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Supporting Information: In the Quest for a Stable Triplet State in Small Polyaromatic Hydrocarbons : An in-silico tool for Rational Design and Prediction

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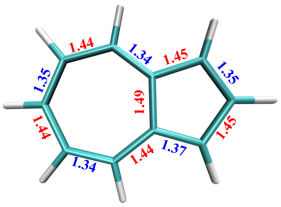
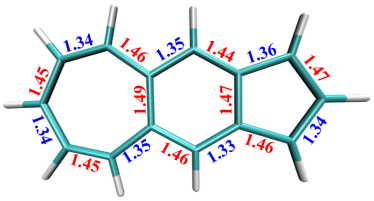
S1 Singlet Geometries

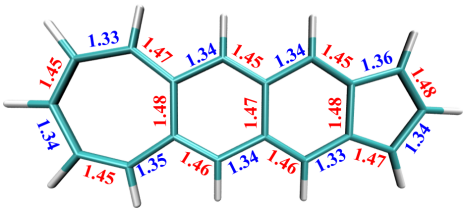
Figure S1 shows the (2e,2o)CASSCF/RB3LYP/6-31G(d) optimized structures of the singlet states of PAHs used for further studies. The red and blue colors denote the long and short bonds respectively and therefore the bond alternation pattern.



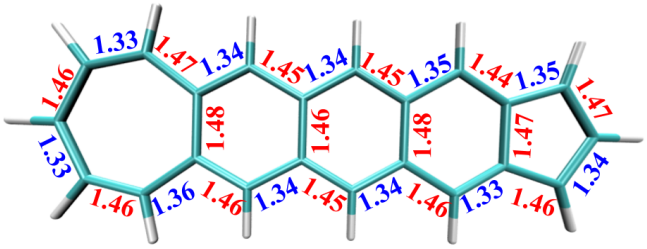
(a) 75 Singlet



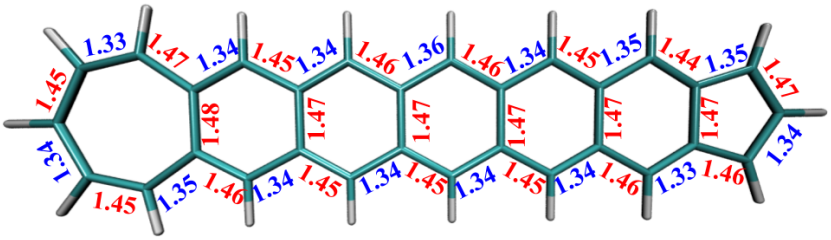
(b) 765 Singlet



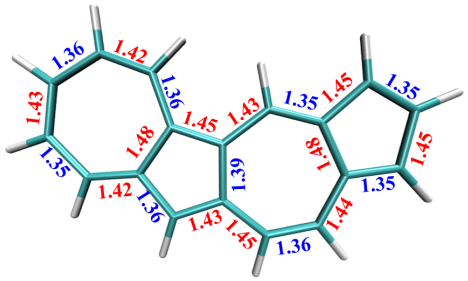
(c) 7665 Singlet



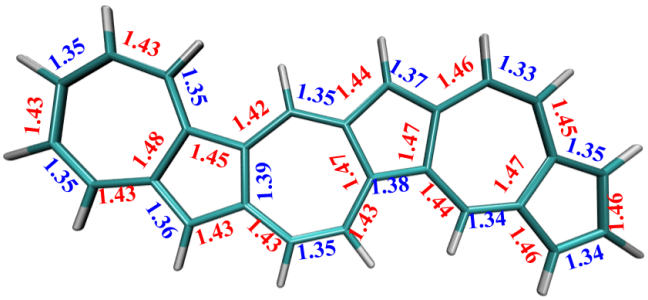
(d) 76665 Singlet



(e) 7666665 Singlet



(f) 7575 Singlet



(g) 757575 Singlet

Figure S1: Singlet optimized geometries of polyazulenes and fused acene-azulenes.

S2 Vertical ST gap

Figure S2 shows the vertical ST gaps of the polyacenes, polyazulenes and fused acene-azulenes at the DMRG/cc-pVDZ level of theory. The polyacenes show a much faster decay in the vertical ST gaps, as compared to both the polyazulenes and fused acene-azulens. Furthermore, the two types of geometries of the fused acene-azulene (i.e. UB3LYP optimized and CAS(2,2) optimized) show a constant shift between each other in the vertical ST gaps (red curve and purple squares). The black squares denote the UB3LYP optimized geometries, where the singlet state retains the C_2 symmetry and a break in bond length alternation along the periphery of the molecule. The red curve denotes the CAS(2,2) optimized geometry which retains the bond length alternation at the cost of C_2 symmetry of the singlet state.

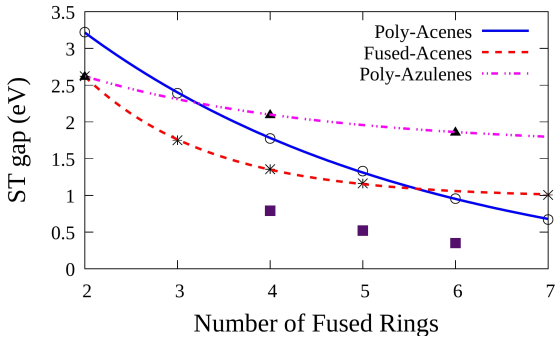


Figure S2: Vertical ST gap of polyacenes, polyazulenes and fused acene-azulenes calculated in DMRG/cc-pVDZ level of theory. The purple squares refer to the UB3LYP optimized geometries of fused acene-azulene with different bond length alternation pattern.

S3 Adiabatic ST gaps

The adiabatic ST gaps for the polyacenes, polyazulenes and fused acene-azulenes are computed at CASSCF/cc-pVDZ and CASPT2/cc-pVDZ with (14o,14e) active spaces. They show the same qualitative trends as the full valence DMRG calculations given in the manuscript. In all the levels of theory, within 5 fused rings in the fused acene-azulene system the ST gap is within 0.1 eV, i.e., computational range of accuracy. In case of CASSCF (without full valence active space), the ST levels do not show any crossover, while in case of CASPT2 the crossover happens around 5 fused rings. In case of DMRG (shown in the manuscript), the crossover is at 6 fused rings.

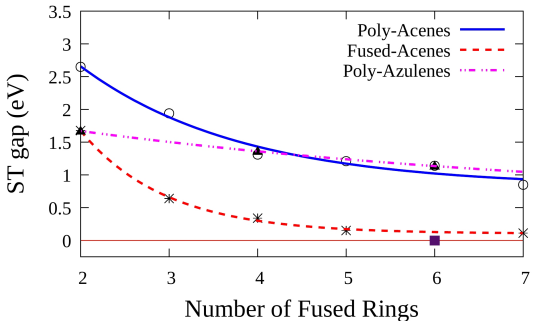


Figure S3: ST gap of polyacenes, polyazulenes and combined azulene-acenes calculated in CASSCF/cc-pVDZ level of theory.

