Supporting information for "Electrocyclic Ring Openings of 2-Furylcarbene and Related Carbenes; A Comparison Between Pseudopericyclic and Coarctate Reactions"

David M. Birney

Table S1. Cartesian coordinates for all stationary points optimized at the B3LYP/6-31G* level. QCISD/6-31G* geometry for **syn-5cTS**.

10 **syn-5a 2-furyl** carbene

C	-0.738261	0.000000	-1.249660
C	0.639436	0.000000	-1.410371
C	1.160496	0.000000	-0.112963
C	0.109471	0.000000	0.818426
O	-1.103923	0.000000	0.016506
H	-1.530237	0.000000	-1.989248
H	1.171790	0.000000	-2.350232
H	2.199453	0.000000	0.185431
C	0.142510	0.000000	2.194235
H	-0.891536	0.000000	2.583992

10 ^{3}**syn-5a** triplet carbene

C	-0.773022	0.000000	-1.240373
C	0.583101	0.000000	-1.438787
C	1.180537	0.000000	-0.158818
C	0.135260	0.000000	0.784931
O	-1.076666	0.000000	0.088297
H	-1.616164	0.000000	-1.914070
H	1.085950	0.000000	-2.395356
H	2.233103	0.000000	0.081950
C	0.127338	0.000000	2.150215
H	-0.608844	0.000000	2.938092

10 **syn-5aTS** 2-furylcarbene transition state

C	-1.395168	0.000000	-0.477422
C	-1.228758	0.000000	0.922399
C	0.129106	0.000000	1.164621
C	0.923443	0.000000	0.000000
O	-0.315560	0.000000	-1.159208
H	-2.346770	0.000000	-1.010843
H	-2.027181	0.000000	1.649922
H	0.601664	0.000000	2.138664
C	2.203087	0.000000	-0.302067
H	2.506503	0.000000	-1.349264

10 ^{3}**syn-5aTS** 2-furylcarbene TS triplet

C	1.358159	-0.648719	-0.002744
C	1.315435	0.732354	-0.004428
C	0.010457	1.256415	0.005285
C	-1.044002	0.348294	0.007756
O	0.253687	-1.342179	0.005978
H	2.278284	-1.237567	-0.006405
H	2.206744	1.346076	-0.007986
H	-0.202617	2.319066	0.021960
C	-2.182865	-0.173659	-0.028033
H	-3.055002	-0.778249	0.077598

10 **anti-5a** 2-furyl carbene, anti conformation

C	-1.316844	0.000000	-0.620312
C	-1.338497	0.000000	0.767409
C	0.005386	0.000000	1.149418
C	0.817571	0.000000	0.000000
O	-0.093664	0.000000	-1.105975
H	-2.126388	0.000000	-1.339082
H	-2.219280	0.000000	1.393156
H	0.396503	0.000000	2.158081
C	2.166297	0.000000	-0.302331
H	2.694994	0.000000	0.670538

10 **anti-5aTS** 2-furylcarbene TS anti conformation

C	-0.650340	0.000002	-1.335938
C	0.768846	0.000003	-1.326622
C	1.165552	0.000000	-0.012405
C	0.130171	-0.000002	0.947217
O	-1.207013	0.000000	-0.200366
H	-1.275303	0.000003	-2.231717
H	1.401757	0.000005	-2.202462
H	2.197490	-0.000001	0.321706
C	-0.267329	-0.000003	2.180718
H	0.450764	-0.000004	2.997573

10 **6a** 2-penten-4-ynal

O	-1.661849	0.000000	-0.585683
C	-0.809160	0.000000	-1.454640
C	0.646256	0.000000	-1.217280
C	1.238065	0.000000	0.000000
C	0.598599	0.000000	1.262304
C	0.168472	0.000000	2.395240
H	-0.270520	0.000000	3.366260
H	-1.095217	0.000000	-2.529036
H	1.279966	0.000000	-2.100404
H	2.327172	0.000000	0.034904

10 ^{3}**6a** 2-penten-4-ynal triplet

O	-0.932755	0.000000	-1.213010
C	-1.522891	0.000000	-0.051116
C	-0.864057	0.000000	1.163978
C	0.542925	0.000000	1.190890
C	1.260359	0.000000	0.000000
C	1.916290	0.000000	-1.041510
H	2.447559	0.000000	-1.964762
H	-2.616140	0.000000	-0.118866
H	-1.443437	0.000000	2.079574
H	1.078303	0.000000	2.134692

