Stretch Effects Induced by Molecular Strains on weakening σ-bonds: Molecular Design of long-lived Diradicals (Biradicals)

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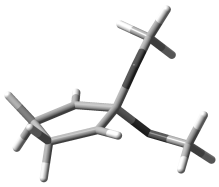
Complete ref. 21:

Gaussian 03, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

All the optimized geometries with Gaussian 03 suite of program are as follows.

singlet 2,2-dimethoxycyclopentane-1,3-diyl (S-**DR1b**)
BS-UB3LYP/6-31G(d), C_2 symmetry

Nuclear repulsion energy: 484.6370085878 Hartree
SCF Done: E(UB3LYP) = -424.273711749 Hartree
Sum of electronic and zero-point Energies = -424.096497 Hartree
S**2 before annihilation 0.8805, after 0.0435
Zero-point correction: 0.177214 Hartree
no imaginary frequency



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H,0,2.2480373307,-0.6911722703,2.4492670078
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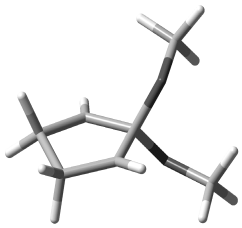
H,0,-2.2480373307,0.6911722703,2.4492670078
H,0,-1.7337418971,1.8771382752,1.2244507727

Triplet 2,2-dimethoxycyclopentane-1,3-diyl (T-**DR1b**)
BS-UB3LYP/6-31G(d), C_2 symmetry

Nuclear repulsion energy: 485.0623448948 Hartree
SCF Done: E(UB3LYP) = -424.268259608 Hartree
Sum of electronic and zero-point Energies = -424.091251 Hartree
S**2 before annihilation 2.0082, after 2.0000
Zero-point correction: 0.177008 Hartree
no imaginary frequency



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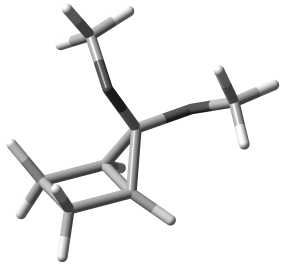
H,0,-1.7290371863,1.9138718607,1.1748705727

5,5-dimethoxybicyclo[2.1.0]pentane (**CP1b**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 494.9543667553 Hartree
SCF Done: E(UB3LYP) = -424.322504593 Hartree
Sum of electronic and zero-point Energies = -424.140102 Hartree
Zero-point correction: 0.182402 Hartree
no imaginary frequency



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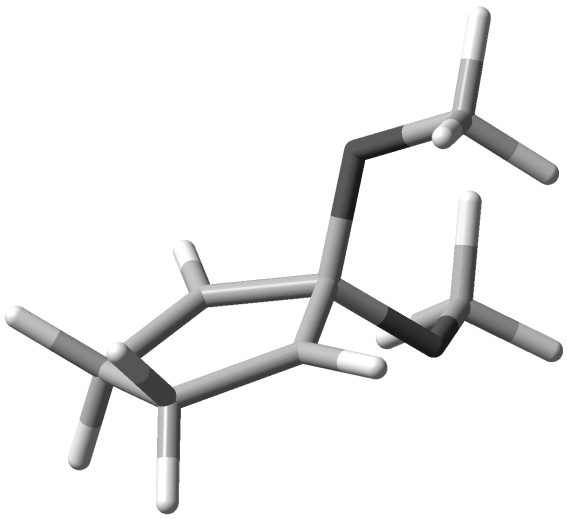
singlet 2,2-dimethoxycyclopentane-1,3-diyl (S-**DR1b**)
BS-UB3LYP/cc-PVDZ, C_2 symmetry

Nuclear repulsion energy: 484.1588877830 Hartree
SCF Done: E(UB3LYP) = -424.292921020 Hartree
Sum of electronic and zero-point Energies = -424.118198 Hartree
S**2 before annihilation 0.8725, after 0.0426
Zero-point correction: 0.174723 Hartree
no imaginary frequency



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C,0,-0.9583334456,1.4318802659,1.6201928268
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H,0,-0.456853352,-3.3788880264,-0.3412401842
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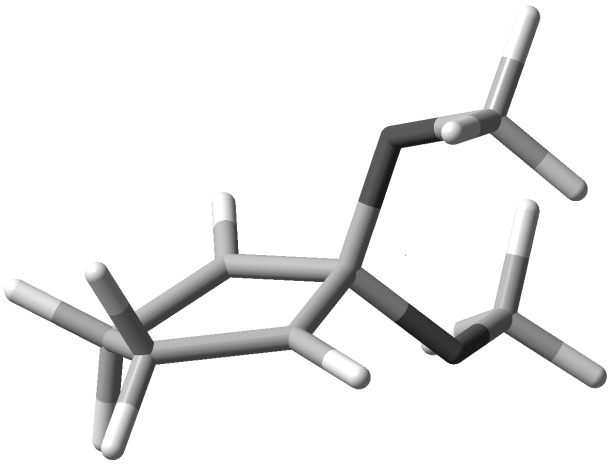
Triplet 2,2-dimethoxycyclopentane-1,3-diyl (T-**DR1b**)
BS-UB3LYP/cc-PVDZ, C_2 symmetry

Nuclear repulsion energy: 484.7067954058 Hartree
SCF Done: E(UB3LYP) = -424.287411406 Hartree
Sum of electronic and zero-point Energies= -424.112920 Hartree
S**2 before annihilation 2.0082, after 2.0000Zero-point correction: 0.174491 Hartree
no imaginary frequency



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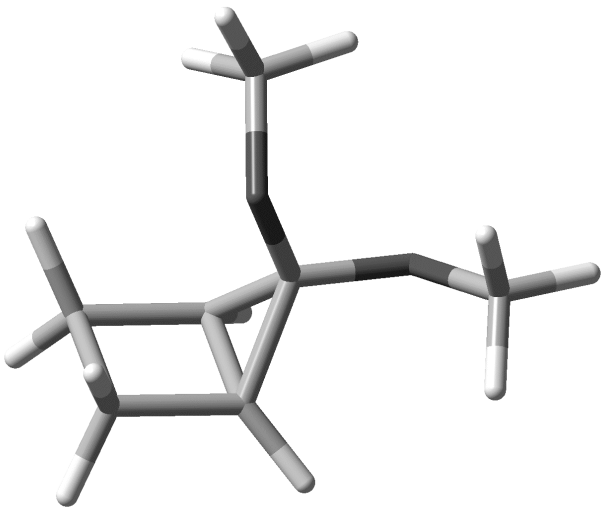
H,0,0.9522213145,0.0074156149,-3.2866448633

5,5-dimethoxybicyclo[2.1.0]pentane (**CP1b**)
RB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 494.4930278473 Hartree
SCF Done: E(RB3LYP) = -424.341093341 Hartree
Sum of electronic and zero-point Energies = -424.161166 Hartree
Zero-point correction: 0.179927 Hartree
no imaginary frequency



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H,0,-3.0986103466,-0.1869804266,1.0059799091
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O,0,1.3935757896,0.6800724444,0.6908108473
C,0,0.9101953976,-2.0924449014,0.0150162138
H,0,1.8872337257,-1.8952066556,0.4877189581
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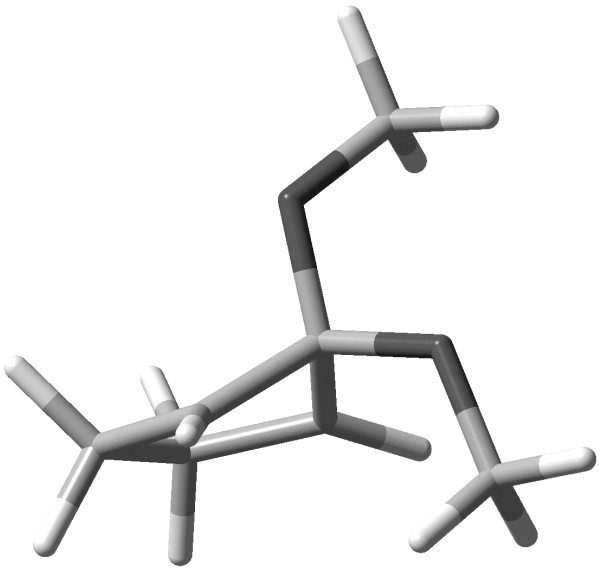
Transition state for the ring-closing reaction (**TS1b**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 486.9966375367 Hartree
SCF Done: E(UB3LYP) = -424.290712541 Hartree
Sum of electronic and zero-point Energies = -424.115735 Hartree
S**2 before annihilation 0.6070, after 0.0164
Zero-point correction: 0.179927 Hartree
1 imaginary frequency: -191.7384



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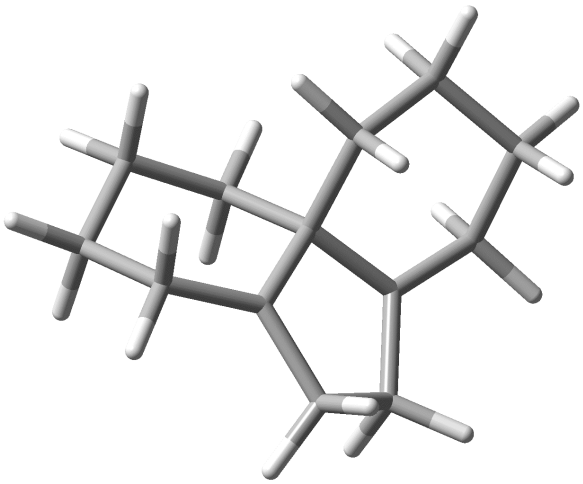
singlet dodecahydrobenzoindene-4,6-diyl (S-**DR2a**)
BS-UB3LYP/cc-PVDZ, C_2 symmetry

Nuclear repulsion energy: 854.5284019382 Hartree
SCF Done: E(UB3LYP) = -507.357450860 Hartree
Sum of electronic and zero-point Energies = -507.060030 Hartree
S**2 before annihilation 1.0045, after 0.0673
Zero-point correction: 0.297482 Hartree
no imaginary frequency



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H,0,1.4861067298,0.296874525,2.6163051109
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C,0,-0.2738773264,2.9888873137,-0.5509526388
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singlet dodecahydrobenzoindene-4,6-diyl (S-**DR2a**)
UCCSD/6-31G(d), C_2 symmetry

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Nuclear repulsion energy: 857.1452201876 Hartree
E(CORR)=     -505.65071507   Hartree

S**2 before annihilation     1.0294,   after
0.2453

S**2, projected HF & approx projected MPn
energies after annihilation of
 unwanted spin states (see manual for
definitions):

 spins       (S**2,0) (S**2,1)    PUHF
PMP2        PMP3        PMP4
 annihilated
 s+1        -0.12684 -0.03224 -503.892510 -
505.544194 -505.647417
 s+1,s+2     0.00234 -0.00101 -503.876376 -
505.528245 -505.631605
 s+1 to s+3 -0.00002  0.00002 -503.876663 -
505.528530 -505.631889
 s+1 to s+4  0.00000  0.00000 -503.876661 -
505.528528 -505.631886
 s+1 to s+5  0.00000  0.00000 -503.876661
 s+1 to s+6 -0.00001  0.00000 -503.876661
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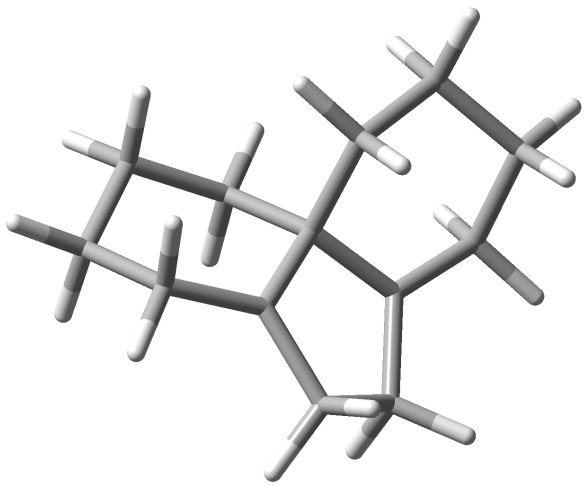


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.117071
2	6	0	0.838628	-0.827375	-0.830574
3	6	0	0.668979	-0.390369	-2.257538
4	6	0	-0.668979	0.390369	-2.257538
5	6	0	-0.838628	0.827375	-0.830574
6	1	0	1.491060	0.276078	-2.579243
7	1	0	0.671257	-1.237883	-2.959608
8	1	0	-1.491060	-0.276078	-2.579243
9	1	0	-0.671257	1.237883	-2.959608
10	6	0	0.846821	0.961207	0.997945
11	1	0	1.374065	0.404414	1.785812
12	1	0	1.622717	1.413035	0.360797
13	6	0	-0.846821	-0.961207	0.997945
14	1	0	-1.622717	-1.413035	0.360797
15	1	0	-1.374065	-0.404414	1.785812
16	6	0	0.000000	2.083888	1.616358
17	1	0	0.648227	2.748066	2.206261
18	1	0	-0.729993	1.661126	2.322966
19	6	0	-1.630365	1.991560	-0.328733
20	1	0	-2.488458	1.648865	0.279449
21	1	0	-2.055144	2.563884	-1.165710
22	6	0	-0.741456	2.896846	0.548170
23	1	0	-1.347651	3.684089	1.019547
24	1	0	-0.004744	3.401499	-0.095252
25	6	0	0.000000	-2.083888	1.616358
26	1	0	-0.648227	-2.748066	2.206261
27	1	0	0.729993	-1.661126	2.322966
28	6	0	1.630365	-1.991560	-0.328733
29	1	0	2.055144	-2.563884	-1.165710
30	1	0	2.488458	-1.648865	0.279449
31	6	0	0.741456	-2.896846	0.548170
32	1	0	1.347651	-3.684089	1.019547
33	1	0	0.004744	-3.401499	-0.095252

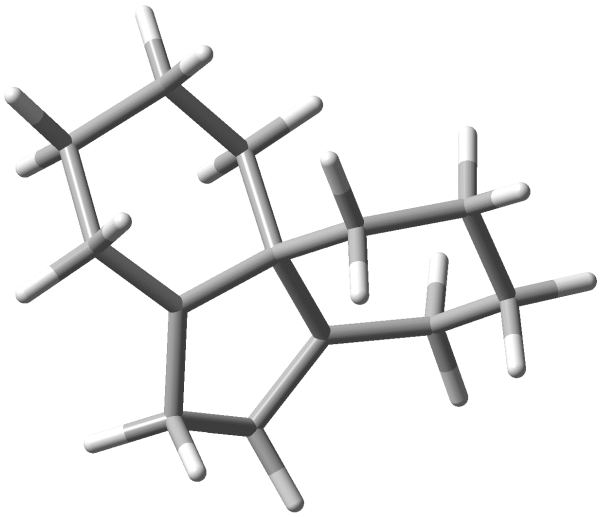
triplet dodecahydrobenzoindene-4,6-diyl (T-**DR2a**)
UB3LYP/ cc-PVDZ, C_2 symmetry

Nuclear repulsion energy: 854.6022655976 Hartree

SCF Done: E(UB3LYP) = -507.357917670 Hartree
Sum of electronic and zero-point Energies=
-507.060392 Hartree

S**2 before annihilation 2.0089, after
2.0000 Zero-point correction: 0.297526 Hartree

no imaginary frequency



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C,0,0.4885936532,0.6031283473,2.2617692712
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C,0,-1.1226818076,0.6296917184,-1.005156754
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C,0,1.1226818076,-0.6296917184,-1.005156754
H,0,2.015074634,-0.7893991688,-0.3742915667
H,0,1.4247159588,0.0733774524,-1.7996661292
C,0,-0.7010480949,1.9745803224,-1.6198624111
H,0,-1.5348260956,2.3831642574,-2.2164998807
H,0,0.1336407418,1.8211050201,-2.3282053571
C,0,0.860566045,2.4288810972,0.3355757686
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H,0,1.0713533197,3.1147084902,1.1731020097
C,0,-0.2772583689,2.9898265958,-0.5500962638
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H,0,-1.1466449639,3.2262859663,0.090445846
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H,0,-0.0397361202,-3.9359014026,-1.0216504283
H,0,1.1466449639,-3.2262859663,0.090445846

triplet dodecahydrobenzoindene-4,6-diyl (T-**DR2a**)
UCCSD/6-31G(d), C_2 symmetry

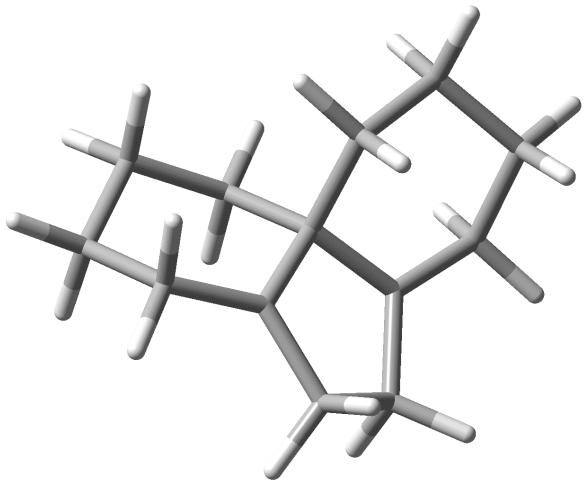
Nuclear repulsion energy: 857.1804414911 Hartree

E(CORR)= -505.65142953 Hartree

S**2 before annihilation 2.0337, after 2.0007

S**2, projected HF & approx projected MPn energies after annihilation of unwanted spin states (see manual for definitions):

spins	(S**2,0)	(S**2,1)	PUHF	PMP2	PMP3	PMP4
annihilated						
s+1	1.99953	2.00020	-503.876825	-505.526175	-505.627934	
s+1,s+2	2.00000	2.00000	-503.876756	-505.526113	-505.627878	
s+1 to s+3	2.00000	2.00000	-503.876756	-505.526113	-505.627878	
s+1 to s+4	2.00000	2.00000	-503.876756	-505.526120	-505.627890	
s+1 to s+5	2.00000	2.00000	-503.876756			
s+1 to s+6	2.00000	2.00000	-503.876756			



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.114366
2	6	0	0.840161	-0.825732	-0.828778
3	6	0	0.671014	-0.386760	-2.256320
4	6	0	-0.671014	0.386760	-2.256320
5	6	0	-0.840161	0.825732	-0.828778
6	1	0	1.491338	0.283470	-2.574590
7	1	0	0.677651	-1.232823	-2.959906
8	1	0	-1.491338	-0.283470	-2.574590
9	1	0	-0.677651	1.232823	-2.959906
10	6	0	0.846464	0.962114	0.998004
11	1	0	1.372135	0.403053	1.785193
12	1	0	1.623390	1.413636	0.362061
13	6	0	-0.846464	-0.962114	0.998004
14	1	0	-1.623390	-1.413636	0.362061
15	1	0	-1.372135	-0.403053	1.785193
16	6	0	0.000000	2.084759	1.616151
17	1	0	0.648687	2.747606	2.207080
18	1	0	-0.731391	1.662615	2.321685
19	6	0	-1.628311	1.993557	-0.329012
20	1	0	-2.487946	1.654437	0.279024
21	1	0	-2.050921	2.565323	-1.167456
22	6	0	-0.738637	2.898569	0.547088
23	1	0	-1.343847	3.687327	1.017155
24	1	0	-0.000333	3.401167	-0.096133
25	6	0	0.000000	-2.084759	1.616151
26	1	0	-0.648687	-2.747606	2.207080
27	1	0	0.731391	-1.662615	2.321685
28	6	0	1.628311	-1.993557	-0.329012
29	1	0	2.050921	-2.565323	-1.167456
30	1	0	2.487946	-1.654437	0.279024
31	6	0	0.738637	-2.898569	0.547088
32	1	0	1.343847	-3.687327	1.017155
33	1	0	0.000333	-3.401167	-0.096133

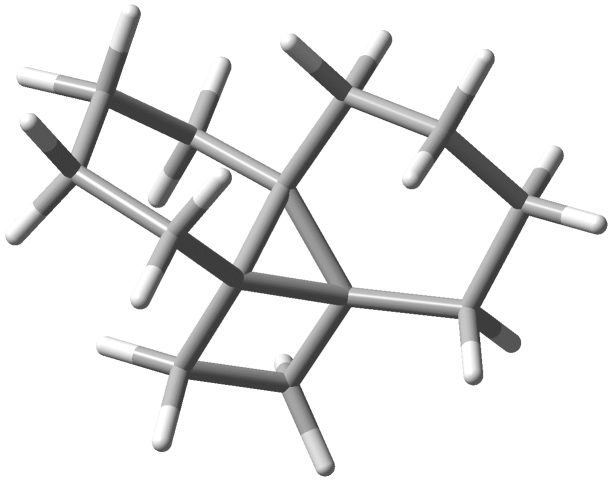
decahydrocyclobuta[2,3]cyclopropa[1,2:1,3]dibenzene (**CP2a**)
UB3LYP/ cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 877.0671000839 Hartree

SCF Done: E(RB3LYP) = -507.361018817 Hartree
Sum of electronic and zero-point Energies= -507.059383 Hartree

