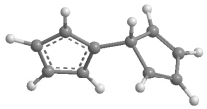
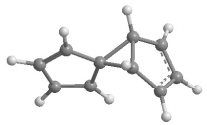
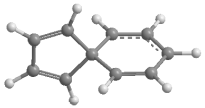
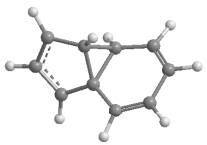
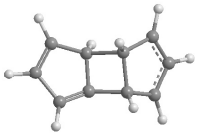
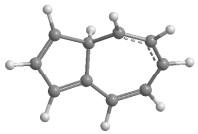
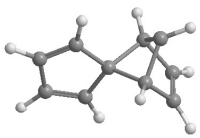
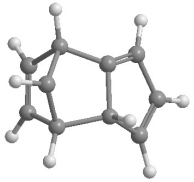
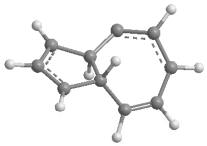
Supporting Information

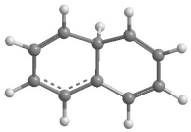
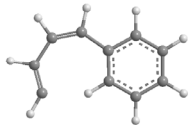
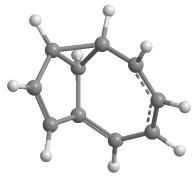
Table S1. B3LYP/6-311G, CCSD(T), MP2, and G3 calculated energies, zero-point energy corrections (ZPE), vibrational frequencies (ν_i), moments of inertia (I_i), rotational constants (B_i), and optimized Cartesian coordinates of all species involved in rearrangements of the 9-H-fulvalenyl radical.**

Species, (point group), electronic state	Energies, a.u. E_{rel}(B3LYP), kcal/mol	i	I_i, a.u.	B_i, GHz	Cartesian coordinates, angstroms				ν_i, cm^{-1}
					Atom	X	Y	Z	
S1, (C_S), $^2A''$  9-H-Fulvalenyl	ZPE = 0.152357 E(B3LYP) = -386.466838532 E(B3LYP+ZPE) = -386.314481 E_{rel}(B3LYP) = 0.0 E(CCSD(T)/6-311G**) = -385.39662483 E(MP2/6-311G**) = -385.25188915 E(MP2/G3large) = -385.47780710 E(G3(MP2,CC) = -385.47018578	A B C	493.5 2067.5 2133.8	3.6573 0.8729 0.8458	C C C C C C C C C C H H H H H H H H	-1.064902 -1.057135 -1.057135 -1.057135 -1.057135 0.097254 0.055137 1.377522 2.276898 1.513075 -1.997563 -1.046464 -1.063060 -1.063060 -1.046464 -0.837765 1.689885 3.356052 1.849758	-0.185648 -1.137352 -2.407149 -2.407149 -1.137352 0.762468 2.159322 2.620917 1.472622 0.348191 0.395507 -0.802071 -3.299079 -3.299079 -0.802071 2.767639 3.657270 1.527094 -0.678433	0.000000 1.179937 0.733585 -0.733585 -1.179937 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 2.207593 1.347250 -1.347250 -2.207593 0.000000 0.000000 0.000000 0.000000	45, 93, 119, 295, 315, 392, 524, 531, 549, 652, 691, 714, 731, 750, 816, 819, 835, 856, 895, 899, 931, 958, 958, 960, 1009, 1017, 1029, 1094, 1111, 1115, 1140, 1214, 1216, 1283, 1304, 1314, 1393, 1414, 1449, 1538, 1564, 1631, 3011, 3188, 3198, 3200, 3213, 3222, 3222, 3227, 3235
S2, (C_S), $^2A''$ 	ZPE = 0.153336 E(B3LYP) = -386.450125145 E(B3LYP+ZPE) = -386.296789 E_{rel}(B3LYP) = 11.1 E(CCSD(T)/6-311G**) = -385.38336604 E(MP2/6-311G**) = -385.22344921 E(MP2/G3large) = -385.44848831 E(G3(MP2,CC) = -385.45506914	A B C	534.3 1665.5 1786.5	3.3779 1.0836 1.0102	C C C C C C C C C C H H H H	1.196059 1.196059 1.196059 1.182921 1.196059 -0.089967 -0.379991 -1.725313 -2.362271 -1.406605 1.698623 1.698623 1.159549 1.128324	-0.020637 -0.020637 -1.439802 -2.235830 -1.439802 0.506087 1.947594 2.112086 0.795447 -0.162345 0.731505 0.731505 -1.786788 -3.317149	0.747788 -0.747788 -1.142948 0.000000 1.142948 0.000000 0.000000 0.000000 0.000000 0.000000 1.341987 -1.341987 -2.166107 0.000000	131, 158, 173, 327, 359, 457, 570, 575, 608, 671, 713, 717, 733, 769, 794, 823, 829, 869, 911, 922, 928, 934, 937, 957, 1007, 1046, 1048, 1082, 1085, 1107, 1113, 1185, 1259, 1284, 1311, 1329, 1337, 1407, 1410, 1470, 1510, 1604, 3175, 3182, 3192, 3194, 3203, 3216, 3218, 3225, 3243

					H	1.159549	-1.786788	2.166107	
					H	0.374791	2.722400	0.000000	
					H	-2.253716	3.056324	0.000000	
					H	-3.431216	0.627373	0.000000	
					H	-1.552593	-1.231355	0.000000	
S3, **(C_{2V}),** **$^2B_1$** 	ZPE = 0.153810 E(B3LYP) = -386.476561725 E(B3LYP+ZPE) = -386.322751 E_{rel}(B3LYP) = -5.2 E(CCSD(T)/6-311G**) = -385.40688393 E(MP2/6-311G**) = -385.25306420 E(MP2/G3large) = -385.47771096 E(G3(MP2,CC) = -385.47772069	A B C	545.6 1723.7 1841.9	3.3076 1.0470 0.9798	C	0.000000	1.256176	0.580661	79, 116, 204, 363, 368, 419, 508, 592, 593, 598, 662, 667, 732, 758, 779, 803, 810, 841, 944, 957, 962, 962, 966, 990, 995, 1054, 1061, 1066, 1130, 1131, 1142, 1200, 1236, 1296, 1322, 1384, 1387, 1442, 1533, 1548, 1591, 1634, 3154, 3156, 3178, 3178, 3185, 3194, 3197, 3221, 3226
					C	0.000000	-1.256176	0.580661	
					C	0.000000	-1.224089	1.943232	
					C	0.000000	0.000000	2.656198	
					C	0.000000	1.224089	1.943232	
					C	0.000000	0.000000	-0.263661	
					C	1.180120	0.000000	-1.236168	
					C	0.734616	0.000000	-2.503595	
					C	-0.734616	0.000000	-2.503595	
					C	-1.180120	0.000000	-1.236168	
					H	0.000000	2.197354	0.042341	
					H	0.000000	-2.197354	0.042341	
					H	0.000000	-2.158167	2.495893	
					H	0.000000	0.000000	3.739082	
					H	0.000000	2.158167	2.495893	
					H	2.205552	0.000000	-0.893823	
					H	1.347508	0.000000	-3.396348	
					H	-1.347508	0.000000	-3.396348	
					H	-2.205552	0.000000	-0.893823	
S4, **(C_1)**  Tricyclyl	ZPE = 0.153889 E(B3LYP) = -386.462862862 E(B3LYP+ZPE) = -386.308974 E_{rel}(B3LYP) = 3.5 E(CCSD(T)/6-311G**) = -385.39472588 E(MP2/6-311G**) = -385.23115003 E(MP2/G3large) = -385.45563738 E(G3(MP2,CC) = -385.46532424	A B C	553.4 1493.8 1790.0	3.2609 1.2082 1.0082	C	-0.853674	1.419653	0.207178	172, 213, 235, 296, 392, 443, 520, 532, 567, 628, 660, 684, 702, 759, 772, 802, 829, 895, 931, 934, 953, 974, 981, 987, 1025, 1047, 1086, 1090, 1092, 1173, 1197, 1205, 1239, 1285, 1340, 1347, 1397, 1424, 1463, 1477, 1561, 1661, 3141, 3152, 3157, 3159, 3170, 3182, 3191, 3207, 3219
					C	-0.131782	-0.971159	-0.531789	
					C	-1.551450	-1.261432	-0.507616	
					C	-2.464955	-0.405756	0.017117	
					C	-2.113524	0.952172	0.359890	
					C	0.278526	0.543546	-0.094012	
					C	0.636256	-0.657256	0.759496	
					C	2.105277	-0.770476	0.674030	
					C	2.599388	0.206480	-0.184489	
					C	1.563538	1.013790	-0.649981	
					H	-0.647497	2.481586	0.291704	
					H	0.466903	-1.422878	-1.315928	
					H	-1.881595	-2.179385	-0.984373	
					H	-3.511634	-0.688803	0.042546	
					H	-2.910039	1.637386	0.628477	
					H	0.102122	-0.856548	1.681303	
					H	2.684111	-1.533838	1.175969	
					H	3.637870	0.307382	-0.473574	
					H	1.654169	1.837721	-1.345058	
S5, **(C_1)**	ZPE = 0.153760 E(B3LYP) = -386.427505520 E(B3LYP+ZPE) = -386.273745 E_{rel}(B3LYP) = 25.6	A B C	489.2 1605.1 1919.4	3.6888 1.1244 0.9403	C	-0.697748	0.960682	0.434351	134, 159, 262, 311, 360, 500, 545, 620, 657, 667, 715, 753, 775, 801, 832, 844, 857, 860, 902, 947, 950, 968, 1005,
					C	-0.591281	-0.583101	0.730989	
					C	-1.907386	-1.142646	0.305971	
					C	-2.636672	-0.157800	-0.357973	

	E(CCSD(T)/6-311G**) = -385.36468136 E(MP2/6-311G**) = -385.19660331 E(MP2/G3large) = -385.41890010 E(G3(MP2,CC) = -385.43321815				C	-1.974108	1.061612	-0.357885	1016, 1022, 1065, 1085, 1104, 1118, 1150, 1169, 1176, 1236, 1251, 1278, 1307, 1310, 1378, 1394, 1459, 1524, 1620, 3043, 3079, 3114, 3178, 3180, 3192, 3202, 3206, 3213
					C	0.644982	0.782480	-0.254559	
					C	1.911313	1.147142	0.053733	
					C	2.756768	-0.045634	-0.027441	
					C	1.992232	-1.150697	-0.221172	
					C	0.580343	-0.714176	-0.405473	
					H	-0.677373	1.644910	1.287754	
					H	-0.219457	-0.857381	1.716631	
					H	-2.198114	-2.178398	0.423065	
					H	-3.599621	-0.326455	-0.825946	
					H	-2.327751	1.974019	-0.819317	
					H	2.231533	2.102121	0.451931	
					H	3.835763	-0.037847	0.073543	
					H	2.360824	-2.153066	-0.398200	
					H	0.123538	-1.115084	-1.312703	
S6, **(C_1)**  9-H-Azulyl	ZPE = 0.154307 E(B3LYP) = -386.492347116 E(B3LYP+ZPE) = -386.338040 E_{rel}(B3LYP) = -14.8 E(CCSD(T)/6-311G**) = -385.41522610 E(MP2/6-311G**) = -385.23506510 E(MP2/G3large) = -385.46055836 E(G3(MP2,CC) = -385.48641236	A B C	646.9 1455.1 2014.5	2.7898 1.2403 0.8959	C	0.643679	1.598462	0.004503	112, 150, 294, 313, 378, 383, 496, 550, 574, 607, 684, 704, 715, 775, 802, 818, 853, 870, 907, 938, 953, 960, 980, 1005, 1033, 1051, 1107, 1130, 1205, 1215, 1235, 1249, 1263, 1337, 1350, 1389, 1421, 1430, 1490, 1542, 1573, 1636, 2932, 3126, 3132, 3145, 3157, 3163, 3189, 3201, 3216
					C	0.460897	-1.552134	-0.238074	
					C	1.785074	-1.300371	-0.331393	
					C	2.484843	-0.107909	0.060886	
					C	1.974775	1.169830	0.186334	
					C	-0.495869	0.792663	0.004447	
					C	-1.799818	1.158571	-0.321965	
					C	-2.678199	0.039248	-0.141228	
					C	-1.975132	-1.035007	0.305076	
					C	-0.524885	-0.659633	0.475969	
					H	0.490105	2.662679	-0.154289	
					H	0.074034	-2.473681	-0.661397	
					H	2.404743	-2.080095	-0.768246	
					H	3.563817	-0.203059	0.141311	
					H	2.706124	1.958211	0.343534	
					H	-2.101346	2.138425	-0.669847	
					H	-3.742223	0.057183	-0.340778	
					H	-2.369059	-2.017202	0.530104	
					H	-0.278389	-0.664775	1.552280	
S7, **(C_S),** **^{2}A'** 	ZPE = 0.153300 E(B3LYP) = -386.357569343 E(B3LYP+ZPE) = -386.204270 E_{rel}(B3LYP) = 69.2 E(CCSD(T)/6-311G**) = -385.32094837 E(MP2/6-311G**) = -385.19127590 E(MP2/G3large) = -385.41253072 E(G3(MP2,CC) = -385.38890320	A B C	563.1 1434.0 1650.6	3.2051 1.2586 1.0934	C	-2.018394	0.110288	0.000000	136, 187, 211, 387, 453, 465, 514, 566, 578, 701, 706, 730, 793, 820, 825, 860, 875, 887, 890, 902, 910, 941, 944, 952, 974, 1000, 1057, 1108, 1117, 1140, 1154, 1173, 1204, 1204, 1221, 1233, 1296, 1324, 1404, 1558, 1593, 1641, 3119, 3130, 3133, 3185, 3198, 3204, 3224, 3230, 3233
					C	-0.967620	-0.340346	1.026591	
					C	-0.967620	-1.837268	0.670886	
					C	-0.967620	-1.837268	-0.670886	
					C	-0.967620	-0.340346	-1.026591	
					C	0.115442	0.219527	0.000000	
					C	1.527815	-0.296574	0.000000	
					C	2.377940	0.745936	0.000000	
					C	1.609146	2.001011	0.000000	
					C	0.295187	1.712584	0.000000	
					H	-3.074732	-0.158338	0.000000	
					H	-0.961691	-0.040315	2.073016	
					H	-0.994531	-2.668128	1.363902	

					H	-0.994531	-2.668128	-1.363902	
					H	-0.961691	-0.040315	-2.073016	
					H	1.787304	-1.345676	0.000000	
					H	3.460578	0.689066	0.000000	
					H	2.047583	2.992375	0.000000	
					H	-0.528222	2.414192	0.000000	
S8, **(C_1)** 	ZPE = 0.154613 E(B3LYP) = -386.404849748 E(B3LYP+ZPE) = -386.250237 E_{rel}(B3LYP) = 40.3 E(CCSD(T)/6-311G**) = -385.35198023 E(MP2/6-311G**) = -385.22164610 E(MP2/G3large) = -385.41183457 E(G3(MP2,CC) = -385.38755570	A B C	640.4 1251.3 1407.0	2.8182 1.4423 1.2827	C C C C C C C C C C H H H H H H H H H	1.094612 1.737948 0.990728 1.305497 1.385345 -0.380574 -1.540138 -2.415711 -1.774514 -0.466939 1.415424 2.800724 1.240814 1.393122 1.522018 -1.764558 -3.428434 -2.207590 -0.589054	1.066167 -0.205094 -1.190745 -0.524642 0.797020 0.704171 1.225001 0.113004 -1.070165 -0.804341 2.030534 -0.282267 -2.246500 -1.046239 1.574637 2.270325 0.237927 -2.050545 -1.150123	-0.486175 -1.024814 -0.128320 1.220141 1.017183 -0.555355 -0.102588 0.291097 0.146122 -0.549753 -0.873498 -1.231504 -0.215271 2.164395 1.758559 0.069135 0.656741 0.295992 -1.589774	157, 210, 371, 379, 441, 480, 560, 613, 646, 704, 725, 760, 789, 825, 836, 848, 860, 888, 900, 940, 945, 951, 961, 971, 1007, 1072, 1086, 1097, 1131, 1155, 1176, 1203, 1233, 1250, 1254, 1287, 1313, 1317, 1376, 1544, 1609, 1643, 2971, 3117, 3126, 3168, 3176, 3185, 3194, 3208, 3211
S9, **(C_1)** 	ZPE = 0.151013 E(B3LYP) = -386.364666450 E(B3LYP+ZPE) = -386.213654 E_{rel}(B3LYP) = 63.3 E(CCSD(T)/6-311G**) = -385.29316858 E(MP2/6-311G**) = -385.11143913 E(MP2/G3large) = -385.33249468 E(G3(MP2,CC) = -385.36321113	A B C	642.5 1456.1 1959.9	2.8091 1.2395 0.9208	C C C C C C C C C C H H H H H H H H H	0.444313 0.440713 1.893236 2.672864 1.901241 -0.626116 -1.822869 -2.437645 -1.869625 -0.560633 0.221129 0.103670 2.266066 3.755379 2.250695 -2.466612 -3.524824 -2.567263 -0.251119	-0.711127 0.673815 1.057239 -0.040328 -1.115895 -1.644912 -1.262118 -0.043012 1.181828 1.561106 -0.508612 0.400462 2.011705 -0.058115 -2.086700 -2.024695 -0.083655 1.890090 2.519941	-0.403961 0.380348 0.415472 0.068575 -0.342026 -0.086983 0.481178 0.117064 -0.339966 -0.237093 -1.479333 1.397102 0.763656 0.113559 -0.661558 0.915289 0.055121 -0.777278 -0.642204	97, 157, 213, 327, 361, 388, 440, 488, 536, 574, 641, 661, 666, 690, 754, 815, 837, 894, 906, 937, 949, 972, 992, 1027, 1048, 1079, 1094, 1108, 1151, 1167, 1207, 1223, 1247, 1281, 1320, 1348, 1392, 1417, 1443, 1459, 1521, 1594, 2819, 2905, 3103, 3117, 3145, 3165, 3183, 3203, 3229
S10, **(C_S),**	ZPE = 0.154450 E(B3LYP) = -386.503165039 E(B3LYP+ZPE) = -386.348715 E_{rel}(B3LYP) = -21.5	A B C	618.9 1475.6 2048.1	2.9162 1.2231 0.8812	C C C	0.230153 -0.545895 -0.246721	1.408675 -0.638764 -1.389141	1.237401 0.000000 1.271999	116, 153, 327, 351, 442, 469, 470, 515, 566, 609, 666, 680, 708, 771, 781, 794, 870, 919,

^{2}A'  9-H-Naphthyl	**E(CCSD(T)/6-311G**) = -385.42544552** **E(MP2/6-311G**) = -385.24340824** **E(MP2/G3large) = -385.46937418** **E(G3(MP2,CC) = -385.49696146**				**C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.065775** **0.230153** **-0.000244** **-0.246721** **0.065775** **0.230153** **0.230153** **0.480717** **-1.660213** **-0.356903** **0.225693** **0.442861** **-0.356903** **0.225693** **0.442861** **0.480717**	**-0.730488** **0.697347** **0.779715** **-1.389141** **-0.730488** **0.697347** **1.408675** **2.465482** **-0.512137** **-2.468587** **-1.281844** **1.199813** **-2.468587** **-1.281844** **1.199813** **2.465482**	**2.409080** **2.419457** **0.000000** **-1.271999** **-2.409080** **-2.419457** **-1.237401** **1.243047** **0.000000** **1.259927** **3.329773** **3.355667** **-1.259927** **-3.329773** **-3.355667** **-1.243047**	**928, 954, 972, 975, 997, 999, 1070, 1074, 1109, 1159, 1174, 1182, 1205, 1259, 1262, 1334, 1341, 1401, 1417, 1469, 1507, 1515, 1632, 1633, 2695, 3148, 3151, 3153, 3156, 3171, 3173, 3187, 3188**
S11, (C_S), ^{2}A'  *cis*-4-phenylbutadienyl	**ZPE = 0.152318** **E(B3LYP) = -386.453966352** **E(B3LYP+ZPE) = -386.301648** **E_{rel}(B3LYP) = 8.1** **E(CCSD(T)/6-311G**) = -385.37025467** **E(MP2/6-311G**) = -385.17357247** **E(MP2/G3large) = -385.40138111** **E(G3(MP2,CC) = -385.44574531**	**A** **B** **C**	**588.4** **2054.2** **2642.6**	**3.0672** **0.8786** **0.6829**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**-0.783955** **-0.677511** **-2.066999** **-2.821485** **-2.170859** **0.000000** **1.451833** **2.507171** **2.639531** **1.744495** **-0.285749** **-0.106402** **-2.563588** **-3.904675** **-2.745909** **1.739747** **3.473582** **3.685908** **1.773767**	**1.788495** **-0.615576** **-0.669523** **0.501863** **1.735382** **0.616120** **0.786065** **-0.062510** **-1.517712** **-2.486365** **2.752627** **-1.539059** **-1.633651** **0.454794** **2.654652** **1.835106** **0.433546** **-1.849328** **-3.566122**	**0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000**	**12, 84, 148, 191, 239, 394, 402, 419, 516, 527, 636, 637, 702, 725, 738, 777, 804, 847, 869, 903, 930, 975, 981, 998, 1005, 1016, 1052, 1110, 1183, 1206, 1213, 1295, 1301, 1355, 1372, 1463, 1486, 1525, 1603, 1621, 1645, 1668, 3002, 3092, 3121, 3150, 3157, 3165, 3176, 3188, 3234**
S12, (C_1) 	**ZPE = 0.154614** **E(B3LYP) = -386.439899850** **E(B3LYP+ZPE) = -386.285286** **E_{rel}(B3LYP) = 18.3** **E(CCSD(T)/6-311G**) = -385.37296071** **E(MP2/6-311G**) = -385.22959153** **E(MP2/G3large) = -385.45376672** **E(G3(MP2,CC) = -385.44252190**	**A** **B** **C**	**758.2** **1151.5** **1483.9**	**2.3802** **1.5673** **1.2162**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H**	**-1.328550** **0.492816** **-0.637962** **-1.786535** **-2.174717** **0.114608** **0.916629** **1.943674** **1.832533** **0.717210** **-1.715677** **0.717221**	**-1.355866** **1.359402** **1.582819** **0.877206** **-0.394340** **-1.099806** **-1.370024** **-0.448830** **0.530772** **0.039570** **-2.309252** **2.240240**	**0.460645** **0.453889** **-0.470693** **-0.573390** **0.042232** **0.379825** **-0.743219** **-0.842430** **0.249470** **1.141347** **0.812044** **1.053339**	**133, 202, 304. 332, 394, 436, 533, 571, 618, 677, 709, 730, 755, 780, 797, 814, 840, 874, 881, 915, 949, 979, 988, 999, 1023, 1029, 1074, 1090, 1166, 1185, 1217, 1247, 1268, 1295, 1332, 1388, 1395, 1427, 1449, 1462, 1609, 1662, 3098, 3116, 3124, 3137, 3138, 3150, 3178, 3188, 3211**

