

Electronic Supporting Information

Detection of diheptacendiyl diradical intermediate in the cycloreversion of diheptacene to heptacene

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1. Experimental Details

The mixture of diheptacenes **B** was synthesized as described previously.¹ For the ESR measurement the diheptacene powder was heated in the dark under an argon atmosphere for 15 min at 315 °C. The ESR spectra were measured on an X-band CW spectrometer (Bruker EMXmicro). Liquid helium was used to cool the sample from 290 to 5 K.

Simulations of ESR spectra were done with EasySpin 6.0.2.²

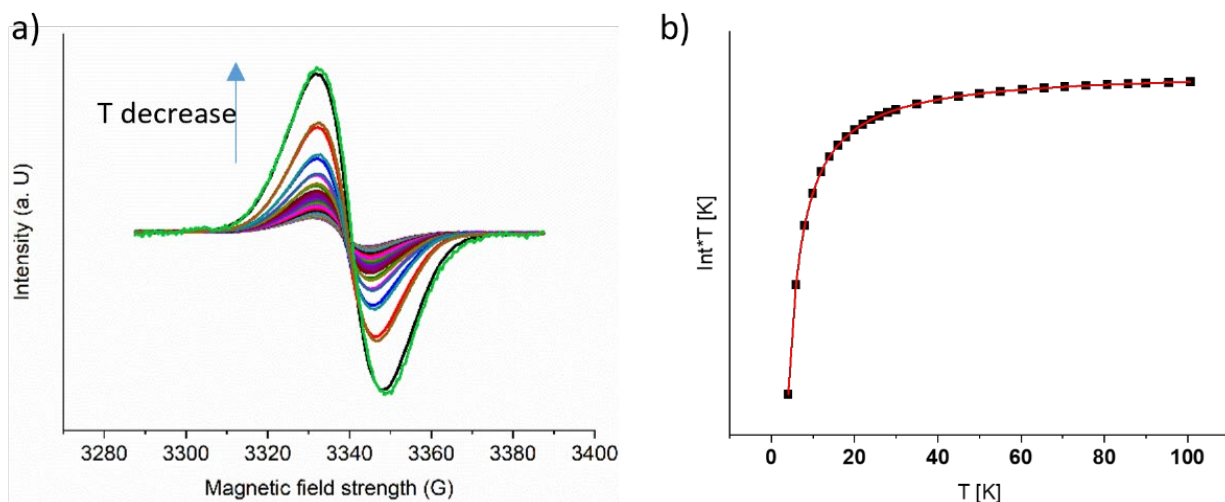


Figure S1. a) Temperature dependent EPR signal of 7,7'-diheptacenyl diradical; signal intensity increases with decreasing temperature. b) Plot of the integrated signal intensity Int multiplied by temperature T vs. T ; the red line is the fit to the data using the Bleaney-Bowers equation.

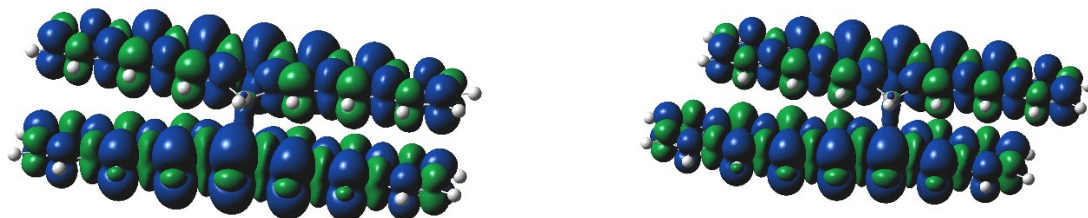


Figure S2. Computed (UM06-2X/def2-SVP, isovalue 0.0004) spin-density of the most stable rotamers of 7,7'-DHD (left) and 6,7'-DHD (right).

Direct dipolar spin-spin coupling is the dominating interaction that is responsible for the zero-field splitting (ZFS) parameters of organic diradicals according to Sinnecker and Neese.³ Computing the ZFS parameters using DFT methods, Sinnecker and Neese found overall good agreement with experiment, although the $|D|$ values of acenes up to tetracene were underestimated.³ We obtain (B3LYP/def2-TZVP, see computational methods below for details) the following $|D|$ values for the three rotamers of 7,7'-DHD: 0.002 cm⁻¹ ($d = 172.9^\circ$), 0.015 cm⁻¹ ($d = 28.7^\circ$), and 0.009 cm⁻¹ ($d = 59.3^\circ$). For the rotamers of the 6,7'-DHD isomer, very similar values were obtained: 0.002 cm⁻¹ ($d = 174.8^\circ$), -0.007 cm⁻¹ ($d = 60.2^\circ$), and -0.015 cm⁻¹ ($d = 26.0^\circ$). Even if theory would underestimate the $|D|$ values by a factor of two as observed by Sinnecker and Neese³ for the acenes, the $|D|$ values of the most stable diradicals are so small

that the absence of the ZFS pattern in the spectra is readily explained. In addition, the intensity of the half-field signal is inversely proportional to the $|D|$ value.⁴ The simulations show that for the small $|D|$ value of the diradical a half-field signal cannot be detected.

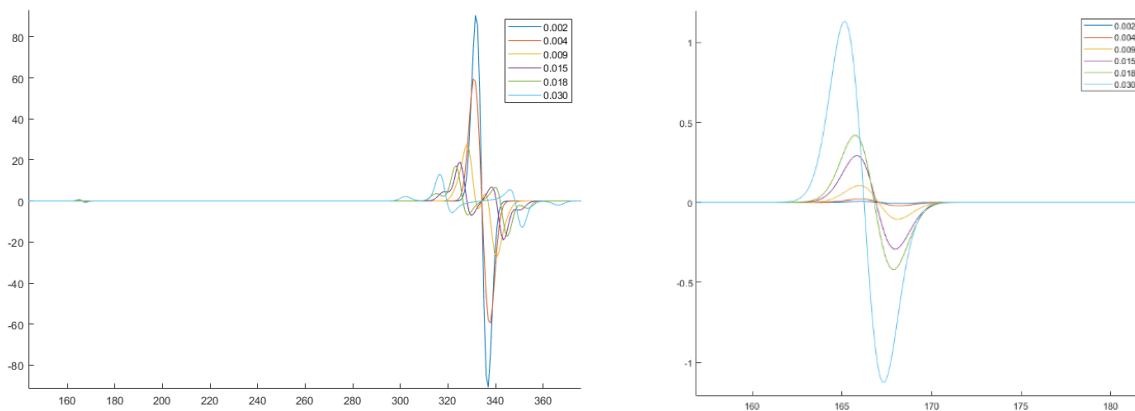


Figure S3. Simulated EPR spectra ($g = 2$, microwave frequency 9.35 GHz) for $|D|$ values given in the inset. Left: full spectrum; right: focus on the half-field range.

2. NMR Spectra

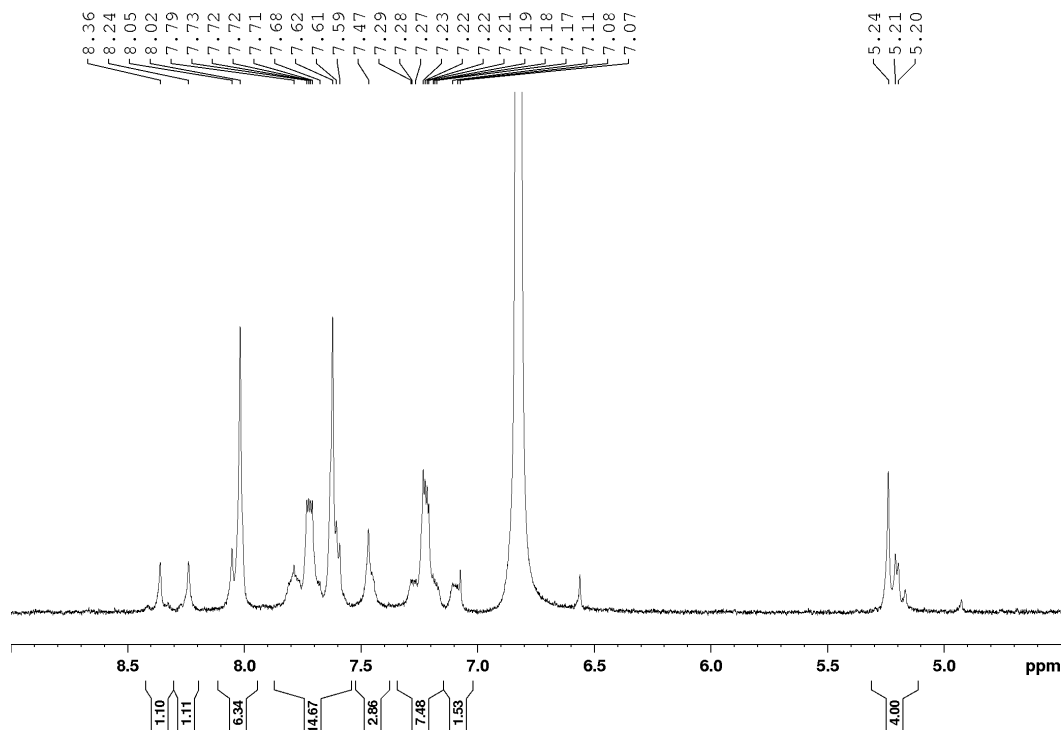


Figure S4. ^1H NMR spectrum of dimer mixture in CDBr_3 at 120 °C. Only the relevant area is shown.

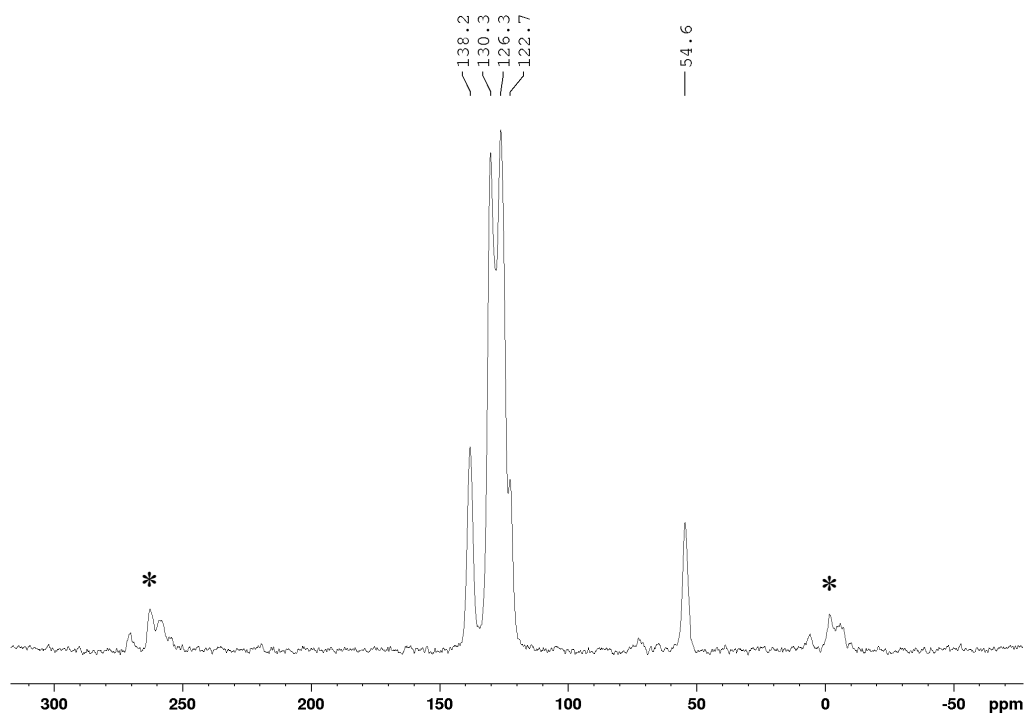


Figure S5. Solid state ^{13}C CP/MAS NMR spectrum of the dimer mixture, 10 kHz rotation speed. The asterisks denote rotational sidebands.

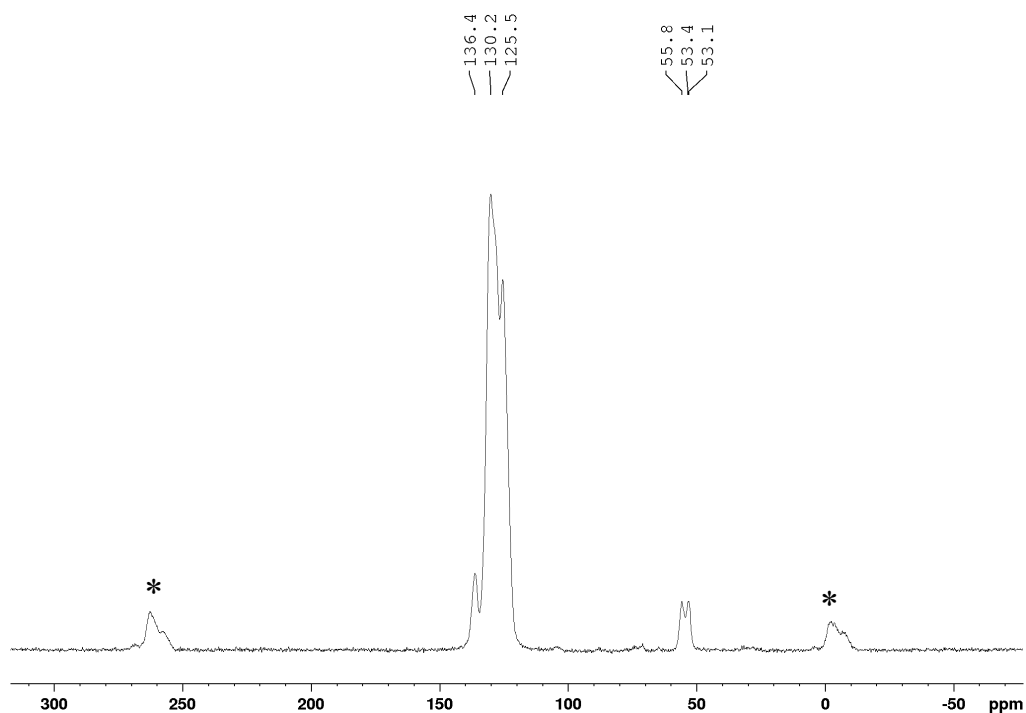


Figure S6. Solid state ^{13}C CP/MAS NMR spectrum of dimer mixture, 10 kHz rotation speed **after** heating the mixture for 30 minutes at 300 °C. The asterisks denote rotational sidebands.

3. Fit of the ESR Intensity Data

The intensity *Int* of the signal centered at ~3340 G was integrated at various temperatures (Table S1), and the intensities were fit to the Bleaney-Bowers equation using Origin 2020b (Table S2).

In the original paper by Bleaney and Bowers⁵ the equation has the following form (*C* is the Curie constant)

$$Int \propto \frac{C}{T} \times \frac{1}{\left(1 + \frac{1}{3} \exp \frac{E_{ST}}{kT}\right)} \quad (1)$$

The equation reflects the fact that there are three degenerate triplet states and one singlet state that can be populated depending on the size of the singlet-triplet energy gap E_{ST} and the temperature. Expanding equation (1) by an $3\exp(E_{ST}/kT)$ term gives equation (2)

$$Int \propto \frac{3C}{T} \times \frac{\exp \frac{E_{ST}}{kT}}{3\exp \frac{E_{ST}}{kT} + 1} \quad (2)$$

This is the form of the Bleaney-Bowers equation given by Abe.⁴ We have used this equation in our work. Note that Iwamura et al.⁶ give an equation that differs from the correct equation by minus signs in the exponents.

Table S1. Bleaney-Bowers equation and parameters A (ΔE_{ST} in J/mol) and C (a.u.) obtained from fit of data using Origin 2020b.

