Bicyclobutane mechanism.

TS1_3

Sum of electronic and zero-point Energies= -385.324176

C	2.025566	1.105610	-0.010306
C	0.705586	1.634923	0.194879
C	-0.381991	-0.646926	0.161104
C	-0.394969	0.825642	0.198261
C	-1.764205	1.219539	-0.004806
C	-2.548534	0.086289	-0.236127
C	0.515294	-1.615346	0.787635
C	1.251861	-1.303906	-0.373824
C	-1.728110	-1.046220	-0.191520
C	2.232581	-0.189221	-0.341207
H	2.872078	1.783032	0.026090
H	0.580311	2.711728	0.274228
H	-2.103797	2.248730	-0.036621
H	-3.609140	0.082638	-0.453487
H	0.214216	-2.597882	1.135536
H	1.375048	-2.045049	-1.167876
H	-2.050898	-2.072589	-0.323417
H	3.243710	-0.532918	-0.558986

TS3_4

Sum of electronic and zero-point Energies= -385.319931

C	-2.133864	0.856136	0.019793
C	-0.903286	1.585984	0.016929
C	0.278135	-0.523975	-0.384097
C	0.299561	0.915538	-0.149188
C	1.672475	1.266546	0.033352
C	2.444746	0.114063	0.012339
C	-0.009323	-1.348596	0.885389
C	-0.968268	-1.343488	-0.259063
C	1.620714	-1.021338	-0.272612
C	-2.184226	-0.506801	-0.105915
H	-3.059423	1.408027	0.147730
H	-0.920727	2.660014	0.181040
H	2.040144	2.267912	0.225624
H	3.517368	0.067407	0.153345
H	-0.023130	-1.045560	1.926261
H	-1.071310	-2.274262	-0.819215
H	1.956884	-2.025878	-0.498462
H	-3.139786	-1.022075	-0.097884

TS4_5

Sum of electronic and zero-point Energies= -385.329567

C	-2.199127	0.727688	0.111120
C	-1.044929	1.538590	0.014757
C	0.197915	-0.485506	-0.481168
C	0.183689	0.927833	-0.211388
C	1.570174	1.340647	-0.028965
C	2.367624	0.243291	0.020887
C	0.561015	-1.298605	0.860791

C	-0.947299	-1.327595	-0.313383
C	1.569355	-1.013482	-0.199569
C	-2.165267	-0.660518	-0.009232
H	-3.150681	1.208400	0.318492
H	-1.119164	2.607938	0.187374
H	1.888943	2.363701	0.132017
H	3.433889	0.231473	0.210568
H	0.420211	-0.901553	1.861623
H	-0.942258	-2.370715	-0.616022
H	1.990907	-1.856517	-0.746966
H	-3.080760	-1.236787	0.069818

TS2_5

Sum of electronic and zero-point Energies= -385.332236

C	-2.357698	0.733909	-0.070213
C	-1.145309	1.434719	0.083798
C	0.013097	-0.690921	0.141302
C	0.049935	0.737388	0.157686
C	1.390560	1.372100	0.127513
C	2.422004	0.577796	-0.215182
C	1.283612	-1.433041	0.562751
C	-1.190020	-1.384833	-0.072292
C	1.985462	-0.809042	-0.480635
C	-2.379885	-0.658159	-0.164113
H	-3.286613	1.291840	-0.138932
H	-1.147566	2.520170	0.113965
H	1.503073	2.440066	0.285861
H	3.446815	0.898266	-0.381617
H	1.568913	-1.553758	1.605692
H	-1.195453	-2.469204	-0.110613
H	1.999407	-1.223991	-1.492915
H	-3.319132	-1.182887	-0.305128

1 (azulene)

Sum of electronic and zero-point Energies= -385.436934

C	2.294245	-0.112931	0.000000
C	1.385533	0.959440	0.000000
C	-0.855800	-0.272227	0.000000
C	0.000000	0.897682	0.000000
C	-0.882358	2.051752	0.000000
C	-2.210260	1.616709	0.000000
C	-0.494488	-1.611373	0.000000
C	0.802917	-2.152129	0.000000
C	-2.222857	0.219423	0.000000
C	2.033653	-1.487202	0.000000
H	3.344618	0.166933	0.000000
H	1.825390	1.954460	0.000000
H	-0.543912	3.081538	0.000000
H	-3.083961	2.255940	0.000000
H	-1.309306	-2.332241	0.000000
H	0.854658	-3.237907	0.000000
H	-3.102013	-0.414637	0.000000

