Supporting Information for: Designing Efficient Solar-Thermal Fuels with [n.n](9,10)Anthracene Cyclophanes: A Theoretical Perspective

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Supplementary Discussion 1: General Information for Quantum-Chemical Calculations

All molecular geometries were optimized in vacuum with M06-2X density functional paired with Pople's split-valence double-ζ + polarization basis set, 6-31++G(d,p) for all atoms. Harmonic vibrational frequencies at the same level of theory were computed to characterize the structures as minimum (all real frequencies) and transition state (one imaginary mode) and also to extract thermo-chemical information e.g. zero-point corrections (ZPC) and thermal correction to enthalpy (H_{corr}). On the gas phase optimized geometries single point gas phase and condensed phase computations were carried out with M06-2X density functional paired with Pople's triple-ζ split valence + polarization basis set, 6-311++G(d,p). However, the single point energy difference between double-ζ and triple-ζ basis set turned out to be less than 0.5 kcal/mol. For condensed phase single point calculations, conductor like polarizable continuum model (PCM) or C-PCM, which gives fairly reliable result for solute-solvent interaction, has been chosen as the solvent model with the Universal Force Field (UFF) radii. The dielectric constant in the C-PCM calculations was set to ϵ=2.3741 to simulate toluene for all bis-anthracene cyclophanes ([n.n]BA]) and corresponding photoproducts ([n.n]PI). However, for density functional calibration for [2.2]BA $\rightarrow$ [2.2]PI photoisomerization, o-dichlorobenzene was used to reproduce the experimentally obtained numbers. Thermal corrections were incorporated from the gas phase frequency calculations at 1 atm pressure and 298 K. All DFT computations were conducted by using Gaussian 09 suite of programs.[S1]

Supplementary Discussion 2: Simulated Spectra of a Series of Lowest Energy [n.n]bis-anthracene intermediates ([n.n]BA, n=2-6)

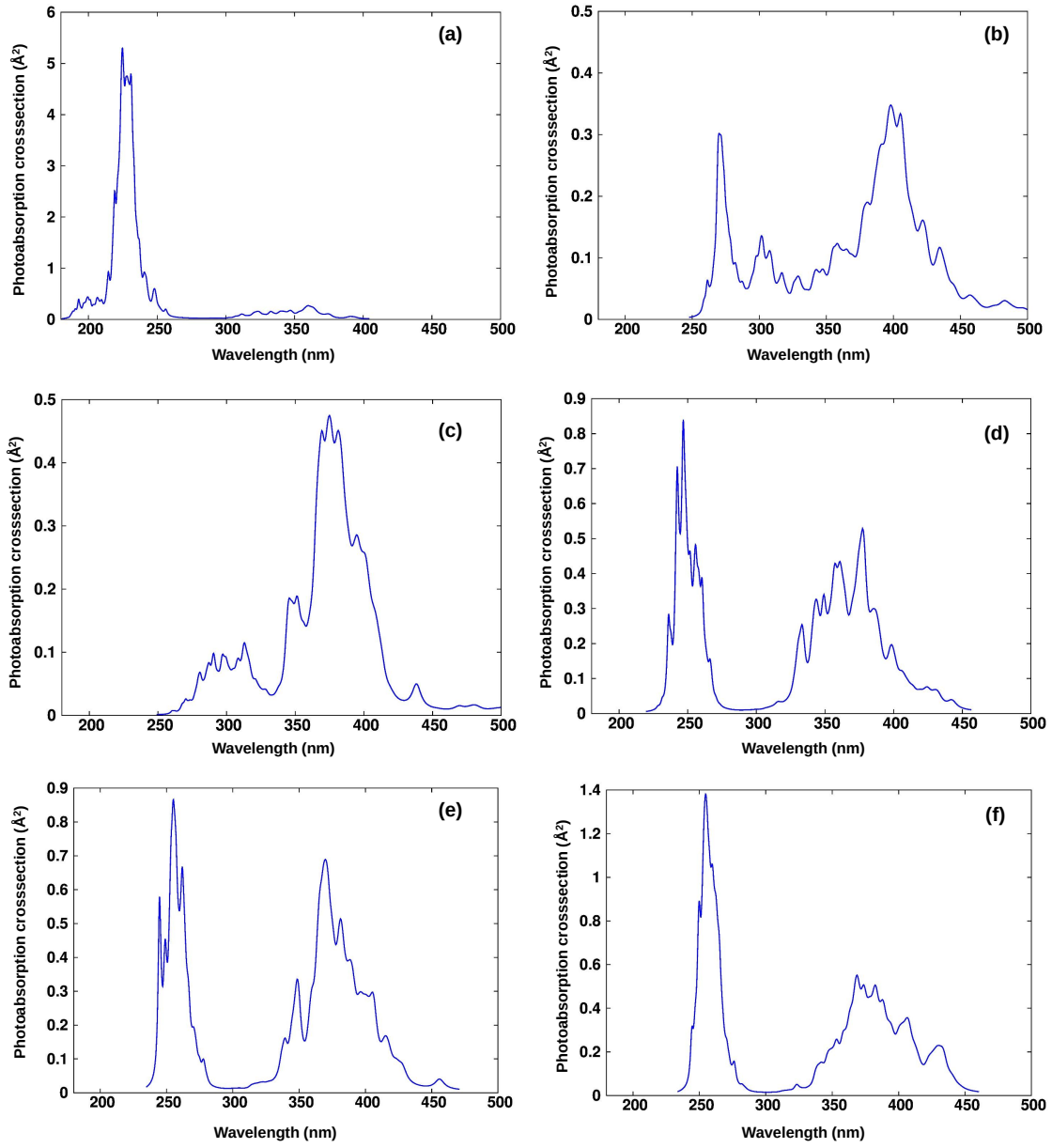


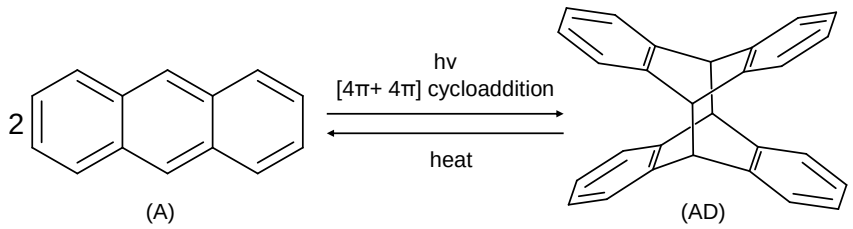
Figure S1: Photoabsorption cross section (Å^2/molecule) as a function of the excitation wavelength (nm) for (a) anthracene monomer; (b) D_2[2.2]BA; (c) C_{2h}[3.3]BA; (d) D_2[4.4]BA; (e) C_{2h}[5.5]BA; and (f) D_2[6.6]BA.

Full photo-absorption spectra, beyond simple vertical transition energies, were further simulated with NEWTON-X program,[S2,S3] interfaced with Gaussian09.[S1] The spectral band shape and the vibrational broadening in the simulated spectra is determined by excitations on nuclear ensemble geometries. The ground state nuclear geometry distributions were generated by Wigner sampling at 300 K temperature. M06-2X/6-31++G(d,p) level of theory was employed to calculate the force constant matrix. Spectra were simulated at TD-CAM-B3LYP/6-31++G(d,p) level of theory with 10 singlet states.

Simulated spectra for anthracene and all lowest energy [n.n]BAs are shown in Fig. S1. It is evident from the simulated spectra that, the characteristic π-π^* absorption onset (λ_{onset}) position remains same in anthracene and all [n.n]BAs. However, a distinct change in photoabsorption cross sections were observed for all [n.n]BAs compared to that of anthracene. The simulated absorption characteristics of [2.2]BA also matches satisfactorily with the experimental spectra.

Supplementary Discussion 3: Benchmarking the Performance of Density Functionals and Basis Sets for Anthracene Based Systems

Choice of Functional in [4π+4π] Photo-dimerization of Anthracene in Gas Phase



Scheme S1: [4π+4π] Photo-dimerization of anthracene (**A**) to produce anthracene photo-dimer (**AD**).

A= Anthracene Monomer;

AD= Anthracene Photo-dimer;

The gas phase reaction energy (ΔE_{rxn}(gas)) is defined as:

$\Delta E_{rxn}(gas) = E(\mathbf{AD}) - 2\times E(\mathbf{A})$

The choice of proper theoretical methods is very very crucial in case of anthrecene photo-dimerization. Grimme et al. proposed that fixed-node diffusion Monte Carlo (FN-DMC) predictions are expected to be accurate for anthracene photo-dimerization.[S4] Please note, DMC is a stochastic method that allows electronic Schrödinger equation to be solved directly and FN approximation is necessary to fulfill the Pauli principle. FN-DMC for anthracene dimerization predicted E_{rxn}(gas)=-9 kcal/mol as shown in Tab. S1 with an error bar of ±2 kcal/mol.[S4] First we performed a more expensive compuation at CCSD(T)/cc-pVTZ level of theory and E_{rxn}(gas) turned out to be -11.2 kcal/mol and nearly falls within the

Table S1: Comparion of ΔE_{rxn}(gas) numbers for different density functionals for anthracene photo dimerization with that of FN-DMC number.

Theoretical Method	$\mathbf{\Delta E_{rxn}(gas)}$ (kcal/mol)
FN-DMC[S4]	-9±2
CCSD(T)/cc-pVTZ	-11.2
M062X/6-311++G(d,p)	**-9.3**
B3PW91-D3/6-311++G(d,p)	**-9.4**
PBE-D3/6-311++G(d,p)	**-10.8**
MP2/cc-pVTZ	-21.1
DLPNO-CCSD(T)/cc-pVTZ/cc-pVTZ/C	-13.6
B3LYP/6-311++G(d,p)	+19.2
B3LYP-D3/6-311++G(d,p)	+3.4
B3PW91/6-311++G(d,p)	+8.3
BP86/6-311++G(d,p)	+13.6
BP86-D3/6-311++G(d,p)	+13.6
PBE/6-311++G(d,p)	-0.1

-9±2 kcal/mol number predicted by FN-DMC. We also compute a comparatively much less expensive DLPNO-CCSD(T)/cc-pVTZ number using ORCA Program Package[S5] which turned out to be -13.6 kcal/mol (deviates from the FN-DMC number). Then we did a calibration study taking a series of density functionals. It must be noted that typically DFT predictions are ascribed error bars of ±2-3 kcal/mol. Given this fact we find M06-2X, B3PW91-D3, and PBE-D3 predictions are closest to the FN-DMC prediction. All other functional choices are expected to overestimate the energy storage for anthracene based systems (as it appears from the above table).

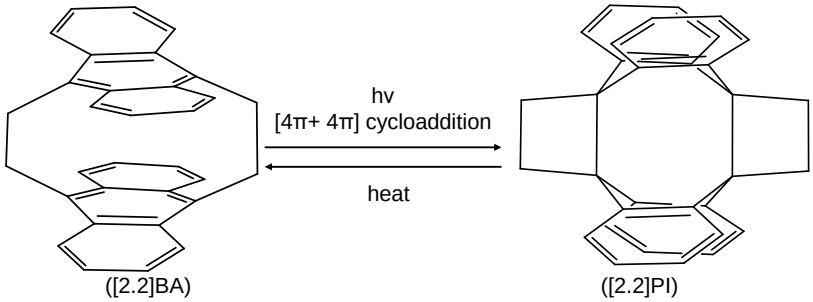
Choice of Basis Set in [4π+4π] Photo-dimerization of Anthracene in Gas Phase

Table S2: Comparion of E_{rxn}(gas) numbers for M06-2X and B3PW91-D3 functionals with different basis sets for anthracene photo-dimerization.

Theoretical Method	**Basis Set**	Δ**E$_{rxn}$(gas)** (kcal/mol)
FN-DMC[S4]	-	**-9±2**
M06-2X	**6-311++G(d,p)**	**-9.3**
	cc-pVTZ	-4.0
	Def2-TZVP	-3.9
B3PW91-D3	**6-311++G(d,p)**	**-9.4**
	cc-pVTZ	-4.5
	Def2-TZVP	-4.9
PBE-D3	**6-311++G(d,p)**	**-10.8**
	cc-pVTZ	-5.9
	Def2-TZVP	-6.2

To check the reliability of Pople's basis set we did a calibration on three best performing functionals for anthracene photo-dimerization: M06-2X, B3PW91-D, and PBE-D3 (see Tab. S2). The table clearly shows that if Dunning and Ahlrichs basis sets are used one would erroneously obtain high energy storage estimates if the FN-DMC numbers are held to be accurate for anthracene based systems.

Choice of Functional in [4π+4π] Photo-dimerization of [2.2]BA → [2.2]PI in Condensed Phase



Scheme S2: [4π+4π] Photo-dimerization of [2.2]BA to produce [2.2]PI.

[2.2]BA= bi[anthracene-9,10-dimethylene]; and **[2.2]PI**= corresponding photo-product;

The solvent-phase reaction enthalpy (ΔH_{rxn}(sol)) is defined as:

H_{rxn}(sol) = H_{sol}(**[2.2]PI**) - H_{sol}(**[2.2]BA**)

H_{sol} = E(o-dichlorobenzene) + H_{corr}

[4π+4π] photo-isomerization enthalpy of [2.2]BA→[2.2]PI in condensed phase (o-dichlorobenzene

Table S3: Comparion of ΔH_{rxn}(sol) numbers for M06-2X, B3PW91-D3, and PBE-D3 functionals against that of experimental values.

Theoretical Method	**ΔH_{rxn}(o-dichlorobenzene)** (kcal/mol)
Experiment	**+8.5**
M06-2X/6-311++G(d,p)	**+8.6**
B3PW91-D3/6-311++G(d,p)	+13.0
PBE-D3/6-311++G(d,p)	+6.9

as solvent) is experimentally known to be +8.5 kcal/mol.[S6,S7] We did a calibration study only considering the three best performing functionals for anthracene photo-dimerization with Pople's triple-ζ 6-311++G(d,p) basis set (see Tab. S3). We found that M06-2X/6-311++G(d,p) prediction (+8.6 kcal/mol) is closest to the experimental predictions, +8.5

kcal/mol. However, B3PW91-D3/6-311++G(d,p) slightly overestimates and PBE-D3/6-311++G(d,p) slightly underestimates the photo-dimerization thermodynamics.

Supplementary Discussion 4: Gas Phase and Condensed Phase Absolute Energies, ZPC, and H_{corr} for [n.n]BA and [n.n]PI (n=2-6)

Table S4: Table of 9C-9'C (d_1) and 10C-10'C (d_2) bond distances in bis-anthracene intermediates or [n.n]BA (n=2-6), single point absolute gas phase energies (E(gas)), single point solvent phase energies (E(solvent:Toluene), zero-point energy corrections (ZPC), and enthalpy corrections (H_{corr}). E(gas) and E(sol) are computed at M06-2X/6-311++G(d,p) and M06-2X/6-311++G(d,p)(CPCM:Toluene) level of theory respectively. ZPC and H_{corr} are computed at M06-2X/6-31++G(d,p) level of theory.

[n.n]BA	P.G. Symm.	d_1=d_2 distance Å	E(gas) (Eh)	E(Toluene) (Eh)	ZPC (Eh/particle)	H_{corr} (Eh/particle)
[2.2]BA	C_2	2.74	-1233.646640	-1233.652723	0.465312	0.488503
	D_2	2.74	-1233.647213	-1233.653320	0.465116	0.488361
[3.3]BA	C_{2h}	3.16	-1312.276822	-1312.283314	0.525787	0.551271
	D_2	3.16	-1312.256872	-1312.262692	0.525176	0.551085
[4.4]BA	C_{2h}	3.81	-1390.892267	-1390.898461	0.583104	0.609247
	D_2	3.81	-1390.894617	-1390.900808	0.584085	0.611666
[5.5]BA	C_{2h}	5.18	-1469.495311	-1469.502963	0.639835	0.670783
	D_2	3.83	-1469.493156	-1469.499191	0.640149	0.670916
[6.6]BA	C_{2h}	6.60	-1548.103259	-1548.110100	0.697183	0.730780
	D_2	6.57	-1548.106296	-1548.113190	0.698176	0.731577

Table S5: Table of 9C-9'C (d_1) and 10C-10'C (d_2) bond distances in photo-products or [n.n]PI (n=2-6), single point absolute gas phase energies (E(gas)), single point solvent phase energies (E(solvent:Toluene), zero-point energy corrections (ZPC), and enthalpy corrections (H_{corr}). E(gas) and E(sol) are computed at M06-2X/6-311++G(d,p) and M06-2X/6-311++G(d,p)(CPCM:Toluene) level of theory respectively. ZPC and H_{corr} are computed at M06-2X/6-31++G(d,p) level of theory.