Bleaney-Bowers Equation		$Int \propto \frac{3C}{T} \times \frac{\exp \frac{\Delta E_{ST}}{RT}}{3\exp \frac{\Delta E_{ST}}{RT} + 1}$
ΔE_{ST}	$-20.2488 \pm 1.07935E-14$	
C	$346384.13092 \pm 9.97218E-12$	
r square (COD)	0.99879	

4. Computational Details

The structures and energies of 7,7',16,16'-tetrahydro-[7,7'-diheptacen]-16,16'-yl diradicals (7,7'-DHD) were computed using the M06-2X⁷ functional in conjunction with the def2-SVP⁸ basis set using Gaussian 16.⁹ The M06-2X functional was employed as it was constructed to take dispersion energy into account that is important for the description of acene dimers.¹⁰ Bendikov et al. employed this functional previously for the study of acene dimerization.^{11, 12} Geometries for the search for minima or transition states were obtained by a scan of the potential energy surface using the dihedral angle $C_{17}-C_{19}-C_{49}-C_{50}$ as scan parameter (see Figure S3). The structures close to minima and maxima of the scan were subsequently fully optimized and harmonic vibrational frequencies were computed analytically to confirm the nature of stationary points as minima or transition states.

The energy of the lowest energy singlet and triplet states of the 7,7'-diheptacenyl diradical (7,7'-DHD) was computed at the triplet geometry obtained at the M06-2X/def2-SVP level using state-

averaged strongly contracted N-electron valence state perturbation theory SC-NEVPT2¹³⁻¹⁵ with Orca 5.0.3.¹⁶⁻¹⁸ The active space was comprised of ten electrons and ten orbitals that were identified in a preceding Hartree-Fock calculation to be the highest occupied and lowest unoccupied orbitals. The def2-SVP basis set along with the recommended fitting basis sets for the utilized resolution of identity (RI) and chain of sphere exchange (COSX) approximations were used.^{8, 19, 20}

The direct dipolar electron spin-spin (SS) contribution to the zero-field splitting tensors of the triplet diradical rotamers were computed using the structures obtained at the M06-2X/def2-SVP level as described above employing the B3LYP^{21, 22} functional in conjunction with the def2-TZVP⁸ basis set. The computations used the spin-unrestricted formalism and unrestricted natural orbitals (UNO) as implemented in Orca 5.

5. Energies of conformers of 7,7',16,16'-tetrahydro-[7,7'-diheptacen]-16,16'-yl

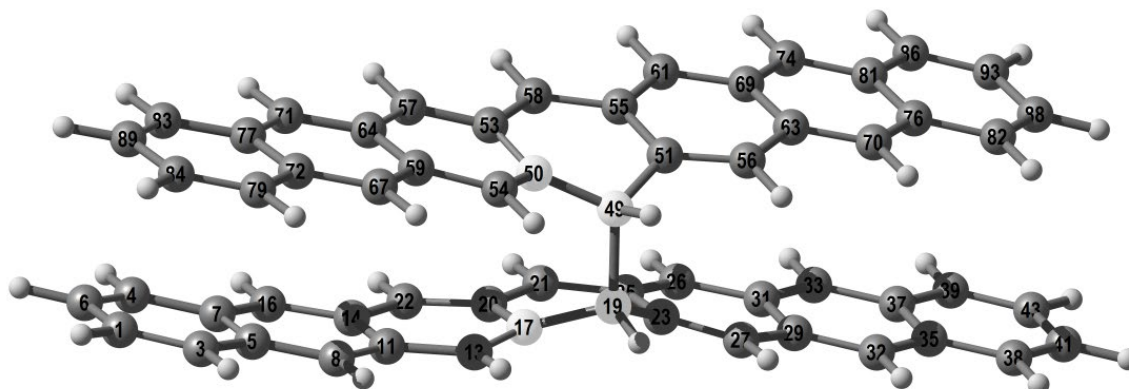


Figure S7. 7,7'-DHD and numbering of atoms used for the scan calculation. The torsional angle involving the bright carbon atoms C₁₇-C₁₉-C₄₉-C₅₀ as kept fix in the scan.

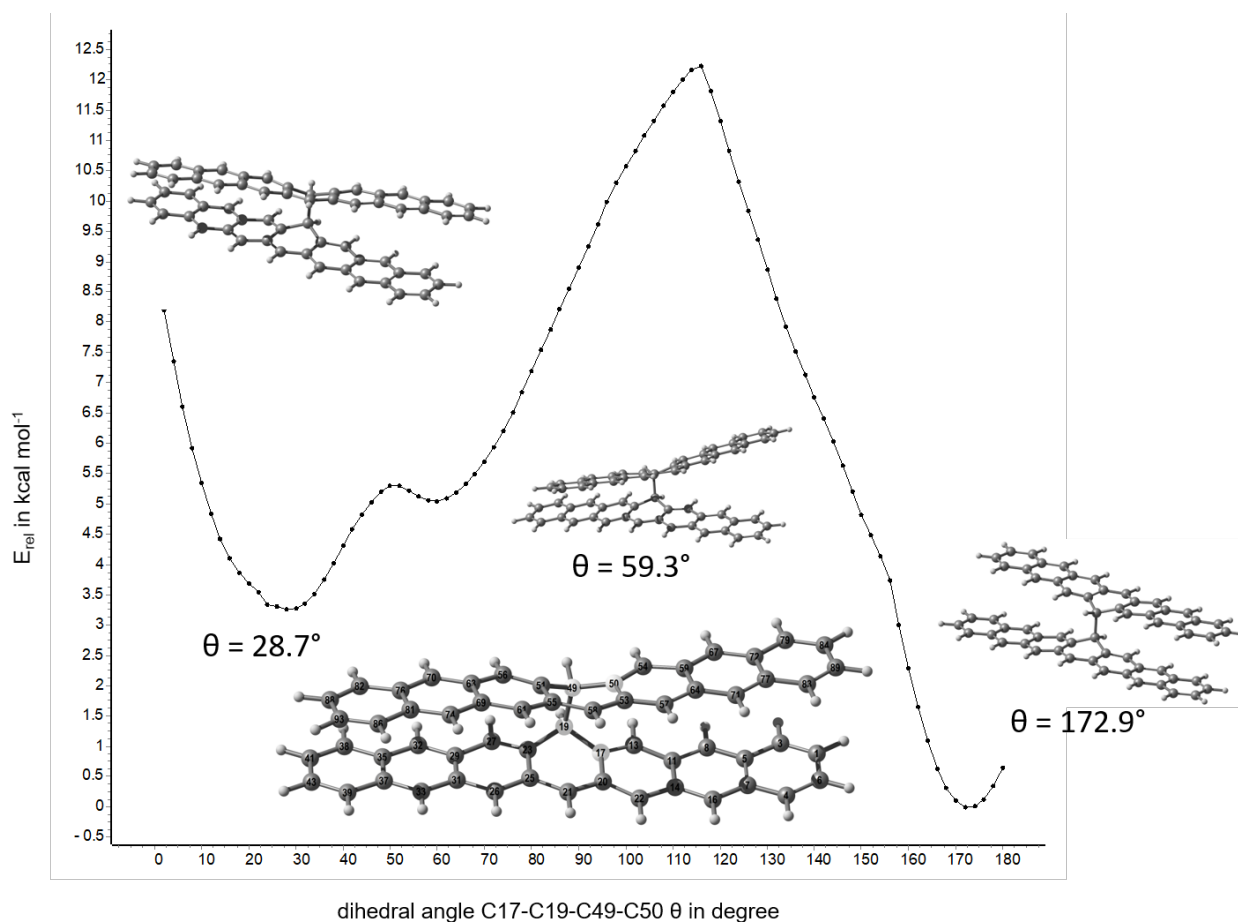


Figure S8. Potential energy diagram for torsion of the heptacenylyl wings of 7,7'-DHD. The torsional angle θ involving the bright carbon atoms C₁₇-C₁₉-C₄₉-C₅₀ was kept fix in the scan. Note that the torsional angles θ are those of the fully optimized structures.

Table S2. Absolute energies E, zero-point energy corrected energies E₀, enthalpies H and Gibbs free energies G at 298.15 K in Hartree and number of imaginary vibrational frequencies (Nimag) of 7,7'-**DHD** conformers as computed at the M06-2X/def2-SVP level of theory.

torsion angle θ C ₁₇ -C ₁₉ -C ₄₉ -C ₅₀ /°	spin state	Nimag ^a	E	E ₀	H	G _{298.15K}
172.9	³ A	0	-2305.53660	-2304.76732	-2304.72542	-2304.83956
115.7	³ A	1	-2305.51710	-2304.74783	-2304.70640	-2304.82119
59.3	³ A	0	-2305.52855	-2304.75901	-2304.71675	-2304.83478
50.9	³ A	1	-2305.52812	-2304.75873	-2304.71741	-2304.83182
28.7	³ A	0	-2305.53140	-2304.76194	-2304.72009	-2304.83440
9.7	³ A	1	-2305.52086	-2304.75209	-2304.71113	-2304.82188
173.1	¹ A	0	-2305.53669	-2304.76745	-2304.72554	-2304.83867
38.2	¹ A	0	-2305.53160	-2304.76208	-2304.72017	-2304.83465

^a Number of imaginary vibrational frequencies.

Table S3. Absolute energies in Hartree and singlet-triplet energy gaps ΔE_{ST} (in kcal mol⁻¹) of 7,7'-**DHD** conformers as computed at the state-averaged SC-NEVPT2/def2-SVP level of theory. The geometries obtained for the triplet states at the M06-2X/def2-SVP level of theory were used for the single point computations.

torsion angle θ C ₁₇ -C ₁₉ - C ₄₉ -C ₅₀ /°	E(triplet)	E(singlet)	ΔE_{ST} ^a
172.9	-2299.18491	-2299.18508	-0.1
28.7	-2299.18194	-2299.18181	0.1

^a A negative value corresponds to a singlet ground state.

6. Energies of conformers of 6,7',17,16'-tetrahydro-[6,7'-diheptacen]-17,16'-yl

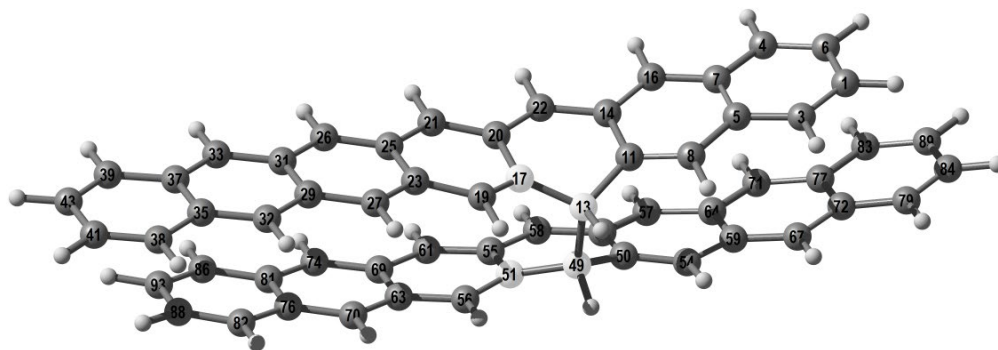


Figure S9. 6,7'-DHD and numbering of atoms used for the scan calculation. The torsional angle involving the bright carbon atoms C₁₇-C₁₃-C₄₉-C₅₁ as kept fix in the scan.

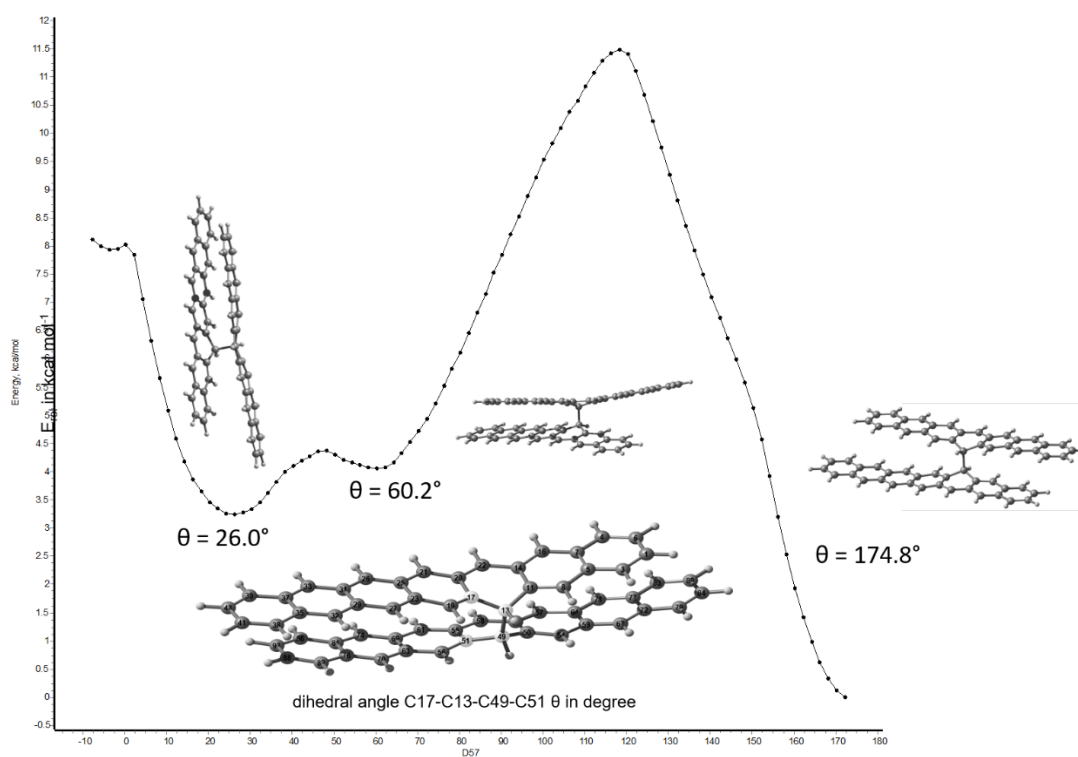


Figure S10. Potential energy diagram for torsion of the heptacenylyl wings of 6,7'-DHD. The torsional angle θ involving the bright carbon atoms C₁₇-C₁₉-C₄₉-C₅₀ was kept fix in the scan. Note that the torsional angles θ given are those of the fully optimized structures.

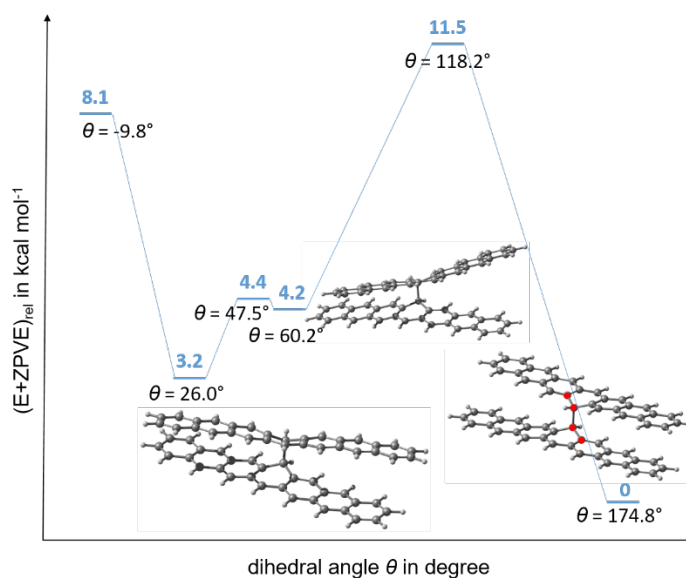


Figure S11. Zero-point vibrational energy (ZPVE) corrected potential energy diagram (E_0 in kcal mol⁻¹) for rotation of the two heptacenyl wings of the triplet state of 6,7'-DHD as computed at the M06-2X/def2-SVP level of theory. The dihedral angle θ involving the red atoms is given in degree.