H	2.911011	-2.128948	0.000000

2 (naphthalene)
Sum of electronic and zero-point Energies= -385.466068

C	-2.452344	-0.696180	0.000000
C	-1.236113	-1.402600	0.000000
C	1.236113	1.402600	0.000000
C	0.000000	-0.716158	0.000000
C	1.236111	-1.402600	0.000000
C	2.452343	-0.696181	0.000000
C	0.000000	0.716157	0.000000
C	-1.236111	1.402601	0.000000
C	2.452344	0.696180	0.000000
C	-2.452343	0.696181	0.000000
H	-3.390234	-1.242136	0.000000
H	-1.242970	-2.489155	0.000000
H	1.242966	2.489154	0.000000
H	1.242966	-2.489155	0.000000
H	3.390233	-1.242137	0.000000
H	-1.242969	2.489155	0.000000
H	3.390235	1.242135	0.000000
H	-3.390233	1.242138	0.000000

3
Sum of electronic and zero-point Energies= -385.330982

C	2.066953	1.010099	-0.054075
C	0.792033	1.618097	0.165824
C	-0.324867	-0.626368	0.032144
C	-0.356398	0.854629	0.170420
C	-1.703940	1.248180	0.056821
C	-2.509526	0.112195	-0.199663
C	0.460748	-1.525156	0.940437
C	1.034161	-1.273983	-0.378658
C	-1.701956	-1.010015	-0.275580
C	2.175604	-0.315215	-0.354272
H	2.957498	1.628714	-0.023149
H	0.729794	2.697797	0.278344
H	-2.062806	2.270275	0.119280
H	-3.582496	0.127401	-0.344874
H	0.170313	-2.428015	1.463344
H	1.068488	-2.073927	-1.118512
H	-2.033621	-2.025184	-0.463566
H	3.155951	-0.751840	-0.531253

4
Sum of electronic and zero-point Energies= -385.334574

C	-2.152569	0.761245	0.109892
C	-0.992750	1.564267	-0.032570
C	0.232628	-0.454623	-0.608057
C	0.240682	0.938651	-0.288988
C	1.620956	1.299634	0.003006
C	2.355107	0.158415	0.130399

C	0.299820	-1.257071	0.774867
C	-0.880632	-1.352881	-0.242525
C	1.510251	-1.047293	-0.158237
C	-2.125630	-0.622081	0.042655
H	-3.094529	1.254175	0.330451
H	-1.049693	2.633033	0.152066
H	1.968977	2.306597	0.200100
H	3.406428	0.105001	0.386373
H	0.198946	-0.783733	1.746420
H	-0.975875	-2.322284	-0.734239
H	1.944004	-1.934981	-0.617796
H	-3.045440	-1.187385	0.153978

5

Sum of electronic and zero-point Energies= -385.343445

C	-2.311874	0.653030	0.044656
C	-1.173009	1.461787	0.149627
C	0.158433	-0.588603	-0.059443
C	0.073616	0.857317	0.052052
C	1.405789	1.426399	-0.065723
C	2.310041	0.449984	-0.320644
C	1.218980	-1.293521	0.936486
C	-1.025229	-1.379760	-0.237054
C	1.652146	-0.905427	-0.373176
C	-2.246871	-0.745352	-0.160254
H	-3.290330	1.123062	0.096264
H	-1.271055	2.537344	0.255934
H	1.629352	2.480469	0.051077
H	3.387493	0.562411	-0.367679
H	1.410512	-0.911115	1.934590
H	-0.948813	-2.455440	-0.362634
H	1.875727	-1.637483	-1.147627
H	-3.165022	-1.314364	-0.259084

Norcaradiene-vinylidene mechanism

TS1_6

Sum of electronic and zero-point Energies= -385.315265

C	2.500980	-0.282711	-0.118999
C	1.650038	-1.207189	0.414743
C	-1.617266	0.978046	0.637379
C	0.204225	-0.945075	0.580408
C	-0.690472	-0.989287	-0.610828
C	-2.026940	-0.877388	-0.708603
C	-0.241040	0.513601	0.361780
C	0.713786	1.392076	-0.191795
C	-2.578974	0.283801	-0.016629
C	2.026450	1.011676	-0.456380
H	3.551254	-0.520589	-0.254297
H	2.003339	-2.186131	0.724822
H	-1.791031	1.869053	1.232063
H	-0.252012	-1.472983	1.424763
H	-2.639461	-1.616375	-1.220266

