REVISED

Supplementary Materials

Table S1. The Activation and Reaction Energies (kcal/mol) for the Bergman Cyclizations of Enediynes **1-3** calculated at the B3LYP/6-31G** (bold) and BLYP/6-31G** Levels.

Enediyne							
	R_{C1-C6}	TS_{C1-C6}	$\Delta E^{\neq}$	$\Delta H^{\neq}$	$\Delta G^{\neq}$	ΔE_r	ΔE_{ST}
	**4.480**	**1.978**	**31.2**	**29.9**	**31.3**	**3.3**	**2.5**
	4.546	2.073	25.4	24.4	26.4	6.8	4.1
	**3.388**	**1.904**	**27.7**	**26.4**	**28.1**	**3.4**	**3.4**
	3.403	1.974	21.4	20.1	22.1	7.5	5.6
	**2.915**	**1.865**	**18.6**	**17.1**	**18.1**	**0.3**	**1.8**
	2.923	1.948	13.0	11.7	12.9	3.5	3.2

Table S2. The Overlap and Fock Matrix Elements of the *In-plane* and *Out-of-plane* π-orbital Interactions in the IRC Path of Reaction **1** calculated at the B3LYP/6-31G** level.

Species	R_{C1C6}	S_{ij}				F_{ij}			
		$\pi_i-\pi_i$	$\pi_i-\pi_i^*$	$\pi_o-\pi_o$	$\pi_o-\pi_o^*$	$\pi_i-\pi_i$	$\pi_i-\pi_i^*$	$\pi_o-\pi_o$	$\pi_o-\pi_o^*$
R	4.480	0.0639	0.0701	0.0157	0.0194	0.0080	0.0087	0.0031	0.0017
IRC1	4.25	0.0775	0.0764	0.0190	0.0220	0.0101	0.0096	0.0036	0.0020
IRC2	4.00	0.0961	0.0791	0.0232	0.0243	0.0128	0.0101	0.0043	0.0022
IRC3	3.75	0.1176	0.0775	0.0282	0.0258	0.0160	0.0096	0.0051	0.0022
IRC4	3.50	0.1436	0.0722	0.0341	0.0258	0.0197	0.0076	0.0061	0.0020
IRC5	3.292	0.1679	0.0594	0.0403	0.0246	0.0236	0.0051	0.0072	0.0016
IRC6	3.177	0.1824	0.0478	0.0443	0.0229	0.026	0.0029	0.0079	0.0012
IRC7	3.022	0.2019	0.0262	0.0498	0.0188	0.0294	0.0015	0.0089	0.0002
IRC8	2.935	0.214	0.0124	0.0533	0.0158	0.0316	0.0044	0.0095	0.0004
IRC9	2.821	0.2316	0.0114	0.0585	0.0103	0.0350	0.0094	0.0105	0.0016
IRC10	2.664	0.2593	0.0471	0.0666	0.0011	0.0408	0.0176	0.0120	0.0036
IRC11	2.553	0.2816	0.0766	0.0739	0.0071	0.0463	0.0249	0.0134	0.0054
IRC12	2.450	0.3040	0.1065	0.0817	0.0161	0.0525	0.0331	0.0149	0.0073
IRC13	2.372	0.3207	0.1303	0.0884	0.0239	0.0580	0.0405	0.0162	0.0091
IRC14	2.285	0.3404	0.1585	0.0971	0.0336	0.0653	0.0502	0.0179	0.0113
IRC15	2.202	0.3596	0.1859	0.1065	0.0439	0.0734	0.0609	0.0198	0.0138
IRC16	2.120	0.3755	0.2118	0.1168	0.0553	0.0825	0.0730	0.0220	0.0166
IRC17	2.070	0.3853	0.2267	0.1238	0.0624	0.0887	0.0812	0.0236	0.0184
TS	1.978	0.4012	0.2521	0.1376	0.0768	0.1017	0.0981	0.0268	0.0223
IRC18	1.907	0.4111	0.2684	0.1493	0.0885	0.1129	0.1127	0.0297	0.0257
IRC19	1.871	0.4154	0.2756	0.1557	0.0948	0.1191	0.1207	0.0313	0.0276
IRC20	1.837	0.4186	0.2810	0.1618	0.1009	0.1252	0.1286	0.0330	0.0296

Table S3. The Overlap and Fock Matrix Elements of the *In-plane* and *Out-of-plane* π-orbital Interactions in the IRC Path of Reaction **2** calculated at the B3LYP/6-31G** level.

Species	d_{C1-C6}	S_{ij}				F_{ij}			
		$\pi_i-\pi_i^*$	$\pi_i-\pi_I$	$\pi_o-\pi_o^*$	$\pi_o-\pi_o$	$\pi_i-\pi_i^*$	$\pi_i-\pi_I$	$\pi_o-\pi_o^*$	$\pi_o-\pi_o$
R	3.388	0.0554	0.1589	0.0221	0.0368	0.0072	0.0204	0.0019	0.0065
IRC1	3.250	0.0355	0.1813	0.0192	0.0432	0.0034	0.0241	0.0012	0.0076
IRC2	3.00	0.0062	0.2088	0.0138	0.0516	0.0023	0.0289	0.0002	0.0090
IRC3	2.874	0.0172	0.2268	0.0086	0.0577	0.0070	0.0323	0.0008	0.0100
IRC4	2.731	0.0485	0.2513	0.0010	0.0657	0.0139	0.0373	0.0023	0.0113
IRC5	2.612	0.0805	0.2752	0.0075	0.0734	0.0217	0.0427	0.0039	0.0126
IRC6	2.474	0.1220	0.3073	0.0197	0.0841	0.0330	0.0511	0.0064	0.0145
IRC7	2.285	0.1830	0.3551	0.0406	0.1025	0.0539	0.0672	0.0108	0.0179
IRC8	2.107	0.2195	0.3653	0.0459	0.0919	0.0744	0.0814	0.0102	0.0150
IRC9	2.006	0.2662	0.4151	0.0800	0.1364	0.0993	0.1032	0.0202	0.0252
IRC10	1.962	0.2805	0.4241	0.0882	0.1453	0.1094	0.1110	0.0226	0.0273
TS	1.904	0.2927	0.4324	0.0979	0.1557	0.1220	0.1210	0.0256	0.0299
IRC11	1.843	0.3052	0.4399	0.1089	0.1671	0.1373	0.1331	0.0292	0.0330

Table S4. The Overlap and Fock Matrix Elements of the *In-plane* and *Out-of-plane* π-orbital Interactions in the IRC Path of Reaction **3** calculated at the B3LYP/6-31G** level.