11 **5b** pyrrolylcarbene

C	-1.3573203206	0.0000926293	-0.6160264171
C	-1.3455771387	0.0001293427	0.7897795468
C	-0.0107297211	0.0000314168	1.1786229017
C	0.8259806468	-0.0000660858	0.0275671682
N	-0.0945393935	-0.0000235979	-1.0615398533
H	0.1916025262	-0.0000578625	-2.0299029006
H	-2.2031979348	0.0001393515	-1.2913903652
H	-2.2240310549	0.0002164235	1.4189091138
H	0.3880471075	0.0000257302	2.1831652084
C	2.2169438449	-0.0001756249	-0.0088171428
H	2.5335712425	-0.0002285259	-1.0767584242

11 **5bTS** pyrrolylcarbene ts

N	0.7629547423	0.5849566873	0.8173415542
H	1.4572791961	0.7968870771	1.5270631325
C	0.1320971906	-1.0050539036	0.0240734923
C	-0.7915107154	-0.317615328	-0.8168678605
H	-1.4039366299	-0.9108696373	-1.4855537521
C	0.087578698	1.5286732859	0.2490103295
H	0.2079639623	2.5881751017	0.4819874477
C	-0.8484169756	1.0418157979	-0.7293345686
H	-1.4995158106	1.6834399713	-1.306368022
C	0.5234643261	-2.2044989684	0.2837945049
H	1.2782509438	-2.5122546268	0.9974249296

11 **6b** 2-penten-4-ynal imine

C	-1.4334294377	0.0045295501	-0.8860169261
C	-1.2400086773	0.0074568107	0.5673895426
C	-0.0719612051	0.0037105069	1.2510104449
H	-2.4903520028	0.0090514473	-1.1916886875
H	-2.1538145588	0.0133446353	1.1573306287
H	-0.132304478	0.0068160148	2.3394317254
C	1.2441035643	-0.0040502857	0.72904044
C	2.4119219699	-0.0103004818	0.4062448526
H	3.4178564895	-0.0159319545	0.0530100035
N	-0.4670733493	-0.0025421882	-1.7259632468
H	-0.8356292887	-0.0035614264	-2.6823510666

12 **syn-5c** cyclopentadienylcarbene

C	0.893580	0.419561	0.659051
H	0.990519	0.475748	1.752474
H	1.921424	0.407688	0.267418
C	0.146264	-0.820295	0.160794
C	-0.894106	-0.350141	-0.632137
H	-1.586455	-1.009508	-1.143818
C	0.112242	1.558165	0.091891
H	0.307868	2.603409	0.308743
C	-0.896560	1.086782	-0.693344
H	-1.611048	1.688229	-1.243114
C	0.398512	-2.200806	0.301539
H	1.418097	-2.325159	0.731533

12 **syn-5cTS** transition state

C	1.004326	0.5554894	0.5846222813
H	1.458568	0.5957632	1.5743090798
H	1.722921	0.2555967	-0.1787151329
C	0.046155	-0.9578393	0.1197708752
C	-0.846733	-0.3305065	-0.7983787661
H	-1.438539	-0.9220416	-1.4890273602
C	0.061958	1.5419504	0.2052138095
H	-0.112089	2.4570577	0.7645229864
C	-0.839935	1.0546931	-0.7586184944
H	-1.534791	1.6669568	-1.3235106935
C	0.343046	-2.1257312	0.5926545275
H	1.291023	-2.4816687	0.9808357229

12 qcisd/6-31G** **syn-5cTS** transition state

C	1.024582	0.548107	0.547219
H	1.498701	0.570943	1.524311
H	1.725591	0.303194	-0.245627
C	0.064056	-0.939082	0.127437
C	-0.843772	-0.324080	-0.812388
H	-1.429637	-0.923245	-1.496512
C	0.048967	1.527354	0.232503
H	-0.174170	2.379907	0.862067
C	-0.849467	1.050945	-0.764292
H	-1.540079	1.666521	-1.323421
C	0.340561	-2.112772	0.598469
H	1.210034	-2.500161	1.105494

