified Seminario method<sup>S17</sup> based on Hessian matrix at  $\omega$ B97XD/def2-TZVP level. For representing OPP, proper GAFF atom types and corresponding bond, angle, and dihedral parameters were assigned. However, we found the rigid structure of cyclooctatetrathiophene linker region between the two loops of OPP cannot be well maintained via GAFF bonded parameters during MD simulation, therefore the bonded parameters related to this region were produced by

modified Seminario method based on Hessian matrix at  $\omega$ B97XD/6-311G(d) level. The assignment of GAFF parameter, the modified Seminario calculation, and the generation of final GROMACS topology files were finished by Sobtop code.<sup>S18</sup>

In our statistical analysis of MD trajectory, the plane of C<sub>18</sub> is defined as the least-square fitted plane for all atoms in the ring. The plane of each loop in OPP is determined as the least-square fitted plane for the linker carbon atoms in phenyl rings, and the center of the loop is defined as the center of these atoms (see **Fig. S1** for illustration). The angular velocity is calculated for the rotation around the normal vector passing through the center of the C<sub>18</sub>.



**Fig. S1.** Definitions of plane and ring of the loops in statistical analysis of MD trajectory. Red/green spheres highlight the atoms used to fit plane of loop-1/loop-2 of OPP. Pink spheres show the center of these atoms, which also correspond to the centers of the two loops.

The DOS analysis were finished by Multiwfn 3.8(dev) code.<sup>S19</sup> All isosurface and molecular structure maps were rendered by VMD software.<sup>S20</sup>

#### Notes and references

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**Table S1** Optimized Cartesian coordinates for all species involved in the present work ( $C_{18}@OPP$ ,  $2C_{18}@OPP$ ,  $C_{18}@OPP^{TS}$ , and  $2C_{18}@OPP^{TS}$ ). The values are given in Å.

$C_{18}@OPP$ (charge = 0, spin multiplicity = 1)			
atom	$x$	$y$	$z$
S	-2.85851431	-0.93088222	2.80017220
S	0.33943849	0.85186407	2.75643388
S	0.33939194	-0.85182038	-2.75656451
S	-2.85849134	0.93106651	-2.80028269
C	-2.68768092	-2.60960541	0.87566585
H	-2.87837508	-3.43832569	0.20332802
C	0.17029879	-2.54916217	-0.84909621
H	0.37734042	-3.37002938	-0.17185243
C	-2.68760679	2.60976271	-0.87575431
H	-2.87825605	3.43847344	-0.20339418
C	0.17047438	2.54918192	0.84892927
H	0.37757647	3.37001896	0.17166962
C	-1.72863204	-1.59440037	0.58917250
C	6.46409880	-4.72080830	-4.70524392
H	5.88771243	-4.30456771	-5.52696833
C	4.53999146	-4.25928415	-3.15920668
C	10.02522377	-5.78672065	-3.99812627
C	5.87229507	-4.84326810	-3.44305989
C	-0.84245308	-1.57862362	-0.59258896
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H	-12.63600233	-7.68119769	2.86437452
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H	-15.07157322	7.45886175	-2.63455469
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C	12.12205518	-6.66932570	-3.14958073
H	12.64413790	-7.39199476	-2.52830679
C	7.93948207	5.81136401	2.62926046
H	8.52363872	6.18003720	1.79119552
C	12.12213291	6.66949239	3.14918418
H	12.64417336	7.39202227	2.52771448
C	10.76061436	4.85652792	4.74019614
H	10.24053880	4.09711363	5.31621566
C	-3.39354913	2.39491298	-2.03085293
C	17.71226136	0.45429178	1.73718558
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C	5.87249330	4.84318751	3.44286149
C	2.11394413	2.99344059	2.44616937
C	6.61901407	5.43490626	2.41968241
H	6.18700662	5.52640206	1.42699954
C	17.28991774	1.56175680	2.45757857
H	16.76611683	1.40983413	3.39662251
C	10.73808966	-6.73324195	-3.25170421
H	10.20065386	-7.50862029	-2.71276100
C	16.23112652	3.99638763	3.85436255
H	16.86111129	3.46710144	4.56422969
C	4.25072667	2.96151153	3.59246465
H	4.99232993	2.41282713	4.16584600
C	7.77981262	5.10962409	4.91727709
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C	3.57762432	4.92860697	2.39577667
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H	-17.24992332	-4.66234675	5.40663322
C	-18.58282746	-3.97001005	3.87756186
H	-19.21493355	-3.43973822	4.58496375
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C	-5.44764572	-2.57853387	3.44335067
H	-5.29342585	-1.56195989	3.79402249
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H	-7.31238009	-2.75112304	4.47615519
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C	12.14247671	4.79266003	4.63902371
H	12.66993101	3.98399234	5.13590116
C	16.23101602	-3.99616857	-3.85484636
H	16.86082998	-3.46669646	-4.56472584
C	12.84511736	5.65664184	3.79101550

C	15.11582477	-4.68479916	-4.31374071
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H	14.89107202	4.68638841	5.37643889
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H	1.64503126	4.86120076	1.47492814
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H	-21.31484413	-2.04657646	-0.97974406
C	-20.61910480	-0.59044306	0.45100301
C	-20.09659296	-0.44286429	1.74080738
H	-19.90312359	0.55236602	2.12986874
C	-19.66144008	-1.54269527	2.46605811
H	-19.14011254	-1.38047942	3.40487796
C	-19.73029816	-2.83306558	1.92925926
C	-20.40949393	-2.99517410	0.71494133
H	-20.54115572	-3.99165128	0.30151785
C	-19.66146162	1.54257068	-2.46612547
H	-19.14013170	1.38036886	-3.40494663
C	-19.73033907	2.83293690	-1.92931898
C	-20.40954521	2.99503122	-0.71500524
H	-20.54122499	3.99150501	-0.30157916
C	-20.84749320	1.89327947	0.01051870
H	-21.31488938	2.04641298	0.97967168
C	-20.61911528	0.59029592	-0.45107592
C	-20.09660069	0.44272993	-1.74088074
H	-19.90311814	-0.55249624	-2.12994660