[n.n]PI	P.G. Symm.	d_1=d_2 distance Å	E(gas) (Eh)	E(Toluene) (Eh)	ZPC (Eh/particle)	H_{corr} (Eh/particle)
[2.2]PI	C_2	-	-	-	-	-
	D_2	1.65	-1233.632311	-1233.639647	0.466563	0.489155
[3.3]PI	C_{2h}	1.66	-1312.275301	-1312.282668	0.528350	0.552249
	D_2	-	-	-	-	-
[4.4]PI	C_2	1.70	-1390.835129	-1390.841227	0.585834	0.611370
	D_2	1.68	-1390.840984	-1390.847180	0.585530	0.610224
[5.5]PI	C_i	1.66	-1469.425276	-1469.431974	0.644351	0.672905
	D_2	1.68	-1469.434553	-1469.441508	0.645220	0.673420
[6.6]PI	C_{2h}	1.66	-1548.024277	-1548.031590	0.703523	0.734418
	D_2	1.66	-1548.024583	-1548.031746	0.703432	0.734508

Table S6: Uniquely defining the energy storage $\Delta E_{storage}$, energy difference between lowest lying photo-product [n.n]PI and lowest lying bis-anthracene intermediate [n.n]BA.

[n.n]anthracenophanes	$\Delta E_{storage}$ is uniquely defined as:
[2.2]anthracenophane	=[E(D_2[2.2]PI) - E(D_2[2.2]PI)]
	= [(-1233.632311) - (-1233.647213)] Eh
	= 9.0 kcal/mol
[3.3]anthracenophane	=[E(C_{2h}[2.2]PI) - E(C_{2h}[2.2]PI)]
	= [(-1312.275301) - (-1312.276822)] Eh
	= 1.0 kcal/mol
[4.4]anthracenophane	=[E(D_2[2.2]PI) - E(D_2[2.2]PI)]
	= [(-1390.840984) - (-1390.894617)] Eh
	= 33.7 kcal/mol
[5.5]anthracenophane	=[E(D_2[2.2]PI) - E(C_{2h}[2.2]PI)]
	= [(-1469.434553) - (-1469.495311)] Eh
	= 38.1 kcal/mol
[6.6]anthracenophane	=[E(D_2[2.2]PI) - E(D_2[2.2]PI)]
	= [(-1548.024583) - (-1548.106296)] Eh
	= 51.3 kcal/mol

Supplementary Discussion 5: $\Delta E_{storage}$ and corresponding energy storage densities at PBE-D3/6-311++G(d,p) and B3PW91-D3/6-311++G(d,p) level of theory

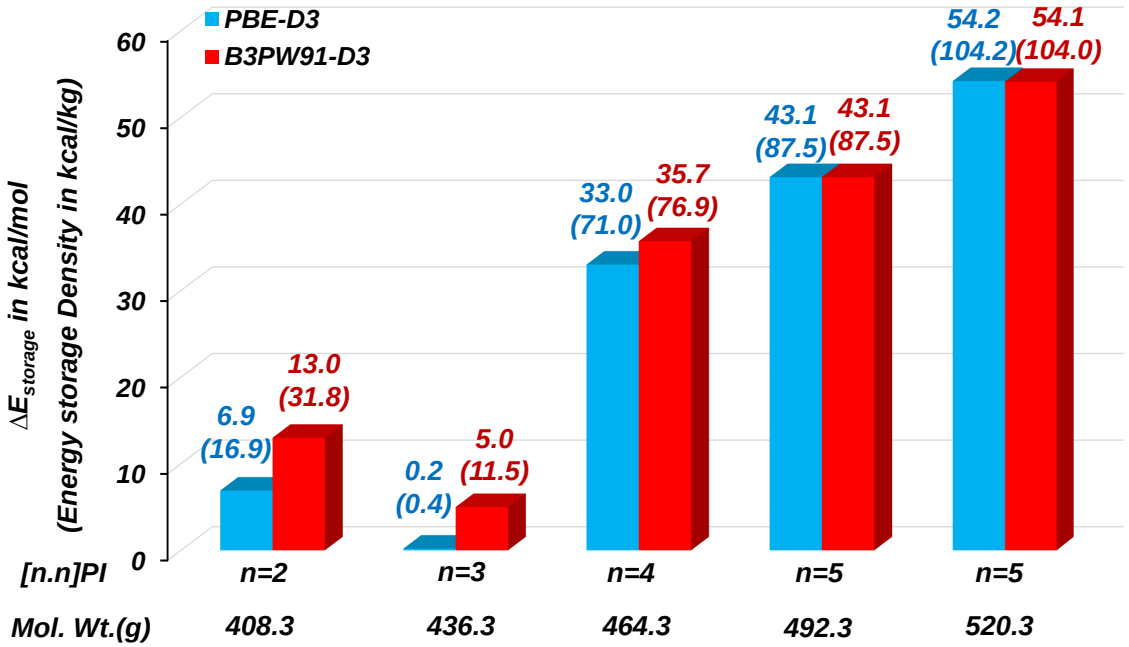
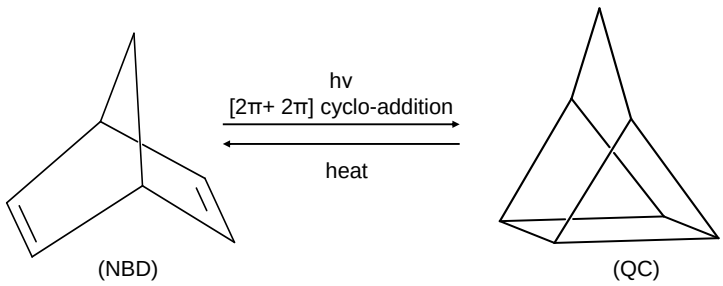


Figure S2: $\Delta E_{storage}$ and corresponding energy storage densities (=$\Delta E_{storage}$/Mol. wt.) at PBE-D3/6-311++G(d,p) and B3PW91-D3/6-311++G(d,p) level of theory.

If we consider the B3PW91-D3/6-311++G(d,p) and PBE-D3/6-311++G(d,p) numbers, the $\Delta E_{storage}$ and corresponding energy storage densities would increase slightly compared to that of M06-2X/6-311++G(d,p) numbers (see Fig. S2). For [6.6]anthracenophane we observe the storage densities greater than 100 kcal/kg.

Supplementary Discussion 6: Benchmarking the Performance of Density Functionals for NBD and AB

[2π+2π] photodimerization Norbornadiene (NBD) to produce Quadricyclane (QC)



Scheme S3: [2π+2π] photodimerization Norbornadiene (NBD) to produce Quadricyclane (QC).

NBD= Norbornadiene; and **QC**= Quadricyclane;

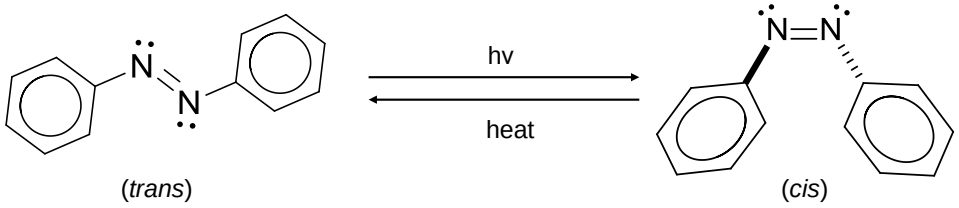
The gas phase reaction energy (E_{rxn}(gas)) is defined as:

E_{rxn}(gas) = E(**QC**) - E(**NBD**) It must be remembered that typically DFT predictions are ascribed error bars of ± 2-3 kcal/mol. CCSD(T)/cc-pVTZ level of computation on NDB→QC system predicted +23.4 kcal/mol as shown in Tab. S7. Given this fact we find DLPNO-CCSD(T), B3LYP, and B3LYP-D3 predictions are closest to the CCSD(T) prediction.

Table S7: Comparion of E_{rxn}(gas) numbers for different density functionals for [2π+2π] cyclo-addition of Norbornadiene (NBD) with that of gold standard CCSD(T) number.

Theoretical Method	**ΔE_{rxn}(gas)** (kcal/mol)
CCSD(T)/cc-pVTZ	**+23.4**
DLPNO-CCSD(T)/cc-pVTZ	**+23.4**
B3LYP/6-311++G(d,p)	**+23.4**
B3LYP-D3/6-311++G(d,p)	**+23.9**
B3PW91-D3/6-311++G(d,p)	+17.0
PBE/6-311++G(d,p)	+14.0
PBE-D3/6-311++G(d,p)	+14.3
M06-2x/6-311++G(d,p)	+15.2

cis-trans photoisomerization of Azo-benzene (AB)



Scheme S4: *trans-cis* isomerization of Azo-benzenewith.

trans= *trans*-Azobenzene; and ***cis***= *cis*-Azobenzene;

The gas phase reaction energy (E_{rxn}(gas)) is defined as:

E_{rxn}(gas) = E(***cis***) - E(***trans***) It must be remembered that typically DFT predictions are

Table S8: Comparion of E_{rxn}(gas) numbers for different density functionals for *E-Z* isomerization of AB with that of gold standard CCSD(T) number.

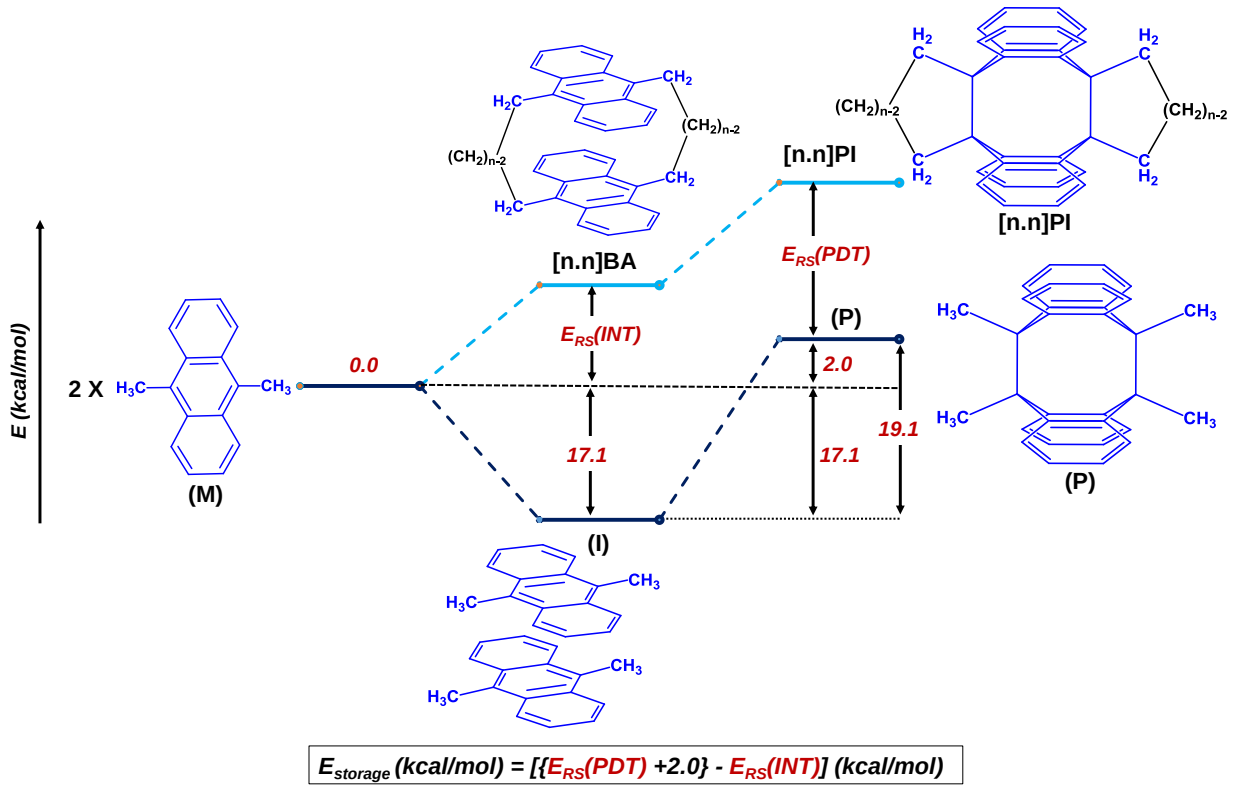
Level of Theory	**ΔE_{rxn}(gas)** (kcal/mol)
CCSD(T)/cc-pVTZ	**+12.1**
M06-2x/6-311++G(d,p)	**+12.2**
DLPNO-CCSD(T)/cc-pVTZ/cc-pVTZ/C	+15.5
B3LYP/6-311++G(d,p)	+15.5
B3LYP-D3/6-311++G(d,p)	+12.8
B3PW91-D3/6-311++G(d,p)	+11.7
PBE/6-311++G(d,p)	+14.6
PBE-D3/6-311++G(d,p)	+12.9

ascribed error bars of ± 2-3 kcal/mol. CCSD(T)/cc-pVTZ for *cis-trans* isomerization of AB predicted +12.1 kcal/mol as shown in Tab. S8. Given this fact we find M06-2x functional prediction is closest to the CCSD(T) prediction.

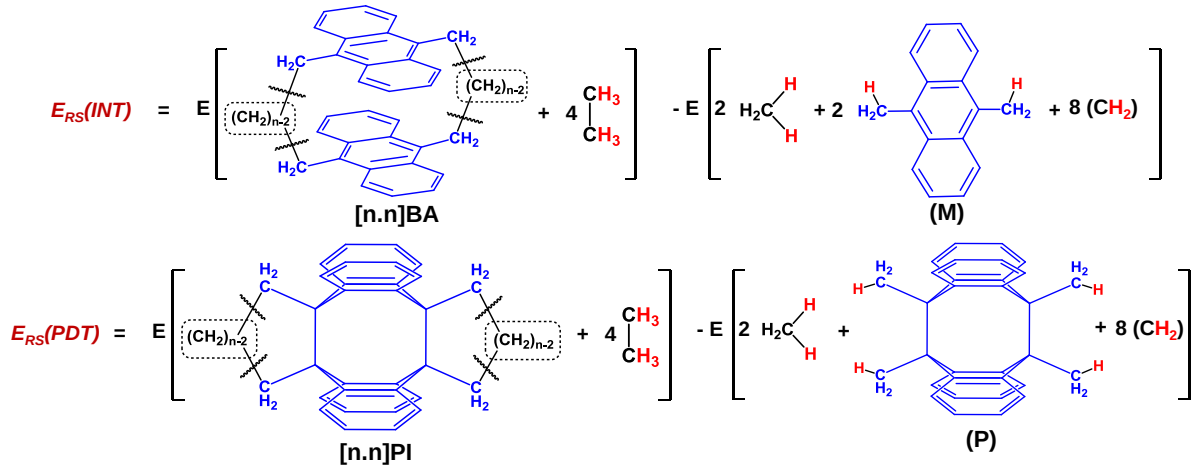
Supplementary Discussion 7: Homodesmotic Approach for Ring-Strain Analysis in this Work

The Homodesmotic Scheme

The 'homodesmotic approach',[S8,S9] was employed to calculate ring-strain (RS) energy in both [n.n]BA (denoted as: E_{RS}(INT)) and [n.n]PI (denoted as: E_{RS}(PDT)) at M06-2X/6-311++G(d,p) level of theory. The homodesmotic scheme ensures that the number of atom and bond types are conserved in the two terms on the left hand side (please see Sch. S5). The evaluation of the ring-strain energy (E_{RS}) requires selecting appropriate reference compounds. For this particular case we have chosen (9,10)-dimethylanthracene (**M**) and the corresponding photo-product (**P**) as the reference compound of [n.n]BA and [n.n]PI respectively (see Sch. S5). As shown in the scheme, we imagined any [n.n]BA and its corresponding photo-product [n.n]BA as a linear methylene-chain ($-(CH_2)_{n\text{-}2}-$) connecting between two **M** and the **P**. It is to be noted here that two **M** can form a slipped-parallel π-stacked C_i symmetry intermediate (**I**) which is 17.1 kcal/mol energetically downhill compared to two free monomers **M**. The photo-dimerized product (**P**) is +2.0 kcal/mol energetically uphill compared to two free **M**s. Therefore, **P** is (17.1+2.0) kcal/mol = 19.1 kcal/mol uphill compared to **I** (see Sch. S5). The stored energy, $\Delta E_{storage}$ in any [n.n]anthracenophane would be simply given by: $\Delta E_{storage}$ = [(E_{RS}(PDT) + 2.0) - E_{RS}(INT))] kcal/mol. Please note, if the π-stacked intermediate (**I**) is chosen as the reference compound in the ring-strain analysis in the [n.n]BA instead of two anthracene monomers (**M**), the E_{RS}(INT) values would be shifted by a constant number +17.1 kcal/mol. Therefore, basically it is a matter of reference molecular fragment.