12 **anti-5c** conf #2 cyclopentadienylcarbene

C	0.9039772484	0.3967854922	0.7010893466
H	1.0142589053	0.4749723746	1.7919835182
H	1.922898917	0.3072382826	0.3026405461
C	0.1074092069	-0.8180678167	0.2289525768
C	-0.9131847358	-0.324177109	-0.5843840404
H	-1.6346559376	-0.9471789686	-1.1032596676
C	0.1769539204	1.5548367071	0.1019039552
H	0.4055656242	2.5943182319	0.3101377682
C	-0.8345088013	1.1076089999	-0.6938564202
H	-1.5116454104	1.7247413909	-1.2735041643
C	0.5729393103	-2.139785872	0.2386880916
H	-0.2779389921	-2.8172937203	0.0176409418

12 **anti-5cTS** cyclopentadienylcarbene ts#2

C	0.163508057	1.271468193	0.1715348827
H	-0.1230767435	2.2030912825	-0.315625289
H	-0.1697097094	1.2377879837	1.2063906274
C	-0.949881902	-0.2115992654	-0.1021711471
C	0.0590544616	-1.1950351616	0.0899093441
H	-0.2066641156	-2.2302868611	0.2808930128
C	1.4151875658	0.6701422961	-0.1110264494
H	2.225698984	1.1709017953	-0.6323583077
C	1.3648502599	-0.7186528903	0.0709073578
H	2.2285007488	-1.3755219112	0.0837918134
C	-2.2059985492	0.0755479073	-0.113026437
H	-3.0350685235	-0.3571987642	-0.6598571635

12 **6c** cis-3,5-hexadien-1-yne

C	-1.1151426677	0.00222549	-0.7935546984
C	-1.1592847098	0.004049738	0.5612688489
C	1.3359806726	-0.0056823745	-1.3930922875
C	0.0286926333	-0.0021682279	-1.701170345
H	-2.0839332766	0.0043706005	-1.2885793841
H	-2.1412419743	0.0073796416	1.0313660783
H	2.0835674255	-0.008807515	-2.1802805031
H	-0.2429381589	-0.0027172803	-2.7558093289
H	1.6933755352	-0.0054453536	-0.3706665663
C	-0.0649715337	0.0020123511	1.4623802406
C	0.8212472572	0.0005510475	2.2907388847
H	1.6120405376	-0.0007082382	3.0045458442

6 **7a (1.5 Å)** propynal 1.5 A

O	-0.885589	-0.692501	0.018169
C	0.359213	0.125520	-0.158776
C	-0.905870	0.607193	-0.038272
C	1.601910	-0.121874	0.125045
H	-1.636074	1.288061	0.403414
H	2.389264	0.586911	-0.116747

6 **8a** propynal singlet

C	0.515859	-0.661038	0.000000
C	-0.008277	0.689236	0.000000
O	-0.179150	-1.657605	0.000000
H	1.621759	-0.725587	0.000000
C	-0.408751	1.830975	0.000000
H	-0.781544	2.831397	0.000000

8 **7c** "cyclopropene carbene"

C	1.041197962	-0.2926042339	0.
C	-0.1247385524	-1.2277367447	0.
C	-0.1430704718	0.3024367225	0.
H	-0.3493146334	-1.7837152288	0.9127954251
H	-0.3493146334	-1.7837152288	-0.9127954251
H	2.1235190652	-0.2193808044	0.
C	-0.9685601325	1.4628673364	0.
H	-0.2538626304	2.3170327808	0.

8 **8c** 3-buten-1-yne

C	0.8359060698	0.0000130845	-1.4854247291
C	0.7909777989	0.000016601	-0.1455032634
H	1.7854506984	0.0000310228	-2.0099493118
H	-0.0677743252	-0.0000078907	-2.0859434866
H	1.7204279689	0.0000389425	0.4225454515
C	-0.4097000343	-0.0000068275	0.620655648
C	-1.4076002893	-0.0000259891	1.3066490907
H	-2.295605612	-0.0000432621	1.8950868693

14 **syn-9a (1.5Å)** c7o carbene fixed 1.5 A

C	-1.525062	-0.551486	-0.859837
C	-1.636743	-0.345220	0.520783
C	-0.601931	0.005641	1.379367
C	-0.427311	-0.308647	-1.703387
C	0.762052	0.177436	0.991080
C	0.710350	0.420572	-1.406978
H	-2.404484	-0.964575	-1.349883
H	-2.605547	-0.551204	0.967651
H	-0.791085	0.022505	2.447316
H	-0.508003	-0.638022	-2.735185
H	1.444772	0.612206	-2.190357
O	0.996884	0.982177	-0.252803
C	1.742222	-0.353403	1.667558
H	2.747809	-0.607689	1.351369