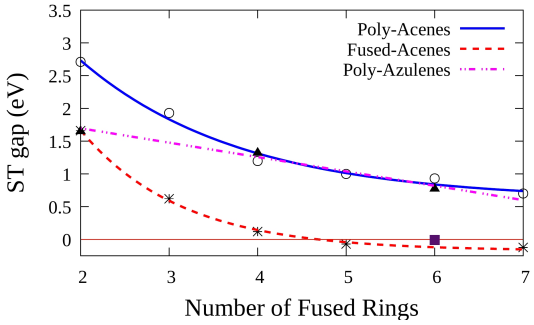


Figure S4: ST gap of polyacenes, polyazulenes and combined azulene-acenes calculated in CASPT2/cc-pVDZ level of theory.

S4 Single reference calculation of ST gaps

The adiabatic ST gaps of the fused acene-azulenes and polyazulenes computed at UB3LYP/6-31G(d) level of theory is shown in Table S1. As expected from earlier results on UB3LYP level calculations of acenes and polyazulenes, the ST gap from UB3LYP is much lower than expected from multireference calulations. The UB3LYP results show a ST crossover for fused acene-azulene at 4 fused rings.

Molecule	ST gap (eV)
75	1.72
765	0.54
7665	-0.12
76665	-0.37
766665	-0.46
75	1.72
7575	1.15
757575	0.97

Table S1: Adiabatic ST gaps of PAHs computed at UB3LYP/6-31G(d) level of theory.

Also from the UB3LYP/6-31G(d) level of calculations we can clearly see that there is no spin contamination in the singlet as well as in the triplet state.

Molecules	S^2 value in	
	Singlet state	Triplet State
75	0.00	2.01
765	0.00	2.03
7665	0.00	2.04
76665	0.00	2.05
766665	0.00	2.06
7575	0.00	2.06
757575	0.00	2.07

Table S2: S^2 value for UB3LYP calculations.

S5 Singlet and Triplet Effect

The singlet states of polyazulenes and fused acene-azulenes show comparable stability. However, the ST gap of the fused acene-azulene is much lower. This points towards a relative destabilization of the triplet states in polyazulenes. Figure S5 shows the energies of the singlet and triplet states of tetracene and its isomers, in both the molecular and model Hamiltonian frameworks. This shows that, as expected, the singlet states of both polyazulenes and fused acene-azulenes are destabilized almost equally with respect to polyacenes. However, the triplet state of polyazulene shows a relative destabilization when compared to fused acene-azulene. This effect is captured in both the Hamiltonians - molecular and model.

We have further dissected the reason for this relative destabilization of the triplet states of polyazulene. The total probability of finding same spins across bonds (in spin Hamiltonian) for all bonds are computed. This probability is 0.2545 for 4-azulene and 0.2406 for 4-fused acene-azulene. This spin frustration

in the triplet state is found to be the reason behind the above mentioned triplet destabilization.

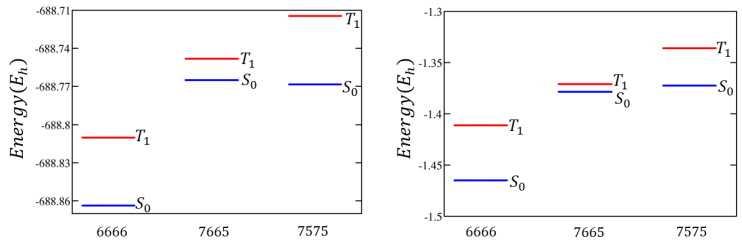


Figure S5: Molecular and model Hamiltonian energies for the singlet and triplet states are compared for 4-fused ring systems, i.e., tetracene, polyazulene and fused acene-azulene.

S6 Kinked versus straight topologies

We have seen that ST gap of polyazulenes are much higher than fused acene-azulenes at various levels of theory (DMRG, CASSCF and CASPT2). One of the reason for that is the spin frustration in triplet state. However, we conjecture that there is another contributing factor. In case of polyacenes and kinked/bent polyacenes (such as anthracene and phenanthrene), it is known that phenanthrene shows higher ST gap. The formation of a stable double bond in phenanthrene is thought to be the cause behind this. However, when the same computation is done with model Hamiltonian, all the bonds are taken to be similar (a priori) and therefore, this effect is supposed to be suppressed. Such model Hamiltonian calculations also show the phenanthrene to have higher ST gap (Table S3) and one of the reasons for such an effect is the kinked or bent topology.[1] We expect such effect to also play a minor role in the higher ST gap of polyazulenes as compared to the fused acene-azulenes.

Hajgató and co-workers have been calculated ab initio ST gap of anthracene, phenanthrene, tetracene, and chrysene at CCSD(T)/cc-pV∞Z^a level of theory. [2] The qualitative trends between their computed straight and bent molecules are similar to that of the model Hamiltonian. Therefore, we expect that along with stable double bond configurations, there is a role of topology in these systems.

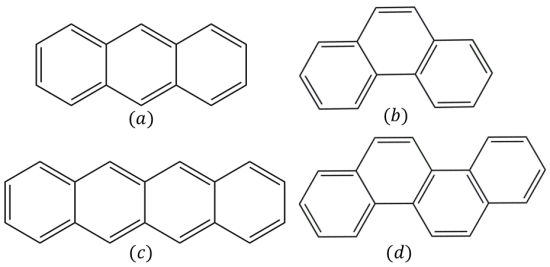


Figure S6: Bent or kinked and straight polyacenes used to understand the effect of topology.

Molecule	Model Hamiltonian ST gap (eV)	Molecular Hamiltonian ST gap (eV)
Anthracene	2.02	2.46
Phenanthrene	2.28	3.54
Tetracene	1.46	1.75
4-Chrysene	1.79	3.24

Table S3: ST gap of straight and bent acenes (model and molecular calculations).

S7 Relative stability of singlet species

In order to ascertain the feasibility of synthesis of the proposed molecules, the stability of the singlet species are compared. In order to do so, an isodesmic reaction of the form,

$$\mathrm{PAH} + n_1\mathrm{CH_4} \rightarrow n_2\mathrm{C_2H_4} + n_3\mathrm{C_2H_6}, \tag{1}$$

is considered. The extra stabilization energy of the PAH with respect to the C-C single and double bonded moieties and appropriate numbers of C-H bonds are considered. This extra stabilization is partly due to the resonance and we tabulate (Table S4) the stabilization energy per π electron. The energies for the moieties on both sides of the reaction is computed with UB3LYP/6-31G(d) level of theory.