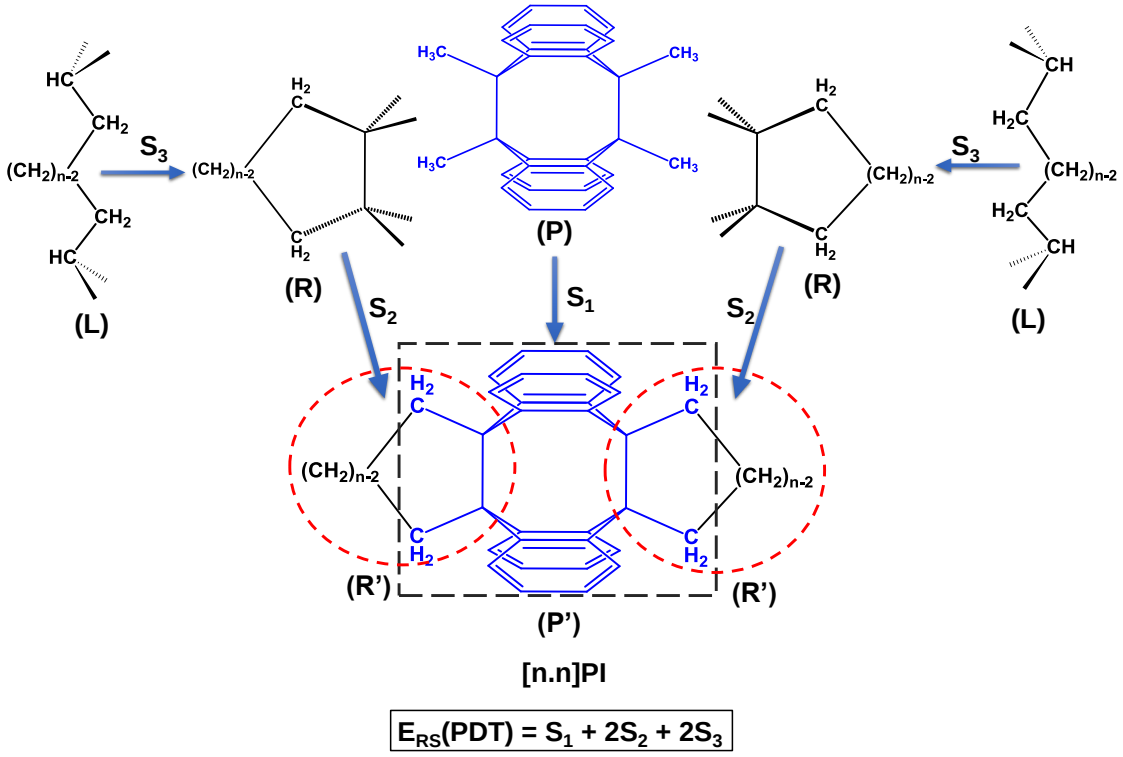
(a)



(b)

Scheme S5: (a) Photo-dimerizationreaction thermodynamics of (9,10)-dimethylanthracene, **M** to yield the corresponding photoproduct, **P** at M06-2X/6-311++G(d,p) level of theory (**I**=π-stacked slipped parallel intermediate formed by two **M**s). E_{RS}(INT))= ring strain in [n.n]BA, and E_{RS}(PDT)=ring strain in [n.n]PI ($E_{storage}$=[(E_{RS}(PDT)+2.0)-E_{RS}(INT)]; (b) Homodesmotic scheme used in this work to evaluate ring-strain energy in the [n.n]BA and [n.n]PI as **M** and **P** as reference compounds.

A More Detailed Analysis of High value of E_{RS}(PDT) in [n.n]PI (n=4-6)



Scheme S6: The total strain energy in [n.n]PI photo-products (E_{RS}(PDT)) can be further decomposed into three major contributors: S_1, S_2, and S_3. S_1 is the deformation strain of the central part of any [n.n]PI w.r.t (9,10)dimethyl-anthracene photo-dimer (**P**). S_2 is the deformation strain of the cyclic ring, formed upon [4π+4π] photo-dimerization, w.r.t. the corresponding most stable cycloalkane conformer. Finally S_3 is the ring strain arising due to ring closure of a linear alkane analog into its cyclic form. Hence, from the above scheme one can clearly say that $E_{RS}(PDT) \approx S_1+2S_2+2S_3$.

The E_{RS}(PDT) in the any [n.n]PI can be further decomposed into strain components arising from three different sources:

- The strain in the central part of the photo-product (S_1) due to geometry deformation w.r.t (9,10)-dimethyl anthracene photo-dimer product, **P**. For evaluation of S_1 we truncated each [n.n]PI mimicking the (9,10)dimethylanthracene photo-product (**P**) by removing the alkyl linkers (and terminating unsaturated bonds with hydrogen), and computed the single point energy difference between the truncated geometry (lets say

P') and the optimized geometry of **P**. This energy difference is denoted as S_1.

- Strain in the (n+2)-membered rings formed by the alkyl chains (**R'**) with respect to the most stable (n+2)-membered cycloalkane conformer (**R**) is denoted as S_2. For evaluation of S_2 we truncated the [n.n]PI only to the (n+2)-membered ring formed upon the photodimerization mimicking the (n+2)-membered 1,1,2,2-tetramethyl cycloalkane and computed the relative strain with respect to the most stable conformation of the 1,1,2,2 tetramethylcyclo-alkane. The energy difference between them is basically S_2.

- S_3 is the strain due to ring closure (**L** $\rightarrow$ **R**) w.r.t linear alkane analogue (**L**). Please note, in the intermediate, the alkyl chain linkers are not exactly in most the stable linear form (**L**). Therefore, the evaluation of S_3 is not at all straight forward. However, for simplicity we have taken the literature values of S_3, which is basically the change in energy due to transforming a linear alkane into a most stable conformation of cycloalkane.

Therefore, $E_{RS}(PDT) \approx S_1+2S_2+2S_3$) (see Sch. S6).

Analysis of E_{RS}(PDT) in [4.4]PI

For [4.4]PI, the truncated central part of the structure (**P'**) closely resemble the (9,10)dimethyl anthracene photo-product (**P**) and S_1 turned out to be negligible (less than 2 kcal/mol). Moreover, for six-membered ring (**R'**), the strain due to ring closure (S_3) with respect to its linear-hexane analogue is assumed to be zero (0.0 kcal/mol). Hence, the main contribution of E_{RS}(PDT) comes from S_2. As we discussed in the manuscript the dihedral angle between four adjacent carbon atoms (ϕ(1-2-3-4)) turned out to be 8.4° (see Fig. S3. The six-membered ring in close to high energy 'Twist-Chair' (TC) conformation and S_2 turned out to be 17.0 kcal/mol w.r.t the most stable 'Full-Chair' (FC) conformation of 1,1,2,2 tetramethyl cyclohexane. Please see Tab. S9.

Table S9: The values of S_1, S_2, and S_3 for [4.4]PI and comparing the value of (S_1+2S_2+2S_3) with E_{RS}(PDT).

[n.n]PI	$\mathbf{S_1}$	$\mathbf{S_2}$	$\mathbf{S_3}$	$\mathbf{S_1+2S_2+2S_3}$	$\mathbf{E_{RS}(PDT)}$
D_2[4.4]PI	+2.0	+17.0	0.0	+36.0	+33.7

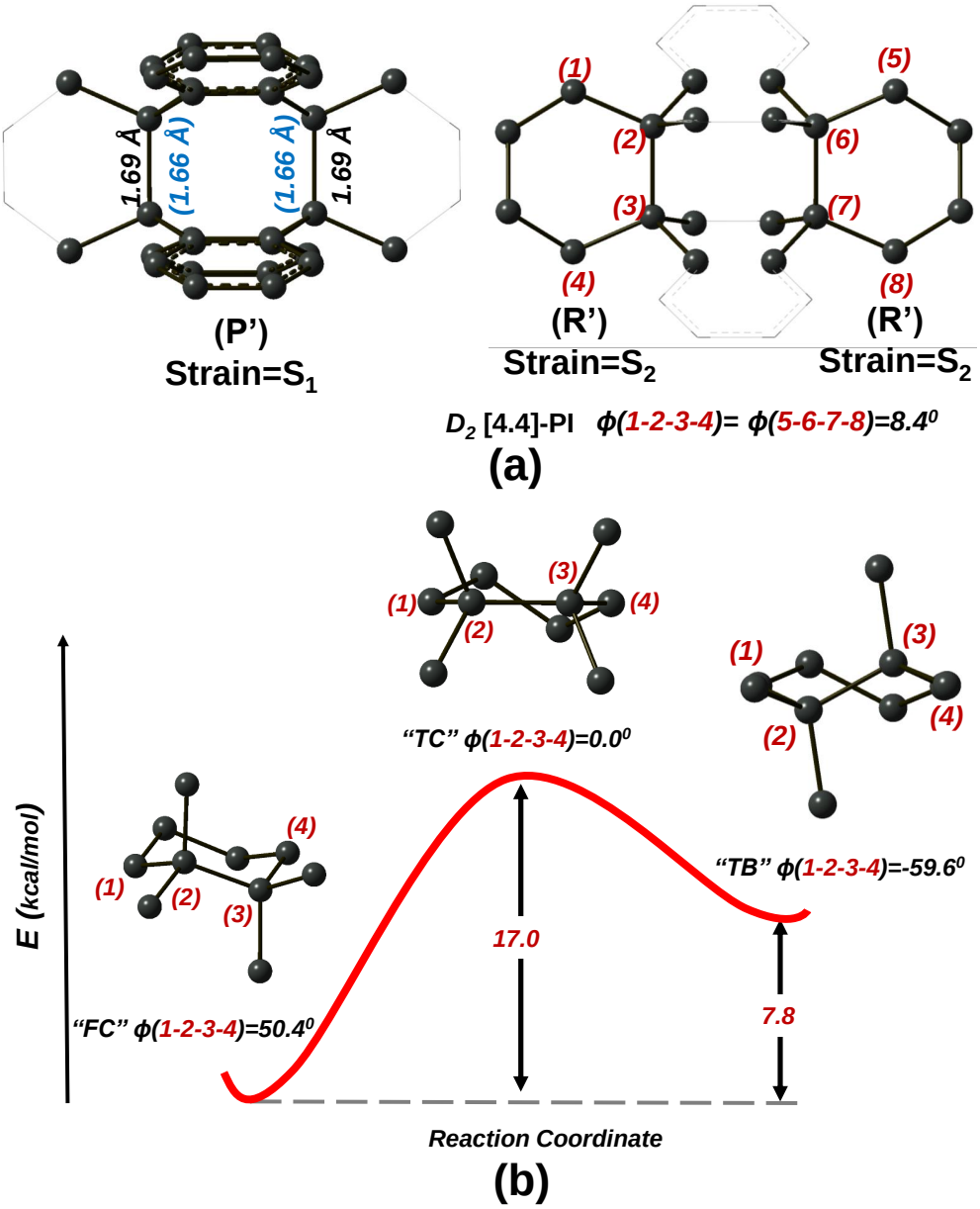


Figure S3: (a) (left) the truncated central part of the ring, **P'** (geometrically very less deviates from **P**) which is the source of comparatively very low value of S_1. The d_1 and d_2 distances in [4.4]PI are written in black, the corresponding d_1 and d_2 distances for **P** are written in the blue parentheses. (right) six-membered rings (**R'**) formed upon photo-dimerization of [4.4]BA is the origin of high of S_2 which turned out to be very high due to near zero dihedral angle between four adjacent carbon atoms. (b) Topomerization of 1,1,2,2 tetramethylcyclohexane between 'Full-Chair (TC)' and 'Twist-Boat (TB)' occurs through a transition state of zero-dihedral angle (ϕ(1-2-3-4)=0.0° transition state which is 17.0 kcal/mol higher compare to the TC conformer. This TS is the 'Twist-Chair (TC)' conformation of cyclohexane.

Analysis of E_{RS}(PDT) in [5.5]PI

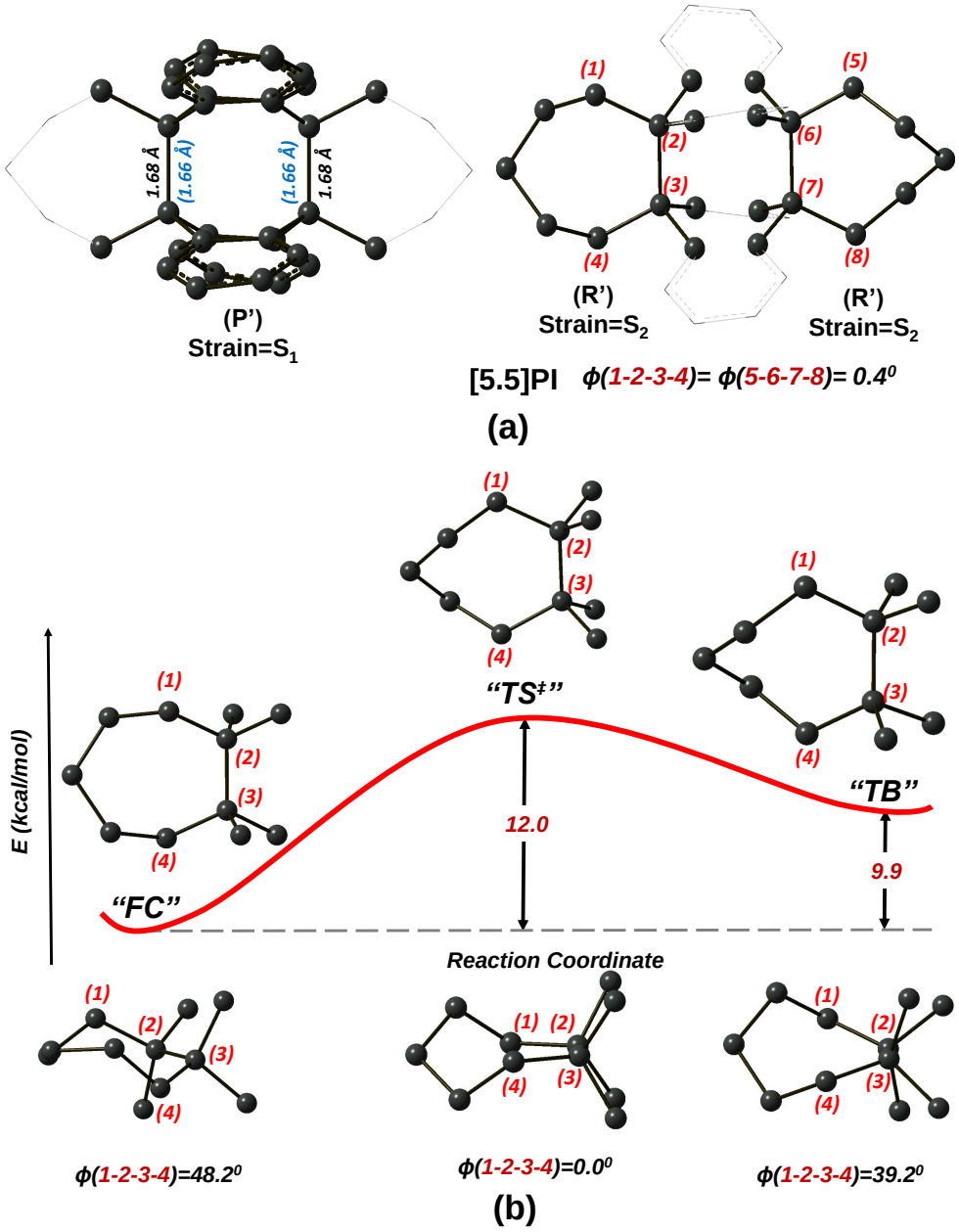


Figure S4: (a) (left) the truncated central part of the ring, **P'** (geometrically very less deviates from **P**) which is the source of comparatively very low value of S_1. The d_1 and d_2 distances in [4.4]PI are written in black, the corresponding d_1 and d_2 distances for **P** are written in the blue parentheses. (right) high strain in the seven-membered ring (**R'**) due to near zero degree dihedral angle between four adjacent carbon atoms is the source of high value of S_2; (b) Topomerization of 1,1,2,2 tetramethylcycloheptane between 'Twist-Chair (TC)' and 'Twist-Boat (TB)' occurs through a transition state of zero-dihedral angle (ϕ(1-2-3-4)=0.0° transition state which is 12.0 kcal/mol higher compared to the TC conformer.

For [5.5]anthracenophane also, the strain in the photo-product can be analyzed in a same fashion. For [5.5]PI, the truncated central part of the structure (**P'**) closely resemble the (9,10)dimethyl anthracene photo-product (**P**) and S_1 turned out to be very negligible (less than 2 kcal/mol). Moreover, for seven-membered ring (**R'**), the strain due to ring closure (S_3) with respect to its linear-heptane analogue is assumed to be ∼6.0 kcal/mol. Hence, here also the main contribution of E_{RS}(PDT) comes from S_2. Please note the most stable conformation of cycloheptane is 'Twist-Chair (TC)'. There are two cycloheptane rings which are formed in the product (D_2[5.5]PI) are locked in a transition state (TS) of 'Twist-Chair (TC)' ↔ 'Twist-Boat (TB)' inter-conversion where four adjacent atoms are held in a zero dihedral angle (ϕ(1-2-3-4)=0.4°) (see Fig S4). The TS is predicted to be 12.0 kcal/mol energetically higher than the corresponding most stable 'TC' conformation in 1,1,2,2-tetramethylcycloheptane. Please see Tab. S10.

Table S10: The values of S_1, S_2, and S_3 for [5.5]PI and comparing the value of (S_1+2S_2+2S_3) with E_{RS}(PDT).