14 **syn-9a (1.6 Å)** c7o carbene 1.6 angstroms

C	-1.519148159	-0.5483405735	-0.8675112489
C	-1.6359116873	-0.3276359303	0.5223804487
C	-0.6158515569	-0.0039857776	1.3926807765
C	-0.4411151832	-0.29997466	-1.7143806432
C	0.765350497	0.1158878	1.0454520073
C	0.7047553019	0.4438446945	-1.4155939601
H	-2.3981531561	-0.9769577868	-1.3456513358
H	-2.6181442514	-0.4999402548	0.9544281815
H	-0.8350855448	0.0457425903	2.4548574746
H	-0.5284811541	-0.6226486504	-2.747947172
H	1.430211426	0.6287125753	-2.2134881039
O	0.982448317	0.9904850765	-0.2766478468
C	1.7873002091	-0.3675672391	1.6538819239
H	2.8177896151	-0.5721589693	1.4095279046

14 **anti-9a** heptadienyl carbene anti

C	-1.4927383378	-0.5864799949	-0.8675286315
C	-1.631884051	-0.3600029901	0.499181358
C	-0.6207154702	0.0791499084	1.3580183048
C	-0.3866627229	-0.3158518526	-1.7038855722
C	0.7431563835	0.2325788604	0.9985504368
C	0.7369565873	0.4249421412	-1.4109708499
H	-2.3509933269	-1.0311457606	-1.3672046021
H	-2.5967280389	-0.5934137469	0.9417704806
H	-0.8436660656	0.149933672	2.4195567331
H	-0.456349261	-0.6473477811	-2.7356697236
H	1.4589726603	0.6322693936	-2.2008768483
O	1.0538886291	0.9896091396	-0.261432832
C	1.7380034217	-0.4161318781	1.5394811362
H	1.8409601348	-0.776394059	2.556809523 2

14 **anti-9aTS** heptadienyl carbene anti config. TS

C	-1.4805244872	-0.5903091098	-0.8833741697
C	-1.6405858158	-0.3462290409	0.487147907
C	-0.650091067	0.0810399637	1.3615788408
C	-0.3792708491	-0.3207509842	-1.709996883
C	0.7300829584	0.1930825363	1.0443537284
C	0.7460219728	0.433823738	-1.4091452365
H	-2.3327215932	-1.0471859078	-1.3829577959
H	-2.6207937198	-0.5553444537	0.9079673442
H	-0.9025495002	0.1868980441	2.4139281923
H	-0.4415977073	-0.6542351589	-2.7418027098
H	1.4696023082	0.632026139	-2.2028026228
O	1.0437046676	0.9952769318	-0.2700959828
C	1.752365679	-0.4032216643	1.5510722842
H	2.0104325249	-0.8089867494	2.516616628

14 **10a** 2,4-heptadien-6ynal

C	1.257363	-0.433342	1.078224
C	1.658391	0.322360	-0.098070
C	1.047697	0.434283	-1.301886
C	0.056771	-0.588021	1.688140
C	-0.155773	-0.181272	-1.714366
C	-1.209453	0.118309	1.427206
H	2.095220	-0.933369	1.567779
H	2.646273	0.774854	-0.022669
H	1.558969	1.015784	-2.067754
H	0.024753	-1.245408	2.555416
H	-2.029375	-0.186752	2.115357
O	-1.400251	0.987688	0.595470
C	-1.160437	-0.701360	-2.148682
H	-2.061189	-1.152354	-2.495278

16 **9c** cycloheptatrienecarbene

C	-1.59888	-0.44633	-0.8958
C	-1.62491	-0.37728	0.48895
C	-0.54152	-0.17207	1.36614
C	-0.46621	-0.34808	-1.75403
C	0.77262	0.23009	1.01435
C	0.72827	0.24616	-1.46849
C	0.98209	1.07715	-0.2641
H	-2.5338	-0.72851	-1.37623
H	-2.57589	-0.61255	0.96211
H	-0.67639	-0.44769	2.40662
H	-0.57135	-0.81054	-2.73396
H	1.55008	0.09958	-2.16643
H	0.2735	1.91308	-0.21123
H	1.9919	1.49356	-0.2736
C	1.72501	-0.2702	1.84845
H	2.68315	-0.54355	1.37994