H	0.413444	2.419462	-0.376054
H	-3.640754	0.502969	0.004557
H	2.710498	1.739295	-0.882044

TS2_6

Sum of electronic and zero-point Energies= -385.344795

C	-2.481695	-0.780760	-0.058843
C	-1.256886	-1.407533	-0.041257
C	-0.021618	0.719674	0.030402
C	0.031383	-0.756803	0.051034
C	2.452148	-0.684593	-0.055927
C	2.405949	0.742624	-0.024314
C	-1.279704	1.346523	0.005859
C	-2.473787	0.629031	-0.038666
C	1.211870	1.421694	0.021104
C	1.310354	-1.432572	-0.020413
H	-3.408067	-1.344787	-0.109894
H	-0.520571	-1.138069	1.108994
H	3.415482	-1.181058	-0.114977
H	3.338523	1.297765	-0.040965
H	-1.314543	2.432266	0.006568
H	-3.421164	1.159813	-0.060902
H	1.191814	2.507382	0.035360
H	1.330445	-2.517023	-0.038067

6

Sum of electronic and zero-point Energies= -385.354921

C	-2.461511	-0.822691	-0.133935
C	-1.267904	-1.425922	-0.024432
C	-0.037773	0.730382	0.091491
C	0.013669	-0.768460	0.251402
C	2.448715	-0.681283	-0.135361
C	2.381027	0.747466	-0.084959
C	-1.301437	1.355179	0.032321
C	-2.464045	0.615836	-0.087379
C	1.185973	1.429396	0.032229
C	1.321135	-1.430384	-0.024058
H	-3.389573	-1.370129	-0.271255
H	3.411150	-1.161432	-0.279459
H	3.304725	1.313477	-0.165851
H	-1.349225	2.439877	0.019729
H	-3.417429	1.131940	-0.167513
H	1.172395	2.515307	0.016861
H	0.016334	-0.850602	1.377491
H	1.344517	-2.515551	-0.033920

Cleavage of the 9,10-bond

TS1_7

Sum of electronic and zero-point Energies= -385.266254

C	-2.128633	-1.013859	-0.163315
C	-0.850387	-1.631401	-0.424551
C	0.874189	1.349700	-0.288248

C	0.352759	-1.380771	0.077055
C	1.604948	-1.304035	0.500747
C	2.553774	-0.285031	0.093875
C	-0.344820	1.477051	0.017666
C	-1.704855	1.457999	0.261590
C	2.227514	0.989964	-0.290308
C	-2.475361	0.284049	0.200009
H	-2.972193	-1.677937	-0.336449
H	-0.894726	-2.483261	-1.110986
H	1.964615	-2.054650	1.208489
H	3.609182	-0.543048	0.131766
H	-2.189221	2.393665	0.520415
H	2.978948	1.704907	-0.605306
H	-3.529441	0.443143	0.411969
H	0.378081	2.555183	-0.127013

TS2_7

Sum of electronic and zero-point Energies= -385.313370

C	2.438654	0.638507	0.224553
C	1.241686	1.417509	0.411169
C	-1.227214	-1.405744	0.461463
C	0.000105	1.121165	0.000108
C	-1.241385	1.417918	-0.410956
C	-2.438302	0.638757	-0.224990
C	-0.000124	-1.123119	0.000402
C	1.226756	-1.405679	-0.461362
C	-2.434862	-0.652418	0.209027
C	2.434790	-0.652705	-0.209239
H	3.379968	1.118438	0.473843
H	1.321476	2.327086	1.011310
H	-1.316218	-2.272668	1.122242
H	-1.321147	2.328189	-1.010022
H	-3.379504	1.118713	-0.474645
H	1.315111	-2.271938	-1.123128
H	-3.376877	-1.156199	0.402358
H	3.376565	-1.156767	-0.403008