C	10.64752949	3.06211431	1.95381990
C	9.43891120	2.90346009	1.85708300
C	8.26021068	2.35282182	1.50903554
C	7.45189566	1.57833672	1.01635395
C	6.98756538	0.51426745	0.33218587
C	6.98628102	-0.51422531	-0.32975361
C	7.45265519	-1.57760112	-1.01362923
C	8.25890023	-2.35346607	-1.50745651
C	9.43850072	-2.90267025	-1.85480555
C	10.64667895	-3.06359678	-1.95300108
C	11.97411441	-2.87274142	-1.83359666
C	13.04707315	-2.37817129	-1.51724149
C	13.94238755	-1.53130899	-0.97338952
C	14.38602632	-0.56972240	-0.36058920
C	14.38492002	0.56875276	0.36038297
C	13.94385755	1.53111321	0.97382203
C	13.04691704	2.37654334	1.51723235
C	11.97528056	2.87301929	1.83508548

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2C<sub>18</sub>@OPP (charge = 0, spin multiplicity = 1)

atom	x	y	z
S	1.65459624	0.84755052	2.73482696
S	-1.65459624	-0.84755052	2.73482696
S	-1.65459624	0.84755052	-2.73482696
S	1.65459624	-0.84755052	-2.73482696
C	1.47876760	2.53999905	0.82133525
H	1.68516560	3.35764579	0.14009489
C	-1.47876760	2.53999905	-0.82133525
H	-1.68516560	3.35764579	-0.14009489
C	1.47876760	-2.53999905	-0.82133525
H	1.68516560	-3.35764579	-0.14009489
C	-1.47876760	-2.53999905	0.82133525
H	-1.68516560	-3.35764579	0.14009489
C	0.45562153	1.57700489	0.58162890
C	-7.78351559	4.70887084	-4.66040077
H	-7.20764951	4.28514967	-5.47864980

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C	-5.86450039	4.24536208	-3.10979455
C	-11.34044360	5.79618170	-3.96664446
C	-7.19377734	4.83423420	-3.39755132
C	-0.45562153	1.57700489	-0.58162890
C	-18.68703696	2.85625033	-1.89900073
C	-19.54921196	0.59455328	-0.44344451
C	-9.87321988	5.62559284	-3.83613266
C	14.16093236	5.67149622	3.76501651
C	13.43708001	6.68187117	3.12030749
H	13.95875273	7.40409402	2.49815621
C	12.05279270	6.74324171	3.22007998
H	11.51493832	7.51664151	2.67873734
C	11.34044360	5.79618170	3.96664446
C	12.07652323	4.86894803	4.71198619
H	11.55739199	4.10893430	5.28800060
C	13.45869087	4.80804195	4.61379400
H	13.98690438	4.00131381	5.11301761
C	7.19377734	-4.83423420	-3.39755132
C	7.93898729	-5.43556021	-2.37902457
H	7.50843180	-5.53010794	-1.38598806
C	9.25705251	-5.81790480	-2.59340106
H	9.84089885	-6.19348142	-1.75822173
C	9.87321988	-5.62559284	-3.83613266
C	9.09602625	-5.10431925	-4.87756308
H	9.52957403	-4.98812774	-5.86687396
C	7.78351559	-4.70887084	-4.66040077
H	7.20764951	-4.28514967	-5.47864980
C	-17.82353892	3.92129823	-2.46575742
C	-2.23005671	2.27960063	-1.93787838
C	-19.78589284	-1.88994316	-0.03513795
H	-20.25133079	-2.02720873	-1.00749421
C	-4.89649372	4.91710093	-2.35565789
H	-5.08024806	5.94011966	-2.03867565
C	-19.54921196	-0.59455328	0.44344451
C	-19.02857722	0.46238008	-1.73510822
H	-18.82604489	-0.52752783	-2.13304206
C	11.34044360	-5.79618170	-3.96664446
C	12.05279270	-6.74324171	-3.22007998

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H	11.51493832	-7.51664151	-2.67873734
C	13.43708001	-6.68187117	-3.12030749
H	13.95875273	-7.40409402	-2.49815621
C	14.16093236	-5.67149622	-3.76501651
C	13.45869087	-4.80804195	-4.61379400
H	13.98690438	-4.00131381	-5.11301761
C	12.07652323	-4.86894803	-4.71198619
H	11.55739199	-4.10893430	-5.28800060
C	-18.68703696	-2.85625033	1.89900073
C	-14.16093236	5.67149622	-3.76501651
C	7.19377734	4.83423420	3.39755132
C	7.78351559	4.70887084	4.66040077
H	7.20764951	4.28514967	5.47864980
C	9.09602625	5.10431925	4.87756308
H	9.52957403	4.98812774	5.86687396
C	9.87321988	5.62559284	3.83613266
C	9.25705251	5.81790480	2.59340106
H	9.84089885	6.19348142	1.75822173
C	7.93898729	5.43556021	2.37902457
H	7.50843180	5.53010794	1.38598806
C	-4.39601034	2.31786432	-3.18088734
H	-4.23753184	1.28470315	-3.47671007
C	-17.04111882	4.68254132	-1.59041202
H	-17.22491657	4.62681492	-0.52149199
C	-15.92679970	-5.37245175	2.04671905
H	-15.26464110	-5.83873687	1.32324216
C	-7.93898729	5.43556021	-2.37902457
H	-7.50843180	5.53010794	-1.38598806
C	-9.87321988	-5.62559284	3.83613266
C	-19.36099653	-3.00206878	0.68008947
H	-19.49876830	-3.99341663	0.25668065
C	-12.07652323	4.86894803	-4.71198619
H	-11.55739199	4.10893430	-5.28800060
C	-15.92679970	5.37245175	-2.04671905
H	-15.26464110	5.83873687	-1.32324216
C	-9.25705251	5.81790480	-2.59340106
H	-9.84089885	6.19348142	-1.75822173
C	-0.43396902	0.58833841	-1.53603133