[n.n]PI	$\mathbf{S_1}$	$\mathbf{S_2}$	$\mathbf{S_3}$	$\mathbf{S_1+2S_2+2S_3}$	$\mathbf{E_{RS}(PDT)}$
D_2[5.5]PI	+2.0	+12.0	+6.0	+38.0	+38.1

Analysis of E_{RS}(PDT) in [6.6]PI

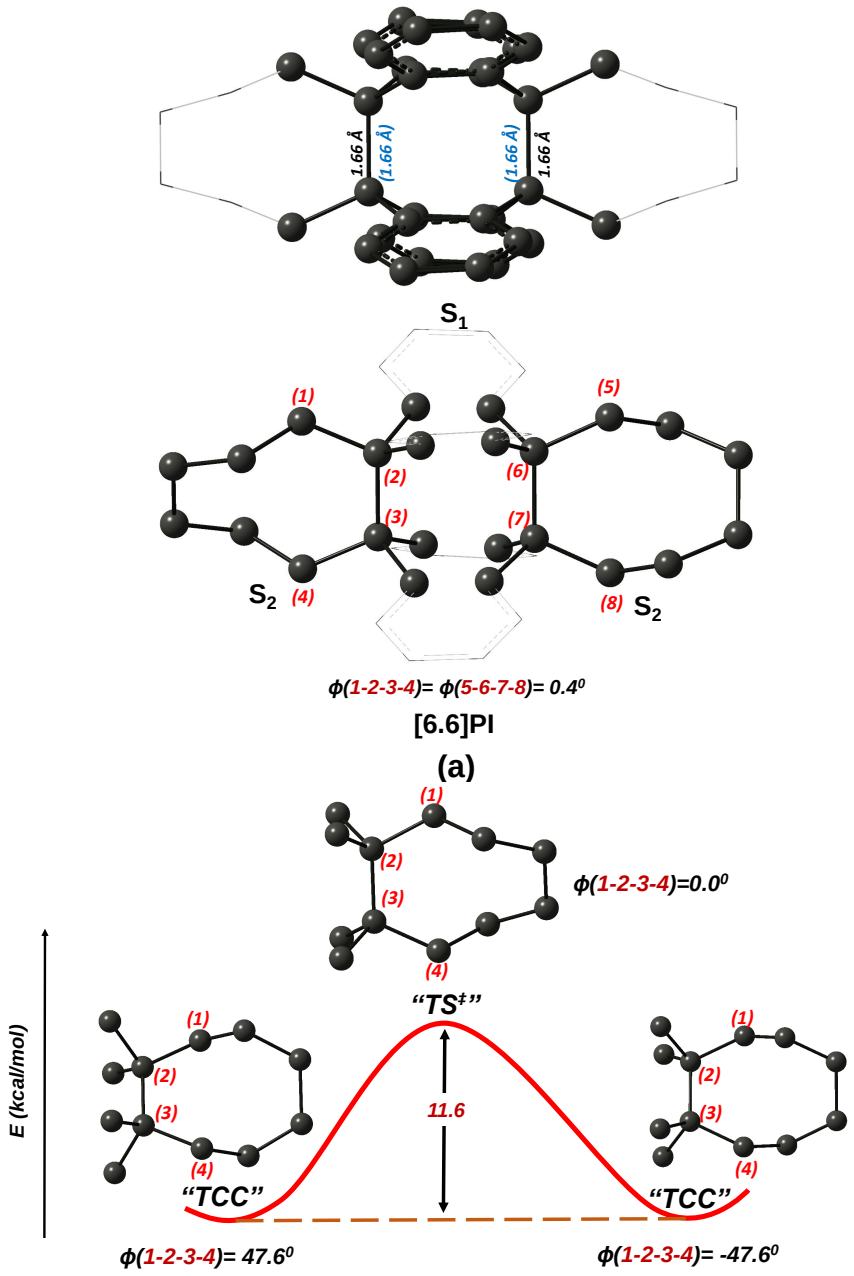


Figure S5: (a) (top) the truncated central part of the ring (**P'**) responsible for the high value of S_1. The d_1 and d_2 distances in [4.4]PI are written in black, the corresponding d_1 and d_2 distances for **P** are written in the blue parentheses. (below) high strain in the eight-membered ring (**R'**) due to near zero degree dihedral angle between four adjacent carbon atoms is the source of high value of S_2; (b) Topomerization of 1,1,2,2 tetramethylcycloctane between two enantiomeric 'Twist-Chair-Chair (TCC)' forms (ϕ(1-2-3-4)=47.6 and -47.6° respectively) occurs through a transition state of zero-dihedral angle (ϕ(1-2-3-4)=0.0° transition state which is 11.4 kcal/mol higher compare to the TCC conformer.

For [6.6]anthracenophane also, the strain in the photo-product can be analyzed in a same fashion. For [6.6]PI, the truncated central part of the structure (**P'**) does not closely resemble the (9,10)dimethyl anthracene photo-product (**P**) and S_1 turned out to be ∼5.9 kcal/mol). Moreover, for eight-membered ring (**R'**), the strain due to ring closure (S_3) with respect to its linear-heptane analogue is assumed to be ∼10.0 kcal/mol. Rest of the main contribution to E_{RS}(PDT) comes from S_2. Please note the most stable conformation of cyclooctane is 'Boat-Chair (BC)'. However, for 1,1,2,2-tetramethyl cyclooctane the 'Twist-Chair-Chair (TCC)' turned out to be the most stable conformation. There are two cyclooctane rings which are formed in the product (D_2[6.6]PI) are locked in a transition state (TS) of Twist-Chair-Chair (TCC:ϕ(1-2-3-4)=47.6°)" ↔ 'Twist-Chair-Chair (TCC:ϕ(1-2-3-4)=-47.6°))' inter-conversion where four adjacent atoms are held in a zero dihedral angle (ϕ(1-2-3-4)=0.4°) (see Fig. S5). The TS is predicted to be 11.4 kcal/mol energetically higher than the corresponding most stable 'TCC' conformation in 1,1,2,2-tetramethylcyclooctane. Please see Tab.S11.

Table S11: The values of S_1, S_2, and S_3 for [6.6]PI and comparing the value of (S_1+2S_2+2S_3) with E_{RS}(PDT).

[n.n]PI	$\mathbf{S_1}$	$\mathbf{S_2}$	$\mathbf{S_3}$	$\mathbf{S_1+2S_2+2S_3}$	$\mathbf{E_{RS}(PDT)}$
D_2[6.6]PI	+5.9	+11.6	+10.0	+49.1	+51.3

Supplementary Discussion 8: Thermal Back Reaction (TBR) for [5.5]PI

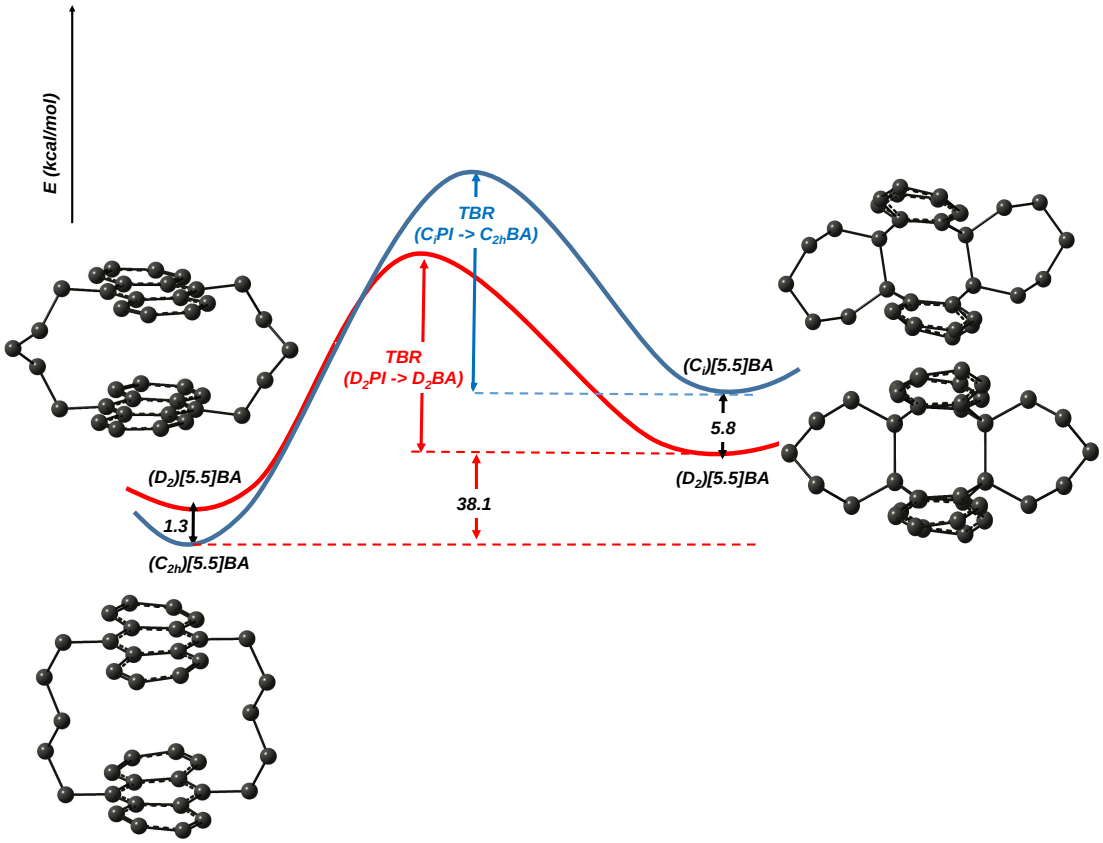


Figure S6: Schematic representation of $\Delta E_{storage}$ and TBR for [5.5]PI.

The energy storage ($\Delta E_{storage}$) is uniquely defined as the difference in energy between lowest energy photo-product/isomer ([n.n]PI) and lowest energy bis-anthracene intermediate ([n.n]BA) among near-degenerate conformers. For [4.4]anthracenophane both BA and PI turned out to be of D_2 symmetry. Therefore, the TBR is also uniquely defined and hence, we studied the linear transit scan for step-wise and concerted C-C bond cleavage of (D_2)[4.4]PI $\rightarrow$ (D_2)[4.4]BA conversion. However, for [5.5]anthracenophane the lowest energy photo-product/isomer [5.5]PI is of D_2 symmetry and bis-anthracene intermediate [5.5]BA is of C_{2h} symmetry. Any linear transit scan for step-wise or concerted C-C bond cleavage does not connect D_2[5.5]PI to C_{2h})[5.5]BA. The linear transit scan starting from

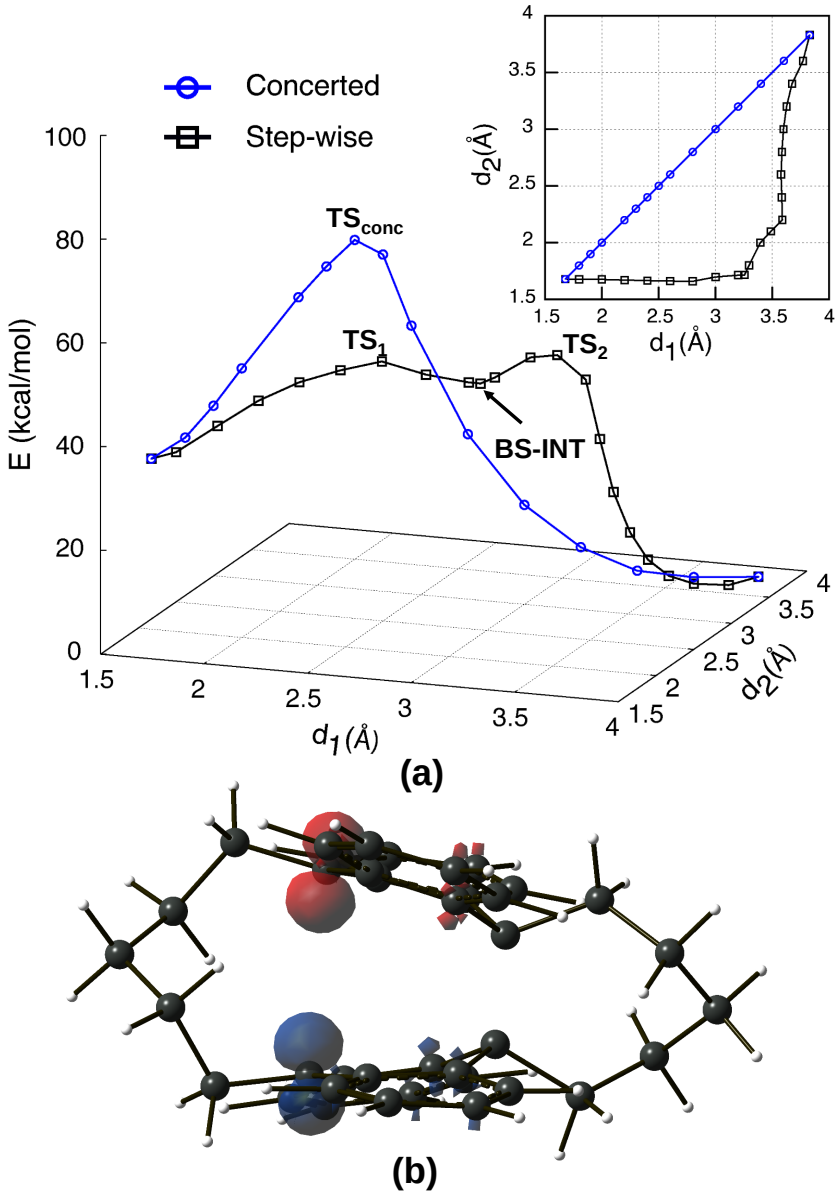


Figure S7: (a) Total energy plot along the reaction coordinate (linear transit scan) for concerted (blue) and step-wise (black) TBR pathway of D_2[5.5]PI calculated at M06-2X/6-31++G(d,p) level of theory. (Inset) d_1(9C-9'C) and d_2(10C-10'C) bond distance correlation diagram for concerted (blue) and step-wise(black). Please note that in step-wise mechanism change in d2 is very negligible up to the BS-INT and after that change in d1 is negligible compared to d2; (b) The spin-density of the broken-symmetry intermediate (BS-INT) at M06-2X/6-31++G(d,p) level of theory (d1=3.25 Å, d2= 1.72 Å). The spin-density is located on the carbon atoms of the broken C-C bond.

D_2[5.5]PI ends up to D_2[5.5]BA and starting from C_i[5.5]PI ends up to C_{2h}[5.5]PI. C_i[5.5]PI is 5.8 kcal/mol energetically higher than D_2[5.5]PI. On the other hand D_2[5.5]BA is only 1.3

kcal/mol higher than C_{2h}[5.5]PI. We predict that the TBR would happen from lowest energy photo-product D_2[5.5]PI to first D_2[5.5]BA and then via some lower-energy conformational changes D_2[5.5]BA would be converted to the lowest energy bis-anthracene intermediate C_{2h}[5.5]BA.

The barrier for C-C bond opening via concerted pathway ($\mathbf{TS_{conc}}$) is 37.5 kcal/mol (see Fig. S7(a)). The 9C-9'C (d_1) and 10C-10'C (d_2) bond distances at $\mathbf{TS_{conc}}$ is predicted to be 2.4 Å. The step-wise C-C bond opening proceeds through a broken-symmetry open shell intermediate. The spin density of the open shell intermediate is exclusively located on the carbon atoms of the cleaved bond. The broken-symmetry intermediate (**BS-INT**) is 20.2 kcal/mol higher compared to the photo-product. For the spin density plot of **BS-INT**, please see Fig. S7(b) The d_1 and d_2 corresponding to the broken-symmetry intermediate if d_1=3.25 Å and d_2=1.72 Å. The first C-C bond cleavage transition state (**TS1**) is 23.3 kcal/mol higher than the photo-product and the second C-C bond cleavage barrier is 3.4 kcal/mol higher than the broken-symmetry intermediate. Therefore, the rate determining barrier (RDB) for the step-wise C-C bond cleavage turned out to be (20.2+3.4)=23.6 kcal/mol attributed to **TS2** (see Fig. S7(a)).

Supplementary Discussion 9: N-Doping Not only Increases Solubility But Also Increases Energy Storage Density

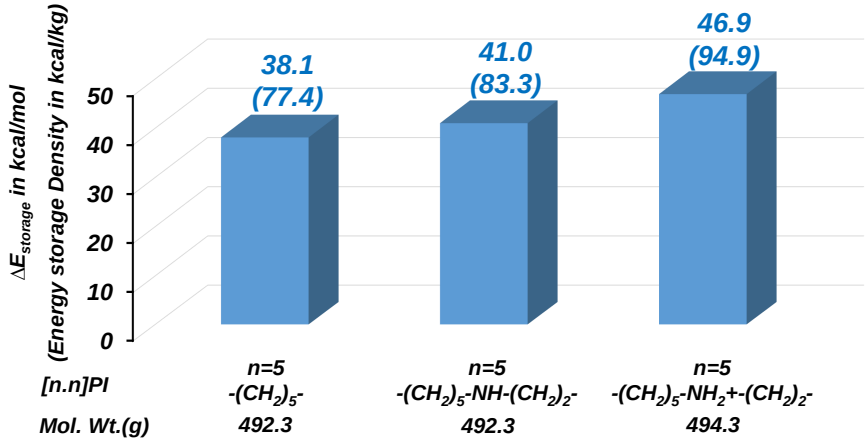


Figure S8: Comparison of $\Delta E_{storage}$ in D_2[5.5]PI with nitrogen doped alkyl chain likers at M06-2x/6-311++G(d,p) level of theory. The values in the parentheses represent the corresponding storage densities.