Table S4. Absolute energies E , zero-point energy corrected energies E_0 , enthalpies H and Gibbs free energies G at 298.15 K in Hartree and number of imaginary vibrational frequencies (Nimag) of 6,7'-DHD conformers as computed at the M06-2X/def2-SVP level of theory.

torsion angle θ C ₁₇ -C ₁₃ -C ₄₉ -C ₅₁ /°	spin state	Nimag ^a	E	E_0	H	$G_{298.15K}$
174.8	³ A	0	-2305.53158	-2304.76234	-2304.72034	-2304.83606
118.2	³ A	1	-2305.51321	-2304.74409	-2304.70262	-2304.81765
60.2	³ A	0	-2305.52505	-2304.75563	-2304.71333	-2304.83165
47.5	³ A	1	-2305.52453	-2304.75527	-2304.71396	-2304.82788
26.0	³ A	0	-2305.52635	-2304.75719	-2304.71527	-2304.83019
-9.8	³ A	1	-2305.51807	-2304.74941	-2304.70848	-2304.81846
174.8	¹ A	0	-2305.53172	-2304.76251	-2304.72051	-2304.83517
43.9	¹ A	0	-2305.52721	-2304.75754	-2304.71551	-2304.83097

^a Number of imaginary vibrational frequencies.

Table S5. Absolute energies in Hartree and singlet-triplet energy gaps ΔE_{ST} (in kcal mol⁻¹) of 6,7'-**DHD** conformers as computed at the state-averaged SC-NEVPT2/def2-SVP level of theory. The geometries obtained for the triplet states at the M06-2X/def2-SVP level of theory were used for the single point computations.

torsion angle θ C ₁₇ -C ₁₃ - C ₄₉ -C ₅₁ /°	E(triplet)	E(singlet)	ΔE_{ST}^a
174.8	-2299.17419	-2299.17424	-0.03
26.0	-2299.1711	-2299.1704	0.5

^a A negative value corresponds to a singlet ground state.

7. Cartesian coordinates

All coordinates were optimized at the M06-2X/def2SVP level of theory and are given in Å, energies are given in Hartree.

7.1 Coordinates associated with the 7,7' isomer

Coordinates of the triplet 7,7'-DHD, torsion 172.9°

C	-8.470573000	-1.040091000	1.372187000
H	-7.128301000	0.252303000	2.429686000
C	-7.232640000	-0.587537000	1.739455000
C	-7.487880000	-2.728687000	-0.064483000
C	-6.048667000	-1.193683000	1.220441000
C	-8.599359000	-2.128145000	0.460003000
C	-6.175967000	-2.282373000	0.292144000
C	-4.765728000	-0.743193000	1.574392000
H	-5.116929000	-3.697112000	-0.946851000
H	-7.583036000	-3.560873000	-0.765336000
C	-3.619437000	-1.318196000	1.035837000
H	-4.668231000	0.100313000	2.262960000
C	-2.313099000	-0.781240000	1.294173000
C	-3.739872000	-2.407569000	0.099602000
H	-2.637486000	-3.827098000	-1.122890000
C	-5.018094000	-2.868476000	-0.240930000
C	-1.202625000	-1.262901000	0.674622000
H	-2.239573000	0.112264000	1.921618000
C	0.082761000	-0.492319000	0.652918000
C	-1.294636000	-2.432851000	-0.182261000
C	-0.096053000	-3.006008000	-0.688326000
C	-2.552958000	-2.962854000	-0.459408000
C	1.290535000	-1.374097000	0.558437000
H	0.149016000	0.171728000	1.527627000
C	1.191228000	-2.557828000	-0.281137000
C	2.358405000	-3.227431000	-0.638980000
C	2.495946000	-0.995414000	1.062565000
H	2.567312000	-0.096645000	1.681901000
C	3.713824000	-1.669888000	0.708031000
H	2.296148000	-4.108606000	-1.282118000
C	3.639755000	-2.795314000	-0.189709000
C	4.955411000	-1.203481000	1.126560000
C	4.827746000	-3.409731000	-0.604168000
H	5.006222000	-0.328587000	1.780542000
C	6.149854000	-1.803971000	0.691768000
H	4.778833000	-4.267032000	-1.280157000
C	6.082098000	-2.936518000	-0.189284000
C	7.430518000	-1.308910000	1.084071000
C	7.304647000	-3.535894000	-0.628472000
H	7.473770000	-0.433298000	1.735731000
C	8.578840000	-1.906756000	0.639265000
H	7.252451000	-4.399639000	-1.294523000
C	8.513918000	-3.037487000	-0.226577000
H	9.438354000	-3.504221000	-0.570072000
H	9.551337000	-1.515903000	0.942273000
H	-9.367339000	-0.563101000	1.770654000
H	-9.593905000	-2.478617000	0.179384000
H	-0.165349000	-3.879845000	-1.340022000
C	0.082759000	0.492248000	-0.652803000
C	1.290532000	1.374025000	-0.558330000
C	-1.202629000	1.262828000	-0.674516000
H	0.149017000	-0.171789000	-1.527522000
C	1.191223000	2.557800000	0.281174000
C	2.495946000	0.995312000	-1.062433000
C	-1.294642000	2.432795000	0.182350000

C	-2.313095000	0.781177000	-1.294083000
C	2.358388000	3.227470000	0.638925000
C	-0.096060000	3.005978000	0.688377000
C	3.713814000	1.669822000	-0.707954000
H	2.567315000	0.096514000	-1.681730000
C	-2.552965000	2.962814000	0.459468000
H	-2.239571000	-0.112324000	-1.921534000
C	-3.619435000	1.318151000	-1.035781000
C	3.639736000	2.795344000	0.189665000
H	2.296120000	4.108703000	1.281984000
H	-0.165351000	3.879858000	1.340017000
C	4.955405000	1.203382000	-1.126444000
H	-2.637494000	3.827083000	1.122918000
C	-3.739876000	2.407536000	-0.099556000
C	-4.765719000	0.743168000	-1.574367000
C	4.827722000	3.409843000	0.604021000
C	6.149838000	1.803939000	-0.691732000
H	5.006219000	0.328414000	-1.780328000
C	-5.018097000	2.868474000	0.240930000
H	-4.668221000	-0.100347000	-2.262927000
C	-6.048662000	1.193690000	-1.220461000
C	6.082073000	2.936605000	0.189170000
H	4.778805000	4.267226000	1.279906000
C	7.430508000	1.308837000	-1.083973000
H	-5.116939000	3.697126000	0.946831000
C	-6.175967000	2.282396000	-0.292184000
C	-7.232631000	0.587559000	-1.739499000
C	7.304619000	3.536068000	0.628253000
C	8.578823000	1.906762000	-0.639259000
H	7.473766000	0.433126000	-1.735501000
C	-7.487880000	2.728749000	0.064388000
H	-7.128290000	-0.252288000	-2.429720000
C	-8.470568000	1.040149000	-1.372280000
C	8.513891000	3.037624000	0.226415000
H	7.252416000	4.399909000	1.294180000
H	9.551324000	1.515875000	-0.942211000
H	-7.583042000	3.560945000	0.765228000
C	-8.599358000	2.128231000	-0.460135000
H	-9.367331000	0.563176000	-1.770774000
H	9.438324000	3.504424000	0.569827000
H	-9.593905000	2.478730000	-0.179551000

Coordinates of the triplet 7,7'-DHD, torsion 115.7°, Nimag=1

C	-6.815684000	-3.334427000	-2.935918000
H	-4.849580000	-4.146170000	-3.187497000
C	-5.448058000	-3.275419000	-2.911487000
C	-6.981531000	-1.029979000	-2.202403000
C	-4.772382000	-2.078380000	-2.524800000
C	-7.593365000	-2.195990000	-2.573998000
C	-5.555350000	-0.929054000	-2.166921000
C	-3.368176000	-1.995730000	-2.469715000
H	-5.497443000	1.126336000	-1.506606000
H	-7.571640000	-0.153743000	-1.925474000
C	-2.723548000	-0.831512000	-2.067501000
H	-2.773250000	-2.876500000	-2.725213000
C	-1.299046000	-0.780596000	-1.868437000
C	-3.507970000	0.327766000	-1.722628000
H	-3.421283000	2.404249000	-1.088432000
C	-4.902773000	0.252668000	-1.785275000
C	-0.692199000	0.312668000	-1.335214000
H	-0.720477000	-1.692128000	-2.042875000
C	0.707570000	0.248871000	-0.777382000
C	-1.456560000	1.530812000	-1.117506000
C	-0.771972000	2.711345000	-0.729323000
C	-2.834191000	1.506720000	-1.297886000
C	1.428137000	1.571577000	-0.846644000
H	1.282620000	-0.502077000	-1.335276000

C	0.646978000	2.787125000	-0.675544000
C	1.312316000	4.000054000	-0.532048000
C	2.783119000	1.643576000	-0.952037000
H	3.365151000	0.729852000	-1.101856000
C	3.490748000	2.891880000	-0.844515000
H	0.732390000	4.916255000	-0.397389000
C	2.730674000	4.092852000	-0.604080000
C	4.875925000	2.968743000	-0.944777000
C	3.406866000	5.311304000	-0.473426000
H	5.450835000	2.057555000	-1.128387000
C	5.557317000	4.191809000	-0.813777000
H	2.832885000	6.223706000	-0.293962000
C	4.803336000	5.389773000	-0.571449000
C	6.979189000	4.282751000	-0.913826000
C	5.506125000	6.628839000	-0.439578000
H	7.548332000	3.369462000	-1.099065000
C	7.616806000	5.486378000	-0.781626000
H	4.929569000	7.537747000	-0.255899000
C	6.869106000	6.676308000	-0.540888000
H	7.392890000	7.627734000	-0.438179000
H	8.703427000	5.541810000	-0.860445000
H	-7.318490000	-4.255810000	-3.233251000
H	-8.682196000	-2.260125000	-2.597343000
H	-1.352019000	3.622751000	-0.566978000
C	0.707569000	-0.248871000	0.777381000
C	1.428135000	-1.571577000	0.846643000
C	-0.692200000	-0.312667000	1.335211000
H	1.282620000	0.502077000	1.335276000
C	0.646976000	-2.787125000	0.675543000
C	2.783118000	-1.643577000	0.952036000
C	-1.456562000	-1.530811000	1.117504000
C	-1.299047000	0.780597000	1.868435000
C	1.312313000	-4.000055000	0.532049000
C	-0.771974000	-2.711344000	0.729321000
C	3.490746000	-2.891881000	0.844514000
H	3.365150000	-0.729852000	1.101855000
C	-2.834193000	-1.506718000	1.297883000
H	-0.720477000	1.692128000	2.042873000
C	-2.723549000	0.831513000	2.067498000
C	2.730671000	-4.092853000	0.604081000
H	0.732387000	-4.916255000	0.397390000
H	-1.352021000	-3.622750000	0.566976000
C	4.875923000	-2.968744000	0.944777000
H	-3.421285000	-2.404247000	1.088430000
C	-3.507972000	-0.327764000	1.722626000
C	-3.368176000	1.995731000	2.469713000
C	3.406863000	-5.311305000	0.473428000
C	5.557314000	-4.191811000	0.813778000
H	5.450833000	-2.057556000	1.128386000
C	-4.902774000	-0.252666000	1.785274000
H	-2.773251000	2.876501000	2.725211000
C	-4.772382000	2.078381000	2.524800000
C	4.803334000	-5.389774000	0.571452000
H	2.832882000	-6.223707000	0.293965000
C	6.979187000	-4.282753000	0.913827000
H	-5.497444000	-1.126334000	1.506607000
C	-5.555350000	0.929056000	2.166922000
C	-5.448058000	3.275420000	2.911487000
C	5.506122000	-6.628841000	0.439581000
C	7.616803000	-5.486381000	0.781628000
H	7.548330000	-3.369463000	1.099064000
C	-6.981531000	1.029980000	2.202405000
H	-4.849580000	4.146171000	3.187496000
C	-6.815685000	3.334428000	2.935920000
C	6.869103000	-6.676310000	0.540891000
H	4.929566000	-7.537749000	0.255903000
H	8.703424000	-5.541813000	0.860446000
H	-7.571641000	0.153744000	1.925478000
C	-7.593365000	2.195990000	2.574001000
H	-7.318490000	4.255810000	3.233254000
H	7.392887000	-7.627736000	0.438183000

H	-8.682196000	2.260125000	2.597348000
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Coordinates of the triplet 7,7'-DHD, torsion 59.3°

C	-7.013883000	-3.551662000	2.450032000
H	-6.858433000	-1.445684000	2.086965000
C	-6.326960000	-2.390338000	2.220129000
C	-4.947295000	-4.814588000	2.564447000
C	-4.900441000	-2.384141000	2.150912000
C	-6.313298000	-4.781085000	2.625095000
C	-4.193592000	-3.622500000	2.324629000
C	-4.169674000	-1.205352000	1.917401000
H	-2.256459000	-4.572167000	2.377849000
H	-4.407330000	-5.754305000	2.697819000
C	-2.780626000	-1.214552000	1.845662000
H	-4.705747000	-0.262777000	1.778025000
C	-2.030389000	-0.024753000	1.551480000
C	-2.067861000	-2.456659000	2.005032000
H	-0.098259000	-3.371073000	2.084650000
C	-2.793120000	-3.628936000	2.249025000
C	-0.680378000	-0.047570000	1.382853000
H	-2.586042000	0.901499000	1.381130000
C	0.055472000	1.134729000	0.801453000
C	0.056051000	-1.277552000	1.628132000
C	1.474252000	-1.250821000	1.614616000
C	-0.647996000	-2.442309000	1.915136000
C	1.510292000	1.196151000	1.199335000
H	-0.447499000	2.062483000	1.112280000
C	2.212627000	-0.044109000	1.486284000
C	3.594611000	-0.020248000	1.630480000
C	2.200409000	2.369167000	1.158042000
H	1.672506000	3.303466000	0.944081000
C	3.626201000	2.425203000	1.336900000
H	4.128667000	-0.955197000	1.815326000
C	4.337456000	1.190038000	1.551903000
C	4.335866000	3.621258000	1.277027000
C	5.731047000	1.221725000	1.685965000
H	3.795476000	4.557330000	1.115019000
C	5.734077000	3.655329000	1.415225000
H	6.271969000	0.286080000	1.847876000
C	6.446631000	2.425133000	1.621849000
C	6.473335000	4.876407000	1.353961000
C	7.870371000	2.471049000	1.758327000
H	5.927318000	5.808992000	1.197356000
C	7.834874000	4.880494000	1.488804000
H	8.408686000	1.534272000	1.916308000
C	8.543214000	3.659612000	1.693809000
H	9.628784000	3.680494000	1.799877000
H	8.387127000	5.820004000	1.440321000
H	-8.103531000	-3.542444000	2.502041000
H	-6.875592000	-5.697792000	2.808620000
H	2.019312000	-2.180525000	1.790421000
C	-0.055491000	1.134797000	-0.801369000
C	-1.510308000	1.196247000	-1.199274000
C	0.680370000	-0.047450000	-1.382832000
H	0.447495000	2.062583000	-1.112118000
C	-2.212629000	-0.043992000	-1.486372000
C	-2.200431000	2.369255000	-1.157911000
C	-0.056051000	-1.277415000	-1.628246000
C	2.030391000	-0.024629000	-1.551359000
C	-3.594608000	-0.020130000	-1.630618000
C	-1.474249000	-1.250688000	-1.614784000
C	-3.626216000	2.425295000	-1.336813000
H	-1.672537000	3.303538000	-0.943858000
C	0.648001000	-2.442151000	-1.915324000
H	2.586038000	0.901602000	-1.380877000
C	2.780632000	-1.214409000	-1.845609000
C	-4.337458000	1.190145000	-1.551952000