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C	-19.36099653	3.00206878	-0.68008947
H	-19.49876830	3.99341663	-0.25668065
C	-12.05279270	-6.74324171	3.22007998
H	-11.51493832	-7.51664151	2.67873734
C	-2.23005671	-2.27960063	1.93787838
C	-15.55457383	-5.32514352	3.39414756
C	-18.60630499	1.57326751	-2.45025675
H	-18.08247498	1.42582717	-3.38999948
C	5.86450039	-4.24536208	-3.10979455
C	5.58223121	-2.94276719	-3.53348075
H	6.32893704	-2.39230060	-4.09850858
C	4.39601034	-2.31786432	-3.18088734
H	4.23753184	-1.28470315	-3.47671007
C	3.43759337	-2.97811304	-2.40222133
C	3.69926767	-4.29978033	-2.01744936
H	2.95790342	-4.85097974	-1.44665261
C	4.89649372	-4.91710093	-2.35565789
H	5.08024806	-5.94011966	-2.03867565
C	-19.78589284	1.88994316	0.03513795
H	-20.25133079	2.02720873	1.00749421
C	-5.86450039	-4.24536208	3.10979455
C	-13.45869087	4.80804195	-4.61379400
H	-13.98690438	4.00131381	-5.11301761
C	0.43396902	-0.58833841	-1.53603133
C	-13.43708001	6.68187117	-3.12030749
H	-13.95875273	7.40409402	-2.49815621
C	-9.25705251	-5.81790480	2.59340106
H	-9.84089885	-6.19348142	1.75822173
C	-13.43708001	-6.68187117	3.12030749
H	-13.95875273	-7.40409402	2.49815621
C	-12.07652323	-4.86894803	4.71198619
H	-11.55739199	-4.10893430	5.28800060
C	2.23005671	-2.27960063	-1.93787838
C	-19.02857722	-0.46238008	1.73510822
H	-18.82604489	0.52752783	2.13304206
C	-7.19377734	-4.83423420	3.39755132
C	-3.43759337	-2.97811304	2.40222133
C	-7.93898729	-5.43556021	2.37902457

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H	-7.50843180	-5.53010794	1.38598806
C	-18.60630499	-1.57326751	2.45025675
H	-18.08247498	-1.42582717	3.38999948
C	-12.05279270	6.74324171	-3.22007998
H	-11.51493832	7.51664151	-2.67873734
C	-17.54820911	-4.01476663	3.83587665
H	-18.17864162	-3.48915766	4.54807218
C	-5.58223121	-2.94276719	3.53348075
H	-6.32893704	-2.39230060	4.09850858
C	-9.09602625	-5.10431925	4.87756308
H	-9.52957403	-4.98812774	5.86687396
C	-4.89649372	-4.91710093	2.35565789
H	-5.08024806	-5.94011966	2.03867565
C	-4.39601034	-2.31786432	3.18088734
H	-4.23753184	-1.28470315	3.47671007
C	-15.55457383	5.32514352	-3.39414756
C	-9.09602625	5.10431925	-4.87756308
H	-9.52957403	4.98812774	-5.86687396
C	2.23005671	2.27960063	1.93787838
C	-3.43759337	2.97811304	-2.40222133
C	-0.43396902	-0.58833841	1.53603133
C	-5.58223121	2.94276719	-3.53348075
H	-6.32893704	2.39230060	-4.09850858
C	0.43396902	0.58833841	1.53603133
C	-11.34044360	-5.79618170	3.96664446
C	17.04111882	4.68254132	1.59041202
H	17.22491657	4.62681492	0.52149199
C	15.92679970	5.37245175	2.04671905
H	15.26464110	5.83873687	1.32324216
C	15.55457383	5.32514352	3.39414756
C	16.43290752	4.70509928	4.29195638
H	16.20804968	4.71115870	5.35508807
C	17.54820911	4.01476663	3.83587665
H	18.17864162	3.48915766	4.54807218
C	17.82353892	3.92129823	2.46575742
C	0.45562153	-1.57700489	-0.58162890
C	-0.45562153	-1.57700489	0.58162890
C	-3.69926767	4.29978033	-2.01744936

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H	-2.95790342	4.85097974	-1.44665261
C	5.86450039	4.24536208	3.10979455
C	4.89649372	4.91710093	2.35565789
H	5.08024806	5.94011966	2.03867565
C	3.69926767	4.29978033	2.01744936
H	2.95790342	4.85097974	1.44665261
C	3.43759337	2.97811304	2.40222133
C	4.39601034	2.31786432	3.18088734
H	4.23753184	1.28470315	3.47671007
C	5.58223121	2.94276719	3.53348075
H	6.32893704	2.39230060	4.09850858
C	-17.82353892	-3.92129823	2.46575742
C	-17.04111882	-4.68254132	1.59041202
H	-17.22491657	-4.62681492	0.52149199
C	-13.45869087	-4.80804195	4.61379400
H	-13.98690438	-4.00131381	5.11301761
C	-17.54820911	4.01476663	-3.83587665
H	-18.17864162	3.48915766	-4.54807218
C	-14.16093236	-5.67149622	3.76501651
C	-16.43290752	4.70509928	-4.29195638
H	-16.20804968	4.71115870	-5.35508807
C	-16.43290752	-4.70509928	4.29195638
H	-16.20804968	-4.71115870	5.35508807
C	-3.69926767	-4.29978033	2.01744936
H	-2.95790342	-4.85097974	1.44665261
C	15.92679970	-5.37245175	-2.04671905
H	15.26464110	-5.83873687	-1.32324216
C	17.04111882	-4.68254132	-1.59041202
H	17.22491657	-4.62681492	-0.52149199
C	17.82353892	-3.92129823	-2.46575742
C	17.54820911	-4.01476663	-3.83587665
H	18.17864162	-3.48915766	-4.54807218
C	16.43290752	-4.70509928	-4.29195638
H	16.20804968	-4.71115870	-5.35508807
C	15.55457383	-5.32514352	-3.39414756
C	-7.78351559	-4.70887084	4.66040077
H	-7.20764951	-4.28514967	5.47864980
C	19.78589284	1.88994316	-0.03513795