Species	d_{C1-C6}	S_{ij}				F_{ij}			
		$\pi_i-\pi_i^*$	$\pi_i-\pi_i$	$\pi_o-\pi_o^*$	$\pi_o-\pi_o$	$\pi_i-\pi_i^*$	$\pi_i-\pi_i$	$\pi_o-\pi_o^*$	$\pi_o-\pi_o$
R	2.915	0.0012	0.2175	0.0096	0.0546	0.0014	0.0288	0.0003	0.0093
IRC1	2.726	0.0390	0.2475	0.0002	0.0649	0.0099	0.0350	0.0022	0.0110
IRC2	2.650	0.0578	0.2614	0.0053	0.0697	0.0143	0.0381	0.0031	0.0118
IRC3	2.500	0.1017	0.2927	0.0180	0.0806	0.0255	0.0459	0.0056	0.0137
IRC4	2.320	0.1590	0.3353	0.0373	0.0973	0.0435	0.0591	0.0096	0.0168
IRC5	2.142	0.2158	0.3763	0.0618	0.1196	0.0676	0.0774	0.0153	0.0213
IRC6	1.997	0.2520	0.3989	0.0880	0.1485	0.0913	0.0958	0.0231	0.0284
IRC7	1.952	0.2676	0.4122	0.0923	0.1497	0.1020	0.1042	0.0237	0.0284
TS	1.865	0.2883	0.4262	0.1067	0.1631	0.1222	0.1198	0.0279	0.0317
IRC8	1.800	0.3000	0.4336	0.1186	0.1751	0.1387	0.1327	0.0319	0.0350

Table S5. The Fock Matrix Elements of the *In-plane* π-orbital Interactions in the IRC Path for cyclization of benzannelated enediyne calculated at the B3LYP/6-31G** level.

Species	d_{C1-C6}	F_{ij}	
		$\pi_i-\pi_i$	$\pi_i-\pi_i^*$
R	4.212	0.0113	0.0109
IRC1	3.950	0.0141	0.011
IRC2	3.550	0.0194	0.0088
IRC3	3.235	0.0247	0.0044
IRC4	3.067	0.0281	0.00015
IRC5	2.837	0.0340	0.00795
IRC6	2.633	0.0416	0.0187
IRC7	2.408	0.0546	0.0361
IRC8	2.218	0.0709	0.0577
IRC9	2.052	0.0902	0.08315
TS	1.924	0.1094	0.1082

Table S6. The Fock Matrix Elements of the *In-plane* π-orbital Interactions in the IRC Path for the cyclization of enediyne **4** calculated at the B3LYP/6-31G** level.

Species	d_{C1-C6}	F_{ij}	
		$\pi_i-\pi_i$	$\pi_i-\pi_i^*$
R	4.291	0.010	0.0106
IRC1	4.000	0.013	0.01075
IRC2	3.750	0.016	0.00995
IRC3	3.500	0.019	0.00765
IRC4	3.250	0.023	0.00325
IRC5	3.000	0.028	0.0036
IRC6	2.750	0.035	0.01375
IRC7	2.500	0.046	0.0291
IRC8	2.250	0.063	0.0531
IRC9	2.000	0.090	0.09055
IRC10	1.975	0.093	0.0952
IRC11	1.950	0.097	0.1
TS	1.926	0.100	0.1046

Table S7. The Fock Matrix Elements of the *In-plane* π-orbital Interactions in the IRC Path for the cyclization of enediyne **8** calculated at the B3LYP/6-31G** level.

Species	d_{C1-C6}	F_{ij}	
		$\pi_i-\pi_i$	$\pi_i-\pi_i^*$
R	3.997	0.014	0.0121
IRC1	3.750	0.0171	0.0116
IRC2	3.500	0.0205	0.00955
IRC3	3.250	0.0245	0.0054
IRC4	3.000	0.0296	0.00435
IRC5	2.750	0.037	0.01165
IRC6	2.500	0.048	0.0273
IRC7	2.250	0.065	0.0516
IRC8	2.000	0.0918	0.0896
IRC9	1.965	0.0965	0.09625
TS	1.934	0.101	0.1024

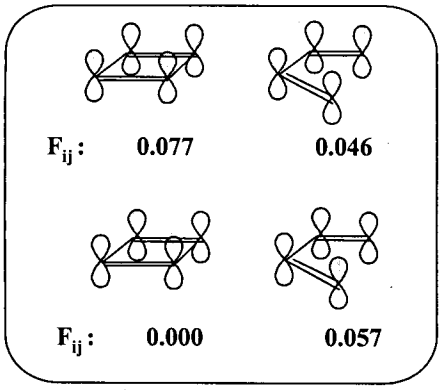


Figure S1. The π-π and π-π* interactions in 1,3-butadiene and cyclobutadiene systems and the corresponding Fock matrix elements.

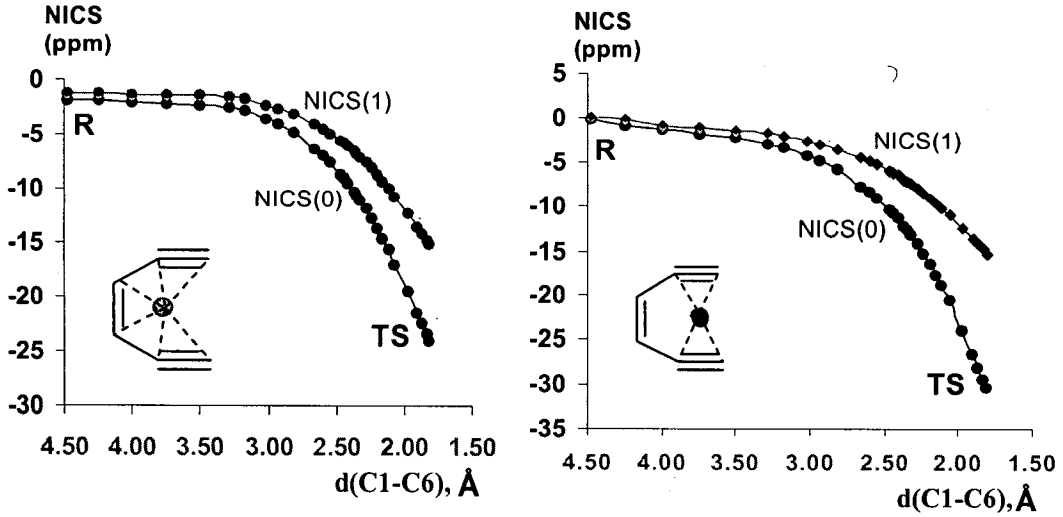
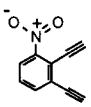
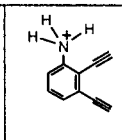
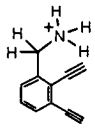
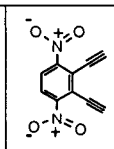
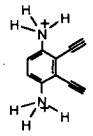
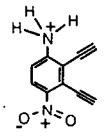


Figure S2. The nucleus independent chemical shift (NICS) changes in the IRC pathway of enediyne cyclization calculated at the UB3LYP/6-311+G**//UB3LYP/6-31G** level for two different reference points in the enediyne plane. NICS(0) values are taken in the enediyne plane, NICS(1) values are for the points which are 1 Å above the plane.