H	-4.128657000	-0.955065000	-1.815561000
H	-2.019301000	-2.180379000	-1.790679000
C	-4.335892000	3.621339000	-1.276860000
H	0.098270000	-3.370898000	-2.084951000
C	2.067869000	-2.456495000	-2.005145000
C	4.169686000	-1.205213000	-1.917268000
C	-5.731046000	1.221838000	-1.686057000
C	-5.734097000	3.655416000	-1.415103000
H	-3.795513000	4.557400000	-1.114751000
C	2.793137000	-3.628752000	-2.249215000
H	4.705756000	-0.262654000	-1.777773000
C	4.900459000	-2.383981000	-2.150859000
C	-6.446638000	2.425235000	-1.621859000
H	-6.271957000	0.286204000	-1.848069000
C	-6.473365000	4.876486000	-1.353756000
H	2.256476000	-4.571965000	-2.378166000
C	4.193612000	-3.622318000	-2.324740000
C	6.326983000	-2.390180000	-2.220000000
C	-7.870375000	2.471155000	-1.758381000
C	-7.834898000	4.880577000	-1.488645000
H	-5.927358000	5.809059000	-1.197050000
C	4.947321000	-4.814387000	-2.564637000
H	6.858453000	-1.445541000	-2.086712000
C	7.013911000	-3.551483000	-2.449983000
C	-8.543226000	3.659709000	-1.693782000
H	-8.408679000	1.534389000	-1.916464000
H	-8.387158000	5.820080000	-1.440100000
H	4.407357000	-5.754087000	-2.698136000
C	6.313327000	-4.780886000	-2.625207000
H	8.103561000	-3.542268000	-2.501931000
H	-9.628792000	3.680595000	-1.799887000
H	6.875626000	-5.697578000	-2.808794000

Coordinates of the triplet 7,7'-DHD, torsion 50.9°, Nimag = 1

C	7.455686000	-2.922679000	-2.105709000
H	7.115257000	-0.837087000	-1.745326000
C	6.668657000	-1.818781000	-1.918137000
C	5.503081000	-4.338772000	-2.358310000
C	5.244169000	-1.922491000	-1.943553000
C	6.863591000	-4.200207000	-2.331143000
C	4.645884000	-3.210077000	-2.162610000
C	4.412778000	-0.804539000	-1.756525000
H	2.794572000	-4.306903000	-2.327729000
H	5.046916000	-5.316181000	-2.528758000
C	3.026769000	-0.922698000	-1.762608000
H	4.865377000	0.175491000	-1.582000000
C	2.175453000	0.202720000	-1.497561000
C	2.421171000	-2.214903000	-1.958721000
H	0.532026000	-3.277381000	-2.126739000
C	3.247785000	-3.325341000	-2.168136000
C	0.826653000	0.072219000	-1.372329000
H	2.652035000	1.167469000	-1.305088000
C	-0.017106000	1.188088000	-0.808279000
C	0.199181000	-1.208859000	-1.650557000
C	-1.218611000	-1.290754000	-1.669909000
C	1.000858000	-2.310778000	-1.928017000
C	-1.453852000	1.147122000	-1.263236000
H	0.433603000	2.152391000	-1.086117000
C	-2.051025000	-0.148093000	-1.551299000
C	-3.430968000	-0.237501000	-1.696203000
C	-2.234053000	2.261726000	-1.239234000
H	-1.785012000	3.235728000	-1.022233000
C	-3.662026000	2.197848000	-1.405868000
H	-3.888411000	-1.213838000	-1.872483000
C	-4.270554000	0.906108000	-1.605236000
C	-4.470353000	3.327741000	-1.324477000

C	-5.664772000	0.816088000	-1.697500000
H	-4.009065000	4.306989000	-1.173293000
C	-5.870594000	3.240305000	-1.419494000
H	-6.126742000	-0.164040000	-1.840040000
C	-6.480139000	1.952856000	-1.605654000
C	-6.710670000	4.392066000	-1.329332000
C	-7.906295000	1.874139000	-1.691758000
H	-6.243004000	5.368749000	-1.188730000
C	-8.071527000	4.277396000	-1.416631000
H	-8.365768000	0.893809000	-1.834022000
C	-8.677592000	2.999700000	-1.599985000
H	-9.763903000	2.925926000	-1.667924000
H	-8.701349000	5.165316000	-1.346413000
H	8.542556000	-2.830633000	-2.085539000
H	7.504986000	-5.069819000	-2.481646000
H	-1.686378000	-2.259296000	-1.858421000
C	0.017112000	1.188113000	0.808239000
C	1.453858000	1.147160000	1.263199000
C	-0.826649000	0.072264000	1.372323000
H	-0.433595000	2.152427000	1.086046000
C	2.051027000	-0.148045000	1.551310000
C	2.234059000	2.261763000	1.239163000
C	-0.199180000	-1.208807000	1.650588000
C	-2.175450000	0.202773000	1.497551000
C	3.430969000	-0.237448000	1.696231000
C	1.218612000	-1.290702000	1.669949000
C	3.662030000	2.197891000	1.405815000
H	1.785020000	3.235758000	1.022126000
C	-1.000861000	-2.310717000	1.928074000
H	-2.652028000	1.167517000	1.305051000
C	-3.026768000	-0.922638000	1.762620000
C	4.270556000	0.906157000	1.605237000
H	3.888410000	-1.213780000	1.872550000
H	1.686377000	-2.259240000	1.858492000
C	4.470358000	3.327780000	1.324395000
H	-0.532031000	-3.277316000	2.126823000
C	-2.421174000	-2.214839000	1.958767000
C	-4.412777000	-0.804476000	1.756522000
C	5.664772000	0.816142000	1.697530000
C	5.870598000	3.240350000	1.419437000
H	4.009071000	4.307023000	1.173168000
C	-3.247792000	-3.325271000	2.168199000
H	-4.865373000	0.175550000	1.581973000
C	-5.244172000	-1.922423000	1.943565000
C	6.480140000	1.952907000	1.605655000
H	6.126741000	-0.163979000	1.840116000
C	6.710675000	4.392107000	1.329245000
H	-2.794582000	-4.306831000	2.327818000
C	-4.645890000	-3.210005000	2.162656000
C	-6.668659000	-1.818712000	1.918130000
C	7.906295000	1.874194000	1.691786000
C	8.071530000	4.277441000	1.416572000
H	6.243010000	5.368784000	1.188599000
C	-5.503091000	-4.338695000	2.358371000
H	-7.115256000	-0.837021000	1.745293000
C	-7.455692000	-2.922605000	2.105716000
C	8.677592000	2.999752000	1.599984000
H	8.365766000	0.893869000	1.834094000
H	8.701353000	5.165359000	1.346330000
H	-5.046930000	-5.316101000	2.528845000
C	-6.863600000	-4.200128000	2.331185000
H	-8.542561000	-2.830558000	2.085532000
H	9.763903000	2.925981000	1.667943000
H	-7.504998000	-5.069736000	2.481700000

Coordinates of the triplet 7,7'-DHD, torsion 28.7°

C	-8.191003000	-1.249827000	1.679998000
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H	-7.420848000	0.741625000	1.489873000
C	-7.189844000	-0.317768000	1.626390000
C	-6.579342000	-3.046043000	1.926837000
C	-5.820346000	-0.709885000	1.722151000
C	-7.880552000	-2.632622000	1.837457000
C	-5.504300000	-2.103925000	1.864289000
C	-4.773829000	0.225311000	1.650467000
H	-3.921246000	-3.562609000	2.023076000
H	-6.338793000	-4.104932000	2.042754000
C	-3.442004000	-0.173497000	1.685224000
H	-5.014565000	1.283992000	1.516932000
C	-2.370087000	0.761006000	1.485216000
C	-3.117395000	-1.571754000	1.815789000
H	-1.491110000	-3.004410000	1.980038000
C	-4.159640000	-2.501171000	1.918154000
C	-1.075396000	0.359881000	1.366180000
H	-2.632904000	1.810352000	1.332506000
C	-0.016523000	1.284012000	0.826982000
C	-0.728198000	-1.029490000	1.605983000
C	0.644464000	-1.389812000	1.642785000
C	-1.746161000	-1.954381000	1.817679000
C	1.360491000	0.969867000	1.344279000
H	-0.288891000	2.318077000	1.081420000
C	1.688550000	-0.430010000	1.576192000
C	3.021735000	-0.794268000	1.727168000
C	2.340686000	1.911268000	1.393468000
H	2.094885000	2.961946000	1.211041000
C	3.728332000	1.557609000	1.541592000
H	3.277263000	-1.847307000	1.866718000
C	4.070721000	0.164629000	1.683314000
C	4.744935000	2.503137000	1.450391000
C	5.418669000	-0.205925000	1.733615000
H	4.486986000	3.558944000	1.333064000
C	6.101830000	2.130877000	1.478602000
H	5.679118000	-1.263392000	1.825496000
C	6.444032000	0.744623000	1.628935000
C	7.154551000	3.087602000	1.347285000
C	7.825407000	0.374289000	1.644930000
H	6.891257000	4.141315000	1.233581000
C	8.466185000	2.695276000	1.363575000
H	8.078622000	-0.682732000	1.749282000
C	8.806370000	1.318881000	1.515721000
H	9.856534000	1.023279000	1.526626000
H	9.259951000	3.436857000	1.262207000
H	-9.233125000	-0.937334000	1.596758000
H	-8.690111000	-3.362685000	1.883909000
H	0.909700000	-2.437917000	1.797661000
C	0.016535000	1.284299000	-0.826479000
C	-1.360505000	0.970360000	-1.343824000
C	1.075415000	0.360390000	-1.366085000
H	0.288862000	2.318447000	-1.080544000
C	-1.688554000	-0.429426000	-1.576270000
C	-2.340714000	1.911777000	-1.392603000
C	0.728216000	-1.028884000	-1.606402000
C	2.370095000	0.761578000	-1.485083000
C	-3.021741000	-0.793625000	-1.727365000
C	-0.644454000	-1.389197000	-1.643281000
C	-3.728358000	1.558176000	-1.540895000
H	-2.094914000	2.962388000	-1.209793000
C	1.746186000	-1.953683000	-1.818474000
H	2.632907000	1.810871000	-1.332011000
C	3.442024000	-0.172839000	-1.685436000
C	-4.070738000	0.165248000	-1.683158000
H	-3.277255000	-1.846607000	-1.867368000
H	-0.909691000	-2.437243000	-1.798551000
C	-4.744963000	2.503673000	-1.449409000
H	1.491138000	-3.003658000	-1.981178000
C	3.117422000	-1.571054000	-1.816461000
C	4.773846000	0.225960000	-1.650495000
C	-5.418683000	-0.205286000	-1.733698000
C	-6.101858000	2.131428000	-1.477886000

H	-4.487019000	3.559438000	-1.331689000
C	4.159670000	-2.500437000	-1.919094000
H	5.014573000	1.284594000	-1.516572000
C	5.820367000	-0.709218000	-1.722386000
C	-6.444051000	0.745230000	-1.628773000
H	-5.679132000	-1.262715000	-1.826023000
C	-7.154587000	3.088106000	-1.346307000
H	3.921282000	-3.561843000	-2.024349000
C	5.504328000	-2.103211000	-1.865000000
C	7.189855000	-0.317142000	-1.626326000
C	-7.825426000	0.374909000	-1.645052000
C	-8.466222000	2.695792000	-1.362887000
H	-6.891301000	4.141775000	-1.232180000
C	6.579372000	-3.045314000	-1.927740000
H	7.420847000	0.742202000	-1.489410000
C	8.191017000	-1.249190000	-1.680117000
C	-8.806398000	1.319458000	-1.515601000
H	-8.078634000	-0.682073000	-1.749821000
H	-9.259993000	3.437339000	-1.261320000
H	6.338831000	-4.104165000	-2.044021000
C	7.880574000	-2.631929000	-1.838075000
H	9.233130000	-0.936732000	-1.596648000
H	-9.856562000	1.023865000	-1.526731000
H	8.690135000	-3.361982000	-1.884667000

Coordinates of the triplet 7,7'-DHD, torsion 9.7°, Nimag = 1

C	8.318275000	-2.253494000	0.156382000
H	7.139192000	-3.051940000	-1.444302000
C	7.140242000	-2.548533000	-0.475024000
C	7.131405000	-1.242186000	2.011928000
C	5.888509000	-2.189751000	0.108119000
C	8.313702000	-1.581721000	1.412530000
C	5.880940000	-1.538290000	1.386551000
C	4.666244000	-2.413653000	-0.550532000
H	4.648935000	-0.721831000	2.959939000
H	7.123594000	-0.729657000	2.976204000
C	3.458434000	-2.011211000	0.004070000
H	4.674284000	-2.868430000	-1.544675000
C	2.235634000	-2.022058000	-0.753266000
C	3.439345000	-1.420028000	1.319226000
H	2.156135000	-0.699541000	2.922449000
C	4.653040000	-1.198178000	1.976284000
C	1.088003000	-1.504889000	-0.247680000
H	2.280922000	-2.329826000	-1.801761000
C	-0.060245000	-1.084428000	-1.108918000
C	1.006817000	-1.120816000	1.152967000
C	-0.275578000	-0.842223000	1.697393000
C	2.183836000	-1.053884000	1.889108000
C	-1.371964000	-1.400166000	-0.451028000
H	-0.000506000	-1.589791000	-2.081856000
C	-1.473326000	-1.075703000	0.964347000
C	-2.732029000	-1.023217000	1.548797000
C	-2.468776000	-1.821886000	-1.134809000
H	-2.385567000	-2.076131000	-2.195541000
C	-3.777145000	-1.833748000	-0.533843000
H	-2.827582000	-0.728018000	2.596562000
C	-3.909612000	-1.364022000	0.823097000
C	-4.917183000	-2.192391000	-1.245405000
C	-5.185422000	-1.262347000	1.386648000
H	-4.816905000	-2.545320000	-2.275362000
C	-6.201868000	-2.095465000	-0.678714000
H	-5.289128000	-0.895033000	2.410733000
C	-6.337010000	-1.616099000	0.667675000
C	-7.380853000	-2.449833000	-1.401798000
C	-7.644831000	-1.517443000	1.235573000
H	-7.275370000	-2.813833000	-2.426229000
C	-8.618272000	-2.343799000	-0.824118000

H	-7.741669000	-1.145377000	2.257631000
C	-8.751453000	-1.873920000	0.514130000
H	-9.744462000	-1.793904000	0.959293000
H	-9.510219000	-2.623089000	-1.387178000
H	9.269654000	-2.521442000	-0.305776000
H	9.261426000	-1.338443000	1.895142000
H	-0.350646000	-0.538951000	2.744136000
C	0.066760000	0.555736000	-1.458956000
C	1.393989000	1.150978000	-1.035777000
C	-1.120820000	1.326540000	-0.937526000
H	0.023681000	0.562428000	-2.556676000
C	1.466875000	1.979284000	0.160733000
C	2.548481000	0.845557000	-1.692411000
C	-1.009132000	2.092030000	0.293604000
C	-2.343174000	1.189752000	-1.520661000
C	2.709489000	2.371264000	0.648206000
C	0.275456000	2.386575000	0.809010000
C	3.847195000	1.218954000	-1.197018000
H	2.509402000	0.232467000	-2.597372000
C	-2.166110000	2.535811000	0.928646000
H	-2.436343000	0.645581000	-2.463924000
C	-3.554197000	1.604442000	-0.870317000
C	3.922774000	1.985995000	0.019722000
H	2.755661000	2.985400000	1.550667000
H	0.352350000	2.985240000	1.719161000
C	5.024745000	0.813783000	-1.818183000
H	-2.080234000	3.091690000	1.865434000
C	-3.459087000	2.249423000	0.413689000
C	-4.805654000	1.293709000	-1.391788000
C	5.177400000	2.314172000	0.546272000
C	6.287261000	1.130622000	-1.285083000
H	4.970649000	0.220011000	-2.734681000
C	-4.635566000	2.538426000	1.117171000
H	-4.873945000	0.792016000	-2.360488000
C	-5.984759000	1.555576000	-0.675434000
C	6.363479000	1.899943000	-0.074661000
H	5.232747000	2.898742000	1.467994000
C	7.501599000	0.710167000	-1.907813000
H	-4.568536000	3.024473000	2.093829000
C	-5.894859000	2.186651000	0.612052000
C	-7.269865000	1.184871000	-1.176314000
C	7.652503000	2.218680000	0.457359000
C	8.717286000	1.035729000	-1.370514000
H	7.439336000	0.118099000	-2.823533000
C	-7.102256000	2.416994000	1.345719000
H	-7.328868000	0.694183000	-2.150202000
C	-8.400987000	1.419010000	-0.443979000
C	8.793343000	1.801097000	-0.170370000
H	7.705512000	2.804229000	1.377631000
H	9.636681000	0.706198000	-1.856931000
H	-7.034047000	2.897430000	2.324145000
C	-8.315065000	2.043831000	0.835489000
H	-9.375283000	1.117113000	-0.831135000
H	9.770365000	2.051708000	0.245775000
H	-9.227004000	2.222220000	1.407563000