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H	20.25133079	2.02720873	-1.00749421
C	19.54921196	0.59455328	0.44344451
C	19.02857722	0.46238008	1.73510822
H	18.82604489	-0.52752783	2.13304206
C	18.60630499	1.57326751	2.45025675
H	18.08247498	1.42582717	3.38999948
C	18.68703696	2.85625033	1.89900073
C	19.36099653	3.00206878	0.68008947
H	19.49876830	3.99341663	0.25668065
C	18.60630499	-1.57326751	-2.45025675
H	18.08247498	-1.42582717	-3.38999948
C	18.68703696	-2.85625033	-1.89900073
C	19.36099653	-3.00206878	-0.68008947
H	19.49876830	-3.99341663	-0.25668065
C	19.78589284	-1.88994316	0.03513795
H	20.25133079	-2.02720873	1.00749421
C	19.54921196	-0.59455328	-0.44344451
C	19.02857722	-0.46238008	-1.73510822
H	18.82604489	0.52752783	-2.13304206
C	-11.95709279	-3.06682207	1.93818199
C	-10.74863336	-2.90614972	1.84302600
C	-9.56833938	-2.35613865	1.49933855
C	-8.75920615	-1.58037528	1.01004654
C	-8.29234143	-0.51500724	0.32956427
C	-8.29234143	0.51500724	-0.32956427
C	-8.75920615	1.58037528	-1.01004654
C	-9.56833938	2.35613865	-1.49933855
C	-10.74863336	2.90614972	-1.84302600
C	-11.95709279	3.06682207	-1.93818199
C	-13.28492107	2.87775302	-1.82022523
C	-14.35830230	2.38262788	-1.50617124
C	-15.25579321	1.53517159	-0.96677609
C	-15.69927565	0.57118641	-0.35762013
C	-15.69927565	-0.57118641	0.35762013
C	-15.25579321	-1.53517159	0.96677609
C	-14.35830230	-2.38262788	1.50617124
C	-13.28492107	-2.87775302	1.82022523
C	11.95709279	-3.06682207	-1.93818199

C	13.28492107	-2.87775302	-1.82022523
C	14.35830230	-2.38262788	-1.50617124
C	15.25579321	-1.53517159	-0.96677609
C	15.69927565	-0.57118641	-0.35762013
C	15.69927565	0.57118641	0.35762013
C	15.25579321	1.53517159	0.96677609
C	14.35830230	2.38262788	1.50617124
C	13.28492107	2.87775302	1.82022523
C	11.95709279	3.06682207	1.93818199
C	10.74863336	2.90614972	1.84302600
C	9.56833938	2.35613865	1.49933855
C	8.75920615	1.58037528	1.01004654
C	8.29234143	0.51500724	0.32956427
C	8.29234143	-0.51500724	-0.32956427
C	8.75920615	-1.58037528	-1.01004654
C	9.56833938	-2.35613865	-1.49933855
C	10.74863336	-2.90614972	-1.84302600

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C<sub>18</sub>@OPPT<sup>S</sup> (charge = 0, spin multiplicity = 1)

atom	<i>x</i>	<i>y</i>	<i>z</i>
S	-0.32514823	-0.91505722	2.76098159
S	2.84327108	0.88907024	2.81944114
S	2.84304291	-0.89066470	-2.81840707
S	-0.32557788	0.91301755	-2.75959793
C	-0.15748280	-2.58128866	0.82654471
H	-0.36071790	-3.39528697	0.13992335
C	2.67428064	-2.59978742	-0.92125300
H	2.86536940	-3.43949636	-0.26277132
C	-0.15790229	2.57930169	-0.82520396
H	-0.36115799	3.39331098	-0.13860031
C	2.67397133	2.59817903	0.92232072
H	2.86482718	3.43792842	0.26382277
C	0.83878454	-1.59325248	0.57177847
C	1.71807742	-1.58737230	-0.61495534
H	-12.79141793	-5.75678102	3.77867736
C	-12.07263828	-6.76334171	3.12148782