We find that doping a hetero-atom like nitrogen (N) in both the alkyl chains of [5.5]anthracenophane slightly increase the $\Delta E_{storage}$ and the corresponding energy storage density. This type of 'N' doped anthracene cyclophanes do exist in the scientific literature.[S10] If the nitrogens can be protonated the $\Delta E_{storage}$ further increases.

Cartesian Coordinates for Optimized Geometries of [n.n]BAs@M06-2X/6-31++G(d,p) (n=2-6)

C_2[2.2]BA

Atom	x	y	z	Atom	x	y	z
C	-0.27582000	3.65768500	0.71062700	C	-3.72070200	2.41411500	-0.71097400
C	0.27582000	2.61530400	1.39599400	H	-2.98501000	1.51372800	-2.47933400
C	0.87704600	1.50929400	0.71811500	H	-4.34154300	3.12233800	1.25043400
C	0.87704600	1.50929400	-0.71811500	H	0.72013000	-4.48992100	-1.24706200
C	0.27582000	2.61530400	-1.39599400	H	-4.34154300	3.12233800	-1.25043400
C	-0.27582000	3.65768500	-0.71062700	C	-0.78904100	-0.07754000	2.79324400
C	1.35288800	0.38623900	1.41966900	C	0.78904100	0.07754000	2.79324400
C	1.35288800	0.38623900	-1.41966900	C	0.78904100	0.07754000	-2.79324400
C	2.16196000	-0.53227300	-0.72218700	C	-0.78904100	-0.07754000	-2.79324400
C	2.16196000	-0.53227300	0.72218700	H	1.22177700	-0.85488400	3.15674000
C	2.95288300	-1.51914700	1.39505700	H	1.04910700	0.84567700	3.53024100
H	2.98501000	-1.51372700	2.47933400	H	-1.04910700	-0.84567700	3.53024100
C	3.72070200	-2.41411500	0.71097400	H	-1.22177700	0.85488400	3.15674000
C	3.72070200	-2.41411500	-0.71097400	H	-1.04910700	-0.84567700	-3.53024100
C	2.95288300	-1.51914700	-1.39505700	H	-1.22177700	0.85488400	-3.15674000
H	-0.72013000	4.48992100	1.24706200	H	1.22177700	-0.85488400	-3.15674000
H	0.27883200	2.62728200	2.48167900	H	1.04910700	0.84567700	-3.53024100
H	0.27883200	2.62728200	-2.48167900				
H	-0.72013000	4.48992100	-1.24706200				
H	4.34154300	-3.12233800	1.25043400				
H	4.34154300	-3.12233800	-1.25043400				
H	2.98501000	-1.51372800	-2.47933400				
C	-1.35288800	-0.38623900	1.41966900				
C	-0.87704600	-1.50929400	0.71811500				
C	-2.16196000	0.53227300	0.72218700				
C	-0.27582000	-2.61530400	1.39599400				
C	-0.87704600	-1.50929400	-0.71811500				
C	-2.16196000	0.53227300	-0.72218700				
C	-2.95288300	1.51914700	1.39505700				
C	0.27582000	-3.65768500	0.71062700				
H	-0.27883200	-2.62728200	2.48167900				
C	-0.27582000	-2.61530400	-1.39599400				
C	-1.35288800	-0.38623900	-1.41966900				
C	-2.95288300	1.51914700	-1.39505700				
H	-2.98501000	1.51372700	2.47933400				
C	-3.72070200	2.41411500	0.71097400				
C	0.27582000	-3.65768500	-0.71062700				
H	0.72013000	-4.48992100	1.24706200				
H	-0.27883200	-2.62728200	-2.48167900				

D_2[2.2]BA

Atom	x	y	z	Atom	x	y	z
C	3.50678300	1.20093500	1.84868100	H	2.10426900	-2.79182800	-1.74539400
C	2.24976700	1.71620700	1.71701600	H	4.70380400	0.61544700	-1.91380800
C	1.10068700	0.86997700	1.59690700	H	-4.70380400	-0.61544700	-1.91380800
C	1.29377400	-0.55774300	1.57319300	H	4.35847700	-1.86225800	-1.97531500
C	2.63720700	-1.04879400	1.66255900	C	0.32131500	2.76205400	-0.72176600
C	3.70238300	-0.20778200	1.81617600	C	-0.32131500	2.76205400	0.72176600
C	-0.18343200	1.40854900	1.39009700	C	0.32131500	-2.76205400	0.72176600
C	0.18343200	-1.40854900	1.39009700	C	-0.32131500	-2.76205400	-0.72176600
C	-1.10068700	-0.86997700	1.59690700	H	1.37751900	3.01539900	-0.62347700
C	-1.29377400	0.55774300	1.57319300	H	-0.14269600	3.56943300	-1.29914700
C	-2.63720700	1.04879400	1.66255900	H	0.14269600	3.56943300	1.29914700
H	-2.81003700	2.11949800	1.65546800	H	-1.37751900	3.01539900	0.62347700
C	-3.70238300	0.20778200	1.81617600	H	1.37751900	-3.01539900	0.62347700
C	-3.50678300	-1.20093500	1.84868100	H	-0.14269600	-3.56943300	1.29914700
C	-2.24976700	-1.71620700	1.71701600	H	0.14269600	-3.56943300	-1.29914700
H	4.35847700	1.86225800	1.97531500	H	-1.37751900	-3.01539900	-0.62347700
H	2.10426900	2.79182800	1.74539400				
H	2.81003700	-2.11949800	1.65546800				
H	4.70380400	-0.61544700	1.91380800				
H	-4.70380400	0.61544700	1.91380800				
H	-4.35847700	-1.86225800	1.97531500				
H	-2.10426900	-2.79182800	1.74539400				
C	0.18343200	1.40854900	-1.39009700				
C	-1.10068700	0.86997700	-1.59690700				
C	1.29377400	0.55774300	-1.57319300				
C	-2.24976700	1.71620700	-1.71701600				
C	-1.29377400	-0.55774300	-1.57319300				
C	1.10068700	-0.86997700	-1.59690700				
C	2.63720700	1.04879400	-1.66255900				
C	-3.50678300	1.20093500	-1.84868100				
H	-2.10426900	2.79182800	-1.74539400				
C	-2.63720700	-1.04879400	-1.66255900				
C	-0.18343200	-1.40854900	-1.39009700				
C	2.24976700	-1.71620700	-1.71701600				
H	2.81003700	2.11949800	-1.65546800				
C	3.70238300	0.20778200	-1.81617600				
C	-3.70238300	-0.20778200	-1.81617600				
H	-4.35847700	1.86225800	-1.97531500				
H	-2.81003700	-2.11949800	-1.65546800				
C	3.50678300	-1.20093500	-1.84868100				

C_{2h}[3.3]BA

Atom	x	y	z	Atom	x	y	z
C	-1.61140600	2.34986000	1.73411900	H	2.23675400	2.68559300	-1.96305100
C	-0.83511700	1.14316100	1.67493400	H	-1.65475100	4.46593700	-1.92866400
C	0.60012500	1.26892700	1.71369500	H	1.65475100	-4.46593700	-1.92866400
C	1.16138700	2.58046500	1.87479300	H	0.83612500	4.67080000	-2.10115400
C	0.38071900	3.69546600	1.96015500	H	2.76867800	2.03544700	0.00000000
C	-1.42536100	-0.13378600	1.58058100	H	4.33087000	1.23388200	0.00000000
C	1.42536100	0.13378600	1.58058100	H	-2.76867800	-2.03544700	0.00000000
C	0.83511700	-1.14316100	1.67493400	H	-4.33087000	-1.23388200	0.00000000
C	-0.60012500	-1.26892700	1.71369500	C	-2.90702200	-0.32080900	1.31420100
C	-1.16138700	-2.58046500	1.87479300	H	-3.35983900	-0.88513200	2.13976800
H	-2.23675400	-2.68559300	1.96305100	H	-3.42380300	0.63945000	1.30465300
C	-0.38071900	-3.69546600	1.96015500	C	-2.90702200	-0.32080900	-1.31420100
C	1.03343800	-3.57731800	1.87428400	H	-3.42380300	0.63945000	-1.30465300
C	1.61140600	-2.34986000	1.73411900	H	-3.35983900	-0.88513200	-2.13976800
H	-2.69190300	2.29519000	1.69575400	C	2.90702200	0.32080900	-1.31420100
H	2.23675400	2.68559300	1.96305100	H	3.42380300	-0.63945000	-1.30465300
H	0.83612500	4.67080000	2.10115400	H	3.35983900	0.88513200	-2.13976800
H	-0.83612500	-4.67080000	2.10115400	C	2.90702200	0.32080900	1.31420100
H	1.65475100	-4.46593700	1.92866400	H	3.35983900	0.88513200	2.13976800
H	2.69190300	-2.29519000	1.69575400	H	3.42380300	-0.63945000	1.30465300
C	3.24841900	1.05477300	0.00000000	C	-1.03343800	3.57731800	1.87428400
C	-3.24841900	-1.05477300	0.00000000	H	-1.65475100	4.46593700	1.92866400
C	-1.42536100	-0.13378600	-1.58058100				
C	-0.60012500	-1.26892700	-1.71369500				
C	-0.83511700	1.14316100	-1.67493400				
C	-1.16138700	-2.58046500	-1.87479300				
C	0.83511700	-1.14316100	-1.67493400				
C	0.60012500	1.26892700	-1.71369500				
C	-1.61140600	2.34986000	-1.73411900				
C	-0.38071900	-3.69546600	-1.96015500				
H	-2.23675400	-2.68559300	-1.96305100				
C	1.61140600	-2.34986000	-1.73411900				
C	1.42536100	0.13378600	-1.58058100				
C	1.16138700	2.58046500	-1.87479300				
H	-2.69190300	2.29519000	-1.69575400				
C	-1.03343800	3.57731800	-1.87428400				
C	1.03343800	-3.57731800	-1.87428400				
H	-0.83612500	-4.67080000	-2.10115400				
H	2.69190300	-2.29519000	-1.69575400				
C	0.38071900	3.69546600	-1.96015500				

D_2[3.3]BA

Atom	x	y	z	Atom	x	y	z
C	3.32758500	1.90949600	-1.64273700	H	1.72721300	-1.85721300	3.03324500
C	2.01194600	1.79356400	-1.98864100	H	4.74876800	-1.95908300	-0.00417500
C	0.98204600	1.64574900	-1.00296600	H	-4.74876800	-1.95908300	0.00417500
C	1.35638800	1.62141400	0.38829100	H	4.08471200	-2.04858500	2.40828900
C	2.75417200	1.72177000	0.69947900	C	-0.74285200	1.14817000	-2.81069500
C	3.70290400	1.86656400	-0.27193400	H	-1.79695200	0.87603000	-2.81001800
C	-0.36231500	1.48772500	-1.38216100	H	-0.66696600	2.04562100	-3.44089900
C	0.36231500	1.48772500	1.38216100	C	0.74285200	-1.14817000	-2.81069500
C	-0.98204600	1.64574900	1.00296600	H	1.79695200	-0.87603000	-2.81001800
C	-1.35638800	1.62141400	-0.38829100	H	0.66696600	-2.04562100	-3.44089900
C	-2.75417200	1.72177000	-0.69947900	C	-0.74285200	-1.14817000	2.81069500
H	-3.07553200	1.72275800	-1.73384700	H	-1.79695200	-0.87603000	2.81001800
C	-3.70290400	1.86656400	0.27193400	H	-0.66696600	-2.04562100	3.44089900
C	-3.32758500	1.90949600	1.64273700	C	0.74285200	1.14817000	2.81069500
C	-2.01194600	1.79356400	1.98864100	H	1.79695200	0.87603000	2.81001800
H	4.08471200	2.04858500	-2.40828900	H	0.66696600	2.04562100	3.44089900
H	1.72721300	1.85721300	-3.03324500	C	0.00000000	0.00000000	3.56163600
H	3.07553200	1.72275800	1.73384700	C	0.00000000	0.00000000	-3.56163600
H	4.74876800	1.95908300	0.00417500	H	0.74627200	0.43681500	-4.23233400
H	-4.74876800	1.95908300	-0.00417500	H	-0.74627200	-0.43681500	-4.23233400
H	-4.08471200	2.04858500	2.40828900	H	-0.74627200	0.43681500	4.23233400
H	-1.72721300	1.85721300	3.03324500	H	0.74627200	-0.43681500	4.23233400
C	0.36231500	-1.48772500	-1.38216100				
C	-0.98204600	-1.64574900	-1.00296600				
C	1.35638800	-1.62141400	-0.38829100				
C	-2.01194600	-1.79356400	-1.98864100				
C	-1.35638800	-1.62141400	0.38829100				
C	0.98204600	-1.64574900	1.00296600				
C	2.75417200	-1.72177000	-0.69947900				
C	-3.32758500	-1.90949600	-1.64273700				
H	-1.72721300	-1.85721300	-3.03324500				
C	-2.75417200	-1.72177000	0.69947900				
C	-0.36231500	-1.48772500	1.38216100				
C	2.01194600	-1.79356400	1.98864100				
H	3.07553200	-1.72275800	-1.73384700				
C	3.70290400	-1.86656400	0.27193400				
C	-3.70290400	-1.86656400	-0.27193400				
H	-4.08471200	-2.04858500	-2.40828900				
H	-3.07553200	-1.72275800	1.73384700				
C	3.32758500	-1.90949600	1.64273700				

C_{2h}[4.4]BA

Atom	x	y	z	Atom	x	y	z
C	1.08927700	4.16468600	0.71030200	C	-1.08927700	-4.16468600	-0.71030200
C	1.31625500	3.00477200	1.39278000	H	-0.90732900	-5.08774200	1.25212400
C	1.55857100	1.76019800	0.71858600	H	-1.30769300	-3.03215200	-2.47580200
C	1.55857100	1.76019800	-0.71858600	C	-2.48837000	3.03475300	-0.71128300
C	1.31625500	3.00477200	-1.39278000	H	-2.29764300	1.90306600	-2.47436200
C	1.08927700	4.16468600	-0.71030200	H	-2.65500900	3.96068100	1.25295200
C	1.80785400	0.56833800	1.43606900	H	-0.90732900	-5.08774200	-1.25212400
C	1.80785400	0.56833800	-1.43606900	H	-2.65500900	3.96068100	-1.25295200
C	2.03738800	-0.62352600	-0.72332500	C	1.79477100	0.62001100	2.95061300
C	2.03738800	-0.62352600	0.72332500	C	-1.79477100	-0.62001100	2.95061300
C	2.28237600	-1.87304800	1.39250800	C	-1.79477100	-0.62001100	-2.95061300
H	2.29764300	-1.90306600	2.47436200	C	1.79477100	0.62001100	-2.95061300
C	2.48837000	-3.03475300	0.71128300	H	-2.32601100	0.22944800	-3.38443900
C	2.48837000	-3.03475300	-0.71128300	H	-2.35653100	-1.50056100	-3.27701800
C	2.28237600	-1.87304800	-1.39250800	H	-0.40393800	-1.07426300	-4.54672900
H	0.90732900	5.08774200	1.25212400	H	0.20327200	-1.40307000	-2.93318500
H	1.30769300	3.03215200	2.47580200	H	-0.20327200	1.40307000	-2.93318500
H	1.30769300	3.03215200	-2.47580200	H	0.40393800	1.07426300	-4.54672900
H	0.90732900	5.08774200	-1.25212400	H	2.32601100	-0.22944800	-3.38443900
H	2.65500900	-3.96068100	1.25295200	H	2.35653100	1.50056100	-3.27701800
H	2.65500900	-3.96068100	-1.25295200	H	2.32601100	-0.22944800	3.38443900
H	2.29764300	-1.90306600	-2.47436200	H	2.35653100	1.50056100	3.27701800
C	0.36500900	0.67864900	-3.52481200	H	-0.20327200	1.40307000	2.93318500
C	0.36500900	0.67864900	3.52481200	H	0.40393800	1.07426300	4.54672900
C	-0.36500900	-0.67864900	-3.52481200	H	-0.40393800	-1.07426300	4.54672900
C	-0.36500900	-0.67864900	3.52481200	H	0.20327200	-1.40307000	2.93318500
C	-1.80785400	-0.56833800	1.43606900	H	-2.32601100	0.22944800	3.38443900
C	-1.55857100	-1.76019800	0.71858600	H	-2.35653100	-1.50056100	3.27701800
C	-2.03738800	0.62352600	0.72332500				
C	-1.31625500	-3.00477200	1.39278000				
C	-1.55857100	-1.76019800	-0.71858600				
C	-2.03738800	0.62352600	-0.72332500				
C	-2.28237600	1.87304800	1.39250800				
C	-1.08927700	-4.16468600	0.71030200				
H	-1.30769300	-3.03215200	2.47580200				
C	-1.31625500	-3.00477200	-1.39278000				
C	-1.80785400	-0.56833800	-1.43606900				
C	-2.28237600	1.87304800	-1.39250800				
H	-2.29764300	1.90306600	2.47436200				
C	-2.48837000	3.03475300	0.71128300				