Table S8. Activation and reaction energies (kcal mol^{-1}), C1-C6 distances in the reactant and the TS, and Fock matrix elements (kcal mol^{-1}) corresponding to the four-electron (π-π) and two-electron (π-π^*) interactions of the *in-plane* acetylenic orbitals for the Bergman cyclizations of various benzannelated enediynes.

Bond length (Å) & Relative Energies (kcal/mol)							
$R_{C1\text{-}C6}$	4.212	3.936	4.291	3.997	3.675	4.283	4.024
$TS_{C1\text{-}C6}$	1.924	1.922	1.926	1.934	1.915	1.894	1.999
$\Delta E^{\neq}$	31.3	27.9	28.4	25.5	25.5	30.8	21.3
ΔE_r	11.0	6.6	11.7	10.0	2.5	11.7	6.7
$F^R_{ij}(\pi i \pi i)$	7.09	9.22	6.59	8.79	11.67	6.59	8.53
$F^{TS}_{ij}(\pi i \pi i)$	68.64	68.84	63.25	63.38	70.41	67.46	55.22
$F^R_{ij}(\pi i \pi i^*)$	6.83	7.21	6.65	7.59	7.03	6.40	6.68
$F^{TS}_{ij}(\pi i \pi i^*)$	67.90	68.21	65.64	64.26	69.15	69.53	57.64
$\Delta F_{ij}(\pi i \pi i)$	61.55	59.62	56.66	54.59	58.74	60.87	46.69
$\Delta F_{ij}(\pi i \pi i^*)$	61.07	61.00	58.99	56.67	62.12	63.13	50.96
$\delta\Delta F_{ij}$	+0.48	-1.38	-2.33	-2.08	-3.38	-2.26	-4.27

Cartesian Coordinates From UB3LYP/6-31G Computations.**

Reactant

3-ene-1,5-diyne (**R1**)
Total energy = -230.88718, Nimag = 0

6	0.000000	1.497422	-0.074561
6	0.000000	0.677267	1.081003
6	0.000000	-0.677267	1.081003
6	0.000000	-1.497422	-0.074561
6	0.000000	-2.239864	-1.031865
6	0.000000	2.239864	-1.031865
1	0.000000	1.189099	2.041006
1	0.000000	-1.189099	2.041006
1	0.000000	-2.873090	-1.888468
1	0.000000	2.873090	-1.888468

cyclodeca-3-ene-1,5-diyne (**R2**)
Total energy = -386.95433, Nimag = 0

6	-1.830153	0.054511	0.538265
6	-1.786058	0.021363	1.956265
6	-0.579369	-0.058307	2.584233
6	0.608104	-0.073645	1.807418
6	1.432751	-0.043014	0.915086
6	-1.571214	0.041249	-0.649176
6	-1.067255	-0.056212	-2.017419
6	0.419990	-0.503349	-2.057222
6	1.441826	0.532261	-1.516603
6	2.264478	0.074876	-0.280694
1	-2.704119	0.048383	2.536641
1	-0.528625	-0.098905	3.668751
1	-1.178936	0.905725	-2.536896
1	-1.669247	-0.777161	-2.586405
1	0.660687	-0.740148	-3.099965
1	0.504047	-1.441419	-1.498076
1	2.156816	0.783743	-2.308351
1	0.929311	1.463750	-1.253276
1	2.760348	-0.881234	-0.498914
1	3.071113	0.798873	-0.104420

cyclonona-3-ene-1,5-diyne (**R3**)
Total Energy = -347.62913, Nimag=0

6	-1.676989	-0.080554	0.371190
6	-1.609642	-0.076953	1.790212
6	-0.374138	-0.076681	2.378181
6	0.769545	-0.079987	1.535485
6	1.383815	-0.085200	0.484487
6	-1.248657	-0.085710	-0.768311
6	-0.499223	-0.095926	-2.024544
6	1.886057	-0.095468	-0.889388
1	-2.506844	-0.076427	2.401653
1	-0.282778	-0.075923	3.460071
1	-1.051947	0.421976	-2.818872
1	-0.372579	-1.132823	-2.370128
1	2.074684	-1.132358	-1.205462
1	2.850928	0.422707	-0.961503
6	0.896649	0.573205	-1.884281
1	0.756009	1.618040	-1.589179
1	1.368018	0.574447	-2.874760

ortho-NH_3^+ (**R4**)
Total energy = -440.2652729, Nimag = 0

6	0.326930	1.773762	0.000126
6	-0.050344	0.399598	0.000156
6	0.894621	-0.661623	0.000067
6	2.288899	-0.386362	0.000053
6	3.479728	-0.177035	0.000090
6	0.556677	2.963862	-0.000339
1	4.531173	0.009027	0.000132
1	0.823023	3.999113	-0.000555
6	-1.412095	0.057276	0.000075
6	-1.881999	-1.245282	-0.000096
6	-0.938186	-2.276443	-0.000134
6	0.423250	-1.987870	-0.000085
1	-2.945277	-1.465748	-0.000156
1	-1.273017	-3.307708	-0.000237
1	1.149150	-2.792918	-0.000184
7	-2.375558	1.192282	0.000152
1	-2.978897	1.190749	0.830667
1	-1.823366	2.071293	0.000263
1	-2.978765	1.190933	-0.830467

para-NH_3^+ (**R5**)
Total Energy = -440.2573805, Nimag = 0

6	1.387392	1.659968	-0.000009
6	0.388574	0.648666	-0.000001
6	0.729281	-0.734798	0.000002
6	2.088096	-1.151100	0.000018
6	3.235725	-1.531911	0.000046
6	2.220148	2.536548	-0.000014
1	4.251979	-1.859011	0.000011
1	2.967228	3.299242	-0.000009
6	-0.969166	1.016464	-0.000017
6	-1.935932	0.025899	-0.000043
6	-1.637025	-1.333847	-0.000040
6	-0.296495	-1.699981	-0.000023
1	-1.226215	2.071774	-0.000015
1	-2.413339	-2.093453	-0.000062
1	-0.025627	-2.749314	-0.000037
7	-3.373621	0.439137	0.000059
1	-3.871793	0.088405	-0.827598
1	-3.870857	0.091454	0.829574
1	-3.459620	1.461492	-0.001793