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C	-12.59770789	-7.47757859	2.49307359
C	-10.68880807	-6.83111106	3.21603841
C	-10.15548456	-7.60125176	2.66562068
C	-9.97008170	-5.89633734	3.97279588
C	-10.70112716	-4.97633170	4.73208454
C	-10.17781145	-4.22779509	5.31946952
C	-12.08330739	-4.90898658	4.63761286
C	-12.60488692	-4.10445355	5.14714537
H	-5.80876284	4.97249274	-3.43942547
C	-6.55562223	5.55005390	-2.40846553
H	-6.12282964	5.63134982	-1.41517702
C	-7.87830262	5.92236772	-2.61029101
C	-8.46161528	6.27725732	-1.76562217
H	-8.49912437	5.74093343	-3.85156955
C	-7.72042729	5.24931695	-4.90644532
H	-8.15762655	5.14591959	-5.89561099
C	-6.40229185	4.86581964	-4.70263610
C	-5.82573075	4.46445348	-5.53162451
H	3.37744537	-2.36771178	-2.07461407
C	-9.96961370	5.89633744	-3.97328805
H	-10.68811421	6.83147037	-3.21675564
C	-10.15460713	7.60153683	-2.66641333
C	-12.07196712	6.76412886	-3.12228519
H	-12.59686491	7.47861456	-2.49401027
C	-12.79100216	5.75766924	-3.77935752
H	-12.08309477	4.90958442	-4.63817043
C	-12.60486777	4.10513239	-5.14763080
C	-10.70088914	4.97649306	-4.73254455
C	-10.17777658	4.22768959	-5.31976946
H	-5.80876178	-4.97401780	3.44003213
C	-6.40243685	-4.86768101	4.70320040
H	-5.82584145	-4.46692479	5.53246024
C	-7.72077570	-5.25070142	4.90662476
C	-8.15810863	-5.14753846	5.89575699
H	-8.49950575	-5.74151230	3.85140294
C	-7.87856138	-5.92267544	2.61014650
C	-8.46189818	-6.27696257	1.76524035
H	-6.55570076	-5.55080428	2.40869175

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C	-6.12278916	-5.63182497	1.41543226
H	1.70117537	-0.58368815	-1.55333145
C	3.37732967	2.36621310	2.07558534
C	-4.47872005	4.37955231	-3.16162891
H	-4.18809712	3.09362571	-3.62847150
C	-4.92254282	2.56535838	-4.22955281
H	-3.01290220	2.45109421	-3.27066091
C	-2.85238586	1.42866666	-3.60065810
C	-2.07295403	3.07611002	-2.44221888
C	-2.33729508	4.38624275	-2.02084071
C	-1.60895669	4.91367867	-1.41209470
H	-3.52352645	5.02084772	-2.36532780
C	-3.71027951	6.03259508	-2.01563811
H	0.86113289	0.61207956	-1.53428765
C	-0.88822582	2.34952906	-1.96142898
C	-0.88774586	-2.35160164	1.96282810
H	1.70129329	0.58190954	1.55451248
C	0.86142758	-0.61398488	1.53557358
H	-15.67084068	-4.76608727	1.59762625
C	-15.85453911	-4.72685597	0.52808081
H	-14.56558595	-5.46577285	2.06184223
C	-13.91705515	-5.95750160	1.34278422
H	-14.18256883	-5.39744474	3.40590182
C	-15.04999041	-4.74897133	4.29496259
H	-14.82435246	-4.74115746	5.35783455
C	-16.15444323	-4.04745758	3.83002789
H	-16.77231672	-3.49967649	4.53646050
C	-16.43274135	-3.96987106	2.45918319
C	0.83847472	1.59135699	-0.57049858
H	1.71789979	1.58560447	0.61613850
C	-4.47849473	-4.38139489	3.16262791
H	-3.52347769	-5.02259280	2.36603540
C	-3.71049577	-6.03414176	2.01591373
H	-2.33712413	-4.38811774	2.02173484
C	-1.60896785	-4.91547188	1.41270155
H	-2.07247231	-3.07820153	2.44359807
C	-3.01219072	-2.45335098	3.27242461
C	-2.85142513	-1.43110330	3.60285741

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H	-4.18750913	-3.09576067	3.63004639
C	-4.92178695	-2.56756856	4.23139857
H	-14.56531649	5.46738493	-2.06253525
C	-13.91675537	5.95917486	-1.34354585
C	-15.67065087	4.76788919	-1.59821134
C	-15.85435967	4.72887635	-0.52865963
H	-16.43256096	3.97153407	-2.45962348
C	-16.15426188	4.04888835	-3.83048599
C	-16.77218549	3.50105938	-4.53683658
H	-15.04973984	4.75020647	-4.29552640
C	-14.82409205	4.74218751	-5.35839442
H	-14.18224709	5.39871847	-3.40655783
C	-18.33380454	-1.88944140	-0.05847934
C	-18.78960406	-2.01559343	-1.03687578
H	-18.09907347	-0.59974652	0.43581622
C	-17.58791529	-0.48609650	1.73334768
H	-17.38205597	0.49777219	2.14410466
C	-17.17979728	-1.60725037	2.44155947
H	-16.66547234	-1.47094773	3.38809308
C	-17.26743316	-2.88687546	1.88104500
C	-17.92565319	-3.01242779	0.65086956
H	-18.06918014	-3.99763982	0.21534490
C	-17.17987152	1.60898961	-2.44189535
C	-16.66566840	1.47261574	-3.38848359
H	-17.26727557	2.88862168	-1.88135993
C	-17.92534563	3.01424181	-0.65110769
H	-18.06871452	3.99946632	-0.21555949
C	-18.33356318	1.89129963	0.05827146
H	-18.78922829	2.01749876	1.03672440
C	-18.09906982	0.60158114	-0.43607453
H	-17.58809277	0.48788471	-1.73366987
C	-17.38241787	-0.49600492	-2.14447040
C	-12.09050012	2.99554685	-1.73828515
H	-13.26158419	2.41769978	-1.41436289
C	-14.05622152	1.61200764	-0.95074901
C	-14.52947092	0.52743866	-0.31042748
C	-14.52780560	-0.52552790	0.31141394
H	-14.05771411	-1.61135409	0.95192547