7

Sum of electronic and zero-point Energies= -385.320044

C	-2.365335	0.629127	-0.260976
C	-1.211316	1.462897	-0.528462
C	1.211334	-1.462946	-0.528411
C	-0.000149	1.375268	-0.000056
C	1.210886	1.462838	0.528699
C	2.365139	0.629559	0.260793
C	0.000156	-1.375169	-0.000035
C	-1.210857	-1.462774	0.528703
C	2.365318	-0.629215	-0.260953
C	-2.365179	-0.629651	0.260702
H	-3.323398	1.066801	-0.528824
H	-1.366629	2.282320	-1.236140
H	1.366526	-2.282202	-1.236307

H	1.365976	2.282114	1.236604
H	3.323129	1.067561	0.528380
H	-1.365829	-2.281837	1.236889
H	3.323347	-1.066733	-0.529170
H	-3.323110	-1.067626	0.528540

Methylene walk

TS1_8

Sum of electronic and zero-point Energies= -385.305800

C	1.859894	1.263158	-0.078846
C	0.515390	1.676854	-0.028034
C	-0.502599	-0.742152	0.016307
C	-0.597205	0.770320	-0.001617
C	-1.927367	1.096741	-0.013724
C	-2.695976	-0.123209	-0.010764
C	0.612091	-1.544738	0.006014
C	1.998693	-1.185046	-0.010103
C	-1.848342	-1.212995	0.011401
C	2.583805	0.066629	-0.026099
H	1.171053	1.694505	1.061440
H	0.316071	2.736782	-0.199503
H	-2.342865	2.097171	-0.034548
H	-3.778783	-0.163614	-0.029754
H	0.423156	-2.615870	0.009247
H	2.691014	-2.023905	0.002558
H	-2.138675	-2.255909	0.015356
H	3.668741	0.137465	-0.012008

TS8_10

Sum of electronic and zero-point Energies= -385.316187

C	1.600318	1.158066	-0.182161
C	0.503900	1.778080	0.503989
C	-0.422625	-0.705294	0.284874
C	-0.528374	0.714588	0.200404
C	-1.847271	1.010850	-0.276308
C	-2.603656	-0.186458	-0.312573
C	0.723858	-1.537484	0.298188
C	1.993551	-1.173385	-0.083182
C	-1.770625	-1.231615	0.042096
C	2.390326	0.172151	-0.511412
H	0.737471	1.957811	1.562423
H	0.187282	2.727327	0.052519
H	-2.219090	2.007473	-0.487380
H	-3.657421	-0.255347	-0.549630
H	0.563373	-2.592140	0.508958
H	2.801575	-1.897788	-0.024536
H	-2.029136	-2.282675	0.091338
H	3.379529	0.338341	-0.937176

TS1_9

Sum of electronic and zero-point Energies= -385.311926

C	-1.954868	-1.239208	-0.188914

C	-0.583158	-1.506735	-0.175890
C	0.591874	0.715150	-0.127260
C	0.564806	-0.776913	0.019847
C	1.891023	-1.196764	0.159942
C	2.741629	-0.057269	0.071228
C	-0.481624	1.563906	-0.064777
C	-1.875693	1.253375	0.139807
C	1.976755	1.082856	-0.117194
C	-2.536571	0.056184	0.131153
H	2.217675	-2.224443	0.263684
H	3.821839	-0.088061	0.144501
H	-0.257521	2.627737	-0.109520
H	-2.501912	2.126256	0.308588
H	2.345045	2.100039	-0.179267
H	-3.608027	0.060623	0.310744
H	-1.406118	-1.967760	0.778462
H	-2.616011	-2.001882	-0.604850

TS9_10

Sum of electronic and zero-point Energies= -385.319063

C	-2.355763	-0.003109	-0.209524
C	-0.763615	-1.294604	-0.243886
C	0.608027	0.750316	0.062688
C	0.457040	-0.683563	-0.255834
C	1.750172	-1.244014	-0.280380
C	2.704181	-0.218971	0.029560
C	-0.436618	1.613689	0.123844
C	-1.781563	1.227600	-0.265734
C	2.048107	0.970033	0.239574
C	-1.899892	-1.237093	0.620415
H	-3.264842	-0.180783	-0.776016
H	1.974330	-2.291313	-0.443435
H	3.775285	-0.373213	0.063843
H	-0.258225	2.663467	0.343379
H	-2.374765	2.014167	-0.730225
H	2.498604	1.935321	0.436987
H	-1.688691	-1.021221	1.675188
H	-2.642157	-2.028135	0.505936