					H	-0.583416	2.505788	-1.044224	
					H	-2.551106	1.307490	-1.216454	
					H	-3.243075	-0.592840	0.076475	
					H	0.669880	-2.108099	-1.496663	
					H	2.675307	-0.396888	-1.637653	
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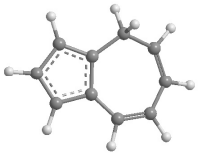
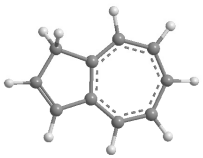
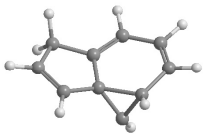
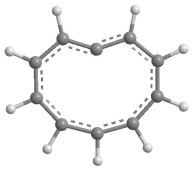
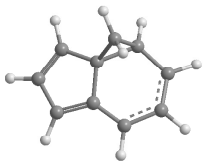
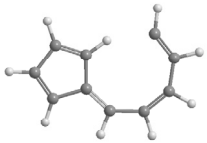
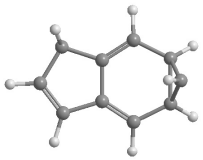
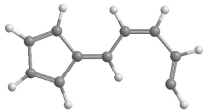
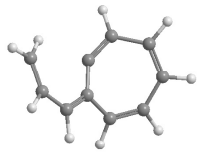
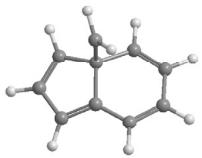
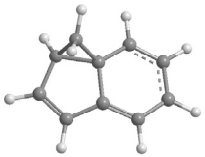
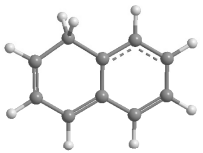
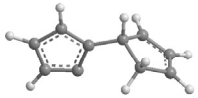
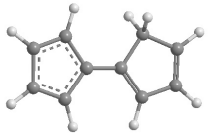
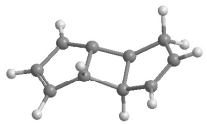
					H	0.784056	-0.001571	2.223654	
S13, (C_1)  4-H-Azulyl	ZPE = 0.154411 E(B3LYP) = -386.493498031 E(B3LYP+ZPE) = -386.339087 E_{rel}(B3LYP) = -15.4 E(CCSD(T)/6-311G**) = -385.41399768 E(MP2/6-311G**) = -385.24014135 E(MP2/G3large) = -385.46743492 E(G3(MP2,CC) = -385.48688025	A B C	668.1 1470.0 2108.3	2.7011 1.2277 0.8560	C	-0.464136	1.630514	0.126494	59, 152, 240, 334, 352, 382, 485, 501, 552, 641, 665, 675, 717, 746, 805, 819, 834, 889, 899, 906, 942, 966, 987, 999, 1013, 1067, 1115, 1213, 1219, 1223, 1272, 1289, 1339, 1377, 1399, 1407, 1448, 1452, 1490, 1539, 1605, 1629, 2912, 3030, 3126, 3136, 3147, 3162, 3194, 3206, 3224
					C	-0.636162	-1.632170	0.250847	
					C	-2.004645	-1.149171	-0.124108	
					C	-2.490879	0.116062	-0.182361	
					C	-1.822302	1.366296	0.006076	
					C	0.600115	0.730484	0.089009	
					C	1.983936	1.118207	-0.000284	
					C	2.733396	-0.019223	-0.133190	
					C	1.840727	-1.174353	-0.099688	
					C	0.556696	-0.744440	0.038897	
					H	-0.190340	2.680124	0.200685	
					H	-0.691386	-1.900277	1.322382	
					H	-2.724457	-1.946792	-0.289966	
					H	-3.553483	0.203505	-0.393834	
					H	-2.472932	2.235746	0.007040	
					H	2.337098	2.139512	-0.013916	
					H	3.807091	-0.070312	-0.255363	
					H	2.162093	-2.206546	-0.154236	
					H	-0.454162	-2.588194	-0.252948	
S14, (C_S), ^{2}A"  1-H-Azulyl	ZPE = 0.153455 E(B3LYP) = -386.504877242 E(B3LYP+ZPE) = -386.351422 E_{rel}(B3LYP) = 23.2 E(CCSD(T)/6-311G**) = -385.42409797 E(MP2/6-311G**) = -385.25420588 E(MP2/G3large) = -385.48254399 E(G3(MP2,CC) = -385.49898107	A B C	645.2 1503.7 2137.8	2.7973 1.2002 0.8442	C	-0.408293	-1.667149	0.000000	115, 167, 234, 331, 363, 404, 426, 493, 561, 570, 634, 665, 675, 741, 758, 802, 859, 891, 923, 929, 948, 950, 978, 981, 995, 1049, 1081, 1129, 1153, 1204, 1243, 1262, 1293, 1347, 1383, 1433, 1449, 1468, 1512, 1557, 1607, 1654, 2999, 3016, 3125, 3130, 3142, 3156, 3169, 3184, 3217
					C	1.360201	0.969061	0.000000	
					C	2.326709	-0.108259	0.000000	
					C	2.114788	-1.449430	0.000000	
					C	0.864239	-2.175241	0.000000	
					C	-0.833755	-0.315148	0.000000	
					C	-2.208791	0.113649	0.000000	
					C	-2.306613	1.466066	0.000000	
					C	-0.929055	2.074785	0.000000	
					C	0.000000	0.867666	0.000000	
					H	-1.212649	-2.400265	0.000000	
					H	1.779146	1.971587	0.000000	
					H	3.364826	0.212214	0.000000	
					H	3.003904	-2.073808	0.000000	
					H	0.954568	-3.256473	0.000000	
					H	-3.045376	-0.575190	0.000000	
					H	-3.221195	2.042307	0.000000	
					H	-0.749907	2.711812	0.876468	
					H	-0.749907	2.711812	-0.876468	
S15, (C_1)	ZPE = 0.152779 E(B3LYP) = -386.419524674 E(B3LYP+ZPE) = -386.266746	A B	682.5 1283.0	2.6442 1.4066	C	-0.603444	-1.435408	1.039023	127, 172, 239, 281, 345, 417, 437, 491, 541, 620, 638, 681,
					C	-0.715726	1.587810	0.186978	

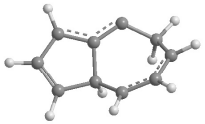
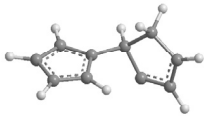
	E_{rel}(B3LYP) = 30.2 E(CCSD(T)/6-311G**) = -385.35273670 E(MP2/6-311G**) = -385.19326247 E(MP2/G3large) = -385.41829249 E(G3(MP2,CC) = -385.42498772	C	1755.8	1.0278	C C C C C C C C H H H H H H H H	-2.020405 -2.214606 -1.191687 0.286817 1.618319 2.480139 1.838985 0.379092 -1.012503 -0.605683 -2.833452 -3.140423 -1.181239 1.839744 3.527181 2.275161 1.986323	1.053381 -0.242322 -1.269197 -0.676205 -1.146957 -0.127249 1.177562 0.796150 -1.189042 2.667696 1.759933 -0.540800 -2.125475 -2.184050 -0.204128 1.526805 1.983678	-0.142511 -0.492872 -0.288475 0.170817 -0.307084 -0.348503 0.078339 0.227763 2.011096 0.216994 -0.272698 -0.974500 -0.961049 -0.524059 -0.613696 1.025328 -0.648268	702, 751, 774, 811, 837, 867, 934, 948, 957, 965, 974, 977, 1008, 1040, 1089, 1113, 1137, 1160, 1194, 1207, 1260, 1288, 1342, 1368, 1389, 1436, 1463, 1581, 1647, 1679, 2989, 3041, 3097, 3146, 3155, 3173, 3179, 3186, 3210
S16, (C_{2V}), $^2A_1$ 	ZPE = 0.153879 E(B3LYP) = -386.404147906 E(B3LYP+ZPE) = -386.250269 E_{rel}(B3LYP) = 40.3 E(CCSD(T)/6-311G**) = -385.30995610 E(MP2/6-311G**) = -385.09774421 E(MP2/G3large) = -385.32341009 E(G3(MP2,CC) = -385.38174298	A B C	962.3 1443.0 2405.3	1.8755 1.2507 0.7503	C C C C C C C C C C H H H H H H H H	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	1.295514 0.000000 1.369497 2.317780 2.352076 0.000000 -1.295514 -2.352076 -2.317780 -1.369497 1.529080 0.000000 1.930140 3.322673 3.349528 -1.529080 -3.349528 -3.322673 -1.930140	-1.748795 1.954013 1.589155 0.550505 -0.844125 -1.353258 -1.748795 -0.844125 0.550505 1.589155 -2.818155 3.042365 2.522239 0.966405 -1.274385 -2.818155 -1.274385 0.966405 2.522239	45, 73, 210, 237, 253, 274, 411, 431, 550, 570, 647, 656, 663, 689, 707, 824, 841, 852, 882, 895, 917, 959, 986, 991, 1006, 1026, 1137, 1142, 1241, 1258, 1288, 1349, 1433, 1458, 1511, 1542, 1553, 1574, 1596, 1601, 1616, 1723, 3037, 3042, 3071, 3093, 3113, 3127, 3134, 3155, 3156
S17, (C_1) 	ZPE = 0.154436 E(B3LYP) = -386.479830655 E(B3LYP+ZPE) = -386.325395 E_{rel}(B3LYP) = -6.8 E(CCSD(T)/6-311G**) = -385.40837434 E(MP2/6-311G**) = -385.24668073 E(MP2/G3large) = -385.47114052 E(G3(MP2,CC) = -385.47839813	A B C	692.0 1234.9 1725.9	2.6079 1.4614 1.0457	C C C C C C C C C C H	-0.802867 -0.469944 -1.013856 -2.133660 -2.040421 0.371493 1.706606 2.501542 1.717054 0.342564 -0.759627	1.610855 -1.491718 -1.239473 -0.289884 1.012307 0.864564 1.264532 0.123928 -0.997581 -0.612916 2.681784	0.254608 0.989597 -0.390053 -0.521600 -0.117735 0.210802 0.063103 -0.273782 -0.327927 0.050759 0.420935	172, 212, 253, 344, 403, 499, 510, 537, 567, 637, 686, 709, 713, 782, 801, 829, 839, 845, 871, 925, 941, 958, 968, 1020, 1026, 1054, 1064, 1094, 1109, 1182, 1212, 1232, 1255, 1331, 1353, 1376, 1399, 1427, 1461, 1478, 1516, 1594, 3124, 3142, 3155, 3168, 3179, 3193, 3207, 3217, 3220

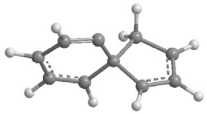
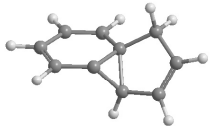
4,9-Cyclopropylyl					H	-0.052190	-2.469956	1.193411	
					H	-0.980888	-2.072121	-1.085057	
					H	-3.063296	-0.667098	-0.933960	
					H	-2.921043	1.643682	-0.172961	
					H	2.064122	2.284407	0.114997	
					H	3.565751	0.153363	-0.468606	
					H	2.043319	-2.010853	-0.518372	
					H	-0.967212	-1.010890	1.822987	
S18, (C_S), $^2A'$ 	**ZPE = 0.150443** **E(B3LYP) = -386.397249566** **E(B3LYP+ZPE) = -386.246807** **E_{rel}(B3LYP) = 42.5** **E(CCSD(T)/6-311G**) = -385.32170723** **E(MP2/6-311G**) = -385.13383421** **E(MP2/G3large) = -385.36050869** **E(G3(MP2,CC) = -385.39793871**	**A** **B** **C**	**672.3** **1934.9** **2271.5**	**2.6845** **0.9327** **0.7945**	C	0.320758	1.413474	-0.199199	**69, 75, 88, 156, 200, 266, 326, 419, 494, 556, 611, 640, 703, 719, 746, 786, 794, 819, 866, 879, 902, 914, 927, 940, 943, 995, 1000, 1057, 1105, 1110, 1179, 1285, 1298, 1312, 1358, 1405, 1444, 1522, 1607, 1609, 1665, 1677, 3063, 3102, 3112, 3143, 3199, 3209, 3227, 3242, 3275**
					C	1.564181	-1.644646	-0.941120	
					C	2.527781	-1.007651	-0.309608	
					C	2.535104	0.291701	0.385675	
					C	1.643182	1.303836	0.403432	
					C	-0.749822	0.603899	-0.028263	
					C	-0.886759	-0.562430	0.853536	
					C	-2.148705	-1.034272	0.720609	
					C	-2.879122	-0.200038	-0.249393	
					C	-2.056350	0.779852	-0.685651	
					H	0.167112	2.309010	-0.801764	
					H	0.511800	-1.575141	-1.159281	
					H	3.506768	-1.493184	-0.304095	
					H	3.473788	0.490154	0.896803	
					H	1.989635	2.225859	0.869368	
					H	-0.109244	-0.940198	1.499535	
					H	-2.574613	-1.878385	1.246696	
					H	-3.907338	-0.358299	-0.545313	
					H	-2.279399	1.557843	-1.402053	
S19, (C_1) 	**ZPE = 0.153312** **E(B3LYP) = -386.427344606** **E(B3LYP+ZPE) = -386.274033** **E_{rel}(B3LYP) = 25.4** **E(CCSD(T)/6-311G**) = -385.35918011** **E(MP2/6-311G**) = -385.22678766** **E(MP2/G3large) = -385.45085673** **E(G3(MP2,CC) = -385.42993717**	**A** **B** **C**	**574.7** **1492.4** **1926.4**	**3.1401** **1.2093** **0.9368**	C	-0.676420	1.468945	-0.230376	**145, 166, 247, 334, 383, 418, 457, 513, 546, 585, 688, 699, 727, 765, 768, 824, 832, 860, 910, 939, 957, 965, 974, 1000, 1030, 1056, 1069, 1117, 1158, 1165, 1192, 1221, 1264, 1310, 1339, 1363, 1380, 1397, 1462, 1622, 1631, 1699, 3007, 3027, 3097, 3104, 3150, 3159, 3183, 3184, 3207**
					C	-0.625433	-1.452156	-0.250927	
					C	-1.957604	-0.821229	-0.257090	
					C	-2.403103	-0.028643	0.889858	
					C	-1.985961	0.801020	-0.243195	
					C	0.454577	0.753620	-0.023696	
					C	1.846189	1.199531	0.043608	
					C	2.680335	0.149106	0.097013	
					C	1.929024	-1.162805	0.061697	
					C	0.479423	-0.716517	-0.028761	
					H	-0.634994	2.534624	-0.432419	
					H	-0.562330	-2.516962	-0.456038	
					H	-2.723665	-1.283146	-0.876885	
					H	-2.007759	-0.031865	1.898032	
					H	-2.768522	1.249346	-0.852244	
					H	2.142973	2.241202	0.048151	
					H	3.759919	0.206497	0.155985	
					H	2.120755	-1.763400	0.960075	
					H	2.227456	-1.781530	-0.793444	
S20,	**ZPE = 0.150349**	**A**	**444.6**	**4.0589**	C	0.000000	0.370171	0.000000	**20, 84, 102, 154, 194, 273,**

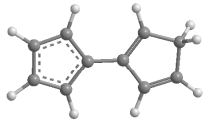
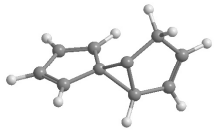
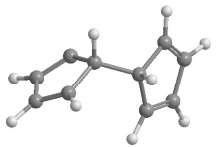
(C_S), $^2A'$ 	**E(B3LYP) = -386.410140725** **E(B3LYP+ZPE) = -386.259792** **E_{rel}(B3LYP) = 34.3** **E(CCSD(T)/6-311G**) = -385.32946349** **E(MP2/6-311G**) = -385.14100815** **E(MP2/G3large) = -385.36745302** **E(G3(MP2,CC) = -385.40555937**	**B** **C**	**2823.5** **3268.1**	**0.6392** **0.5522**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.383996** **-0.928640** **-1.745849** **-1.352812** **0.377742** **1.766751** **1.751692** **0.353218** **-0.465796** **0.784832** **1.093454** **-1.509386** **-2.815157** **-2.138742** **2.630729** **2.612725** **0.045055** **-1.545325**	**3.487201** **3.358493** **2.146525** **0.848156** **-0.937707** **-1.409404** **-2.763271** **-3.219484** **-2.140617** **1.122776** **4.301004** **4.288994** **2.333135** **0.099673** **-0.760050** **-3.417868** **-4.256598** **-2.151437**	**0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000**	**360, 428, 434, 558, 633, 636, 638, 714, 769, 770, 783, 814, 864, 871, 916, 921, 932, 948, 975, 1005, 1006, 1096, 1105, 1139, 1188, 1280, 1284, 1309, 1352, 1394, 1459, 1516, 1590, 1603, 1638, 1667, 3013, 3129, 3152, 3172, 3198, 3207, 3225, 3234, 3243**
S21, (C_1) 	**ZPE = 0.151497** **E(B3LYP) = -386.427142326** **E(B3LYP+ZPE) = -386.275646** **E_{rel}(B3LYP) = 24.4** **E(CCSD(T)/6-311G**) = -385.34233847** **E(MP2/6-311G**) = -385.14529318** **E(MP2/G3large) = -385.37192420** **E(G3(MP2,CC) = -385.41747249**	**A** **B** **C**	**652.5** **1898.0** **2405.2**	**2.7659** **0.9508** **0.7503**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.740356** **0.930523** **2.092525** **2.550175** **2.008735** **-0.394076** **-1.632813** **-2.852763** **-3.117562** **-0.079506** **0.536592** **0.915027** **2.675784** **3.486846** **2.725144** **-1.683085** **-3.654226** **-2.393076** **-4.082580**	**-1.484988** **1.614544** **1.270747** **-0.001442** **-1.212016** **-0.567668** **-1.045247** **-0.314232** **0.974243** **0.756048** **-2.460534** **2.580426** **2.081866** **-0.126625** **-2.024249** **-2.111678** **-0.894518** **1.606958** **1.408416**	**-0.442782** **-0.416255** **0.381032** **0.530254** **-0.045483** **-0.239688** **0.167729** **0.371760** **0.066090** **-0.538986** **-0.879142** **-0.916953** **0.810387** **1.066126** **-0.143544** **0.369212** **0.824055** **-0.432170** **0.300008**	**69, 97, 144, 216, 278, 308, 356, 404, 417, 534, 583, 590, 628, 708, 762, 791, 808, 843, 856, 904, 908, 938, 980, 998, 1007, 1013, 1039, 1109, 1173, 1232, 1248, 1289, 1315, 1341, 1414, 1446, 1457, 1462, 1561, 1619, 1636, 1705, 3117, 3122, 3125, 3133, 3137, 3143, 3152, 3159, 3227**
S22, (C_1) 	**ZPE = 0.151791** **E(B3LYP) = -386.439566735** **E(B3LYP+ZPE) = -386.287776** **E_{rel}(B3LYP) = 16.8** **E(CCSD(T)/6-311G**) = -385.37278512** **E(MP2/6-311G**) = -385.18499448** **E(MP2/G3large) = -385.40891772** **E(G3(MP2,CC) = -385.44491736**	**A** **B** **C**	**724.2** **1259.8** **1640.3**	**2.4920** **1.4326** **1.1003**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C**	**-1.062546** **0.170771** **-0.887533** **-2.067019** **-2.169464** **0.228358** **1.460606** **2.388565** **1.744580** **0.324298**	**1.484046** **-1.333881** **-1.221794** **-0.558094** **0.781028** **0.872760** **1.404923** **0.337279** **-0.847916** **-0.639478**	**0.318400** **1.400040** **-0.640414** **-0.591290** **-0.043434** **0.175145** **-0.036215** **-0.394074** **-0.414158** **0.053499**	**145, 162, 192, 261, 285, 383, 417, 519, 537, 554, 575, 586, 664, 699, 722, 747, 806, 819, 862, 876, 945, 951, 957, 974, 979, 1007, 1030, 1079, 1151, 1166, 1173, 1213, 1245, 1318, 1380, 1385, 1433, 1437, 1508, 1550, 1613, 1652, 3136, 3156, 3162, 3177, 3186, 3188, 3199,**