Coordinates of the singlet 7,7'-DHD, torsion 173.1°

C	-8.472787000	-1.050189000	1.361935000
H	-7.133059000	0.243471000	2.421105000
C	-7.235765000	-0.596416000	1.730680000
C	-7.486755000	-2.737660000	-0.073855000
C	-6.050608000	-1.201187000	1.212730000
C	-8.599400000	-2.138298000	0.449430000
C	-6.175629000	-2.290104000	0.284331000
C	-4.768572000	-0.749297000	1.568068000
H	-5.113700000	-3.704244000	-0.952824000
H	-7.580299000	-3.569916000	-0.774836000

C	-3.621103000	-1.323010000	1.030715000
H	-4.672786000	0.094597000	2.256422000
C	-2.315731000	-0.784253000	1.290091000
C	-3.739198000	-2.412911000	0.094811000
H	-2.633561000	-3.831624000	-1.125716000
C	-5.016554000	-2.875305000	-0.247037000
C	-1.203807000	-1.265036000	0.672456000
H	-2.244116000	0.109763000	1.917047000
C	0.080659000	-0.493051000	0.652618000
C	-1.293579000	-2.435413000	-0.184084000
C	-0.093666000	-3.007189000	-0.688829000
C	-2.550877000	-2.967055000	-0.462435000
C	1.289459000	-1.373315000	0.558827000
H	0.145298000	0.170669000	1.527693000
C	1.192413000	-2.557162000	-0.280590000
C	2.361076000	-3.225094000	-0.637769000
C	2.494225000	-0.992619000	1.063344000
H	2.563907000	-0.093641000	1.682576000
C	3.713236000	-1.665470000	0.709945000
H	2.300480000	-4.106277000	-1.281048000
C	3.641364000	-2.791164000	-0.187717000
C	4.953834000	-1.197339000	1.129419000
C	4.830627000	-3.403976000	-0.601198000
H	5.002942000	-0.322330000	1.783377000
C	6.149518000	-1.796542000	0.696025000
H	4.783439000	-4.261373000	-1.277181000
C	6.084005000	-2.929159000	-0.185116000
C	7.429084000	-1.300083000	1.089806000
C	7.307705000	-3.527047000	-0.623018000
H	7.470614000	-0.424323000	1.741397000
C	8.578650000	-1.896734000	0.646443000
H	7.257257000	-4.390806000	-1.289183000
C	8.515992000	-3.027363000	-0.219587000
H	9.441332000	-3.493078000	-0.562028000
H	9.550336000	-1.504771000	0.950601000
H	-9.370505000	-0.574220000	1.759484000
H	-9.593266000	-2.489784000	0.167674000
H	-0.161189000	-3.881202000	-1.340472000
C	0.080659000	0.493051000	-0.652618000
C	1.289459000	1.373315000	-0.558827000
C	-1.203807000	1.265036000	-0.672456000
H	0.145298000	-0.170669000	-1.527693000
C	1.192413000	2.557162000	0.280590000
C	2.494225000	0.992619000	-1.063344000
C	-1.293579000	2.435413000	0.184084000
C	-2.315731000	0.784252000	-1.290090000
C	2.361076000	3.225094000	0.637769000
C	-0.093667000	3.007189000	0.688829000
C	3.713236000	1.665470000	-0.709945000
H	2.563907000	0.093641000	-1.682576000
C	-2.550877000	2.967055000	0.462435000
H	-2.244116000	-0.109763000	-1.917047000
C	-3.621103000	1.323010000	-1.030715000
C	3.641364000	2.791164000	0.187717000
H	2.300480000	4.106277000	1.281048000
H	-0.161189000	3.881202000	1.340472000
C	4.953834000	1.197339000	-1.129419000
H	-2.633561000	3.831624000	1.125716000
C	-3.739198000	2.412911000	-0.094811000
C	-4.768572000	0.749296000	-1.568068000
C	4.830627000	3.403976000	0.601198000
C	6.149518000	1.796542000	-0.696025000
H	5.002942000	0.322330000	-1.783377000
C	-5.016554000	2.875305000	0.247037000
H	-4.672786000	-0.094598000	-2.256422000
C	-6.050608000	1.201187000	-1.212730000
C	6.084005000	2.929159000	0.185116000
H	4.783439000	4.261373000	1.277181000
C	7.429084000	1.300083000	-1.089806000
H	-5.113700000	3.704244000	0.952824000
C	-6.175629000	2.290104000	-0.284331000

C	-7.235765000	0.596416000	-1.730680000
C	7.307705000	3.527047000	0.623018000
C	8.578650000	1.896734000	-0.646443000
H	7.470614000	0.424323000	-1.741397000
C	-7.486755000	2.737660000	0.073855000
H	-7.133059000	-0.243471000	-2.421105000
C	-8.472787000	1.050189000	-1.361935000
C	8.515992000	3.027363000	0.219587000
H	7.257257000	4.390806000	1.289183000
H	9.550336000	1.504771000	-0.950601000
H	-7.580299000	3.569916000	0.774836000
C	-8.599400000	2.138298000	-0.449430000
H	-9.370505000	0.574220000	-1.759484000
H	9.441332000	3.493078000	0.562028000
H	-9.593266000	2.489784000	-0.167674000

Coordinates of the singlet 7,7'-DHD, torsion 38.2°

C	-7.874688000	-1.964661000	1.532357000
H	-7.277316000	0.093883000	1.486538000
C	-6.958000000	-0.948797000	1.555144000
C	-6.118052000	-3.629066000	1.711078000
C	-5.560094000	-1.228308000	1.655782000
C	-7.447784000	-3.323712000	1.616619000
C	-5.126323000	-2.596686000	1.723813000
C	-4.599103000	-0.205185000	1.658496000
H	-3.426208000	-3.921851000	1.827298000
H	-5.789225000	-4.668638000	1.771740000
C	-3.237471000	-0.490048000	1.686322000
H	-4.928294000	0.835031000	1.577325000
C	-2.254022000	0.542694000	1.531067000
C	-2.793860000	-1.860279000	1.742454000
H	-1.048763000	-3.151841000	1.854519000
C	-3.753842000	-2.880330000	1.778712000
C	-0.932130000	0.257524000	1.378994000
H	-2.608806000	1.569586000	1.416627000
C	0.022940000	1.276281000	0.822953000
C	-0.459684000	-1.101650000	1.578385000
C	0.936339000	-1.338953000	1.612933000
C	-1.394761000	-2.122002000	1.736375000
C	1.443281000	1.073511000	1.280715000
H	-0.324539000	2.283471000	1.095155000
C	1.890385000	-0.289797000	1.534746000
C	3.250732000	-0.541070000	1.667592000
C	2.349017000	2.089025000	1.267521000
H	2.015747000	3.111855000	1.066432000
C	3.763859000	1.850749000	1.387380000
H	3.593198000	-1.567522000	1.819693000
C	4.218023000	0.495032000	1.567718000
C	4.701652000	2.869761000	1.244105000
C	5.591973000	0.230392000	1.586484000
H	4.359240000	3.898361000	1.104228000
C	6.083278000	2.604922000	1.247642000
H	5.935763000	-0.800801000	1.701210000
C	6.536001000	1.252479000	1.418653000
C	7.055440000	3.637009000	1.070658000
C	7.942456000	0.988649000	1.394495000
H	6.708210000	4.664742000	0.945383000
C	8.392779000	3.347095000	1.054397000
H	8.278889000	-0.043327000	1.515426000
C	8.842405000	2.003036000	1.215724000
H	9.912178000	1.789610000	1.197985000
H	9.124005000	4.144840000	0.916587000
H	-8.939288000	-1.739193000	1.452317000
H	-8.191928000	-4.121490000	1.603541000
H	1.295505000	-2.359357000	1.762867000
C	-0.022942000	1.276278000	-0.822984000
C	-1.443282000	1.073497000	-1.280753000

C	0.932131000	0.257502000	-1.378998000
H	0.324537000	2.283463000	-1.095193000
C	-1.890382000	-0.289812000	-1.534789000
C	-2.349022000	2.089008000	-1.267569000
C	0.459686000	-1.101675000	-1.578367000
C	2.254027000	0.542663000	-1.531067000
C	-3.250727000	-0.541088000	-1.667638000
C	-0.936338000	-1.338972000	-1.612945000
C	-3.763865000	1.850728000	-1.387426000
H	-2.015757000	3.111840000	-1.066480000
C	1.394762000	-2.122032000	-1.736320000
H	2.608813000	1.569557000	-1.416660000
C	3.237477000	-0.490084000	-1.686297000
C	-4.218024000	0.495009000	-1.567758000
H	-3.593190000	-1.567544000	-1.819723000
H	-1.295506000	-2.359378000	-1.762861000
C	-4.701661000	2.869737000	-1.244149000
H	1.048763000	-3.151872000	-1.854450000
C	2.793863000	-1.860314000	-1.742398000
C	4.599109000	-0.205222000	-1.658495000
C	-5.591972000	0.230361000	-1.586500000
C	-6.083285000	2.604891000	-1.247666000
H	-4.359252000	3.898339000	-1.104278000
C	3.753843000	-2.880368000	-1.778637000
H	4.928304000	0.834996000	-1.577361000
C	5.560100000	-1.228348000	-1.655774000
C	-6.536004000	1.252443000	-1.418656000
H	-5.935758000	-0.800835000	-1.701213000
C	-7.055451000	3.636974000	-1.070675000
H	3.426206000	-3.921890000	-1.827200000
C	5.126325000	-2.596726000	-1.723760000
C	6.958008000	-0.948837000	-1.555176000
C	-7.942457000	0.988604000	-1.394466000
C	-8.392788000	3.347052000	-1.054389000
H	-6.708225000	4.664709000	-0.945414000
C	6.118051000	-3.629108000	-1.711014000
H	7.277328000	0.093845000	-1.486607000
C	7.874694000	-1.964701000	-1.532376000
C	-8.842408000	2.002988000	-1.215691000
H	-8.278885000	-0.043375000	-1.515381000
H	-9.124016000	4.144794000	-0.916573000
H	5.789222000	-4.668681000	-1.771643000
C	7.447786000	-3.323754000	-1.616587000
H	8.939297000	-1.739233000	-1.452363000
H	-9.912179000	1.789557000	-1.197931000
H	8.191928000	-4.121534000	-1.603502000

Coordinates of centrosymmetric diheptacene D7A, D_{2h}

C	7.810251000	4.561736000	0.714179000
H	6.745882000	4.047161000	2.498006000
C	6.749769000	4.049403000	1.406053000
C	6.749769000	4.049403000	-1.406053000
C	5.618398000	3.503221000	0.718582000
C	7.810251000	4.561736000	-0.714179000
C	5.618398000	3.503221000	-0.718582000
C	4.517162000	2.972766000	1.401798000
H	4.516949000	2.973579000	-2.494652000
H	6.745882000	4.047161000	-2.498006000
C	3.419698000	2.442665000	0.718748000
H	4.516949000	2.973579000	2.494652000
C	2.284054000	1.900351000	1.405172000
C	3.419698000	2.442665000	-0.718748000
H	2.283209000	1.907539000	-2.498282000
C	4.517162000	2.972766000	-1.401798000
C	1.223660000	1.384046000	0.720822000
H	2.283209000	1.907539000	2.498282000
C	0.000000000	0.802705000	1.395810000

C	1.223660000	1.384046000	-0.720822000
C	0.000000000	0.802705000	-1.395810000
C	2.284054000	1.900351000	-1.405172000
C	-1.223660000	1.384046000	0.720822000
H	0.000000000	1.111973000	2.448794000
C	-1.223660000	1.384046000	-0.720822000
C	-2.284054000	1.900351000	-1.405172000
C	-2.284054000	1.900351000	1.405172000
H	-2.283209000	1.907539000	2.498282000
C	-3.419698000	2.442665000	0.718748000
H	-2.283209000	1.907539000	-2.498282000
C	-3.419698000	2.442665000	-0.718748000
C	-4.517162000	2.972766000	1.401798000
C	-4.517162000	2.972766000	-1.401798000
H	-4.516949000	2.973579000	2.494652000
C	-5.618398000	3.503221000	0.718582000
H	-4.516949000	2.973579000	-2.494652000
C	-5.618398000	3.503221000	-0.718582000
C	-6.749769000	4.049403000	1.406053000
C	-6.749769000	4.049403000	-1.406053000
H	-6.745882000	4.047161000	2.498006000
C	-7.810251000	4.561736000	0.714179000
H	-6.745882000	4.047161000	-2.498006000
C	-7.810251000	4.561736000	-0.714179000
H	-8.665980000	4.974807000	-1.250179000
H	-8.665980000	4.974807000	1.250179000
H	8.665980000	4.974807000	1.250179000
H	8.665980000	4.974807000	-1.250179000
H	0.000000000	1.111973000	-2.448794000
C	0.000000000	-0.802705000	1.395810000
C	1.223660000	-1.384046000	0.720822000
C	-1.223660000	-1.384046000	0.720822000
H	0.000000000	-1.111973000	2.448794000
C	1.223660000	-1.384046000	-0.720822000
C	2.284054000	-1.900351000	1.405172000
C	-1.223660000	-1.384046000	-0.720822000
C	-2.284054000	-1.900351000	1.405172000
C	2.284054000	-1.900351000	-1.405172000
C	0.000000000	-0.802705000	-1.395810000
C	3.419698000	-2.442665000	0.718748000
H	2.283209000	-1.907539000	2.498282000
C	-2.284054000	-1.900351000	-1.405172000
H	-2.283209000	-1.907539000	2.498282000
C	-3.419698000	-2.442665000	0.718748000
C	3.419698000	-2.442665000	-0.718748000
H	2.283209000	-1.907539000	-2.498282000
H	0.000000000	-1.111973000	-2.448794000
C	4.517162000	-2.972766000	1.401798000
H	-2.283209000	-1.907539000	-2.498282000
C	-3.419698000	-2.442665000	-0.718748000
C	-4.517162000	-2.972766000	1.401798000
C	4.517162000	-2.972766000	-1.401798000
C	5.618398000	-3.503221000	0.718582000
H	4.516949000	-2.973579000	2.494652000
C	-4.517162000	-2.972766000	-1.401798000
H	-4.516949000	-2.973579000	2.494652000
C	-5.618398000	-3.503221000	0.718582000
C	5.618398000	-3.503221000	-0.718582000
H	4.516949000	-2.973579000	-2.494652000
C	6.749769000	-4.049403000	1.406053000
H	-4.516949000	-2.973579000	-2.494652000
C	-5.618398000	-3.503221000	-0.718582000
C	-6.749769000	-4.049403000	1.406053000
C	6.749769000	-4.049403000	-1.406053000
C	7.810251000	-4.561736000	0.714179000
H	6.745882000	-4.047161000	2.498006000
C	-6.749769000	-4.049403000	-1.406053000
H	-6.745882000	-4.047161000	2.498006000
C	-7.810251000	-4.561736000	0.714179000
C	7.810251000	-4.561736000	-0.714179000
H	6.745882000	-4.047161000	-2.498006000

H	8.665980000	-4.974807000	1.250179000
H	-6.745882000	-4.047161000	-2.498006000
C	-7.810251000	-4.561736000	-0.714179000
H	-8.665980000	-4.974807000	1.250179000
H	8.665980000	-4.974807000	-1.250179000
H	-8.665980000	-4.974807000	-1.250179000