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C	-13.26058786	-2.41556298	1.41384230
H	-12.09109995	-2.99624509	1.73847452
C	-10.88811332	-3.18856604	1.84555142
H	-9.56184442	-2.98641082	1.73932706
C	-8.49633968	-2.46380614	1.44325327
H	-7.63164490	-1.57166305	0.92402974
C	-7.21528618	-0.58036082	0.34028392
H	-7.21374690	0.57956280	-0.34424925
C	-7.63300795	1.57013702	-0.92716395
H	-8.49527572	2.46435037	-1.44682488
C	-9.56235751	2.98498688	-1.74076409
H	-10.88808495	3.19021655	-1.84766833
C	15.19129581	-5.61321549	-3.94782285
H	14.50713070	-6.68837825	-3.36765933
C	15.05441385	-7.41555166	-2.77366485
C	13.12873181	-6.81271818	-3.49806652
H	12.61933367	-7.63786575	-3.00747867
C	12.38364003	-5.86644057	-4.21261542
C	13.08489424	-4.86267820	-4.88972563
C	12.53672990	-4.10501832	-5.44198326
C	14.46060999	-4.73904937	-4.76052202
H	14.95927980	-3.88631954	-5.21190005
C	8.19004580	5.08129611	3.72388656
C	8.93930014	5.66323153	2.69627665
C	8.50051129	5.76757846	1.70781072
H	10.27233256	6.00204483	2.88922309
C	10.85513398	6.36002715	2.04539751
H	10.90393603	5.77840685	4.11808008
C	10.12267742	5.29646238	5.17553400
C	10.57033402	5.16324041	6.15663126
H	8.79189586	4.95014548	4.98102214
C	8.21589839	4.54946698	5.81085796
H	12.38305720	5.86674458	4.21268999
C	13.12786375	6.81320407	3.49808433
C	12.61823187	7.63825744	3.00758076
C	14.50627317	6.68916027	3.36750854
C	15.05333174	7.41646704	2.77347050
H	15.19073441	5.61412420	3.94755701

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C	14.46033148	4.73978039	4.76031942
C	14.95923609	3.88714282	5.21161246
H	13.08460441	4.86311192	4.88968897
C	12.53666603	4.10531821	5.44198728
H	8.19051629	-5.08187189	-3.72337869
C	8.79220167	-4.95063168	-4.98058396
C	8.21602957	-4.55009709	-5.81036789
H	10.12303531	-5.29667267	-5.17522904
C	10.57055834	-5.16338550	-6.15637826
H	10.90451035	-5.77841923	-4.11784472
C	10.27308685	-6.00215807	-2.88891358
C	10.85605565	-6.35999228	-2.04514088
H	8.94000342	-5.66362095	-2.69583316
C	8.50134141	-5.76803302	-1.70731777
H	6.86449331	4.48325259	3.43059221
C	6.57380868	3.19740130	3.89863727
H	7.29113839	2.68539141	4.53338521
C	5.42808993	2.52891397	3.49510913
C	5.27394846	1.50661913	3.82876291
H	4.51668540	3.12472672	2.61496683
C	4.77094496	4.44005806	2.20236994
H	4.06137280	4.94960408	1.55738019
C	5.92736612	5.10149104	2.59484617
H	6.10777122	6.11418088	2.24447849
C	18.04460054	-4.62118269	-1.72624504
H	18.22587799	-4.59358743	-0.65576360
C	16.93550324	-5.30547527	-2.20383428
H	16.27592047	-5.80028891	-1.49679338
C	16.57156180	-5.23362650	-3.55269144
C	17.44829018	-4.58200560	-4.42951423
H	17.22813058	-4.56408328	-5.49361890
C	18.55946662	-3.89794328	-3.95157978
H	19.19075063	-3.35341833	-4.64881569
C	18.83259611	-3.83979566	-2.57905304
C	6.86487458	-4.48408887	-3.42995525
H	5.92795081	-5.10250361	-2.59411240
C	6.10859038	-6.11515409	-2.24375160
H	4.77143842	-4.44129253	-2.20152872

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C	4.06202674	-4.95096909	-1.55646556
C	4.51688396	-3.12601516	-2.61411075
H	5.42808564	-2.53002886	-3.49434550
C	5.27371523	-1.50776655	-3.82799198
H	6.57389398	-3.19829716	-3.89798137
C	7.29106166	-2.68615310	-4.53280418
C	16.93477218	5.30677631	2.20333382
H	16.27499293	5.80146808	1.49639106
C	18.04394024	4.62271262	1.72558170
H	18.22507480	4.59516963	0.65507470
C	18.83220828	3.84146871	2.57826876
C	18.55925717	3.89954332	3.95083453
H	19.19074539	3.35513409	4.64797582
C	17.44800749	4.58337327	4.42893195
H	17.22799554	4.56538823	5.49306617
C	16.57102796	5.23483051	3.55223875
C	20.82195775	-1.89208459	-0.02522430
H	21.28967609	-2.06290384	0.94081141
C	20.59258381	-0.58089737	-0.46242364
C	20.06952083	-0.40960749	-1.74906799
C	19.87522759	0.59261670	-2.11934507
C	19.63506017	-1.49601083	-2.49469692
C	19.11338878	-1.31669481	-3.43021158
C	19.70526422	-2.79614926	-1.98219742
C	20.38476220	-2.98039033	-0.77120125
C	20.51734020	-3.98434172	-0.37657516
C	19.63513410	1.49784552	2.49378625
C	19.11364193	1.31842212	3.42938010
C	19.70499582	2.79799952	1.98127777
C	20.38426954	2.98237946	0.77017721
C	20.51658210	3.98635803	0.37553105
C	20.82157119	1.89416383	0.02413149
C	21.28910532	2.06507979	-0.94197633
C	20.59253359	0.58292965	0.46136513
C	20.06970277	0.41153165	1.74808979
C	19.87567215	-0.59073247	2.11839624