Molecule	Stabilization energy per π electron (in kcal/mol)
6-6	12.19
7-5	8.21
6-6-6	12.39
7-6-5	8.30
7-5-6	10.13
6-6-6-6	12.42
7-6-6-5	8.94
7-5-7-5	9.35
7-5-6-6	10.87
6-6-6-6-6	12.40
7-6-6-6-5	9.44

Table S4: Stabilization energy per π electron for the PAH systems.

We notice that this stability index of the acenes remain almost constant throughout the series. The polyazulenes and fused acene-azulenes are less stable than acenes as expected. It is important to note that the fused acene-azulenes (7-5-6 and 7-5-6-6) with stability indices, 10.13 and 10.87, have been synthesized.[3] Therefore, we expect that the polyazulenes and fused acene-azulenes which have stability indices not too different than these molecules are feasible.

S8 Correlation between HOMO-LUMO gap and ST gap

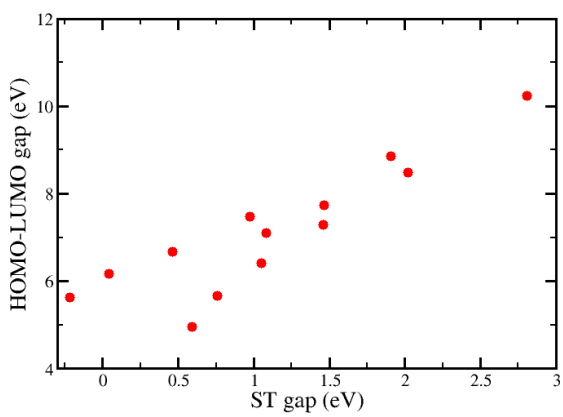


Figure S7: Correlation between HOMO-LUMO gap and ST gap

The HOMO-LUMO gaps are not very correlated with the ST gaps. However, there is some early indication of the ST gaps from the HOMO-LUMO gaps.

S9 Corrletion between diradical nature and ST gap

The diradical character of a molecule can be find out by calculating it's natural orbital occupation number (NOON) of lowest unoccupied natural orbital (LUNO).[4] The more the value of NOON of LUNO the more diradical nature of the nmolecule. While earlier work on polyacenes showed that there is strong relationship between the diradical nature and ST gap, in our work on polyazulenes and fused acene-azulenes, we notice that there is no correlation between them.

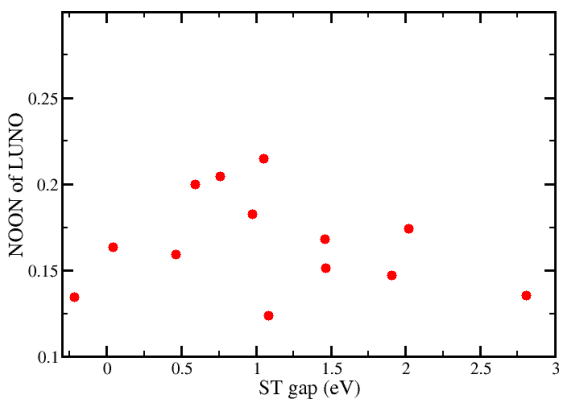


Figure S8: Correlation between diradical nature and ST gap

S10 Dipole moment values for Polyazulenes and Fused acene-azulenes

Molecules	Dipole moment (Debye)
75	0.55
765	0.91
7665	1.15
76665	1.44
7666665	1.93
7575	1.96
757575	4.00

Table S5: Dipole moment of the molecules calculated in CASSCF/cc-pVDZ level of theory.

S11 Optimized geometries of Azulenes and Fused acene-azulene in cartesian coordinate

All these geometries are optimized at (2e,2o)CASSCF/RB3LYP/6-31G(d) level of theory.

S11.1 75 singlet

DMRG/cc-pVDG(M=1500)= -383.410551
CASSCF(10e,10o)/cc-pVDG= -383.442188
CASPT2/cc-pVDG energy= -383.493745

Atom	X	Y	Z
C	0.0000000000	0.0240064216	-2.4942387877
C	0.0000000000	-1.2847628599	-1.8904536593
C	0.0000000000	-1.6156150040	-0.5872086388
C	0.0000000000	1.2404648612	-1.9165910733
C	0.0000000000	-0.7495033013	0.5589903522
C	0.0000000000	1.5687975526	-0.5158463343
C	0.0000000000	0.7376815424	0.5413663621
H	0.0000000000	0.0156581131	-3.5710281768
H	0.0000000000	-2.1014107970	-2.5914050432
H	0.0000000000	-2.6683173659	-0.3574139743
H	0.0000000000	2.0872022567	-2.5807223343
H	0.0000000000	2.6235830483	-0.2957266469
C	0.0000000000	-1.1373589702	1.8693777270
H	0.0000000000	-2.1485096034	2.2285675073
C	0.0000000000	0.0504942506	2.7073099461
H	0.0000000000	0.0373179335	3.7807191710
C	0.0000000000	1.1493209071	1.9307655033
H	0.0000000000	2.1709510143	2.2583122198

S11.2 75 Triplet

DMRG/cc-pVDG(M=1500)= -383.340407
CASSCF(10e,10o)/cc-pVDG= -383.380608
CASPT2/cc-pVDG energy= -383.432719

Atom	X	Y	Z
C	0.0000000000	0.0297030368	-2.5178664820
C	0.0000000000	-1.2750153473	-1.8801557581
C	0.0000000000	-1.5907430121	-0.5751814490

C	0.0000000000	1.2513709520	-1.9351858711
C	0.0000000000	-0.6811190532	0.5431872145
C	0.0000000000	1.6100142050	-0.5620989566
C	0.0000000000	0.7174922129	0.5334181137
H	0.0000000000	0.0068487116	-3.5930910146
H	0.0000000000	-2.1045703608	-2.5670230149
H	0.0000000000	-2.6376332679	-0.3233324659
H	0.0000000000	2.0876697998	-2.6149549499
H	0.0000000000	2.6606658276	-0.3359442211
C	0.0000000000	-1.1192213273	1.9439864235
H	0.0000000000	-2.1488046024	2.2479037090
C	0.0000000000	-0.0434096852	2.7502872929
H	0.0000000000	-0.0326950215	3.8216246924
C	0.0000000000	1.1251083274	1.9017774208
H	0.0000000000	2.1443386042	2.2374234364

S11.3 765 Singlet

DMRG/cc-pVDG(M=1500)= -536.079102
CASSCF(14e,14o)/cc-pVDZ= -536.125782
CASPT2/cc-pVDG energy= -536.198042