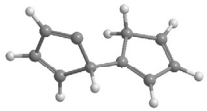
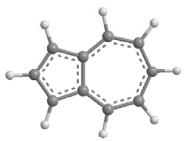
9-Methylyl					H	-1.138654	2.523218	0.621348	3216, 3253
					H	0.501980	-2.360062	1.499406	
					H	-0.818905	-2.227869	-1.038996	
					H	-2.964944	-1.028127	-0.977892	
					H	-3.148670	1.243547	0.010865	
					H	1.716015	2.456021	0.011850	
					H	3.439456	0.488758	-0.605894	
					H	2.179334	-1.821902	-0.594872	
					H	-0.549315	-0.946830	2.109188	
S23, (C_1)  1,9-Cyclopropylyl	ZPE = 0.154489 E(B3LYP) = -386.481155128 E(B3LYP+ZPE) = -386.326666 E_{rel}(B3LYP) = -7.6 E(CCSD(T)/6-311G**) = -385.40992790 E(MP2/6-311G**) = -385.24570223 E(MP2/G3large) = -385.47065527 E(G3(MP2,CC) = -385.48039194	A B C	664.1 1284.3 1761.8	2.7174 1.4052 1.0244	C	-1.238477	1.425382	0.243509	148, 204, 339, 359, 416, 435, 519, 541, 579, 657, 689, 708, 737, 755, 789, 809, 838, 862, 914, 931, 936, 955, 965, 1002, 1026, 1035, 1062, 1097, 1117, 1162, 1199, 1217, 1265, 1312, 1335, 1376, 1408, 1441, 1467, 1528, 1542, 1595, 3113, 3147, 3154, 3158, 3173, 3188, 3188, 3208, 3210
					C	1.243966	-1.249343	0.969215	
					C	-0.991728	-1.361736	-0.341759	
					C	-2.216776	-0.766300	-0.268135	
					C	-2.360034	0.610857	0.077652	
					C	0.032721	0.879505	0.134575	
					C	1.308528	1.505327	-0.079880	
					C	2.236859	0.580623	-0.445306	
					C	1.671475	-0.798271	-0.401501	
					C	0.201927	-0.592519	0.012445	
					H	-1.360648	2.494728	0.385615	
					H	1.101020	-2.311026	1.135760	
					H	-0.893835	-2.412829	-0.592279	
					H	-3.107879	-1.345419	-0.485541	
					H	-3.352995	1.039694	0.142754	
					H	1.486449	2.569665	0.009537	
					H	3.268667	0.786543	-0.699583	
					H	1.960858	-1.547384	-1.130859	
					H	1.567595	-0.675128	1.829703	
S24, (C_S), ^{2}A"  1-H-Naphthyl	ZPE = 0.155639 E(B3LYP) = -386.543591946 E(B3LYP+ZPE) = -386.387953 E_{rel}(B3LYP) = -46.1 E(CCSD(T)/6-311G**) = -385.46216244 E(MP2/6-311G**) = -385.28721642 E(MP2/G3large) = -385.51529491 E(G3(MP2,CC) = -385.53460193	A B C	599.0 1513.9 2102.1	3.0127 1.1921 0.8586	C	-1.367679	-1.324149	0.000000	83, 171, 250, 358, 429, 471, 485, 506, 541, 613, 661, 714, 748, 752, 792, 795, 871, 921, 932, 954, 959, 967, 985, 1057, 1092, 1139, 1175, 1179, 1201, 1202, 1234, 1277, 1309, 1356, 1393, 1439, 1445, 1473, 1516, 1559, 1599, 1630, 2955, 2956, 3149, 3152, 3158, 3171, 3172, 3183, 3187
					C	1.351720	1.378016	0.000000	
					C	-1.170946	1.446288	0.000000	
					C	-2.424848	0.839190	0.000000	
					C	-2.519274	-0.555296	0.000000	
					C	-0.089006	-0.725145	0.000000	
					C	1.106951	-1.516899	0.000000	
					C	2.374959	-0.912706	0.000000	
					C	2.525747	0.447863	0.000000	
					C	0.000000	0.691391	0.000000	
					H	-1.436181	-2.407220	0.000000	
					H	1.417358	2.052895	0.868000	
					H	-1.101649	2.530268	0.000000	
					H	-3.322196	1.447390	0.000000	
					H	-3.491931	-1.034560	0.000000	
					H	1.017884	-2.597076	0.000000	
					H	3.257165	-1.545053	0.000000	
					H	3.516447	0.889134	0.000000	
					H	1.417358	2.052895	-0.868000	

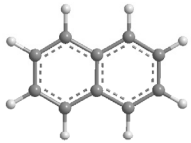
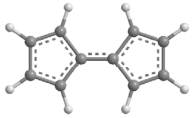
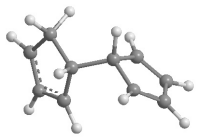
S25, (C_1) 	**ZPE = 0.150072** **E(B3LYP) = -386.361722338** **E(B3LYP+ZPE) = -386.211650** **E_{rel}(B3LYP) = 64.5** **E(CCSD(T)/6-311G**) = -385.23439339** **E(MP2/6-311G**) = -385.12577315** **E(MP2/G3large) = -385.34580324** **E(G3(MP2,CC) = -385.30435148**	**A** **B** **C**	**483.0** **2156.7** **2215.7**	**3.7368** **0.8368** **0.8145**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H** **H**	**-0.693517** **-1.386707** **-2.573007** **-2.765710** **-1.579028** **0.736414** **1.889697** **3.017211** **2.557453** **1.185514** **-0.731646** **-0.998894** **-3.261041** **-3.631699** **-1.858784** **1.959555** **4.058008** **3.162061** **-1.027477**	**0.704301** **-0.332166** **-0.751201** **-0.125257** **0.733781** **0.335230** **1.000901** **0.156306** **-1.072566** **-0.967987** **1.685444** **-0.656844** **-1.461686** **-0.239780** **1.752435** **1.984723** **0.430310** **-1.894449** **0.311796**	**0.298455** **1.155990** **0.561299** **-0.655086** **-0.999819** **0.093103** **0.413809** **0.070547** **-0.462087** **-0.429153** **0.789699** **2.111709** **1.003671** **-1.293893** **-1.288717** **0.858073** **0.196329** **-0.811465** **-1.847761**	**49, 53, 111, 182, 330, 357, 445, 532, 580, 619, 649, 677, 710, 720, 761, 780, 806, 828, 854, 921, 938, 943, 949, 961, 1011, 1039, 1078, 1106, 1139, 1173, 1201, 1239, 1261, 1290, 1297, 1315, 1347, 1395, 1431, 1470, 1484, 1545, 2996, 3013, 3044, 3184, 3187, 3206, 3207, 3220, 3241**
S26, (C_S), ^{2}A"  1-H-Fulvalenyl	**ZPE = 0.153207** **E(B3LYP) = -386.494211401** **E(B3LYP+ZPE) = -386.341005** **E_{rel}(B3LYP) = -16.6** **E(CCSD(T)/6-311G**) = -385.41546219** **E(MP2/6-311G**) = -385.25144246** **E(MP2/G3large) = -385.47924381** **E(G3(MP2,CC) = -385.49005654**	**A** **B** **C**	**428.2** **2145.6** **2562.7**	**4.2149** **0.8411** **0.7042**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H** **H**	**0.000000** **-1.058075** **-0.551040** **0.810228** **1.287502** **-0.074417** **1.043018** **0.539803** **-0.924499** **-1.291275** **1.905095** **-2.107049** **-1.168693** **1.466320** **1.905095** **2.086412** **1.112378** **-1.588168** **-2.298858**	**0.660427** **1.573229** **2.912232** **2.891908** **1.468103** **-0.734852** **-1.659165** **-2.927688** **-2.852201** **-1.542941** **1.243385** **1.310725** **3.801167** **3.751444** **1.243385** **-1.378823** **-3.845465** **-3.706162** **-1.153974**	**0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.000000** **0.877894** **0.000000** **0.000000** **0.000000** **-0.877894** **0.000000** **0.000000** **0.000000** **0.000000**	**100, 108, 153, 240, 383, 397, 443, 533, 558, 642, 689, 703, 759, 778, 814, 828, 844, 889, 890, 908, 922, 958, 963, 970, 1030, 1047, 1094, 1112, 1118, 1145, 1149, 1260, 1282, 1303, 1339, 1389, 1401, 1430, 1481, 1511, 1553, 1563, 3026, 3051, 3195, 3198, 3208, 3214, 3223, 3224, 3231**
S27, (C_1) 	**ZPE = 0.153416** **E(B3LYP) = -386.405068826** **E(B3LYP+ZPE) = -386.251653** **E_{rel}(B3LYP) = 39.4** **E(CCSD(T)/6-311G**) = -385.33928332** **E(MP2/6-311G**) = -385.18048798** **E(MP2/G3large) = -385.40152761** **E(G3(MP2,CC) = -385.40690696**	**A** **B** **C**	**474.2** **1695.6** **2066.0**	**3.8063** **1.0644** **0.8736**	**C** **C** **C** **C** **C** **C** **C** **C** **C**	**-0.656517** **-0.628360** **-1.957691** **-2.716690** **-2.034087** **0.663119** **1.936433** **2.835134** **2.154268**	**0.747919** **-0.754764** **-1.184352** **-0.122279** **1.219022** **0.733305** **1.234016** **0.091714** **-1.091253**	**0.354818** **0.578192** **0.009549** **-0.288109** **-0.008819** **-0.208357** **-0.044470** **0.016669** **-0.039347**	**107, 135, 239, 288, 372, 425, 529, 570, 653, 696, 727, 759, 793, 812, 834, 862, 896, 917, 921, 936, 968, 977, 999, 1011, 1024, 1077, 1104, 1109, 1131, 1157, 1173, 1230, 1237, 1247, 1289, 1316, 1351, 1364, 1423, 1466, 1547, 1640, 2978, 3025,**

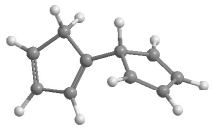
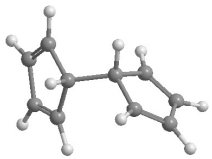
					C	0.716014	-0.770420	-0.316032	3046, 3049, 3165, 3177, 3189, 3197, 3206
					H	-2.551445	1.752601	0.802069	
					H	-0.438890	-1.096221	1.600092	
					H	-2.275051	-2.216055	-0.095658	
					H	-3.732892	-0.176821	-0.663268	
					H	-2.037181	1.887733	-0.875564	
					H	2.216991	2.251008	0.196960	
					H	3.910772	0.180992	0.116541	
					H	2.607637	-2.072927	-0.092672	
					H	0.430333	-1.127761	-1.313054	
S28, (C_1) 	ZPE = 0.150571 E(B3LYP) = -386.377776585 E(B3LYP+ZPE) = -386.227206 E_{rel}(B3LYP) = 54.8 E(CCSD(T)/6-311G**) = -385.30494344 E(MP2/6-311G**) = -385.12029603 E(MP2/G3large) = -385.34235669 E(G3(MP2,CC) = -385.37643310	A B C	645.5 1473.6 1990.2	2.7957 1.2247 0.9068	C	0.632504	-1.567591	-0.220292	112, 138, 175, 271, 343, 358, 459, 485, 540, 555, 595, 612, 671, 710, 779, 790, 813, 820, 896, 923, 949, 967, 972, 1026, 1044, 1069, 1082, 1110, 1143, 1186, 1196, 1227, 1253, 1272, 1330, 1366, 1409, 1459, 1463, 1488, 1503, 1539, 2906, 2938, 3084, 3131, 3154, 3167, 3189, 3207, 3221
					C	0.476420	1.587350	-0.096914	
					C	1.795020	1.261821	-0.352357	
					C	2.444671	0.043862	-0.161008	
					C	1.906396	-1.189621	0.494404	
					C	-0.495379	-0.837503	-0.132937	
					C	-1.842971	-1.171825	-0.382402	
					C	-2.696152	-0.070626	-0.108498	
					C	-1.971672	1.009796	0.315768	
					C	-0.526107	0.642350	0.441786	
					H	1.679693	-1.003124	1.557070	
					H	0.128236	2.572786	-0.387998	
					H	2.391705	2.034585	-0.830746	
					H	3.410302	-0.062654	-0.646118	
					H	2.651133	-1.985360	0.456139	
					H	-2.165034	-2.153522	-0.701051	
					H	-3.770733	-0.087003	-0.240031	
					H	-2.356876	2.004025	0.501859	
					H	-0.304801	0.432179	1.505578	
S29, (C_1) 	ZPE = 0.150375 E(B3LYP) = -386.362934135 E(B3LYP+ZPE) = -386.212559 E_{rel}(B3LYP) = 64.0 E(CCSD(T)/6-311G**) = -385.27849431 E(MP2/6-311G**) = -385.11533644 E(MP2/G3large) = -385.33836289 E(G3(MP2,CC) = -385.35114576	A B C	508.1 2019.3 2129.4	3.5516 0.8938 0.8476	C	-0.691948	-0.909584	-0.100798	25, 62, 118, 224, 273, 359, 467, 531, 548, 640, 661, 702, 711, 725, 744, 782, 855, 867, 894, 899, 917, 932, 944, 970, 1000, 1030, 1084, 1094, 1120, 1178, 1212, 1222, 1245, 1282, 1291, 1322, 1352, 1418, 1437, 1445, 1479, 1556, 3012, 3050, 3068, 3190, 3198, 3210, 3211, 3222, 3233
					C	-1.386553	-0.212718	-1.232064	
					C	-2.450821	0.592441	-0.850238	
					C	-2.645692	0.443889	0.509180	
					C	-1.642718	-0.522741	1.103709	
					C	0.704028	-0.367093	-0.017134	
					C	1.899420	-1.076670	-0.187363	
					C	2.951115	-0.165042	-0.063765	
					C	2.397686	1.163872	0.166187	
					C	1.041536	1.052070	0.185178	
					H	-1.070091	-0.077916	1.920978	
					H	-0.653449	-1.993301	-0.239429	
					H	-3.043775	1.212840	-1.509424	
					H	-3.438324	0.906932	1.083544	
					H	-2.141943	-1.409851	1.511938	
					H	1.985819	-2.140058	-0.357720	
					H	4.006599	-0.400982	-0.106581	
					H	2.977730	2.066323	0.295980	

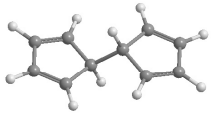
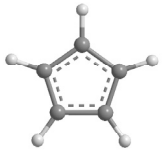
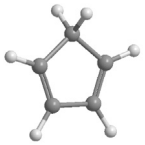
					H	0.321114	1.845472	0.323361	
S30, (C_1) 	ZPE = 0.149750 E(B3LYP) = -386.371951937 E(B3LYP+ZPE) = -386.222202 E_{rel}(B3LYP) = 58.0 E(CCSD(T)/6-311G**) = -385.29346196 E(MP2/6-311G**) = -385.12510685 E(MP2/G3large) = -385.34599154 E(G3(MP2,CC) = -385.36459665	A B C	539.4 1779.2 1875.2	3.3461 1.0144 0.9624	C C C C C C C C C C H H H H H H H H H H	0.224354 1.172936 2.495352 2.604240 1.247882 -0.653792 -0.601750 -1.963355 -2.687905 -1.996111 1.123767 0.803007 3.336617 3.529367 1.049049 -0.066463 -2.514932 -3.760293 -2.551231	-0.039325 -0.327924 -0.182162 0.139063 0.174363 -1.216893 1.198452 1.190004 -0.006679 -1.251760 -0.637503 -0.579598 -0.303223 0.308865 1.109618 2.084632 2.112361 0.027463 -2.185448	0.031342 -1.147525 -0.764112 0.578664 1.223041 0.247222 -0.251168 -0.168291 0.052975 0.087630 1.950109 -2.131384 -1.436654 1.113715 1.757373 -0.580600 -0.321394 0.212580 0.097586	56, 76, 148, 275, 313, 369, 436, 483, 556, 560, 617, 633, 670, 690, 765, 777, 804, 851, 872, 903, 946, 952, 954, 982, 1019, 1033, 1062, 1078, 1108, 1122, 1159, 1218, 1271, 1281, 1302, 1319, 1388, 1402, 1459, 1476, 1522, 1550, 3006, 3042, 3140, 3143, 3161, 3175, 3181, 3205, 3223
S31, (C_1) 	ZPE = 0.153750 E(B3LYP) = -386.430793062 E(B3LYP+ZPE) = -386.277043 E_{rel}(B3LYP) = 23.5 E(CCSD(T)/6-311G**) = -385.36209952 E(MP2/6-311G**) = -385.20340017 E(MP2/G3large) = -385.42754113 E(G3(MP2,CC) = -385.43249048	A B C	550.8 1533.8 1864.3	3.2765 1.1766 0.9680	C C C C C C C C C C H H H H H H H	-0.201339 -0.755302 -2.221434 -2.602599 -1.454717 0.180590 0.912392 2.198283 2.531690 1.539051 -1.335704 -0.389498 -2.877388 -3.612904 -1.602732 0.691244 3.006028 3.575013 1.786257	0.462395 -0.881558 -0.845167 0.207423 1.129896 -0.902734 1.318657 0.905385 -0.403142 -1.300183 1.283963 -1.211557 -1.628264 0.394325 2.123896 2.329663 1.571336 -0.684599 -2.324593	0.005719 0.712099 0.454033 -0.268205 -0.587566 -0.427035 0.431553 0.309444 -0.199454 -0.494195 -1.666436 1.681044 0.817240 -0.612119 -0.144635 0.763157 0.594491 -0.290104 -0.760990	82, 186, 218, 351, 378, 398, 438, 488, 587, 634, 668, 694, 721, 749, 811, 835, 912, 934, 941, 950, 961, 974, 979, 990, 998, 1047, 1094, 1137, 1152, 1171, 1187, 1230, 1263, 1315, 1361, 1374, 1415, 1443, 1472, 1505, 1627, 1672, 3000, 3035, 3125, 3135, 3140, 3165, 3171, 3180, 3196
S32, (C_S), ^{2}A"	ZPE = 0.152779 E(B3LYP) = -386.486505413 E(B3LYP+ZPE) = -386.333726 E_{rel}(B3LYP) = -12.1 E(CCSD(T)/6-311G**) = -385.40977727 E(MP2/6-311G**) = -385.24420721 E(MP2/G3large) = -385.47216702 E(G3(MP2,CC) = -385.48495808	A B C	428.8 2162.0 2579.8	4.2087 0.8347 0.6996	C C C C C C C C	0.000000 -1.212724 -0.870041 0.630282 1.091249 0.022057 -1.121387 -0.661180	0.654998 1.499257 2.796390 2.929914 1.504664 -0.761730 -1.639930 -2.929017	0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	80, 108, 158, 261, 369, 385, 438, 548, 579, 643, 696, 701, 732, 735, 783, 807, 834, 884, 905, 913, 922, 940, 958, 977, 991, 1045, 1076, 1105, 1125, 1127, 1144, 1255, 1286, 1296, 1352, 1369, 1418, 1430, 1486,

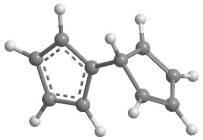
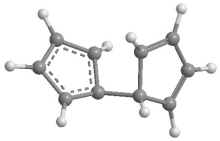
 2-H-Fulvalenyl					C	0.806299	-2.903813	0.000000	1492, 1558, 1623, 2997, 3013, 3199, 3201, 3210, 3220, 3224, 3230, 3235
					C	1.213452	-1.606939	0.000000	
					H	2.129545	1.204802	0.000000	
					H	-2.221066	1.108767	0.000000	
					H	-1.547530	3.639677	0.000000	
					H	0.998905	3.482685	0.876149	
					H	0.998905	3.482685	-0.876149	
					H	-2.154667	-1.326700	0.000000	
					H	-1.265447	-3.826241	0.000000	
					H	1.440949	-3.779334	0.000000	
					H	2.232364	-1.249104	0.000000	
S33, **(C_1)** 	ZPE = 0.153477 E(B3LYP) = -386.408241387 E(B3LYP+ZPE) = -386.254765 E_{rel}(B3LYP) = 37.5 E(CCSD(T)/6-311G**) = -385.34386775 E(MP2/6-311G**) = -385.18815450 E(MP2/G3large) = -385.41280037 E(G3(MP2,CC) = -385.41503662	A B C	525.0 1734.7 1831.7	3.4378 1.0404 0.9853	C	0.776812	-0.700044	0.823389	122, 148, 155, 293, 360, 388, 550, 564, 607, 643, 709, 733, 755, 778, 807, 825, 881, 903, 918, 928, 937, 954, 965, 982, 1004, 1031, 1038, 1105, 1118, 1130, 1158, 1207, 1254, 1282, 1323, 1346, 1365, 1418, 1459, 1512, 1609, 1636, 2997, 3059, 3171, 3180, 3193, 3204, 3205, 3226, 3234
					C	0.800831	-0.972835	-0.614682	
					C	1.874985	-0.104907	-1.170631	
					C	2.490137	0.571945	-0.192707	
					C	1.896239	0.252675	1.171137	
					C	-0.464763	-0.269937	0.126869	
					C	-0.896786	1.119011	-0.118831	
					C	-2.249601	1.136178	-0.172018	
					C	-2.759927	-0.223338	0.017091	
					C	-1.717295	-1.065901	0.183884	
					H	2.643020	-0.224651	1.820559	
					H	0.523068	-1.907147	-1.086471	
					H	2.124280	-0.062882	-2.223700	
					H	3.315656	1.261016	-0.327074	
					H	1.539984	1.139356	1.704262	
					H	-0.227564	1.957440	-0.241096	
					H	-2.868197	2.007486	-0.343717	
					H	-3.806922	-0.496072	0.015970	
					H	-1.747121	-2.131632	0.360267	
S34, **(C_1)** 	ZPE = 0.153239 E(B3LYP) = -386.402492586 E(B3LYP+ZPE) = -386.249254 E_{rel}(B3LYP) = 40.9 E(CCSD(T)/6-311G**) = -385.34112296 E(MP2/6-311G**) = -385.18112419 E(MP2/G3large) = -385.40323564 E(G3(MP2,CC) = -385.40999541	A B C	548.9 1915.1 1926.1	3.2882 0.9424 0.9370	C	0.717466	-0.504881	-0.640417	74, 95, 130, 228, 312, 390, 497, 553, 653, 684, 719, 769, 780, 798, 817, 827, 847, 877, 925, 944, 956, 957, 976, 992, 1003, 1034, 1073, 1111, 1114, 1134, 1180, 1196, 1223, 1258, 1300, 1319, 1337, 1400, 1544, 1557, 1634, 1643, 2978, 3000, 3181, 3188, 3198, 3206, 3215, 3215, 3226
					C	1.825914	-1.066307	0.217301	
					C	2.680078	-0.080235	0.542398	
					C	2.203496	1.184582	-0.034670	
					C	1.060443	0.964082	-0.706785	
					C	-0.711323	-0.834829	-0.142718	
					C	-1.839497	-0.291339	-1.006681	
					C	-2.690626	0.424102	-0.248675	
					C	-2.222550	0.449514	1.158523	
					C	-1.092008	-0.253954	1.187429	
					H	0.809472	-0.932395	-1.651803	
					H	1.898715	-2.109529	0.494525	
					H	3.579642	-0.183465	1.135870	
					H	2.705272	2.137118	0.078576	
					H	0.460456	1.692538	-1.233723	
					H	-1.919337	-0.486373	-2.068406	
					H	-3.593583	0.915241	-0.591495	