ortho-NMe_2H^+ (**R6**)
Total Energy = -518.90045, Nimag = 0

6	0.464420	0.000148	-1.735068
6	0.458970	0.000064	-0.309043
6	1.658171	0.000125	0.453437
6	2.925231	0.000278	-0.191978
6	4.014484	0.000427	-0.716819
6	0.391406	0.000078	-2.944830
1	4.975621	0.000549	-1.181510
1	0.386453	0.000103	-4.013415
6	-0.766748	-0.000080	0.381433
6	-0.849927	-0.000174	1.765891
6	0.337504	-0.000118	2.502761
6	1.569722	0.000027	1.857230
1	-1.806980	-0.000288	2.276939
1	0.294486	-0.000190	3.586275
1	2.487740	0.000069	2.433650
7	-1.998400	-0.000137	-0.450906
1	-1.643203	-0.000062	-1.422320
6	-2.821428	-1.253515	-0.284996
1	-3.642405	-1.227638	-1.002476
1	-2.178578	-2.113415	-0.469998
1	-3.211856	-1.288229	0.731156
6	-2.821623	1.253096	-0.284871
1	-2.178912	2.113114	-0.469803
1	-3.642607	1.227156	-1.002341
1	-3.212041	1.287655	0.731292

para-NMe_2H^+ (**R7**)
Total energy = -518.89329, Nimag = 0

6	-2.117561	1.664732	-0.000901
6	-1.124917	0.646423	-0.000362
6	-1.474135	-0.733858	0.000369
6	-2.835274	-1.144556	0.000596
6	-3.984496	-1.520487	0.000799
6	-2.943980	2.547314	-0.001375
1	-5.002106	-1.842720	0.000978
1	-3.685991	3.314683	-0.001793
6	0.234947	1.003837	-0.000588
6	1.209463	0.017252	-0.000137
6	0.890872	-1.340436	0.000583
6	-0.451224	-1.700980	0.000824
1	0.494276	2.059379	-0.001143
1	1.654182	-2.111438	0.000964
1	-0.726044	-2.749392	0.001371
7	2.636523	0.449076	-0.000296
1	2.616097	1.473204	-0.001173
6	3.375492	0.037438	1.253244
1	4.375442	0.472239	1.227564
1	2.817101	0.400973	2.115117
1	3.438045	-1.049348	1.278988
6	3.375968	0.035404	-1.252872
1	2.817851	0.397435	-2.115554
1	4.375861	0.470356	-1.227548
1	3.438695	-1.051407	-1.276773

ortho-$CH_2NH_3^+$ (**R8**)
Total Enerdy = -479.58154, Nimag = 0

6	-2.291314	1.140349	0.000000
6	-1.416799	0.016531	0.000000
6	0.000000	0.194495	0.000000
6	0.496014	1.538477	0.000000
6	0.884556	2.687700	0.000000
6	-3.064590	2.069993	0.000000
1	1.163199	3.719284	0.000000
1	-3.747515	2.890105	0.000000
6	-1.951882	-1.279942	0.000000
6	-1.115624	-2.390490	0.000000
6	0.266614	-2.221909	0.000000
6	0.834800	-0.944253	0.000000
1	-3.029271	-1.398841	0.000000
1	-1.537661	-3.389633	0.000000
1	0.911028	-3.097179	0.000000
6	2.356400	-0.952216	0.000000
1	2.740401	-1.469437	0.883603
1	2.740401	-1.469437	-0.883603
7	3.032155	0.404179	0.000000
1	2.746659	0.966403	-0.810472
1	2.746659	0.966403	0.810472
1	4.051959	0.300669	0.000000

1-NH_3^+,4-OMe (**R9**)
Total Energy = -554.78775, Nimag = 0

6	-0.706110	0.000089	-2.174875
6	-0.659343	-0.000257	-0.748624
6	0.575339	-0.000136	-0.036349
6	1.769249	-0.000063	-0.814064
6	2.719215	0.000002	-1.563067
6	-0.864492	0.000305	-3.376685
1	3.573250	0.000048	-2.203474
1	-0.931799	0.000565	-4.443310
6	-1.867127	-0.000129	-0.041588
6	-1.919942	0.000081	1.346705
6	-0.725675	0.000108	2.043563
6	0.525037	0.000004	1.386927
1	-2.864769	0.000169	1.882051
1	-0.715430	0.000262	3.127083
7	-3.117527	-0.000337	-0.841755
1	-3.697019	0.828970	-0.666675
1	-2.843839	0.001001	-1.843195
1	-3.695396	-0.831235	-0.668801
8	1.551342	0.000130	2.242737
6	2.941268	0.000164	1.869335
1	3.193983	-0.895388	1.300029
1	3.193865	0.895599	1.299789
1	3.474592	0.000325	2.819224

1-NH_3^+, 4-NO_2 (**R10**)
Total Energy = -644.73902 , Nimag = 0

6	-0.667768	0.000082	-2.438038
6	-0.682690	0.000037	-1.013304
6	0.519165	0.000095	-0.239574
6	1.750782	0.000200	-0.939831
6	2.724569	0.000319	-1.657719
6	-0.759487	0.000020	-3.646532
1	3.616634	0.000416	-2.245212
1	-0.773654	0.000022	-4.715873
6	-1.914290	-0.000104	-0.345239
6	-2.043708	-0.000193	1.034153
6	-0.875047	-0.000144	1.790070
6	0.367921	-0.000012	1.164031
1	-3.013919	-0.000307	1.520810
1	-0.905279	-0.000215	2.872239
7	-3.130767	-0.000166	-1.200707
1	-3.714217	0.830741	-1.045410
1	-2.819245	-0.000122	-2.191571
1	-3.714110	-0.831153	-1.045443
7	1.553415	-0.000005	2.066321
8	1.321763	0.000056	3.271141
8	2.659308	-0.000054	1.546741

1-NH_3^+ Naphthalene (**R11**)
Total Energy = -593.91734 , Nimag = 0

6	-0.824240	0.292492	-0.000076
6	0.593172	0.038368	0.000101
6	1.044097	-1.328034	0.000216
6	0.087934	-2.379735	0.000089
6	-1.255408	-2.120684	-0.000121
6	-1.733584	-0.781449	-0.000172
1	-1.979432	-2.927039	-0.000238
6	1.631316	1.014871	0.000184
6	2.972659	0.704193	0.000412
6	3.383112	-0.641367	0.000539
6	2.428132	-1.631978	0.000432
1	3.717972	1.495722	0.000459
1	4.439727	-0.882686	0.000700
1	2.725159	-2.675997	0.000508
7	1.302334	2.471305	-0.000057
1	1.684032	2.939347	-0.828528
1	0.262061	2.612790	-0.000328
1	1.683681	2.939540	0.828464
1	0.446252	-3.404251	0.000153
6	-1.373652	1.612188	-0.000158
6	-1.868433	2.721188	-0.000366
1	-2.353692	3.673300	-0.000517
6	-3.137447	-0.555248	-0.000408
6	-4.338371	-0.409914	-0.000588
1	-5.397807	-0.279206	-0.000759