Zero-point correction: 0.301635 Hartree

no imaginary frequency



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C,0,-1.2943078711,0.634633304,1.9777513033
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H,0,-2.078356316,1.3663740107,1.7223228183
H,0,-1.5597969351,0.1573064375,2.9328611082
C,0,-0.3652882844,1.7314133948,-0.8778371868
H,0,-0.6911864948,2.4532684267,-0.1151037881
H,0,-0.9955294975,1.9087648787,-1.7674306344
C,0,1.1380136945,1.9731723026,-1.2576580748
H,0,1.3096834066,3.0548600947,-1.3910576447
H,0,1.3168067456,1.5281385506,-2.250724606
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H,0,3.1930519737,1.4174734415,-0.7935253062
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C,0,1.9530350276,0.0273116498,0.3777518219
H,0,2.65872713,-0.1324707711,1.2118715915
H,0,2.1245422999,-0.7805456272,-0.3489389472
C,0,-0.2267049236,-0.7032405384,-1.5282993178
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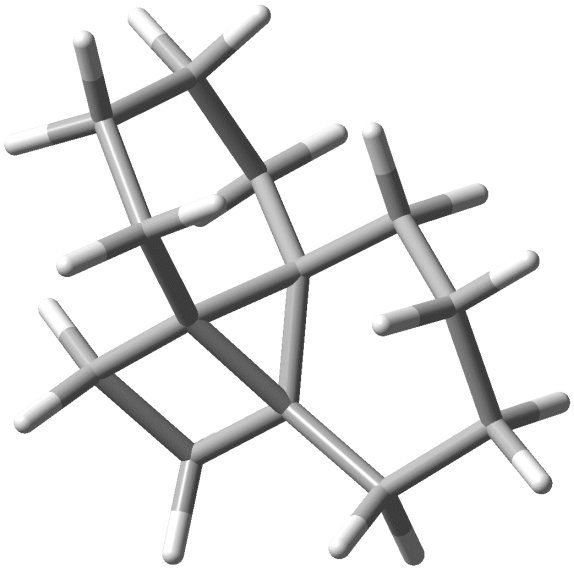
H,0,-2.674906257,-1.6382196657,1.2321665635
H,0,-1.0405960553,-0.5009857605,-2.2500629219
C,0,-0.2793061667,-2.194830626,-1.1727452201
H,0,-0.211815636,-2.7857563454,-2.101718471
H,0,0.5906008406,-2.484946801,-0.5563981855
C,0,-1.5724782367,-2.5152701582,-0.4260021696
H,0,-1.6768639697,-3.5986807694,-0.25180602
H,0,-2.4267230614,-2.2151808122,-1.0598036479

decahydrocyclobuta[2,3]cyclopropa[1,2:1,3]dibenzene (**CP2a**)
CCSD/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 881.0499847105 Hartree
E(CORR)= -505.66018655 Hartree



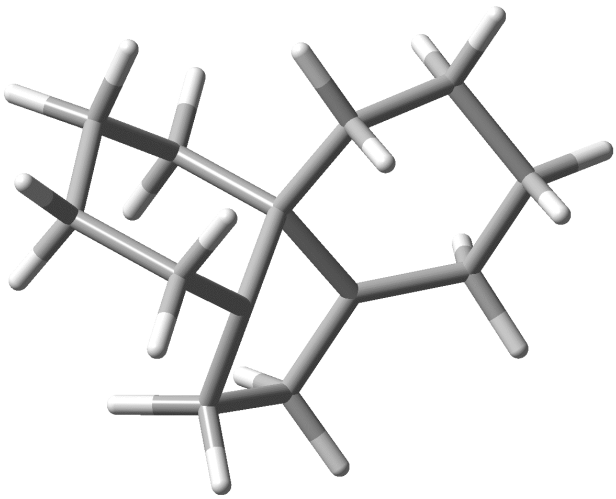
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.029012	-0.167191	-0.618556
2	6	0	0.414407	0.547553	0.651837
3	6	0	0.987629	1.942780	0.346441
4	6	0	-0.289015	2.315646	-0.440186
5	6	0	-0.886942	0.945651	-0.136014
6	1	0	1.080754	2.526678	1.272036
7	1	0	1.942470	2.013245	-0.189890
8	1	0	-0.164047	2.535703	-1.509003
9	1	0	-0.854999	3.135665	0.018978
10	6	0	1.219325	-0.235215	-1.558731
11	1	0	1.566911	0.759977	-1.858567
12	1	0	1.008301	-0.786507	-2.487619
13	6	0	2.324579	-0.991335	-0.748937
14	1	0	3.298487	-0.846614	-1.238628
15	1	0	2.121265	-2.067674	-0.820403
16	6	0	2.493834	-0.619267	0.761748
17	1	0	3.078136	-1.417404	1.242509
18	1	0	3.113421	0.284990	0.829196
19	6	0	1.189420	-0.350022	1.581178
20	1	0	1.449271	0.129001	2.536989
21	1	0	0.669665	-1.284621	1.818840
22	6	0	-0.599976	-1.559175	-0.431274
23	1	0	0.145663	-2.282696	-0.078639
24	6	0	-2.372812	0.797706	0.127575
25	1	0	-2.578068	1.173501	1.141622
26	1	0	-2.909500	1.469150	-0.560379
27	1	0	-0.899058	-1.905439	-1.434233
28	6	0	-1.837996	-1.623573	0.469686
29	1	0	-2.233188	-2.649252	0.458653
30	1	0	-1.577304	-1.398633	1.514349
31	6	0	-2.890888	-0.634969	-0.020920
32	1	0	-3.838913	-0.755594	0.521193
33	1	0	-3.102722	-0.845004	-1.080075

Transition state for the ring-closing reaction (**TS2a**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 863.5917958884 Hartree
SCF Done: E(UB3LYP) = -507.340607989 Hartree
Sum of electronic and zero-point Energies =-507.041948Hartree
S**2 before annihilation 0.3327, after 0.0039

Zero-point correction: 0.298660 Hartree
1 imaginary frequency: -400.6326



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C,0,0.3566062986,2.2478584674,0.5589776176
C,0,-0.9890137121,2.052999487,-0.1608973857
C,0,-0.7904854305,0.6600724128,-0.7130999539
H,0,0.2479801089,2.37729074,1.6562134402
H,0,0.9168130968,3.1218520159,0.1900444566
H,0,-1.1101473631,2.7904810258,-0.972335817
H,0,-1.8805495346,2.1626827182,0.4925113885
C,0,-0.8272469357,-0.6188157837,1.4328863448
H,0,-0.2976481391,-1.3051515297,2.1180833388
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C,0,0.6501785793,-1.4405098405,-0.4836451283
H,0,0.6378203253,-1.2896155299,-1.5773184154
H,0,0.0471659825,-2.3382733629,-0.2848652239
C,0,-2.1140366541,-1.3003083822,0.8947389627
H,0,-2.8224126065,-1.4648951752,1.7247313415
H,0,-1.8597125408,-2.3080864887,0.5221137705
C,0,-1.9178371593,-0.0568573374,-1.4010719544
H,0,-1.5666188295,-0.9318980819,-1.972153045
H,0,-2.4823980101,0.5850938551,-2.0981794796
C,0,-2.8453633621,-0.5285847256,-0.2347138743
H,0,-3.6561405374,-1.1608173246,-0.6375213489
H,0,-3.3378079738,0.3608406078,0.1960573779
C,0,2.1041777008,-1.6876900126,-0.0616863789
H,0,2.4721898706,-2.62536695,-0.5112128232
H,0,2.1660177399,-1.821426956,1.0353060162
C,0,2.5024603255,0.793920645,0.1506611173
H,0,2.9766459668,1.6697703388,-0.3266045957
H,0,2.8515436625,0.8138860792,1.2093652484
C,0,2.984943645,-0.5129687246,-0.4932457227
H,0,4.0418303847,-0.6897151851,-0.2344226865
H,0,2.9371535547,-0.4184641851,-1.5930732273

singlet decahydrocyclopentadipyran-4,6-diyl (S-**DR2b**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

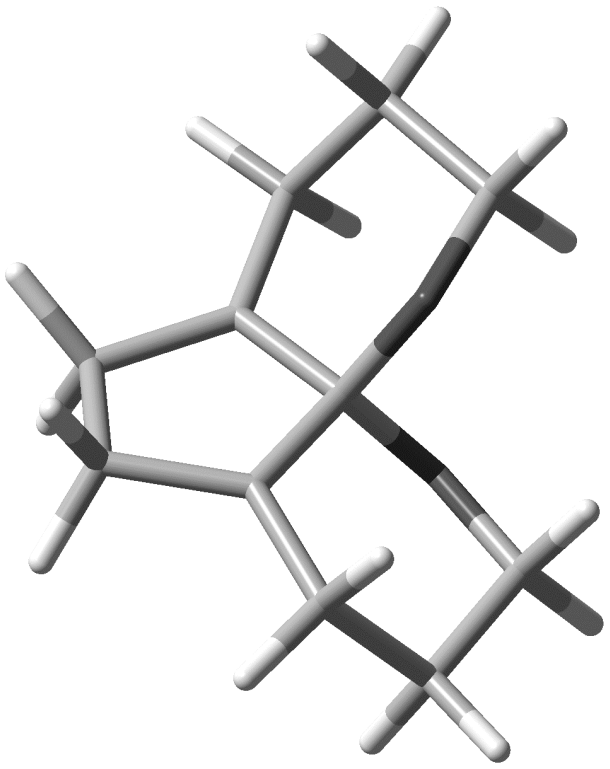
Nuclear repulsion energy: 878.6534846595 Hartree
SCF Done: E(UB3LYP) = -579.168502412 Hartree

Sum of electronic and zero-point Energies=
-578.918701

S**2 before annihilation 0.8989, after
0.0476

Zero-point correction: 0.24980 Hartree

no imaginary frequency:



C,0,-0.0000013108,-0.0596422881,0.0000515532
C,0,0.6595187185,2.2949161534,-0.4120941934
C,0,-0.6581524899,2.2952481125,0.412423386
C,0,-1.0639441758,0.8613660017,0.4998776647
H,0,1.4483137049,2.9248427288,0.0405521083
H,0,0.4772731587,2.728512056,-1.4173186387
H,0,-1.4465292049,2.9258214714,-0.0400449131
H,0,-0.4756039558,2.7284480202,1.4177663646
O,0,0.4922380323,-0.9085682599,1.0605983447
O,0,-0.4925890121,-0.9085803114,-1.0602804715
C,0,-2.8221093727,-0.6700328148,-0.3303915294
H,0,-3.7135693023,-1.2539584674,-0.0430835443
C,0,-1.6732815322,-1.6213116292,-0.6765139151
H,0,-1.9333286345,-2.2532793112,-1.5393142347
H,0,-1.4523527396,-2.281138262,0.1830284738
C,0,1.672594751,-1.6219291482,0.6769732499
H,0,1.4513369319,-2.2818863109,-0.1823849364
H,0,1.9323945373,-2.2537873285,1.5399294783
C,0,2.8218458274,-0.6712676041,0.3305453113
H,0,3.7130202603,-1.2556781892,0.0433338262
H,0,3.0817008659,-0.0864404373,1.2298293846
C,0,2.4103966092,0.2951865738,-0.8071639969
H,0,2.3716467658,-0.2750243462,-1.7575360168
H,0,3.1634348863,1.0886674985,-0.9429074561
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H,0,-3.0816386939,-0.0853176106,-1.2298415877
C,0,-2.4102886297,0.2965228802,0.8070915755
H,0,-2.3719496676,-0.2734386588,1.7576360927
H,0,-3.1629381239,1.0904255664,0.9425363676

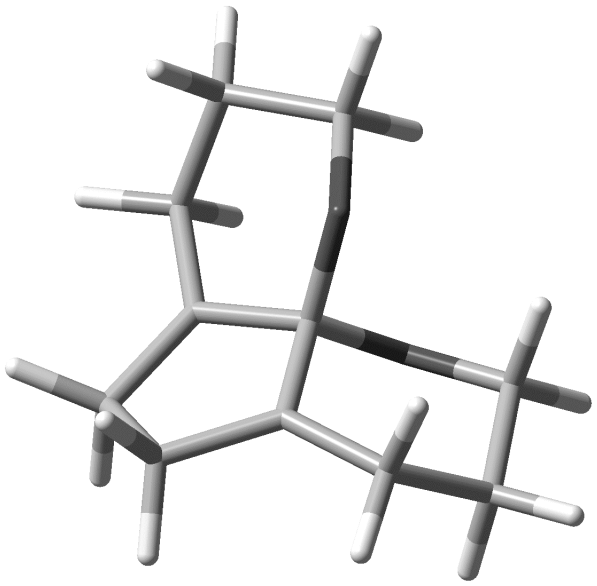
singlet decahydrocyclopentadipyran-4,6-diyl (S-**DR2b**)
UCCSD/6-31G(d), C_2 symmetry

Nuclear repulsion energy: 881.1927587380 Hartree

E(CORR)= -577.35356364 Hartree

S**2 before annihilation 1.0101, after 0.2232

spins	(S**2,0)	(S**2,1)	PUHF	PMP2	PMP3	PMP4
annihilated						
s+1	-0.11495	-0.02826	-575.532924	-577.267001	-577.348880	
s+1,s+2	0.00199	-0.00088	-575.517949	-577.252239	-577.334313	
s+1 to s+3	-0.00002	0.00002	-575.518198	-577.252486	-577.334557	
s+1 to s+4	0.00000	0.00000	-575.518197	-577.252484	-577.334554	
s+1 to s+5	0.00000	0.00000	-575.518197			
s+1 to s+6	0.00000	0.00000	-575.518197			



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.061893
2	6	0	0.224512	0.743754	-2.290782
3	6	0	-0.224512	-0.743754	-2.290782
4	6	0	-0.136829	-1.168089	-0.857532
5	1	0	-0.394132	1.372963	-2.948848
6	1	0	1.257286	0.825102	-2.672646
7	1	0	0.394132	-1.372963	-2.948848
8	1	0	-1.257286	-0.825102	-2.672646
9	8	0	-1.159539	0.121433	0.896424
10	8	0	1.159539	-0.121433	0.896424
11	6	0	1.202259	-2.558403	0.678211
12	1	0	1.220448	-3.490015	1.262275
13	6	0	1.155151	-1.358399	1.623797
14	1	0	2.046034	-1.324753	2.261120
15	1	0	0.266232	-1.408684	2.268735
16	6	0	-1.155151	1.358399	1.623797
17	1	0	-0.266232	1.408684	2.268735
18	1	0	-2.046034	1.324753	2.261120
19	6	0	-1.202259	2.558403	0.678211
20	1	0	-1.220448	3.490015	1.262275
21	1	0	-2.135187	2.509828	0.100071
22	6	0	0.000000	2.541849	-0.289277
23	1	0	0.913240	2.813110	0.268315
24	1	0	-0.124034	3.291664	-1.082597
25	6	0	0.136829	1.168089	-0.857532
26	1	0	2.135187	-2.509828	0.100071
27	6	0	0.000000	-2.541849	-0.289277
28	1	0	-0.913240	-2.813110	0.268315
29	1	0	0.124034	-3.291664	-1.082597

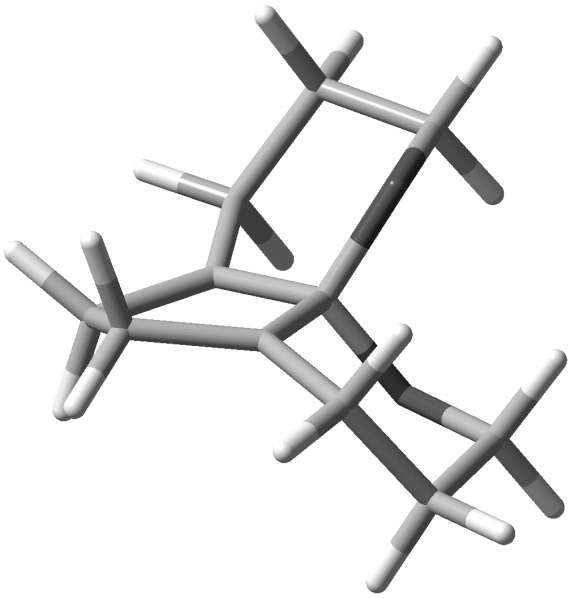
triplet decahydrocyclopentadipyran-4,6-diyl (T-**DR2b**)
UB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 877.8225663665 Hartree
SCF Done: E(UB3LYP) = -579.164572556 Hartree

Sum of electronic and zero-point Energies= -578.914753

S**2 before annihilation 2.0085, after 2.0000
Zero-point correction: 0.249820 Hartree

no imaginary frequency:



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C,0,-0.8290287573,0.8320585571,2.027988781
C,0,-1.1607203225,-0.0001018056,0.8259443546
H,0,1.1489537836,1.7769579202,2.444550867
H,0,0.1382643542,2.6659991996,1.2979629692
H,0,-1.6682511902,1.4760947823,2.3437105581
H,0,-0.5938512378,0.1873056186,2.9015781003
O,0,0.5255069006,-1.4166165409,-0.1534733794
O,0,-0.3528485092,0.3350212402,-1.4395654426
C,0,-2.7389949803,-0.0979964021,-1.0857032454
H,0,-3.6036211071,-0.6409551479,-1.5047453318
C,0,-1.4993198237,-0.3676387065,-1.9376420524
H,0,-1.6387822916,-0.0066605058,-2.9677027806
H,0,-1.2870726951,-1.4523285762,-1.9745962376
C,0,1.7975506129,-1.4991932984,-0.8102262724
H,0,1.703143541,-1.1493984496,-1.8550597711
H,0,2.0501158553,-2.5700655199,-0.8248528955
C,0,2.8647803926,-0.6903371494,-0.0739626802
H,0,3.8319592814,-0.7879080849,-0.5964803953
H,0,2.9884134524,-1.1058541696,0.9410030918
C,0,2.4413094193,0.795102551,0.0232134778
H,0,2.5542110678,1.2545206477,-0.9811239948
H,0,3.1084284786,1.3520738225,0.7016138936
C,0,1.020310433,0.8789670728,0.4652905882
H,0,-2.9693340834,0.9806736508,-1.124708149
C,0,-2.4850486731,-0.5199503888,0.3814898386
H,0,-2.4932109137,-1.6290541029,0.4300412387
H,0,-3.297528069,-0.1695015849,1.0391895853

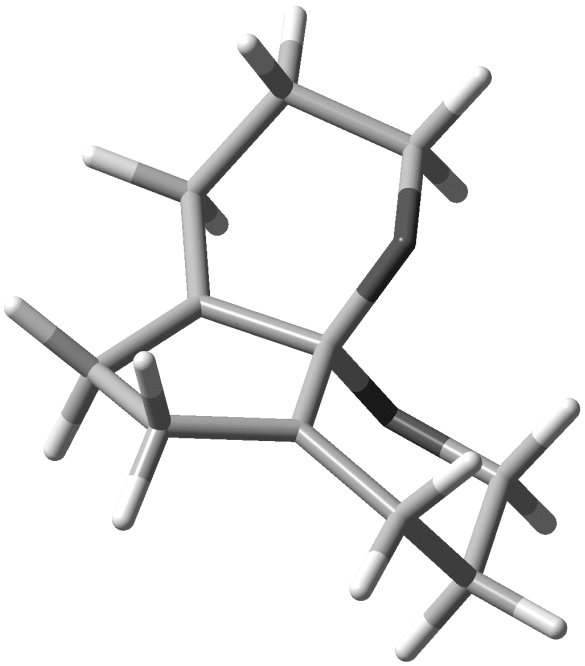
triplet decahydrocyclopentadipyran-4,6-diyl (T-**DR2b**)
UCCSD/6-31G(d), C_2 symmetry

Nuclear repulsion energy: 880.4973926191 Hartree

E(CORR)= -577.35083990 Hartree

S**2 before annihilation 2.0310, after 2.0006

spins	(S**2,0)	(S**2,1)	PUHF	PMP2	PMP3	PMP4
annihilated						
s+1	1.99961	2.00018	-575.513707	-577.244251	-577.325289	
s+1,s+2	2.00000	2.00000	-575.513648	-577.244198	-577.325242	
s+1 to s+3	2.00000	2.00000	-575.513648	-577.244198	-577.325242	
s+1 to s+4	2.00000	2.00000	-575.513648	-577.244194	-577.325235	
s+1 to s+5	2.00000	2.00000	-575.513648			
s+1 to s+6	2.00000	2.00000	-575.513648			



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.072505
2	6	0	0.278194	0.725575	-2.272242
3	6	0	-0.278194	-0.725575	-2.272242
4	6	0	-0.165771	-1.174166	-0.843430
5	1	0	-0.266534	1.386399	-2.962109
6	1	0	1.331077	0.727714	-2.606404
7	1	0	0.266534	-1.386399	-2.962109
8	1	0	-1.331077	-0.727714	-2.606404
9	8	0	-1.160277	0.139770	0.897373
10	8	0	1.160277	-0.139770	0.897373
11	6	0	1.211414	-2.572177	0.659415
12	1	0	1.241515	-3.510005	1.232789
13	6	0	1.156379	-1.383425	1.615549
14	1	0	2.043918	-1.348483	2.257175
15	1	0	0.264106	-1.440422	2.255454
16	6	0	-1.156379	1.383425	1.615549
17	1	0	-0.264106	1.440422	2.255454
18	1	0	-2.043918	1.348483	2.257175
19	6	0	-1.211414	2.572177	0.659415
20	1	0	-1.241515	3.510005	1.232789
21	1	0	-2.140024	2.507611	0.075985
22	6	0	0.000000	2.552446	-0.295467
23	1	0	0.902158	2.846222	0.269749
24	1	0	-0.123151	3.288177	-1.102095
25	6	0	0.165771	1.174166	-0.843430
26	1	0	2.140024	-2.507611	0.075985
27	6	0	0.000000	-2.552446	-0.295467
28	1	0	-0.902158	-2.846222	0.269749
29	1	0	0.123151	-3.288177	-1.102095