Atom	X	Y	Z
C	0.0000000000	-1.5157178165	-1.7200651345
C	0.0000000000	-0.7181247299	-0.6313874777
C	0.0000000000	0.7696614421	-0.6095734644
C	0.0000000000	-1.2268824894	-3.1380650180
C	0.0000000000	1.5889065317	-1.8222866677
C	0.0000000000	-0.0352158923	-3.7423317705
C	0.0000000000	1.2730247381	-3.1202650881
H	0.0000000000	-2.5710730440	-1.5085154444
H	0.0000000000	-2.0981294079	-3.7693247033
H	0.0000000000	2.6438533650	-1.6077963786
H	0.0000000000	-0.0316887749	-4.8186152103
H	0.0000000000	2.1003209005	-3.8084438905
C	0.0000000000	-1.4070884603	0.6611637275
C	0.0000000000	1.4254976297	0.5686791055
H	0.0000000000	2.5012395268	0.5748476302
H	0.0000000000	-2.4828872070	0.6456351616
C	0.0000000000	-0.7392409396	1.8145269475
C	0.0000000000	0.7309015374	1.8303303639
C	0.0000000000	-1.1717405561	3.2093665089
C	0.0000000000	1.1354541988	3.1290278084
C	0.0000000000	-0.0709598724	3.9743128690

H	0.0000000000	-2.1913611463	3.5416873832
H	0.0000000000	-0.0523466952	5.0479012484
H	0.0000000000	2.1435971620	3.4958428536

S11.4 765 Triplet

DMRG/cc-pVDG(M=1500)= -536.043263
CASSCF(14e,14o)/cc-pVDG= -536.097394
CASPT2/cc-pVDG energy= -536.175306

Atom	X	Y	Z
C	0.0000000000	-1.5616952882	-1.8005708855
C	0.0000000000	-0.7045105945	-0.6129442038
C	0.0000000000	0.7116791933	-0.6180231411
C	0.0000000000	-1.2646182240	-3.1139300757
C	0.0000000000	1.5636825127	-1.8053487011
C	0.0000000000	0.0009186796	-3.7586734731
C	0.0000000000	1.2615785301	-3.1218958198
H	0.0000000000	-2.6116670331	-1.5657805807
H	0.0000000000	-2.1122931225	-3.7787074044
H	0.0000000000	2.6145346057	-1.5748172178
H	0.0000000000	-0.0023827912	-4.8327428391
H	0.0000000000	2.1082807078	-3.7880120243
C	0.0000000000	-1.3833062012	0.6155206537
C	0.0000000000	1.3947585214	0.6085698709
H	0.0000000000	2.4703215882	0.6033776038
H	0.0000000000	-2.4589362690	0.6128275083
C	0.0000000000	-0.6963000237	1.8057165633
C	0.0000000000	0.7097607580	1.8011498857
C	0.0000000000	-1.1281458723	3.2024185913
C	0.0000000000	1.1409551256	3.1856753894
C	0.0000000000	-0.0294019417	3.9992509024
H	0.0000000000	-2.1497555052	3.5303908902
H	0.0000000000	-0.0289249006	5.0715389981
H	0.0000000000	2.1554675449	3.5316608689

S11.5 7665 Singlet

DMRG/cc-pVDG(M=1500)= -688.765128
CASSCF(14e,14o)/cc-pVDG= -688.762373
CASPT2/cc-pVDG energy= -688.829345

Atom	X	Y	Z

C	4.9672468473	-0.0449524585	0.0000000000
C	4.3497324417	1.2697910292	0.0000000000
C	3.0561317102	1.5956953324	0.0000000000
C	4.3567974952	-1.2322210228	0.0000000000
C	1.8411682114	0.7739366621	0.0000000000
C	2.9360256256	-1.5167951838	0.0000000000
C	1.8580080527	-0.7057646544	0.0000000000
H	6.0433727298	-0.0456234771	0.0000000000
H	5.0437728313	2.0923278001	0.0000000000
H	2.8449451812	2.6512548671	0.0000000000
H	4.9844019836	-2.1062637437	0.0000000000
H	2.7158923012	-2.5703849779	0.0000000000
C	0.6615377219	1.4172529858	0.0000000000
C	0.5532380722	-1.3589198074	0.0000000000
H	0.5532260341	-2.4347752144	0.0000000000
C	-0.6345467961	0.7624579207	0.0000000000
C	-0.6185316490	-0.7084064026	0.0000000000
C	-1.8904439737	-1.4277605347	0.0000000000
H	-1.8656235738	-2.5039889418	0.0000000000
C	-3.0378230911	-0.7504227354	0.0000000000
C	-1.7959779156	1.4398699443	0.0000000000
H	-1.7988582767	2.5160736300	0.0000000000
C	-3.0533388853	0.7261075470	0.0000000000
C	-4.4382849698	-1.1807293054	0.0000000000
H	-4.7695034886	-2.2007521971	0.0000000000
C	-4.3530882244	1.1252009397	0.0000000000
H	-4.7206639626	2.1331689852	0.0000000000
C	-5.2024279831	-0.0827778527	0.0000000000
H	-6.2758583262	-0.0623898820	0.0000000000
H	0.6543892373	2.4931678667	0.0000000000

S11.6 7665 Triplet

DMRG/cc-pVDZ(M=1500)= -688.748079
CASSCF(14e,14o)/cc-pVDZ= -688.750035
CASPT2/cc-pVDZ energy= -688.825070

Atom	X	Y	Z
C	4.9721950071	0.0011774365	0.0000000000
C	4.3371913304	1.2696301764	0.0000000000
C	3.0255321218	1.5739812843	0.0000000000
C	4.3332401104	-1.2679410024	0.0000000000
C	1.8336606983	0.7234318937	0.0000000000
C	3.0221605852	-1.5692223353	0.0000000000

C	1.8311863889	-0.7155301253	0.0000000000
H	6.0463617280	-0.0004610281	0.0000000000
H	5.0079001064	2.1124334301	0.0000000000
H	2.7945057311	2.6247987229	0.0000000000
H	5.0025223795	-2.1118539732	0.0000000000
H	2.7885619104	-2.6194901726	0.0000000000
C	0.6259012610	1.3757643488	0.0000000000
C	0.6222807738	-1.3649257463	0.0000000000
H	0.6134616184	-2.4407312357	0.0000000000
C	-0.6187360088	0.7117973488	0.0000000000
C	-0.6212648921	-0.6984262072	0.0000000000
C	-1.8574574666	-1.4075874735	0.0000000000
H	-1.8473178396	-2.4836995231	0.0000000000
C	-3.0202819262	-0.7106405590	0.0000000000
C	-1.8524316518	1.4238443410	0.0000000000
H	-1.8408074841	2.4998768719	0.0000000000
C	-3.0185007189	0.7274152310	0.0000000000
C	-4.4201200037	-1.1310761470	0.0000000000
H	-4.7528309419	-2.1509713403	0.0000000000
C	-4.4061798157	1.1449778423	0.0000000000
H	-4.7589695163	2.1567877903	0.0000000000
C	-5.2118028682	-0.0299259361	0.0000000000
H	-6.2845187827	-0.0316442042	0.0000000000
H	0.6194735267	2.4515874101	0.0000000000