2C <sub>18</sub> @OPP <sup>TS</sup> (charge = 0, spin multiplicity = 1)			
atom	x	y	z
S	-1.64083093	0.91181485	-2.73807244
S	1.63943089	-0.80518650	-2.75190002
S	1.63907906	0.80557986	2.75395591
S	-1.64080525	-0.91218448	2.73991798
C	-1.46700361	2.57164519	-0.79633960
H	-1.66971929	3.38195056	-0.10529783
C	1.46478461	2.52962326	0.86928051
H	1.67127884	3.35889729	0.20225465
C	-1.46647550	-2.57195648	0.79818476
H	-1.66895442	-3.38228812	0.10710557
C	1.46540977	-2.52930460	-0.86726160
H	1.67205848	-3.35856191	-0.20026109
C	-0.46039802	1.59077975	-0.55838135
C	0.44431152	1.56858711	0.60985999
H	-14.10880395	5.77513431	-3.74656787
C	-13.38876808	6.77824228	-3.08549587
C	-13.91320597	7.49174160	-2.45570169
C	-12.00462434	6.84309036	-3.17771106
C	-11.47064724	7.61064392	-2.62434063
C	-11.28670015	5.90826367	-3.93525889
C	-12.01885259	4.99247685	-4.69862646
C	-11.49671621	4.24375790	-5.28676973
C	-13.40133684	4.92847564	-4.60709381
C	-13.92396737	4.12666082	-5.11982244
H	-7.13126251	-4.96692630	3.39083032
C	-7.87665359	-5.55176891	2.36299686
H	-7.44485189	-5.63433051	1.36936953
C	-9.19717197	-5.93008064	2.56819012
C	-9.77993794	-6.29014062	1.72535595
H	-9.81697818	-5.74807473	3.80993544
C	-9.03878515	-5.24966768	4.86204845
H	-9.47439804	-5.14593057	5.85185401
C	-7.72321288	-4.85960003	4.65472724
C	-7.14724430	-4.45274403	5.48144131
H	2.21371575	2.25214635	1.98277126
C	-11.28674450	-5.90846052	3.93474589

H	-12.00465228	-6.84308317	3.17693359
C	-11.47066444	-7.61059306	2.62351207
C	-13.38878073	-6.77810179	3.08455903
H	-13.91320136	-7.49146288	2.45459431
C	-14.10881427	-5.77504356	3.74570633
H	-13.40137568	-4.92854735	4.60641839
C	-13.92400605	-4.12676464	5.11919832
C	-12.01890837	-4.99269411	4.69812934
C	-11.49676579	-4.24413124	5.28646659
H	-7.13149937	4.96614488	-3.39017164
C	-7.72323685	4.85842135	-4.65413528
H	-7.14718842	4.45112777	-5.48057806
C	-9.03868503	5.24867993	-4.86186359
C	-9.47411461	5.14465450	-5.85171864
H	-9.81698623	5.74765403	-3.81009624
C	-9.19738126	5.93001058	-2.56830074
C	-9.78022936	6.29050035	-1.72570847
H	-7.87697020	5.55153745	-2.36271215
C	-7.44533519	5.63441725	-1.36903890
H	0.42218492	0.56375978	1.54685442
C	2.21432744	-2.25164345	-1.98071372
C	-5.80373423	-4.36938240	3.11092508
H	-5.51931902	-3.07985515	3.57170747
C	-6.25835580	-2.55052814	4.16622237
H	-4.34349382	-2.43655300	3.21737267
C	-4.18657780	-1.41217718	3.54306528
C	-3.39667597	-3.06450735	2.39903293
C	-3.65661752	-4.37659504	1.98109964
C	-2.92318397	-4.90555005	1.37982667
H	-4.84361549	-5.01196098	2.32172912
C	-5.02629096	-6.02589670	1.97622654
H	-0.43985207	-0.61679172	1.52923522
C	-2.20592999	-2.34096361	1.92868065
C	-2.20631308	2.34048077	-1.92689351
H	0.42241798	-0.56365285	-1.54485875
C	-0.43990368	0.61669256	-1.52729500
H	-16.98931898	4.77622905	-1.57137525
C	-17.17295560	4.73126268	-0.50204047

H	-15.88375277	5.47791011	-2.03187101
C	-15.23484652	5.96542809	-1.31027459
H	-15.50073438	5.41634457	-3.37624252
C	-16.36858290	4.77332763	-4.26882626
H	-16.14277349	4.77095396	-5.33169277
C	-17.47339418	4.06994392	-3.80763779
H	-18.09158365	3.52627368	-4.51696453
C	-17.75147350	3.98489010	-2.43718135
C	-0.46005676	-1.59087907	0.56031498
H	0.44472121	-1.56848436	-0.60787125
C	-5.80408724	4.36854375	-3.10983955
H	-4.84395154	5.01138599	-2.32087988
C	-5.02656676	6.02548214	-1.97581603
H	-3.65698880	4.37609423	-1.97998482
C	-2.92350750	4.90525284	-1.37894816
H	-3.39710982	3.06383354	-2.39740664
C	-4.34398384	2.43556447	-3.21543998
C	-4.18711657	1.41103836	-3.54068351
H	-5.51977290	3.07878667	-3.57004309
C	-6.25884878	2.54925750	-4.16433040
H	-15.88360211	-5.47753397	2.03089504
C	-15.23462575	-5.96494151	1.30928748
C	-16.98916859	-4.77585161	1.57041010
C	-17.17274107	-4.73076157	0.50106976
H	-17.75145005	-3.98468551	2.43626726
C	-17.47344239	-4.06986804	3.80672701
C	-18.09170055	-3.52630277	4.51607502
H	-16.36862576	-4.77325833	4.26790625
C	-16.14288907	-4.77100145	5.33078846
H	-15.50069829	-5.41614782	3.37531048
C	-19.65224282	1.89007373	0.06883053
C	-20.10797620	2.01057750	1.04797066
H	-19.41753859	0.60325543	-0.43290996
C	-18.90639723	0.49704914	-1.73107158
H	-18.70052167	-0.48445293	-2.14744701
C	-18.49834172	1.62224789	-2.43284489
H	-17.98403774	1.49138977	-3.38015255
C	-18.58605703	2.89864606	-1.86501774