Coordinates of heptacene, D_{2h}

C	0.000000000	8.561911000	0.720143000
H	0.000000000	7.391033000	2.504598000
C	0.000000000	7.392929000	1.412459000
C	0.000000000	7.392929000	-1.412459000
C	0.000000000	6.123249000	0.727386000
C	0.000000000	8.561911000	-0.720143000
C	0.000000000	6.123249000	-0.727386000
C	0.000000000	4.923276000	1.409009000
H	0.000000000	4.925476000	-2.502028000
H	0.000000000	7.391033000	-2.504598000
C	0.000000000	3.674503000	0.727714000
H	0.000000000	4.925476000	2.502028000
C	0.000000000	2.460588000	1.409520000
C	0.000000000	3.674503000	-0.727714000
H	0.000000000	2.461779000	-2.502412000
C	0.000000000	4.923276000	-1.409009000
C	0.000000000	1.224979000	0.728164000
H	0.000000000	2.461779000	2.502412000
C	0.000000000	0.000000000	1.409610000
C	0.000000000	1.224979000	-0.728164000
C	0.000000000	0.000000000	-1.409610000
C	0.000000000	2.460588000	-1.409520000
C	0.000000000	-1.224979000	0.728164000
H	0.000000000	0.000000000	2.502483000
C	0.000000000	-1.224979000	-0.728164000
H	0.000000000	0.000000000	-2.502483000
C	0.000000000	-2.460588000	-1.409520000
C	0.000000000	-2.460588000	1.409520000
H	0.000000000	-2.461779000	2.502412000
C	0.000000000	-3.674503000	0.727714000
H	0.000000000	-2.461779000	-2.502412000
C	0.000000000	-3.674503000	-0.727714000
C	0.000000000	-4.923276000	1.409009000
C	0.000000000	-4.923276000	-1.409009000
H	0.000000000	-4.925476000	2.502028000
C	0.000000000	-6.123249000	0.727386000
H	0.000000000	-4.925476000	-2.502028000
C	0.000000000	-6.123249000	-0.727386000
C	0.000000000	-7.392929000	1.412459000
C	0.000000000	-7.392929000	-1.412459000
H	0.000000000	-7.391033000	2.504598000
C	0.000000000	-8.561911000	0.720143000
H	0.000000000	-7.391033000	-2.504598000
C	0.000000000	-8.561911000	-0.720143000
H	0.000000000	-9.514102000	-1.253122000
H	0.000000000	-9.514102000	1.253122000
H	0.000000000	9.514102000	1.253122000
H	0.000000000	9.514102000	-1.253122000

7.2 Coordinates associated with the 6,7' isomer

Coordinates of the triplet 6,7'-DHD, torsion 174.8°

6	-7.129728000	-1.870454000	1.367561000
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1	-5.929160000	-0.369109000	2.326343000
6	-5.941591000	-1.254043000	1.685709000
6	-5.963009000	-3.488390000	-0.009179000
6	-4.715743000	-1.727446000	1.153941000
6	-7.138003000	-2.999697000	0.511586000
6	-4.719511000	-2.862241000	0.288578000
6	-3.487889000	-1.040900000	1.374837000
1	-3.487327000	-4.211389000	-0.879617000
1	-5.967923000	-4.359645000	-0.667804000
6	-2.323874000	-1.435383000	0.773196000
1	-3.506752000	-0.118595000	1.963749000
6	-1.118023000	-0.544633000	0.732907000
6	-2.296180000	-2.636292000	-0.022348000
1	-1.026876000	-4.006739000	-1.142700000
6	-3.492178000	-3.312438000	-0.257870000
6	0.168544000	-1.308230000	0.666849000
1	-1.118873000	0.147064000	1.588527000
6	1.326129000	-0.797100000	1.155577000
6	0.187480000	-2.522126000	-0.144908000
6	1.422764000	-3.072522000	-0.500507000
6	-1.039133000	-3.107457000	-0.522772000
6	2.612804000	-1.344104000	0.805051000
1	1.306564000	0.121063000	1.750092000
6	2.654196000	-2.495235000	-0.078102000
6	3.891183000	-2.975833000	-0.503266000
6	3.785951000	-0.732162000	1.192887000
1	3.745341000	0.157066000	1.827865000
6	5.050588000	-1.190912000	0.738631000
1	3.930496000	-3.844174000	-1.165393000
6	5.102507000	-2.345370000	-0.128473000
6	6.240269000	-0.530105000	1.074560000
6	6.353897000	-2.785886000	-0.597320000
1	6.193587000	0.360934000	1.706510000
6	7.476586000	-0.962414000	0.591766000
1	6.398893000	-3.660890000	-1.250428000
6	7.534927000	-2.122728000	-0.261489000
6	8.693695000	-0.272106000	0.901484000
6	8.814761000	-2.549028000	-0.750762000
1	8.638252000	0.613317000	1.538578000
6	9.890395000	-0.706569000	0.408078000
1	8.858279000	-3.432231000	-1.391391000
6	9.951445000	-1.866229000	-0.428261000
1	10.917503000	-2.200881000	-0.809017000
1	10.810504000	-0.173092000	0.651120000
1	-8.071352000	-1.480153000	1.757425000
1	-8.086226000	-3.479569000	0.263953000
1	1.448846000	-3.968581000	-1.125148000
6	-1.206057000	0.399469000	-0.599586000
6	-0.065644000	1.370008000	-0.556436000
6	-2.544533000	1.073738000	-0.614170000
1	-1.107633000	-0.283754000	-1.456359000
6	-0.232937000	2.562691000	0.258917000
6	1.152625000	1.070693000	-1.083096000
6	-2.704584000	2.256439000	0.215412000
6	-3.628315000	0.495961000	-1.197042000
6	0.890513000	3.320814000	0.578705000
6	-1.541071000	2.927157000	0.682723000
6	2.324106000	1.844574000	-0.778718000
1	1.276687000	0.164402000	-1.683182000
6	-3.992061000	2.700172000	0.507488000
1	-3.501923000	-0.407209000	-1.801721000
6	-4.965329000	0.940357000	-0.919569000
6	2.189471000	2.975029000	0.105391000
1	0.778605000	4.207315000	1.207685000
1	-1.661270000	3.809106000	1.315791000
6	3.585235000	1.470902000	-1.231202000
1	-4.126896000	3.572359000	1.151891000
6	-5.146136000	2.041381000	-0.007037000
6	-6.076187000	0.262257000	-1.409732000
6	3.339507000	3.679679000	0.482725000
6	4.742273000	2.167308000	-0.840739000

1	3.684264000	0.594063000	-1.877104000
6	-6.446433000	2.406851000	0.362939000
1	-5.930587000	-0.590142000	-2.078506000
6	-7.379489000	0.612619000	-1.019811000
6	4.614255000	3.296882000	0.037445000
1	3.244752000	4.538358000	1.152111000
6	6.044983000	1.768920000	-1.269623000
1	-6.591471000	3.240786000	1.054339000
6	-7.567025000	1.708708000	-0.111418000
6	-8.523683000	-0.112786000	-1.470783000
6	5.801138000	3.986146000	0.442172000
6	7.158166000	2.452711000	-0.860649000
1	6.136357000	0.894523000	-1.918278000
6	-8.897582000	2.039291000	0.298238000
1	-8.370951000	-0.951651000	-2.153059000
6	-9.780960000	0.226966000	-1.049839000
6	7.032639000	3.577225000	0.007165000
1	5.703473000	4.846526000	1.107524000
1	8.147976000	2.130305000	-1.187591000
1	-9.039014000	2.876255000	0.985245000
6	-9.969970000	1.320352000	-0.153787000
1	-10.647280000	-0.336600000	-1.399271000
1	7.928869000	4.113110000	0.323956000
1	-10.978788000	1.580954000	0.169748000

Coordinates of the triplet 6,7'-DHD, torsion 118.2°, Nimag = 1

6	-6.020388000	0.883513000	3.440821000
1	-4.334118000	2.215928000	3.467868000
6	-4.704458000	1.220949000	3.211055000
6	-5.649485000	-1.330615000	2.535516000
6	-3.811123000	0.292229000	2.623968000
6	-6.497035000	-0.404379000	3.096902000
6	-4.287910000	-1.008777000	2.283926000
6	-2.471915000	0.646186000	2.281158000
1	-3.741893000	-2.945526000	1.474943000
1	-6.012849000	-2.323716000	2.262987000
6	-1.649531000	-0.223369000	1.620136000
1	-2.135861000	1.668932000	2.474173000
6	-0.367439000	0.234864000	0.972802000
6	-2.086199000	-1.575694000	1.378738000
1	-1.500555000	-3.535688000	0.641517000
6	-3.392016000	-1.933758000	1.694738000
6	0.674333000	-0.851625000	0.907994000
1	0.034601000	1.088419000	1.534456000
6	2.003094000	-0.576632000	0.934680000
6	0.213018000	-2.219242000	0.676654000
6	1.155463000	-3.205071000	0.379296000
6	-1.157190000	-2.516388000	0.833260000
6	3.001514000	-1.589029000	0.678437000
1	2.342883000	0.444575000	1.128798000
6	2.551698000	-2.933138000	0.364368000
6	3.496470000	-3.917206000	0.085731000
6	4.352162000	-1.309578000	0.700817000
1	4.688312000	-0.297316000	0.938708000
6	5.326923000	-2.304653000	0.419691000
1	3.161311000	-4.930469000	-0.148199000
6	4.883901000	-3.642321000	0.102347000
6	6.701846000	-2.028124000	0.440145000
6	5.845371000	-4.630137000	-0.178056000
1	7.036970000	-1.016390000	0.681521000
6	7.651476000	-3.012714000	0.160746000
1	5.511618000	-5.642590000	-0.418086000
6	7.210737000	-4.348388000	-0.156987000
6	9.058995000	-2.740078000	0.178973000
6	8.199715000	-5.348188000	-0.442161000
1	9.388767000	-1.727616000	0.420672000

6	9.966803000	-3.720552000	-0.098458000
1	7.862279000	-6.358457000	-0.682403000
6	9.529816000	-5.046175000	-0.414278000
1	10.271098000	-5.816030000	-0.633164000
1	11.034844000	-3.499093000	-0.080904000
1	-6.700737000	1.609655000	3.888271000
1	-7.541767000	-0.660115000	3.279806000
1	0.818172000	-4.227578000	0.193926000
6	-0.616834000	0.771270000	-0.549968000
6	-0.214040000	2.222373000	-0.602289000
6	-2.039248000	0.541628000	-0.989950000
1	0.055775000	0.187157000	-1.191797000
6	-1.224524000	3.220453000	-0.285274000
6	1.073672000	2.603222000	-0.823296000
6	-3.031104000	1.542182000	-0.629943000
6	-2.432894000	-0.633328000	-1.547884000
6	-0.833733000	4.545373000	-0.124488000
6	-2.589744000	2.826740000	-0.219670000
6	1.493193000	3.974486000	-0.701773000
1	1.825428000	1.851966000	-1.081195000
6	-4.379644000	1.215401000	-0.708358000
1	-1.684073000	-1.379228000	-1.828563000
6	-3.822315000	-0.992624000	-1.650725000
6	0.513947000	4.960321000	-0.318274000
1	-1.585362000	5.299944000	0.119575000
1	-3.337805000	3.575495000	0.051061000
6	2.808691000	4.368468000	-0.922829000
1	-5.130241000	1.945287000	-0.395762000
6	-4.811053000	-0.059363000	-1.171294000
6	-4.226395000	-2.243768000	-2.101736000
6	0.912005000	6.294145000	-0.173342000
6	3.210635000	5.708310000	-0.778618000
1	3.549672000	3.620075000	-1.215058000
6	-6.157091000	-0.437998000	-1.160590000
1	-3.474823000	-2.952554000	-2.459044000
6	-5.579767000	-2.630107000	-2.087287000
6	2.238308000	6.692331000	-0.393647000
1	0.171108000	7.044045000	0.114574000
6	4.558221000	6.124499000	-1.003467000
1	-6.905741000	0.264191000	-0.785759000
6	-6.565260000	-1.706080000	-1.600868000
6	-6.006401000	-3.917849000	-2.532732000
6	2.657272000	8.052506000	-0.249888000
6	4.922125000	7.435495000	-0.855814000
1	5.293888000	5.372948000	-1.297296000
6	-7.935999000	-2.113009000	-1.577212000
1	-5.254089000	-4.616530000	-2.904755000
6	-7.328347000	-4.272098000	-2.496228000
6	3.957449000	8.413247000	-0.473285000
1	1.915072000	8.798157000	0.042415000
1	5.954857000	7.740089000	-1.031123000
1	-8.681907000	-1.407498000	-1.205399000
6	-8.306831000	-3.356639000	-2.010398000
1	-7.640304000	-5.259282000	-2.840154000
1	4.263976000	9.454095000	-0.360236000
1	-9.356141000	-3.654278000	-1.987350000

Coordinates of the triplet 6,7'-DHD, torsion 60.2°

6	5.861786000	2.052614000	3.288713000
1	5.610277000	0.075328000	2.481878000
6	5.127751000	1.016032000	2.756900000
6	3.877171000	3.432015000	3.438296000
6	3.733123000	1.152264000	2.546045000
6	5.227981000	3.270945000	3.635691000
6	3.093896000	2.382138000	2.883018000
6	2.955865000	0.110683000	1.961124000

1	1.199330000	3.433739000	2.960748000
1	3.385298000	4.370268000	3.703388000
6	1.624530000	0.272173000	1.685700000
1	3.463734000	-0.812363000	1.668031000
6	0.873076000	-0.731503000	0.845000000
6	0.956200000	1.483582000	2.091145000
1	-0.952227000	2.516517000	2.239781000
6	1.701518000	2.509717000	2.664052000
6	-0.615634000	-0.735732000	1.096384000
1	1.276331000	-1.737425000	1.035017000
6	-1.373024000	-1.820132000	0.789740000
6	-1.259712000	0.498928000	1.535663000
6	-2.652560000	0.568570000	1.541969000
6	-0.462074000	1.586636000	1.944035000
6	-2.815640000	-1.789753000	0.825898000
1	-0.890295000	-2.746189000	0.462868000
6	-3.465232000	-0.543440000	1.187969000
6	-4.856935000	-0.479558000	1.189371000
6	-3.582215000	-2.889922000	0.497759000
1	-3.090502000	-3.826903000	0.224756000
6	-5.001296000	-2.839173000	0.499613000
1	-5.348717000	0.457328000	1.461888000
6	-5.652764000	-1.599079000	0.853397000
6	-5.787211000	-3.953017000	0.166683000
6	-7.059126000	-1.545547000	0.854915000
1	-5.293671000	-4.890589000	-0.100903000
6	-7.181432000	-3.892913000	0.169788000
1	-7.553841000	-0.609074000	1.123937000
6	-7.833656000	-2.656075000	0.523662000
6	-7.993300000	-5.025720000	-0.168279000
6	-9.268228000	-2.612241000	0.522818000
1	-7.495416000	-5.960056000	-0.435513000
6	-9.355038000	-4.940816000	-0.156736000
1	-9.758982000	-1.674690000	0.791883000
6	-10.002863000	-3.713772000	0.194777000
1	-11.092751000	-3.666387000	0.198558000
1	-9.960504000	-5.810490000	-0.415824000
1	6.935280000	1.938407000	3.445839000
1	5.818432000	4.084134000	4.060510000
1	-3.137425000	1.501572000	1.838180000
6	1.143811000	-0.476792000	-0.715618000
6	2.620086000	-0.616271000	-0.998132000
6	0.571330000	0.852995000	-1.141225000
1	0.598604000	-1.284895000	-1.225515000
6	3.450388000	0.576938000	-1.012931000
6	3.198686000	-1.843774000	-1.107468000
6	1.429521000	2.026599000	-1.105330000
6	-0.751857000	0.992725000	-1.425704000
6	4.832424000	0.437067000	-1.060289000
6	2.832934000	1.856144000	-0.984507000
6	4.623817000	-2.013776000	-1.190943000
1	2.573800000	-2.741993000	-1.098285000
6	0.857403000	3.287074000	-1.241845000
1	-1.396911000	0.110691000	-1.466812000
6	-1.366570000	2.283371000	-1.570478000
6	5.456879000	-0.838444000	-1.141871000
1	5.460467000	1.330796000	-1.043662000
1	3.469176000	2.742957000	-0.952793000
6	5.216712000	-3.269260000	-1.288581000
1	1.496988000	4.171810000	-1.200382000
6	-0.539932000	3.457372000	-1.448893000
6	-2.736969000	2.424696000	-1.762430000
6	6.848433000	-0.989381000	-1.187548000
6	6.612803000	-3.422104000	-1.336950000
1	4.583474000	-4.159256000	-1.325792000
6	-1.135944000	4.720246000	-1.547388000
1	-3.361255000	1.530214000	-1.835958000
6	-3.338863000	3.692774000	-1.850474000
6	7.446490000	-2.253296000	-1.283586000
1	7.482329000	-0.100005000	-1.151469000
6	7.232713000	-4.705497000	-1.436073000