9-NH_3^+-cyclodeca-3-ene-1,5-diyne (**R12**)
Total Energy = -442.67480 , Nimag = 0

6	-1.620221	0.138203	0.807537
6	-1.660336	0.126353	2.222673
6	-0.466984	0.098048	2.883539
6	0.740232	0.112144	2.144418
6	1.598943	0.178721	1.287327
6	-1.349599	0.116156	-0.378383
6	-0.757884	0.033911	-1.694864
6	0.734811	-0.372032	-1.692186
6	1.687113	0.729089	-1.144901
6	2.477262	0.332066	0.131499
1	-2.605590	0.151420	2.753284
1	-0.446968	0.091777	3.969670
1	-0.911604	0.942191	-2.290025
1	1.021250	-0.614913	-2.723585
1	0.833486	-1.288428	-1.099532
1	2.411818	0.983269	-1.923503
1	1.125532	1.644111	-0.930669
1	3.042105	-0.592477	-0.047148
1	3.226612	1.106989	0.333447
7	-1.543621	-1.060635	-2.492932
1	-1.452415	-1.963190	-2.013582
1	-2.541941	-0.829497	-2.524536
1	-1.196965	-1.162765	-3.453253

Transition State

TS1, S^2 = 0.000
Total Energy = -230.83752, Nimag = 1

6	0.000000	1.370526	0.001937
6	0.000000	0.701064	-1.221515
6	0.000000	-0.701064	-1.221515
6	0.000000	-1.370526	0.001937
6	0.000000	-0.988995	1.208385
6	0.000000	0.988995	1.208385
1	0.000000	1.210477	-2.178871
1	0.000000	-1.210477	-2.178871
1	0.000000	-1.262274	2.246029

TS2, S^2 = 0.000
Total Energy = -386.90969, Nimag = 1

6	-0.001216	0.705223	2.635807
6	0.001216	-0.705223	2.635807
6	-0.008925	1.360685	1.417435
6	0.008925	-1.360685	1.417435
6	0.000000	0.952098	0.199817
6	0.000000	-0.952098	0.199817
6	0.082168	1.554377	-1.171177
6	-0.082168	-1.554377	-1.171177
6	-0.365263	0.670994	-2.338467
6	0.365263	-0.670994	-2.338467
1	0.002044	1.211430	3.594853
1	-0.002044	-1.211430	3.594853
1	-0.510293	2.475436	-1.154238
1	0.510293	-2.475436	-1.154238
1	1.123244	1.862759	-1.342413
1	-1.123244	-1.862759	-1.342413
1	-0.174830	1.211548	-3.272366
1	0.174830	-1.211548	-3.272366
1	-1.448577	0.501361	-2.286327
1	1.448577	-0.501361	-2.286327

TS3, S^2 = 0.000
Total Energy = -347.59946, Nimag = 1

6	-2.272529	0.705038	0.378030
6	-2.272221	-0.706122	0.378307
6	-1.076370	1.372849	0.149315
6	-1.075849	-1.373390	0.149259
6	0.103691	-0.932615	-0.073361
6	0.103376	0.932607	-0.073375
6	1.531047	-1.230185	-0.387969
6	1.530615	1.230995	-0.387724
6	2.361324	0.000514	0.012390
1	-3.212761	1.207677	0.577074
1	-3.212218	-1.209125	0.577514
1	1.852633	-2.136547	0.134352
1	1.851682	2.137223	0.135161
1	1.634116	-1.423930	-1.465442
1	1.633844	1.425386	-1.465062
1	3.347369	0.000699	-0.460842
1	2.506826	0.000473	1.098017

TS4, S^2 = 0.000
TOTAL ENERGY = -440.2200137,
Nimag = 1

6	-1.044661	1.415669	0.000010
6	-0.066739	0.399000	-0.000039
6	-0.461054	-1.016777	-0.000047
6	-1.844144	-1.210163	-0.000038
6	-2.911312	-0.549291	0.000037
6	-2.312745	1.281590	0.000035
1	-3.985590	-0.547720	0.000018
1	-3.250146	1.812080	0.000023
6	1.308973	0.659023	-0.000026
6	2.294858	-0.310969	0.000019
6	1.893651	-1.652401	0.000042
6	0.545805	-1.995926	-0.000008
1	3.348961	-0.050744	0.000041
1	2.645645	-2.433152	0.000089
1	0.256009	-3.040063	-0.000016
7	1.644057	2.108026	-0.000006
1	2.172415	2.396152	-0.831309
1	0.716812	2.592432	-0.000414
1	2.171699	2.396306	0.831700

TS5, S^2 = 0.000
TOTAL ENERGY = -440.2090312,
Nimag =-1

6	0.522715	2.051225	0.000000
6	0.000000	0.753095	0.000000
6	0.971021	-0.379733	0.000000
6	2.326760	-0.037694	0.000000
6	2.955626	1.059828	0.000000
6	1.708769	2.496171	0.000000
1	3.930059	1.515736	0.000000
1	2.309760	3.388763	0.000000
6	-1.368802	0.443235	0.000000
6	-1.775140	-0.879514	0.000000
6	-0.895226	-1.957945	0.000000
6	0.467925	-1.691341	0.000000
1	-2.084980	1.258559	0.000000
1	-1.248315	-2.985476	0.000000
1	1.171626	-2.514653	0.000000
7	-3.245611	-1.158205	0.000000
1	-3.708581	-0.765527	0.829088
1	-3.708581	-0.765527	-0.829088
1	-3.423598	-2.168402	0.00000