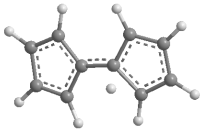
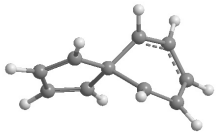
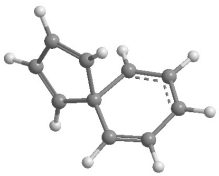
					H	-2.724023	0.951889	1.973991	
					H	-0.804978	-1.929430	-0.091765	
S35, **(C_1)** 	**ZPE = 0.152959** **E(B3LYP) = -386.408755384** **E(B3LYP+ZPE) = -386.255796** **E_{rel}(B3LYP) = 36.8** **E(CCSD(T)/6-311G**) = -385.34490751** **E(MP2/6-311G**) = -385.18495926** **E(MP2/G3large) = -385.40712373** **E(G3(MP2,CC) = -385.41411299**	**A** **B** **C**	**469.4** **2155.5** **2239.1**	**3.8447** **0.8373** **0.8060**	C C C C C C C C C C H H H H H H H H	-0.672105 -1.762024 -2.972098 -2.623775 -1.125029 0.767121 1.596195 2.696821 2.721747 1.617019 -0.799783 -1.756673 -3.979682 -3.289808 -0.700289 1.295478 3.467767 3.502646 0.797120	-0.313703 -1.102804 -0.303257 0.976146 1.096541 -0.728051 -0.592987 0.142109 0.578161 0.090124 1.792778 -2.165645 -0.698431 1.806313 1.475088 -1.045348 0.389923 1.169490 -1.777844	-0.136726 -0.232096 -0.012120 0.216576 0.156784 -0.271107 1.007887 0.770813 -0.647156 -1.208111 -0.626723 -0.442292 -0.037000 0.408006 1.095217 1.943356 1.490690 -1.104950 -0.594772	**49, 96, 127, 285, 290, 387, 413, 502, 554, 668, 695, 774, 778, 808, 825, 837, 877, 883, 919, 944, 946, 953, 961, 975, 993, 1016, 1107, 1122, 1129, 1170, 1192, 1210, 1225, 1280, 1322, 1328, 1388, 1416, 1543, 1575, 1634, 1656, 3010, 3021, 3046, 3183, 3185, 3197, 3212, 3217, 3220**
AZ, **(C_{2V}),** **$^1A_1$**  Azulene	**ZPE = 0.145451** **E(B3LYP) = -385.930867730** **E(B3LYP+ZPE) = -385.785416** **E(CCSD(T)/6-311G**) = -384.85198627** **E(MP2/6-311G**) = -384.73966184** **E(MP2/G3large) = -384.97035416** **E(G3(MP2,CC) = -384.93724759**	**A** **B** **C**	**632.0** **1438.0** **2070.1**	**2.85541** **1.25500** **0.87182**	C C C C C C C C C C H H H H H H H H	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	0.749633 -0.749633 1.148409 -1.148409 1.592432 -1.592432 1.263804 -1.263804 0.000000 0.000000 0.000000 0.000000 2.172524 -2.172524 2.656321 -2.656321 2.103905 -2.103905	0.553208 0.553208 1.899320 1.899320 -0.551625 -0.551625 -1.907998 -1.907998 2.704613 -2.499250 3.787071 -3.586206 2.245658 2.245658 -0.324086 -0.324086 -2.595518 -2.595518	**163, 170, 320, 338, 412, 429, 498, 575, 612, 679, 724, 741, 744, 782, 796, 833, 875, 915, 940, 961, 975, 993, 1008, 1023, 1064, 1081, 1186, 1238, 1243, 1301, 1322, 1335, 1420, 1428, 1487, 1489, 1532, 1580, 1633, 1644, 3129, 3132, 3139, 3159, 3168, 3196, 3213, 3222**
NP, **(D_{2h}),** **^1A_g**	**ZPE = 0.146928** **E(B3LYP) = -385.984930544** **E(B3LYP+ZPE) = -385.838003** **E(CCSD(T)/6-311G**) = -384.90987012** **E(MP2/6-311G**) = -384.79552163** **E(MP2/G3large) = -385.02573266** **E(G3(MP2,CC) = -384.99315315**	**A** **B** **C**	**576.9** **1462.6** **2039.5**	**3.12815** **1.23394** **0.88488**	C C C C C C C C	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	0.000000 0.000000 1.243465 -1.243465 1.243465 -1.243465 2.429373 -2.429373	0.715661 -0.715661 1.400275 1.400275 -1.400275 -1.400275 0.707395 0.707395	**174, 186, 366, 396, 480, 488, 519, 520, 635, 636, 729, 773, 787, 799, 809, 850, 897, 951, 957, 974, 993, 1000, 1036, 1046, 1151, 1169, 1172, 1185, 1232, 1270, 1287, 1391, 1399, 1418, 1491, 1492, 1549, 1614,**

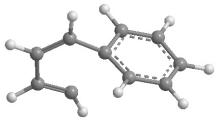
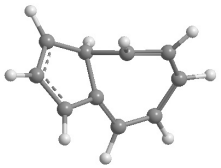
 Naphthalene					C	0.0	2.429373	-0.707395	1641, 1671, 3156, 3158, 3160, 3164, 3174, 3175, 3187, 3188
					C	0.0	-2.429373	-0.707395	
					H	0.0	1.241873	2.485452	
					H	0.0	-1.241873	2.485452	
					H	0.0	1.241873	-2.485452	
					H	0.0	-1.241873	-2.485452	
					H	0.0	3.372182	1.242827	
					H	0.0	-3.372182	1.242827	
					H	0.0	3.372182	-1.242827	
					H	0.0	-3.372182	-1.242827	
FL **(D_{2h}),** **^1A_g**  Fulvalene	ZPE = 0.143399 E(B3LYP) = -385.890861786 E(B3LYP+ZPE) = -385.747463 E(CCSD(T)/6-311G**) = -384.82333903 E(MP2/6-311G**) = -384.69944937 E(MP2/G3large) = -384.92779177 E(G3(MP2,CC) = -384.90828243	A B C	427.3 2063.1 2490.4	4.22348 0.87478 0.72468	C	0.0	0.000000	0.680770	100, 120, 159, 248, 400, 445, 523, 579, 609, 659, 717, 722, 773, 797, 809, 817, 841, 903, 923, 931, 940, 942, 948, 1001, 1026, 1101, 1108, 1110, 1138, 1143, 1238, 1321, 1322, 1378, 1391, 1529, 1533, 1607, 1611, 1682, 3202, 3203, 3213, 3215, 3236, 3240, 3242, 3246
					C	0.0	1.177500	1.562500	
					C	0.0	0.738500	2.840330	
					C	0.0	-0.738500	2.840330	
					C	0.0	-1.177500	1.562500	
					C	0.0	0.000000	-0.680770	
					C	0.0	-1.177500	-1.562500	
					C	0.0	-0.738500	-2.840330	
					C	0.0	0.738500	-2.840330	
					C	0.0	1.177500	-1.562500	
					H	0.0	-2.202660	1.225400	
					H	0.0	2.202660	1.225400	
					H	0.0	1.352100	3.731000	
					H	0.0	-1.352100	3.731000	
					H	0.0	-2.202660	-1.225400	
					H	0.0	-1.352100	-3.731000	
					H	0.0	1.352100	-3.731000	
					H	0.0	2.202660	-1.225400	
A1, **(C_1)**  **1,9,10-** **Trihydrofulvalenyl**	ZPE = 0.175883 E(B3LYP) = -387.683166793 E(B3LYP+ZPE) = -387.507284 E(CCSD(T)/6-311G**) = -386.60796001 E(MP2/6-311G**) = -386.45687020 E(MP2/G3large) = -386.68157709 E(G3(MP2,CC) = -386.65678390	A B C	581.2 1971.9 1980.0	3.10544 0.91521 0.91148	H	2.359771	1.928788	0.147149	54, 89, 115, 210, 295, 354, 442, 550, 584, 639, 679, 699, 723, 743, 800, 816, 839, 850, 909, 939, 946, 954, 955, 956, 1003, 1035, 1042, 1071, 1076, 1107, 1115, 1135, 1160, 1200, 1230, 1282, 1300, 1308, 1323, 1341, 1400, 1404, 1475, 1483, 1554, 1640, 2969, 2979, 2999, 3022, 3179, 3184, 3194, 3204, 3211, 3217, 3220
					H	1.440107	1.235563	1.464509	
					C	2.193509	-1.170294	-0.370115	
					C	2.721903	-0.189423	0.456111	
					C	1.827563	1.022395	0.459652	
					C	0.676930	0.659160	-0.534391	
					C	1.012875	-0.749308	-0.962476	
					H	2.643988	-2.143061	-0.529595	
					H	3.633704	-0.269713	1.032982	
					H	0.722551	1.329614	-1.403712	
					H	0.396353	-1.327875	-1.636711	
					C	-0.749606	0.822101	0.063131	
					C	-1.094794	-0.107283	1.202482	
					C	-2.242171	-0.751537	0.923987	
					C	-2.728692	-0.327468	-0.395773	
					C	-1.873736	0.573273	-0.912829	
					H	-0.495850	-0.216675	2.096075	
					H	-2.741242	-1.472779	1.558868	
					H	-3.637070	-0.689399	-0.860915	

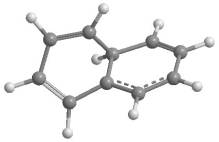
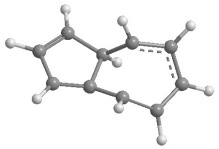
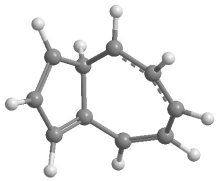
					H	-1.956733	1.074046	-1.868635	
					H	-0.828258	1.861798	0.421312	
A2, (C_1)  1,10-Dihydrofulvalene	ZPE = 0.165578 E(B3LYP) = -387.102193854 E(B3LYP+ZPE) = -386.936616 E(CCSD(T)/6-311G**) = -386.03306275 E(MP2/6-311G**) = -385.89921171 E(MP2/G3large) = -386.12548218 E(G3(MP2,CC) = -386.09375521	A B C	489.3 2115.6 2356.9	3.68820 0.85305 0.76574	H H C C C C C H H H C C C C C H H H H H	1.865080 1.522313 2.645589 2.978215 1.747883 0.662185 1.213102 3.316852 3.957923 0.687207 -0.774806 -1.531325 -2.671116 -2.758165 -1.668069 -1.177729 -3.418000 -3.583136 -1.440715 -0.790758	-1.367581 -1.976830 0.873813 -0.369745 -1.060767 -0.019450 1.092682 1.613341 -0.825584 2.010237 -0.268038 -1.175109 -0.572922 0.747713 0.947541 -2.151473 -0.981447 1.436973 1.819349 -0.751288	1.450123 -0.160276 -0.512343 -0.122105 0.401785 0.246596 -0.282644 -0.930514 -0.162219 -0.511700 0.625707 -0.330321 -0.709265 -0.070943 0.689815 -0.631750 -1.378269 -0.199526 1.287867 1.618580	48, 93, 142, 255, 339, 384, 413, 528, 568, 671, 692, 722, 795, 813, 825, 828, 878, 911, 921, 936, 952, 954, 959, 960, 1008, 1015, 1035, 1109, 1112, 1121, 1126, 1151, 1210, 1254, 1265, 1307, 1323, 1384, 1397, 1416, 1557, 1576, 1641, 1658, 2949, 3010, 3034, 3186, 3189, 3197, 3207, 3216, 3220, 3222
S0$_{cis}$, (C_2), ^{1}A  *cis*-9,10-Dihydrofulvalene	ZPE = 0.165939 E(B3LYP) = -387.097777115 E(B3LYP+ZPE) = -386.931838 E(CCSD(T)/6-311G**) = -386.03108576 E(MP2/6-311G**) = -385.89746412 E(MP2/G3large) = -386.12349936 E(G3(MP2,CC) = -386.09118200	A B C	560.3 1930.6 1940.8	3.22084 0.93480 0.92988	C C C C C C C C C C C H H H H H H H H H H	-0.269402 -1.083110 -0.584881 0.584881 0.793058 0.269402 1.083110 0.584881 -0.584881 -0.793058 -0.901815 -1.934088 -0.968741 1.172471 1.572997 1.934088 0.968741 -1.172471 -1.572997 0.901815	0.728110 1.116668 2.247935 2.674323 1.800169 -0.728110 -1.116668 -2.247935 -2.674323 -1.800169 0.836969 0.550457 2.773253 3.559624 1.841432 -0.550457 -2.773253 -3.559624 -1.841432 -0.836969	0.767391 -0.443454 -0.972579 -0.191780 0.809095 0.767391 -0.443454 -0.972579 -0.191780 0.809095 1.663356 -0.795388 -1.837853 -0.400280 1.558126 -0.795388 -1.837853 -0.400280 1.558126 1.663356	77, 97, 130, 246, 305, 398, 549, 562, 651, 692, 719, 728, 781, 803, 817, 825, 854, 877, 918, 956, 956, 958, 958, 998, 1005, 1025, 1037, 1069, 1111, 1111, 1122, 1134, 1195, 1195, 1268, 1296, 1316, 1321, 1400, 1401, 1555, 1556, 1641, 1641, 2972, 2978, 3185, 3185, 3196, 3197, 3212
S0$_{trans}$, (C_{2h}), ^1A_g	ZPE = 0.166106 E(B3LYP) = -387.098225348 E(B3LYP+ZPE) = -386.932119 E(CCSD(T)/6-311G**) = -386.03099792	A B C	471.2 2041.3 2423.2	3.82973 0.88411 0.74478	C C C C C	0.429238 0.170320 -0.170320 -0.170320 0.170320	0.649855 1.560443 2.783600 2.783600 1.560443	0.000000 1.177483 0.734602 -0.734602 -1.177483	79, 98, 171, 172, 351, 402, 555, 576, 581, 694, 719, 726, 758, 815, 818, 818, 852, 919, 922, 955, 957, 957, 958, 1004, 1010, 1018, 1055, 1065, 1109,

 ***trans*-9,10-Dihydrofulvalene**	E(MP2/6-311G**) = -385.89710652 E(MP2/G3large) = -386.12306240 E(G3(MP2,CC) = -386.09084780				C C C C C H H H H H H H H H	-0.429238 -0.170320 0.170320 0.170320 -0.170320 1.485369 0.266879 -0.403844 -0.403844 0.266879 -0.266879 0.403844 0.403844 -0.266879 -1.485369	-0.649855 -1.560443 -2.783600 -2.783600 -1.560443 0.341323 1.250870 3.644542 3.644542 1.250870 -1.250870 -3.644542 -3.644542 -1.250870 -0.341323	0.000000 1.177483 0.734602 -0.734602 -1.177483 0.000000 2.208895 1.348186 -1.348186 -2.208895 2.208895 1.348186 -1.348186 -2.208895 0.000000	**1122, 1127, 1149, 1171, 1218, 1257, 1285, 1313, 1315, 1398, 1404, 1555, 1557, 1641, 1642, 2989, 3003, 3186, 3187, 3196, 3198, 3216, 3221, 3222, 3226**
c-C_5H_5 (C_{2V}), $^2B_1$  **Cyclopentadienyl**	ZPE = 0.077704 E(B3LYP) = -193.512983250 E(B3LYP+ZPE) = -193.435279 E(CCSD(T)/6-311G**) = -192.96785740 E(MP2/6-311G**) = -192.88363418 E(MP2/G3large) = -192.99696881 E(G3(MP2,CC) = -193.00348802	A B C	194.1 212.0 406.1	9.30036 8.51141 4.44421	C C C C C H H H H H	0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0	0.741277 1.169009 0.000000 -1.169009 -0.741277 1.357995 2.190729 0.000000 -2.190729 -1.357995	-0.946378 0.352883 1.186344 0.352883 -0.946378 -1.834653 0.702061 2.269063 0.702061 -1.834653	**77, 500, 516, 681, 719, 816, 847, 892, 899, 929, 944, 1059, 1072, 1143, 1217, 1295, 1386, 1490, 1534, 3200, 3204, 3216, 3232, 3240**
c-C_5H_6 (C_{2V}), $^1A_1$  **Cyclopentadiene**	ZPE = 0.092158 E(B3LYP) = -194.153720460 E(B3LYP+ZPE) = -194.061562 E(CCSD(T)/6-311G**) = -193.60871246 E(MP2/6-311G**) = -193.53596012 E(MP2/G3large) = -193.65006691 E(G3(MP2,CC) = -193.63066125	A B C	213.0 219.2 421.1	8.47494 8.23256 4.28579	H H C C C C C H H H H	-0.876973 0.876973 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000	0.000000 0.000000 0.734440 1.179487 0.000000 -1.179487 -0.734440 1.346962 2.210199 -2.210199 -1.346962	1.877302 1.877302 -0.989270 0.280863 1.215703 0.280863 -0.989270 -1.881938 0.607971 0.607971 -1.881938	**348, 524, 681, 713, 817, 819, 918, 924, 954, 956, 971, 1012, 1112, 1126, 1130, 1266, 1315, 1397, 1415, 1553, 1639, 3011, 3033, 3187**
H_2, ($D_{\infty h}$), $^1\Sigma_g^+$	ZPE = 0.010067 E(B3LYP) = -1.17957102175 E(B3LYP+ZPE) = -1.169504 E(CCSD(T)/6-311G**) = -1.16833998 E(MP2/6-311G**) = -1.16024855 E(MP2/G3large) = -1.16275945 E(G3(MP2,CC) = -1.16078388	A B C	0.00000 0.99666 0.99666	1810.8	H H	0.0 0.0	0.0 0.0	0.372107 -0.372107	**4419**
H, ^2S	ZPE = 0.0 E(B3LYP) = -0.502155930011								

	E(CCSD(T)/6-311G**) = -0.49980982 E(MP2/6-311G**) = -0.49980982 E(MP2/G3large) = -0.49981792 E(G3(MP2,CC) = -0.49981792								
TS S1-S2, (C_1) 	ZPE = 0.152344 E(B3LYP) = -386.445912363 E(B3LYP+ZPE) = -386.293569 E_{rel}(B3LYP) = 13.1 E(CCSD(T)/6-311G**) = -385.37519909 E(MP2/6-311G**) = -385.21490885 E(MP2/G3large) = -385.44145286 E(G3(MP2,CC) = -385.44939910	A B C	540.0 1695.4 1815.9	3.3422 1.0645 0.9938	C C C C C C C C C C H H H H H H H H H	0.844211 0.948644 1.900559 2.438088 1.856254 -0.482996 -1.693435 -2.736502 -2.219948 -0.872421 0.734754 0.552465 2.150913 3.169299 2.029721 -1.740959 -3.776570 -2.820551 -0.193796	-0.836506 -0.908735 0.054967 0.690654 0.179626 -0.269670 -1.057892 -0.195425 1.168217 1.132464 -1.735696 -1.706672 0.284186 1.488523 0.500082 -2.135785 -0.468236 2.057196 1.970198	-0.722173 0.760580 1.171681 0.020411 -1.112510 -0.216108 -0.093042 0.094459 0.109603 -0.070909 -1.321531 1.367111 2.197794 0.042739 -2.129977 -0.163546 0.213333 0.246487 -0.104362	426*i*, 125, 142, 171, 346, 407, 519, 571, 586, 642, 705, 731, 751, 757, 804, 815, 831, 858, 891, 904, 912, 945, 960, 984, 1012, 1051, 1071, 1085, 1091, 1102, 1119, 1196, 1247, 1287, 1313, 1317, 1348, 1410, 1419, 1478, 1506, 1568, 3135, 3196, 3197, 3208, 3218, 3221, 3227, 3244, 3250
TS S1-S5, (C_1) 	ZPE = 0.152440 E(B3LYP) = -386.420671692 E(B3LYP+ZPE) = -386.268232 E_{rel}(B3LYP) = 29.0 E(CCSD(T)/6-311G**) = -385.35211910 E(MP2/6-311G**) = -385.17966258 E(MP2/G3large) = -385.40389369 E(G3(MP2,CC) = -385.42391021	A B C	498.4 1643.2 1901.9	3.6210 1.0983 0.9489	C C C C C C C C C C H H H H H H H H H	-0.720713 -0.698457 -1.919347 -2.617692 -1.949777 0.629659 1.875682 2.759769 2.041157 0.670926 -0.720619 -0.160366 -2.209224 -3.546024 -2.245553 2.131199 3.828632 2.450253 0.044461	0.979066 -0.462552 -1.087786 -0.203466 0.990666 0.725069 1.115857 -0.021647 -1.139660 -0.740818 1.770127 -0.715010 -2.103297 -0.447478 1.830863 2.063370 0.009171 -2.112640 -1.223472	0.365543 0.887430 0.472438 -0.386440 -0.507690 -0.258444 0.145594 0.032542 -0.328201 -0.521320 1.119595 1.791508 0.705832 -0.888414 -1.120855 0.601533 0.206110 -0.563311 -1.260699	479*i*, 139, 171, 237, 340, 372, 520, 584, 654, 668, 731, 749, 771, 794, 816, 827, 850, 874, 891, 918, 926, 952, 964, 993, 1031, 1048, 1055, 1067, 1096, 1114, 1143, 1183, 1240, 1278, 1287, 1307, 1330, 1400, 1406, 1455, 1485, 1575, 3063, 3184, 3188, 3189, 3198, 3203, 3212, 3216, 3221
TS S1-S26, (C_1)	ZPE = 0.149020 E(B3LYP) = -386.435072552 E(B3LYP+ZPE) = -386.286052 E_{rel}(B3LYP) = 17.8	A B C	426.8 2148.6 2559.4	4.2288 0.8399 0.7051	C C C	0.688680 1.556217 2.857576	0.015884 1.165385 0.738675	0.137823 0.072708 -0.092451	1187*i*, 43, 116, 152, 300, 389, 422, 540, 587, 616, 663, 675, 693, 737, 767, 782, 845, 848,