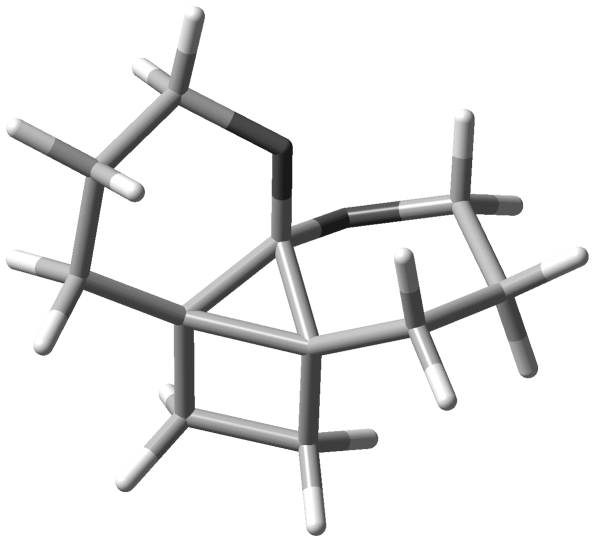
octahydrocyclobuta[2,3]cyclopropa[1,2-*b*:1,3-*b*′]dipyran (**CP2b**)
UB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 898.1459967287 Hartree
SCF Done: E(UB3LYP) = -579.166001285 Hartree

Sum of electronic and zero-point Energies= -578.912665

Zero-point correction: 0.253336 Hartree

no imaginary frequency:



C,0,0.0122347931,-0.6036121827,-0.0281193788
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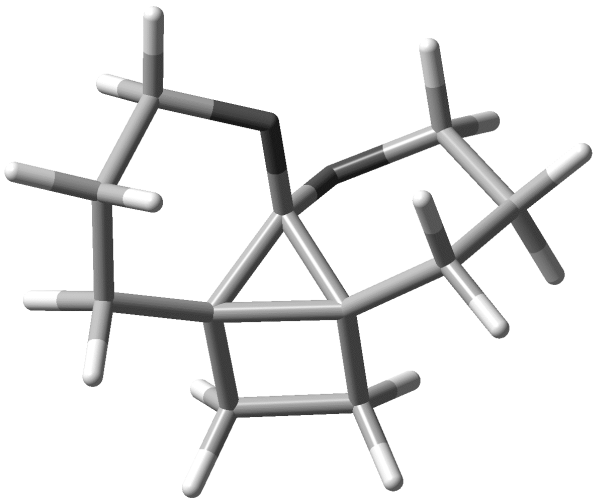
C,0,-0.7799073488,0.1913734495,2.1906759178
C,0,-1.0346690286,0.196598052,0.6903770337
H,0,1.4566907688,-0.036017085,2.3379513638
H,0,0.8685868951,1.6543576107,2.4072873999
H,0,-1.3963425637,0.9350931516,2.7166756333
H,0,-0.9103187613,-0.7892175285,2.6744800319
O,0,0.8303313473,-1.6705459095,0.3519498819
O,0,-0.1988607661,-0.6207552907,-1.4287470891
C,0,-2.4269310431,0.3015091368,-1.4320590853
H,0,-3.4595336714,0.1562940538,-1.7907513199
C,0,-1.5443516626,-0.873754933,-1.8323106677
H,0,-1.5078361611,-1.0053144041,-2.9238407287
H,0,-1.9106463907,-1.8184955684,-1.3840953012
C,0,2.1092523446,-1.4118444319,-0.3122023968
H,0,1.994370479,-1.7003718036,-1.3694883017
H,0,2.8228732579,-2.1005565029,0.1618292443
C,0,2.6575829637,0.0493308767,-0.2341532982
H,0,3.464065146,0.12410541,-0.9837958769
H,0,3.1357075006,0.2004021506,0.7473414222
C,0,1.6055565026,1.1920258295,-0.4496082038
H,0,1.2881505654,1.2369534205,-1.4993940844
H,0,2.038935892,2.167084338,-0.1718015223
C,0,0.4837194264,0.7283829105,0.4547769661
H,0,-2.032485192,1.2102935434,-1.917657277
C,0,-2.3984343357,0.4557419846,0.0936532234
H,0,-3.0906933649,-0.2791822788,0.5491163516
H,0,-2.7574843117,1.4522289618,0.4018760533

octahydrocyclobuta[2,3]cyclopropa[1,2-*b*:1,3-*b*']dipyran (**CP2b**)
CCSD/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 901.8769103624 Hartree
E(CORR)= -577.35674957 Hartree



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.025942	-0.192436	-0.441739
2	6	0	-1.090238	1.947144	0.075038
3	6	0	0.250915	2.258424	-0.631925
4	6	0	0.857313	0.967103	-0.103828
5	1	0	-1.955494	1.830635	-0.587219
6	1	0	-1.335152	2.681332	0.852988
7	1	0	0.754053	3.144150	-0.225557
8	1	0	0.219813	2.337072	-1.725659
9	8	0	-0.961680	-0.411834	-1.453646
10	8	0	0.504277	-1.418088	0.018381
11	6	0	2.706842	-0.628625	0.556337
12	1	0	3.784184	-0.800409	0.424793
13	6	0	1.890043	-1.598341	-0.283739
14	1	0	2.111499	-2.643255	-0.040595
15	1	0	2.068282	-1.445908	-1.360166
16	6	0	-2.021151	-1.171055	-0.786220
17	1	0	-1.677301	-2.207969	-0.702076
18	1	0	-2.869954	-1.139691	-1.477189
19	6	0	-2.478078	-0.658473	0.617487
20	1	0	-3.071633	-1.468934	1.065051
21	1	0	-3.165911	0.184793	0.476983
22	6	0	-1.346199	-0.201454	1.594851
23	1	0	-0.783517	-1.057913	1.976330
24	1	0	-1.775887	0.341350	2.448123
25	6	0	-0.514207	0.656242	0.671540
26	1	0	2.466458	-0.810733	1.612315
27	6	0	2.333615	0.803626	0.163165
28	1	0	2.858205	1.075145	-0.768001
29	1	0	2.654106	1.526771	0.926202

Transition state for the ring-closing reaction (**TS2b**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

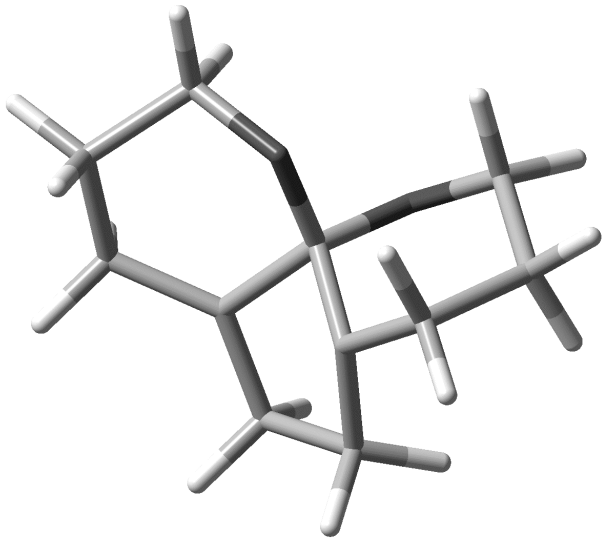
Nuclear repulsion energy: 888.7073768999 Hartree
SCF Done: E(UB3LYP) = -579.154853988 Hartree

Sum of electronic and zero-point Energies =-578.904018Hartree

S**2 before annihilation 0.1533, after 0.0007

Zero-point correction: 0.250836 Hartree

1 imaginary frequency: -388.2754



C,0,0.0148091147,-0.1303715044,-0.1862455882
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C,0,0.3771784304,2.2644648846,-0.5443425733
C,0,1.0171297396,0.9609860277,-0.1822317786
H,0,-1.8649824873,2.1888385083,-0.4789266076
H,0,-1.084826841,2.8224954499,0.9836050601
H,0,0.944587007,3.1309850163,-0.1698580558
H,0,0.2668402878,2.3880497488,-1.6396123086
O,0,-0.691119316,-0.5306548917,-1.3742430937
O,0,0.4833682014,-1.3079639821,0.4721085703
C,0,2.8121058888,-0.6614067585,0.5069397887
H,0,3.8336442224,-0.9804909752,0.2420279179
C,0,1.788600781,-1.6971983068,0.0503489231
H,0,1.9766112258,-2.6789365584,0.5100608356
H,0,1.8121243861,-1.8230980783,-1.0501777259
C,0,-1.8445064651,-1.2879032047,-0.9543793071
H,0,-1.5128444722,-2.2791912348,-0.5992180402
H,0,-2.4536989639,-1.4327197067,-1.8592874932
C,0,-2.7066819151,-0.6140866231,0.1474913428
H,0,-3.4714214176,-1.3414650362,0.4732517725
H,0,-3.2496215192,0.2397498035,-0.2922869803
C,0,-1.887104533,-0.0998212664,1.3784188022
H,0,-1.4713631798,-0.952339079,1.9360678737
H,0,-2.5232975145,0.4884843008,2.0589335953
C,0,-0.794125892,0.6897164483,0.7185798542
H,0,2.7574421526,-0.5876242714,1.6060075218
C,0,2.4885717957,0.7033772387,-0.121749806
H,0,2.8711824626,0.7230734076,-1.1665218268
H,0,3.0117860209,1.5226261374,0.400846892

Transition state for the migration reaction (**TS2b**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

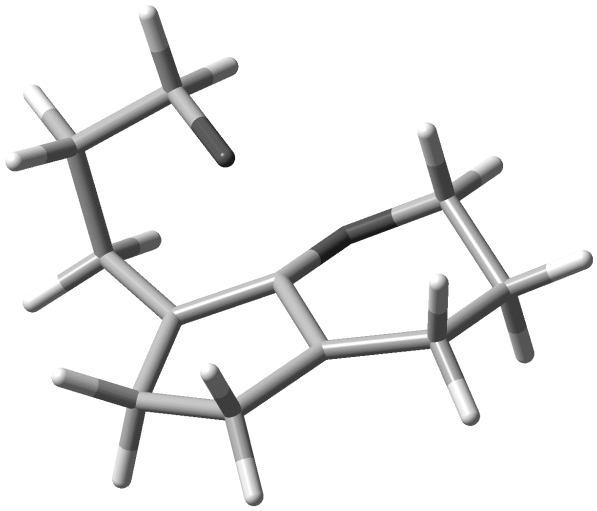
Nuclear repulsion energy: 874.2784951877 Hartree
SCF Done: E(UB3LYP) = -579.151491602 Hartree

Sum of electronic and zero-point Energies =-578.903164Hartree

S**2 before annihilation 0.6920, after 0.0323

Zero-point correction: 0.248327 Hartree

1 imaginary frequency: -566.4544



C,0,-0.164239898,0.0360016962,-0.2942987842
C,0,0.8862188711,2.1845307054,-0.2473351218
C,0,-0.4958974124,2.2854851099,0.4520773892
C,0,-1.157646972,0.9840800558,0.147989365
H,0,1.7203733144,2.4913127527,0.4085776184
H,0,0.9336681867,2.8490708394,-1.1314508291
H,0,-1.0863015779,3.1614254547,0.1306308037
H,0,-0.3475126164,2.3905510258,1.5461357617
O,0,0.6575087272,-0.6216959123,1.2813679027
O,0,-0.5331456746,-1.1216774498,-0.9129122994
C,0,-2.8791573716,-0.7402700128,-0.3064265927
H,0,-3.7629220969,-1.2400061329,0.1226463284
C,0,-1.7003451911,-1.7131319538,-0.3060215351
H,0,-1.9155337059,-2.6074606131,-0.9063132902
H,0,-1.433373266,-2.0137530324,0.7212622969
C,0,1.7097163298,-1.4637555396,0.92528984
H,0,1.380329711,-2.3074218763,0.2748009276
H,0,2.135911472,-1.9229609702,1.8438551357
C,0,2.8279617042,-0.688964877,0.1981124292
H,0,3.6593051275,-1.3537673908,-0.1001422435
H,0,3.2359802718,0.0692456914,0.8894449835
C,0,2.2514592641,0.0343155186,-1.0551247477
H,0,2.0094984794,-0.7245564266,-1.8195041557
H,0,2.9978309383,0.7235718627,-1.4820899904
C,0,1.0073838873,0.7507662379,-0.6578985782
H,0,-3.1215835748,-0.4799782391,-1.3509243596
C,0,-2.5386074549,0.539372177,0.4842554595
H,0,-2.6002692072,0.3280482301,1.5734231672
H,0,-3.2790752649,1.3352400692,0.290190119

singlet 1,7-dioxaspiro[5.5]undecane-5,11-diyl (S-**DR3**)
BS-UB3LYP/cc-PVDZ, C_2 symmetry

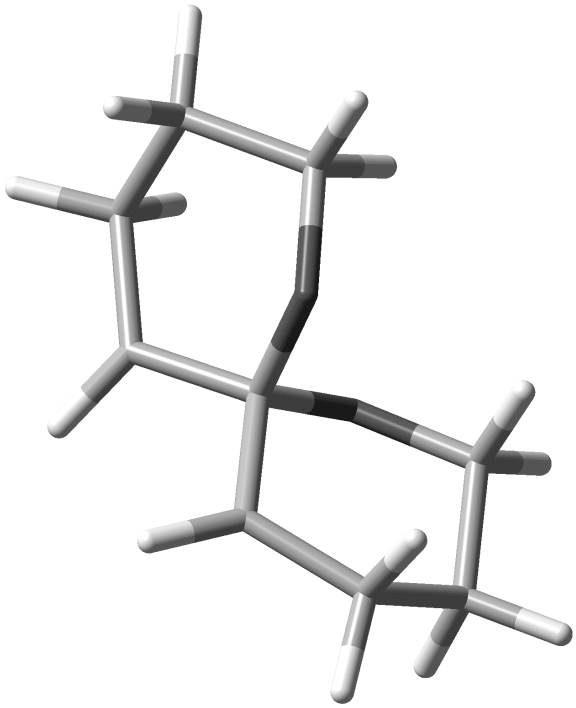
Nuclear repulsion energy: 670.6670606767 Hartree
SCF Done: E(UB3LYP) = -501.731238073 Hartree

Sum of electronic and zero-point Energies= -501.517853

S**2 before annihilation 0.9933, after 0.0563

Zero-point correction: 0.213385 Hartree

no imaginary frequency:



C,0,0.,0.,0.4457185297
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O,0,1.0727333954,0.4767386881,-0.3926480667
C,0,-0.8231949777,2.4330025877,0.6206630304
H,0,-1.7489318597,2.3623449028,0.0087491626
H,0,-1.0088487213,3.2176857173,1.3719994189
C,0,0.3502743432,2.8122419918,-0.3035822078
H,0,1.223786291,3.0973166391,0.3074924359
H,0,0.0873524596,3.6768670659,-0.936397824
C,0,0.7284199378,1.6223478017,-1.18188526
H,0,1.6219280659,1.837236162,-1.7872273199
H,0,-0.1036895507,1.3729138227,-1.8662967345
C,0,-0.7284199378,-1.6223478017,-1.18188526
H,0,0.1036895507,-1.3729138227,-1.8662967345
H,0,-1.6219280659,-1.837236162,-1.7872273199
C,0,-0.3502743432,-2.8122419918,-0.3035822078
H,0,-0.0873524596,-3.6768670659,-0.936397824
H,0,-1.223786291,-3.0973166391,0.3074924359
C,0,0.8231949777,-2.4330025877,0.6206630304
H,0,1.7489318597,-2.3623449028,0.0087491626
H,0,1.0088487213,-3.2176857173,1.3719994189
C,0,0.5631327624,-1.1164838515,1.2738568345
H,0,0.9569838964,-0.8814881114,2.2645285507
H,0,-0.9569838964,0.8814881114,2.2645285507

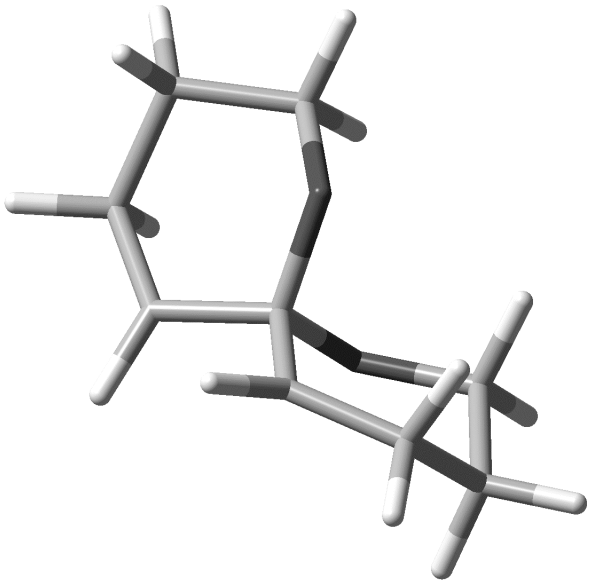
triplet 1,7-dioxaspiro[5.5]undecane-5,11-diyl (T-**DR3**)
UB3LYP/cc-PVDZ, C_2 symmetry

Nuclear repulsion energy: 668.8168887459 Hartree
SCF Done: E(UB3LYP) = -501.731670149 Hartree

Sum of electronic and zero-point Energies= -501.517929

S**2 before annihilation 2.0077, after 2.0000
Zero-point correction: 0.213746 Hartree

no imaginary frequency:



C,0,0.,0.,0.3845574409
C,0,-0.6144263897,1.0869753389,1.2214079082
O,0,-1.0580665978,-0.510317065,-0.4465073465
O,0,1.0580665978,0.510317065,-0.4465073465
C,0,-0.8075094306,2.451547331,0.6473666436
H,0,-1.7410112073,2.4588202827,0.0411235256
H,0,-0.9622160101,3.1957285731,1.446641895
C,0,0.3704094851,2.8428234861,-0.2612853012
H,0,1.2568527435,3.0730463073,0.3543185635
H,0,0.1281486558,3.7433066617,-0.8504367645
C,0,0.7074604207,1.6830087826,-1.1920745417
H,0,1.5870988444,1.9048833705,-1.8146980475
H,0,-0.1462762543,1.4640036345,-1.8603700438
C,0,-0.7074604207,-1.6830087826,-1.1920745417
H,0,0.1462762543,-1.4640036345,-1.8603700438
H,0,-1.5870988444,-1.9048833705,-1.8146980475
C,0,-0.3704094851,-2.8428234861,-0.2612853012
H,0,-0.1281486558,-3.7433066617,-0.8504367645
H,0,-1.2568527435,-3.0730463073,0.3543185635
C,0,0.8075094306,-2.451547331,0.6473666436
H,0,1.7410112073,-2.4588202827,0.0411235256
H,0,0.9622160101,-3.1957285731,1.446641895
C,0,0.6144263897,-1.0869753389,1.2214079082
H,0,1.1481628359,-0.7815526678,2.1243460739
H,0,-1.1481628359,0.7815526678,2.1243460739

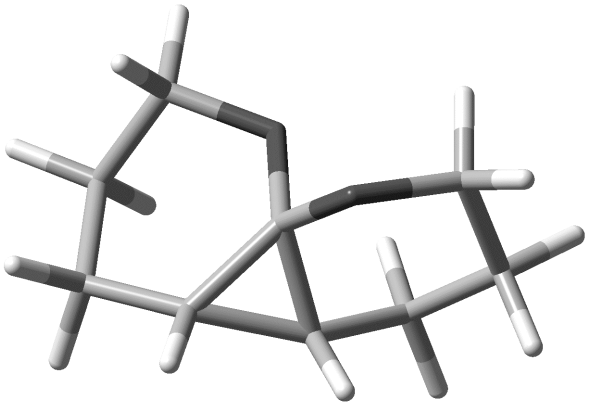
cis octahydrocyclopropa[1,2-*b*:1,3-*b*′]dipyran (**CP3**)
RB3LYP/cc-PVDZ, C_1 symmetry

Nuclear repulsion energy: 685.1924248047 Hartree
SCF Done: E(RB3LYP) = -501.755863798 Hartree

Sum of electronic and zero-point Energies= -501.536403

S**2 before annihilation 2.0078, after 2.0000
Zero-point correction: 0.219461 Hartree

no imaginary frequency:



C,0,-0.0767062099,-0.7245114444,0.303754083
C,0,0.5745148037,0.0094823436,1.4519313263
C,0,-0.7812106009,0.4771181671,0.8591148462
O,0,-0.9118617113,-1.8357258573,0.2138871601
C,0,-1.9235333693,-1.4435241232,-0.7732495668
H,0,-2.722831588,-2.1916444265,-0.6755442599
H,0,-1.4662806125,-1.5486734323,-1.7700056987
C,0,-2.5312042581,-0.0064359827,-0.6349170108
H,0,-3.3019070302,-0.0243068197,0.1555341748
H,0,-3.0595662281,0.2042224092,-1.5809159821
C,0,-1.5268001707,1.1463879072,-0.2823594642
H,0,-2.0787527589,2.0599880293,-0.0074157473
H,0,-0.8686891056,1.3758236768,-1.1304961999
O,0,0.5576059682,-0.498479033,-0.9410903281
C,0,1.9817667096,-0.4393491759,-0.9230824788
H,0,2.2866933495,-0.3769880151,-1.9781365991
H,0,2.4032903067,-1.3715180857,-0.4968731087
C,0,1.9681341413,0.6082323461,1.3262637828
H,0,2.6649608281,-0.0734816413,1.8471496344
H,0,2.0035853796,1.5674003146,1.8695092637
C,0,2.4336047306,0.7750356101,-0.1239612053
H,0,3.5295983573,0.8892787863,-0.1677872411
H,0,1.9895165264,1.6767208711,-0.5794164003
H,0,0.3827136354,-0.3966604829,2.4486343255
H,0,-1.5246410926,0.1396080586,1.5904726945

singlet 1,3-diphenylcyclopentane-1,3-diyl (S-**DR4a**)
BS-UB3LYP/6-31G(d), C_2 symmetry