1	-0.512079000	5.613560000	-1.463458000
6	-2.516832000	4.866049000	-1.744642000
6	-4.745187000	3.852658000	-2.041790000
6	8.866853000	-2.420708000	-1.332782000
6	8.594828000	-4.825680000	-1.480354000
1	6.594735000	-5.590778000	-1.476316000
6	-3.139628000	6.150550000	-1.839184000
1	-5.364619000	2.956821000	-2.121304000
6	-5.305253000	5.098636000	-2.126217000
6	9.423466000	-3.665956000	-1.427982000
1	9.497806000	-1.530421000	-1.293335000
1	9.055505000	-5.811569000	-1.556472000
1	-2.512228000	7.040795000	-1.760254000
6	-4.490070000	6.263947000	-2.023858000
1	-6.380672000	5.206865000	-2.274160000
1	10.507857000	-3.779377000	-1.465004000
1	-4.951914000	7.249819000	-2.094296000

Coordinates of the triplet 6,7'-DHD, torsion 47.5°, Nimag = 1

6	6.347813000	1.623871000	2.947396000
1	5.918060000	-0.343949000	2.195814000
6	5.514792000	0.628233000	2.488937000
6	4.468246000	3.128932000	3.208832000
6	4.119775000	0.850424000	2.372771000
6	5.816903000	2.884755000	3.315084000
6	3.584181000	2.123817000	2.727311000
6	3.241185000	-0.146893000	1.859625000
1	1.769134000	3.297718000	2.901461000
1	4.056227000	4.100694000	3.488981000
6	1.908043000	0.097073000	1.661283000
1	3.670362000	-1.106184000	1.558989000
6	1.037364000	-0.874773000	0.901474000
6	1.349563000	1.357183000	2.079409000
1	-0.474304000	2.528614000	2.273874000
6	2.191387000	2.338636000	2.591668000
6	-0.424015000	-0.783779000	1.263227000
1	1.404216000	-1.896100000	1.082472000
6	-1.273392000	-1.818491000	1.041867000
6	-0.954199000	0.520163000	1.658716000
6	-2.337668000	0.708387000	1.681810000
6	-0.065399000	1.555171000	1.994941000
6	-2.709453000	-1.655554000	1.073150000
1	-0.877378000	-2.794247000	0.744077000
6	-3.243759000	-0.337394000	1.364315000
6	-4.620156000	-0.131542000	1.305272000
6	-3.572706000	-2.686575000	0.763269000
1	-3.170581000	-3.678490000	0.542374000
6	-4.979800000	-2.492089000	0.702293000
1	-5.020656000	0.864687000	1.508408000
6	-5.513180000	-1.176741000	0.972981000
6	-5.862314000	-3.531782000	0.375337000
6	-6.903610000	-0.975645000	0.895051000
1	-5.459254000	-4.526930000	0.171621000
6	-7.241765000	-3.326837000	0.301809000
1	-7.306994000	0.019569000	1.098147000
6	-7.775285000	-2.013768000	0.567329000
6	-8.151413000	-4.383258000	-0.032412000
6	-9.194671000	-1.820337000	0.485993000
1	-7.743367000	-5.376101000	-0.232530000
6	-9.495583000	-4.156417000	-0.099254000
1	-9.595389000	-0.825056000	0.688754000
6	-10.025524000	-2.853633000	0.164313000
1	-11.102939000	-2.692578000	0.106403000
1	-10.176482000	-4.969583000	-0.354520000
1	7.420661000	1.444068000	3.029642000
1	6.485298000	3.664891000	3.682640000

1	-2.737465000	1.694686000	1.928660000
6	1.177852000	-0.685325000	-0.700422000
6	2.637655000	-0.606949000	-1.062701000
6	0.379772000	0.497948000	-1.184525000
1	0.739273000	-1.604199000	-1.116610000
6	3.257799000	0.707752000	-1.134011000
6	3.404372000	-1.726077000	-1.163165000
6	1.021895000	1.800615000	-1.225936000
6	-0.950994000	0.392522000	-1.447195000
6	4.643989000	0.794160000	-1.204497000
6	2.438884000	1.867091000	-1.135585000
6	4.838020000	-1.661706000	-1.265787000
1	2.935746000	-2.713407000	-1.109840000
6	0.237919000	2.936311000	-1.397999000
1	-1.434391000	-0.587685000	-1.441517000
6	-1.786151000	1.549502000	-1.604596000
6	5.467089000	-0.364515000	-1.254243000
1	5.118743000	1.777889000	-1.222131000
1	2.921351000	2.846523000	-1.154598000
6	5.629103000	-2.804585000	-1.329065000
1	0.714525000	3.919311000	-1.415131000
6	-1.176873000	2.853595000	-1.544855000
6	-3.168213000	1.437257000	-1.712575000
6	6.864311000	-0.285883000	-1.297523000
6	7.032335000	-2.727547000	-1.375720000
1	5.151082000	-3.787433000	-1.337444000
6	-1.995735000	3.986508000	-1.623824000
1	-3.625336000	0.443906000	-1.728856000
6	-3.993701000	2.573544000	-1.758059000
6	7.662571000	-1.436912000	-1.356571000
1	7.342833000	0.696393000	-1.284024000
6	7.854691000	-3.893773000	-1.437729000
1	-1.540240000	4.979354000	-1.589862000
6	-3.391206000	3.877164000	-1.722324000
6	-5.416985000	2.470909000	-1.827494000
6	9.091161000	-1.369992000	-1.400206000
6	9.218589000	-3.789901000	-1.478436000
1	7.371018000	-4.872665000	-1.452628000
6	-4.243210000	5.025462000	-1.774293000
1	-5.866066000	1.475142000	-1.845384000
6	-6.198936000	3.593560000	-1.868900000
6	9.845332000	-2.509238000	-1.459195000
1	9.566987000	-0.387305000	-1.386438000
1	9.834966000	-4.688685000	-1.526251000
1	-3.784527000	6.016250000	-1.752820000
6	-5.602440000	4.888693000	-1.845246000
1	-7.284820000	3.503440000	-1.923142000
1	10.933793000	-2.444015000	-1.492673000
1	-6.239623000	5.773513000	-1.882647000

Coordinates of the triplet 6,7'-DHD, torsion 26.0°

6	6.959855000	-0.377596000	2.353589000
1	6.141777000	-1.969987000	1.166421000
6	5.931645000	-1.089764000	1.779044000
6	5.384420000	1.199667000	3.304047000
6	4.586761000	-0.672401000	1.937298000
6	6.680819000	0.777304000	3.125507000
6	4.301710000	0.493638000	2.709068000
6	3.511606000	-1.337896000	1.281137000
1	2.726948000	1.769405000	3.480054000
1	5.167512000	2.088737000	3.900108000
6	2.227059000	-0.867166000	1.335857000
1	3.747474000	-2.203606000	0.657727000
6	1.161680000	-1.389738000	0.406582000
6	1.919193000	0.251821000	2.187748000
1	0.324641000	1.512993000	2.961789000
6	2.955467000	0.908589000	2.846627000

6	-0.227958000	-1.270253000	0.971372000
1	1.383439000	-2.440473000	0.172426000
6	-1.244329000	-2.065920000	0.552945000
6	-0.513307000	-0.105997000	1.809264000
6	-1.841689000	0.240844000	2.053153000
6	0.553267000	0.639885000	2.346631000
6	-2.630186000	-1.721735000	0.778885000
1	-1.030885000	-2.932474000	-0.080500000
6	-2.924084000	-0.513919000	1.528520000
6	-4.245890000	-0.105982000	1.675586000
6	-3.664519000	-2.436382000	0.209589000
1	-3.443609000	-3.337582000	-0.368356000
6	-5.017299000	-2.010153000	0.318911000
1	-4.466332000	0.808827000	2.230957000
6	-5.311948000	-0.819902000	1.082036000
6	-6.068544000	-2.691350000	-0.312829000
6	-6.643631000	-0.381055000	1.177167000
1	-5.847852000	-3.591656000	-0.891833000
6	-7.389096000	-2.242368000	-0.226731000
1	-6.862212000	0.530048000	1.739680000
6	-7.682527000	-1.056325000	0.538227000
6	-8.468848000	-2.918835000	-0.884104000
6	-9.039409000	-0.595072000	0.598657000
1	-8.244668000	-3.820324000	-1.458111000
6	-9.747328000	-2.447863000	-0.799454000
1	-9.254596000	0.307319000	1.174955000
6	-10.037154000	-1.264899000	-0.048462000
1	-11.065046000	-0.903300000	0.004964000
1	-10.558595000	-2.971994000	-1.306649000
1	7.993133000	-0.695723000	2.205967000
1	7.502398000	1.333037000	3.580306000
1	-2.060891000	1.130933000	2.647348000
6	1.208613000	-0.641343000	-1.069979000
6	2.602122000	-0.137134000	-1.324415000
6	0.167594000	0.438910000	-1.186024000
1	0.962732000	-1.444341000	-1.778812000
6	2.923295000	1.203389000	-0.854273000
6	3.590764000	-0.950607000	-1.782268000
6	0.503361000	1.776600000	-0.730008000
6	-1.107918000	0.154679000	-1.562759000
6	4.257184000	1.578390000	-0.753758000
6	1.869688000	2.095117000	-0.515782000
6	4.979248000	-0.580848000	-1.696103000
1	3.347423000	-1.958327000	-2.132676000
6	-0.519906000	2.702491000	-0.544908000
1	-1.358671000	-0.843336000	-1.930310000
6	-2.183057000	1.089601000	-1.382683000
6	5.312813000	0.703130000	-1.132294000
1	4.508626000	2.568060000	-0.365192000
1	2.127859000	3.090196000	-0.146855000
6	6.000988000	-1.456516000	-2.049107000
1	-0.277680000	3.703154000	-0.178756000
6	-1.880797000	2.378987000	-0.813718000
6	-3.502988000	0.744710000	-1.651142000
6	6.657471000	1.039565000	-0.949473000
6	7.354643000	-1.126733000	-1.851754000
1	5.749097000	-2.432151000	-2.473016000
6	-2.935433000	3.258506000	-0.539004000
1	-3.727125000	-0.243313000	-2.062653000
6	-4.563387000	1.621054000	-1.362099000
6	7.687691000	0.150029000	-1.285918000
1	6.909601000	2.007422000	-0.509315000
6	8.411886000	-2.027690000	-2.184124000
1	-2.715704000	4.238747000	-0.108344000
6	-4.270718000	2.905819000	-0.790228000
6	-5.924814000	1.261789000	-1.596469000
6	9.065253000	0.467532000	-1.069465000
6	9.719582000	-1.688890000	-1.962915000
1	8.154904000	-2.996218000	-2.618262000
6	-5.360137000	3.781670000	-0.485380000
1	-6.140777000	0.271476000	-2.006315000

6	-6.941388000	2.125987000	-1.289701000
6	10.050712000	-0.423653000	-1.395425000
1	9.313214000	1.438517000	-0.635659000
1	10.517047000	-2.387352000	-2.220418000
1	-5.137991000	4.760031000	-0.053965000
6	-6.653314000	3.404184000	-0.727801000
1	-7.978055000	1.831913000	-1.463316000
1	11.097779000	-0.169572000	-1.224287000
1	-7.473615000	4.083503000	-0.490430000

Coordinates of the triplet 6,7'-DHD, torsion -9.8°, Nimag = 1

6	7.250550000	-2.685651000	-0.684768000
1	5.872804000	-3.040807000	-2.294575000
6	6.001521000	-2.699546000	-1.264722000
6	6.326101000	-1.810154000	1.372263000
6	4.863069000	-2.256866000	-0.545959000
6	7.415034000	-2.227907000	0.644857000
6	5.022983000	-1.818321000	0.802489000
6	3.575489000	-2.150404000	-1.151665000
1	3.994833000	-1.118759000	2.578718000
1	6.448164000	-1.453877000	2.397396000
6	2.501001000	-1.656138000	-0.464831000
1	3.475107000	-2.399200000	-2.212313000
6	1.212013000	-1.261842000	-1.125562000
6	2.622248000	-1.349586000	0.939577000
1	1.536764000	-0.705650000	2.718418000
6	3.880165000	-1.400206000	1.528811000
6	0.043206000	-1.609295000	-0.263081000
1	1.121316000	-1.763161000	-2.098222000
6	-1.128050000	-2.064677000	-0.762734000
6	0.148550000	-1.200070000	1.135220000
6	-1.033104000	-1.009613000	1.854010000
6	1.436336000	-1.016625000	1.675985000
6	-2.359996000	-1.931288000	-0.022906000
1	-1.187899000	-2.391562000	-1.804701000
6	-2.307268000	-1.279675000	1.274225000
6	-3.499187000	-0.903567000	1.884636000
6	-3.576782000	-2.241896000	-0.587740000
1	-3.607572000	-2.734859000	-1.562885000
6	-4.800432000	-1.849463000	0.017597000
1	-3.469021000	-0.380372000	2.843530000
6	-4.753947000	-1.127476000	1.266715000
6	-6.038287000	-2.073920000	-0.598687000
6	-5.951907000	-0.633154000	1.809775000
1	-6.071168000	-2.624581000	-1.542357000
6	-7.224249000	-1.571880000	-0.059374000
1	-5.917901000	-0.065056000	2.742841000
6	-7.176910000	-0.820818000	1.169082000
6	-8.487830000	-1.741160000	-0.712332000
6	-8.395885000	-0.270498000	1.685152000
1	-8.520062000	-2.312238000	-1.642739000
6	-9.625477000	-1.193391000	-0.191803000
1	-8.353976000	0.301752000	2.614365000
6	-9.578690000	-0.445205000	1.026592000
1	-10.498580000	-0.016986000	1.427656000
1	-10.580707000	-1.325932000	-0.702243000
1	8.121310000	-3.018785000	-1.251796000
1	8.412062000	-2.198591000	1.087114000
1	-0.988199000	-0.619683000	2.873710000
6	1.173633000	0.383364000	-1.471145000
6	2.407401000	1.079383000	-0.949155000
6	-0.116960000	1.061620000	-1.048089000
1	1.215891000	0.390713000	-2.568947000
6	2.342822000	1.847952000	0.283524000
6	3.620477000	0.866142000	-1.528973000
6	-0.132778000	1.915828000	0.132409000
6	-1.293162000	0.824591000	-1.696706000

6	3.523758000	2.207607000	0.927562000
6	1.080659000	2.238146000	0.787898000
6	4.854456000	1.197903000	-0.872330000
1	3.681837000	0.320105000	-2.473775000
6	-1.341294000	2.420915000	0.600058000
1	-1.300115000	0.190430000	-2.587891000
6	-2.560758000	1.315533000	-1.220219000
6	4.796463000	1.837583000	0.416550000
1	3.470850000	2.764150000	1.866350000
1	1.041522000	2.848547000	1.692613000
6	6.085991000	0.811908000	-1.390769000
1	-1.340903000	3.059540000	1.486615000
6	-2.578028000	2.129043000	-0.031906000
6	-3.767011000	0.996308000	-1.838495000
6	5.984580000	2.042032000	1.129264000
6	7.276330000	0.993236000	-0.666945000
1	6.126730000	0.313665000	-2.362788000
6	-3.800882000	2.596045000	0.464176000
1	-3.761112000	0.364734000	-2.731101000
6	-4.999601000	1.453247000	-1.335964000
6	7.221167000	1.613951000	0.626706000
1	5.943510000	2.521146000	2.110715000
6	8.538223000	0.548154000	-1.165143000
1	-3.808691000	3.218786000	1.362329000
6	-5.014454000	2.277341000	-0.159429000
6	-6.243773000	1.125304000	-1.956736000
6	8.435153000	1.753737000	1.371346000
6	9.678254000	0.695963000	-0.422737000
1	8.570611000	0.075262000	-2.149026000
6	-6.272112000	2.743072000	0.339397000
1	-6.230523000	0.488612000	-2.844384000
6	-7.428567000	1.587788000	-1.450699000
6	9.624486000	1.305386000	0.865854000
1	8.391615000	2.224499000	2.355790000
1	10.636047000	0.348019000	-0.812541000
1	-6.276892000	3.370749000	1.233205000
6	-7.441822000	2.409320000	-0.285567000
1	-8.371443000	1.320693000	-1.930174000
1	10.541885000	1.415760000	1.446051000
1	-8.395604000	2.764289000	0.107700000