TS10_11

Sum of electronic and zero-point Energies= -385.332293

C	2.041400	0.714823	0.051835
C	0.712699	1.168232	-0.188471
C	-0.135952	-1.085564	-0.212903
C	-0.271150	0.271762	-0.568990
C	-1.659297	0.728608	-0.323139
C	-2.318471	-0.411245	0.224380
C	1.170615	-1.576839	-0.004909
C	2.256438	-0.658002	0.047873
C	-1.446949	-1.503737	0.226414
C	-0.227632	2.118260	0.405879
H	2.847133	1.409676	0.264894

H	-2.200271	1.475239	-0.894594
H	-3.374799	-0.462653	0.459664
H	1.354067	-2.632463	0.173876
H	3.260106	-1.043141	0.195605
H	-1.709136	-2.508003	0.542563
H	-0.237804	2.240691	1.487943
H	-0.669500	2.922866	-0.177766

TS11_12

Sum of electronic and zero-point Energies= -385.318404

C	-2.149153	-0.793134	-0.037005
C	-0.856581	-1.260771	-0.337929
C	0.093839	0.977699	-0.181734
C	0.215645	-0.408287	-0.582983
C	1.611491	-0.860597	-0.318630
C	2.305946	0.410728	0.054990
C	-1.177467	1.470334	0.060473
C	-2.288458	0.582314	0.109444
C	1.441039	1.456057	0.087602
C	0.678146	-1.528497	0.712576
H	-2.999558	-1.462719	0.037300
H	2.112506	-1.566862	-0.976710
H	3.370894	0.455984	0.248052
H	-1.332766	2.522706	0.280704
H	-3.275060	0.991458	0.309084
H	1.686086	2.475963	0.360255
H	0.557151	-1.077145	1.692716
H	0.634064	-2.614471	0.647775

TS12_13

Sum of electronic and zero-point Energies= -385.321964

C	-2.380668	-0.827804	-0.195056
C	-1.108405	-1.374472	-0.142280
C	-0.038848	0.753152	0.164808
C	0.041695	-0.668886	0.097103
C	2.031798	-0.697696	-0.459314
C	2.312006	0.720014	-0.253983
C	-1.288825	1.346678	0.117222
C	-2.455526	0.558995	-0.048203
C	1.253508	1.466122	0.124840
C	1.363293	-1.425490	0.578168
H	-3.265747	-1.430736	-0.371753
H	2.245113	-1.174965	-1.417845
H	3.290044	1.122453	-0.504895
H	-1.380004	2.427055	0.175279
H	-3.423681	1.049234	-0.099920
H	1.311740	2.538981	0.276958
H	1.589261	-1.137364	1.606381
H	1.253108	-2.498339	0.435969

TS6_13

Sum of electronic and zero-point Energies= -385.345674

C	-2.465860	-0.822671	-0.058888
C	-1.262303	-1.426811	-0.008164
C	-0.052373	0.716594	0.033365
C	-0.008778	-0.753854	0.057386
C	2.467965	-0.644133	-0.065392
C	2.393192	0.757166	-0.037905
C	-1.323930	1.348924	0.016784
C	-2.486605	0.613949	-0.030983
C	1.168617	1.415976	0.011857
C	1.309122	-1.416691	-0.036955
H	-3.394908	-1.382176	-0.123213
H	3.429263	-1.142962	-0.130143
H	3.310107	1.337419	-0.060926
H	-1.363628	2.433764	0.025346
H	-3.447433	1.119802	-0.053441
H	1.144029	2.502303	0.017475
H	0.561302	-1.097290	1.105628
H	1.326980	-2.501549	-0.067357

8

Sum of electronic and zero-point Energies= -385.324426

C	1.908618	1.226365	-0.035827
C	0.559646	1.744026	0.088664
C	-0.507420	-0.743243	0.042034
C	-0.589315	0.779895	0.008220
C	-1.903184	1.101956	-0.055686
C	-2.688359	-0.134166	-0.050706
C	0.604260	-1.567518	0.049847
C	1.970161	-1.218295	-0.014269
C	-1.847252	-1.225070	0.019924
C	2.584211	0.056315	-0.079315
H	0.528924	2.271901	1.063150
H	0.423669	2.561828	-0.639517
H	-2.326445	2.098293	-0.094720
H	-3.771000	-0.170036	-0.102465
H	0.401583	-2.635327	0.080851
H	2.659163	-2.061159	-0.021859
H	-2.134704	-2.268211	0.028856
H	3.670608	0.081125	-0.151606