	E(CCSD(T)/6-311G**) = -385.35632534 E(MP2/6-311G**) = -385.20588849 E(MP2/G3large) = -385.43639131 E(G3(MP2,CC) = -385.43780815				C	2.898616	-0.676522	-0.138011	872, 892, 894, 914, 943, 969, 1030, 1038, 1082, 1089, 1098, 1116, 1136, 1182, 1231, 1288, 1308, 1364, 1422, 1440, 1479, 1518, 1528, 1537, 2071, 3203, 3204, 3213, 3223, 3228, 3235, 3240, 3248
					C	1.601792	-1.167412	-0.014595	
					C	-0.753754	0.001064	0.045387	
					C	-1.604813	-1.163878	0.024937	
					C	-2.900281	-0.730137	-0.050843	
					C	-2.898634	0.737423	-0.080513	
					C	-1.603526	1.168441	-0.019604	
					H	1.054854	-0.638217	1.150626	
					H	1.221730	2.186708	0.173354	
					H	3.726232	1.382423	-0.126879	
					H	3.787304	-1.285020	-0.222830	
					H	1.256866	-2.187601	-0.081404	
					H	-1.271006	-2.190611	0.058418	
					H	-3.784829	-1.351039	-0.088881	
					H	-3.781772	1.357858	-0.144456	
					H	-1.260621	2.191963	-0.026978	
TS S2-S3, (C_1)	ZPE = 0.151413 E(B3LYP) = -386.413417119 E(B3LYP+ZPE) = -386.262004 E_{rel}(B3LYP) = 32.9	A	550.9	3.2760	C	0.681042	-0.906930	-0.834070	700*i*, 130, 164, 184, 382, 402, 470, 538, 566, 604, 639, 656, 710, 733, 739, 771, 813, 839, 861, 870, 910, 941, 953, 959, 994, 1022, 1037, 1090, 1104, 1123, 1140, 1175, 1248, 1296, 1315, 1366, 1397, 1401, 1424, 1558, 1565, 1641, 3163, 3166, 3175, 3183, 3188, 3198, 3203, 3216, 3241
		B	1680.2	1.0741	C	0.708756	-0.491606	1.108579	
		C	1734.4	1.0405	C	1.877412	0.390761	1.097061	
	E(CCSD(T)/6-311G**) = -385.34675049 E(MP2/6-311G**) = -385.16970488 E(MP2/G3large) = -385.39563057 E(G3(MP2,CC) = -385.42126318				C	2.448906	0.574487	-0.122112	
					C	1.882886	-0.284037	-1.133360	
					C	-0.361415	-0.254927	0.108090	
					C	-1.633027	-1.035624	0.251133	
					C	-2.678546	-0.219944	0.031611	
					C	-2.181997	1.133283	-0.265549	
					C	-0.839072	1.135802	-0.220653	
					H	0.367859	-1.816453	-1.331733	
					H	0.596731	-1.291872	1.831561	
					H	2.237508	0.845097	2.013281	
					H	3.295045	1.224329	-0.304344	
					H	2.448454	-0.572731	-2.012730	
					H	-1.661073	-2.089449	0.494486	
					H	-3.724014	-0.497959	0.066756	
					H	-2.815323	1.982672	-0.488123	
					H	-0.174866	1.968773	-0.393539	
TS S3-S4, (C_1)	ZPE = 0.152674 E(B3LYP) = -386.453149516 E(B3LYP+ZPE) = -386.300475 E_{rel}(B3LYP) = 8.8	A	553.3	3.2618	C	-0.837502	1.392028	0.232893	564*i*, 150, 222, 244, 401, 406, 453, 562, 578, 622, 660, 696, 711, 751, 772, 807, 830, 870, 884, 899, 935, 942, 970, 972, 988, 1043, 1070, 1090, 1108, 1159, 1164, 1199, 1234, 1276, 1298, 1358, 1410, 1432, 1462, 1483, 1518, 1623, 3156, 3160, 3181, 3190, 3193, 3207, 3210, 3221, 3244
		B	1541.5	1.1708	C	-0.209392	-0.915365	-0.630832	
		C	1767.3	1.0212	C	-1.568009	-1.260177	-0.514158	
	E(CCSD(T)/6-311G**) = -385.38175919 E(MP2/6-311G**) = -385.20909960 E(MP2/G3large) = -385.43385675 E(G3(MP2,CC) = -385.45384234				C	-2.489076	-0.393605	0.040397	
					C	-2.113885	0.957381	0.354692	
					C	0.269585	0.453378	-0.098056	
					C	0.757692	-0.554392	0.914066	
					C	2.144732	-0.682394	0.762718	
					C	2.585176	0.207573	-0.261080	
					C	1.522358	0.904654	-0.769304	
					H	-0.582206	2.434215	0.384808	
					H	0.461336	-1.467282	-1.274109	

					H	-1.895935	-2.210621	-0.922668	
					H	-3.526939	-0.690095	0.133112	
					H	-2.892467	1.658298	0.637182	
					H	0.147701	-0.918564	1.725089	
					H	2.771834	-1.368675	1.315121	
					H	3.608167	0.289077	-0.605870	
					H	1.538435	1.619158	-1.580690	
TS S3-S11, (C_S), $^2A'$	ZPE = 0.151213 E(B3LYP) = -386.439329224 E(B3LYP+ZPE) = -386.288116 E_{rel}(B3LYP) = 16.5  E(CCSD(T)/6-311G**) = -385.36220796 E(MP2/6-311G**) = -385.17002746 E(MP2/G3large) = -385.39607130 E(G3(MP2,CC) = -385.43703880	A B C	596.2 1805.5 1848.1	3.0268 0.9996 0.9765	C	0.496426	-0.505335	1.218892	483*i*, 97, 113, 174, 320, 339, 415, 428, 511, 598, 625, 660, 676, 706, 738, 742, 815, 828, 872, 889, 891, 968, 979, 986, 994, 1000, 1035, 1097, 1147, 1173, 1187, 1200, 1238, 1286, 1342, 1390, 1455, 1490, 1566, 1590, 1601, 1670, 3084, 3158, 3163, 3163, 3177, 3181, 3187, 3190, 3241
					C	0.496426	-0.505335	-1.218892	
					C	0.496426	-1.888752	-1.209657	
					C	0.477817	-2.592894	0.000000	
					C	0.496426	-1.888752	1.209657	
					C	0.405572	0.236842	0.000000	
					C	0.757350	1.691928	0.000000	
					C	-0.220459	2.605354	0.000000	
					C	-1.594538	2.081437	0.000000	
					C	-1.715431	0.766622	0.000000	
					H	0.529801	0.038959	2.155852	
					H	0.529801	0.038959	-2.155852	
					H	0.531890	-2.430667	-2.148687	
					H	0.485150	-3.676670	0.000000	
					H	0.531890	-2.430667	2.148687	
					H	1.807935	1.962237	0.000000	
					H	-0.026323	3.672144	0.000000	
					H	-2.442271	2.767959	0.000000	
					H	-2.523962	0.051059	0.000000	
TS S4-S6, (C_1)	ZPE = 0.153298 E(B3LYP) = -386.462543601 E(B3LYP+ZPE) = -386.309246 E_{rel}(B3LYP) = 3.3  E(CCSD(T)/6-311G**) = -385.39253640 E(MP2/6-311G**) = -385.22719054 E(MP2/G3large) = -385.45198754 E(G3(MP2,CC) = -385.46403540	A B C	560.7 1484.8 1796.6	3.2189 1.2155 1.0045	C	-0.303340	0.589203	-0.076329	281*i*, 181, 219, 263, 384, 442, 467, 537, 565, 631, 666, 689, 706, 751, 774, 818, 841, 895, 919, 937, 946, 970, 976, 996, 1021, 1055, 1093, 1100, 1107, 1178, 1204, 1208, 1244, 1287, 1341, 1360, 1398, 1433, 1468, 1491, 1528, 1639, 3139, 3143, 3153, 3158, 3167, 3179, 3192, 3209, 3220
					C	-0.611192	-0.633419	0.744483	
					C	-2.083105	-0.787703	0.667262	
					C	-2.602732	0.183585	-0.174521	
					C	-1.584038	1.025483	-0.633911	
					C	0.843914	1.436941	0.167994	
					C	2.100429	0.952437	0.363290	
					C	2.457272	-0.397476	0.041613	
					C	1.557601	-1.264201	-0.514160	
					C	0.145629	-1.038148	-0.511134	
					H	0.670715	2.508294	0.168575	
					H	-0.081980	-0.801693	1.677109	
					H	-2.635869	-1.579055	1.154638	
					H	-3.644114	0.263964	-0.459572	
					H	-1.697948	1.856266	-1.317053	
					H	2.898145	1.643300	0.614147	
					H	3.508446	-0.664758	0.058589	
					H	1.920389	-2.131961	-1.057513	
					H	-0.460418	-1.494566	-1.286445	
TS S4-S10, (C_1)	ZPE = 0.152866 E(B3LYP) = -386.443999677 E(B3LYP+ZPE) = -386.291134	A B	574.3 1488.7	3.1423 1.2123	C	-0.851923	1.407867	0.293337	709*i*, 158, 200, 264, 382, 430, 444, 512, 581, 605, 653, 679,
					C	-0.106375	-0.835023	-0.615359	

	E_{rel}(B3LYP) = 14.7 E(CCSD(T)/6-311G**) = -385.37197297 E(MP2/6-311G**) = -385.19511124 E(MP2/G3large) = -385.42024515 E(G3(MP2,CC) = -385.44424089	C	1797.2	1.0042	C C C C C C C C H H H H H H H H H	-1.537713 -2.463615 -2.125365 0.195253 0.716752 2.105059 2.563430 1.540272 -0.604120 0.415649 -1.829615 -3.499686 -2.901366 0.191342 2.743923 3.608292 1.660923	-1.215858 -0.391812 0.942985 0.580778 -0.999210 -0.785358 0.271264 1.075374 2.429913 -1.205729 -2.178554 -0.709422 1.583668 -1.400769 -1.269571 0.457842 1.986584	-0.533105 0.002254 0.439160 -0.224033 0.669519 0.668252 -0.175245 -0.590199 0.561848 -1.500399 -0.940104 0.057091 0.840266 1.527800 1.398056 -0.387996 -1.164050	694, 714, 742, 799, 821, 857, 901, 933, 954, 978, 993, 998, 1028, 1040, 1104, 1126, 1151, 1173, 1197, 1225, 1272, 1302, 1349, 1375, 1399, 1424, 1472, 1523, 1538, 1657, 3049, 3153, 3160, 3166, 3173, 3178, 3182, 3190, 3203
TS S5-S6, (C_1) 	ZPE = 0.151840 E(B3LYP) = -386.395835285 E(B3LYP+ZPE) = -386.243995 E_{rel}(B3LYP) = 44.2 E(CCSD(T)/6-311G**) = -385.32814648 E(MP2/6-311G**) = -385.14429315 E(MP2/G3large) = -385.36788059 E(G3(MP2,CC) = -385.39989392	A B C	529.7 1557.1 1885.7	3.4070 1.1591 0.9570	C C C C C C C C C C H H H H H H H H	-0.669291 -0.552408 -1.913268 -2.542824 -1.896883 0.635511 1.930141 2.718356 1.910097 0.498872 -0.715915 -0.121080 -2.488752 -3.490841 -2.266073 2.304340 3.798088 2.230628 0.039792	1.179720 -0.863268 -1.132661 -0.148501 1.050610 0.813978 1.107761 -0.102714 -1.146928 -0.643729 1.940936 -1.227842 -1.858667 -0.308222 1.914502 2.012780 -0.149610 -2.142207 -0.867286	0.415261 0.694573 0.407380 -0.412815 -0.420044 -0.108965 0.183337 -0.048346 -0.353826 -0.447046 1.198149 1.622977 0.973915 -0.914573 -0.965971 0.643845 0.032224 -0.632958 -1.414667	762*i*, 147, 186, 293, 338, 364, 468, 545, 579, 648, 658, 702, 726, 768, 793, 830, 842, 879, 908, 919, 935, 957, 963, 1002, 1006, 1023, 1052, 1112, 1128, 1137, 1182, 1220, 1230, 1284, 1319, 1340, 1372, 1385, 1415, 1515, 1534, 1610, 3056, 3069, 3139, 3146, 3155, 3180, 3181, 3200, 3209
TS S6-S12, (C_1) 	ZPE = 0.153322 E(B3LYP) = -386.436500069 E(B3LYP+ZPE) = -386.283178 E_{rel}(B3LYP) = 19.6 E(CCSD(T)/6-311G**) = -385.36538989 E(MP2/6-311G**) = -385.18991376 E(MP2/G3large) = -385.41525111 E(G3(MP2,CC) = -385.43740524	A B C	747.8 1191.6 1560.7	2.4133 1.5145 1.1564	C C C C C C C C C C H	-1.219078 0.311970 -0.834833 -1.919362 -2.166422 0.187750 1.041558 2.078061 1.894758 0.724349 -1.498980	-1.421014 1.447231 1.561268 0.733609 -0.560605 -1.031060 -1.356875 -0.409311 0.584108 0.182751 -2.403982	0.480625 0.392792 -0.474808 -0.566185 0.048941 0.365543 -0.674540 -0.770714 0.227251 1.072366 0.850139	513*i*, 139, 207, 306, 392, 414, 437, 537, 604, 612, 689, 725, 745, 761, 808, 816, 834, 873, 887, 920, 947, 966, 970, 979, 1007, 1054, 1086, 1102, 1153, 1187, 1213, 1255, 1270, 1298, 1339, 1381, 1408, 1422, 1469, 1499, 1550, 1635, 3093, 3120, 3129, 3136, 3145, 3155, 3192, 3209, 3226

					H	0.635218	2.376907	0.851802	
					H	-0.905922	2.499600	-1.019921	
					H	-2.744686	1.109575	-1.165568	
					H	-3.206908	-0.871578	0.092978	
					H	0.851476	-2.142939	-1.394585	
					H	2.844602	-0.389167	-1.533571	
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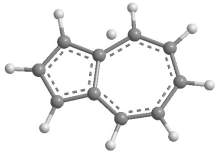
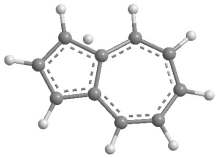
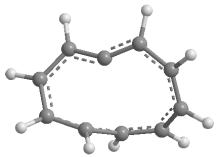
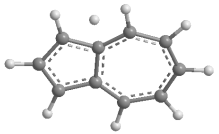
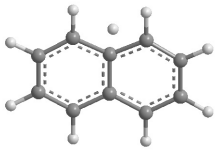
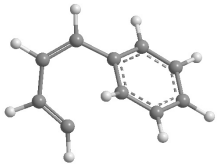
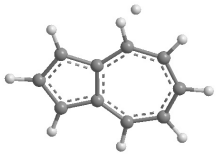
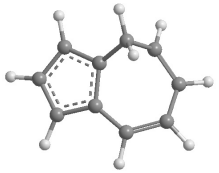
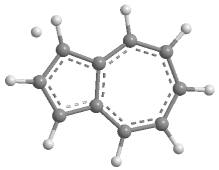
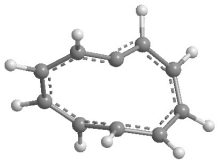
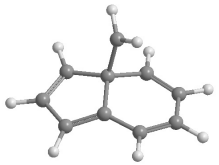
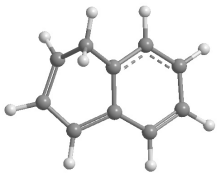
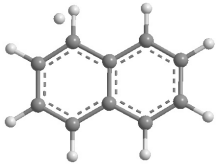
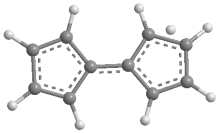
					H	0.778809	0.161305	2.159818	
TS S6-S13, (C_1) 	ZPE = 0.150286 E(B3LYP) = -386.432580104 E(B3LYP+ZPE) = -386.282294 E_{rel}(B3LYP) = 20.2 E(CCSD(T)/6-311G**) = -385.34672944 E(MP2/6-311G**) = -385.16604002 E(MP2/G3large) = -385.39719999 E(G3(MP2,CC) = -385.42760341	A B C	652.7 1479.8 2121.9	2.7650 1.2196 0.8505	C C C C C C C C C C H H H H H H H H	2.742355 1.957357 0.582666 0.566188 1.890567 -0.594937 -0.573238 -1.899100 -1.954441 -2.522839 3.821888 2.296758 2.223070 -0.345840 -0.334809 -2.594175 -2.645431 -3.607300 0.018376	0.012275 -1.122799 -0.708639 0.760671 1.159862 -1.625316 1.632240 1.300081 -1.246677 0.011948 0.032617 -2.149240 2.188532 -2.675028 2.691797 2.134659 -2.081627 0.032106 -1.215695	-0.062571 0.004372 0.045796 0.021849 -0.051233 -0.009577 0.045355 0.018179 -0.073995 -0.048891 -0.111747 0.019698 -0.095760 -0.109993 0.071278 0.032073 -0.142127 -0.086115 1.086988	1709*i*, 141, 175, 284, 329, 387, 415, 486, 565, 573, 648, 672, 692, 725, 755, 771, 826, 842, 851, 896, 905, 927, 942, 975, 1029, 1047, 1071, 1098, 1183, 1223, 1231, 1265, 1277, 1364, 1386, 1408, 1443, 1450, 1484, 1506, 1559, 1623, 2114, 3135, 3145, 3155, 3167, 3182, 3201, 3210, 3227
TS S6-S14, (C_1) 	ZPE = 0.150871 E(B3LYP) = -386.454431580 E(B3LYP+ZPE) = -386.303561 E_{rel}(B3LYP) = 6.9 E(CCSD(T)/6-311G**) = -385.37047492 E(MP2/6-311G**) = -385.21636538 E(MP2/G3large) = -385.44739328 E(G3(MP2,CC) = -385.45063183	A B C	644.4 1483.3 2115.2	2.8006 1.2167 0.8532	C C C C C C C C C C H H H H H H H H	2.735004 0.525636 0.533936 -2.541010 1.954355 -0.595633 -1.923798 1.873387 -0.606743 -1.937522 3.814411 -3.625636 2.271946 -0.341976 -2.611447 2.187673 -0.376452 -2.635699 1.211519	0.055174 -0.697201 0.744712 -0.005838 -1.108707 -1.614550 -1.274789 1.157613 1.617900 1.269763 0.082308 -0.012756 -2.140300 -2.667829 -2.111812 2.193238 2.679139 2.102680 -0.989127	-0.077807 0.078678 0.003409 -0.008367 0.027282 -0.045459 -0.074497 -0.090217 0.032099 0.038248 -0.087421 -0.022041 -0.028680 -0.111538 -0.168554 -0.113905 0.029301 0.060535 1.142081	1222*i*, 121, 188, 311, 335, 391, 419, 498, 573, 596, 657, 673, 707, 754, 765, 772, 818, 863, 895, 912, 916, 933, 974, 977, 1039, 1078, 1108, 1135, 1189, 1212, 1241, 1247, 1274, 1343, 1384, 1413, 1455, 1468, 1473, 1529, 1573, 1602, 2015, 3130, 3134, 3154, 3158, 3170, 3198, 3218, 3236
TS S6-S16,	ZPE = 0.150167	A	733.9	2.4591	C	0.896778	1.637157	0.071082	474*i*, 131, 166, 216, 226, 301,