Coordinates of the singlet 6,7'-DHD, torsion 174.8°

6	-7.128099000	-1.874849000	1.365278000
1	-5.928990000	-0.371321000	2.322465000
6	-5.940499000	-1.257308000	1.683252000
6	-5.959703000	-3.494032000	-0.008589000
6	-4.714136000	-1.730592000	1.152647000
6	-7.135246000	-3.005369000	0.510941000
6	-4.716774000	-2.866517000	0.288740000
6	-3.486869000	-1.042879000	1.373103000
1	-3.483215000	-4.215739000	-0.877874000
1	-5.963737000	-4.366182000	-0.666029000
6	-2.322258000	-1.437102000	0.772381000
1	-3.506732000	-0.119910000	1.960955000
6	-1.117385000	-0.545126000	0.731677000
6	-2.293620000	-2.638649000	-0.022128000
1	-1.023341000	-4.008707000	-1.141815000
6	-3.488969000	-3.316232000	-0.256945000
6	0.169932000	-1.307219000	0.664374000
1	-1.118393000	0.146391000	1.587484000
6	1.327757000	-0.794065000	1.151114000
6	0.189660000	-2.521759000	-0.145991000
6	1.425456000	-3.071400000	-0.501867000
6	-1.036343000	-3.108891000	-0.522681000
6	2.614586000	-1.340687000	0.801060000
1	1.307800000	0.124563000	1.744882000
6	2.656470000	-2.492987000	-0.080533000

6	3.893821000	-2.973874000	-0.504828000
6	3.787608000	-0.727965000	1.188376000
1	3.746694000	0.161988000	1.822321000
6	5.052603000	-1.187721000	0.735940000
1	3.933472000	-3.842993000	-1.165902000
6	5.104957000	-2.343177000	-0.129893000
6	6.242211000	-0.527420000	1.072871000
6	6.356658000	-2.784785000	-0.596808000
1	6.195279000	0.364146000	1.704056000
6	7.479062000	-0.961198000	0.592411000
1	6.401967000	-3.660434000	-1.249025000
6	7.537768000	-2.122189000	-0.259815000
6	8.696252000	-0.271891000	0.903799000
6	8.817970000	-2.549995000	-0.746659000
1	8.640571000	0.613998000	1.540234000
6	9.893435000	-0.707865000	0.412811000
1	8.861730000	-3.433677000	-1.386609000
6	9.954795000	-1.868073000	-0.422652000
1	10.921177000	-2.203917000	-0.801534000
1	10.813633000	-0.175145000	0.657166000
1	-8.070160000	-1.484518000	1.754052000
1	-8.083039000	-3.486234000	0.263592000
1	1.451914000	-3.968026000	-1.125674000
6	-1.207812000	0.400174000	-0.600561000
6	-0.068016000	1.371286000	-0.557936000
6	-2.546719000	1.073560000	-0.613481000
1	-1.109836000	-0.282793000	-1.457606000
6	-0.235392000	2.564211000	0.256703000
6	1.150651000	1.071517000	-1.083898000
6	-2.706689000	2.256772000	0.215384000
6	-3.630995000	0.494849000	-1.194666000
6	0.888189000	3.322949000	0.575873000
6	-1.543098000	2.928422000	0.681245000
6	2.322004000	1.845511000	-0.779766000
1	1.274820000	0.165055000	-1.683676000
6	-3.994046000	2.700224000	0.508293000
1	-3.504920000	-0.408828000	-1.798670000
6	-4.967893000	0.939320000	-0.916854000
6	2.187076000	2.976933000	0.103130000
1	0.776094000	4.209769000	1.204364000
1	-1.663186000	3.810693000	1.313884000
6	3.583335000	1.470833000	-1.230750000
1	-4.128573000	3.572763000	1.152281000
6	-5.148321000	2.040971000	-0.004999000
6	-6.079019000	0.261315000	-1.406646000
6	3.337094000	3.681925000	0.480224000
6	4.740396000	2.167550000	-0.840450000
1	3.682575000	0.593232000	-1.875582000
6	-6.448538000	2.406786000	0.365130000
1	-5.933704000	-0.591450000	-2.075023000
6	-7.382167000	0.612269000	-1.016876000
6	4.612079000	3.298327000	0.036131000
1	3.242113000	4.541362000	1.148600000
6	6.043158000	1.768137000	-1.267764000
1	-6.593293000	3.241107000	1.056118000
6	-7.569296000	1.708768000	-0.108815000
6	-8.526724000	-0.112505000	-1.468141000
6	5.798792000	3.987851000	0.440666000
6	7.156361000	2.452220000	-0.858920000
1	6.134744000	0.892825000	-1.915156000
6	-8.899818000	2.040021000	0.300582000
1	-8.374294000	-0.951508000	-2.150315000
6	-9.783871000	0.228063000	-1.047618000
6	7.030561000	3.577959000	0.007085000
1	5.700894000	4.849193000	1.104736000
1	8.146310000	2.128975000	-1.184630000
1	-9.040970000	2.877158000	0.987435000
6	-9.972460000	1.321638000	-0.151625000
1	-10.650447000	-0.334975000	-1.397264000
1	7.926709000	4.114061000	0.323730000
1	-10.981210000	1.582828000	0.171649000

Coordinates of the singlet 6,7'-DHD, torsion 43.9°

6	6.459254000	1.613978000	2.613096000
1	5.953145000	-0.416565000	2.124465000
6	5.585459000	0.595746000	2.308549000
6	4.631771000	3.199842000	2.736028000
6	4.193623000	0.845955000	2.201041000
6	5.975201000	2.928299000	2.832953000
6	3.704349000	2.170357000	2.409434000
6	3.275050000	-0.173093000	1.822144000
1	1.929608000	3.411676000	2.497400000
1	4.256106000	4.211391000	2.904015000
6	1.947112000	0.092877000	1.614139000
1	3.669832000	-1.170725000	1.613841000
6	1.050722000	-0.902586000	0.924474000
6	1.428762000	1.402033000	1.919211000
1	-0.360252000	2.628911000	2.057468000
6	2.315739000	2.410866000	2.287916000
6	-0.405788000	-0.750672000	1.284590000
1	1.394648000	-1.921019000	1.157854000
6	-1.287142000	-1.770152000	1.121798000
6	-0.897932000	0.589716000	1.602443000
6	-2.272505000	0.818560000	1.626131000
6	0.022321000	1.627775000	1.847547000
6	-2.717296000	-1.560479000	1.138733000
1	-0.921450000	-2.771948000	0.876212000
6	-3.211328000	-0.215437000	1.367543000
6	-4.578682000	0.033473000	1.286276000
6	-3.612076000	-2.575286000	0.861903000
1	-3.241393000	-3.588492000	0.687301000
6	-5.009844000	-2.335366000	0.770582000
1	-4.947563000	1.050860000	1.438659000
6	-5.501504000	-0.992918000	0.980522000
6	-5.923869000	-3.356022000	0.467052000
6	-6.882361000	-0.745567000	0.865029000
1	-5.553265000	-4.372049000	0.310060000
6	-7.292573000	-3.105302000	0.356920000
1	-7.251805000	0.271667000	1.018189000
6	-7.783728000	-1.764116000	0.559053000
6	-8.233550000	-4.141393000	0.044433000
6	-9.193631000	-1.524171000	0.438949000
1	-7.857865000	-5.155302000	-0.107682000
6	-9.566618000	-3.869855000	-0.060801000
1	-9.562007000	-0.508037000	0.594133000
6	-10.054428000	-2.539256000	0.139965000
1	-11.123928000	-2.342707000	0.052395000
1	-10.271255000	-4.667843000	-0.298974000
1	7.528951000	1.412217000	2.685274000
1	6.676768000	3.726718000	3.079506000
1	-2.642118000	1.829275000	1.815628000
6	1.200515000	-0.797118000	-0.698160000
6	2.656975000	-0.674735000	-1.057203000
6	0.363834000	0.334635000	-1.225829000
1	0.796783000	-1.751236000	-1.067077000
6	3.223662000	0.663197000	-1.156780000
6	3.471027000	-1.763283000	-1.115793000
6	0.948847000	1.663901000	-1.259469000
6	-0.958604000	0.167562000	-1.499477000
6	4.604382000	0.806160000	-1.209681000
6	2.357671000	1.790262000	-1.174748000
6	4.902399000	-1.640334000	-1.194979000
1	3.043633000	-2.767447000	-1.036676000
6	0.104103000	2.764668000	-1.381900000
1	-1.394622000	-0.834512000	-1.502493000
6	-1.848697000	1.284840000	-1.630013000
6	5.475801000	-0.318003000	-1.211038000
1	5.038547000	1.808386000	-1.240223000

1	2.800823000	2.788131000	-1.198285000
6	5.742930000	-2.749872000	-1.200488000
1	0.530522000	3.770851000	-1.371959000
6	-1.304995000	2.614981000	-1.519691000
6	-3.225113000	1.107479000	-1.734707000
6	6.868745000	-0.180404000	-1.220717000
6	7.142197000	-2.613806000	-1.212301000
1	5.307335000	-3.752257000	-1.187759000
6	-2.183065000	3.707055000	-1.534610000
1	-3.632393000	0.093672000	-1.784097000
6	-4.107252000	2.198842000	-1.709257000
6	7.716244000	-1.297064000	-1.219249000
1	7.304358000	0.821743000	-1.224858000
6	8.015084000	-3.744729000	-1.212261000
1	-1.778687000	4.719645000	-1.460011000
6	-3.571707000	3.529405000	-1.615540000
6	-5.525456000	2.023918000	-1.749041000
6	9.141470000	-1.169763000	-1.224765000
6	9.373865000	-3.583200000	-1.217998000
1	7.574038000	-4.743695000	-1.207954000
6	-4.483832000	4.632459000	-1.589647000
1	-5.922831000	1.007601000	-1.805203000
6	-6.364722000	3.104076000	-1.710383000
6	9.944812000	-2.276358000	-1.223986000
1	9.574387000	-0.167326000	-1.230846000
1	10.028996000	-4.455474000	-1.218369000
1	-4.076927000	5.643937000	-1.527706000
6	-5.835027000	4.427091000	-1.634697000
1	-7.445700000	2.959440000	-1.741659000
1	11.030055000	-2.165007000	-1.228884000
1	-6.518086000	5.277517000	-1.611150000

Coordinates of planosymmetric diheptacene D7A, C_s

1	-2.065896000	6.563571000	2.497619000
6	-2.066159000	6.563196000	1.404836000
6	-2.066159000	6.563196000	-1.404836000
6	-1.895785000	5.341598000	0.722038000
6	-1.895785000	5.341598000	-0.722038000
6	-1.725775000	4.116984000	1.405053000
1	-1.726618000	4.116698000	-2.497768000
1	-2.065896000	6.563571000	-2.497619000
6	-1.557886000	2.920713000	0.722874000
1	-1.726618000	4.116698000	2.497768000
6	-1.386943000	1.667564000	1.408078000
6	-1.557886000	2.920713000	-0.722874000
1	-1.394155000	1.668471000	-2.501155000
6	-1.725775000	4.116984000	-1.405053000
6	-1.218978000	0.504149000	0.723871000
1	-1.394155000	1.668471000	2.501155000
6	-1.039948000	-0.840282000	1.395201000
6	-1.218978000	0.504149000	-0.723871000
6	-1.039948000	-0.840282000	-1.395201000
6	-1.386943000	1.667564000	-1.408078000
6	-1.964879000	-1.826961000	0.714809000
1	-1.335914000	-0.748450000	2.448064000
6	-1.964879000	-1.826961000	-0.714809000
6	-2.779639000	-2.691263000	-1.399776000
6	-2.779639000	-2.691263000	1.399776000
1	-2.785123000	-2.690029000	2.493030000
6	-3.628167000	-3.603412000	0.712152000
1	-2.785123000	-2.690029000	-2.493030000
6	-3.628167000	-3.603412000	-0.712152000
6	-4.477581000	-4.510288000	1.400771000
6	-4.477581000	-4.510288000	-1.400771000
1	-4.474312000	-4.506368000	2.492788000
6	-5.287765000	-5.377716000	0.708411000
1	-4.474312000	-4.506368000	-2.492788000

6	-5.287765000	-5.377716000	-0.708411000
1	-1.335914000	-0.748450000	-2.448064000
6	0.489516000	-1.329895000	1.395928000
6	1.416424000	-0.341758000	0.720848000
6	0.670452000	-2.672421000	0.720925000
1	0.784041000	-1.423779000	2.448990000
6	1.416424000	-0.341758000	-0.720848000
6	2.230739000	0.511546000	1.405147000
6	0.670452000	-2.672421000	-0.720925000
6	0.837382000	-3.839973000	1.405191000
6	2.230739000	0.511546000	-1.405147000
6	0.489516000	-1.329895000	-1.395928000
6	3.092430000	1.428668000	0.718730000
1	2.237063000	0.508808000	2.498261000
6	0.837382000	-3.839973000	-1.405191000
1	0.843980000	-3.841466000	2.498307000
6	1.005913000	-5.087157000	0.718726000
6	3.092430000	1.428668000	-0.718730000
1	2.237063000	0.508808000	-2.498261000
1	0.784041000	-1.423779000	-2.448990000
6	3.930534000	2.313535000	1.401807000
1	0.843980000	-3.841466000	-2.498307000
6	1.005913000	-5.087157000	-0.718726000
6	1.173241000	-6.294398000	1.401754000
6	3.930534000	2.313535000	-1.401807000
6	4.770040000	3.201983000	0.718575000
1	3.931156000	2.313169000	2.494658000
6	1.173241000	-6.294398000	-1.401754000
1	1.174098000	-6.294417000	2.494612000
6	1.339048000	-7.505535000	0.718550000
6	4.770040000	3.201983000	-0.718575000
1	3.931156000	2.313169000	-2.494658000
6	5.633356000	4.114538000	1.406076000
1	1.174098000	-6.294417000	-2.494612000
6	1.339048000	-7.505535000	-0.718550000
6	1.509949000	-8.750144000	1.406017000
6	5.633356000	4.114538000	-1.406076000
6	6.442970000	4.969961000	0.714193000
1	5.629915000	4.111624000	2.498024000
6	1.509949000	-8.750144000	-1.406017000
1	1.509257000	-8.745711000	2.497976000
6	1.670290000	-9.917002000	0.714172000
6	6.442970000	4.969961000	-0.714193000
1	5.629915000	4.111624000	-2.498024000
1	7.095753000	5.660498000	1.250122000
1	1.509257000	-8.745711000	-2.497976000
6	1.670290000	-9.917002000	-0.714172000
1	1.799521000	-10.858388000	1.250187000
1	7.095753000	5.660498000	-1.250122000
1	1.799521000	-10.858388000	-1.250187000
6	-2.233723000	7.762589000	0.722640000
6	-2.233723000	7.762589000	-0.722640000
6	-2.408304000	9.013624000	-1.409045000
6	-2.570538000	10.175724000	-0.717203000
6	-2.570538000	10.175724000	0.717203000
6	-2.408304000	9.013624000	1.409045000
1	-2.407597000	9.009754000	-2.500969000
1	-2.701826000	11.117914000	-1.251272000
1	-2.701826000	11.117914000	1.251272000
1	-2.407597000	9.009754000	2.500969000
1	-5.934631000	-6.070897000	-1.248070000
1	-5.934631000	-6.070897000	1.248070000

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