TS6, S^2 = 0.000
Total Energy = -518.85512, Nimag = 1

6	0.394258	0.072865	-1.712576
6	0.395462	0.010232	-0.303204
6	1.670454	-0.033340	0.430990
6	2.798268	-0.006412	-0.392272
6	3.094110	0.045339	-1.611852
6	1.391547	0.100077	-2.505245
1	3.861603	0.071980	-2.362965
1	1.688182	0.143777	-3.539526
6	-0.776655	-0.014040	0.466024
6	-0.790080	-0.075684	1.849455
6	0.433416	-0.116563	2.528143
6	1.637303	-0.095837	1.833411
1	-1.720170	-0.092711	2.408227
1	0.440668	-0.165059	3.611166
1	2.575020	-0.128178	2.375376
7	-2.033067	0.031985	-0.328391
1	-1.666354	0.072199	-1.302151
6	-2.839421	1.281206	-0.090786
1	-3.205844	1.277805	0.935249
1	-2.194286	2.143148	-0.257410
1	-3.677840	1.291630	-0.788171
6	-2.860763	-1.219478	-0.202028
1	-3.227578	-1.301120	0.820621
1	-3.698909	-1.153473	-0.896687
1	-2.230415	-2.074088	-0.445355

TS7, S^2 = 0.000
Total Energy = -518.84491, Nimag = 1

6	0.187101	0.000000	-2.658973
6	0.204285	0.000000	-1.259370
6	1.531970	0.000000	-0.588062
6	2.653393	0.000000	-1.423416
6	2.814535	0.000000	-2.677957
6	1.110075	0.000000	-3.526808
1	3.537980	0.000000	-3.473855
1	1.322743	0.000000	-4.581422
6	-0.939729	0.000000	-0.444179
6	-0.824418	0.000000	0.935407
6	0.410729	0.000000	1.586376
6	1.565815	0.000000	0.817591
1	-1.912001	0.000000	-0.928546
1	0.489672	0.000000	2.668322
1	2.531441	0.000000	1.308452
7	-2.084687	0.000000	1.733601
1	-2.846193	0.000000	1.048519
6	-2.255164	1.252946	2.562146
1	-3.237924	1.229281	3.034586
1	-1.473908	1.277909	3.320121
1	-2.163873	2.114856	1.902248
6	-2.255164	-1.252946	2.562146
1	-1.473908	-1.277909	3.320121
1	-3.237924	-1.229281	3.034586
1	-2.163873	-2.114856	1.902248

TS8, S^2 = 0.000
Total Energy = -479.54089, Nimag = 1

6	0.221913	1.574906	0.000000
6	0.000000	0.171885	0.000000
6	-1.406052	-0.295288	0.000000
6	-2.359172	0.724423	0.000000
6	-2.468792	1.972355	0.000000
6	-0.617793	2.532598	0.000000
1	-3.093457	2.845131	0.000000
1	-0.727706	3.603458	0.000000
6	1.003782	-0.818555	0.000000
6	0.678572	-2.176513	0.000000
6	-0.649360	-2.599566	0.000000
6	-1.680198	-1.668898	0.000000
1	1.472545	-2.918814	0.000000
1	-0.878370	-3.659480	0.000000
1	-2.713115	-1.996023	0.000000
6	2.495714	-0.517680	0.000000
1	2.979296	-0.942178	0.884207
1	2.979296	-0.942178	-0.884207
7	2.851180	0.951198	0.000000
1	2.421963	1.432882	-0.801507
1	2.421963	1.432882	0.801507
1	3.867648	1.087930	0.000000

TS9, S^2 = 0.000
Total Energy = -554.74687, Nimag = 1

6	1.476683	1.793245	-0.000071
6	0.980529	0.470637	0.000073
6	-0.472110	0.227347	-0.000200
6	-1.228703	1.401221	-0.000574
6	-1.099376	2.648776	-0.000746
6	0.820664	2.885014	-0.000375
1	-1.552667	3.621930	-0.000996
1	0.898769	3.958973	-0.000636
6	1.822729	-0.642837	0.000484
6	1.368099	-1.954269	0.000729
6	-0.000254	-2.179268	0.000503
6	-0.923698	-1.117013	0.000024
1	2.055177	-2.795027	0.001060
1	-0.397705	-3.187094	0.000664
7	3.269186	-0.312908	0.000622
1	3.762302	-0.658360	-0.830575
1	3.294828	0.733493	0.000858
1	3.762287	-0.658881	0.831604
8	-2.206527	-1.504702	-0.000166
6	-3.290955	-0.569089	-0.000489
1	-3.273030	0.054985	0.898024
1	-3.272750	0.054656	-0.899224
1	-4.192549	-1.181361	-0.000516

TS10, S^2 = 0.000
Total Energy = -644.70300, Nimag = 1

6	-2.321924	0.967922	-0.000010
6	-1.263022	0.026554	0.000046
6	0.121860	0.465869	0.000027
6	0.306994	1.848280	-0.000148
6	-0.330987	2.924023	-0.000275
6	-2.208622	2.238018	-0.000007
1	-0.336236	3.997982	-0.000414
1	-2.735524	3.177038	0.000013
6	-1.481489	-1.356894	-0.000024
6	-0.479599	-2.314139	-0.000065
6	0.849097	-1.876646	0.000027
6	1.116762	-0.514834	0.000064
1	-0.702482	-3.376272	-0.000098
1	1.675391	-2.576556	0.000046
7	-2.920150	-1.717813	-0.000071
1	-3.201956	-2.248205	0.832240
1	-3.409919	-0.784742	-0.000407
1	-3.201788	-2.248914	-0.831979
7	2.524879	-0.053527	0.000136
8	2.708196	1.163460	0.000004
8	3.394928	-0.912194	0.000287

TS11, , S^2 = 0.000
Total Energy = -593.88339, Nimag = 1

6	-1.181790	0.073434	-2.835924
6	-1.222115	0.044056	-1.438809
6	0.072777	0.016640	-0.819207
6	1.226894	0.021955	-1.662032
6	1.285574	0.048538	-2.936236
6	-0.521966	0.088601	-3.887348
1	1.897809	0.061068	-3.820224
1	-0.372861	0.109593	-4.948222
6	-2.398080	0.039898	-0.642415
6	-2.306633	0.009739	0.724379
6	-1.048568	-0.018174	1.389331
6	0.153063	-0.014725	0.610082
1	-3.364564	0.060868	-1.131440
1	-3.210543	0.006785	1.324816
6	-0.969051	-0.049177	2.805186
6	1.385858	-0.043430	1.325697
6	1.442100	-0.073257	2.699268
6	0.246690	-0.076189	3.449862
1	-1.891147	-0.051383	3.377837
1	0.297411	-0.099787	4.532625
1	2.401045	-0.094595	3.209547
7	2.642807	-0.040658	0.549621
1	3.203820	-0.879527	0.719725
1	2.328976	-0.013677	-0.557933
1	3.221884	0.777810	0.754923