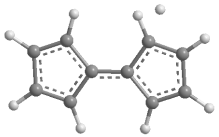
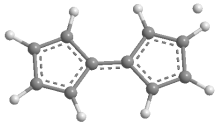
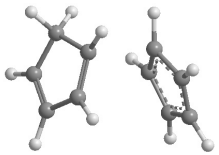
(C_1) 	**E(B3LYP) = -386.384957548** **E(B3LYP+ZPE) = -386.234791** **E_{rel}(B3LYP) = 50.0** **E(CCSD(T)/6-311G**) = -385.30735102** **E(MP2/6-311G**) = -385.11087635** **E(MP2/G3large) = -385.33696979** **E(G3(MP2,CC) = -385.38327746**	**B** **C**	**1453.0** **1928.8**	**1.2421** **0.9357**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.183851** **1.514013** **2.371810** **2.103736** **-0.304930** **-1.645381** **-2.517979** **-2.008871** **-0.686370** **1.032417** **-0.300759** **2.017193** **3.365496** **2.887996** **-1.959674** **-3.567478** **-2.621530** **-0.293591**	**-1.405194** **-1.217261** **-0.366937** **0.922526** **1.083364** **1.233086** **0.230136** **-0.834852** **-1.189801** **2.691054** **-1.941869** **-1.697856** **-0.745701** **1.513108** **2.125379** **0.298573** **-1.141615** **-1.654424**	**-0.563511** **-0.658334** **0.160418** **0.472432** **-0.034530** **-0.486008** **-0.195342** **0.644893** **0.624560** **-0.199431** **-1.377463** **-1.496239** **0.388686** **0.938083** **-1.026277** **-0.459671** **1.488981** **1.529375**	**353, 403, 450, 521, 544, 608, 653, 733, 747, 768, 799, 802, 854, 910, 938, 943, 963, 979, 985, 1000, 1043, 1071, 1153, 1215, 1222, 1262, 1272, 1360, 1391, 1423, 1448, 1492, 1568, 1599, 1661, 1701, 3017, 3098, 3105, 3106, 3124, 3129, 3138, 3151, 3178**
TS S6-AZ, (C_1) 	**ZPE = 0.146814** **E(B3LYP) = -386.428506378** **E(B3LYP+ZPE) = -386.281693** **E_{rel}(B3LYP) = 20.6** **E(CCSD(T)/6-311G**) = -385.34442338** **E(MP2/6-311G**) = -385.15049822** **E(MP2/G3large) = -385.37881817** **E(G3(MP2,CC) = -385.42592933**	**A** **B** **C**	**651.2** **1456.5** **2074.3**	**2.7713** **1.2391** **0.8700**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.572149** **0.556775** **1.906807** **2.507319** **1.924784** **-0.538440** **-1.878614** **-2.695081** **-1.907307** **-0.545346** **0.351401** **0.317926** **2.590866** **3.593870** **2.619012** **-2.218355** **-3.775057** **-2.257140** **-0.640797**	**1.603450** **-1.590091** **-1.264888** **-0.003514** **1.262947** **0.766198** **1.165444** **0.021370** **-1.126582** **-0.736170** **2.668105** **-2.648934** **-2.103275** **-0.010727** **2.097111** **2.190676** **0.029996** **-2.149046** **-0.662892**	**0.007093** **-0.067089** **-0.098101** **-0.021023** **0.031296** **0.004945** **-0.080013** **-0.091626** **-0.005384** **0.080487** **-0.019861** **-0.129764** **-0.186440** **-0.027543** **0.058406** **-0.127644** **-0.160094** **-0.000860** **2.030285**	**756*i*, 158, 175, 285, 333, 349, 402, 414, 430, 502, 576, 607, 670, 712, 736, 748, 779, 799, 830, 870, 914, 942, 958, 961, 988, 1006, 1038, 1064, 1085, 1182, 1239, 1243, 1289, 1314, 1333, 1402, 1424, 1482, 1490, 1516, 1570, 1617, 1632, 3132, 3136, 3143, 3160, 3169, 3199, 3216, 3226**
TS S10-NP, (C_S), ^{2}A'	**ZPE = 0.148688** **E(B3LYP) = -386.474439208** **E(B3LYP+ZPE) = -386.325752** **E_{rel}(B3LYP) = -7.1** **E(CCSD(T)/6-311G**) = -385.39399417** **E(MP2/6-311G**) = -385.20641000** **E(MP2/G3large) = -385.43457678** **E(G3(MP2,CC) = -385.47347295**	**A** **B** **C**	**598.0** **1477.8** **2046.9**	**3.0179** **1.2212** **0.8817**	**H** **C** **C** **C** **C** **C** **C** **C** **C** **C**	**-1.633527** **0.000000** **-0.183554** **-0.286082** **-0.286082** **-0.096411** **-0.096411** **0.238774** **0.238774** **0.312676**	**1.124465** **0.723714** **-0.716756** **-1.386110** **-1.386110** **-0.715634** **-0.715634** **0.664222** **0.664222** **1.360713**	**0.000000** **0.000000** **0.000000** **1.242465** **-1.242465** **2.427539** **-2.427539** **2.427869** **-2.427869** **1.255202**	**1052*i*, 166, 171, 348, 376, 458, 476, 493, 520, 554, 568, 623, 638, 724, 745, 784, 802, 812, 837, 903, 943, 955, 972, 988, 993, 1027, 1036, 1149, 1159, 1176, 1181, 1217, 1265, 1277, 1379, 1383, 1412, 1478, 1485, 1532, 1587, 1637, 1656, 3158, 3160, 3163, 3166, 3177,**

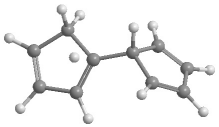
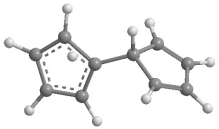
					C	0.312676	1.360713	-1.255202	3178, 3189, 3190
					H	-0.493940	-2.451216	1.244156	
					H	-0.493940	-2.451216	-1.244156	
					H	-0.165906	-1.247625	3.369419	
					H	-0.165906	-1.247625	-3.369419	
					H	0.448313	1.161193	3.368443	
					H	0.448313	1.161193	-3.368443	
					H	0.565211	2.415390	1.248903	
					H	0.565211	2.415390	-1.248903	
TS S11-S10, (C_1)	ZPE = 0.151850 E(B3LYP) = -386.446367013 E(B3LYP+ZPE) = -386.294517 E_{rel}(B3LYP) = 12.5	A B C	655.3 1617.1 2076.7	2.7541 1.1160 0.8690	C	-0.065534	-0.708680	0.302845	375*i*, 105, 150, 231, 292, 395, 414, 437, 515, 538, 618, 644, 703, 732, 751, 769, 818, 836, 863, 891, 939, 954, 974, 986, 999, 1024, 1041, 1089, 1178, 1188, 1196, 1227, 1265, 1328, 1336, 1428, 1455, 1513, 1557, 1593, 1613, 1650, 3048, 3138, 3157, 3162, 3166, 3169, 3179, 3188, 3211
	E(CCSD(T)/6-311G**) = -385.36488105 E(MP2/6-311G**) = -385.16900984 E(MP2/G3large) = -385.39571295 E(G3(MP2,CC) = -385.43973416				C	-1.154740	-1.375372	-0.271270	
					C	-2.355656	-0.714501	-0.506544	
					C	-2.498959	0.633044	-0.145223	
					C	-1.457175	1.300643	0.474192	
					C	-0.219428	0.652807	0.689841	
					C	1.242283	-1.344514	0.406009	
					C	2.396824	-0.711858	0.097878	
					C	2.483919	0.632339	-0.475368	
					C	1.520187	1.540695	-0.457859	
					H	-1.043412	-2.415330	-0.561057	
					H	-3.181583	-1.241984	-0.969825	
					H	-3.440532	1.141340	-0.321562	
					H	-1.587387	2.322988	0.811354	
					H	0.451864	1.053060	1.439262	
					H	1.274949	-2.403658	0.647267	
					H	3.324009	-1.273579	0.151078	
					H	3.412587	0.853677	-1.009466	
					H	1.439176	2.535873	-0.874048	
TS S13-AZ, (C_1)	ZPE = 0.146572 E(B3LYP) = -386.430091537 E(B3LYP+ZPE) = -386.283520 E_{rel}(B3LYP) = 19.4	A B C	662.8 1456.6 2090.9	2.7231 1.2390 0.8632	C	0.518540	1.628084	0.052353	648*i*, 160, 163, 236, 288, 338, 359, 410, 446, 496, 582, 611, 676, 724, 740, 742, 781, 803, 833, 877, 913, 936, 958, 978, 996, 1009, 1016, 1059, 1079, 1184, 1236, 1241, 1299, 1317, 1332, 1417, 1425, 1481, 1482, 1525, 1570, 1607, 1635, 3132, 3138, 3143, 3161, 3170, 3197, 3215, 3224
	E(CCSD(T)/6-311G**) = -385.34482069 E(MP2/6-311G**) = -385.15179967 E(MP2/G3large) = -385.38048758 E(G3(MP2,CC) = -385.42693660				C	0.565316	-1.562642	-0.038014	
					C	1.924553	-1.203513	-0.095734	
					C	2.491155	0.065882	-0.070412	
					C	1.878535	1.320062	0.008051	
					C	-0.574255	0.769943	0.021998	
					C	-1.926072	1.154220	0.025968	
					C	-2.716286	-0.000846	-0.036250	
					C	-1.893165	-1.140779	-0.075605	
					C	-0.557813	-0.726032	-0.042427	
					H	0.276152	2.687300	0.103017	
					H	0.353977	-2.622431	-0.154131	
					H	2.622456	-2.032970	-0.147956	
					H	3.576642	0.086139	-0.115768	
					H	2.553800	2.169772	0.027080	
					H	-2.283371	2.173801	0.060238	
					H	-3.798412	-0.015067	-0.052990	
					H	-2.227598	-2.167990	-0.114662	
					H	0.663317	-2.104830	1.895615	

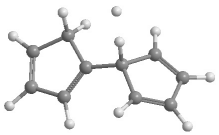
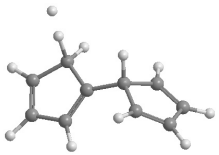
TS S13-S17, (C_1) 	**ZPE = 0.153522** **E(B3LYP) = -386.471646693** **E(B3LYP+ZPE) = -386.318125** **E_{rel}(B3LYP) = -2.3** **E(CCSD(T)/6-311G**) = -385.39644303** **E(MP2/6-311G**) = -385.23131870** **E(MP2/G3large) = -385.45765724** **E(G3(MP2,CC) = -385.46925956**	**A** **B** **C**	**691.6** **1290.1** **1779.4**	**2.6096** **1.3989** **1.0142**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**-0.724482** **-0.576932** **-1.279791** **-2.168475** **-1.986988** **0.428904** **1.768033** **2.548889** **1.762823** **0.431819** **-0.621758** **-0.263930** **-1.264886** **-3.007258** **-2.797104** **2.100972** **3.591352** **2.084273** **-1.044457**	**1.582245** **-1.476988** **-1.255587** **-0.170374** **1.096879** **0.801433** **1.221006** **0.086550** **-1.050105** **-0.638207** **2.649475** **-2.502379** **-2.065154** **-0.332044** **1.813306** **2.249942** **0.105753** **-2.074598** **-1.025417**	**0.337151** **0.890912** **-0.397168** **-0.589519** **-0.055146** **0.259469** **-0.027278** **-0.344116** **-0.233685** **0.198170** **0.509481** **1.070009** **-1.118546** **-1.261031** **-0.142323** **-0.061896** **-0.630119** **-0.362516** **1.764208**	**382*i*, 170, 216, 274, 347, 413, 486, 523, 557, 633, 669, 706, 717, 726, 783, 824, 849, 852, 868, 892, 950, 954, 975, 1024, 1042, 1072, 1108, 1133, 1190, 1201, 1220, 1231, 1258, 1317, 1378, 1399, 1414, 1456, 1476, 1490, 1509, 1594, 3079, 3140, 3150, 3152, 3169, 3174, 3199, 3209, 3224**
TS S14-AZ, (C_1) 	**ZPE = 0.146557** **E(B3LYP) = -386.433673618** **E(B3LYP+ZPE) = -386.287116** **E_{rel}(B3LYP) = 17.2** **E(CCSD(T)/6-311G**) = -385.34850246** **E(MP2/6-311G**) = -385.15360755** **E(MP2/G3large) = -385.38223309** **E(G3(MP2,CC) = -385.43057100**	**A** **B** **C**	**657.1** **1472.3** **2097.4**	**2.7465** **1.2258** **0.8605**	**C** **C** **C** **C** **C** **C** **C** **C** **C** **C** **H** **H** **H** **H** **H** **H** **H** **H**	**0.627037** **0.539912** **1.905252** **2.531300** **1.974613** **-0.497800** **-1.835776** **-2.673033** **-1.900781** **-0.537830** **0.427618** **0.281461** **2.568935** **3.617404** **2.684217** **-2.149535** **-3.754093** **-2.271998** **-2.201382**	**1.597592** **-1.582014** **-1.292643** **-0.046748** **1.231773** **0.784342** **1.223901** **0.108443** **-1.072299** **-0.707280** **2.666419** **-2.637936** **-2.151267** **-0.077140** **2.051987** **2.258125** **0.139452** **-2.078060** **-1.641988**	**0.039532** **-0.071820** **-0.043139** **0.014935** **0.053777** **-0.014036** **-0.038347** **-0.089241** **-0.078206** **-0.057748** **0.070700** **-0.104202** **-0.063563** **0.033159** **0.097960** **-0.016067** **-0.119160** **-0.206953** **2.013872**	**230*i*, 152, 165, 220, 244, 322, 340, 412, 428, 500, 574, 609, 681, 728, 744, 747, 790, 817, 835, 877, 914, 939, 961, 976, 994, 1010, 1027, 1064, 1080, 1183, 1236, 1243, 1290, 1323, 1336, 1419, 1423, 1480, 1487, 1523, 1579, 1625, 1642, 3133, 3136, 3143, 3161, 3170, 3202, 3219, 3230**
TS S16-S10, (C_1)	**ZPE = 0.149786** **E(B3LYP) = -386.391961842** **E(B3LYP+ZPE) = -386.242176** **E_{rel}(B3LYP) = 45.4** **E(CCSD(T)/6-311G**) = -385.31506162** **E(MP2/6-311G**) = -385.10865130** **E(MP2/G3large) = -385.33277096** **E(G3(MP2,CC) = -385.38939528**	**A** **B** **C**	**709.4** **1439.0** **1773.5**	**2.5442** **1.2542** **1.0176**	**C** **C** **C** **C** **C** **C** **C** **C** **C**	**0.744150** **0.162805** **1.530787** **2.392429** **2.009621** **-0.253772** **-0.646379** **-1.868225** **-2.454409**	**1.538491** **-1.113812** **-1.068268** **-0.329984** **0.870361** **1.036767** **-1.327612** **-0.796866** **0.232067**	**-0.304598** **0.645950** **0.769655** **-0.122942** **-0.621151** **0.408020** **-0.603048** **-0.829441** **0.018241**	**794*i*, 136, 163, 227, 264, 345, 346, 393, 425, 478, 532, 615, 645, 702, 739, 767, 797, 821, 864, 875, 916, 935, 948, 962, 976, 992, 1028, 1066, 1151, 1201, 1213, 1244, 1296, 1361, 1386, 1419, 1448, 1461, 1530, 1587, 1608, 1735, 3058, 3082,**

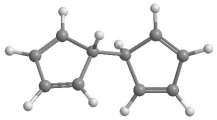
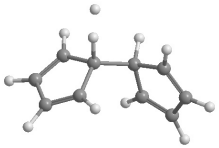
					C	-1.631449	1.093645	0.691159	3113, 3123, 3137, 3140, 3159, 3170, 3171
					H	0.630370	2.546689	-0.710673	
					H	-0.370665	-1.456208	1.534655	
					H	1.969400	-1.418924	1.701741	
					H	3.412658	-0.669271	-0.282200	
					H	2.705430	1.433552	-1.234107	
					H	-0.263906	-2.084034	-1.281875	
					H	-2.450800	-1.173941	-1.665065	
					H	-3.530888	0.278494	0.143396	
					H	-2.014952	1.734923	1.483055	
TS S17-S22, (C_1) 	ZPE = 0.151402 E(B3LYP) = -386.439400956 E(B3LYP+ZPE) = -386.287999 E_{rel}(B3LYP) = 16.6 E(CCSD(T)/6-311G**) = -385.37034682 E(MP2/6-311G**) = -385.18484946 E(MP2/G3large) = -385.40904752 E(G3(MP2,CC) = -385.44314287	A B C	717.5 1251.5 1653.8	2.5153 1.4420 1.0913	C	-1.020924	1.512239	0.297223	227*i*, 160, 198, 262, 351, 395, 413, 525, 539, 558, 562, 585, 655, 701, 721, 744, 807, 821, 862, 872, 928, 948, 955, 967, 984, 1007, 1024, 1081, 1149, 1164, 1182, 1217, 1250, 1317, 1377, 1388, 1432, 1439, 1443, 1539, 1592, 1634, 3145, 3158, 3166, 3180, 3188, 3190, 3201, 3217, 3265
					C	0.058235	-1.368859	1.340989	
					C	-0.901845	-1.212259	-0.614427	
					C	-2.077884	-0.518658	-0.574804	
					C	-2.146251	0.825006	-0.062022	
					C	0.255185	0.877282	0.174100	
					C	1.507173	1.382002	-0.007061	
					C	2.413713	0.296419	-0.356751	
					C	1.742370	-0.874726	-0.402561	
					C	0.325082	-0.632131	0.039787	
					H	-1.078239	2.558574	0.578523	
					H	0.356846	-2.405405	1.426730	
					H	-0.851181	-2.222649	-1.002475	
					H	-2.986821	-0.986623	-0.936318	
					H	-3.113027	1.314486	-0.021589	
					H	1.786099	2.426358	0.051753	
					H	3.471329	0.424554	-0.549951	
					H	2.156166	-1.856883	-0.586992	
					H	-0.670289	-0.970310	2.033483	
TS S23-S24, (C_1) 	ZPE = 0.153754 E(B3LYP) = -386.473893724 E(B3LYP+ZPE) = -386.320140 E_{rel}(B3LYP) = -3.6 E(CCSD(T)/6-311G**) = -385.40042212 E(MP2/6-311G**) = -385.23119718 E(MP2/G3large) = -385.45739788 E(G3(MP2,CC) = -385.47286882	A B C	658.3 1319.1 1817.6	2.7416 1.3682 0.9929	C	-1.252773	1.401847	0.211601	538*i*, 168, 201, 361, 372, 413, 459, 523, 559, 591, 698, 706, 710, 740, 745, 807, 833, 863, 912, 929, 937, 958, 975, 1030, 1068, 1075, 1109, 1142, 1148, 1172, 1204, 1216, 1282, 1323, 1346, 1389, 1437, 1461, 1476, 1534, 1580, 1586, 3073, 3154, 3156, 3160, 3169, 3174, 3178, 3188, 3199
					C	1.343120	-1.304964	0.784058	
					C	-1.034487	-1.382322	-0.191125	
					C	-2.261163	-0.760397	-0.279799	
					C	-2.387593	0.622107	-0.033192	
					C	0.008315	0.822851	0.247241	
					C	1.275682	1.503663	0.056025	
					C	2.219121	0.678417	-0.458542	
					C	1.827569	-0.739401	-0.487757	
					C	0.133035	-0.627337	0.156937	
					H	-1.346574	2.479766	0.299514	
					H	1.247567	-2.386045	0.836573	
					H	-0.954393	-2.457194	-0.314569	
					H	-3.143059	-1.344873	-0.517130	
					H	-3.363699	1.090435	-0.081078	
					H	1.399110	2.569975	0.197855	
					H	3.185876	1.004749	-0.824520	
					H	2.033754	-1.384293	-1.334133	

					H	1.716457	-0.859303	1.704802	
TS S24-NP, (C_1) 	ZPE = 0.148342 E(B3LYP) = -386.484503428 E(B3LYP+ZPE) = -386.336161 E_{rel}(B3LYP) = -13.6 E(CCSD(T)/6-311G**) = -385.40249259 E(MP2/6-311G**) = -385.21710750 E(MP2/G3large) = -385.44683000 E(G3(MP2,CC) = -385.48387309	A B C	603.2 1486.3 2062.4	2.9922 1.2143 0.8751	C C C C C C C C C C H H H H H H H H H	-1.290042 1.253427 -1.237357 -2.437760 -2.464036 -0.035710 1.195175 2.397911 2.430979 -0.011778 -1.307449 1.272031 -1.215993 -3.369923 -3.416244 1.171756 3.327173 3.382405 1.351379	1.402102 -1.355938 -1.394194 -0.723187 0.688400 0.739602 1.449180 0.782533 -0.623417 -0.687789 2.486124 -2.428367 -2.478359 -1.276121 1.206388 2.533084 1.340625 -1.138825 -1.908297	0.046057 -0.042243 -0.068217 -0.046207 0.014100 0.018314 0.023361 -0.046104 -0.102225 -0.035574 0.089980 -0.198449 -0.104629 -0.072520 0.034545 0.065342 -0.064286 -0.163082 1.845530	650*i*, 169, 177, 274, 347, 372, 414, 482, 511, 518, 521, 629, 638, 737, 772, 788, 800, 808, 863, 901, 948, 961, 979, 996, 1003, 1037, 1048, 1145, 1166, 1169, 1185, 1227, 1265, 1285, 1382, 1390, 1416, 1484, 1488, 1544, 1600, 1623, 1661, 3159, 3161, 3164, 3170, 3176, 3179, 3189, 3191
TS S26-S32, (C_1) 	ZPE = 0.149541 E(B3LYP) = -386.442409744 E(B3LYP+ZPE) = -386.292869 E_{rel}(B3LYP) = 13.6 E(CCSD(T)/6-311G**) = -385.36161225 E(MP2/6-311G**) = -385.21105097 E(MP2/G3large) = -385.44217166 E(G3(MP2,CC) = -385.44319194	A B C	421.6 2152.5 2564.9	4.2807 0.8384 0.7036	C C C C C C C C C C H H H H H H H H H	-0.668014 -1.528060 -2.854653 -2.907077 -1.509659 0.755381 1.621986 2.915295 2.906002 1.607861 -1.221307 -1.182185 -3.716447 -3.768127 -2.297446 1.292609 3.805080 3.787526 1.265928	0.019828 1.157935 0.766744 -0.653099 -1.128793 0.009201 1.167646 0.725935 -0.738797 -1.162924 -2.154417 2.178086 1.413642 -1.281218 -1.122240 2.195484 1.340716 -1.364790 -2.187317	-0.030313 0.016261 0.013576 -0.043812 -0.081688 -0.009455 -0.031804 -0.010493 0.028701 0.026544 -0.255513 0.107598 0.084233 -0.221821 0.996420 -0.069181 -0.021619 0.056848 0.057934	1291*i*, 71, 112, 154, 291, 390, 437, 548, 582, 607, 652, 690, 732, 742, 771, 780, 847, 851, 872, 893, 921, 925, 976, 992, 1013, 1048, 1071, 1083, 1100, 1128, 1136, 1229, 1250, 1295, 1325, 1381, 1394, 1428, 1479, 1499, 1538, 1543, 2093, 3198, 3208, 3213, 3222, 3223, 3231, 3236, 3243
TS S26-FL, (C_1)	ZPE = 0.144128 E(B3LYP) = -386.393133136 E(B3LYP+ZPE) = -386.249006 E_{rel}(B3LYP) = 41.1 E(CCSD(T)/6-311G**) = -385.32106594 E(MP2/6-311G**) = -385.14439655 E(MP2/G3large) = -385.37431513 E(G3(MP2,CC) = -385.40685651	A B C	457.0 2091.9 2510.4	3.94868 0.86272 0.71892	C C C C C C C C	-0.657684 -1.527399 -2.811846 -2.830109 -1.553319 0.703256 1.572316 2.854386	-0.033761 -1.215573 -0.792772 0.674321 1.133908 -0.018935 1.166738 0.741988	-0.022987 0.032532 -0.025265 -0.121231 -0.103825 -0.017632 -0.071816 -0.046862	192*i*, 98, 113, 153, 162, 172, 251, 400, 445, 521, 577, 612, 664, 720, 734, 774, 796, 809, 815, 841, 903, 922, 931, 941, 943, 950, 1004, 1028, 1100, 1108, 1111, 1138, 1142, 1238, 1321, 1322, 1380, 1391, 1503, 1533, 1595, 1610, 1683, 3203