D_2[4.4]BA

Atom	x	y	z	Atom	x	y	z
C	3.59018900	1.03440700	1.92652700	C	-3.71329200	-0.37816400	-1.82280500
C	2.35486600	1.60984900	1.97291500	H	-4.48035600	1.65481600	-1.96386700
C	1.14675000	0.83222500	1.91498400	H	-2.71934200	-2.23387200	-1.73026300
C	1.27301600	-0.60244700	1.86955000	C	3.59018900	-1.03440700	-1.92652700
C	2.59635400	-1.16008400	1.80455900	H	2.29227400	-2.68798600	-2.05094600
C	3.71329200	-0.37816400	1.82280500	H	4.69683200	0.83382700	-1.76086600
C	-0.12996400	1.43013800	1.90026800	H	-4.69683200	-0.83382700	-1.76086600
C	0.12996400	-1.43013800	1.90026800	H	4.48035600	-1.65481600	-1.96386700
C	-1.14675000	-0.83222500	1.91498400	H	1.02323500	4.48048200	-0.53900800
C	-1.27301600	0.60244700	1.86955000	H	1.40061200	2.84191500	-0.03238400
C	-2.59635400	1.16008400	1.80455900	H	-1.40061200	2.84191500	0.03238400
H	-2.71934200	2.23387200	1.73026300	H	-1.02323500	4.48048200	0.53900800
C	-3.71329200	0.37816400	1.82280500	H	-1.02323500	-4.48048200	-0.53900800
C	-3.59018900	-1.03440700	1.92652700	H	-1.40061200	-2.84191500	-0.03238400
C	-2.35486600	-1.60984900	1.97291500	H	1.40061200	-2.84191500	0.03238400
H	4.48035600	1.65481600	1.96386700	H	1.02323500	-4.48048200	0.53900800
H	2.29227400	2.68798600	2.05094600	C	-0.31487100	2.93429600	1.88103600
H	2.71934200	-2.23387200	1.73026300	H	-1.13544700	3.20289600	2.55298400
H	4.69683200	-0.83382700	1.76086600	H	0.56132100	3.44611600	2.28458000
H	-4.69683200	0.83382700	1.76086600	C	0.31487100	2.93429600	-1.88103600
H	-4.48035600	-1.65481600	1.96386700	H	1.13544700	3.20289600	-2.55298400
H	-2.29227400	-2.68798600	2.05094600	H	-0.56132100	3.44611600	-2.28458000
C	0.61305500	-3.46597200	0.46550100	C	-0.31487100	-2.93429600	-1.88103600
C	-0.61305500	3.46597200	0.46550100	H	-1.13544700	-3.20289600	-2.55298400
C	-0.61305500	-3.46597200	-0.46550100	H	0.56132100	-3.44611600	-2.28458000
C	0.61305500	3.46597200	-0.46550100	C	0.31487100	-2.93429600	1.88103600
C	0.12996400	1.43013800	-1.90026800	H	1.13544700	-3.20289600	2.55298400
C	-1.14675000	0.83222500	-1.91498400	H	-0.56132100	-3.44611600	2.28458000
C	1.27301600	0.60244700	-1.86955000				
C	-2.35486600	1.60984900	-1.97291500				
C	-1.27301600	-0.60244700	-1.86955000				
C	1.14675000	-0.83222500	-1.91498400				
C	2.59635400	1.16008400	-1.80455900				
C	-3.59018900	1.03440700	-1.92652700				
H	-2.29227400	2.68798600	-2.05094600				
C	-2.59635400	-1.16008400	-1.80455900				
C	-0.12996400	-1.43013800	-1.90026800				
C	2.35486600	-1.60984900	-1.97291500				
H	2.71934200	2.23387200	-1.73026300				
C	3.71329200	0.37816400	-1.82280500				

C_{2h}[5.5]BA

Atom	x	y	z	Atom	x	y	z
C	1.84419800	2.16556400	2.41354700	H	3.20243600	-1.43439800	-2.83286000
C	0.88498800	1.10252100	2.53781400	H	3.88434900	2.76029600	-2.33965900
C	1.38616200	-0.24679000	2.61424900	H	-3.88434900	-2.76029600	-2.33965900
C	2.80805000	-0.43432500	2.69988100	H	4.74927400	0.43542300	-2.69051200
C	3.68026700	0.61142500	2.62317200	H	-0.01485900	-3.54429000	0.00000000
C	-0.50289900	1.34509100	2.58882800	H	0.53475900	-1.87206800	0.00000000
C	0.50289900	-1.34509100	2.58882800	H	0.01485900	3.54429000	0.00000000
C	-0.88498800	-1.10252100	2.53781400	H	-0.53475900	1.87206800	0.00000000
C	-1.38616200	0.24679000	2.61424900	C	-1.05863400	2.75440800	2.58203100
C	-2.80805000	0.43432500	2.69988100	H	-1.79514800	2.85439200	3.38772400
H	-3.20243600	1.43439800	2.83286000	H	-0.27540200	3.47193000	2.82826900
C	-3.68026700	-0.61142500	2.62317200	C	-1.05863400	2.75440800	-2.58203100
C	-3.18817200	-1.93385200	2.44282600	H	-0.27540200	3.47193000	-2.82826900
C	-1.84419800	-2.16556400	2.41354700	H	-1.79514800	2.85439200	-3.38772400
H	1.49889600	3.18281600	2.27947600	C	1.05863400	-2.75440800	-2.58203100
H	3.20243600	-1.43439800	2.83286000	H	0.27540200	-3.47193000	-2.82826900
H	4.74927400	0.43542300	2.69051200	H	1.79514800	-2.85439200	-3.38772400
H	-4.74927400	-0.43542300	2.69051200	C	1.05863400	-2.75440800	2.58203100
H	-3.88434900	-2.76029600	2.33965900	H	1.79514800	-2.85439200	3.38772400
H	-1.49889600	-3.18281600	2.27947600	H	0.27540200	-3.47193000	2.82826900
C	0.88487100	-2.91231100	0.00000000	C	3.18817200	1.93385200	2.44282600
C	-0.88487100	2.91231100	0.00000000	H	3.88434900	2.76029600	2.33965900
C	-0.50289900	1.34509100	-2.58882800	C	-1.72312700	3.16199000	-1.25386200
C	-1.38616200	0.24679000	-2.61424900	H	-2.66023300	2.60543100	-1.13525100
C	0.88498800	1.10252100	-2.53781400	H	-2.00002500	4.22282600	-1.31243800
C	-2.80805000	0.43432500	-2.69988100	C	-1.72312700	3.16199000	1.25386200
C	-0.88498800	-1.10252100	-2.53781400	H	-2.00002500	4.22282600	1.31243800
C	1.38616200	-0.24679000	-2.61424900	H	-2.66023300	2.60543100	1.13525100
C	1.84419800	2.16556400	-2.41354700	C	1.72312700	-3.16199000	1.25386200
C	-3.68026700	-0.61142500	-2.62317200	H	2.00002500	-4.22282600	1.31243800
H	-3.20243600	1.43439800	-2.83286000	H	2.66023300	-2.60543100	1.13525100
C	-1.84419800	-2.16556400	-2.41354700	C	1.72312700	-3.16199000	-1.25386200
C	0.50289900	-1.34509100	-2.58882800	H	2.66023300	-2.60543100	-1.13525100
C	2.80805000	-0.43432500	-2.69988100	H	2.00002500	-4.22282600	-1.31243800
H	1.49889600	3.18281600	-2.27947600				
C	3.18817200	1.93385200	-2.44282600				
C	-3.18817200	-1.93385200	-2.44282600				
H	-4.74927400	-0.43542300	-2.69051200				
H	-1.49889600	-3.18281600	-2.27947600				
C	3.68026700	0.61142500	-2.62317200				

D_2[5.5]BA

Atom	x	y	z	Atom	x	y	z
C	-1.90677000	3.54033800	-1.19065200	C	1.84078600	-3.72570100	0.21727500
C	-1.94194000	2.28096600	-1.71362000	H	1.93065500	-4.40266400	-1.84986800
C	-1.89602400	1.10737500	-0.88493100	H	1.78957600	-2.80989300	2.11619300
C	-1.86224200	1.29750700	0.54336300	C	1.90677000	3.54033800	1.19065200
C	-1.83083300	2.64311900	1.04655100	H	1.99687400	2.17308900	2.78988100
C	-1.84078600	3.72570100	0.21727500	H	1.80261500	4.72869200	-0.63117200
C	-1.90459300	-0.19536700	-1.42311400	H	1.80261500	-4.72869200	0.63117200
C	-1.90459300	0.19536700	1.42311400	H	1.93065500	4.40266400	1.84986800
C	-1.89602400	-1.10737500	0.88493100	C	-2.03955400	-0.46261300	-2.90970800
C	-1.86224200	-1.29750700	-0.54336300	H	-2.86327400	-1.17420200	-3.03373700
C	-1.83083300	-2.64311900	-1.04655100	H	-2.36751000	0.43520100	-3.43644000
H	-1.78957600	-2.80989300	-2.11619300	C	2.03955400	0.46261300	-2.90970800
C	-1.84078600	-3.72570100	-0.21727500	H	2.86327400	1.17420200	-3.03373700
C	-1.90677000	-3.54033800	1.19065200	H	2.36751000	-0.43520100	-3.43644000
C	-1.94194000	-2.28096600	1.71362000	C	2.03955400	-0.46261300	2.90970800
H	-1.93065500	4.40266400	-1.84986800	H	2.86327400	-1.17420200	3.03373700
H	-1.99687400	2.17308900	-2.78988100	H	2.36751000	0.43520100	3.43644000
H	-1.78957600	2.80989300	2.11619300	C	-2.03955400	0.46261300	2.90970800
H	-1.80261500	4.72869200	0.63117200	H	-2.86327400	1.17420200	3.03373700
H	-1.80261500	-4.72869200	-0.63117200	H	-2.36751000	-0.43520100	3.43644000
H	-1.93065500	-4.40266400	1.84986800	C	0.00000000	0.00000000	4.43930100
H	-1.99687400	-2.17308900	2.78988100	C	0.00000000	0.00000000	-4.43930100
C	-0.78391800	1.02846000	3.61997000	H	-0.12710000	-1.49136100	-2.87839500
C	-0.78391800	-1.02846000	-3.61997000	H	-1.10014500	-1.83179600	-4.29703600
C	0.78391800	-1.02846000	3.61997000	H	-0.70138300	0.52687900	-5.10093700
C	0.78391800	1.02846000	-3.61997000	H	0.70138300	-0.52687900	-5.10093700
C	1.90459300	0.19536700	-1.42311400	H	0.12710000	1.49136100	-2.87839500
C	1.89602400	-1.10737500	-0.88493100	H	1.10014500	1.83179600	-4.29703600
C	1.86224200	1.29750700	-0.54336300	H	0.12710000	-1.49136100	2.87839500
C	1.94194000	-2.28096600	-1.71362000	H	1.10014500	-1.83179600	4.29703600
C	1.86224200	-1.29750700	0.54336300	H	0.70138300	0.52687900	5.10093700
C	1.89602400	1.10737500	0.88493100	H	-0.70138300	-0.52687900	5.10093700
C	1.83083300	2.64311900	-1.04655100	H	-0.12710000	1.49136100	2.87839500
C	1.90677000	-3.54033800	-1.19065200	H	-1.10014500	1.83179600	4.29703600
H	1.99687400	-2.17308900	-2.78988100				
C	1.83083300	-2.64311900	1.04655100				
C	1.90459300	-0.19536700	1.42311400				
C	1.94194000	2.28096600	1.71362000				
H	1.78957600	2.80989300	-2.11619300				
C	1.84078600	3.72570100	-0.21727500				

C_{2h}[6.6]BA

Atom	x	y	z	Atom	x	y	z
C	-2.79247000	4.59771500	0.71066200	C	2.79247000	-4.59771500	-0.71066200
C	-1.69404000	4.16181300	1.39311600	H	3.66731700	-4.94329700	1.25258400
C	-0.51297300	3.69997800	0.71837000	H	1.72141200	-4.16690800	-2.47589700
C	-0.51297300	3.69997800	-0.71837000	C	-4.04019900	-1.93550300	-0.71161000
C	-1.69404000	4.16181300	-1.39311600	H	-2.96513700	-2.34110300	-2.47594500
C	-2.79247000	4.59771500	-0.71066200	H	-4.91727400	-1.59551900	1.25336500
C	0.61481100	3.24320500	1.43648700	H	3.66731700	-4.94329700	-1.25258400
C	0.61481100	3.24320500	-1.43648700	H	-4.91727400	-1.59551900	-1.25336500
C	1.75382000	2.82235800	-0.72290400	C	0.52597400	3.15632800	2.94633500
C	1.75382000	2.82235800	0.72290400	C	-0.52597400	-3.15632800	2.94633500
C	2.93958600	2.36039800	1.39389100	C	-0.52597400	-3.15632800	-2.94633500
H	2.96513700	2.34110300	2.47594500	C	0.52597400	3.15632800	-2.94633500
C	4.04019900	1.93550300	0.71161000	H	-1.51587500	-3.11639300	-3.40472800
C	4.04019900	1.93550300	-0.71161000	H	-0.07000700	-4.07097400	-3.33612100
C	2.93958600	2.36039800	-1.39389100	H	0.59318400	-2.05613600	-4.44730100
H	-3.66731700	4.94329700	1.25258400	H	1.21588600	-1.88303000	-2.81014200
H	-1.72141200	4.16690800	2.47589700	H	-1.21588600	1.88303000	-2.81014200
H	-1.72141200	4.16690800	-2.47589700	H	-0.59318400	2.05613600	-4.44730100
H	-3.66731700	4.94329700	-1.25258400	H	1.51587500	3.11639300	-3.40472800
H	4.91727400	1.59551900	1.25336500	H	0.07000700	4.07097400	-3.33612100
H	4.91727400	1.59551900	-1.25336500	H	1.51587500	3.11639300	3.40472800
H	2.96513700	2.34110300	-2.47594500	H	0.07000700	4.07097400	3.33612100
C	-0.29136500	1.92941200	-3.39954800	H	-1.21588600	1.88303000	2.81014200
C	-0.29136500	1.92941200	3.39954800	H	-0.59318400	2.05613600	4.44730100
C	0.29136500	-1.92941200	-3.39954800	H	0.59318400	-2.05613600	4.44730100
C	0.29136500	-1.92941200	3.39954800	H	1.21588600	-1.88303000	2.81014200
C	-0.61481100	-3.24320500	1.43648700	H	-1.51587500	-3.11639300	3.40472800
C	0.51297300	-3.69997800	0.71837000	H	-0.07000700	-4.07097400	3.33612100
C	-1.75382000	-2.82235800	0.72290400	C	0.46388300	0.60761700	-3.24822800
C	1.69404000	-4.16181300	1.39311600	C	-0.46388300	-0.60761700	-3.24822800
C	0.51297300	-3.69997800	-0.71837000	C	0.46388300	0.60761700	3.24822800
C	-1.75382000	-2.82235800	-0.72290400	C	-0.46388300	-0.60761700	3.24822800
C	-2.93958600	-2.36039800	1.39389100	H	1.02701500	0.60402000	2.30604500
C	2.79247000	-4.59771500	0.71066200	H	1.20738800	0.51755700	4.05378000
H	1.72141200	-4.16690800	2.47589700	H	-1.02701500	-0.60402000	2.30604500
C	1.69404000	-4.16181300	-1.39311600	H	-1.20738800	-0.51755700	4.05378000
C	-0.61481100	-3.24320500	-1.43648700	H	1.20738800	0.51755700	-4.05378000
C	-2.93958600	-2.36039800	-1.39389100	H	1.02701500	0.60402000	-2.30604500
H	-2.96513700	-2.34110300	2.47594500	H	-1.20738800	-0.51755700	-4.05378000
C	-4.04019900	-1.93550300	0.71161000	H	-1.02701500	-0.60402000	-2.30604500