9

Sum of electronic and zero-point Energies= -385.352467

C	-0.673646	-2.284584	0.000000
C	0.563088	-1.511790	0.000000
C	0.000000	0.931285	0.000000
C	0.938111	-0.231323	0.000000
C	2.263360	0.322333	0.000000
C	2.175519	1.713056	0.000000
C	-1.374983	0.908564	0.000000
C	-2.267378	-0.218341	0.000000
C	0.818070	2.087760	0.000000
C	-1.988126	-1.548640	0.000000

H	3.173806	-0.265018	0.000000
H	3.015005	2.396910	0.000000
H	-1.866184	1.880222	0.000000
H	-3.321712	0.044198	0.000000
H	0.445777	3.106759	0.000000
H	-2.842362	-2.224027	0.000000
H	-0.664212	-2.974482	0.863000
H	-0.664212	-2.974482	-0.863000

10

Sum of electronic and zero-point Energies= -385.414787

C	1.757038	-1.174315	0.000000
C	1.400754	0.241939	0.000000
C	-0.971225	-0.485864	0.000000
C	0.000000	0.563273	0.000000
C	-0.716941	1.813435	0.000000
C	-2.088792	1.543962	0.000000
C	-0.587587	-1.809507	0.000000
C	0.804373	-2.151591	0.000000
C	-2.279699	0.149584	0.000000
C	2.384655	1.197486	0.000000
H	2.811372	-1.433762	0.000000
H	-0.274202	2.802514	0.000000
H	-2.875466	2.287306	0.000000
H	-1.330372	-2.603112	0.000000
H	1.090648	-3.197736	0.000000
H	-3.232825	-0.366555	0.000000
H	2.160142	2.259827	0.000000
H	3.435247	0.921118	0.000000

11

Sum of electronic and zero-point Energies= -385.343952

C	1.818907	1.049157	0.172982
C	0.443564	1.221649	-0.183408
C	0.080061	-1.099486	-0.331261
C	-0.267426	0.189388	-0.763948
C	-1.651497	0.579270	-0.350428
C	-2.092676	-0.675418	0.326979
C	1.477249	-1.358518	-0.071266
C	2.328903	-0.261024	0.126487
C	-1.114673	-1.651602	0.265904
C	-0.848967	1.816454	0.363746
H	2.440148	1.875113	0.506849
H	-2.375230	0.951628	-1.080072
H	-3.086916	-0.834533	0.732844
H	1.851286	-2.372525	0.036651
H	3.378802	-0.435882	0.338846
H	-1.187898	-2.640614	0.705488
H	-0.885539	1.815340	1.456295
H	-1.175323	2.782260	-0.031617

12
Sum of electronic and zero-point Energies= -385.338470

C	-2.256405	-0.860791	-0.220674
C	-0.989723	-1.348464	-0.324172
C	0.007210	0.857756	0.079236
C	0.175500	-0.584499	-0.110919
C	1.668096	-0.800051	-0.436049
C	2.247515	0.583683	-0.339253
C	-1.273937	1.378172	0.208950
C	-2.379422	0.525781	0.066522
C	1.304472	1.500648	-0.022062
C	1.276685	-1.344409	0.864888
H	-3.138848	-1.477610	-0.358873
H	1.919423	-1.474384	-1.250439
H	3.315086	0.759287	-0.413161
H	-1.428623	2.440574	0.367958
H	-3.379116	0.945820	0.148126
H	1.476582	2.554893	0.160704
H	1.472132	-0.787027	1.776235
H	1.083425	-2.408506	0.970641

13
Sum of electronic and zero-point Energies= -385.386909

C	-2.554878	-0.479249	0.000000
C	-1.404012	-1.234623	0.000000
C	0.000000	0.687779	0.000000
C	-0.121123	-0.748351	0.000000
C	2.399212	-0.878979	0.000000
C	2.476775	0.487865	0.000000
C	-1.167756	1.503689	0.000000
C	-2.425038	0.931626	0.000000
C	1.288419	1.253226	0.000000
C	1.109366	-1.600016	0.000000
H	-3.538929	-0.940912	0.000000
H	3.306119	-1.478778	0.000000
H	3.437156	0.992144	0.000000
H	-1.054776	2.583802	0.000000
H	-3.315461	1.552349	0.000000
H	1.371542	2.338729	0.000000
H	1.094279	-2.292569	0.861008
H	1.094279	-2.292569	-0.861008