TS12, , S^2 = 0.000
Total Energy = -442.63708, Nimag = 1

6	-2.754241	0.039194	-0.431915
6	-2.756956	-0.002325	0.970659
6	-1.523638	0.118646	-1.087896
6	-1.534870	0.029424	1.614093
6	-0.335169	0.153050	-0.599645
6	-0.292923	0.083514	1.368927
6	1.034622	0.226696	-1.170718
6	1.072666	0.040232	1.961510
6	2.187137	-0.285391	-0.309684
6	2.216424	0.461808	1.030257
1	-3.712139	0.043712	-0.939737
1	-3.707121	-0.025233	1.492310
1	1.069566	0.681199	2.849522
1	1.253451	1.246391	-1.510601
1	1.251526	-0.982367	2.319523
1	3.130627	-0.134556	-0.845975
1	3.165558	0.258078	1.532548
1	2.072305	-1.362876	-0.131230
1	2.181584	1.543049	0.852636
7	0.956191	-0.587807	-2.481579
1	0.098729	-0.292946	-2.970733
1	1.778606	-0.463976	-3.082729
1	0.845665	-1.584910	-2.268003

Didehydroarene Product

P1, S^2 = 0.950
Total Energy = -230.88193, Nimag = 0

6	0.000000	1.341582	0.000003
6	0.000000	0.711159	-1.221038
6	0.000000	-0.711159	-1.221038
6	0.000000	- 1.341582	0.000003
6	0.000000	-0.711197	1.221015
6	0.000000	0.711197	1.221015
1	0.000000	1.248317	-2.165790
1	0.000000	-1.248317	-2.165790
1	0.000000	-1.248110	2.165911
1	0.000000	1.248110	2.165911

P2, S^2 = 0.964
Total Energy = -386.94902, Nimag = 0

6	-1.840582	0.212939	-1.998050
6	-1.822347	0.157867	-0.628575
6	-0.711456	0.045266	0.182140
6	0.555313	-0.022351	-0.482391
6	0.526768	0.033673	-1.860800
6	-0.582696	0.145538	-2.657926
6	-0.813796	-0.033151	1.697469
6	1.854474	-0.121164	0.302058
6	1.649950	-0.560484	1.756800
6	0.517340	0.240490	2.407669
1	-0.533923	0.182667	-3.742350
1	-2.755056	0.304090	-2.576963
1	2.343959	0.862957	0.286990
1	2.536011	-0.803888	-0.216536
1	-1.586652	0.662331	2.041807
1	-1.168712	-1.037398	1.969074
1	2.585520	-0.435273	2.313101
1	1.403310	-1.630207	1.790229
1	0.424467	-0.008773	3.470517
1	0.753267	1.311769	2.353763

P3, S^2 = 0.917
Total Energy = -347.62868, Nimag = 0

6	-1.744038	-0.025149	-1.668742
6	-1.709825	-0.074146	-0.294995
6	-0.568226	-0.017491	0.456865
6	0.680910	0.108499	-0.238045
6	0.643972	0.163360	-1.604572
6	-0.504158	0.099922	-2.358541
6	-0.323923	-0.034010	1.953096
6	1.818943	0.182220	0.760989
1	-0.501771	0.134657	-3.444071
1	-2.665817	-0.083668	-2.240125
1	2.143602	1.225413	0.876911
1	2.695147	-0.390717	0.443313
1	-0.552989	0.953279	2.377223
1	-0.955720	-0.759198	2.474511
6	1.185527	-0.354811	2.066615
1	1.642061	0.070873	2.964364
1	1.320394	-1.440996	2.111854

P4, S^2 = 0.933
Total Energy =-440.24671, Nimag = 0

6	-1.105454	1.344131	-0.000509
6	-0.077357	0.398833	0.000154
6	-0.463046	-1.012673	0.000460
6	-1.838703	-1.251390	0.000491
6	-2.822085	-0.324632	-0.000138
6	-2.428976	1.072308	-0.000371
1	-3.879665	-0.569584	-0.000272
1	-3.202135	1.834429	-0.000344
6	1.307081	0.677210	-0.000313
6	2.285475	-0.285080	-0.000545
6	1.894951	-1.643489	-0.000244
6	0.561193	-1.994458	0.000311
1	3.339618	-0.022456	-0.000913
1	2.659929	-2.411378	-0.000589
1	0.270835	-3.039320	0.000367
7	1.672509	2.124002	0.000546
1	2.228143	2.388833	-0.821665
1	0.796812	2.671899	-0.015183
1	2.200417	2.395000	0.839003

P5 , S^2 = 0.957
TOTAL ENERGY=-440.2427197,
Nimag = 0

6	-2.312138	0.004939	0.000000
6	-0.964809	-0.360188	0.000000
6	0.000000	0.742890	0.000000
6	-0.526057	2.035917	0.000000
6	-1.842141	2.355631	0.000000
6	-2.797190	1.269463	0.000000
1	-2.206574	3.378379	0.000000
1	-3.858111	1.500428	0.000000
6	-0.482799	-1.695881	0.000000
6	0.866535	-1.969082	0.000000
6	1.766342	-0.884013	0.000000
6	1.384047	0.432657	0.000000
1	-1.200538	-2.508523	0.000000
1	1.220885	-2.995689	0.000000
1	2.104158	1.246223	0.000000
7	3.228397	-1.198535	0.000000
1	3.501112	-1.743011	0.828165
1	3.501112	-1.743011	-0.828165
1	3.788427	-0.339045	0.000000

P6, S^2 = 0.933
Total Energy = -518.88235, Nimag = 0

6	0.339295	0.004049	-1.737082
6	0.380006	0.001726	-0.340713
6	1.702795	0.005000	0.286341
6	2.781904	0.010135	-0.599024
6	2.723336	0.012304	-1.949146
6	1.408570	0.009055	-2.563102
1	3.599340	0.016324	-2.590193
1	1.335753	0.010740	-3.646277
6	-0.745245	-0.003540	0.517625
6	-0.642948	-0.005628	1.887572
6	0.640770	-0.002427	2.480024
6	1.779029	0.002733	1.702997
1	-1.523168	-0.009664	2.522698
1	0.721039	-0.004094	3.561147
1	2.759683	0.005154	2.165919
7	-2.071441	-0.006598	-0.161945
1	-1.831835	-0.004687	-1.165065
6	-2.873809	1.243611	0.101806
1	-3.773306	1.217445	-0.514470
1	-3.142218	1.271753	1.156916
1	-2.258694	2.105993	-0.152428
6	-2.866744	-1.261883	0.098787
1	-3.135013	-1.294137	1.153813
1	-3.766403	-1.239245	-0.517391
1	-2.246849	-2.120210	-0.157559