16 **9cTS** cycloheptatrienecarbene transition state

C	-1.6225947028	-0.3913458845	-0.9355507993
C	-1.6160339696	-0.3719715765	0.4957043104
C	-0.59210302	-0.2430737592	1.3977529066
C	-0.56109025	-0.2667369424	-1.8066574513
C	0.7971304075	0.0415328368	1.1687430774
C	0.7259363399	0.220808842	-1.4953081682
C	1.0045379511	1.0484429979	-0.3955409569
H	-2.5788004385	-0.6653068833	-1.37644689
H	-2.5785318974	-0.6101508256	0.9444343294
H	-0.8111687708	-0.4928018042	2.4318620075
H	-0.7240719798	-0.5949371629	-2.8323667886
H	1.5498946536	-0.0803872601	-2.1398783594
H	0.2320360502	1.7543678485	-0.0977415208
H	2.0038888242	1.4689150472	-0.337176582
C	1.8626219024	-0.1218760192	1.8571400716
H	2.9163256073	-0.2743819295	1.6896158629

16 **10c** 3,5,7-octatriene-1-yne

C	0.6	0.	0.65
C	0.68079	-0.55777	1.85017
H	1.52404	0.	0.05642
H	1.60481	-0.55775	2.44379
C	-0.69567	-0.00003	-0.18238
C	-1.90156	-0.00006	0.36886
H	-0.53993	-0.00005	-1.26954
H	-2.82558	-0.0001	-0.22476
C	-2.11993	-0.00003	1.8933
C	-1.26521	0.55781	2.73966
H	-3.17343	-0.00003	2.20365
H	-1.42094	0.55782	3.82683
H	-0.34421	1.05728	2.41033
C	-0.17157	-1.77223	2.26268
C	-0.83298	-2.71462	2.58277
H	-1.42023	-3.55134	2.86696

16 ***s*-trans-*s*-trans10c** 3,5,7-octatrien-1-yne

C	-0.625	0.	-1.7
C	-0.625	0.	-0.37408
H	0.29904	0.	-2.29359
H	-1.54901	-0.00002	-2.29362
H	0.29901	0.00003	0.21953
C	-1.9207	-0.00003	0.45825
C	-1.9207	-0.00003	1.78416
H	-2.84471	-0.00005	-0.13537
H	-2.84473	-0.00005	2.37775
C	-0.62503	0.00001	2.61654
C	-0.66455	0.00007	3.94187
H	0.30307	0.00001	2.02932
H	0.24136	0.00012	4.56276
C	-1.98448	0.00008	4.73521
C	-3.00871	0.00008	5.35082
H	-3.91808	0.00009	5.8974

12 **11**

C	-0.300603	-0.000002	-0.516219
C	1.080873	0.000003	-0.677394
C	1.603583	0.000006	0.617136
C	0.548726	0.000002	1.546133
O	-0.657795	-0.000002	0.764037
H	1.597935	0.000005	-1.625247
H	2.642386	0.000010	0.915667
C	0.592445	0.000003	2.930675
H	-0.440690	0.000000	3.322695
C	-1.371298	-0.000007	-1.534034
O	-1.132384	-0.000003	-2.724652
H	-2.400554	-0.000014	-1.125980

12 **^{3}11**

C	-0.2905352456	-0.0000014995	-0.5397942663
C	1.0972557966	0.0000037784	-0.6599337848
C	1.6198140416	0.0000064118	0.6281852595
C	0.5199017654	0.0000025636	1.529090861
O	-0.65242068	-0.0000020428	0.7817437776
H	1.6311659209	0.0000053311	-1.5989550206
H	2.6578176038	0.0000105272	0.9269339598
C	0.4676897213	0.0000032948	2.8845502216
H	-0.2846589615	-0.000000348	3.6571729014
C	-1.3377804439	-0.0000061941	-1.5380350172
O	-1.1093198916	-0.000004749	-2.7416492059
H	-2.3684738026	-0.0000113062	-1.1302880574