D_2[6.6]BA

Atom	x	y	z	Atom	x	y	z
C	-3.41009900	3.30073900	1.52447900	C	3.73165100	-3.27879600	0.13891200
C	-2.10602800	3.30840900	1.92246700	H	4.20408300	-3.30876600	2.26470700
C	-1.01968200	3.30045100	0.98127900	H	3.00584700	-3.24679100	-1.84073300
C	-1.34596200	3.28871000	-0.42291600	C	-3.41010000	-3.30067600	-1.52448000
C	-2.73503000	3.27043500	-0.79217300	H	-1.89175200	-3.31380700	-2.98347600
C	-3.73165100	3.27879600	0.13891200	H	-4.77032800	-3.26765600	0.17622300
C	0.32713900	3.27111500	1.39876400	H	4.77032800	-3.26773500	-0.17622400
C	-0.32713900	3.27111500	-1.39876500	H	-4.20408400	-3.30868600	-2.26470800
C	1.01968300	3.30043200	-0.98128000	H	-1.48145100	-1.63407100	4.22483700
C	1.34596200	3.28869100	0.42291500	H	-1.78215800	-1.28486600	2.52440500
C	2.73503000	3.27039400	0.79217200	H	1.78215800	1.28486600	2.52440500
H	3.00584700	3.24674900	1.84073200	H	1.48145100	1.63407100	4.22483700
C	3.73165100	3.27873300	-0.13891300	H	1.48145300	-1.63406700	-4.22483500
C	3.41010000	3.30067600	-1.52448000	H	1.78216000	-1.28486500	-2.52440200
C	2.10602900	3.30836600	-1.92246800	H	-1.78216000	1.28486500	-2.52440200
H	-4.20408300	3.30876600	2.26470700	H	-1.48145300	1.63406700	-4.22483500
H	-1.89175100	3.31385200	2.98347500	C	0.70310100	3.12775600	2.85907600
H	-3.00584700	3.24679100	-1.84073300	H	1.56522600	3.76161100	3.08357700
H	-4.77032800	3.26773500	-0.17622400	H	-0.09203500	3.49349200	3.51145600
H	4.77032800	3.26765600	0.17622300	C	-0.70310100	-3.12775600	2.85907600
H	4.20408400	3.30868600	-2.26470800	H	-1.56522600	-3.76161100	3.08357700
H	1.89175200	3.31380700	-2.98347600	H	0.09203500	-3.49349200	3.51145600
C	-1.02791600	1.66488200	-3.22576200	C	0.70310300	-3.12775400	-2.85907600
C	1.02791300	1.66488300	3.22576400	H	1.56522800	-3.76161100	-3.08357600
C	1.02791600	-1.66488200	-3.22576200	H	-0.09203200	-3.49348900	-3.51145700
C	-1.02791300	-1.66488300	3.22576400	C	-0.70310300	3.12775400	-2.85907600
C	-0.32713900	-3.27111500	1.39876400	H	-1.56522800	3.76161100	-3.08357600
C	1.01968200	-3.30045100	0.98127900	H	0.09203200	3.49348900	-3.51145700
C	-1.34596200	-3.28869100	0.42291500	C	0.19024900	-0.73972800	3.18881300
C	2.10602800	-3.30840900	1.92246700	C	-0.19024900	0.73972800	3.18881300
C	1.34596200	-3.28871000	-0.42291600	C	0.19024800	0.73972800	-3.18880900
C	-1.01968300	-3.30043200	-0.98128000	C	-0.19024800	-0.73972800	-3.18880900
C	-2.73503000	-3.27039400	0.79217200	H	-0.85110300	0.96435100	4.03895700
C	3.41009900	-3.30073900	1.52447900	H	-0.77461800	0.93814700	2.28191800
H	1.89175100	-3.31385200	2.98347500	H	0.85110300	-0.96435100	4.03895700
C	2.73503000	-3.27043500	-0.79217300	H	0.77461800	-0.93814700	2.28191800
C	0.32713900	-3.27111500	-1.39876500	H	0.85110200	0.96435200	-4.03895400
C	-2.10602900	-3.30836600	-1.92246800	H	0.77461600	0.93814900	-2.28191500
H	-3.00584700	-3.24674900	1.84073200	H	-0.85110200	-0.96435200	-4.03895400
C	-3.73165100	-3.27873300	-0.13891300	H	-0.77461600	-0.93814900	-2.28191500

Cartesian Coordinates for Optimized Geometries of [n.n]PIs@M06-2X/6-31++G(d,p) (n=2-6)

D_2[2.2]PI

Atom	x	y	z	Atom	x	y	z
C	-3.31031600	2.48677200	1.04928900	H	4.09407700	-2.90671300	1.67202800
C	-2.14661500	1.98304500	1.63697900	H	2.58269500	-1.89051700	-2.20465900
C	-1.14065900	1.44747900	0.84412000	C	-3.31031600	-2.48677200	-1.04928900
C	-1.28643300	1.38915300	-0.55536400	H	-2.03380100	-2.01196200	-2.71687400
C	-2.44594900	1.90154100	-1.12890700	H	-4.35341300	-2.84289300	0.79670600
C	-3.45574500	2.44852700	-0.33101100	H	4.35341300	-2.84289300	-0.79670600
C	0.12545200	0.81396600	1.35808900	H	-4.09407700	-2.90671300	-1.67202800
C	-0.12545200	0.81396600	-1.35808900	C	-0.32386600	-0.69545800	2.88016500
C	1.14065900	1.44747900	-0.84412000	C	0.32386600	0.69545800	2.88016500
C	1.28643300	1.38915300	0.55536400	C	-0.32386600	0.69545800	-2.88016500
C	2.44594900	1.90154100	1.12890700	C	0.32386600	-0.69545800	-2.88016500
H	2.58269500	1.89051700	2.20465900	H	-1.38456300	-0.62389800	3.12638600
C	3.45574500	2.44852700	0.33101100	H	0.12414500	-1.46918200	3.50859600
C	3.31031600	2.48677200	-1.04928900	H	-0.12414500	1.46918200	3.50859600
C	2.14661500	1.98304500	-1.63697900	H	1.38456300	0.62389800	3.12638600
H	-4.09407700	2.90671300	1.67202800	H	-1.38456300	0.62389800	-3.12638600
H	-2.03380100	2.01196200	2.71687400	H	0.12414500	1.46918200	-3.50859600
H	-2.58269500	1.89051700	-2.20465900	H	-0.12414500	-1.46918200	-3.50859600
H	-4.35341300	2.84289300	-0.79670600	H	1.38456300	-0.62389800	-3.12638600
H	4.35341300	2.84289300	0.79670600				
H	4.09407700	2.90671300	-1.67202800				
H	2.03380100	2.01196200	-2.71687400				
C	-0.12545200	-0.81396600	1.35808900				
C	1.14065900	-1.44747900	0.84412000				
C	-1.28643300	-1.38915300	0.55536400				
C	2.14661500	-1.98304500	1.63697900				
C	1.28643300	-1.38915300	-0.55536400				
C	-1.14065900	-1.44747900	-0.84412000				
C	-2.44594900	-1.90154100	1.12890700				
C	3.31031600	-2.48677200	1.04928900				
H	2.03380100	-2.01196200	2.71687400				
C	2.44594900	-1.90154100	-1.12890700				
C	0.12545200	-0.81396600	-1.35808900				
C	-2.14661500	-1.98304500	-1.63697900				
H	-2.58269500	-1.89051700	2.20465900				
C	-3.45574500	-2.44852700	0.33101100				
C	3.45574500	-2.44852700	-0.33101100				

C_{2h}[3.3]PI

Atom	x	y	z	Atom	x	y	z
C	-1.67670700	2.13393800	1.90922700	H	2.12556200	2.68399700	-1.85827800
C	-0.86463700	1.12315800	1.39210500	H	-1.79858800	4.09114500	-2.79046800
C	0.53013500	1.31303400	1.37822400	H	1.79858800	-4.09114500	-2.79046800
C	1.05618100	2.51074400	1.86497500	H	0.67211800	4.43736300	-2.74130000
C	0.23408800	3.51644700	2.36940300	H	3.09972600	2.26665100	0.00000000
C	-1.41335400	-0.18831700	0.82866700	H	4.56029000	1.26382700	0.00000000
C	1.41335400	0.18831700	0.82866700	H	-3.09972600	-2.26665100	0.00000000
C	0.86463700	-1.12315800	1.39210500	H	-4.56029000	-1.26382700	0.00000000
C	-0.53013500	-1.31303400	1.37822400	C	-2.90096900	-0.43082800	1.16620500
C	-1.05618100	-2.51074400	1.86497500	H	-3.03079700	-0.87258200	2.15689800
H	-2.12556200	-2.68399700	1.85827800	H	-3.44267400	0.51636500	1.16796400
C	-0.23408800	-3.51644700	2.36940300	C	-2.90096900	-0.43082800	-1.16620500
C	1.13927000	-3.32489300	2.39512000	H	-3.44267400	0.51636500	-1.16796400
C	1.67670700	-2.13393800	1.90922700	H	-3.03079700	-0.87258200	-2.15689800
H	-2.75164800	2.01550600	1.94932400	C	2.90096900	0.43082800	-1.16620500
H	2.12556200	2.68399700	1.85827800	H	3.44267400	-0.51636500	-1.16796400
H	0.67211800	4.43736300	2.74130000	H	3.03079700	0.87258200	-2.15689800
H	-0.67211800	-4.43736300	2.74130000	C	2.90096900	0.43082800	1.16620500
H	1.79858800	-4.09114500	2.79046800	H	3.03079700	0.87258200	2.15689800
H	2.75164800	-2.01550600	1.94932400	H	3.44267400	-0.51636500	1.16796400
C	3.46682600	1.23604100	0.00000000	C	-1.13927000	3.32489300	2.39512000
C	-3.46682600	-1.23604100	0.00000000	H	-1.79858800	4.09114500	2.79046800
C	-1.41335400	-0.18831700	-0.82866700				
C	-0.53013500	-1.31303400	-1.37822400				
C	-0.86463700	1.12315800	-1.39210500				
C	-1.05618100	-2.51074400	-1.86497500				
C	0.86463700	-1.12315800	-1.39210500				
C	0.53013500	1.31303400	-1.37822400				
C	-1.67670700	2.13393800	-1.90922700				
C	-0.23408800	-3.51644700	-2.36940300				
H	-2.12556200	-2.68399700	-1.85827800				
C	1.67670700	-2.13393800	-1.90922700				
C	1.41335400	0.18831700	-0.82866700				
C	1.05618100	2.51074400	-1.86497500				
H	-2.75164800	2.01550600	-1.94932400				
C	-1.13927000	3.32489300	-2.39512000				
C	1.13927000	-3.32489300	-2.39512000				
H	-0.67211800	-4.43736300	-2.74130000				
H	2.75164800	-2.01550600	-1.94932400				
C	0.23408800	3.51644700	-2.36940300				

C_2[4.4]PI

Atom	x	y	z	Atom	x	y	z
C	3.34642000	-2.39128300	-0.50415600	C	-3.44614200	2.21329100	0.87048200
C	2.49323800	-1.57383400	-1.23673500	H	-3.92629700	3.15778400	-1.00869800
C	1.71528900	-0.58096400	-0.63061700	H	-2.70558700	1.16985100	2.57034500
C	1.75825400	-0.45977500	0.76632300	C	-0.04461500	-4.11094100	0.49810200
C	2.64850700	-1.25933300	1.49191300	H	-0.02413600	-3.00167500	2.29312900
C	3.44614200	-2.21329100	0.87048200	H	-0.06726300	-4.97178000	-1.47850500
C	0.78831700	0.32036800	-1.46512700	H	-4.11825600	2.82686600	1.46237800
C	0.73052400	0.42793800	1.46469000	H	0.23522400	-5.02815700	1.00670000
C	0.57939100	1.72602600	0.63589400	C	1.42695100	0.47755200	-2.88547600
C	0.68984600	1.68475700	-0.76912800	C	-1.42695100	-0.47755200	-2.88547600
C	0.50618200	2.86826300	-1.49325500	C	-1.25480800	-0.79954000	2.88681700
H	0.53334300	2.86683000	-2.57489600	C	1.25480800	0.79954000	2.88681700
C	0.20752200	4.07840100	-0.87783100	H	-0.97408900	-1.81899300	3.13390400
C	0.04461500	4.11094100	0.49810200	H	-2.34699700	-0.81998100	2.83779600
C	0.22269700	2.94242600	1.23074500	H	-1.17972700	-0.39047000	4.98830600
H	3.92629700	-3.15778400	-1.00869800	H	-1.08299200	1.07666300	4.01302600
H	2.41972200	-1.74028700	-2.30661100	H	1.08299200	-1.07666300	4.01302600
H	2.70558700	-1.16985100	2.57034500	H	1.17972700	0.39047000	4.98830600
H	4.11825600	-2.82686600	1.46237800	H	0.97408900	1.81899300	3.13390400
H	0.06726300	4.97178000	-1.47850500	H	2.34699700	0.81998100	2.83779600
H	-0.23522400	5.02815700	1.00670000	H	1.46914800	1.52927100	-3.15468700
H	0.02413600	3.00167500	2.29312900	H	2.47403700	0.17892900	-2.82693200
C	0.76066100	-0.02826300	4.06678600	H	0.79047500	-1.30852000	-3.97234700
C	0.73052400	-0.21358600	-4.04995800	H	1.23575800	0.06958300	-4.97970600
C	-0.76066100	0.02826300	4.06678600	H	-1.23575800	-0.06958300	-4.97970600
C	-0.73052400	0.21358600	-4.04995800	H	-0.79047500	1.30852000	-3.97234700
C	-0.78831700	-0.32036800	-1.46512700	H	-1.46914800	-1.52927100	-3.15468700
C	-1.71528900	0.58096400	-0.63061700	H	-2.47403700	-0.17892900	-2.82693200
C	-0.68984600	-1.68475700	-0.76912800				
C	-2.49323800	1.57383400	-1.23673500				
C	-1.75825400	0.45977500	0.76632300				
C	-0.57939100	-1.72602600	0.63589400				
C	-0.50618200	-2.86826300	-1.49325500				
C	-3.34642000	2.39128300	-0.50415600				
H	-2.41972200	1.74028700	-2.30661100				
C	-2.64850700	1.25933300	1.49191300				
C	-0.73052400	-0.42793800	1.46469000				
C	-0.22269700	-2.94242600	1.23074500				
H	-0.53334300	-2.86683000	-2.57489600				
C	-0.20752200	-4.07840100	-0.87783100				

D_2[4.4]PI

Atom	x	y	z	Atom	x	y	z
C	3.65007000	0.35604400	1.93382500	C	-3.46389600	-1.00011300	-2.16018700
C	2.58021300	1.13521500	1.50173200	H	-4.61928700	0.81808900	-2.09357900
C	1.30962600	0.59528200	1.26851400	H	-2.10827700	-2.63461900	-2.00355400
C	1.16116000	-0.79813500	1.39610700	C	3.65007000	-0.35604400	-1.93382500
C	2.22552800	-1.56576200	1.87503500	H	2.78302400	-2.18204100	-1.31604000
C	3.46389600	-1.00011300	2.16018700	H	4.27662000	1.62173400	-2.52286800
C	0.09561000	1.45668700	0.83590300	H	-4.27662000	-1.62173400	-2.52286800
C	-0.09561000	-1.45668700	0.83590300	H	4.61928700	-0.81808900	-2.09357900
C	-1.30962600	-0.59528200	1.26851400	H	0.05442900	4.98456200	-1.24616000
C	-1.16116000	0.79813500	1.39610700	H	1.39905300	4.03640200	-0.60972600
C	-2.22552800	1.56576200	1.87503500	H	-1.39905300	4.03640200	0.60972600
H	-2.10827700	2.63461900	2.00355400	H	-0.05442900	4.98456200	1.24616000
C	-3.46389600	1.00011300	2.16018700	H	-0.05442900	-4.98456200	-1.24616000
C	-3.65007000	-0.35604400	1.93382500	H	-1.39905300	-4.03640200	-0.60972600
C	-2.58021300	-1.13521500	1.50173200	H	1.39905300	-4.03640200	0.60972600
H	4.61928700	0.81808900	2.09357900	H	0.05442900	-4.98456200	1.24616000
H	2.78302400	2.18204100	1.31604000	C	0.27088900	2.87803700	1.45162400
H	2.10827700	-2.63461900	2.00355400	H	-0.09488400	2.83293500	2.48213100
H	4.27662000	-1.62173400	2.52286800	H	1.32810200	3.11109900	1.54208600
H	-4.27662000	1.62173400	2.52286800	C	-0.27088900	2.87803700	-1.45162400
H	-4.61928700	-0.81808900	2.09357900	H	0.09488400	2.83293500	-2.48213100
H	-2.78302400	-2.18204100	1.31604000	H	-1.32810200	3.11109900	-1.54208600
C	0.30563800	-4.07067600	0.69651800	C	0.27088900	-2.87803700	-1.45162400
C	-0.30563800	4.07067600	0.69651800	H	-0.09488400	-2.83293500	-2.48213100
C	-0.30563800	-4.07067600	-0.69651800	H	1.32810200	-3.11109900	-1.54208600
C	0.30563800	4.07067600	-0.69651800	C	-0.27088900	-2.87803700	1.45162400
C	-0.09561000	1.45668700	-0.83590300	H	0.09488400	-2.83293500	2.48213100
C	-1.30962600	0.59528200	-1.26851400	H	-1.32810200	-3.11109900	1.54208600
C	1.16116000	0.79813500	-1.39610700				
C	-2.58021300	1.13521500	-1.50173200				
C	-1.16116000	-0.79813500	-1.39610700				
C	1.30962600	-0.59528200	-1.26851400				
C	2.22552800	1.56576200	-1.87503500				
C	-3.65007000	0.35604400	-1.93382500				
H	-2.78302400	2.18204100	-1.31604000				
C	-2.22552800	-1.56576200	-1.87503500				
C	0.09561000	-1.45668700	-0.83590300				
C	2.58021300	-1.13521500	-1.50173200				
H	2.10827700	2.63461900	-2.00355400				
C	3.46389600	1.00011300	-2.16018700				