P7, S^2 = 0.956

Total Energy = -518.87819, Nimag = 0

6	-0.422714	0.013825	-2.968310
6	-0.432835	0.008998	-1.572068
6	0.877642	-0.003862	-0.918803
6	1.994828	-0.009997	-1.756515
6	1.970080	-0.005054	-3.110398
6	0.676715	0.007766	-3.758697
1	2.866635	-0.010201	-3.722720
1	0.630835	0.011872	-4.843473
6	-1.598945	0.015511	-0.762831
6	-1.518956	0.010063	0.611408
6	-0.243978	-0.002294	1.218509
6	0.925653	-0.009209	0.498313
1	-2.568249	0.024994	-1.248696
1	-2.427817	0.015246	1.203368
1	1.898168	-0.018790	0.984567
7	-0.144420	-0.008382	2.706856
1	0.858068	-0.017513	2.916422
6	-0.701854	1.246789	3.339107
1	-0.504028	1.215193	4.411204
1	-0.214446	2.106371	2.880661
1	-1.774498	1.283003	3.155841
6	-0.722854	-1.258459	3.330252
1	-0.524368	-1.237879	4.402494
1	-1.795985	-1.275257	3.147001
1	-0.250080	-2.122839	2.865543

P8, S^2 = 0.777

Total Energy = -479.56556, Nimag = 0

6	-2.339110	0.844351	0.000000
6	-1.426420	-0.209639	0.000000
6	0.000000	0.169038	0.000000
6	0.244575	1.549823	0.000000
6	-0.670193	2.543711	0.000000
6	-2.071616	2.165405	0.000000
1	-0.418354	3.599967	0.000000
1	-2.826932	2.944494	0.000000
6	-1.776281	-1.581703	0.000000
6	-0.805823	-2.557640	0.000000
6	0.557671	-2.205004	0.000000
6	0.963726	-0.882700	0.000000
1	-2.828388	-1.843955	0.000000
1	-1.085200	-3.605397	0.000000
1	1.303536	-2.995983	0.000000
6	2.468058	-0.659887	0.000000
1	2.936132	-1.100206	0.884807
1	2.936132	-1.100206	-0.884807
7	2.887118	0.796708	0.000000
1	2.498620	1.290392	-0.813235
1	2.498620	1.290392	0.813235
1	3.908477	0.889014	0.000000

P9, S^2 = 0.931

Total Energy = -554.77320, Nimag = 0

6	-0.860687	-0.000358	-2.064714
6	-0.798327	-0.000249	-0.669105
6	0.539603	0.000179	-0.065384
6	1.592640	0.000473	-0.980486
6	1.512394	0.000419	-2.329544
6	0.187309	-0.000159	-2.915949
1	2.376938	0.000746	-2.985627
1	0.089803	-0.000372	-3.997210
6	-1.913722	-0.000350	0.192763
6	-1.802640	-0.000059	1.565402
6	-0.531351	0.000322	2.145541
6	0.628710	0.000402	1.367664
1	-2.680987	-0.000150	2.204925
1	-0.418516	0.000577	3.222777
7	-3.249343	-0.001023	-0.464683
1	-3.808152	0.827344	-0.227472
1	-3.095884	0.001740	-1.485783
1	-3.805308	-0.832546	-0.231772
8	1.769613	0.000935	2.067221
6	3.067198	-0.000074	1.457294
1	3.217278	-0.898213	0.851647
1	3.218271	0.897310	0.850767
1	3.768309	-0.000039	2.291872

P10, S^2 = 0.909

Total Energy = -644.72693, Nimag = 0

6	-0.038394	-0.000400	-1.911139
6	-0.050967	-0.000120	-0.520332
6	1.259685	0.000368	0.135532
6	2.386429	0.000503	-0.688274
6	2.365565	0.000218	-2.038640
6	1.066830	-0.000259	-2.690400
1	3.257422	0.000331	-2.657912
1	1.033178	-0.000487	-3.775720
6	-1.187806	-0.000249	0.325882
6	-1.111183	0.000061	1.699893
6	0.149302	0.000530	2.333206
6	1.274717	0.000666	1.547003
1	-2.026326	-0.000061	2.278617
1	0.206922	0.000780	3.417437
7	2.628821	0.001150	2.172119
1	3.327512	0.001252	1.409682
1	2.789734	0.832222	2.754010
1	2.790215	-0.829681	2.754229
7	-2.537354	-0.000740	-0.296165
8	-3.497877	-0.000886	0.463735
8	-2.590124	-0.001005	-1.522287

P11, S^2 = 0.860

Total Energy = -593.90729, Nimag = 0

6	-2.937981	-0.003646	-1.824381
6	-2.922522	-0.004402	-0.443513
6	-1.709090	-0.002890	0.282017
6	-0.464751	-0.000493	-0.416646
6	-0.538475	0.000196	-1.830470
6	-1.725282	-0.001311	-2.533652
6	-1.712945	-0.003742	1.715972
6	0.779451	0.001062	0.326409
6	0.721310	0.000108	1.789416
6	-0.558671	-0.002319	2.434755
6	1.944164	0.001687	2.437324
6	3.178425	0.003993	1.886047
6	3.239063	0.004936	0.441716
6	2.057557	0.003438	-0.221389
1	-2.671026	-0.005590	2.225472
1	-3.876461	-0.004835	-2.367018
1	-3.856724	-0.006201	0.109145
1	-1.727454	-0.000697	-3.620197
1	-0.578867	-0.002984	3.518666
1	4.105564	0.005153	2.449957
1	4.212610	0.006764	-0.038144
7	0.730027	0.002681	-2.604974
1	0.820736	-0.827418	-3.199991
1	0.818083	0.833768	-3.199011
1	1.541838	0.003566	-1.905694

P12, S^2 = 0.953

Total Energy = -442.67595, Nimag = 0

6	-2.144179	0.041833	-1.976918
6	-2.152632	0.057056	-0.607527
6	-1.064250	0.089386	0.234781
6	0.208627	0.113406	-0.420771
6	0.219203	0.103665	-1.802014
6	-0.874928	0.067345	-2.622496
6	-1.171998	0.087555	1.749481
6	1.488973	0.186398	0.381616
6	1.337456	-0.216901	1.846189
6	0.126257	0.516989	2.443134
1	-0.816346	0.066384	-3.706206
1	-3.049958	0.019845	-2.575549
1	1.939805	1.182267	0.302103
1	-1.996766	0.740446	2.048766
1	-1.450659	-0.923096	2.076181
1	2.251940	0.019346	2.400851
1	1.174578	-1.301514	1.918489
1	0.065994	0.305998	3.513775
1	0.269244	1.599753	2.343423
7	2.510324	-0.732834	-0.314701
1	3.452167	-0.639955	0.080007
1	2.217590	-1.712743	-0.233517
1	2.534966	-0.507288	-1.318264