S11.7 76665 Singlet

DMRG/cc-pVDZ(M=1500)= -841.452535
CASSCF(14e,14o)/cc-pVDZ= -841.401575
CASPT2/cc-pVDZ energy= -841.466698

Atom	X	Y	Z
C	4.2610628721	-1.5901940950	0.0000000000
C	3.0430764511	-0.7701574395	0.0000000000
C	3.0551841795	0.7128454392	0.0000000000
C	5.5524658320	-1.2611101789	0.0000000000
C	4.1431245947	1.5338932562	0.0000000000
C	6.1751957673	0.0556200663	0.0000000000
C	5.5702229466	1.2417261262	0.0000000000
H	4.0517625872	-2.6460843690	0.0000000000
H	6.2470112052	-2.0833724553	0.0000000000
H	3.9230423117	2.5873489537	0.0000000000
H	7.2513324778	0.0511864808	0.0000000000
H	6.1999115691	2.1144397036	0.0000000000

C	1.8673023297	-1.4185966398	0.0000000000
C	1.7449161264	1.3638860797	0.0000000000
H	1.7376760940	2.4397473090	0.0000000000
H	1.8629176833	-2.4944177992	0.0000000000
C	0.5708229238	-0.7631324522	0.0000000000
C	0.5810442796	0.7004789966	0.0000000000
C	-0.5935072405	-1.4280655450	0.0000000000
C	-0.7015925641	1.3836446826	0.0000000000
H	-0.6938984663	2.4600533312	0.0000000000
H	-0.5978941234	-2.5044649128	0.0000000000
C	-1.8816134898	-0.7539451017	0.0000000000
C	-1.8686611489	0.7215362025	0.0000000000
C	-3.0502785249	-1.4237387812	0.0000000000
C	-3.1422005454	1.4378795893	0.0000000000
H	-3.0581243471	-2.4999236371	0.0000000000
H	-3.1168258545	2.5141031077	0.0000000000
C	-4.2915876354	0.7615855334	0.0000000000
C	-4.3026003173	-0.7108234237	0.0000000000
C	-5.5887704874	-1.1117843710	0.0000000000
C	-5.6905306990	1.1884303601	0.0000000000
H	-6.0284538326	2.2059420318	0.0000000000
H	-5.9478432733	-2.1232420485	0.0000000000
C	-6.4455685390	0.0794706298	0.0000000000
H	-7.5187566540	0.0478256713	0.0000000000

S11.8 76665 Triplet

DMRG/cc-pVDZ(M=1500)= -841.451106
CASSCF(14e,14o)/cc-pVDZ= -841.396031
CASPT2/cc-pVDZ enengy= -841.469346

Atom	X	Y	Z
C	4.2244804483	-1.5730002841	0.0000000000
C	3.0280335799	-0.7281497355	0.0000000000
C	3.0263365134	0.7284382237	0.0000000000
C	5.5349226977	-1.2674371047	0.0000000000
C	4.2215586761	1.5757564301	0.0000000000
C	6.1687882070	0.0029177114	0.0000000000
C	5.5320286068	1.2728392043	0.0000000000
H	3.9954924907	-2.6242772347	0.0000000000
H	6.2069340239	-2.1090663695	0.0000000000
H	3.9903944671	2.6265562811	0.0000000000
H	7.2430253075	0.0040452246	0.0000000000
H	6.2025834665	2.1156323846	0.0000000000

C	1.8326428848	-1.3792885572	0.0000000000
C	1.8297932704	1.3770965247	0.0000000000
H	1.8191217576	2.4527137757	0.0000000000
H	1.8241759439	-2.4549247313	0.0000000000
C	0.5728639429	-0.7108233572	0.0000000000
C	0.5711384560	0.7061404934	0.0000000000
C	-0.6399734772	-1.3948889996	0.0000000000
C	-0.6432306412	1.3875278592	0.0000000000
H	-0.6421836303	2.4639081438	0.0000000000
H	-0.6367684511	-2.4712677089	0.0000000000
C	-1.8524912523	-0.7210259278	0.0000000000
C	-1.8542243705	0.7115235708	0.0000000000
C	-3.1060544758	-1.4269738967	0.0000000000
C	-3.1103178116	1.4152761016	0.0000000000
H	-3.0963716821	-2.5029437378	0.0000000000
H	-3.1015034664	2.4913458573	0.0000000000
C	-4.2634104880	0.7202244864	0.0000000000
C	-4.2629132028	-0.7316358307	0.0000000000
C	-5.6499678712	-1.1440683378	0.0000000000
C	-5.6634663871	1.1365941662	0.0000000000
H	-5.9989386546	2.1554587490	0.0000000000
H	-6.0061846876	-2.1545073801	0.0000000000
C	-6.4519955801	0.0332574939	0.0000000000
H	-7.5249541222	0.0356168122	0.0000000000

S11.9 766665 Singlet

DMRG/cc-pVDZ(M=1500)= -994.148047
CASSCF(14e,14o)/cc-pVDZ= -994.039565
CASPT2/cc-pVDZ enengy= -994.108297

Atom	X	Y	Z
C	5.4467493029	-1.5781612555	0.0000000000
C	4.2504578368	-0.7337379956	0.0000000000
C	4.2520644868	0.7327542323	0.0000000000
C	6.7575413890	-1.2749190606	0.0000000000
C	5.4514422561	1.5741428548	0.0000000000
C	7.3933392383	-0.0054516796	0.0000000000
C	6.7606126705	1.2672306868	0.0000000000
H	5.2165043682	-2.6291372353	0.0000000000
H	7.4283095326	-2.1174467005	0.0000000000
H	5.2240102542	2.6257530159	0.0000000000
H	8.4676183014	-0.0067268024	0.0000000000
H	7.4341564664	2.1075208917	0.0000000000