C_i[5.5]PI

Atom	x	y	z	Atom	x	y	z
C	-3.63819100	0.66973300	1.95355700	C	3.63819100	-0.66973300	-1.95355700
C	-2.85893100	-0.30609700	1.34027600	H	3.60033500	-2.55832600	-2.99794700
C	-1.47720300	-0.15391700	1.15871400	H	3.36989100	1.19887900	-1.00424900
C	-0.92126700	1.09881700	1.46558200	C	-3.00323200	1.94755600	-2.04330200
C	-1.68173700	2.02682700	2.18461100	H	-1.46819800	3.13956300	-1.18930300
C	-3.03155200	1.81730800	2.44513300	H	-4.37840100	0.49689500	-2.84999100
C	-0.55725800	-1.32432400	0.68553500	H	4.70487400	-0.50789700	-2.07295100
C	0.49332700	1.38616100	0.96953100	H	-3.65899300	2.79893900	-2.19676500
C	1.32656300	0.22183000	1.50566400	C	-1.24699700	-2.56974900	1.37874000
C	0.85128400	-1.08522800	1.27025700	C	-1.01367400	-2.73620700	-1.49548100
C	1.73831500	-2.14033900	1.49020700	C	1.24699700	2.56974900	-1.37874000
H	1.46819800	-3.13956300	1.18930300	C	1.01367400	2.73620700	1.49548100
C	3.00323200	-1.94755600	2.04330200	C	-0.98867400	-4.77189400	0.06802800
C	3.40892800	-0.66785900	2.39230400	C	0.98867400	4.77189400	-0.06802800
C	2.57462900	0.40902900	2.10119600	H	0.17817500	-4.20872700	1.79901300
H	-4.70487400	0.50789700	2.07295100	H	-1.49327900	-4.51704000	2.13298900
H	-3.36989100	-1.19887900	1.00424900	H	-0.20581800	-4.68860600	-1.93407600
H	-1.22915000	2.93964000	2.54777600	H	0.74033500	-3.81888800	-0.74556900
H	-3.60033500	2.55832600	2.99794700	H	1.49327900	4.51704000	-2.13298900
H	3.65899300	-2.79893900	2.19676500	H	-0.17817500	4.20872700	-1.79901300
H	4.37840100	-0.49689500	2.84999100	H	1.34028100	2.25930600	-2.42463600
H	2.93132400	1.40821200	2.31962100	H	2.26628800	2.61025700	-0.99304700
C	0.28556900	4.02949100	1.06136500	H	-1.01212400	-2.66659900	-2.58986000
C	-0.82352200	-4.05017700	1.39957800	H	-2.06520500	-2.84352900	-1.20926200
C	0.82352200	4.05017700	-1.39957800	H	-1.34028100	-2.25930600	2.42463600
C	-0.28556900	-4.02949100	-1.06136500	H	-2.26628800	-2.61025700	0.99304700
C	-0.49332700	-1.38616100	-0.96953100	H	1.01212400	2.66659900	2.58986000
C	0.92126700	-1.09881700	-1.46558200	H	2.06520500	2.84352900	1.20926200
C	-1.32656300	-0.22183000	-1.50566400	H	-0.74033500	3.81888800	0.74556900
C	1.68173700	-2.02682700	-2.18461100	H	0.20581800	4.68860600	1.93407600
C	1.47720300	0.15391700	-1.15871400	H	-2.05725000	-4.87119200	-0.16940700
C	-0.85128400	1.08522800	-1.27025700	H	-0.59182800	-5.79016400	0.15286700
C	-2.57462900	-0.40902900	-2.10119600	H	2.05725000	4.87119200	0.16940700
C	3.03155200	-1.81730800	-2.44513300	H	0.59182800	5.79016400	-0.15286700
H	1.22915000	-2.93964000	-2.54777600				
C	2.85893100	0.30609700	-1.34027600				
C	0.55725800	1.32432400	-0.68553500				
C	-1.73831500	2.14033900	-1.49020700				
H	-2.93132400	-1.40821200	-2.31962100				
C	-3.40892800	0.66785900	-2.39230400				

D_2[5.5]PI

Atom	x	y	z	Atom	x	y	z
C	0.76150800	3.49124700	-2.24551800	C	-0.61273900	-3.58294200	2.08040900
C	1.41031000	2.31424000	-1.88836100	H	1.33380700	-4.32900900	2.63138600
C	0.72110000	1.20832700	-1.37730800	H	-2.38613700	-2.58721900	1.50429700
C	-0.68351800	1.26672000	-1.30539800	C	-0.76095000	3.49135900	2.24554900
C	-1.31622800	2.47383200	-1.62389400	H	-2.48334000	2.28534000	2.00995900
C	-0.61220000	3.58317700	-2.07981200	H	1.14347000	4.50113800	2.31146300
C	1.46977400	-0.02653700	-0.83941700	H	-1.14343800	-4.50095500	2.31224600
C	-1.46979000	0.02647300	-0.83937700	H	-1.33376000	4.32922500	2.63074300
C	-0.72112500	-1.20834400	-1.37738800	C	2.87721600	-0.05376400	-1.51657300
C	0.68349200	-1.26673900	-1.30553400	C	2.87725600	0.05331700	1.51650300
C	1.31620600	-2.47377500	-1.62430800	C	-2.87722900	-0.05334300	1.51656700
H	2.38572700	-2.58760700	-1.50428700	C	-2.87724400	0.05373500	-1.51650900
C	0.61216900	-3.58304900	-2.08038500	C	-4.89017100	0.00012400	0.00000300
C	-0.76154800	-3.49110400	-2.24601600	C	4.89017000	-0.00040600	-0.00003600
C	-1.41034400	-2.31416000	-1.88864100	H	5.54321000	-0.66743100	-0.57615300
H	1.33445500	4.32902800	-2.63069500	H	5.54334700	0.66650800	0.57605300
H	2.48370800	2.28495700	-2.00990700	H	-5.54332700	0.66707300	-0.57606900
H	-2.38573700	2.58766600	-1.50377800	H	-5.54323100	-0.66686500	0.57613900
H	-1.14275100	4.50132900	-2.31143900	H	4.61605900	-1.21229400	1.77246000
H	1.14272000	-4.50115000	-2.31221500	H	3.61349100	-1.69082900	0.42105100
H	-1.33450000	-4.32881500	-2.63133900	H	4.61619200	1.21161700	-1.77246200
H	-2.48374200	-2.28484500	-2.01018500	H	3.61370500	1.69020800	-0.42101200
C	-4.01020100	-0.81784600	-0.94830600	H	-4.61608900	1.21221100	1.77236900
C	4.01021800	0.81769300	-0.94825800	H	-3.61355100	1.69063600	0.42089700
C	-4.01014600	0.81818600	0.94818900	H	-4.61616300	-1.21170500	-1.77255100
C	4.01012700	-0.81833800	0.94823900	H	-3.61364600	-1.69040000	-0.42116000
C	1.46979500	0.02624500	0.83937700	H	3.27133200	-1.06580000	-1.54123900
C	0.72093800	-1.20845300	1.37739800	H	2.69348400	0.19413000	-2.56648600
C	0.68371500	1.26661100	1.30540000	H	3.27152400	1.06529700	1.54107200
C	1.40997600	-2.31437300	1.88866900	H	2.69351400	-0.19446400	2.56644200
C	-0.68368900	-1.26662800	1.30553600	H	-2.69347800	0.19459700	2.56646600
C	-0.72091200	1.20843900	1.37731500	H	-3.27144700	-1.06533900	1.54129500
C	1.31661900	2.47362000	1.62390100	H	-2.69352100	-0.19400000	-2.56646200
C	0.76099100	-3.49121200	2.24604900	H	-3.27141100	1.06575600	-1.54101800
H	2.48337600	-2.28522800	2.01022600				
C	-1.31659700	-2.47356000	1.62431700				
C	-1.46978000	-0.02630700	0.83941800				
C	-1.40994100	2.31445700	1.88838700				
H	2.38614700	2.58728300	1.50377900				
C	0.61277200	3.58307300	2.07983200				

C_{2h}[6.6]PI

Atom	x	y	z	Atom	x	y	z
C	-3.12472500	2.71412700	0.69245200	C	3.12472500	-2.71412700	-0.69245200
C	-2.06336500	2.12367000	1.37110200	H	3.94044400	-3.16224800	1.25121700
C	-0.98511700	1.52911100	0.70566300	H	2.11442700	-2.13236400	-2.45084200
C	-0.98511700	1.52911100	-0.70566300	C	-3.80098300	-1.80470400	-0.69260300
C	-2.06336500	2.12367000	-1.37110200	H	-2.65868500	-1.51376200	-2.44611600
C	-3.12472500	2.71412700	-0.69245200	H	-4.69490600	-2.06048000	1.25285800
C	0.15601700	0.81574400	1.47087100	H	3.94044400	-3.16224800	-1.25121700
C	0.15601700	0.81574400	-1.47087100	H	-4.69490600	-2.06048000	-1.25285800
C	1.44809500	1.13981700	-0.70345200	C	0.23780000	1.45126700	2.89202500
C	1.44809500	1.13981700	0.70345200	C	-0.23780000	-1.45126700	2.89202500
C	2.62850300	1.48385500	1.36958700	C	-0.23780000	-1.45126700	-2.89202500
H	2.65868500	1.51376200	2.44611600	C	0.23780000	1.45126700	-2.89202500
C	3.80098300	1.80470400	0.69260300	C	-0.39861400	-0.65439400	5.31668400
C	3.80098300	1.80470400	-0.69260300	C	0.39861400	0.65439400	5.31668400
C	2.62850300	1.48385500	-1.36958700	C	0.39861400	0.65439400	-5.31668400
H	-3.94044400	3.16224800	1.25121700	C	-0.39861400	-0.65439400	-5.31668400
H	-2.11442700	2.13236400	2.45084200	H	-0.28565300	1.49469100	5.49915300
H	-2.11442700	2.13236400	-2.45084200	H	1.09030700	0.63858600	6.16694800
H	-3.94044400	3.16224800	-1.25121700	H	-1.09030700	-0.63858600	6.16694800
H	4.69490600	2.06048000	1.25285800	H	0.28565300	-1.49469100	5.49915300
H	4.69490600	2.06048000	-1.25285800	H	0.28565300	-1.49469100	-5.49915300
H	2.65868500	1.51376200	-2.44611600	H	-1.09030700	-0.63858600	-6.16694800
C	1.17713800	0.96132700	-4.03078300	H	-0.28565300	1.49469100	-5.49915300
C	1.17713800	0.96132700	4.03078300	H	1.09030700	0.63858600	-6.16694800
C	-1.17713800	-0.96132700	-4.03078300	H	-1.87939300	-1.76828700	-4.26659600
C	-1.17713800	-0.96132700	4.03078300	H	-1.80046400	-0.11015100	-3.74297100
C	-0.15601700	-0.81574400	1.47087100	H	1.80046400	0.11015100	-3.74297100
C	0.98511700	-1.52911100	0.70566300	H	1.87939300	1.76828700	-4.26659600
C	-1.44809500	-1.13981700	0.70345200	H	-1.80046400	-0.11015100	3.74297100
C	2.06336500	-2.12367000	1.37110200	H	-1.87939300	-1.76828700	4.26659600
C	0.98511700	-1.52911100	-0.70566300	H	1.80046400	0.11015100	3.74297100
C	-1.44809500	-1.13981700	-0.70345200	H	1.87939300	1.76828700	4.26659600
C	-2.62850300	-1.48385500	1.36958700	H	-0.45053000	-2.51071100	-2.70691500
C	3.12472500	-2.71412700	0.69245200	H	0.75549400	-1.44059400	-3.32330600
H	2.11442700	-2.13236400	2.45084200	H	-0.75549400	1.44059400	-3.32330600
C	2.06336500	-2.12367000	-1.37110200	H	0.45053000	2.51071100	-2.70691500
C	-0.15601700	-0.81574400	-1.47087100	H	0.45053000	2.51071100	2.70691500
C	-2.62850300	-1.48385500	-1.36958700	H	-0.75549400	1.44059400	3.32330600
H	-2.65868500	-1.51376200	2.44611600	H	-0.45053000	-2.51071100	2.70691500
C	-3.80098300	-1.80470400	0.69260300	H	0.75549400	-1.44059400	3.32330600

D_2[6.6]PI

Atom	x	y	z	Atom	x	y	z
C	-0.82864800	3.48641000	2.23534500	C	0.55397700	-3.55304300	-2.17462100
C	-1.47099900	2.31782200	1.83793000	H	-1.41416600	-4.33176400	-2.58327000
C	-0.76771700	1.20122100	1.37240500	H	2.34168700	-2.53096200	-1.69054300
C	0.63858000	1.26451700	1.31989600	C	0.82864800	3.48641000	-2.23534500
C	1.26673600	2.44584900	1.72615700	H	2.55072100	2.31526700	-1.89578800
C	0.55397700	3.55304300	2.17462100	H	-1.08438100	4.45221600	-2.47221600
C	-1.46704600	-0.05723200	0.83046300	H	1.08438100	-4.45221600	-2.47221600
C	1.46704600	0.05723200	0.83046300	H	1.41416600	4.33176400	-2.58327000
C	0.76771700	-1.20122100	1.37240500	H	-4.23113700	1.79035500	-1.86555900
C	-0.63858000	-1.26451700	1.31989600	H	-3.68234200	1.79367800	-0.21390400
C	-1.26673600	-2.44584900	1.72615700	H	-3.68234200	-1.79367800	0.21390400
H	-2.34168700	-2.53096200	1.69054300	H	-4.23113700	-1.79035500	1.86555900
C	-0.55397700	-3.55304300	2.17462100	H	4.23113700	-1.79035500	-1.86555900
C	0.82864800	-3.48641000	2.23534500	H	3.68234200	-1.79367800	-0.21390400
C	1.47099900	-2.31782200	1.83793000	H	3.68234200	1.79367800	0.21390400
H	-1.41416600	4.33176400	2.58327000	H	4.23113700	1.79035500	1.86555900
H	-2.55072100	2.31526700	1.89578800	C	-2.88365300	-0.14158400	1.47264500
H	2.34168700	2.53096200	1.69054300	H	-2.69525100	-0.29402900	2.54169600
H	1.08438100	4.45221600	2.47221600	H	-3.34279300	0.83661300	1.41235700
H	-1.08438100	-4.45221600	2.47221600	C	-2.88365300	0.14158400	-1.47264500
H	1.41416600	-4.33176400	2.58327000	H	-2.69525100	0.29402900	-2.54169600
H	2.55072100	-2.31526700	1.89578800	H	-3.34279300	-0.83661300	-1.41235700
C	3.99551100	1.12939100	1.02407600	C	2.88365300	-0.14158400	-1.47264500
C	-3.99551100	-1.12939100	1.02407600	H	2.69525100	-0.29402900	-2.54169600
C	3.99551100	-1.12939100	-1.02407600	H	3.34279300	0.83661300	-1.41235700
C	-3.99551100	1.12939100	-1.02407600	C	2.88365300	0.14158400	1.47264500
C	-1.46704600	0.05723200	-0.83046300	H	2.69525100	0.29402900	2.54169600
C	-0.76771700	-1.20122100	-1.37240500	H	3.34279300	-0.83661300	1.41235700
C	-0.63858000	1.26451700	-1.31989600	C	-5.28922300	0.38356700	-0.66512700
C	-1.47099900	-2.31782200	-1.83793000	C	-5.28922300	-0.38356700	0.66512700
C	0.63858000	-1.26451700	-1.31989600	C	5.28922300	0.38356700	0.66512700
C	0.76771700	1.20122100	-1.37240500	C	5.28922300	-0.38356700	-0.66512700
C	-1.26673600	2.44584900	-1.72615700	H	-6.12793700	-1.08932500	0.65512200
C	-0.82864800	-3.48641000	-2.23534500	H	-5.49627800	0.31819100	1.48480300
H	-2.55072100	-2.31526700	-1.89578800	H	-6.12793700	1.08932500	-0.65512200
C	1.26673600	-2.44584900	-1.72615700	H	-5.49627800	-0.31819100	-1.48480300
C	1.46704600	-0.05723200	-0.83046300	H	6.12793700	1.08932500	0.65512200
C	1.47099900	2.31782200	-1.83793000	H	5.49627800	-0.31819100	1.48480300
H	-2.34168700	2.53096200	-1.69054300	H	6.12793700	-1.08932500	-0.65512200
C	-0.55397700	3.55304300	-2.17462100	H	5.49627800	0.31819100	-1.48480300

References

(S1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A. *Gaussian 09*, revision A.01. Gaussian, Inc.: Wallingford, CT, **2009**.

(S2) Ruckenbauer, M.; Fazzi, D.; Arbelo-Gonzalez, W.; Barbatti, M. Tutorial for NEWTON-X, version 2.0, www.newtonx.org, **2016**.

(S3) Crespo-Otero, R.; Barbatti, M. *Theor. Chem. Acc.* **2012**, *131*, 1237.

(S4) Grimme, S.; Diedrich, C.; Korth, M. *Angew. Chem. Int. Ed.* **2006**, *45*, 625-629.

(S5) Neese, F. The Orca Program System. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2*, 73-78.

(S6) Jones, G.; Reinhard, T. E.; Bergmark, W. R. *Sol. Energy.* **1978**, *20*, 241-248.

(S7) Mau, A. W. H. Mau, Albert WH. *J. Chem. Soc., Faraday Trans. 1* **1978**, *74*, 603-612.

(S8) De Lio, A. M.; Durfey, B. L.; Gille, A. L.; Gilbert, T. M. *J. Phys. Chem. A* **2014**, *118*, 6050-6059.

(S9) Khoury, P. R.; Goddard, J. D.; Tam, W. *Tetrahedron.* **2004**, *60*, 8103-8112.

(S10) Usui, M.; Nishiwaki, T.; Anda, K.; Hida, M. *Chem. Lett.* **1984**, *13*, 1561-1564.