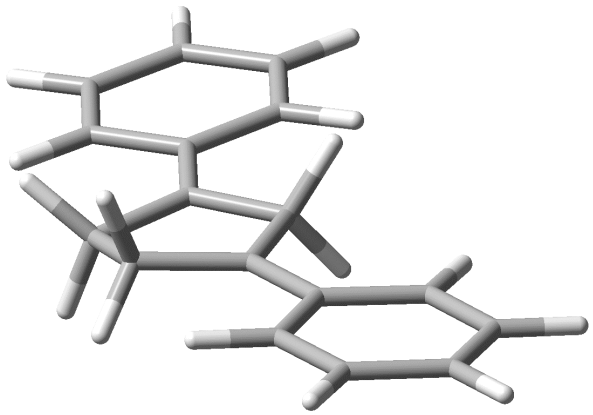
Nuclear repulsion energy: 1040.8102473352 Hartree
SCF Done: E(UB3LYP) = -657.379245278 Hartree

Sum of electronic and zero-point Energies= -657.103288

S**2 before annihilation 1.0485, after 0.4283

Zero-point correction: 0.275957 Hartree

no imaginary frequency:



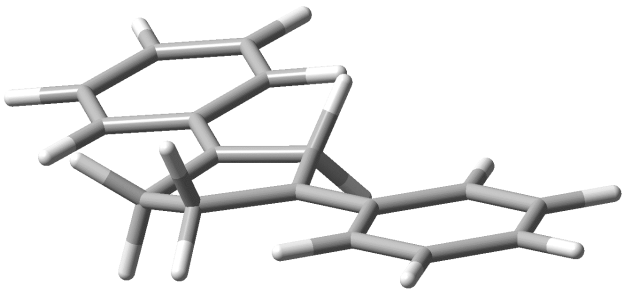
C,0,1.1660992209,-0.1601780435,-0.4485868552
C,0,-0.0253283822,-0.0462488307,0.4717096551
H,0,0.0111551767,0.8753977626,1.081302752
H,0,-0.0529239693,-0.8685364819,1.2102538605
C,0,-1.2288302883,-0.0673092784,-0.4396438789
C,0,-2.5752628973,-0.0439968803,0.0089171116
C,0,-5.2693750794,0.0027918631,0.9117584361
C,0,-3.6684137768,-0.0240237238,-0.9057985279
C,0,-2.89684139,-0.036189082,1.397732356
C,0,-4.2142089325,-0.014355199,1.8327211979
C,0,-4.9816247741,-0.0016991209,-0.4593014106
H,0,-3.4688608427,-0.0225594125,-1.9730648483
H,0,-2.0947302674,-0.0491996935,2.1294377879
H,0,-4.4260962627,-0.0100384661,2.89909775
H,0,-5.7930580982,0.0136805361,-1.1827922694
H,0,-6.2993194965,0.0205221577,1.2567162986
C,0,2.5183039542,-0.1188135966,-0.0191426047
C,0,5.2240576099,-0.0354179795,0.8454224195
C,0,2.8580644391,0.0768844868,1.3514550758
C,0,3.5993839631,-0.2739018599,-0.9352715258
C,0,4.9183545126,-0.2318310779,-0.5075721984
C,0,4.1810410373,0.1177470864,1.7676458163
H,0,2.0656014905,0.1979294011,2.0837773269
H,0,3.3858557408,-0.4317272036,-1.9880671401
H,0,5.720247582,-0.3540259421,-1.2315439888
H,0,4.4068919203,0.2697082877,2.8202486773
H,0,6.2584515581,-0.0034092315,1.1757256174
C,0,-0.7977442138,-0.0604420802,-1.8841904413
H,0,-0.978017899,0.9279404431,-2.33831211
H,0,-1.3612584939,-0.7768298774,-2.4960881559
C,0,0.7161238196,-0.3782827678,-1.8707492804
H,0,1.2708765032,0.2401384546,-2.5883732752
H,0,0.8913865357,-1.42272465,-2.177423628

triplet 1,3-diphenylcyclopentane-1,3-diyl (T-**DR4a**)
UB3LYP/6-31G(d), C_2 symmetry

Nuclear repulsion energy: 1040.7409382234 Hartree
SCF Done: E(UB3LYP) = -657.379621807 Hartree

Sum of electronic and zero-point Energies= -657.103730

S**2 before annihilation 2.0543, after 2.0018
Zero-point correction: 0.275892 Hartree



no imaginary frequency:

C,0,1.166620474,-0.1608492545,-0.4478505822
C,0,-0.0253590328,-0.0465872795,0.4672331075
H,0,0.0113676815,0.8743072758,1.0793274489
H,0,-0.0531660101,-0.8677644392,1.2081440555
C,0,-1.2293438701,-0.0665537424,-0.4390066918
C,0,-2.5762222738,-0.0449500273,0.009945567
C,0,-5.2712500745,0.0005715362,0.9108747542
C,0,-3.6685593485,-0.0201590892,-0.9052769549
C,0,-2.8990435253,-0.0429961718,1.3983741091
C,0,-4.216606055,-0.0216507622,1.8324859976
C,0,-4.9823062221,0.0016496124,-0.4597205415
H,0,-3.4682848763,-0.0143201752,-1.972380044
H,0,-2.0976863303,-0.0602840478,2.1309213818
H,0,-4.4291553703,-0.0218619276,2.8987439848
H,0,-5.7930050781,0.0209204328,-1.1839480041
H,0,-6.3014151923,0.0177218569,1.2551836541
C,0,2.5192760815,-0.117724433,-0.0182769107
C,0,5.2259200045,-0.0333277153,0.8441944124
C,0,2.8602691771,0.0836937545,1.3510655317
C,0,3.5995408097,-0.2776224309,-0.9341939474
C,0,4.9190347269,-0.2351661712,-0.5075100269
C,0,4.1834289053,0.1249243824,1.7663122964
H,0,2.0685670723,0.2090707634,2.0835865068
H,0,3.3852976294,-0.4397387999,-1.9861786939
H,0,5.7201874086,-0.3612955831,-1.2316336444
H,0,4.4099361366,0.2813351799,2.8181266337
H,0,6.2605257922,-0.000829346,1.1737662736
C,0,-0.7965636043,-0.0536690795,-1.8839504613
H,0,-0.9674351336,0.9402412053,-2.3297079391
H,0,-1.3649917661,-0.7602643156,-2.5021775761
C,0,0.7149512109,-0.3849787605,-1.8694991645
H,0,1.2745438002,0.2228148269,-2.5920198036
H,0,0.8809268527,-1.4336572748,-2.1669547288

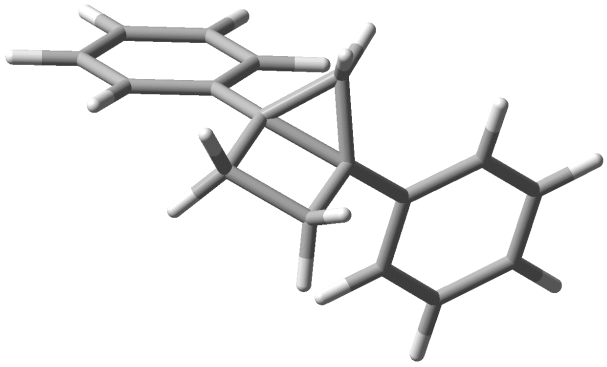
1,4-diphenylbicyclo[2.1.0]pentane (**CP4a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 1106.5971397315 Hartree
SCF Done: E(RB3LYP) = -657.393937239 Hartree

Sum of electronic and zero-point Energies= -657.114922

S**2 before annihilation 2.0078, after 2.0000
Zero-point correction: 0.279015 Hartree

no imaginary frequency:



C,0,-1.9678332027,-1.0378841629,1.5593856199
H,0,-2.1870058428,-1.9091473066,2.1887168082
H,0,-2.3071226232,-0.1375633001,2.0798279235
C,0,-2.4787210749,-1.0909980463,0.0875299973
H,0,-3.0785449281,-0.2155150892,-0.1760585752
H,0,-3.0266815815,-1.9918974028,-0.2162837913
C,0,-1.0321198031,-1.0006089357,-0.4336042829
C,0,-0.2397358561,-2.1246935006,0.1611540841
H,0,0.7924884464,-2.2098957831,-0.1684549843
H,0,-0.7142356532,-3.0836124171,0.3790566622
C,0,-0.5233604299,-0.930586433,1.0501431713
C,0,0.5396187878,-0.1020608032,1.6693968946
C,0,2.5422285008,1.4641316608,2.8967728864
C,0,0.4095973742,0.3254235252,3.00012311
C,0,1.6938037367,0.2789984699,0.9622136611
C,0,2.681169909,1.0521480521,1.5689975516
C,0,1.4011227613,1.0960021263,3.6091281832
H,0,-0.4718757422,0.0425366848,3.5691737398
H,0,1.8139966127,-0.0187655056,-0.0754428715
H,0,3.5622292276,1.3378794861,0.9998255281
H,0,1.2787112604,1.4079260004,4.6433908102
H,0,3.3141952697,2.0663250475,3.3682775449
C,0,-0.6145183853,-0.2349270015,-1.638843684
C,0,0.128799367,1.2252703412,-3.9326489754
C,0,-0.9708898006,1.1168143374,-1.7805515173
C,0,0.1204425327,-0.8384006697,-2.6703671822
C,0,0.4902797711,-0.1163927076,-3.806425935
C,0,-0.6046527129,1.8395388635,-2.9143240701
H,0,-1.5301537865,1.6066704774,-0.987377319
H,0,0.393930531,-1.8865674327,-2.5835623006
H,0,1.0569999711,-0.6051282217,-4.5948942638
H,0,-0.8862574357,2.8858351389,-3.0011246648
H,0,0.4160947993,1.7891445079,-4.8161497588

Transition state for the ring-closing reaction (**TS4a**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

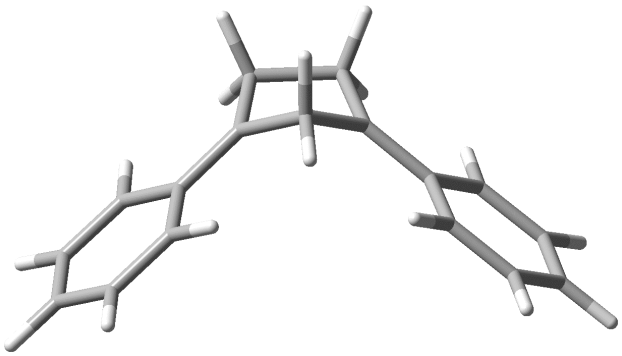
Nuclear repulsion energy: 1068.2404847279 Hartree
SCF Done: E(UB3LYP) = -657.370746088 Hartree

Sum of electronic and zero-point Energies= -657.094131

S**2 before annihilation 0.5527, after 0.0899

Zero-point correction: 0.276615 Hartree

1 imaginary frequency: -201.0799



C,0,-0.7332992924,2.536534811,0.0029007639
H,0,-0.2997879224,3.3178644008,0.6487206633
H,0,-0.3485644523,2.7126025694,-1.0052067401
C,0,-2.2830064011,2.5364379554,0.0025990432
H,0,-2.6671981283,2.7117232944,-1.005840544
H,0,-2.7170417345,3.3181411851,0.647646397
C,0,-2.5801639767,1.1457000468,0.5230079923
C,0,-1.5081012323,0.786563097,1.5127056076
H,0,-1.5081493515,-0.2630001265,1.8054081563
H,0,-1.5080480933,1.3989935413,2.4335767601
C,0,-0.4361482367,1.1456404284,0.5228520291
C,0,0.635177956,0.2993142336,0.0948799686
C,0,2.7923857398,-1.3555983184,-0.7452465412
C,0,1.5361817821,0.7069077146,-0.9284809067
C,0,0.8730591312,-0.9747681324,0.6823411435
C,0,1.9223310814,-1.7818707741,0.2643552479
C,0,2.5903554127,-0.1014771961,-1.3317245183
H,0,1.4041509728,1.6729090523,-1.4043732489
H,0,0.2291621751,-1.3254181075,1.4820708531
H,0,2.0709851171,-2.750324067,0.7354857789
H,0,3.2603193812,0.2457876904,-2.1143837737
H,0,3.6155658105,-1.9876618975,-1.0660722599
C,0,-3.6514629256,0.2992888888,0.0951624819
C,0,-5.8087213672,-1.3558307391,-0.7443946994
C,0,-3.888827192,-0.974947654,0.6824376545
C,0,-4.5530759551,0.70700806,-0.927625149
C,0,-5.6072687641,-0.101494619,-1.3305985985
C,0,-4.9381098692,-1.782165423,0.2647119817
H,0,-3.2444560624,-1.3256622598,1.481774847
H,0,-4.4215693062,1.673212101,-1.4032308141
H,0,-6.2777033315,0.2458613753,-2.1128168198
H,0,-5.0863133993,-2.7507791651,0.7356517297
H,0,-6.6319097757,-1.9879900663,-1.0650094861

singlet 1,3-di([1,1'-biphenyl]-3-yl)cyclopentane-1,3-diyl (S-**DR5a**)
BS-UB3LYP/6-31G(d), C_1 symmetry

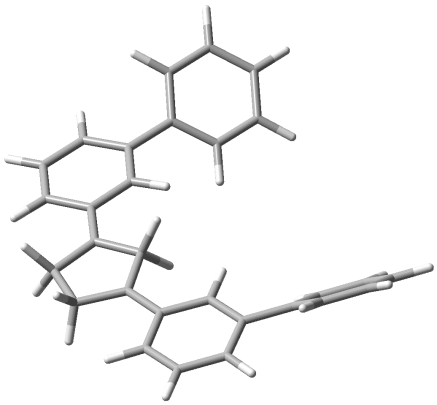
Nuclear repulsion energy: 2300.3028882507 Hartree
SCF Done: E(UB3LYP) = -1119.49351956 Hartree

Sum of electronic and zero-point Energies= -1119.055603

S**2 before annihilation 1.0481, after 0.4338

Zero-point correction: 0.437917 Hartree

no imaginary frequency:



C,0,-1.2653913496,0.799011789,3.5985389151
H,0,-0.6362184677,1.2703908405,4.3685912102
H,0,-2.2917064463,1.1297071596,3.8176495824
C,0,-0.8384077605,1.2105993377,2.2125295947
C,0,-0.4463873239,0.0115881164,1.3859085967
H,0,0.5993090687,0.0798059525,1.0323433455
H,0,-1.0475702143,-0.0648194967,0.4609737077
C,0,-0.6561720234,-1.1762968696,2.2911886606
C,0,-1.1507975169,-0.744669187,3.6483122865
H,0,-0.4661798307,-1.0682347916,4.4467490956
H,0,-2.1193297895,-1.2083482986,3.8886932349
C,0,-0.4219640839,-2.5248593344,1.9120373451
C,0,0.0551420933,-5.2096121872,1.145707921
C,0,0.0507133087,-2.8568069049,0.6116313888
C,0,-0.6437494125,-3.6017340515,2.8171401858
C,0,-0.4062042892,-4.9124833986,2.4319110502
C,0,0.28873575,-4.1750730588,0.2180851039
H,0,0.2602875291,-2.0566125072,-0.09104136
H,0,-1.0034039162,-3.3936676759,3.8200409551
H,0,-0.5893842172,-5.72097639,3.135268606
H,0,0.2071892504,-6.2430679437,0.8491310185
C,0,-0.8107666595,2.5512193391,1.7443389218
C,0,-0.7449884526,5.2210493091,0.8006880176
C,0,-1.1963960627,3.6390520556,2.5785861751
C,0,-0.3900057801,2.8649201341,0.4217555892
C,0,-0.3539758014,4.1752907548,-0.0588598092
C,0,-1.1597010208,4.9424849222,2.1067730764
H,0,-1.5231440846,3.4451647249,3.5954911222
H,0,-0.0590624996,2.0614092747,-0.2284974057
H,0,-1.4657554717,5.7582403799,2.7570049638
H,0,-0.7509082666,6.2438560753,0.4360830324
C,0,0.7802487444,-4.4813325574,-1.1514766884
C,0,1.7166642529,-5.0618445203,-3.7483823668
C,0,0.3112171449,-3.7655362813,-2.265852205
C,0,1.7276818942,-5.4961191583,-1.3680829943
C,0,2.1905547819,-5.7836254023,-2.6513984512
C,0,0.7746307883,-4.0509566347,-3.5493615046
H,0,-0.4423407604,-2.9956116869,-2.1247337489
H,0,2.1225060653,-6.0466438761,-0.5185662672
H,0,2.9297776141,-6.5678458911,-2.7931175965
H,0,0.3913739573,-3.4885071886,-4.3968997081
H,0,2.0774205045,-5.285507966,-4.7487338802
C,0,0.089468113,4.4619730082,-1.4489161081
C,0,0.9346779382,5.0060804232,-4.0847037381
C,0,0.8721191357,5.592544242,-1.7380714785
C,0,-0.2617206722,3.6114763258,-2.5107577613
C,0,0.1568417342,3.8790094561,-3.8133896782
C,0,1.2898142901,5.8620747814,-3.0406417098
H,0,1.1759642178,6.2513478569,-0.9291851462
H,0,-0.8897883439,2.7469028037,-2.3143132262
H,0,-0.1337375003,3.2103265115,-4.6196049559
H,0,1.9015295708,6.7385336958,-3.2385305917
H,0,1.2602902707,5.2157339886,-5.1000343224

triplet 1,3-di([1,1'-biphenyl]-3-yl)cyclopentane-1,3-diyl (T-**DR4a**)
UB3LYP/6-31G(d), C_1 symmetry

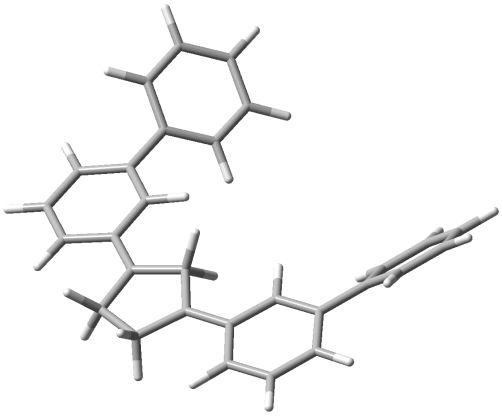
Nuclear repulsion energy: 2299.9117867302 Hartree
SCF Done: E(UB3LYP) = -1119.49387328 Hartree

Sum of electronic and zero-point Energies= -1119.056058

S**2 before annihilation 2.0551, after 2.0019

Zero-point correction: 0.437816 Hartree

no imaginary frequency:



C,0,-1.2666398587,0.7994903597,3.5983010598
H,0,-0.6370673707,1.2711445692,4.367645268
H,0,-2.2927318858,1.1307282622,3.8169532282
C,0,-0.8395061543,1.2112313528,2.2112442415
C,0,-0.4506001262,0.0113952725,1.3899255155
H,0,0.5946492543,0.0794375101,1.0324604381
H,0,-1.050899372,-0.0649810531,0.4634788627
C,0,-0.6572038311,-1.1771827939,2.2899354739
C,0,-1.1521588193,-0.7453732806,3.6480445913
H,0,-0.4673612467,-1.069435042,4.445914409
H,0,-2.1205545078,-1.2093827503,3.8877345917
C,0,-0.4217970066,-2.5259970955,1.9104337418
C,0,0.0568031661,-5.2115056458,1.1467363658
C,0,0.0506707792,-2.8591266398,0.6103735815
C,0,-0.6426500666,-3.6020272521,2.816420743
C,0,-0.4043911881,-4.9132528752,2.432469902
C,0,0.2894195105,-4.1774927038,0.2180710445
H,0,0.2595328125,-2.0596929784,-0.0934998997
H,0,-1.0021824669,-3.3932984467,3.8192201892
H,0,-0.5870021187,-5.7209905398,3.1368504039
H,0,0.2094924608,-6.2451211608,0.8510714243
C,0,-0.8106757896,2.5522641782,1.7426972209
C,0,-0.7434144516,5.2232541893,0.8016653547
C,0,-1.1950654336,3.6394788958,2.5779442893
C,0,-0.3904347711,2.8671129442,0.4203392519
C,0,-0.3536413271,4.1777819482,-0.0590206245
C,0,-1.1576763425,4.9435813635,2.1073966685
H,0,-1.5214882734,3.4449559571,3.594824951
H,0,-0.0604670366,2.064148665,-0.2312171741
H,0,-1.4629063377,5.7587584494,2.7587489916
H,0,-0.7486812717,6.2463844335,0.4379785881
C,0,0.7808030251,-4.4847214516,-1.1513257571
C,0,1.717185307,-5.0671006673,-3.7478650749
C,0,0.3107408403,-3.7706734337,-2.2663888345
C,0,1.7292119903,-5.4987826807,-1.3670897264
C,0,2.1920692174,-5.7872029742,-2.6502067945
C,0,0.7741411775,-4.0569867365,-3.5497084101
H,0,-0.4436765013,-3.0014623804,-2.1259496368
H,0,2.1247715772,-6.047999023,-0.5170713864
H,0,2.932047003,-6.5708336259,-2.7912554859
H,0,0.3900576611,-3.4958860163,-4.3977692223
H,0,2.0779183202,-5.2914893407,-4.7480630033
C,0,0.0893840674,4.4654024233,-1.4490221717
C,0,0.9340039885,5.0113557334,-4.0846564865
C,0,0.8731706667,5.5954002224,-1.7373663534
C,0,-0.2632884622,3.6164812694,-2.5116332278
C,0,0.1549901616,3.8848980285,-3.814178741
C,0,1.2905758373,5.8658360541,-3.0398430475
H,0,1.1780968533,6.253013294,-0.9279215205
H,0,-0.8923633936,2.7524865118,-2.3158500077
H,0,-0.1367646056,3.2174280518,-4.6209775954
H,0,1.903176917,6.7418235165,-3.2370841653
H,0,1.2593774231,5.2217251318,-5.0999160445