C	3.0596252450	-1.3813799699	0.0000000000
C	3.0633368716	1.3834700225	0.0000000000
H	3.0553452201	2.4590235515	0.0000000000
H	3.0488137229	-2.4569038762	0.0000000000
C	1.7904408664	-0.7124682701	0.0000000000
C	1.7918702339	0.7178304732	0.0000000000
C	0.5941370054	-1.3920632184	0.0000000000
C	0.5974019444	1.3998654941	0.0000000000
H	0.5981839253	2.4761125656	0.0000000000
H	0.5926485989	-2.4683069191	0.0000000000
C	-0.6340909396	-0.7083885375	0.0000000000
C	-0.6328292490	0.7187695528	0.0000000000
C	-1.8713312663	-1.3874657328	0.0000000000
C	-1.8683972094	1.3995460699	0.0000000000
H	-1.8694473321	-2.4637747203	0.0000000000
H	-1.8650774770	2.4758509509	0.0000000000
C	-3.0655458330	0.7295214585	0.0000000000
C	-3.0666113391	-0.7158761610	0.0000000000
C	-4.3285615618	1.4327429453	0.0000000000
C	-4.3320915702	-1.4187452634	0.0000000000
H	-4.3206914549	2.5086437473	0.0000000000
H	-4.3237004899	-2.4947679237	0.0000000000
C	-5.4803696954	0.7363391001	0.0000000000
C	-5.4798417726	-0.7239818967	0.0000000000
C	-6.8803273104	-1.1384926159	0.0000000000
C	-6.8664888105	1.1451425074	0.0000000000
H	-7.2251425892	2.1546020308	0.0000000000
H	-7.2168562605	-2.1569415752	0.0000000000
C	-7.6669812462	-0.0348500972	0.0000000000
H	-8.7400635373	-0.0375291199	0.0000000000

S11.10 766665 Triplet

DMRG/cc-pVDZ(M=1500)= -994.147487
CASSCF(14e,14o)/cc-pVDZ= -994.039635
CASPT2/cc-pVDZ enengy= -994.108585

Atom	X	Y	Z
C	5.4473405097	-1.5778193222	0.0000000000
C	4.2504376120	-0.7340047739	0.0000000000
C	4.2519248793	0.7324360937	0.0000000000
C	6.7578003040	-1.2738574826	0.0000000000
C	5.4502546559	1.5740100630	0.0000000000
C	7.3931101677	-0.0035566612	0.0000000000

C	6.7603185308	1.2676041298	0.0000000000
H	5.2177056237	-2.6289288886	0.0000000000
H	7.4290774756	-2.1159563416	0.0000000000
H	5.2225302135	2.6255303496	0.0000000000
H	8.4673822858	-0.0046203149	0.0000000000
H	7.4331043133	2.1085078131	0.0000000000
C	3.0599248248	-1.3820542311	0.0000000000
C	3.0625811884	1.3827822772	0.0000000000
H	3.0542114364	2.4583101859	0.0000000000
H	3.0495301944	-2.4575811768	0.0000000000
C	1.7904009882	-0.7136231172	0.0000000000
C	1.7918686636	0.7167625116	0.0000000000
C	0.5942548970	-1.3932162921	0.0000000000
C	0.5970790139	1.3988031729	0.0000000000
H	0.5978647758	2.4750363095	0.0000000000
H	0.5928404781	-2.4694629354	0.0000000000
C	-0.6342139465	-0.7096902730	0.0000000000
C	-0.6327768272	0.7176805283	0.0000000000
C	-1.8712991651	-1.3883119743	0.0000000000
C	-1.8683125467	1.3987681014	0.0000000000
H	-1.8697423166	-2.4646201721	0.0000000000
H	-1.8646929611	2.4750605879	0.0000000000
C	-3.0654696433	0.7289386050	0.0000000000
C	-3.0667627631	-0.7164934647	0.0000000000
C	-4.3282331174	1.4326759036	0.0000000000
C	-4.3320226758	-1.4187454939	0.0000000000
H	-4.3198978480	2.5085731789	0.0000000000
H	-4.3240423597	-2.4947673089	0.0000000000
C	-5.4802254548	0.7366361510	0.0000000000
C	-5.4799329216	-0.7236109715	0.0000000000
C	-6.8798202351	-1.1374831348	0.0000000000
C	-6.8663542872	1.1457273992	0.0000000000
H	-7.2245117941	2.1553915801	0.0000000000
H	-7.2169752624	-2.1557175473	0.0000000000
C	-7.6665019644	-0.0326122721	0.0000000000
H	-8.7395921490	-0.0351552670	0.0000000000

S11.11 7666665 Singlet

DMRG/cc-pVDZ(M=1500)= -1146.828624
CASSCF(14e,14o)/cc-pVDZ= -1146.689040
CASPT2/cc-pVDZ enengy= -1146.748035

Atom	X	Y	Z

C	0.0000000000	-1.5454434519	-6.5796318629
C	0.0000000000	-0.7258656217	-5.5066203857
C	0.0000000000	0.7547165534	-5.5065002469
C	0.0000000000	-1.2744476989	-8.0018735084
C	0.0000000000	1.5634631705	-6.7313121358
C	0.0000000000	-0.0951368174	-8.6280273551
C	0.0000000000	1.2237688039	-8.0213008783
H	0.0000000000	-2.5969569356	-6.3498036252
H	0.0000000000	-2.1556143367	-8.6197379739
H	0.0000000000	2.6211192336	-6.5313008572
H	0.0000000000	-0.1067590624	-9.7039499597
H	0.0000000000	2.0407496707	-8.7221218471
C	0.0000000000	-1.3627409004	-4.1950387258
C	0.0000000000	1.4151320799	-4.3361856790
H	0.0000000000	2.4908818845	-4.3424169554
H	0.0000000000	-2.4384054379	-4.1797636893
C	0.0000000000	-0.6930461392	-3.0324299580
C	0.0000000000	0.7723469566	-3.0336309139
C	0.0000000000	-1.3651575773	-1.7451751114
C	0.0000000000	1.4520249132	-1.8782052591
H	0.0000000000	2.5283250976	-1.8856566076
H	0.0000000000	-2.4415074878	-1.7416512711
C	0.0000000000	-0.6887050483	-0.5854112231
C	0.0000000000	0.7841292399	-0.5831819280
C	0.0000000000	-1.3618530757	0.7012110401
C	0.0000000000	1.4580752473	0.5943340056
H	0.0000000000	-2.4382364949	0.7001917919
H	0.0000000000	2.5340888083	0.5982861585
C	0.0000000000	0.7751511683	1.8829393330
C	0.0000000000	-0.6922200768	1.8658727587
C	0.0000000000	1.4283235023	3.0544646581
C	0.0000000000	-1.3798870866	3.1458674231
H	0.0000000000	2.5047221198	3.0669422201
H	0.0000000000	-2.4562301792	3.1313259510
C	0.0000000000	0.7469332285	4.3378026459
C	0.0000000000	-0.7262931342	4.3180147048
C	0.0000000000	1.4129786913	5.5093828718
C	0.0000000000	-1.4485900334	5.5878437922
H	0.0000000000	2.4891212704	5.5215471121
H	0.0000000000	-2.5246725178	5.5577766531
C	0.0000000000	0.6943630991	6.7576567502
C	0.0000000000	-0.7770627292	6.7403712392
C	0.0000000000	1.0906533668	8.0458211172
C	0.0000000000	-1.2089545023	8.1375156030
H	0.0000000000	2.1008515525	8.4084738461
H	0.0000000000	-2.2277809604	8.4715069658