					C	2.870184	-0.733787	0.023393	1533, 1595, 1610, 1683, 3203, 3205, 3214, 3217, 3238
					C	1.597496	-1.186118	0.041743	
					H	-1.474412	1.802411	2.209066	
					H	-1.181353	-2.234694	0.111882	
					H	-3.694583	-1.417320	-0.004139	
					H	-3.726073	1.275789	-0.190950	
					H	-1.228778	2.156916	-0.210392	
					H	1.223962	2.187101	-0.116123	
					H	3.738570	1.364461	-0.071293	
					H	3.767471	-1.336925	0.054655	
					H	1.271499	-2.213787	0.089001	
TS S32-FL, (C_1)	ZPE = 0.143951 E(B3LYP) = -386.393043505 E(B3LYP+ZPE) = -386.249092 E_{rel}(B3LYP) = 41.0	A	450.8	4.00380	C	-0.631155	0.023791	-0.047413	197*i*, 93, 102, 125, 157, 161, 255, 400, 445, 526, 579, 609, 660, 718, 722, 776, 796, 809, 818, 841, 902, 922, 930, 938, 942, 948, 1000, 1027, 1100, 1109, 1110, 1138, 1143, 1238, 1321, 1322, 1378, 1391, 1517, 1531, 1597, 1609, 1674, 3203, 3207, 3214, 3218, 3237
	E(CCSD(T)/6-311G**) = -385.32129443 E(MP2/6-311G**) = -385.14570524 E(MP2/G3large) = -385.37574424 E(G3(MP2,CC) = -385.40738243	B	2125.0	0.84927	C	-1.497629	1.212685	-0.029273	
		C	2536.2	0.71159	C	-2.780888	0.794451	-0.074187	
					C	-2.801469	-0.682456	-0.122935	
					C	-1.524473	-1.138539	-0.111973	
					C	0.731004	0.005246	-0.015395	
					C	1.627074	1.169918	0.041611	
					C	2.899037	0.713807	0.057366	
					C	2.880148	-0.762323	0.011449	
					C	1.597121	-1.183682	-0.031915	
					H	-1.202141	-2.167770	-0.146196	
					H	-1.146792	2.232236	0.016645	
					H	-3.663170	1.419679	-0.071956	
					H	-3.696895	-1.282456	-0.205854	
					H	-3.394168	-1.041868	2.238169	
					H	1.303512	2.199165	0.065638	
					H	3.797236	1.315101	0.096998	
					H	3.762638	-1.387678	0.013384	
					H	1.247161	-2.203787	-0.070839	
TS A1, (C_1)	ZPE = 0.173197 E(B3LYP) = -387.650214538 E(B3LYP+ZPE) = -387.477017	A	702.7	2.56820	H	2.835068	-1.375705	-0.599247	457*i*, 35, 92, 126, 170, 204, 358, 504, 563, 574, 673, 706, 724, 754, 787, 801, 805, 824, 849, 887, 891, 907, 930, 952, 957, 964, 981, 1014, 1045, 1057, 1091, 1097, 1115, 1134, 1143, 1278, 1282, 1303, 1311, 1371, 1401, 1423, 1439, 1468, 1542, 1567, 2991, 3072, 3182, 3192, 3194, 3198, 3203, 3217, 3219, 3228, 3229
	E(CCSD(T)/6-311G**) = -386.56589535 E(MP2/6-311G**) = -386.38521542 E(MP2/G3large) = -386.61359376 E(G3(MP2,CC) = -386.62107668	B	1763.0	1.02368	H	1.581035	-0.882035	-1.723869	
		C	1802.2	1.00140	C	1.783121	1.077281	0.773027	
					C	2.327312	0.701851	-0.418568	
					C	1.953900	-0.725247	-0.708509	
					C	0.959497	-1.045786	0.394065	
					C	1.009069	0.002646	1.312591	
					H	1.910395	2.041589	1.247883	
					H	2.942841	1.311301	-1.065978	
					H	0.736225	-2.065544	0.676502	
					H	0.489304	0.025133	2.259644	
					C	-1.014047	-0.924184	-0.616802	
					C	-1.059590	0.371166	-1.246745	
					C	-1.885949	1.171393	-0.502384	
					C	-2.433220	0.389325	0.603058	
					C	-1.941429	-0.876255	0.519931	
					H	-0.524077	0.654610	-2.140900	

					H	-2.114211	2.211192	-0.697486	
					H	-3.115179	0.767527	1.352845	
					H	-2.151907	-1.703840	1.183010	
					H	-0.781473	-1.837359	-1.150381	
TS A1-A2, (C_1) 	ZPE = 0.167151 E(B3LYP) = -387.604456430 E(B3LYP+ZPE) = -387.437305 E(CCSD(T)/6-311G**) = -386.53011712 E(MP2/6-311G**) = -386.37012700 E(MP2/G3large) = -386.59754372 E(G3(MP2,CC) = -386.59038284	A B C	520.6 2123.0 2313.5	3.46638 0.85010 0.78010	H H C C C C C H H H H C C C C C H H H H H	-1.925477 -1.489843 -2.579633 -2.943587 -1.749839 -0.651139 -1.164519 -3.224032 -3.929012 -1.037903 -0.611594 0.790681 1.501422 2.636658 2.762393 1.700934 1.126984 3.356590 3.591945 1.500746 0.821369	1.269233 1.973563 -0.819536 0.378782 1.027794 0.001103 -1.050817 -1.518877 0.822865 -1.055619 -1.929895 0.270915 1.189357 0.603198 -0.717227 -0.932917 2.162578 1.024415 -1.394985 -1.807096 0.749908	1.523348 -0.026236 -0.672267 -0.175135 0.468118 0.293037 -0.399443 -1.189293 -0.207199 2.209159 -0.702909 0.645947 -0.334093 -0.750715 -0.118373 0.677837 -0.620153 -1.441077 -0.275184 1.281686 1.638384	268*i*, 70, 99, 143, 251, 301, 329, 354, 384, 424, 527, 568, 673, 693, 723, 794, 814, 825, 830, 877, 907, 917, 933, 952, 957, 961, 962, 1008, 1019, 1035, 1109, 1115, 1121, 1132, 1149, 1210, 1252, 1269, 1307, 1324, 1387, 1396, 1414, 1544, 1556, 1628, 1642, 2970, 3017, 3046, 3187, 3193, 3198, 3209, 3218, 3222, 3224
TS A2-S0, (C_1) 	ZPE = 0.162232 E(B3LYP) = -387.056619310 E(B3LYP+ZPE) = -386.894387 E(CCSD(T)/6-311G**) = -385.98361162 E(MP2/6-311G**) = -385.85780459 E(MP2/G3large) = -386.08637426 E(G3(MP2,CC) = -386.04994929	A B C	491.3 2134.2 2242.8	3.67320 0.84565 0.80469	H H C C C C C H H H C C C C C H H H H H	1.376666 1.753454 2.538855 2.953526 1.838813 0.674363 1.175495 3.192900 3.962364 0.587655 -0.765360 -1.454994 -2.603980 -2.757584 -1.700080 -1.049099 -3.314864 -3.600641 -1.516299 -0.786458	-0.174794 -1.990623 0.883219 -0.353317 -0.981353 -0.060338 1.071663 1.614829 -0.739254 1.941910 -0.453533 -1.032655 -0.371667 0.684533 0.665167 -1.853517 -0.568962 1.361434 1.317529 -1.218877	1.422332 0.866836 -0.606933 -0.095925 0.488867 0.317419 -0.362694 -1.063616 -0.086751 -0.615636 0.556502 -0.663881 -0.881594 0.130632 0.959466 -1.238576 -1.673795 0.186146 1.802231 1.349673	1212*i*, 61, 100, 130, 296, 354, 397, 554, 603, 677, 678, 725, 757, 787, 810, 813, 839, 858, 898, 909, 939, 951, 954, 959, 1006, 1037, 1065, 1071, 1102, 1112, 1126, 1156, 1205, 1239, 1277, 1303, 1312, 1355, 1397, 1456, 1491, 1515, 1560, 1643, 2062, 2973, 3189, 3196, 3199, 3213, 3219, 3225, 3225, 3232
TS A2-S26, (C_1)	ZPE = 0.164944 E(B3LYP) = -387.603556691 E(B3LYP+ZPE) = -387.438612	A B	521.0 2151.6	3.46371 0.83880	H H	1.773132 1.442213	-1.568676 -1.918845	1.212207 -0.476054	328*i*, 52, 99, 149, 160, 166, 258, 357, 387, 413, 529, 567,

	E(CCSD(T)/6-311G**) = -386.52758704 E(MP2/6-311G**) = -386.36901871 E(MP2/G3large) = -386.59689083 E(G3(MP2,CC) = -386.59051517	C	2414.2	0.74755	C	2.725778	0.880874	-0.402993	669, 693, 724, 797, 811, 826, 826, 877, 909, 920, 942, 951, 954, 958, 959, 1008, 1016, 1040, 1106, 1113, 1120, 1125, 1154, 1196, 1257, 1266, 1307, 1323, 1383, 1398, 1417, 1553, 1565, 1636, 1649, 2317, 3013, 3037, 3189, 3191, 3199, 3207, 3220, 3221, 3225
					C	2.979687	-0.421987	-0.181773	
					C	1.701171	-1.108279	0.217562	
					C	0.678453	0.005223	0.191881	
					C	1.304069	1.147676	-0.168051	
					H	3.445899	1.630180	-0.706329	
					H	3.933376	-0.923806	-0.270539	
					H	0.835643	2.116709	-0.278182	
					C	-0.764506	-0.197989	0.533075	
					C	-1.536013	-1.146430	-0.360705	
					C	-2.690384	-0.564135	-0.729487	
					C	-2.763386	0.782093	-0.146398	
					C	-1.649870	1.018908	0.570139	
					H	-1.189840	-2.135717	-0.625175	
					H	-3.456423	-1.004499	-1.355043	
					H	-3.595075	1.462447	-0.278193	
					H	-1.411658	1.913116	1.129020	
					H	-0.809297	-0.656697	1.574567	
					H	-0.877957	-1.289944	2.934224	
TS A2-S1, (C_1) 	ZPE = 0.163497 E(B3LYP) = -387.599881579 E(B3LYP+ZPE) = -387.436385 E(CCSD(T)/6-311G**) = -386.51966409 E(MP2/6-311G**) = -386.35818056 E(MP2/G3large) = -386.58630035 E(G3(MP2,CC) = -386.58428687	A B C	523.0 2157.1 2377.0	3.45064 0.83666 0.75925	H	1.910318	-1.337545	1.364605	942*i*, 48, 92, 141, 209, 235, 310, 369, 394, 523, 541, 578, 673, 703, 723, 793, 813, 818, 829, 874, 906, 938, 940, 946, 953, 961, 970, 1008, 1013, 1035, 1100, 1110, 1117, 1120, 1150, 1209, 1250, 1263, 1298, 1307, 1322, 1381, 1398, 1519, 1557, 1568, 1637, 1645, 2951, 3078, 3187, 3194, 3198, 3211, 3217, 3223, 3225
					H	1.523679	-1.994516	-0.251901	
					C	2.598722	0.979219	-0.503378	
					C	2.943680	-0.303029	-0.268454	
					C	1.736396	-1.029914	0.216872	
					C	0.635179	-0.011383	0.188323	
					C	1.169777	1.161727	-0.218524	
					H	3.258144	1.765033	-0.849069	
					H	3.921574	-0.749320	-0.379717	
					H	0.634923	2.095657	-0.327787	
					C	-0.788761	-0.323487	0.566743	
					C	-1.551704	-1.127644	-0.472394	
					C	-2.706304	-0.503557	-0.759629	
					C	-2.798090	0.734388	0.026621	
					C	-1.695746	0.863655	0.785032	
					H	-1.191551	-2.057455	-0.890602	
					H	-3.460900	-0.844855	-1.456973	
					H	-3.634691	1.420749	-0.006824	
					H	-1.468209	1.664425	1.475195	
					H	-0.775229	-0.915324	1.498890	
					H	2.023056	-1.686701	2.456907	
TS S0$_{cis}$-S0$_{trans}$, (C_2), ^{1}A	ZPE = 0.165709 E(B3LYP) = -387.090674422 E(B3LYP+ZPE) = -386.924966 E(CCSD(T)/6-311G**) = -386.02273688 E(MP2/6-311G**) = -385.88824609 E(MP2/G3large) = -386.11412263 E(G3(MP2,CC) = -386.08290442	A B C	485.3 2081.8 2333.9	3.71856 0.86691 0.77326	C	0.378852	0.689362	-0.423599	76*i*, 106, 127, 241, 307, 395, 549, 557, 623, 693, 722, 729, 774, 813, 817, 827, 846, 895, 922, 954, 954, 956, 957, 995, 1007, 1017, 1047, 1062, 1109, 1112, 1127, 1151, 1183, 1189, 1270, 1271, 1311, 1312, 1396,
					C	0.702059	1.294205	0.923840	
					C	0.275181	2.568413	0.959640	
					C	-0.378852	2.896795	-0.315864	
					C	-0.338689	1.821794	-1.121471	
					C	-0.378852	-0.689362	-0.423599	
					C	-0.702059	-1.294205	0.923840	

					C	-0.275181	-2.568413	0.959640	1397, 1558, 1558, 1641, 1642, 2989, 2993, 3186, 3186, 3196, 3196, 3212, 3213, 3223, 3225
					C	0.378852	-2.896795	-0.315864	
					C	0.338689	-1.821794	-1.121471	
					H	1.336366	0.533743	-0.942536	
					H	1.227569	0.760194	1.703037	
					H	0.393498	3.259935	1.784195	
					H	-0.812804	3.859769	-0.553388	
					H	-0.732805	1.746637	-2.126586	
					H	-1.227569	-0.760194	1.703037	
					H	-0.393498	-3.259935	1.784195	
					H	0.812804	-3.859769	-0.553388	
					H	0.732805	-1.746637	-2.126586	
					H	-1.336366	-0.533743	-0.942536	
TS S0$_{cis}$-S1, (C_1) 	ZPE = 0.164454 E(B3LYP) = -387.597617931 E(B3LYP+ZPE) = -387.433164 E(CCSD(T)/6-311G**) = -386.52143757 E(MP2/6-311G**) = -386.38541349 E(MP2/G3large) = -386.61237285 E(G3(MP2,CC) = -386.58394292	A	588.4	3.06725	C	0.736948	0.326173	-0.731440	596*i*, 78, 98, 133, 216, 237, 271, 326, 399, 550, 563, 656, 691, 722, 730, 785, 804, 816, 826, 856, 880, 925, 950, 953, 956, 958, 998, 1005, 1026, 1043, 1076, 1107, 1111, 1121, 1131, 1180, 1210, 1263, 1287, 1312, 1315, 1398, 1399, 1544, 1553, 1628, 1640, 1820, 2980, 3187, 3189, 3198, 3200, 3216, 3217, 3226, 3229
		B	1978.2	0.91230	C	1.151566	-1.116133	-0.550321	
		C	2000.6	0.90209	C	2.296243	-1.165546	0.153608	
					C	2.709742	0.199860	0.505170	
					C	1.813630	1.075715	0.016571	
					C	-0.705285	0.635674	-0.284462	
					C	-1.073003	0.345111	1.141002	
					C	-2.254113	-0.301318	1.165614	
					C	-2.720025	-0.512074	-0.212351	
					C	-1.819778	0.006973	-1.069356	
					H	0.811603	0.584100	-1.799955	
					H	0.588128	-1.949828	-0.945240	
					H	2.840046	-2.060644	0.427582	
					H	3.602632	0.444850	1.066426	
					H	1.838543	2.153425	0.106710	
					H	-0.468028	0.640354	1.986274	
					H	-2.788394	-0.624769	2.049690	
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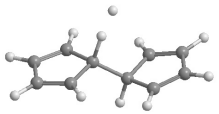
					H	-1.877080	0.020601	-2.149427	
					H	-0.833662	1.790053	-0.426500	
					H	-0.882564	3.039628	-0.641340	
TS S0$_{trans}$-S1, (C_1) 	ZPE = 0.164092 E(B3LYP) = -387.597009296 E(B3LYP+ZPE) = -387.432917 E(CCSD(T)/6-311G**) = -386.51974400 E(MP2/6-311G**) = -386.38295474 E(MP2/G3large) = -386.60992400 E(G3(MP2,CC) = -386.58262126	A	490.7	3.67815	C	0.668326	0.000016	-0.498851	763*i*, 75, 101, 166, 184, 239, 264, 365, 399, 556, 573, 590, 691, 718, 726, 762, 811, 817, 818, 854, 918, 929, 948, 952, 956, 958, 1004, 1011, 1023, 1056, 1085, 1107, 1120, 1124, 1158, 1175, 1190, 1245, 1271, 1311, 1315, 1397, 1404, 1536, 1556, 1626, 1642, 1647, 2976, 3188, 3191, 3199, 3202, 3219, 3224, 3225, 3230
		B	2094.1	0.86183	C	1.574328	-1.178647	-0.226928	
		C	2456.7	0.73461	C	2.795729	-0.734454	0.117480	
					C	2.795728	0.734466	0.117506	
					C	1.574327	1.178671	-0.226885	
					C	-0.654472	-0.000001	0.295493	
					C	-1.565799	-1.177189	0.113193	
					C	-2.820333	-0.734325	-0.099721	
					C	-2.820331	0.734346	-0.099683	
					C	-1.565796	1.177196	0.113253	
					H	0.396524	0.000035	-1.566977	
					H	1.265057	-2.209902	-0.324446	
					H	3.655564	-1.347806	0.355110	

H	**3.655562**	**1.347811**	**0.355159**
H	**1.265054**	**2.209929**	**-0.324364**
H	**-1.244011**	**-2.206674**	**0.180676**
H	**-3.700221**	**-1.348483**	**-0.242407**
H	**-3.700218**	**1.348513**	**-0.242340**
H	**-1.244006**	**2.206678**	**0.180786**
H	**-0.331764**	**-0.000041**	**1.434914**
H	**0.092218**	**-0.000538**	**2.564749**

TABLE S2. RRKM and TST calculated high-pressure limit thermal rate constants (in units of s^{-1} and $cm^3\ s^{-1}\ mol^{-1}$ for unimolecular and bimolecular steps, respectively) for all studied reactions within the 300-3000K temperature range.