12 **11TS**

C	-0.146025	0.000000	-0.594734
C	1.209237	0.000000	-0.201673
C	1.228774	0.000000	1.176741
C	-0.046849	0.000000	1.777883
O	-1.001135	0.000000	0.360271
H	2.047328	0.000000	-0.882123
H	2.114910	0.000000	1.799101
C	-0.553218	0.000000	2.990514
H	-1.632428	0.000000	3.137144
C	-0.640769	0.000000	-2.009604
O	0.114417	0.000000	-2.957380
H	-1.742965	0.000000	-2.112011

12 ^{3}**11TS** Triplet

C	-0.3721421701	-0.0032785544	0.5439581986
C	1.0388882163	-0.0050977294	0.4951561475
C	1.5423046129	0.0031872968	-0.7853940221
C	0.6120371115	0.0120937918	-1.8434914703
O	-1.0214212103	0.0057151669	-0.5866259342
H	1.6325555829	-0.0123983851	1.3993040457
H	2.6015362864	0.0031820943	-1.0162256575
C	0.1638627413	0.0210310697	-3.0096527017
H	-0.4173153512	0.0282482592	-3.904485173
C	-1.1246943854	-0.0111055563	1.811827156
O	-0.5728897505	-0.0196271572	2.90462234
H	-2.2238255899	-0.0087179557	1.7030156911

12 **12** 2-oxo-3-hexen-5-ynal

O	1.223143	0.808603	0.000000
C	0.000000	0.809029	0.000000
C	-0.870497	-0.373546	0.000000
C	-0.428536	-1.653159	0.000000
C	0.914861	-2.095468	0.000000
C	2.022722	-2.586766	0.000000
H	3.019677	-2.963741	0.000000
H	-1.937477	-0.178924	0.000000
H	-1.175883	-2.446232	0.000000
C	-0.707624	2.171022	0.000000
O	-1.910119	2.308873	0.000000
H	0.003936	3.022415	0.000000

12 ^{3}**12** 2-oxo-3-hexen-5-ynal triplet

O	1.24762590	0.69288153	0.0
C	-0.01625030	0.77570411	0.0
C	-0.90304219	-0.34932504	0.0
C	-0.47547872	-1.64819827	0.0
C	0.8715954	-2.05339239	0.0
C	2.02135909	-2.45275153	0.0
H	3.03946571	-2.76726582	0.0
H	-1.95855147	-0.09807869	0.0
H	-1.22857757	-2.43344186	0.0
C	-0.65483468	2.13376287	0.0
O	-1.86845867	2.29349460	0.0
H	0.05423396	2.97297874	0.0

Table S2. Absolute energies (Hartree), dipole moments (Debye), zero point energies (ZPE, kcal/mol), and low frequencies (cm^{-1}) of all stationary points. Geometries are at the B3LYP/6-31G(d,p) level, or at the MP2(full)/6-31G(d) level for G2(MP2) calculations.

	B3LYP/6-31G(d,p)				MP2	MP4(SDQ)	CCSD(T)	
	energy	dipole	low freq	ZPE		6-311+G(d,p)		G2 (0 K)
syn-5a	-268.02116	4.417	227.7	45.4	-267.31765	-267.34761	-267.39157	-267.55417
^{3}syn-5a	-268.01551	0.9717	251.0	44.7	-267.28979	-267.33637	-267.38334	
syn-5aTS	-268.01766	3.8258	-490.0	44.4	-267.30881	-267.33779	-267.38497	-267.55110
^{3}syn-5aTS	-267.97673	0.8582	-290.0	42.0	-267.21399	-267.27240	-267.33412	
anti-5a	-268.01855	4.9251	209.5	45.6				
anti-5aTS	-268.00887	4.3787	-544.0	44.3				
6a	-268.05906	2.425	121.7	44.6	-267.36749	-267.39643	-267.43766	-267.59811
^{3}6a	-267.97823	0.9006	147.6	42.4	-267.22862	-267.28490	-267.33876	