C	0.0000000000	-0.1032556818	8.8978547157
H	0.0000000000	-0.0759112505	9.9710648008

S11.12 7666665 Triplet

DMRG/cc-pVDZ(M=1500)= -1146.836937
CASSCF(14e,14o)/cc-pVDZ= -1146.684733
CASPT2/cc-pVDZ enengy= -1146.752550

Atom	X	Y	Z
C	0.0000000000	-1.5834441381	-6.6647409620
C	0.0000000000	-0.7412843755	-5.4672582051
C	0.0000000000	0.7311661082	-5.4692765624
C	0.0000000000	-1.2793685351	-7.9753331908
C	0.0000000000	1.5700446870	-6.6688897244
C	0.0000000000	-0.0091605201	-8.6101981356
C	0.0000000000	1.2624596995	-7.9788265314
H	0.0000000000	-2.6346652475	-6.4355892599
H	0.0000000000	-2.1213479181	-8.6466922458
H	0.0000000000	2.6218820010	-6.4425957697
H	0.0000000000	-0.0106535491	-9.6845349667
H	0.0000000000	2.1027252668	-8.6523407561
C	0.0000000000	-1.3887772729	-4.2798231447
C	0.0000000000	1.3818623291	-4.2835468797
H	0.0000000000	2.4573653296	-4.2760258268
H	0.0000000000	-2.4642551966	-4.2694195967
C	0.0000000000	-0.7216924989	-3.0043315704
C	0.0000000000	0.7182250980	-3.0062960770
C	0.0000000000	-1.3995114451	-1.8186415672
C	0.0000000000	1.3993053293	-1.8224864889
H	0.0000000000	2.4754740778	-1.8234529260
H	0.0000000000	-2.4756799688	-1.8167231511
C	0.0000000000	-0.7157410164	-0.5756039539
C	0.0000000000	0.7189233710	-0.5775338463
C	0.0000000000	-1.3924103265	0.6424172223
C	0.0000000000	1.3989773278	0.6385295255
H	0.0000000000	-2.4686095670	0.6438999060
H	0.0000000000	2.4751753373	0.6370494067
C	0.0000000000	0.7221217763	1.8511138400
C	0.0000000000	-0.7122400947	1.8529839282
C	0.0000000000	1.4038248671	3.0996067665
C	0.0000000000	-1.3906496959	3.1035693674
H	0.0000000000	2.4800711871	3.0953416362
H	0.0000000000	-2.4669047895	3.1020713293

C	0.0000000000	0.7356538907	4.2876469578
C	0.0000000000	-0.7196316324	4.2893210838
C	0.0000000000	1.4377078299	5.5556852091
C	0.0000000000	-1.4196220699	5.5603694394
H	0.0000000000	2.5135806237	5.5481732202
H	0.0000000000	-2.4956396748	5.5536439356
C	0.0000000000	0.7414494230	6.7052766438
C	0.0000000000	-0.7237957487	6.7051444124
C	0.0000000000	1.1491499113	8.0904608830
C	0.0000000000	-1.1355679698	8.1049223277
H	0.0000000000	2.1585528369	8.4492358312
H	0.0000000000	-2.1532414730	8.4436279156
C	0.0000000000	-0.0292506370	8.8900192395
H	0.0000000000	-0.0313675268	9.9631915112

S11.13 7575 Singlet

DMRG/cc-pVDZ(M=1500)= -688.768365
CASSCF(14e,14o)/cc-pVDZ= -688.755921
CASPT2/cc-pVDZ enengy= -688.829396

Atom	X	Y	Z
C	-1.0644283900	-4.4755066928	0.0000000000
C	0.3594239444	-4.5339271523	0.0000000000
C	1.2463553483	-3.5114560988	0.0000000000
C	-1.8791597426	-3.3925280819	0.0000000000
C	1.0004291085	-2.1101552965	0.0000000000
C	-1.5349556756	-2.0099698930	0.0000000000
C	-0.3097071213	-1.4284260498	0.0000000000
H	-1.5563525573	-5.4329254528	0.0000000000
H	0.7755985916	-5.5259845908	0.0000000000
H	2.2885831755	-3.7827074678	0.0000000000
H	-2.9360337484	-3.5932899699	0.0000000000
H	-2.3844582758	-1.3515753138	0.0000000000
C	1.9611048276	-1.1441210554	0.0000000000
H	3.0205074456	-1.3161536143	0.0000000000
C	1.3536076919	0.1472223526	0.0000000000
C	-0.0298475806	-0.0054785384	0.0000000000
C	2.1468836398	1.3597380159	0.0000000000
C	-1.0310616688	1.0172365692	0.0000000000
H	3.2112061800	1.1995324066	0.0000000000
H	-2.0518421080	0.6771391612	0.0000000000
C	-0.8742122911	2.3561279220	0.0000000000
C	1.7220619508	2.6467961602	0.0000000000

H	2.4866221680	3.4054918425	0.0000000000
C	0.3694664155	3.1508490479	0.0000000000
C	-1.9611867197	3.3156497210	0.0000000000
C	0.0112758395	4.4568184876	0.0000000000
H	-3.0021067658	3.0547325539	0.0000000000
H	0.6863528436	5.2918793604	0.0000000000
C	-1.4330783694	4.5558387066	0.0000000000
H	-1.9816711860	5.4785637409	0.0000000000

S11.14 7575 Triplet

DMRG/cc-pVDZ(M=1500)= -688.714600
CASSCF(14e,14o)/cc-pVDZ= -688.705928
CASPT2/cc-pVDZ enengy= -688.780500