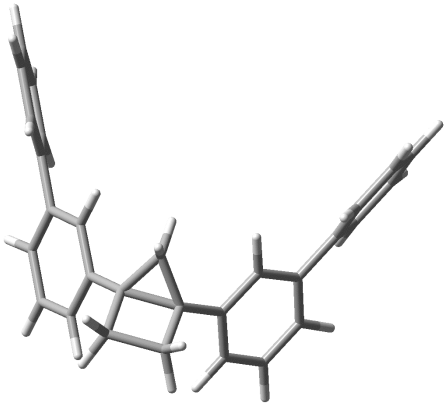
1,4-di([1,1'-biphenyl]-3-yl)bicyclo[2.1.0]pentane (**CP5a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 2392.1474694261 Hartree
SCF Done: E(RB3LYP) = -1119.50735152 Hartree

Sum of electronic and zero-point Energies= -1119.066361

S**2 before annihilation 2.0078, after 2.0000
Zero-point correction: 0.440990 Hartree

no imaginary frequency:



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C,0,-0.7879675293,-2.5022959847,-0.9150586798
C,0,-0.7788960637,-4.0089339325,-1.2282609191
C,0,0.7788791641,-4.0089543531,-1.22823151
C,0,0.787989828,-2.5023032094,-0.9150726665
H,0,-0.0000147066,-0.701827272,-1.897623457
H,0,-1.1963914976,-4.6184294666,-0.4219412553
H,0,-1.2755265108,-4.2906722976,-2.1652147135
H,0,1.2755238264,-4.2907190922,-2.1651679851
H,0,1.1963372002,-4.6184545127,-0.4218946426
C,0,-1.7546755233,-1.8327021055,-0.0041820152
C,0,-3.5857063829,-0.589461778,1.7334350029
C,0,-2.387325144,-0.6344363293,-0.3576952627
C,0,-2.0618991859,-2.4029538225,1.2426728518
C,0,-2.9681287793,-1.784605713,2.1004257975
C,0,-3.3033041561,0.0047461059,0.4937911332
H,0,-2.1532611217,-0.1787226858,-1.3149256963
H,0,-1.5824079412,-3.3304913233,1.5441159939
H,0,-3.1997632381,-2.2383440354,3.0606625631
H,0,-4.31110944,-0.1285962913,2.3978209733
C,0,1.7547178667,-1.8327169792,-0.0042107709
C,0,3.5857765579,-0.5894997097,1.7333946405
C,0,2.3873382332,-0.6344291065,-0.3577040041
C,0,2.0619863815,-2.4030017589,1.2426179129
C,0,2.9682301347,-1.7846659632,2.1003644801
C,0,3.3033282923,0.0047433177,0.4937782162
H,0,2.1532436989,-0.178689598,-1.3149141891
H,0,1.5825210392,-3.3305579067,1.5440453244
H,0,3.1999004661,-2.2384318857,3.060579521
H,0,4.3111911743,-0.1286434486,2.3977742487
C,0,3.9599019338,1.2745885764,0.0872676767
C,0,5.2065509419,3.6857739089,-0.6809410727
C,0,4.3679315174,1.4863057216,-1.2406391227
C,0,4.1910889865,2.2985313857,1.021557922
C,0,4.8077851736,3.4900009337,0.6425449783
C,0,4.983380035,2.6780462622,-1.6209477275
H,0,4.223925712,0.698186371,-1.9745248254
H,0,3.8601851364,2.167677159,2.0481586237
H,0,4.9684055251,4.2708869853,1.3814398957
H,0,5.2973894832,2.815600694,-2.6524627429
H,0,5.6865631108,4.6146931968,-0.9768871163
C,0,-3.9599134769,1.274564993,0.0872558942
C,0,-5.2066339574,3.6856977543,-0.6810017414
C,0,-4.3679896788,1.4862254209,-1.240645609
C,0,-4.1910902239,2.2985376924,1.0215158788
C,0,-4.8078216268,3.4899813667,0.6424786533
C,0,-4.9834738498,2.677939811,-1.6209784256
H,0,-4.2239920396,0.6980816953,-1.9745067192
H,0,-3.8601514532,2.1677274451,2.0481109139
H,0,-4.9684334713,4.2708916107,1.3813498609
H,0,-5.2975191846,2.815450085,-2.6524884101
H,0,-5.6866737784,4.614596793,-0.9769665378

Transition state for the ring-closing reaction (**TS5a**)
BS-UB3LYP/cc-PVDZ, C_1 symmetry

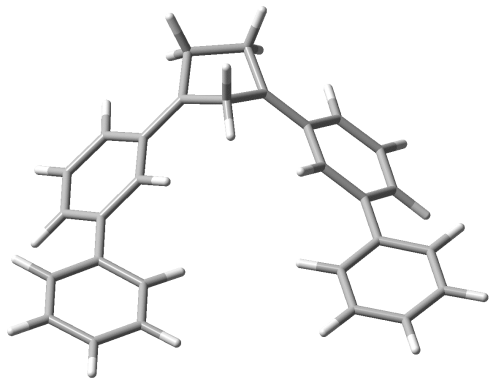
Nuclear repulsion energy: 2382.1996853661 Hartree
SCF Done: E(UB3LYP) = -1119.48505312 Hartree

Sum of electronic and zero-point Energies= -1119.046390

S**2 before annihilation 0.5560, after 0.0932

Zero-point correction: 0.438663 Hartree

1 imaginary frequency: -194.9910



C,0,0.7747244987,-4.2292225085,-0.787292484
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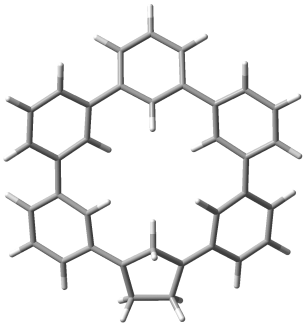
H,0,1.1593155341,-4.7202914949,0.1105617569
C,0,1.0724779129,-2.7452789751,-0.8325012702
C,0,-0.0001093349,-2.0840526026,-1.6517667231
H,0,-0.000187658,-2.3621531459,-2.7219116935
H,0,-0.0001346088,-0.9963124303,-1.5856777578
C,0,-1.0725266007,-2.7453459283,-0.8323508577
C,0,-0.7746898828,-4.2292758402,-0.7872723455
H,0,-1.2086248674,-4.7609940582,-1.6500295613
H,0,-1.1592311044,-4.7204682657,0.1105347741
C,0,-2.1457695216,-2.0836096977,-0.1547183025
C,0,-4.3023548277,-0.7841484871,1.1532890587
C,0,-2.3928247721,-0.6940963285,-0.3190627469
C,0,-3.0387560014,-2.7979769874,0.6903550367
C,0,-4.0938039302,-2.1548672185,1.3218399483
C,0,-3.4447404095,-0.037309082,0.3239337484
H,0,-1.7694707024,-0.1227860416,-0.9979834007
H,0,-2.9000564186,-3.8625809095,0.8445824041
H,0,-4.7587047559,-2.7237539645,1.966887606
H,0,-5.1113748676,-0.2875149201,1.680458116
C,0,2.1457505423,-2.0834499097,-0.1550016875
C,0,4.3023674926,-0.783792667,1.1527570311
C,0,3.038760072,-2.7976929252,0.6901495147
C,0,2.3928163576,-0.6939636256,-0.3195750286
C,0,3.4447487597,-0.0370773109,0.3232944012
C,0,4.0938173924,-2.1544856664,1.3215193599
H,0,2.9000563326,-3.8622720364,0.8445497276
H,0,1.7694601815,-0.1227641637,-0.9985854282
H,0,4.7587274145,-2.7232721726,1.9666458717
H,0,5.1113980027,-0.2870854166,1.6798406643
C,0,-3.662550432,1.4198588694,0.1234703004
C,0,-4.0782945237,4.1829099017,-0.2623281795
C,0,-2.5785053879,2.3106056996,0.0513107514
C,0,-4.9599617322,1.9451372716,0.0005824377
C,0,-5.16600286,3.3107638534,-0.1900645104
C,0,-2.7831963488,3.6762386529,-0.1405975945
H,0,-1.5683093289,1.9291197722,0.1733046727
H,0,-5.8121044671,1.2716334232,0.0297007416
H,0,-6.1785828711,3.6929023352,-0.2908188514
H,0,-1.9292571596,4.3473360492,-0.1852962075
H,0,-4.2384827108,5.2473836026,-0.4109691374
C,0,3.662562681,1.4200556004,0.1225934089
C,0,4.0783174369,4.1830453782,-0.2636678765
C,0,4.9599703109,1.9452969796,-0.0004993651
C,0,2.5785278679,2.3108126258,0.0503995989
C,0,2.7832229205,3.6764120459,-0.1417391147
C,0,5.166016835,3.3108910161,-0.1913723836
H,0,5.8121073435,1.2717870463,0.0286414158
H,0,1.5683345881,1.929367516,0.172542681
H,0,1.9292890159,4.347514371,-0.1864647863
H,0,6.1785947655,3.6929947648,-0.2922791679
H,0,4.2385085372,5.2474932964,-0.4124891047

singlet cyclopentane-1,3-diyl derivative (S-**DR6a**)
BS-UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3243.0807821107 Hartree
SCF Done: E(UB3LYP) = -1349.35054342 Hartree
Sum of electronic and zero-point Energies= -1348.851253
S**2 before annihilation 1.0102, after 0.4089
Zero-point correction: 0.499291 Hartree
no imaginary frequency:



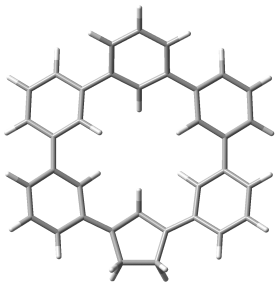
C,0,-3.4074056734,-1.1581478434,0.7982962678
C,0,-2.6459632007,-1.2503390022,-0.5001338825
H,0,-1.7220543553,-0.6680401392,-0.4861938483
H,0,-3.2349016125,-0.8581671116,-1.3539622194
C,0,-2.3938186655,-2.7320210479,-0.6237258799
C,0,-4.1799787511,-2.4376220059,1.0102705582
H,0,-5.2470982214,-2.3153629671,0.7644526485
H,0,-4.1473859352,-2.7664550339,2.0562141183
C,0,-3.5045379668,-3.4831654091,0.0699394731
H,0,-3.123760744,-4.3397008307,0.6398253248
H,0,-4.2297951234,-3.8965993169,-0.6491602397
C,0,-3.2798742158,-0.0832449422,1.7200501993
C,0,-2.871480325,2.0310534483,3.577819627
C,0,-2.377558396,0.9864081559,1.464886766
C,0,-4.0003076884,-0.0280876431,2.9481090391
C,0,-3.8021367835,1.0174312011,3.8400685245
C,0,-2.133615089,2.0104362555,2.3791366623
H,0,-1.8444701466,1.0136224643,0.5228286616
H,0,-4.7141672767,-0.8104390716,3.1880798766
H,0,-4.3638967701,1.0381263134,4.7706550197
H,0,-2.6937226454,2.8110536103,4.3125826193
C,0,-1.213377074,-3.2934963027,-1.1829539307
C,0,1.2309595978,-4.3434546684,-2.1882940565
C,0,-0.162919063,-2.4551270412,-1.6487513935
C,0,-0.9938104989,-4.6983246391,-1.2743915843
C,0,0.1985743262,-5.1981122528,-1.7807873621
C,0,1.057637984,-2.9487690368,-2.1076376363
H,0,-0.3035674234,-1.3815308543,-1.6447997281
H,0,-1.7682057747,-5.3857502356,-0.9472328231
H,0,0.3428531433,-6.2739890941,-1.8413289355
H,0,2.1756022311,-4.7551495341,-2.5318608512
C,0,2.1367981931,-1.9852537931,-2.4556375664
C,0,4.1111221374,-0.0729007089,-3.0633415985
C,0,2.3180175619,-0.8442538051,-1.6594152162
C,0,2.9859853322,-2.1655623051,-3.5578251614
C,0,3.9640646382,-1.2145102757,-3.8513898137
C,0,3.2840403203,0.130776684,-1.9463600028
H,0,1.7138251903,-0.7363354361,-0.7647868094
H,0,2.8616761458,-3.0335998664,-4.1995608011
H,0,4.6052184836,-1.3536223346,-4.7180122408
H,0,4.8546865603,0.6732365071,-3.3290552568
C,0,-1.0803638236,3.0145869205,2.0686396747
C,0,0.9474295958,4.8442179416,1.3868287982
C,0,-1.2246233903,4.3785551255,2.3640154724
C,0,0.1065343482,2.5925299592,1.450706452
C,0,1.1267873955,3.4834517464,1.0879456431
C,0,-0.2140253648,5.2792610453,2.0253106018
H,0,-2.1378340355,4.7366490677,2.8315349659
H,0,0.2550530284,1.5304383104,1.286506499
H,0,-0.3426282618,6.336689701,2.2415746173
H,0,1.7068539082,5.5658477055,1.0991939625
C,0,3.414191252,1.3270147075,-1.0709665798
C,0,3.6157896453,3.5447496902,0.6551492152
C,0,2.2796544675,1.8823034795,-0.4595097657
C,0,4.6597271601,1.9223855546,-0.8133238705
C,0,4.7516477696,3.0250973916,0.0352444934
C,0,2.3546085277,2.9737050547,0.4194733847
H,0,1.3043080924,1.471945931,-0.699509815
H,0,5.5603346097,1.502984102,-1.252681094
H,0,5.7236246296,3.4675556731,0.237405725
H,0,3.7116780203,4.3760208017,1.3478450718

triplet cyclopentane-1,3-diyl derivative (T-**DR6a**)
UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3240.3633745499 Hartree
SCF Done: E(UB3LYP) = -1349.35018073 Hartree

Sum of electronic and zero-point Energies= -1348.851144
S**2 before annihilation 2.0567, after 2.0020

Zero-point correction: 0.499036 Hartree
no imaginary frequency:



C,0,-3.3460315771,-1.1751883299,0.8915189647
C,0,-2.4373166211,-1.2991454604,-0.2978865181
H,0,-1.4603693902,-0.8414550944,-0.1078234391
H,0,-2.8399766732,-0.7612681972,-1.1815805542
C,0,-2.3155102069,-2.7745375394,-0.5515391691
C,0,-4.1229343452,-2.4565776479,1.0752750871
H,0,-5.1836472067,-2.3298220767,0.8080947143
H,0,-4.1175836553,-2.7865495106,2.1226398883
C,0,-3.4384654843,-3.5078250889,0.1421613496
H,0,-3.0635590153,-4.3665937695,0.7153857189
H,0,-4.1611602445,-3.9230364321,-0.577168495
C,0,-3.3053860348,-0.0544228893,1.7653045258
C,0,-2.9794493857,2.1397974728,3.5435877734
C,0,-2.3965580389,1.0077616634,1.5034413216
C,0,-4.0896184322,0.0567654549,2.9480163672
C,0,-3.9275505941,1.1409145013,3.8021899985
C,0,-2.1882442598,2.0697878761,2.3805819644
H,0,-1.8272148796,0.9963550946,0.5830880878
H,0,-4.8141406431,-0.7158754251,3.1891143925
H,0,-4.5317191691,1.2030913709,4.703938584
H,0,-2.8319395315,2.9465321019,4.2558647202
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C,0,1.2084423274,-4.3661503418,-2.341611187
C,0,-0.14328566,-2.4947797109,-1.6674280677
C,0,-0.9992417726,-4.7412022854,-1.3869727179
C,0,0.1728822335,-5.2269122826,-1.9540329355
C,0,1.0576114119,-2.9746465823,-2.1854137984
H,0,-0.272951949,-1.4218772,-1.6087401582
H,0,-1.7731113549,-5.4349254622,-1.0708250298
H,0,0.3003510893,-6.2996674028,-2.0764359001
H,0,2.1379072758,-4.7739015175,-2.7286095972
C,0,2.1334216692,-1.9983143214,-2.5085856356
C,0,4.0918930541,-0.0556183106,-3.0736815385
C,0,2.3122980873,-0.8772245774,-1.68178329
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C,0,3.9494719428,-1.1771291395,-3.8906983102
C,0,3.268156646,0.1130330493,-1.948054712
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H,0,2.8562875384,-2.9918075175,-4.2851276219
H,0,4.5875342971,-1.2885995628,-4.76357529
H,0,4.8283478886,0.703037312,-3.3232101834
C,0,-1.1162228383,3.0529011453,2.0654164982
C,0,0.941538956,4.8420625309,1.3627315694
C,0,-1.2458807167,4.4249596013,2.3276593598
C,0,0.0735119905,2.6027526061,1.4701308124
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C,0,3.5987562537,3.4978969902,0.6931421227
C,0,2.2579304576,1.8493565133,-0.4387134612
C,0,4.6416932575,1.8767229315,-0.775785713
C,0,4.7361001159,2.9716717015,0.082113585
C,0,2.3346407287,2.9391611573,0.4434923766
H,0,1.2812644949,1.4464023154,-0.68741369
H,0,5.541904397,1.4545691618,-1.2133236922
H,0,5.7099195532,3.4045689308,0.2957670104
H,0,3.6943329322,4.3265767469,1.3889833499

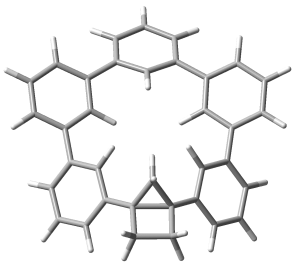
bicyclo[2.1.0]pentane derivative (**CP6a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3300.3040266082 Hartree

SCF Done: E(RB3LYP) = -1349.36176163 Hartree

Sum of electronic and zero-point Energies= -1348.859799

Zero-point correction: 0.501963 Hartree



no imaginary frequency:

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H,0,-4.8573122729,-2.5992932602,1.3688505541
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C,0,-3.0570818175,0.1501480204,3.8340472425
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H,0,-1.7981207711,0.9580894544,0.282257372
H,0,-4.0064651542,-1.5661149272,2.9756477153
H,0,-3.4191340693,-0.074360665,4.8341109953
H,0,-1.999164683,1.9268817601,4.4509053118
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C,0,0.9937739255,-2.7575250064,-1.5676093233
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H,0,0.3261033751,-5.8965014907,-0.4343391435
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C,0,4.1028158949,-0.1771921172,-3.0512855163
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C,0,2.9152170356,-2.2957083484,-3.1728373576
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C,0,3.2989496069,0.232311419,-1.976569583
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C,0,-1.14266424,4.0125517338,2.5354722349
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C,0,1.1793710492,3.5272943129,1.0051449082
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H,0,-2.043480732,4.2138196905,3.1091256821
H,0,0.5188585833,1.4781455434,1.0506676272
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C,0,3.4524966357,1.5310402467,-1.2703122607
C,0,3.6333516435,3.8174248593,0.3728679875
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C,0,4.7547507946,3.3360496245,-0.3067349394
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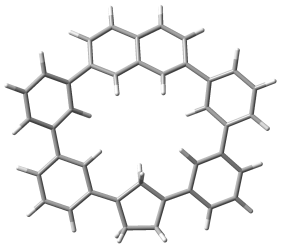
H,0,5.5835407752,1.7851679983,-1.5505711395
H,0,5.7127215254,3.8321378562,-0.1739554195
H,0,3.7340511499,4.6602593474,1.051171385

singlet cyclopentane-1,3-diyl derivative (S-**DR7a**)
BS-UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3778.4946677300 Hartree
SCF Done: E(UB3LYP) = -1502.99192484 Hartree
Sum of electronic and zero-point Energies= -1502.446329
S**2 before annihilation 1.0477, after 0.4389
Zero-point correction: 0.545596 Hartree
no imaginary frequency:



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H,0,-1.5751471515,-0.9143798833,0.0541929225
C,0,-2.266137765,-2.9795814796,0.0672305728
C,0,-4.2643449325,-2.3364692594,1.3261776245
H,0,-5.1911499894,-1.9478088543,0.8797867464
H,0,-4.5554909176,-2.7233189931,2.3148937116
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H,0,-4.2655086516,-3.6390812662,-0.4448859616
C,0,-3.4355516876,0.0055277059,2.0617304566
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C,0,-0.121172917,-3.1556329821,-1.1731585733
C,0,-1.8368018911,-4.8297015882,-1.5376328554
C,0,-1.0166381813,-5.43665998,-2.4772228467
C,0,0.7061443628,-3.7515285339,-2.1324894631
H,0,0.2442372039,-2.2922952722,-0.6284739116
H,0,-2.8117946192,-5.2558347485,-1.3231741337
H,0,-1.3614283065,-6.330200577,-2.9915833414
H,0,0.8446445683,-5.3737585404,-3.5605501213
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C,0,2.2429097965,-1.7883963313,-2.2743687217
C,0,3.1266762199,-3.9261922239,-2.8997908295
C,0,4.3563521073,-3.3195094571,-3.1619832913
C,0,3.4881230917,-1.1700675414,-2.4676335577
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H,0,5.1870347028,-3.9277052094,-3.5106129285
H,0,5.5276928601,-1.5084980699,-3.1025200557
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C,0,-0.5068410675,3.1929701602,1.7177396648
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C,0,-0.3272244618,5.1635798595,3.6368982689
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H,0,-0.26011192,5.9380942563,4.396570864
H,0,1.5319735761,5.7293427217,2.6995338914
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H,0,1.4770669304,1.6499732211,1.0297129826
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C,0,3.4595746371,3.0315054846,-1.3992837109
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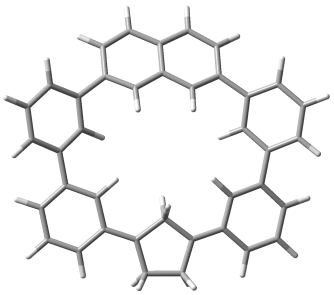
H,0,2.1780241134,5.7989221131,0.1594219229
H,0,4.7657134281,3.3220693751,-3.1072170904
H,0,3.7457087188,5.1702864956,-1.6255782564
C,0,3.6002143199,0.2627500939,-2.0919960177
H,0,2.4180518541,-0.0548301421,-0.3368504371
C,0,4.3011800097,1.2497497148,-2.8461632468
H,0,4.8560833376,0.9466599016,-3.7303111084
C,0,4.2424118056,2.585607533,-2.5015325271

triplet cyclopentane-1,3-diyl derivative (T-**DR7a**)
UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3778.2033765261 Hartree
SCF Done: E(UB3LYP) = -1502.99224271 Hartree
Sum of electronic and zero-point Energies= -1502.446752
S**2 before annihilation 2.0559, after 2.0020
Zero-point correction: 0.545491 Hartree
no imaginary frequency:



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C,0,-4.2695959242,-2.3323790038,1.3186261982
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H,0,-4.5621086011,-2.7192644597,2.3066610859
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H,0,-3.6158043343,-4.4078509285,0.9754131226
H,0,-4.2682726785,-3.6358632655,-0.454063043
C,0,-3.4360635294,0.0074052769,2.062682186
C,0,-3.8843536678,2.5666034671,3.2039074379
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C,0,-4.7000524516,0.3582357856,2.6177328722
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C,0,-1.4173629367,-3.6486909388,-0.862887951
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H,0,0.8519305399,-5.3825857243,-3.5521043446
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C,0,2.9166767123,0.6776464382,-0.9653111269
H,0,2.1770911696,5.7993421441,0.158542392
H,0,4.7637471793,3.3224760653,-3.1089758821
H,0,3.7437902857,5.1706345001,-1.6273045853
C,0,3.5987614761,0.2629981385,-2.0936386943
H,0,2.4157022754,-0.0545168585,-0.3391004603
C,0,4.2996893938,1.2500762087,-2.8477348906
H,0,4.8551866385,0.9469514489,-3.7314975773
C,0,4.2403447553,2.5859902266,-2.5034071149

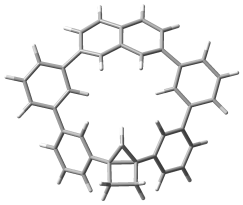
bicyclo[2.1.0]pentane derivative (**CP7a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3864.9589798963 Hartree

SCF Done: E(RB3LYP) = -1502.99347520 Hartree
Sum of electronic and zero-point Energies= -1502.445054

Zero-point correction: 0.548421 Hartree

no imaginary frequency:



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C,0,-2.8876136687,-4.0297504412,1.7120485182
H,0,-2.3428300962,-4.8300768181,2.2287700009
H,0,-3.6284476991,-4.490602147,1.0532003532
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C,0,-3.9477536346,2.2389491815,1.5884133677
C,0,-2.1932155728,0.6340352617,1.991431341
C,0,-4.3816626827,-0.1359193681,1.3675220664
C,0,-4.8202020854,1.1854569279,1.3092817303
C,0,-2.6116554623,1.9746564698,1.9184925032
H,0,-1.1751463574,0.4269023072,2.3055850759
H,0,-5.0766307816,-0.9400575099,1.1418903238
H,0,-5.8499004363,1.398444434,1.0337324147
H,0,-4.2921014147,3.2670429978,1.515693083
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C,0,-2.0553451536,-3.8501306276,-2.7021006969
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H,0,-3.5134011456,-3.7872957921,-1.1268272628
H,0,-2.7680148491,-4.2143455717,-3.4376434285
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H,0,-0.4614524194,-1.5760373519,1.6605728778
H,0,-0.8500511734,-2.8106449635,2.9427170209

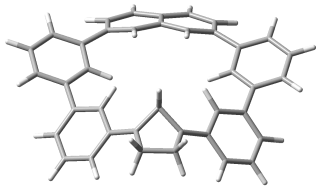
bicyclo[2.1.0]pentane derivative (**CP7a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 3811.6582286603 Hartree

SCF Done: E(RB3LYP) = -1502.97806518 Hartree
Sum of electronic and zero-point Energies= -1502.431616
S**2 before annihilation 0.3035, after 0.0218

Zero-point correction: 0.546449 Hartree

1 imaginary frequency: -402.1308



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H,0,-1.1844313237,1.8776653658,-1.2284911459
C,0,-2.4307488716,4.5708197186,0.4270226106
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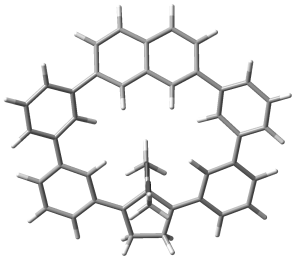
C,0,-1.2618193234,5.2801326812,0.6185498373

singlet cyclopentane-1,3-diyl derivative (S-**DR7b**)
BS-UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 4784.4187859664 Hartree
SCF Done: E(UB3LYP) = -1731.421219 Hartree
Sum of electronic and zero-point Energies= -1502.446329
S**2 before annihilation 0.8971, after 0.2761Zero-point correction: 0.611365 Hartree
no imaginary frequency:



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H,0,0.3644033364,-2.1710867992,2.9976062488
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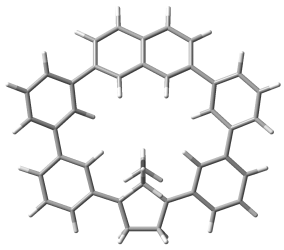
H,0,-1.4032181403,-2.0697784979,3.2058731957

triplet cyclopentane-1,3-diyl derivative (T-**DR7b**)
UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 4781.2842705812 Hartree
SCF Done: E(UB3LYP) = -1732.02794838 Hartree
Sum of electronic and zero-point Energies= -1731.416925
S**2 before annihilation 2.0550, after 2.0019
Zero-point correction: 0.611023 Hartree
no imaginary frequency:



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C,0,4.5127056194,1.3721164316,-2.8598975768
H,0,5.0938746065,1.0651663723,-3.725786375
C,0,4.4606166957,2.7074577093,-2.5123937212
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O,0,-0.6051527149,-1.4358240696,1.3901724911
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H,0,-0.7135988058,-3.3690733666,2.1861469807
H,0,-1.4256114576,-2.0802312317,3.2052113707

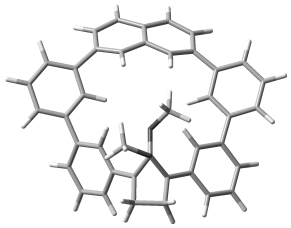
bicyclo[2.1.0]pentane derivative (**CP7b**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 4796.2614176856 Hartree

SCF Done: E(RB3LYP) = -1732.02317567 Hartree
Sum of electronic and zero-point Energies= -1731.408859

Zero-point correction: 0.614316 Hartree

no imaginary frequency:



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C,0,-2.1080562507,0.9285957087,1.6522136948
C,0,-4.2281348926,0.2649800618,0.728089331
C,0,-4.6183801006,1.6002218642,0.6671457057
C,0,-2.4820739434,2.2828688081,1.5772351129
H,0,-1.1305203964,0.6721640803,2.0431226902
H,0,-4.9115864298,-0.5017725146,0.3758388936
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H,0,-4.058224646,3.6514889441,1.0343317817
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C,0,-0.5608615587,-3.8414945068,-3.2723607808
C,0,-0.365442198,-2.5587518943,-1.2339746301
C,0,-2.2647408047,-3.9883767279,-1.5614622515
C,0,-1.7754882355,-4.3425190538,-2.8168950689
C,0,0.1709072241,-2.9474794369,-2.4754944886
H,0,0.1801326826,-1.8466996565,-0.6332664589
H,0,-3.1954515358,-4.4324268095,-1.2304125949
H,0,-2.3465074505,-5.0268003671,-3.4391992407
H,0,-0.1878014831,-4.1279613141,-4.2511846162
C,0,1.5128890474,-2.4664704727,-2.9126595825
C,0,4.0851797259,-1.5483585837,-3.6585912743
C,0,1.9738604744,-1.1973026372,-2.5476652105
C,0,2.3742371322,-3.2730884292,-3.6783910637
C,0,3.6354883555,-2.8095147402,-4.0542296675
C,0,3.2580577536,-0.7289551784,-2.8788076461
H,0,1.3022013012,-0.5312184896,-2.0174559436
H,0,2.0679053427,-4.2759654866,-3.9613085042
H,0,4.2867322424,-3.4514521328,-4.6418980833
H,0,5.0842762966,-1.2157886181,-3.928017663
C,0,-1.4866640388,3.3449725574,1.8948518993
C,0,0.504271739,5.3147897532,2.2634154208
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C,0,-0.2417455384,3.2572551684,1.2705004838
C,0,0.7719550868,4.2154202831,1.4356716739
C,0,-0.7384811339,5.4229974543,2.8953613639
H,0,-2.6904452378,4.5607374407,3.2186665543
H,0,-0.0859438576,2.4449296288,0.5711037016
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H,0,1.2622815657,6.0774196399,2.4233832139
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H,0,1.9559136105,1.8901663935,1.0100477221
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C,0,3.6399045791,0.6153764677,-2.3756152683
H,0,2.742734443,0.2330829787,-0.4718155767
C,0,4.2934168925,1.6090698027,-3.1640080618
H,0,4.6799599448,1.3390267773,-4.143358447
C,0,4.3687030273,2.9203808374,-2.7386168107
C,0,-2.094823944,-2.8450874395,0.6544323126
C,0,-2.6851289904,-1.5467661138,1.4978693411
C,0,-1.374212017,-2.2000276884,1.8231165124
O,0,-1.2394227172,-2.9617688524,2.9913127954
O,0,-0.2338150701,-1.431234821,1.5604356562
C,0,0.9958546034,-2.155550275,1.6992123113
H,0,1.2269879391,-2.3506403026,2.7507719163
H,0,1.7701859326,-1.5141725454,1.2714627933
H,0,0.9695058093,-3.106592809,1.1578542643
C,0,-1.21391705,-2.1785700267,4.1842077016
H,0,-0.3166114348,-1.5500112429,4.2377989677
H,0,-1.2109462916,-2.8857725439,5.016894387
H,0,-2.097932556,-1.532425504,4.2563299367

singlet diradical in (2,7)pyrenophane (S-**DR8a**)
BS-UB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 2203.6708780908 Hartree

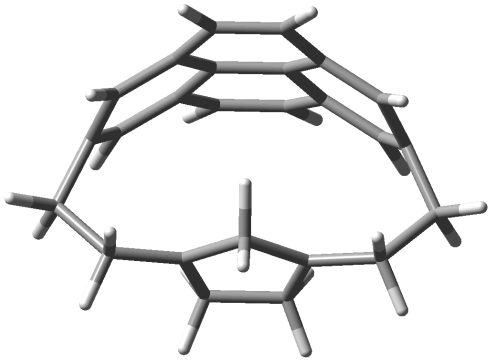
SCF Done: E(UB3LYP) = -965.784293116 Hartree

Sum of electronic and zero-point Energies= -965.391221

S**2 before annihilation 1.0074, after 0.0659

Zero-point correction: 0.393072 Hartree

no imaginary frequency:



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C,0,-2.5460908297,1.0151752509,-1.2105212092
C,0,-1.3314349016,1.5802579027,1.2618703301
C,0,-1.3350418021,1.7192157186,-1.1978613088
C,0,-2.5368903488,0.8687171183,1.1927708318
C,0,-0.6400891324,1.8381734291,0.0427820685
C,0,-0.6052060956,1.9997093451,-2.4142851318
H,0,-2.9652112775,0.479293506,2.1145823544
C,0,0.7540884545,1.9454683767,-2.4166895114
H,0,-1.1573143798,2.1137320668,-3.3442542679
H,0,1.3102374789,2.015266204,-3.3486199949
C,0,1.4635505393,1.607561778,-1.2028097277
C,0,2.6146065977,0.8092748949,-1.2196321641
C,0,0.7846710884,1.7813502254,0.0402627841
C,0,3.0548485285,0.178436672,-0.0473133821
H,0,3.0234585842,0.5044773859,-2.1816217338
C,0,2.6023004323,0.6637920188,1.1837040853
H,0,3.0015135158,0.2414026266,2.1040635951
C,0,1.4575882861,1.4690596711,1.2569424942
C,0,0.7515564852,1.6659249735,2.5010162893
H,0,1.3083490712,1.6262925889,3.4342959141
C,0,-0.6075841725,1.720100178,2.5034162981
H,0,-1.1624680948,1.7247767385,3.4386605849
C,0,3.6352300263,-1.2154569678,-0.1150385071
H,0,3.9722112683,-1.5267204873,0.880598573
H,0,4.5001222387,-1.2904751703,-0.7873712877
C,0,-3.7208241887,-0.9220342592,-0.1021435025
H,0,-4.0779573289,-1.2057005053,0.8947133089
H,0,-4.5913379464,-0.9277896361,-0.7713741169
C,0,2.5358079748,-2.2238994935,-0.6472661317
H,0,2.9343492435,-3.237919675,-0.4640192605
H,0,2.5008939828,-2.1081330715,-1.7378496123
C,0,-2.7070910301,-2.0146764487,-0.6382439541
H,0,-2.6668270716,-1.9016770497,-1.7289324962
H,0,-3.1844988622,-2.9937954798,-0.453689424
C,0,-1.2879573122,-2.029778921,-0.1218370925
C,0,1.1217668118,-2.1259040832,-0.1259890823
C,0,-0.0779572914,-1.9102446553,-1.0226069687
H,0,-0.0401092265,-0.9383550061,-1.5458515863
H,0,-0.1092319961,-2.659056864,-1.8441964795
C,0,0.6835063848,-2.4928221794,1.2672951184
H,0,1.1060352634,-1.813631767,2.0240900475
H,0,1.0423915007,-3.498254322,1.5494649242
C,0,-0.8755594066,-2.4313577622,1.269777367
H,0,-1.3115062783,-3.4057799652,1.5522638091
H,0,-1.2410383951,-1.7218667562,2.0284610233

triplet diradical (T-**DR8a**)
UB3LYP/6-31G(d), C_1symmetry

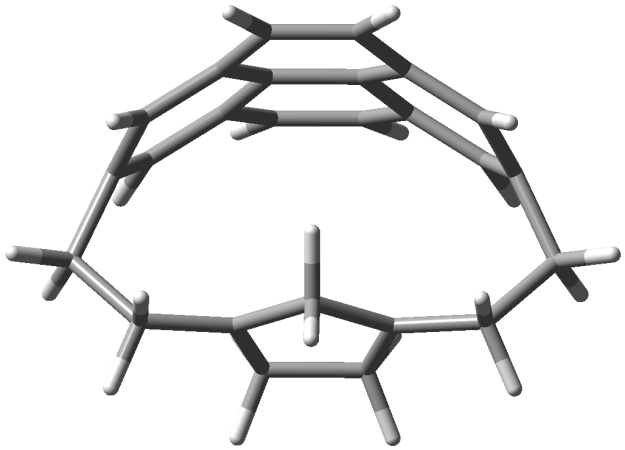
Nuclear repulsion energy: 2203.8056287139 Hartree

SCF Done: E(UB3LYP) = -965.785219775 Hartree
Sum of electronic and zero-point Energies= -965.392216

S**2 before annihilation 2.0091, after 2.0001

Zero-point correction: 0.393003 Hartree

no imaginary frequency:



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C,0,-1.3313859331,1.5801469588,1.2613248821
C,0,-1.3350228308,1.7196506502,-1.1983648265
C,0,-2.5366383736,0.8683091868,1.1920525334
C,0,-0.6400792854,1.838463602,0.0422963763
C,0,-0.6051807348,2.0004601349,-2.4147284904
H,0,-2.9648481065,0.4785624204,2.1137745375
C,0,0.7541243736,1.9462206682,-2.4171316591
H,0,-1.1572764527,2.1147519458,-3.3446744927
H,0,1.310283997,2.0162892381,-3.3490379094
C,0,1.4635658827,1.6079997707,-1.2033107665
C,0,2.614444841,0.8094259058,-1.2202913908
C,0,0.7846814096,1.7816411838,0.0397783339
C,0,3.0544515606,0.178168448,-0.0481097949
H,0,3.0233121629,0.5048160511,-2.182338549
C,0,2.6020113243,0.6634060947,1.1829904761
H,0,3.0010853841,0.2407019788,2.1032612161
C,0,1.4575253678,1.4689533057,1.256399559
C,0,0.7515375795,1.665635376,2.5005230497
H,0,1.3083298265,1.6257661667,3.4337909347
C,0,-0.6075956819,1.7198106995,2.5029219248
H,0,-1.1624997189,1.7242516991,3.43815355
C,0,3.634336736,-1.2158964456,-0.1160553413
H,0,3.9716771553,-1.527276715,0.8794259835
H,0,4.4989131315,-1.2911414295,-0.7887771118
C,0,-3.7199729001,-0.922545938,-0.1031652039
H,0,-4.0774793,-1.2062950406,0.893536584
H,0,-4.5901882489,-0.9285537855,-0.7727898687
C,0,2.5344486596,-2.2238924986,-0.6477709973
H,0,2.9331497988,-3.2380303686,-0.4659220124
H,0,2.4981717914,-2.1072030087,-1.7382438904
C,0,-2.7057379829,-2.0147860509,-0.6387455076
H,0,-2.6640453768,-1.9009891874,-1.7293297688
H,0,-3.1833185791,-2.9940068193,-0.4555737737
C,0,-1.2871217084,-2.0305747165,-0.1205058748
C,0,1.1208764771,-2.1266265889,-0.1246572567
C,0,-0.0778901517,-1.9088668505,-1.015150121
H,0,-0.0400419109,-0.9367799752,-1.5417386666
H,0,-0.1090078661,-2.6534552371,-1.8438014236
C,0,0.6838351548,-2.494102832,1.2696978383
H,0,1.1063186234,-1.8144631144,2.0259498703
H,0,1.0433318133,-3.4992760929,1.5513523501
C,0,-0.8759743419,-2.4325845678,1.2721902726
H,0,-1.3125465,-3.4066724737,1.5542034549
H,0,-1.2413342695,-1.7226080099,2.0303132037

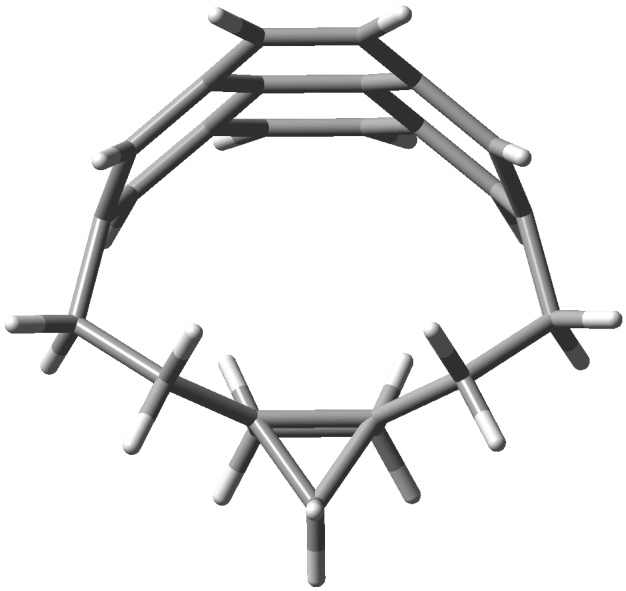
Ring-closd compound (**CP8a**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 2198.9198057563 Hartree

SCF Done: E(RB3LYP) = -965.786481938 Hartree
Sum of electronic and zero-point Energies= -965.389698

Zero-point correction: 0.396784 Hartree

no imaginary frequency:



C,0,-2.7958689308,0.2830108472,-0.2517405179
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C,0,-1.4241928397,1.6788539994,1.1855588884
C,0,-1.3332598657,1.9384914354,-1.259743167
C,0,-2.4832638722,0.7724541083,1.020908361
C,0,-0.7134426395,2.0774779169,0.0175399993
C,0,-0.588540232,2.3671303355,-2.4275872086
H,0,-2.88607473,0.2769622559,1.901958967
C,0,0.7685429321,2.3655948537,-2.3782444662
H,0,-1.1145523089,2.5255428142,-3.3659885296
H,0,1.3616736743,2.5227413054,-3.2759537909
C,0,1.4255175855,1.9354264837,-1.1594196737
C,0,2.488767221,1.0269051932,-1.1905365468
C,0,0.7148692519,2.0759106782,0.0694765462
C,0,2.807392571,0.2768856535,-0.0478801367
H,0,2.8891338439,0.728219753,-2.1581285335
C,0,2.4043474443,0.7672670531,1.1987034229
H,0,2.7410551374,0.2710478949,2.1066741598
C,0,1.3380439923,1.6759138708,1.2860249974
C,0,0.5908371382,1.8360221383,2.5162789954
H,0,1.1147843817,1.788279729,3.467945479
C,0,-0.767991004,1.8374470718,2.4668595847
H,0,-1.3597852991,1.7908855012,3.3779474695
C,0,3.1900108061,-1.1781592772,-0.2157309092
H,0,3.5122983122,-1.6103916952,0.7391746752
H,0,4.0287197599,-1.2915306001,-0.9160459267
C,0,-3.1685233932,-1.1711809081,-0.4472250975
H,0,-3.5603327365,-1.6026775098,0.4816611106
H,0,-3.9543521767,-1.2826984736,-1.206676589
C,0,-1.9465420222,-2.025198325,-0.957996419
H,0,-1.5247209478,-1.5181949072,-1.8351734913
H,0,-2.3863880369,-2.9584094565,-1.3370317221
C,0,2.006522092,-2.0295329923,-0.8140337475
H,0,2.4707143453,-2.9637474641,-1.160128911
H,0,1.6507440358,-1.5216940236,-1.7195487349
C,0,-0.8082775668,-2.4353221611,0.0023408642
C,0,0.800521173,-2.4371249063,0.0609249542
C,0,0.0081252385,-3.6544673738,-0.3344567377
H,0,-0.0161488121,-4.5438106981,0.3047489966
H,0,0.0467171924,-3.8911664881,-1.3986970309
C,0,-0.8375825655,-2.3445891464,1.5336660138
H,0,-1.3428435204,-3.1796469321,2.0388526427
H,0,-1.2513269573,-1.4068482011,1.907712725
C,0,0.7187061669,-2.3468276022,1.5903373138
H,0,1.1067428592,-1.4102913251,1.9937506416
H,0,1.183587397,-3.1833550506,2.1306716271

singlet diradical in (2,7)pyrenophane (S-**DR8b**)
BS-UB3LYP/6-31G(d), C_1 symmetry