Reaction	Deg*	Temperature, K								
		300	500	600	700	800	900	1000	1100	1200
S1 → S2	2	7.45E2	4.25E6	3.72E7	1.76E8	5.66E8	1.4E9	2.9E9	5.23E9	8.67E9
S2 → S1	2	4.16E10	5.43E11	1.05E12	1.7E12	2.42E12	3.2E12	4.01E12	4.81E12	5.63E12
S1 → S5	2	1.1E-9	2.47E-1	3.01E1	9.34E2	1.23E4	9.17E4	4.55E5	1.69E6	5.08E6
S5 → S1	1	4.11E8	2.58E10	7.49E10	1.61E11	2.9E11	4.59E11	6.61E11	8.93E11	1.15E12
S1 → S26	2	3.16E-2	2.22E4	6.59E5	7.57E6	4.76E7	2.0E8	6.34E8	1.64E9	3.65E9
S26 → S1	2	5.95E-11	2.06E-1	5.22E1	2.78E3	5.51E4	5.72E5	3.74E6	1.75E7	6.34E7
S2 → S3	1	2.93E-3	5.39E3	2.07E5	2.83E6	2.02E7	9.36E7	3.19E8	8.74E8	2.02E9
S3 → S2	1	7.4E-14	1.72E-3	7.07E-1	5.25E1	1.34E3	1.68E4	1.27E5	6.71E5	2.68E6
S3 → S4	4	1.11E2	2.57E6	3.26E7	2.0E8	7.86E8	2.3E9	5.41E9	1.1E10	1.97E10
S4 → S3	1	4.41E7	6.0E9	2.1E10	5.19E10	1.03E11	1.76E11	2.7E11	3.88E11	5.19E11
S3 → S11	2	4.81E-6	2.04E2	1.71E4	4.1E5	4.48E6	2.87E7	1.28E8	4.34E8	1.2E9
S11 → S3	2	7.23E7	2.7E9	6.79E9	1.34E10	2.24E10	3.34E10	4.65E10	6.05E10	7.6E10
S4 → S6	1	1.3E12	2.59E12	3.08E12	3.51E12	3.86E12	4.15E12	4.42E12	4.66E12	4.85E12
S6 → S4	1	1.46E2	2.17E6	2.43E7	1.39E8	5.13E8	1.42E9	3.22E9	6.32E9	1.11E10
S4 → S10	1	1.96E3	1.48E7	1.41E8	7.03E8	2.37E9	6.06E9	1.29E10	2.41E10	4.04E10
S10 → S4	2	3.34E-15	4.0E-4	2.45E-1	2.43E1	7.74E2	1.14E4	9.89E4	5.79E5	2.53E6
S5 → S6	1	4.72E-3	6.81E3	2.46E5	3.21E6	2.23E7	1.01E8	3.38E8	9.13E8	2.08E9
S6 → S5	1	1.48E-27	1.01E-11	9.52E-8	6.71E-5	9.29E-3	4.33E-1	9.33E0	1.17E2	9.48E2

S6 → S12	1	1.3E-10	1.29E-1	2.33E1	9.64E2	1.59E4	1.4E5	7.99E5	3.34E6	1.09E7
S12 → S6	1	3.32E10	3.46E11	6.36E11	9.91E11	1.39E12	1.81E12	2.23E12	2.66E12	3.08E12
S6 → S13	1	2.38E-14	1.09E-3	5.18E-1	4.3E1	1.2E3	1.61E4	1.29E5	7.16E5	2.99E6
S13 → S6	2	1.45E-14	7.3E-4	3.58E-1	3.04E1	8.59E2	1.18E4	9.59E4	5.36E5	2.28E6
S6 → S14	1	4.62E-4	1.46E3	6.33E4	9.52E5	7.36E6	3.62E7	1.3E8	3.74E8	9.04E8
S14 → S6	2	1.38E-9	7.6E-1	1.19E2	4.42E3	6.74E4	5.62E5	3.1E6	1.25E7	4.05E7
S6 → AZ + H	1	1.78E-15	3.21E-4	2.28E-1	2.57E1	9.09E2	1.48E4	1.39E5	8.79E5	4.1E6
AZ + H → S6	--	2.54E-16	2.74E-14	9.63E-14	2.44E-13	5.08E-13	9.14E-13	1.49E-12	2.26E-12	3.23E-12
S10 → NP + H	1	1.77E2	3.68E6	4.7E7	3.0E8	1.23E9	3.73E9	9.08E9	1.91E10	3.56E10
NP + H → S10	--	9.67E-20	2.66E-16	2.09E-15	9.39E-15	3E-14	7.56E-14	1.61E-13	3.03E-13	5.23E-13
S11 → S10	4	3.12E9	1.73E10	3.19E10	5.0E10	7.01E10	9.11E10	1.13E11	1.35E11	1.56E11
S10 → S11	2	1.68E-13	8.92E-3	4.51E0	3.93E2	1.13E4	1.54E5	1.25E6	6.97E6	2.91E7
S13 → S17	1	1.34E4	2.36E7	1.57E8	6.11E8	1.7E9	3.8E9	7.22E9	1.22E10	1.9E10
S17 → S13	1	3.94E8	2.46E10	7.03E10	1.49E11	2.59E11	4.04E11	5.74E11	7.62E11	9.64E11
S13 → AZ + H	2	4.07E-15	5.77E-4	3.9E-1	4.24E1	1.46E3	2.33E4	2.16E5	1.35E6	6.26E6
AZ + H → S13	--	9.55E-16	7.32E-14	2.38E-13	5.71E-13	1.13E-12	1.97E-12	3.12E-12	4.62E-12	6.48E-12
S14 → AZ + H	2	7.33E-19	4.75E-6	8.13E-3	1.69E0	9.48E1	2.2E3	2.74E4	2.18E5	1.23E6
AZ + H → S14	--	3.42E-14	7.62E-13	1.8E-12	3.42E-12	5.7E-12	8.63E-12	1.22E-11	1.65E-11	2.14E-11
S17 → S22	1	5.33E-4	2.85E3	1.45E5	2.43E6	2.02E7	1.06E8	4.0E8	1.19E9	2.93E9
S22 → S17	1	4.77E11	1.05E12	1.28E12	1.48E12	1.65E12	1.8E12	1.93E12	2.05E12	2.15E12
S17 → S23	1	5.33E-4	2.85E3	1.45E5	2.43E6	2.02E7	1.06E8	4.0E8	1.19E9	2.93E9
S23 → S17	1	7.19E-5	8.86E2	5.55E4	1.08E6	1.02E7	5.8E7	2.35E8	7.41E8	1.92E9

S23 → S24	1	2.66E9	7.32E10	1.71E11	3.12E11	4.91E11	7.01E11	9.29E11	1.18E12	1.42E12
S24 → S23	1	1.96E-16	4.15E-5	2.95E-2	3.25E0	1.11E2	1.76E3	1.6E4	9.76E4	4.41E5
S24 → NP + H	2	7.78E-11	2.14E-1	5.35E1	2.86E3	5.78E4	6.08E5	4.05E6	1.91E7	7.06E7
NP + H → S24	--	4.61E-15	2.24E-13	6.46E-13	1.42E-12	2.65E-12	4.35E-12	6.66E-12	9.48E-12	1.29E-11
S26 → S32	2	1.26E-8	4.06E0	5.62E2	1.93E4	2.76E5	2.21E6	1.18E7	4.66E7	1.46E8
S32 → S26	2	2.33E-6	8.41E1	6.7E3	1.55E5	1.65E6	1.04E7	4.6E7	1.56E8	4.34E8
S26 → FL + H	2	3.32E-25	1.47E-9	1.33E-5	9.22E-3	1.27E0	6.02E1	1.33E3	1.67E4	1.4E5
FL + H → S26	--	3.16E-11	7.96E-11	1.09E-10	1.41E-10	1.76E-10	2.13E-10	2.53E-10	2.93E-10	3.38E-10
S32 → FL + H	2	1.41E-22	6.02E-8	3.02E-4	1.38E-1	1.38E1	5.06E2	9.14E3	9.86E4	7.2E5
FL + H → S32	--	7.43E-11	1.59E-10	2.09E-10	2.64E-10	3.22E-10	3.84E-10	4.5E-10	5.19E-10	5.92E-10
c-C_5H_5 + c-C_5H_6 → A1	--	1.38E-21	5.26E-19	2.66E-18	9.08E-18	2.38E-17	5.26E-17	1.02E-16	1.81E-16	2.99E-16
A1 → c-C_5H_5 + c-C_5H_6	1	6.31E-4	3.34E3	1.7E5	2.85E6	2.41E7	1.27E8	4.82E8	1.44E9	3.6E9
A1 → A2 + H	1	2.42E-18	7.23E-6	1.04E-2	1.96E0	1.02E2	2.23E3	2.68E4	2.05E5	1.13E6
A2 + H → A1	--	2.76E-13	1.29E-12	2.03E-12	2.92E-12	3.95E-12	5.05E-12	6.33E-12	7.61E-12	9.05E-12
A2 → S0$_{cis}$	1	8.8E-8	7.56E0	7.48E2	2.02E4	2.44E5	1.69E6	8.07E6	2.9E7	8.44E7
S0$_{cis}$ → A2	4	8.6E-6	2.76E2	2.14E4	4.84E5	5.12E6	3.22E7	1.41E8	4.76E8	1.31E9
A2 + H → S1 + H_2	--	1.51E-15	7.07E-14	2.03E-13	4.51E-13	8.54E-13	1.44E-12	2.24E-12	3.27E-12	4.56E-12
S1 + H_2→ A1 + H	--	1.92E-33	3.99E-25	5.04E-23	1.67E-21	2.41E-20	1.98E-19	1.09E-18	4.49E-18	1.51E-17
A2 + H → S26 + H_2	--	9.07E-13	4.8E-12	7.9E-12	1.17E-11	1.63E-11	2.15E-11	2.73E-11	3.36E-11	4.06E-11
S26 + H_2→ A2 + H	--	2.61E-39	2.84E-28	1.72E-25	1.75E-23	5.78E-22	9.03E-21	8.33E-20	5.23E-19	2.46E-18
S0$_{cis}$ → S0$_{trans}$	2	6.5E8	2.3E10	5.6E10	1.06E11	1.72E11	2.48E11	3.34E11	4.28E11	5.26E11
S0$_{trans}$ → S0$_{cis}$	2	4.6E8	1.87E10	4.74E10	9.18E10	1.52E11	2.24E11	3.06E11	3.92E11	4.88E11

$S0_{cis}$ + H → S1 + H_2	--	2.39E-14	5.42E-13	1.31E-12	2.53E-12	4.32E-12	6.69E-12	9.71E-12	1.34E-11	1.78E-11
S1 + H_2 → $S0_{cis}$ + H	--	6.25E-34	1.7E-25	2.29E-23	7.91E-22	1.17E-20	9.7E-20	5.43E-19	2.27E-18	7.63E-18
$S0_{trans}$+H → S1+H_2	--	8.43E-15	2.82E-13	7.49E-13	1.57E-12	2.84E-12	4.61E-12	6.92E-12	9.86E-12	1.35E-11
S1+H_2 → $S0_{trans}$ + H	--	1.56E-34	7.13E-26	1.1E-23	4.18E-22	6.66E-21	5.89E-20	3.45E-19	1.5E-18	5.23E-18

TABLE S2. Continued.

Reaction	Deg*	Temperature, K										
		1300	**1400**	**1500**	**1700**	**1900**	**2000**	**2200**	**2400**	**2600**	**2800**	**3000**
S1 → S2	2	1.31E10	1.89E10	2.57E10	4.31E10	6.46E10	7.67E10	1.03E11	1.33E11	1.64E11	1.97E11	2.3E11
S2 → S1	2	6.38E12	7.18E12	7.91E12	9.29E12	1.05E13	1.11E13	1.22E13	1.32E13	1.41E13	1.49E13	1.57E13
S1 → S5	2	1.28E7	2.84E7	5.64E7	1.75E8	4.3E8	6.31E8	1.22E9	2.12E9	3.36E9	5.01E9	7.08E9
S5 → S1	1	1.42E12	1.71E12	2.0E12	2.6E12	3.21E12	3.5E12	4.09E12	4.64E12	5.14E12	5.64E12	6.13E12
S1 → S26	2	7.15E9	1.28E10	2.12E10	4.88E10	9.49E10	1.26E11	2.05E11	3.1E11	4.4E11	5.91E11	7.67E11
S26 → S1	2	1.9E8	4.86E8	1.1E9	4.21E9	1.23E10	1.94E10	4.25E10	8.25E10	1.44E11	2.32E11	3.51E11
S2 → S3	1	4.11E9	7.61E9	1.29E10	3.09E10	6.15E10	8.27E10	1.37E11	2.1E11	3.0E11	4.07E11	5.31E11
S3 → S2	1	8.66E6	2.38E7	5.7E7	2.4E8	7.47E8	1.22E9	2.8E9	5.64E9	1.02E10	1.69E10	2.61E10
S3 → S4	4	3.25E10	4.97E10	7.2E10	1.32E11	2.14E11	2.64E11	3.77E11	5.04E11	6.52E11	8.08E11	9.7E11
S4 → S3	1	6.68E11	8.32E11	1.0E12	1.36E12	1.74E12	1.94E12	2.32E12	2.69E12	3.06E12	3.43E12	3.74E12
S3 → S11	2	2.86E9	5.98E9	1.14E10	3.28E10	7.56E10	1.08E11	1.99E11	3.33E11	5.14E11	7.49E11	1.03E12
S11 → S3	2	9.23E10	1.08E11	1.25E11	1.59E11	1.92E11	2.08E11	2.39E11	2.68E11	2.95E11	3.23E11	3.46E11

S4 → S6	1	5.01E12	5.19E12	5.33E12	5.54E12	5.73E12	5.83E12	5.98E12	6.11E12	6.21E12	6.33E12	6.38E12
S6 → S4	1	1.77E10	2.67E10	3.81E10	6.81E10	1.08E11	1.31E11	1.84E11	2.43E11	3.08E11	3.78E11	4.51E11
S4 → S10	1	6.25E10	9.1E10	1.27E11	2.15E11	3.31E11	3.96E11	5.42E11	7.04E11	8.74E11	1.06E12	1.25E12
S10 → S4	2	8.84E6	2.57E7	6.55E7	3.02E8	1.01E9	1.69E9	4.1E9	8.59E9	1.6E10	2.75E10	4.36E10
S5 → S6	1	4.2E9	7.66E9	1.29E10	3.06E10	6.04E10	8.04E10	1.33E11	2.01E11	2.86E11	3.89E11	5.06E11
S6 → S5	1	5.63E3	2.59E4	9.81E4	8.71E5	4.88E6	1.02E7	3.62E7	1.04E8	2.54E8	5.49E8	1.07E9
S6 → S12	1	3.01E7	7.13E7	1.52E8	5.21E8	1.39E9	2.1E9	4.28E9	7.77E9	1.29E10	1.99E10	2.9E10
S12 → S6	1	3.49E12	3.89E12	4.27E12	4.97E12	5.6E12	5.9E12	6.43E12	6.94E12	7.41E12	7.84E12	8.17E12
S6 → S13	1	1.01E7	2.85E7	7.09E7	3.16E8	1.04E9	1.71E9	4.11E9	8.53E9	1.58E10	2.69E10	4.28E10
S13 → S6	2	7.73E6	2.21E7	5.51E7	2.48E8	8.22E8	1.37E9	3.29E9	6.92E9	1.29E10	2.2E10	3.52E10
S6 → S14	1	1.91E9	3.62E9	6.37E9	1.61E10	3.36E10	4.59E10	7.9E10	1.24E11	1.82E11	2.52E11	3.38E11
S14 → S6	2	1.09E8	2.54E8	5.32E8	1.82E9	4.78E9	7.21E9	1.47E10	2.66E10	4.42E10	6.8E10	9.9E10
S6 → AZ + H	1	1.51E7	4.66E7	1.24E8	6.26E8	2.25E9	3.88E9	1.0E10	2.19E10	4.29E10	7.61E10	1.26E11
AZ + H → S6	--	4.41E-12	5.84E-12	7.44E-12	1.14E-11	1.62E-11	1.89E-11	2.52E-11	3.21E-11	4.0E-11	4.86E-11	5.79E-11
S10 → NP + H	1	6.05E10	9.56E10	1.43E11	2.77E11	4.7E11	5.87E11	8.68E11	1.21E12	1.59E12	2.03E12	2.48E12
NP + H → S10	--	8.35E-13	1.26E-12	1.81E-12	3.36E-12	5.56E-12	6.9E-12	1.03E-11	1.44E-11	1.94E-11	2.52E-11	3.18E-11
S11 → S10	4	1.77E11	1.97E11	2.17E11	2.52E11	2.87E11	3.02E11	3.3E11	3.57E11	3.81E11	4.03E11	4.23E11
S10 → S11	2	9.77E7	2.77E8	6.82E8	3.0E9	9.7E9	1.59E10	3.75E10	7.71E10	1.42E11	2.38E11	3.73E11
S13 → S17	1	2.77E10	3.82E10	5.04E10	7.96E10	1.15E11	1.34E11	1.74E11	2.18E11	2.63E11	3.08E11	3.57E11
S17 → S13	1	1.18E12	1.41E12	1.64E12	2.1E12	2.56E12	2.78E12	3.2E12	3.62E12	4.01E12	4.36E12	4.71E12
S13 → AZ + H	2	2.29E7	7.0E7	1.85E8	9.23E8	3.3E9	5.69E9	1.45E10	3.21E10	6.22E10	1.1E11	1.82E11
AZ + H → S13	--	8.69E-12	1.13E-11	1.42E-11	2.15E-11	3.0E-11	3.48E-11	4.57E-11	5.8E-11	7.12E-11	8.6E-11	1.02E-10

S14 → AZ + H	2	5.32E6	1.88E7	5.62E7	3.44E8	1.45E9	2.65E9	7.64E9	1.84E10	3.9E10	7.38E10	1.29E11
AZ + H → S14	--	2.7E-11	3.33E-11	3.99E-11	5.53E-11	7.28E-11	8.17E-11	1.03E-10	1.25E-10	1.49E-10	1.74E-10	2.02E-10
S17 → S22	1	6.34E9	1.23E10	2.18E10	5.6E10	1.18E11	1.62E11	2.82E11	4.44E11	6.54E11	9.1E11	1.21E12
S22 → S17	1	2.23E12	2.32E12	2.39E12	2.52E12	2.62E12	2.66E12	2.75E12	2.81E12	2.87E12	2.93E12	2.96E12
S17 → S23	1	6.34E9	1.23E10	2.18E10	5.6E10	1.18E11	1.62E11	2.82E11	4.44E11	6.54E11	9.1E11	1.21E12
S23 → S17	1	4.32E9	8.7E9	1.58E10	4.28E10	9.37E10	1.31E11	2.34E11	3.78E11	5.7E11	8.07E11	1.09E12
S23 → S24	1	1.68E12	1.93E12	2.18E12	2.66E12	3.12E12	3.34E12	3.75E12	4.12E12	4.5E12	4.82E12	5.11E12
S24 → S23	1	1.59E6	4.73E6	1.23E7	5.91E7	2.04E8	3.44E8	8.54E8	1.82E9	3.49E9	6.03E9	9.72E9
S24 → NP + H	2	2.14E8	5.52E8	1.27E9	4.99E9	1.48E10	2.35E10	5.24E10	1.03E11	1.82E11	2.96E11	4.52E11
NP + H → S24	--	1.7E-11	2.17E-11	2.69E-11	3.91E-11	5.37E-11	6.15E-11	7.93E-11	9.89E-11	1.21E-10	1.44E-10	1.69E-10
S26 → S32	2	3.9E8	8.99E8	1.86E9	6.2E9	1.61E10	2.41E10	4.86E10	8.79E10	1.44E11	2.21E11	3.19E11
S32 → S26	2	1.03E9	2.17E9	4.14E9	1.21E10	2.81E10	4.03E10	7.55E10	1.27E11	1.97E11	2.89E11	4.02E11
S26 → FL + H	2	8.44E5	3.97E6	1.52E7	1.4E8	8.06E8	1.71E9	6.21E9	1.83E10	4.58E10	1.01E11	1.98E11
FL + H → S26	--	3.82E-10	4.33E-10	4.81E-10	5.85E-10	6.96E-10	7.55E-10	8.77E-10	1.0E-9	1.13E-9	1.27E-9	1.41E-9
S32 → FL + H	2	3.86E6	1.64E7	5.76E7	4.6E8	2.38E9	4.8E9	1.62E10	4.44E10	1.04E11	2.18E11	4.12E11
FL + H → S32	--	6.65E-10	7.48E-10	8.24E-10	9.95E-10	1.18E-9	1.27E-9	1.48E-9	1.68E-9	1.9E-9	2.11E-9	2.34E-9
$c\text{-}C_5H_5 + c\text{-}C_5H_6 \rightarrow A1$	--	4.63E-16	6.86E-16	9.86E-16	1.82E-15	3.08E-15	3.9E-15	5.98E-15	8.75E-15	1.23E-14	1.66E-14	2.2E-14
$A1 \rightarrow c\text{-}C_5H_5 + c\text{-}C_5H_6$	1	7.81E9	1.51E10	2.7E10	6.96E10	1.48E11	2.03E11	3.52E11	5.6E11	8.23E11	1.15E12	1.53E12
A1 → A2 + H	1	4.83E6	1.66E7	4.93E7	2.94E8	1.22E9	2.23E9	6.32E9	1.51E10	3.18E10	6.0E10	1.04E11
A2 + H → A1	--	1.06E-11	1.22E-11	1.38E-11	1.74E-11	2.13E-11	2.33E-11	2.75E-11	3.2E-11	3.66E-11	4.15E-11	4.67E-11
A2 → $S0_{cis}$	1	2.09E8	4.57E8	9.01E8	2.77E9	6.73E9	9.86E9	1.9E10	3.29E10	5.21E10	7.78E10	1.1E11
$S0_{cis}$ → A2	4	3.1E9	6.52E9	1.24E10	3.58E10	8.32E10	1.2E11	2.24E11	3.76E11	5.8E11	8.52E11	1.18E12

A2+H→S1+H_2	--	6.12E-12	7.98E-12	1.01E-11	1.52E-11	2.15E-11	2.5E-11	3.31E-11	4.25E-11	5.27E-11	6.42E-11	7.69E-11
S1+H_2→A1+H	--	4.25E-17	1.05E-16	2.32E-16	8.94E-16	2.66E-15	4.29E-15	9.91E-15	2.05E-14	3.83E-14	6.67E-14	1.08E-13
A2+H→S26+H_2	--	4.81E-11	5.64E-11	6.47E-11	8.38E-11	1.04E-10	1.15E-10	1.38E-10	1.64E-10	1.9E-10	2.17E-10	2.48E-10
S26+H_2→A2+H	--	9.34E-18	2.96E-17	8.1E-17	4.42E-16	1.73E-15	3.14E-15	8.85E-15	2.15E-14	4.65E-14	9.09E-14	1.63E-13
S0$_{cis}$ → S0$_{trans}$	2	6.24E11	7.26E11	8.26E11	1.01E12	1.2E12	1.29E12	1.46E12	1.62E12	1.76E12	1.9E12	2.02E12
S0$_{trans}$ → S0$_{cis}$	2	5.84E11	6.84E11	7.82E11	9.72E11	1.15E12	1.24E12	1.42E12	1.58E12	1.73E12	1.86E12	2.0E12
S0$_{cis}$+H→S1+H_2	--	2.28E-11	2.86E-11	3.5E-11	5.01E-11	6.78E-11	7.71E-11	9.89E-11	1.23E-10	1.49E-10	1.77E-10	2.09E-10
S1+H_2→S0$_{cis}$+H	--	2.16E-17	5.36E-17	1.18E-16	4.57E-16	1.36E-15	2.19E-15	5.07E-15	1.04E-14	1.95E-14	3.37E-14	5.49E-14
S0$_{trans}$+H→S1+H_2	--	1.78E-11	2.27E-11	2.83E-11	4.16E-11	5.79E-11	6.68E-11	8.7E-11	1.1E-10	1.36E-10	1.64E-10	1.93E-10
S1+H_2→S0$_{trans}$+H	--	1.52E-17	3.88E-17	8.79E-17	3.51E-16	1.08E-15	1.77E-15	4.17E-15	8.75E-15	1.67E-14	2.94E-14	4.8E-14

[*] **Reaction path degeneracy.**