	syn-5c	**syn-5cTS**	**anti-5c**	**anti-5cTS**	**6c**
QCISD(T)/6-311G(d,p)	-231.49461	-231.485172	-231.493563	-231.47655	-231.54884
MP2/6-311+G(3df,2p)	-231.54744	-231.53645	-231.546884	-231.53060	-231.60541
MP2/6-311G(d,p)	-231.40551	-231.39192	-231.40473	-231.38675	-231.4639
MP2(Full)/6-31G(d)	-231.30955	-231.29448	-231.30841	-231.28945	-231.36913
CISD + Δ MP2	-231.63655	-231.629701	-231.635713	-231.62041	-231.69035
B3LYP/6-31G(d,p)	-232.09303	-232.079427	-232.09270	-232.07360	-232.14371
+ ZPE	-231.99844	-231.98600	-231.99772	-231.98034	-232.04866
QCISD/6-31g(d,p) //QCISD/6-31G(d,p)		-231.359938			

syn-5cTS constrained	1.85A	1.80 A	1.75 Å	1.75 Å 125°	1.72 Å	1.72 Å 125°	1.7 Å	1.70 Å 125°
QCISD(T)/6-311G(D,P)	-231.48333	-231.481466	-231.479986	-231.47845	-231.47909	-231.47959	-231.47841	-231.4798
MP2/6-311+G(3df,2p)	-231.54804	-231.546007	-231.54421	-231.53663	-231.54318	-231.53652	-231.54248	-231.536
MP2/6-311G(d,p)	-231.40435	-231.402206	-231.400376	-231.39199	-231.39938	-231.39173	-231.39876	-231.39112
MP2(Full)/6-31G(d)	-231.30704	-231.304793	-231.302919	-231.29392	-231.30194	-231.29368	-231.30134	-231.29309
CISD + Δ MP2	-231.62703	-231.625266	-231.623819	-231.6231	-231.62289	-231.62438	-231.62213	-231.62468

	B3LYP/6-31G(d,p)	+ZPE	low freq
5b	-248.17154	-248.08595	232.0
5bTS	-248.14914	-248.06643	-546.4
6b	-248.18345	-248.09974	82.5
7c	-154.59407	-154.53659	-824.5302
7c (1.65 Å)	-154.62959		
8c	-154.74043	-154.67933	228.4795
syn-9a (1.5 Å)	-345.40805		
syn-9a (1.6 Å)	-345.41005		
anti-9a	-345.40566	66.1	145.1
anti-9aTS	-345.40550	65.6	-276.9
10a	-345.45730	65.7	82.0
9c	-309.51032	81.7	122.2
9cTS	-309.49965	80.5	-557.0
10c	-309.53893	80.7	72.3
***s*-trans-*s*-trans10c**	-309.55689	80.8	56.2

	b3lyp/6-31G**	relative energy, kcal/mol
7a 1.5	-190.49693	95.3
7a 1.6	-190.52315	78.8
7a 1.7	-190.54761	63.5
7a 1.8	-190.57359	47.2
7a 1.9	-190.59776	32.0
7a 2.0	-190.61782	19.4
7a 2.1	-190.63298	9.9
8a	-190.6488	0.0

	B3LYP/6-31G(d,p)				G2(MP2)			
	energy	dipole	low freq	ZPE	0 K	free energy	low freq	ZPE
11	-381.34045	1.4188	111.7	51.1	-380.72493	-380.75608	115.1	55.6
^{3}11	-381.34519	3.2479	124.7	50.8	-380.71664	-380.74881	131.4	53.7
11TS	-381.33525	1.1057	-505.9	50.1	-380.72031	-380.75195	-780.1	53.9
^{3}11TS	-381.30734	3.6559	-365.7	48.6	-380.67207		-510.0	50.2
12	-381.37836	1.911	51.6	50.6	-380.76908	-380.80266	38.2	55.3
^{3}12	-381.31306	1.3338	76.5	48.9	-380.67589	-380.70994	73.8	51.5

	11	**^{3}11**	**11 TS**	**^{3}11 TS**	**12**	**^{3}12**
QCISD(T)/6-311G(D,P)	-380.468697	-380.46476	-380.46114	-380.415343	-380.5174	-380.42418
MP2/6-311+G(3df,2p)	-380.614985	-380.58274	-380.6041	-380.510104	-380.6603	-380.52506
MP2/6-311G(d,p)	-380.379617	-380.34985	-380.36824	-380.277251	-380.42999	-380.29539
MP2(Full)/6-31G(d)	-380.235234	-380.20835	-380.22495	-380.134583	-380.28547	-380.1494
ZPE (Hartree)	0.088633	0.085562	0.085894	0.08007	0.088067	0.082131