Atom	X	Y	Z
C	-1.0177689713	-4.5344612782	0.0000000000
C	0.3249591331	-4.5671193579	0.0000000000
C	1.2562544036	-3.4773301293	0.0000000000
C	-1.9017692224	-3.3749909375	0.0000000000
C	0.9602367646	-2.1071592732	0.0000000000
C	-1.5990015757	-2.0692378757	0.0000000000
C	-0.2968617844	-1.4486525923	0.0000000000
H	-1.5242165070	-5.4837161136	0.0000000000
H	0.7774712217	-5.5443181151	0.0000000000
H	2.2981110159	-3.7410615849	0.0000000000
H	-2.9503481591	-3.6177359307	0.0000000000
H	-2.4379869158	-1.3982268762	0.0000000000
C	1.9602641844	-1.1190194237	0.0000000000
H	3.0154824252	-1.3117899320	0.0000000000
C	1.3763112011	0.1964574906	0.0000000000
C	-0.0676403100	0.0017824882	0.0000000000
C	2.1180232562	1.3376605538	0.0000000000
C	-1.0286915397	0.9575996707	0.0000000000
H	3.1869253751	1.2111792857	0.0000000000
H	-2.0530556627	0.6304043457	0.0000000000
C	-0.8772510235	2.3733522815	0.0000000000
C	1.6612169459	2.6846139367	0.0000000000
H	2.4381065802	3.4308521468	0.0000000000
C	0.3884133465	3.1462226503	0.0000000000
C	-1.8961203639	3.2790743493	0.0000000000
C	0.0098467810	4.5343390728	0.0000000000
H	-2.9432738095	3.0439210652	0.0000000000
H	0.7010362936	5.3544756902	0.0000000000

C	-1.3437043915	4.6050252760	0.0000000000
H	-1.9255917215	5.5072698968	0.0000000000

S11.15 757575 Singlet

DMRG/cc-pVDZ(M=1500)= -994.119896
CASSCF(14e,14o)/cc-pVDZ= -994.016504
CASPT2/cc-pVDZ enengy= -994.081251

Atom	X	Y	Z
C	-1.0146978406	-4.4554095951	0.0000000000
C	0.4134235120	-4.5003346994	0.0000000000
C	1.2907123339	-3.4729969806	0.0000000000
C	-1.8386431308	-3.3822708776	0.0000000000
C	1.0315987063	-2.0699426125	0.0000000000
C	-1.5051851140	-1.9941396436	0.0000000000
C	-0.2860225172	-1.4045943273	0.0000000000
H	-1.4963390104	-5.4178908664	0.0000000000
H	0.8372274992	-5.4890754487	0.0000000000
H	2.3352183719	-3.7347067943	0.0000000000
H	-2.8937073544	-3.5916698325	0.0000000000
H	-2.3598149823	-1.3423061287	0.0000000000
C	1.9837179731	-1.0985235201	0.0000000000
H	3.0443525842	-1.2618641736	0.0000000000
C	1.3647638485	0.1910449387	0.0000000000
C	-0.0200263653	0.0243153721	0.0000000000
C	2.1270765159	1.4053323133	0.0000000000
C	-1.0138827720	1.0381150749	0.0000000000
H	3.1940115631	1.2634073095	0.0000000000
H	-2.0351134946	0.6999465181	0.0000000000
C	-0.8637668992	2.3847101945	0.0000000000
C	1.6983115957	2.6833563159	0.0000000000
H	2.4789488842	3.4209802691	0.0000000000
C	0.3595084496	3.1954344716	0.0000000000
C	-1.9628642812	3.3171974405	0.0000000000
C	-0.0104055094	4.5234116727	0.0000000000
H	-2.9985234340	3.0356432535	0.0000000000
C	-1.4766492372	4.5947138059	0.0000000000
C	-2.3337569047	5.7746075232	0.0000000000
C	0.9038856768	5.6370345058	0.0000000000
H	-3.3868953109	5.5490673201	0.0000000000
H	1.9491990220	5.3849277926	0.0000000000
C	0.6320330111	6.9516907973	0.0000000000
C	-1.9921354688	7.0625834992	0.0000000000

H	-2.7963090044	7.7795109481	0.0000000000
C	-0.6661352476	7.6514742352	0.0000000000
C	1.6515039500	8.0001875224	0.0000000000
C	-0.4044732280	8.9756583558	0.0000000000
H	2.7084377803	7.8141033458	0.0000000000
H	-1.1407156727	9.7576770277	0.0000000000
C	1.0373611233	9.1920530848	0.0000000000
H	1.5103001082	10.1554486818	0.0000000000

S11.16 757575 Triplet

DMRG/cc-pVDZ(M=1500)= -994.080063
CASSCF(14e,14o)/cc-pVDZ= -993.974797
CASPT2/cc-pVDZ enengy= -994.052481

Atom	X	Y	Z
C	-1.0021410136	-4.4769883630	0.0000000000
C	0.3526503607	-4.5207965287	0.0000000000
C	1.2681267325	-3.4317687256	0.0000000000
C	-1.8709607325	-3.3460409414	0.0000000000
C	1.0098624214	-2.0986467036	0.0000000000
C	-1.5631747857	-2.0249752876	0.0000000000
C	-0.2875652363	-1.3981896744	0.0000000000
H	-1.5037788363	-5.4294873820	0.0000000000
H	0.8016460356	-5.4984267478	0.0000000000
H	2.3091587207	-3.7078662715	0.0000000000
H	-2.9202324291	-3.5838227394	0.0000000000
H	-2.4087888480	-1.3619186381	0.0000000000
C	2.0110601802	-1.0801789443	0.0000000000
H	3.0680480257	-1.2648082477	0.0000000000
C	1.4137075340	0.1418152392	0.0000000000
C	-0.0332204127	-0.0360823746	0.0000000000
C	2.1653134494	1.3841183252	0.0000000000
C	-1.0164815482	0.9950305570	0.0000000000
H	3.2331245774	1.2483967167	0.0000000000
H	-2.0438450916	0.6830873578	0.0000000000
C	-0.8264951485	2.3802253702	0.0000000000
C	1.7263973025	2.6526049916	0.0000000000
H	2.4964825729	3.4014274779	0.0000000000
C	0.3811851767	3.1450094923	0.0000000000
C	-1.8981832365	3.2847823006	0.0000000000
C	0.0263943362	4.5718991311	0.0000000000
H	-2.9349730457	3.0090402679	0.0000000000
C	-1.4278428414	4.6425470993	0.0000000000

C	-2.2618577250	5.7218332225	0.0000000000
C	0.9041227583	5.6057055880	0.0000000000
H	-3.3166254666	5.5076637982	0.0000000000
H	1.9522898269	5.3656999396	0.0000000000
C	0.6362407990	7.0024160598	0.0000000000
C	-1.9166268436	7.0978908132	0.0000000000
H	-2.7522153027	7.7781389511	0.0000000000
C	-0.6850468627	7.6669064976	0.0000000000
C	1.5799690794	7.9898171272	0.0000000000
C	-0.4230149806	9.0786520371	0.0000000000
H	2.6428402701	7.8399429030	0.0000000000
H	-1.1791965072	9.8395428503	0.0000000000
C	0.9223720826	9.2630027050	0.0000000000
H	1.4268043821	10.2107088404	0.0000000000

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