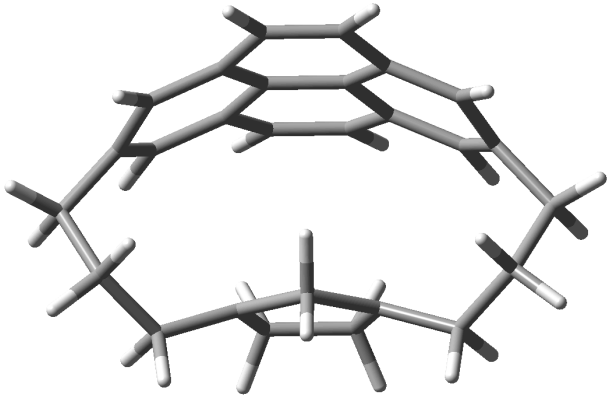
Nuclear repulsion energy: 2507.4034270069 Hartree

SCF Done: E(UB3LYP) = -1044.43831937 Hartree
Sum of electronic and zero-point Energies= -1043.986971

S**2 before annihilation 0.9983, after 0.0637

Zero-point correction: 0.451348 Hartree

no imaginary frequency:



C,0,-3.2134825882,0.8126160519,-0.1502309484
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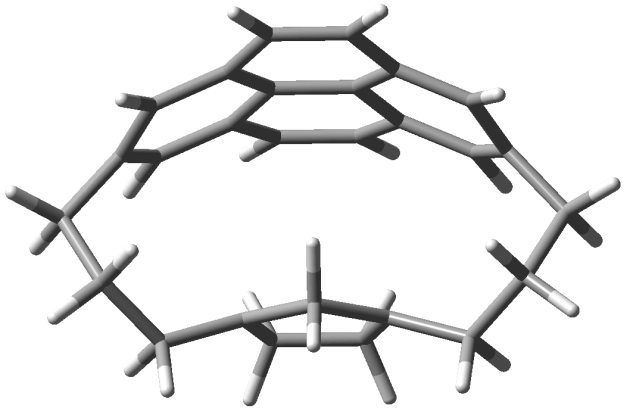
C,0,-2.6316886298,1.3685710631,-1.2981147199
C,0,-1.3451653272,1.6174546598,1.1873629483
C,0,-1.3362249079,1.8928408239,-1.2637029426
C,0,-2.6393857052,1.0821274435,1.0943528551
C,0,-0.6366079899,1.8812143933,-0.0201391703
C,0,-0.5969862398,2.1932738692,-2.4653608993
H,0,-3.1262635696,0.7224925899,1.9987382795
C,0,0.7619695122,2.1388346939,-2.467719359
H,0,-1.1469749794,2.3533028852,-3.3897655907
H,0,1.3197893177,2.2544813136,-3.3940475185
C,0,1.4789673859,1.7800808355,-1.2685844278
C,0,2.7281979683,1.1538340756,-1.3073995834
C,0,0.7849749616,1.8243078878,-0.0226018979
C,0,3.26761758,0.5529838784,-0.161441469
H,0,3.2000693029,0.9834669791,-2.2736832606
C,0,2.7212860868,0.8674996679,1.0850795928
H,0,3.1809769172,0.4699937288,1.9878388682
C,0,1.4743630971,1.5046341607,1.1824818307
C,0,0.7499443887,1.5944930784,2.4249068283
H,0,1.3008249184,1.5073104109,3.3586161803
C,0,-0.6115945493,1.6489481873,2.4272630049
H,0,-1.164448765,1.605913982,3.3628817163
C,0,4.2138450677,-0.61129506,-0.3302505323
H,0,4.6627990455,-0.891989665,0.6311879269
H,0,5.0406014991,-0.3494840555,-1.004996361
C,0,-4.25047608,-0.2721228081,-0.3156463223
H,0,-4.7172188048,-0.5160700176,0.6473464482
H,0,-5.0558814213,0.0551394552,-0.9876380436
C,0,3.4790057515,-1.8399839273,-0.9463854847
H,0,4.252296078,-2.5565397665,-1.2563265732
H,0,2.9730588527,-1.5209552307,-1.8661068278
C,0,-3.6184738628,-1.5556422088,-0.9340511139
H,0,-3.0917560813,-1.2780711559,-1.8555575612
H,0,-4.4476997811,-2.2079697491,-1.2412076599
C,0,-2.685939012,-2.4295696113,-0.0421493751
H,0,-2.6108151382,-3.3965521255,-0.5751233635
H,0,-3.2353876764,-2.6528334179,0.8842163857
C,0,2.4825279961,-2.6366850809,-0.0512732708
H,0,3.0155240595,-2.9035245793,0.8731741005
H,0,2.3283738734,-3.5943546158,-0.5840533509
C,0,-1.2864448501,-2.0061819644,0.3321330646
C,0,1.1227466008,-2.102687196,0.327857344
C,0,-0.082331504,-2.025502904,-0.5969457907
H,0,-0.0482081664,-1.1435108529,-1.2630994571
H,0,-0.1182921166,-2.8929685221,-1.2901072153
C,0,0.6930017196,-2.0908694202,1.7719225413
H,0,1.1281751911,-1.2419916948,2.3212274979
H,0,1.0556890156,-2.9917926966,2.2952595838
C,0,-0.8520194568,-2.0301420923,1.7746530334
H,0,-1.282359862,-2.9007291278,2.2981328443
H,0,-1.2175106511,-1.1506771188,2.3266203991

triplet diradical (T-**DR8b**)
UB3LYP/6-31G(d), C_1symmetry



Nuclear repulsion energy: 2506.6029377729 Hartree

SCF Done: E(UB3LYP) = -1044.43872317 Hartree
Sum of electronic and zero-point Energies= -1043.987540

S**2 before annihilation 2.0090, after 2.0001

Zero-point correction: 0.451183 Hartree

no imaginary frequency:

C,0,-3.2154064834,0.8163179962,-0.1526582403
H,0,-3.1206677634,1.2450262798,-2.2641611044
C,0,-2.6329044942,1.3738105337,-1.2993241808
C,0,-1.3452986609,1.6141504809,1.1865568734
C,0,-1.3363441749,1.8954717685,-1.2638934217
C,0,-2.640361694,1.081192282,1.0924141338
C,0,-0.6366364581,1.8799912268,-0.0204257172
C,0,-0.5968184368,2.1978306077,-2.4648367084
H,0,-3.1276542331,0.719985543,1.9959417511
C,0,0.762189848,2.1433868399,-2.4671953713
H,0,-1.1466874268,2.3599053217,-3.3889658949
H,0,1.3200555295,2.2610794206,-3.3932479249
C,0,1.4793160728,1.7826910164,-1.2687748048
C,0,2.7298401849,1.1589473438,-1.308610552
C,0,0.7849237842,1.8230899664,-0.0228874276
C,0,3.2698343012,0.556510995,-0.1638681844
H,0,3.2023698748,0.9916234026,-2.2751129951
C,0,2.7221969857,0.8665013068,1.0831441273
H,0,3.1821718394,0.4674002534,1.9850469033
C,0,1.4742494658,1.5013452222,1.1816784929
C,0,0.7496889613,1.5875141693,2.4242054605
H,0,1.3005404982,1.4982341464,3.3577289575
C,0,-0.6118848515,1.6419593097,2.426559998
H,0,-1.1648797084,1.5968239841,3.3619917295
C,0,4.2171507005,-0.6064529357,-0.3346845345
H,0,4.6691911168,-0.8862488784,0.6255788436
H,0,5.0415949181,-0.3440123384,-1.0119910342
C,0,-4.2534017988,-0.2670065765,-0.3200864872
H,0,-4.7231715068,-0.5097988263,0.6417354446
H,0,-5.0564452032,0.0607062936,-0.9946610949
C,0,3.4816801393,-1.8362681304,-0.9477355778
H,0,4.2550680251,-2.5523668994,-1.2585288327
H,0,2.9737507699,-1.5186430666,-1.8669007687
C,0,-3.6208580682,-1.5517120614,-0.9353896595
H,0,-3.0922666583,-1.2757157713,-1.8563469883
H,0,-4.4501502757,-2.2035745998,-1.2433936428
C,0,-2.6912448013,-2.4255326336,-0.0404868806
H,0,-2.622806389,-3.3961009164,-0.5674449831
H,0,-3.2409023883,-2.6406779017,0.8876680984
C,0,2.4881184099,-2.6331119298,-0.0496562138
H,0,3.0219735144,-2.8919121534,0.8765730946
H,0,2.3403570957,-3.5948725876,-0.5764780665
C,0,-1.2890013295,-2.0074222311,0.3330930087
C,0,1.1251758115,-2.1041540881,0.3287911995
C,0,-0.083106892,-2.0449339686,-0.5855090724
H,0,-0.0495325109,-1.1759020027,-1.2711187658
H,0,-0.1194602306,-2.9222591525,-1.2675130505
C,0,0.6940220436,-2.0938108377,1.7744458336
H,0,1.1270772596,-1.2438525462,2.3230875426
H,0,1.0594429098,-2.9939829779,2.2969414639
C,0,-0.8532699631,-2.033196493,1.777188765
H,0,-1.2860516124,-2.9030871926,2.299592682
H,0,-1.2168139866,-1.1530772435,2.3287325474

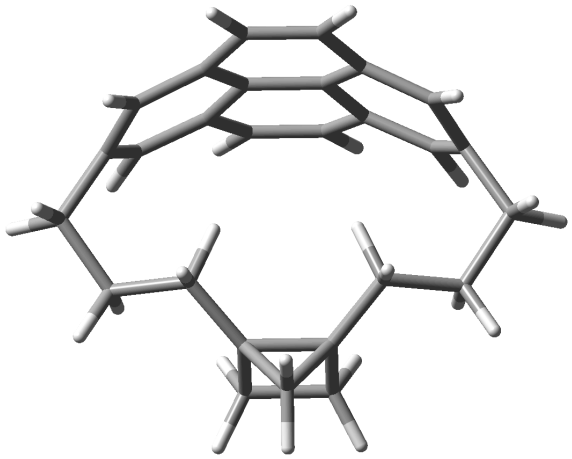
Ring-closd compound (**CP8b**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 2489.1868289758 Hartree

SCF Done: E(RB3LYP) = -1044.47173080 Hartree
Sum of electronic and zero-point Energies= -1044.016396

Zero-point correction: 0.455335 Hartree

no imaginary frequency:



C,0,-3.2076398942,0.7967394237,0.2680907096
H,0,-3.1489437664,1.0154703685,-1.8786097602
C,0,-2.6846227595,1.2952263348,-0.9343787956
C,0,-1.4111242706,1.8896406098,1.5022856747
C,0,-1.4340209586,1.9267970333,-0.9626419279
C,0,-2.6584486702,1.2466402631,1.4734774205
C,0,-0.7263982278,2.0844994313,0.2673039651
C,0,-0.7150074427,2.1515578302,-2.1943443773
H,0,-3.0975530803,0.9203159891,2.4144413759
C,0,0.6457111296,2.1619585023,-2.2056146501
H,0,-1.2754589084,2.1941118604,-3.1253132614
H,0,1.1899505264,2.212956093,-3.1457329566
C,0,1.3883777056,1.9483668968,-0.9860186149
C,0,2.6487753759,1.3359727911,-0.9785538529
C,0,0.6988955797,2.0953919576,0.2554992121
C,0,3.1991837607,0.8456742748,0.2150241751
H,0,3.1016100746,1.0632192001,-1.9303814079
C,0,2.6632289687,1.287288009,1.429399389
H,0,3.1227882953,0.9678224239,2.3629198529
C,0,1.4068782836,1.9111679609,1.4789457385
C,0,0.68739789,2.0791444537,2.717070376
H,0,1.2476192288,2.0927129098,3.6489833629
C,0,-0.6738856105,2.0687472327,2.7283453358
H,0,-1.2187371635,2.0738762998,3.6694107124
C,0,4.0432737267,-0.4122601934,0.1878211883
H,0,4.439011431,-0.6156136692,1.1904805337
H,0,4.9049765199,-0.3267848233,-0.487313708
C,0,-4.03277968,-0.4739264501,0.2547145489
H,0,-4.4086961133,-0.6831752593,1.2637681359
H,0,-4.9067588695,-0.4016798163,-0.4060322327
C,0,3.1651101362,-1.6191808872,-0.2981806548
H,0,3.7290463097,-2.5485490188,-0.1420569309
H,0,3.0429234445,-1.5147142805,-1.3828313401
C,0,-3.1444894998,-1.6673631808,-0.2459482768
H,0,-3.0418164932,-1.5610957856,-1.3324438968
H,0,-3.6915675681,-2.6051985413,-0.0807381205
C,0,-1.7263662424,-1.7555664031,0.3735068687
H,0,-1.8074446301,-2.0174221985,1.4371538937
H,0,-1.2828958075,-0.7553815861,0.3451476176
C,0,1.758896586,-1.7288207454,0.3445638918
H,0,1.2998191839,-0.7355217221,0.3234749733
H,0,1.8614590348,-1.9891081468,1.4067399207
C,0,-0.7645798449,-2.7130584353,-0.3321664035
C,0,0.8003392933,-2.7010569668,-0.3451488634
C,0,0.0319870044,-3.7920094146,0.3583059074
H,0,0.0366996472,-4.8173560692,-0.0212710086
H,0,0.0405412638,-3.7300380919,1.445615637
C,0,-0.7713602855,-3.0069484936,-1.8418871605
H,0,-1.1843692033,-2.1893839874,-2.4406970749
H,0,-1.2638991356,-3.9400255801,-2.1464974977
C,0,0.7865996332,-2.9950254823,-1.8548013012
H,0,1.177064371,-2.1713070155,-2.4602660101
H,0,1.2882528113,-3.9204918852,-2.167647142

singlet diradical in (2,7)pyrenophane (S-**DR8c**)
BS-UB3LYP/6-31G(d), C_1 symmetry

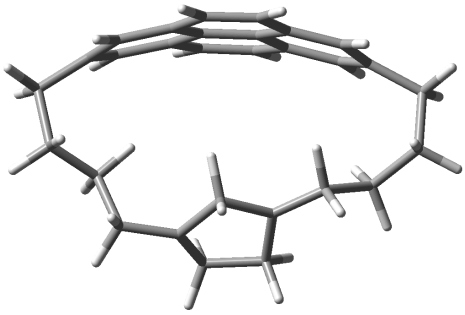
Nuclear repulsion energy: 2755.6323987033 Hartree

SCF Done: E(UB3LYP) = -1123.09518752 Hartree
Sum of electronic and zero-point Energies= -1122.585915

S**2 before annihilation 1.0051, after 0.0624

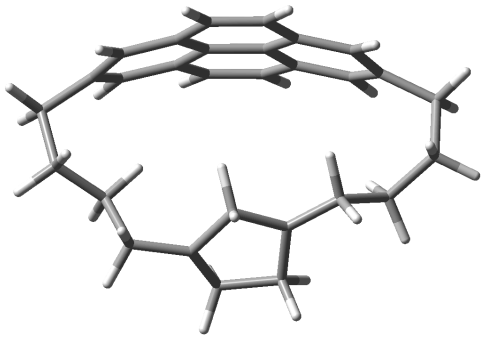
Zero-point correction: 0.509272 Hartree

no imaginary frequency:



C,0,-3.3621764845,1.3979314664,0.3287422282
H,0,-3.3115326007,1.8117364543,-1.787847756
C,0,-2.7408948668,1.8016027936,-0.8607312572
C,0,-1.2554436973,1.7289942661,1.5284965428
C,0,-1.3664180262,2.0758262561,-0.910975338
C,0,-2.6297101074,1.447865794,1.51858424
C,0,-0.5972514294,1.9677630543,0.2868766172
C,0,-0.6706211819,2.3270714464,-2.1466476257
H,0,-3.1160377054,1.1818231092,2.4551566211
C,0,0.6894798824,2.2946909451,-2.2095597522
H,0,-1.2583138469,2.483572239,-3.0482842497
H,0,1.1984883793,2.4233224854,-3.1619552998
C,0,1.4836858589,2.0125843803,-1.0415210441
C,0,2.8377357735,1.6556183648,-1.1167095254
C,0,0.8247166351,1.9462966039,0.2232776449
C,0,3.5419881734,1.2242752678,0.0153458347
H,0,3.3114778572,1.6028646684,-2.0954938539
C,0,2.9401260946,1.3537153127,1.270768573
H,0,3.4923718931,1.0546724729,2.1596185287
C,0,1.5865326663,1.6983239342,1.4029262669
C,0,0.8995596894,1.6443870432,2.6654612882
H,0,1.4898938737,1.5278335123,3.5712819641
C,0,-0.4609905564,1.6539633659,2.724782387
H,0,-0.9714305778,1.5464887089,3.6790121732
C,0,4.7819300889,0.3689342745,-0.141051268
H,0,5.2754788173,0.2485811859,0.8312927336
H,0,5.5130536072,0.8313111671,-0.8170874441
C,0,-4.7296398045,0.7493777376,0.3119554128
H,0,-5.1032100761,0.6801425169,1.3411566758
H,0,-5.4513846053,1.36360876,-0.2429976012
C,0,4.3907534166,-1.029102966,-0.7147937527
H,0,5.2789903963,-1.6756635923,-0.7169153082
H,0,4.1076648235,-0.8919961106,-1.767592384
C,0,-4.7154450348,-0.6758124169,-0.3173961812
H,0,-4.6471795117,-0.5751956212,-1.4088187364
H,0,-5.6974465359,-1.1250989939,-0.1221144484
C,0,3.218845254,-1.7129461451,0.0143882423
H,0,2.4281675092,-0.972835,0.1590762124
H,0,3.5274153213,-2.0234837072,1.0219681287
C,0,2.5878918716,-2.9264537097,-0.7402373014
H,0,3.1211815209,-3.8497697568,-0.4738620214
H,0,2.7447165805,-2.780044823,-1.8199043622
C,0,-3.5838917763,-1.6235581765,0.1693851085
H,0,-3.1396137625,-1.2344841183,1.0933410483
H,0,-4.0067114008,-2.6034813057,0.4237527661
C,0,-2.4730230357,-1.8086680109,-0.8918459344
H,0,-2.2319393545,-0.8264064349,-1.318879005
H,0,-2.9116744903,-2.3810359477,-1.7354917327
C,0,1.1159975098,-3.0637800145,-0.4837811915
C,0,-1.1916595321,-2.4433560909,-0.4492137197
C,0,0.096717972,-2.2111954376,-1.1981236891
H,0,0.3701507523,-1.1381007584,-1.214698723
H,0,0.0176800096,-2.4856672606,-2.2722337265
C,0,0.4977811938,-3.7196183788,0.7211800375
H,0,0.7849816499,-3.1957877189,1.6519328425
H,0,0.8251114769,-4.7614322888,0.8556308925
C,0,-1.0352433255,-3.5972698504,0.5025900945
H,0,-1.4271450698,-4.5342308057,0.061492189
H,0,-1.5857389818,-3.4606650458,1.4434917686

triplet diradical (T-**DR8c**)
UB3LYP/6-31G(d), C_1symmetry



Nuclear repulsion energy: 2755.6214077812 Hartree

SCF Done: E(UB3LYP) = -1123.09598162 Hartree
Sum of electronic and zero-point Energies= -1122.586764

S**2 before annihilation 2.0087, after 2.0000

Zero-point correction: 0.509217 Hartree

no imaginary frequency:

C,0,-3.3629496225,1.4000793019,0.3256967395
H,0,-3.310021547,1.8047693926,-1.7925993846
C,0,-2.7402200388,1.7980061042,-0.8649363189
C,0,-1.2569397363,1.7341193546,1.5259133656
C,0,-1.3655544656,2.0713598903,-0.9149998785
C,0,-2.6314912396,1.4544539472,1.5159742322
C,0,-0.5975014795,1.9676399147,0.2839702902
C,0,-0.6685591212,2.3181579098,-2.1508951681
H,0,-3.1188745955,1.1927126751,2.4532064867
C,0,0.6916161325,2.2858754334,-2.2123664124
H,0,-1.2553953481,2.4715843502,-3.0536220394
H,0,1.201544431,2.4115150047,-3.1646748846
C,0,1.4847197979,2.0076555331,-1.0426390639
C,0,2.8389356388,1.6509252911,-1.1153523981
C,0,0.8245166855,1.945319996,0.2217271809
C,0,3.5421283117,1.2227634539,0.0185961924
H,0,3.3137614779,1.5958276818,-2.0934818547
C,0,2.9388136154,1.3552456155,1.2729741105
H,0,3.4901140592,1.0587186219,2.16324733
C,0,1.5851696944,1.7006914504,1.4028324279
C,0,0.8970663872,1.651381649,2.6649275776
H,0,1.4865227111,1.537320819,3.5716369911
C,0,-0.4635246926,1.6626094485,2.7230984217
H,0,-0.9748419375,1.5589457412,3.6772797648
C,0,4.7833435187,0.3686160536,-0.1347286871
H,0,5.2741973188,0.2479609106,0.8389406312
H,0,5.5159633598,0.8323728558,-0.8082143394
C,0,-4.7310315621,0.7527579574,0.3106379382
H,0,-5.1052559088,0.68805084,1.3398906295
H,0,-5.4518949008,1.3653863498,-0.2472088438
C,0,4.395131078,-1.0289114016,-0.7113180898
H,0,5.2849444915,-1.6732607057,-0.7162165188
H,0,4.1110288048,-0.8893663428,-1.763509281
C,0,-4.7175661488,-0.6750762071,-0.3129042179
H,0,-4.6505996317,-0.5788285445,-1.4047908171
H,0,-5.6993261432,-1.1236489662,-0.1147997196
C,0,3.2254131323,-1.7180495317,0.0168539191
H,0,2.4378308995,-0.9775496009,0.175708421
H,0,3.5394133042,-2.0419961953,1.0184996543
C,0,2.5866104928,-2.9196594116,-0.7500486644
H,0,3.1190697789,-3.8478454457,-0.4994785712
H,0,2.7384847654,-2.7590922645,-1.8283747137
C,0,-3.5850009225,-1.6203194718,0.1764680745
H,0,-3.1349398868,-1.2238514192,1.0943503503
H,0,-4.0077009946,-2.5973487077,0.4418503994
C,0,-2.4794060103,-1.8166265173,-0.8888866321
H,0,-2.2446403147,-0.8395565547,-1.3306498977
H,0,-2.9208217193,-2.4036216654,-1.7207497289
C,0,1.1153119261,-3.0593960418,-0.4894052888
C,0,-1.1932396611,-2.4391023447,-0.4413915921
C,0,0.0943919832,-2.1969514275,-1.1806291399
H,0,0.3694243151,-1.1226589914,-1.1834840147
H,0,0.0134716703,-2.4479877445,-2.2622416764
C,0,0.5002742818,-3.727159819,0.7118986486
H,0,0.7878032564,-3.207625904,1.6450230518
H,0,0.8300586613,-4.7688192714,0.8391322324
C,0,-1.0335550077,-3.6067254825,0.4949931605
H,0,-1.422762574,-4.5370557145,0.0378189529
H,0,-1.5846616008,-3.4866927524,1.4376514926

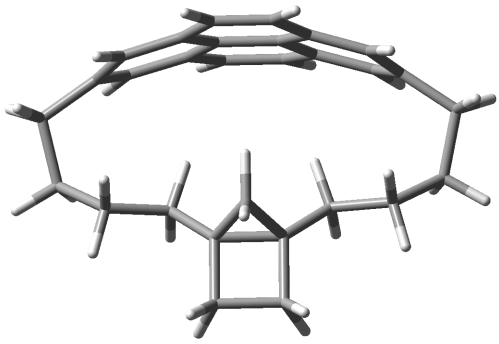
Ring-closd compound (**CP8c**)
RB3LYP/6-31G(d), C_1 symmetry

Nuclear repulsion energy: 2805.4784947502Hartree

SCF Done: E(RB3LYP) = -1123.14196048 Hartree
Sum of electronic and zero-point Energies= -1122.628704

Zero-point correction: 0.513256 Hartree

no imaginary frequency:



C,0,-3.3419788544,1.4171460234,-0.0249394991
H,0,-3.2530201633,1.70563952,-2.1599212622
C,0,-2.7101006719,1.7865802018,-1.2197765699
C,0,-1.2946412762,1.9134898808,1.2085209994
C,0,-1.3460732642,2.1057867106,-1.251479042
C,0,-2.6596398398,1.5933626477,1.1820902646
C,0,-0.6070764901,2.0717026504,-0.0305788611
C,0,-0.6216386866,2.2906174543,-2.4828997665
H,0,-3.1637476592,1.3649138935,2.1189713919
C,0,0.7375465837,2.220765544,-2.5144324306
H,0,-1.1878478043,2.4120922558,-3.4033172906
H,0,1.2700415266,2.2857756706,-3.4603394424
C,0,1.4954076124,1.9597561405,-1.3174003702
C,0,2.819549437,1.5023978278,-1.3480622701
C,0,0.8140720135,1.9986664093,-0.0635488858
C,0,3.4648336244,1.0673271358,-0.1828545895
H,0,3.3072513624,1.3684910669,-2.3121165851
C,0,2.8607029621,1.3096595376,1.054020848
H,0,3.381541279,1.0285353437,1.9671234702
C,0,1.5383791241,1.7678944996,1.1427961769
C,0,0.8321454241,1.8401636214,2.3943716594
H,0,1.402296087,1.7605317438,3.3168574621
C,0,-0.5275918153,1.9100437968,2.4259170452
H,0,-1.0596205115,1.8870552553,3.3739729207
C,0,4.6584074545,0.146788996,-0.2693602856
H,0,5.1586610071,0.0967302309,0.7059654222
H,0,5.3990617455,0.520918875,-0.9887245935
C,0,-4.6263046949,0.6239507665,-0.0539611585
H,0,-5.0834026393,0.6230830254,0.9435760263
H,0,-5.35720605,1.0737101355,-0.7391811703
C,0,4.2443782854,-1.2911156848,-0.7022811696
H,0,5.1518887864,-1.9081889743,-0.6647261571
H,0,3.942880223,-1.264450116,-1.7583666312
C,0,-4.3822389891,-0.8477681777,-0.5021617852
H,0,-4.1287453098,-0.8496065798,-1.5711173132
H,0,-5.3454833842,-1.3687054327,-0.4212329269
C,0,3.1248420547,-1.9816259353,0.1234601789
H,0,3.1373404614,-1.6146573017,1.1585443405
H,0,3.357726924,-3.0532401069,0.1839034127
C,0,1.6937018718,-1.8393428687,-0.4518797001
H,0,1.7089943425,-2.1853454763,-1.4972451844
H,0,1.4049233446,-0.7845157136,-0.4824702806
C,0,-3.30236187,-1.6513101663,0.2725658323
H,0,-3.2292909144,-1.2874292569,1.3062349164
H,0,-3.640781667,-2.6935586482,0.3462927195
C,0,-1.8923321196,-1.6550677184,-0.368701587
H,0,-1.4987171335,-0.6353124142,-0.4151510359
H,0,-1.9913422028,-1.9952181099,-1.4114073952
C,0,0.6514264782,-2.6270280899,0.3138040692
C,0,-0.9019506614,-2.5472072183,0.349829738
C,0,-0.0725077975,-2.1014958741,1.530419398
H,0,-0.0800741082,-2.6698057482,2.4633576791
H,0,-0.0138390032,-1.0247201832,1.6740585924
C,0,0.5750630831,-4.1629596083,0.3296749995
H,0,1.0615754134,-4.6625995242,1.1776151002
H,0,0.945856582,-4.6162732129,-0.596355473
C,0,-0.9826773778,-4.0829169374,0.3657761374
H,0,-1.4403485795,-4.4936535589,-0.5410573201
H,0,-1.4781096448,-4.5321104739,1.2364694113

singlet oxyallyl derivative (S-**DR9**)
BS-UB3LYP/6-31G(d), C_s symmetry

Nuclear repulsion energy: 3809.7193733470 Hartree

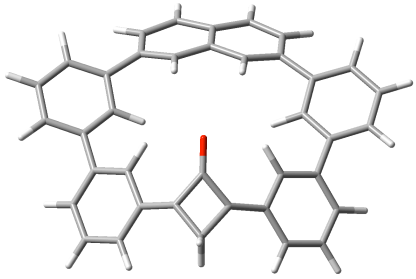
SCF Done: E(UB3LYP) = -1537.69551718 Hartree

Sum of electronic and zero-point Energies= -1537.194583

S**2 before annihilation 0.0000, after 0.0000

Zero-point correction: 0.500934 Hartree

no imaginary frequency:



H,0,4.810268219,3.3675287787,-0.6904437258
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C,0,5.1098648245,1.2604959234,-0.4984578144
C,0,2.616748651,1.221469488,0.7507667066
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C,0,3.0974548557,2.4224316504,0.2609711839
C,0,3.2836795628,0.,0.511578524
C,0,5.1098648245,-1.2604959234,-0.4984578144
H,0,1.6532472983,-1.1831265813,1.2504192418
H,0,1.6532472983,1.1831265813,1.2504192418
C,0,4.3985584643,-2.4305090817,-0.3243123771
H,0,6.0850242381,-1.2881352993,-0.9795036073
H,0,4.810268219,-3.3675287787,-0.6904437258
C,0,3.0974548557,-2.4224316504,0.2609711839
C,0,2.616748651,-1.221469488,0.7507667066
C,0,2.1706643168,-3.5840961976,0.2323889285
C,0,0.2277865701,-5.6301054838,0.1302805052
C,0,0.8184692408,-3.3085728439,-0.0217899421
C,0,2.5422113677,-4.9248937836,0.4100490353
C,0,1.5739606963,-5.9312479268,0.3523575399
C,0,-0.1701085193,-4.29664931,-0.0531133675
H,0,0.5313605072,-2.2879038136,-0.2437507706
H,0,3.5782926905,-5.1819819331,0.6144842385
H,0,1.8703992056,-6.9658188746,0.5045438691
H,0,-0.5113180857,-6.4269918485,0.1224301303
C,0,2.1706643168,3.5840961976,0.2323889285
C,0,0.2277865701,5.6301054838,0.1302805052
C,0,2.5422113677,4.9248937836,0.4100490353
C,0,0.8184692408,3.3085728439,-0.0217899421
C,0,-0.1701085193,4.29664931,-0.0531133675
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C,0,-1.5760243354,-3.8674760421,-0.2859854222
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C,0,-2.0279434866,-2.6714586107,0.2857238081
C,0,-2.4635860535,-4.5870260281,-1.1050350922
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H,0,-1.3893946439,-2.1130486129,0.9615837319
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C,0,-3.7223927307,-0.9403499903,0.6794374316
C,0,-3.7223927307,0.9403499903,0.6794374316
C,0,-4.8808112892,0.,0.4143222965
H,0,-5.2802686589,0.,-0.6080877441
H,0,-5.7011363347,0.,1.1399605738
C,0,-2.9093386495,0.,1.4307433477
O,0,-1.8489154231,0.,2.0544226862

triplet oxyallyl derivative (T-**DR9**)
UB3LYP/6-31G(d), C_s symmetry

Nuclear repulsion energy: 3793.4539041041 Hartree

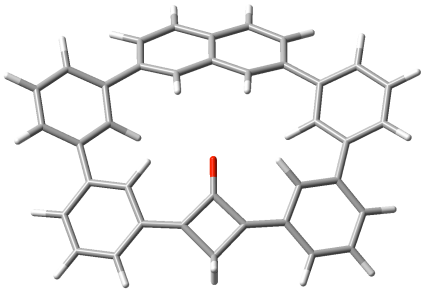
SCF Done: E(UB3LYP) = -1537.67278911 Hartree

Sum of electronic and zero-point Energies= -1537.174265

S**2 before annihilation 2.0567, after 2.0021

Zero-point correction: 0.498524 Hartree

no imaginary frequency:



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C,0,4.3265134224,2.4401036652,-0.3888969596
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C,0,5.0195208119,1.2606475589,-0.5717657729
C,0,2.4279350149,1.2262010944,0.4573183753
C,0,4.4173272509,0.,-0.3006918602
C,0,2.9878815584,2.4424859344,0.1044501697
C,0,3.0950355395,0.,0.2367179604
C,0,5.0195208119,-1.2606475589,-0.5717657729
H,0,1.4281522149,-1.1854200106,0.8790293128
H,0,1.4281522149,1.1854200106,0.8790293128
C,0,4.3265134224,-2.4401036652,-0.3888969596
H,0,6.031026027,-1.2855798792,-0.9711039522
H,0,4.7927164078,-3.3829907201,-0.663177923
C,0,2.9878815584,-2.4424859344,0.1044501697
C,0,2.4279350149,-1.2262010944,0.4573183753
C,0,2.1382602265,-3.6605732031,0.1934991114
C,0,0.3243530107,-5.812504989,0.4534997518
C,0,0.7711060085,-3.5150694043,-0.0787607429
C,0,2.596084392,-4.9362873049,0.5578604168
C,0,1.6927779448,-5.9970813348,0.6704395968
C,0,-0.1603890078,-4.5485500979,0.0843352486
H,0,0.4217106417,-2.5583973415,-0.4462617561
H,0,3.6474361286,-5.0963049685,0.782364494
H,0,2.0574373163,-6.9777246584,0.9651449729
H,0,-0.3628186178,-6.6421079885,0.5987268937
C,0,2.1382602265,3.6605732031,0.1934991114
C,0,0.3243530107,5.812504989,0.4534997518
C,0,2.596084392,4.9362873049,0.5578604168
C,0,0.7711060085,3.5150694043,-0.0787607429
C,0,-0.1603890078,4.5485500979,0.0843352486
C,0,1.6927779448,5.9970813348,0.6704395968
H,0,3.6474361286,5.0963049685,0.782364494
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H,0,2.0574373163,6.9777246584,0.9651449729
H,0,-0.3628186178,6.6421079885,0.5987268937
C,0,-1.5982061884,-4.216885651,-0.1202962635
C,0,-4.2486141006,-3.3522993127,-0.6680102464
C,0,-2.0206522848,-2.9300799158,0.2094643927
C,0,-2.5457490597,-5.0957827701,-0.6813674858
C,0,-3.8567536503,-4.6598193417,-0.9306606187
C,0,-3.319068445,-2.4422309836,-0.0973987764
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H,0,-2.2544391952,-6.1054592247,-0.9577208081
H,0,-4.57008798,-5.352948409,-1.3688947685
H,0,-5.2560253992,-3.0222034712,-0.9066209222
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C,0,-2.5457490597,5.0957827701,-0.6813674858
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H,0,-4.57008798,5.352948409,-1.3688947685
H,0,-5.2560253992,3.0222034712,-0.9066209222
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C,0,-4.579431996,0.,-0.2710985284
H,0,-4.8826438755,0.,-1.32796506
H,0,-5.4952193209,0.,0.3387727283
C,0,-2.5988362572,0.,0.5326231238
O,0,-1.4519693356,0.,0.9967643333

singlet oxyallyl derivative (S-**DR11**)
BS-UB3LYP/6-31G(d), C_s symmetry

Nuclear repulsion energy: 1016.8733969973 Hartree

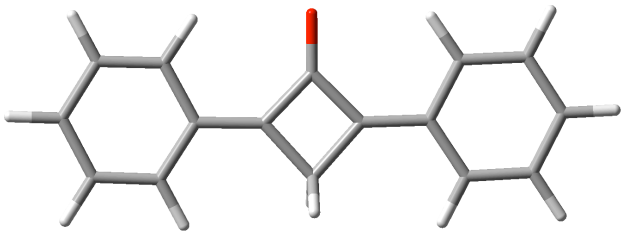
SCF Done: E(UB3LYP) = -692.081050356 Hartree

Sum of electronic and zero-point Energies= -691.850807

S**2 before annihilation 0.3849, after 0.0300

Zero-point correction: 0.230244 Hartree

no imaginary frequency:



C,0,1.2570962261,0.,0.4390293524
H,0,2.165712853,0.,-0.1839991948
H,0,1.5739707604,0.,1.4941864333
C,0,0.1836668939,1.0211759996,0.06051658
C,0,0.1836668939,-1.0211759996,0.06051658
C,0,0.15366438,2.4392880788,0.0523479134
C,0,0.0400654052,5.2428787316,0.0168107612
C,0,1.2740011523,3.21106469,0.449483524
C,0,-1.0293649028,3.1070471585,-0.3645442196
C,0,-1.0761597314,4.4938575641,-0.378820812
C,0,1.2128717451,4.597894036,0.4301605421
H,0,2.1811606572,2.7054932395,0.7691624985
H,0,-1.8802330745,2.5038169152,-0.6661097898
H,0,-1.9825045788,5.0009423985,-0.6982202477
H,0,2.0752743211,5.1840236565,0.735838424
H,0,-0.0033522375,6.3286435988,0.003248252
C,0,0.15366438,-2.4392880788,0.0523479134
C,0,0.0400654052,-5.2428787316,0.0168107612
C,0,-1.0293649028,-3.1070471585,-0.3645442196
C,0,1.2740011523,-3.21106469,0.449483524
C,0,1.2128717451,-4.597894036,0.4301605421
C,0,-1.0761597314,-4.4938575641,-0.378820812
H,0,-1.8802330745,-2.5038169152,-0.6661097898
H,0,2.1811606572,-2.7054932395,0.7691624985
H,0,2.0752743211,-5.1840236565,0.735838424
H,0,-1.9825045788,-5.0009423985,-0.6982202477
H,0,-0.0033522375,-6.3286435988,0.003248252
C,0,-0.8008773861,0.,-0.2881123397
O,0,-1.9668325136,0.,-0.7008510135

triplet oxyallyl derivative (T-**DR11**)
UB3LYP/6-31G(d), C_s symmetry

Nuclear repulsion energy: 1012.8490519977 Hartree

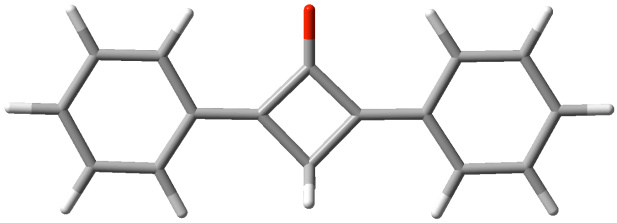
SCF Done: E(UB3LYP) = -692.067452243 Hartree

Sum of electronic and zero-point Energies= -691.839007

S**2 before annihilation 2.0565, after 2.0021

Zero-point correction: 0.228446 Hartree

no imaginary frequency:



C,0,1.1999866685,0.,0.4227443182
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C,0,0.1609947637,1.054856969,0.0557796615
C,0,0.1609947637,-1.054856969,0.0557796615
C,0,0.1411479161,2.4660749821,0.0490248924
C,0,0.0684912264,5.2846378418,0.0239223773
C,0,1.2722150584,3.2298325874,0.448719215
C,0,-1.0310295106,3.1626817857,-0.3649192445
C,0,-1.0569611951,4.5487020387,-0.3737984425
C,0,1.2303434663,4.6159472796,0.4342096992
H,0,2.1741774657,2.7139771761,0.7672238186
H,0,-1.8966029557,2.5837133788,-0.6708021467
H,0,-1.9573964925,5.0675321434,-0.6917800865
H,0,2.1029371084,5.1857972258,0.7425617984
H,0,0.0408556335,6.3706615659,0.0143986161
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C,0,0.0684912264,-5.2846378418,0.0239223773
C,0,-1.0310295106,-3.1626817857,-0.3649192445
C,0,1.2722150584,-3.2298325874,0.448719215
C,0,1.2303434663,-4.6159472796,0.4342096992
C,0,-1.0569611951,-4.5487020387,-0.3737984425
H,0,-1.8966029557,-2.5837133788,-0.6708021467
H,0,2.1741774657,-2.7139771761,0.7672238186
H,0,2.1029371084,-5.1857972258,0.7425617984
H,0,-1.9573964925,-5.0675321434,-0.6917800865
H,0,0.0408556335,-6.3706615659,0.0143986161
C,0,-0.8166227425,0.,-0.2895729769
O,0,-1.9808650405,0.,-0.7008117681

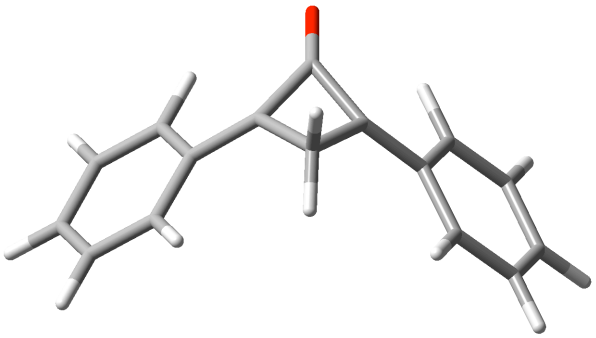
bicyclo[1.1.0]butan-2-one derivative (**CP11**)
RB3LYP/6-31G(d), C_s symmetry

Nuclear repulsion energy: 1153.4144680999 Hartree

SCF Done: E(RB3LYP) = -731.426638908 Hartree
Sum of electronic and zero-point Energies= -731.166231

Zero-point correction: 0.260408 Hartree

no imaginary frequency:



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C,0,-4.4852676647,-1.656383251,2.2423809029
C,0,-3.3711263233,-1.0772470319,2.8558587051
C,0,-2.3000162989,-0.7874382731,0.6841122098
H,0,-3.4802065563,-1.5004771415,-0.9960785261
H,0,-5.3273732322,-1.9912917504,2.8424666936
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H,0,-1.4145497606,-0.1938881386,2.5512346083
C,0,4.1312260892,1.9615855302,-1.9228048818
C,0,2.7500204361,1.5491700838,0.4816102842
C,0,4.7053334461,2.3471231222,-0.7048905541
C,0,2.8750923644,1.3733473838,-1.9437660372
C,0,2.1505783072,1.151173767,-0.7430713043
C,0,4.0097052636,2.1377647278,0.4889902538
H,0,5.6896579036,2.8078900215,-0.6905063477
H,0,2.4432831412,1.0799258234,-2.8956389966
H,0,4.4548203341,2.4367901356,1.4342872834
H,0,2.1923923311,1.3771192807,1.3946076345
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H,0,-1.2668533845,-1.5283991233,-1.9234890183
H,0,-2.0054621822,0.0530701342,-2.076696327
C,0,0.1862150841,0.1094546729,-2.0403806812
H,0,0.7906103768,-0.6311472645,-2.5841185979
H,0,0.052262219,0.9505712318,-2.7361189009
C,0,0.0232386722,0.2682331196,0.3933107838
O,0,0.3008405265,0.5134922097,1.5920880958
H,0,-5.3800541779,-2.2549470332,0.3693181101
H,0,4.6689926336,2.1227020172,-2.853288813
C,0,-1.1911016599,-0.3476649254,-0.1183188101
C,0,0.8491253362,0.5409767343,-0.7725431371