C	-19.24416557	3.01713101	-0.63407765
H	-19.38768039	3.99983205	-0.19290758
C	-18.49841729	-1.62207692	2.43198687
C	-17.98414135	-1.49122736	3.37931182
H	-18.58609445	-2.89846891	1.86414146
C	-19.24417858	-3.01695674	0.63319037
H	-19.38766161	-3.99965716	0.19200837
C	-19.65224531	-1.88989955	-0.06972401
H	-20.10795556	-2.01040165	-1.04887505
C	-19.41754811	-0.60308160	0.43202130
H	-18.90644629	-0.49687542	1.73019982
C	-18.70058581	0.48462653	2.14658256
C	-13.40481279	-3.00409992	1.71798604
H	-14.57569471	-2.42384905	1.39764671
C	-15.37397854	-1.61766910	0.94115242
C	-15.84576911	-0.52837321	0.30778566
C	-15.84695754	0.52860170	-0.30724759
H	-15.37335316	1.61718797	-0.94048366
C	-14.57684245	2.42450125	-1.39806723
H	-13.40505917	3.00315878	-1.71798757
C	-12.20230655	3.19662760	-1.82577823
H	-10.87641670	2.99138457	-1.72136409
C	-9.80841170	2.47025283	-1.43174292
H	-8.94355277	1.57502697	-0.91819847
C	-8.52324961	0.58173919	-0.34065484
H	-8.52412545	-0.58173840	0.33782791
C	-8.94237011	-1.57557219	0.91591854
H	-9.80858633	-2.46964366	1.42921058
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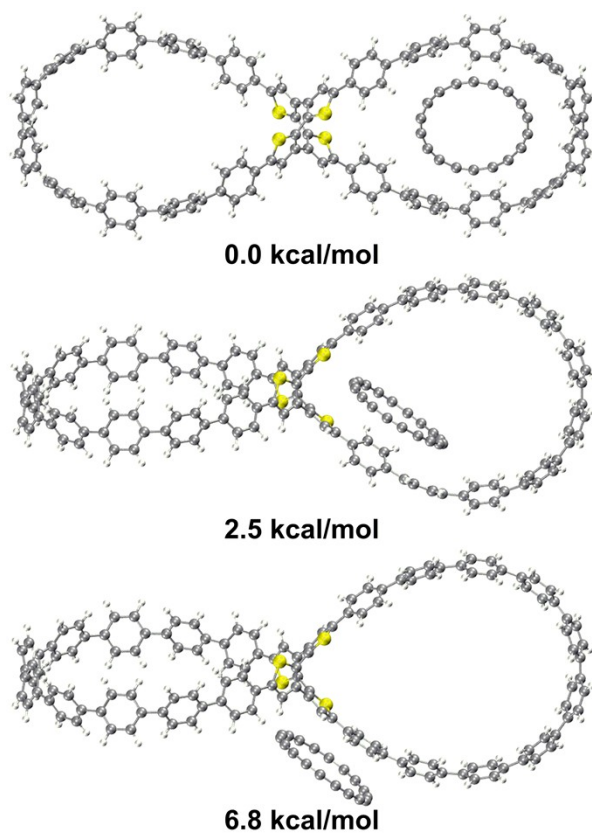
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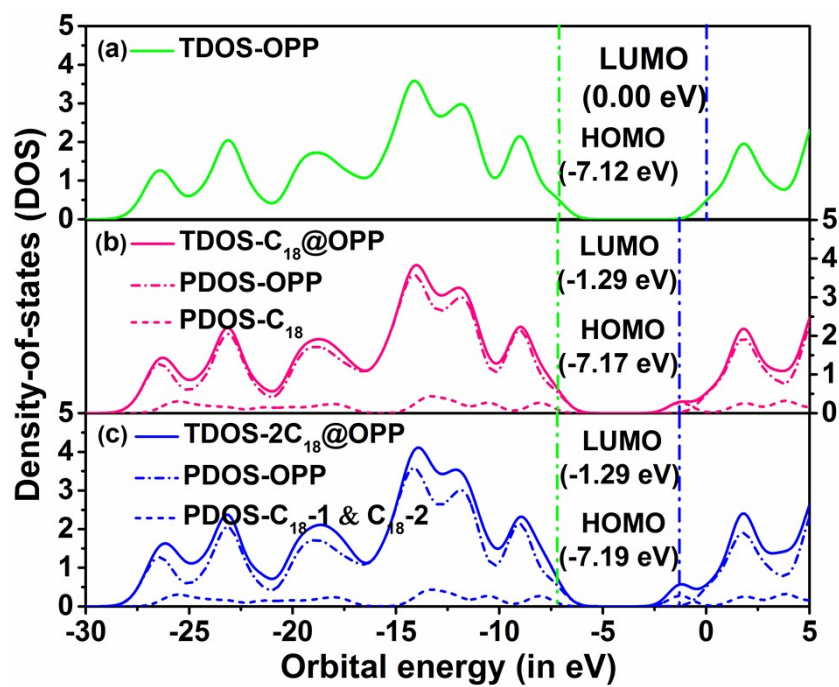


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C	13.27255806	2.84409054	1.87390794
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C	9.55640247	2.32931708	1.54152895
C	10.73639402	2.87300331	1.89612134

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**Fig. S2.** Comparison of different complexation schemes between  $C_{18}$  and OPP. Relative electronic energies of different  $C_{18}@OPP$  configurations evaluated at  $\omega B97X-V/def2-TZVP$  level, with the first one as a reference.



**Fig. S3.** DOS maps and energy levels of FMOs of (a) OPP, (b) C<sub>18</sub>@OPP, and (c) 2C<sub>18</sub>@OPP.