Hydrogen shift

TS1_14
Sum of electronic and zero-point Energies= -385.303362

C	1.927244	1.220711	-0.019483
C	0.575478	1.571956	0.043468
C	-0.587718	-0.775155	0.008406
C	-0.565751	0.763793	0.054439
C	-1.895840	1.141672	0.003044
C	-2.723010	-0.019869	-0.059094

C	0.591265	-1.535053	-0.013701
C	1.961379	-1.317185	-0.035136
C	-1.958180	-1.175554	-0.049153
C	2.541162	-0.045619	-0.061606
H	2.615841	2.060426	-0.040495
H	0.371780	2.640994	0.061477
H	-2.252042	2.164821	-0.014222
H	-3.804752	0.000855	-0.124434
H	-0.059950	-1.423568	1.086861
H	2.612473	-2.187448	-0.013079
H	-2.308007	-2.198540	-0.088332
H	3.628491	-0.035722	-0.094880

TS14_15

Sum of electronic and zero-point Energies= -385.315870

C	2.089019	0.868553	0.144203
C	0.848106	1.534177	0.161916
C	-0.576461	-0.432598	0.923386
C	-0.408917	0.898070	0.258892
C	-1.594429	1.161210	-0.475088
C	-2.415214	0.025647	-0.475292
C	0.099324	-1.249954	-0.040000
C	1.324827	-1.469301	-0.516093
C	-1.856168	-0.966383	0.354384
C	2.321220	-0.468993	-0.193214
H	2.970376	1.502362	0.186638
H	0.858068	2.605300	-0.030857
H	-0.329810	-0.547161	1.983558
H	-1.786775	2.069132	-1.037490
H	-3.334455	-0.079012	-1.039698
H	1.585121	-2.294905	-1.172471
H	-2.303114	-1.908295	0.645501
H	3.352752	-0.749997	-0.393742

TS2_15

Sum of electronic and zero-point Energies= -385.313977

C	2.208322	0.734105	0.076597
C	1.039999	1.382841	0.373557
C	-0.799027	-0.418882	1.116655
C	-0.259148	0.700441	0.239155
C	-1.378062	1.161915	-0.598234
C	-2.372062	0.211490	-0.573996
C	-0.049513	-0.870794	-0.031951
C	1.142619	-1.448386	-0.444831
C	-1.968967	-0.828192	0.313749
C	2.265179	-0.620407	-0.388257
H	3.143921	1.278958	0.155213
H	1.046364	2.440766	0.620229
H	-0.551493	-0.665588	2.145586
H	-1.334139	2.037751	-1.235396
H	-3.257979	0.187070	-1.195800
H	1.204053	-2.479775	-0.778757

H	-2.455291	-1.785852	0.458967
H	3.228520	-1.038119	-0.664706

14
Sum of electronic and zero-point Energies= -385.339394

C	1.980988	1.154750	0.165708
C	0.632056	1.542509	0.047069
C	-0.566023	-0.748030	0.415983
C	-0.503629	0.731648	0.048329
C	-1.805569	1.135737	-0.244947
C	-2.702080	0.025893	-0.183380
C	0.525845	-1.534871	-0.164868
C	1.844728	-1.350798	-0.308499
C	-2.004839	-1.097783	0.163112
C	2.517328	-0.113482	-0.016814
H	2.697676	1.963484	0.274965
H	0.454952	2.607169	-0.099109
H	-0.457643	-0.843331	1.519768
H	-2.100455	2.159220	-0.456184
H	-3.766483	0.078499	-0.377882
H	2.460759	-2.173919	-0.667612
H	-2.406072	-2.095621	0.299383
H	3.604431	-0.168946	-0.023492

15
Sum of electronic and zero-point Energies= -385.332241

C	2.098110	0.712791	0.069584
C	0.963878	1.533036	0.156266
C	-0.549035	-0.220251	1.105494
C	-0.348365	1.007346	0.315664
C	-1.486122	1.213314	-0.535885
C	-2.214362	0.043875	-0.574849
C	-0.151614	-1.202700	0.104395
C	1.001808	-1.509648	-0.516122
C	-1.638498	-0.965706	0.356649
C	2.134990	-0.658239	-0.270305
H	3.054351	1.227567	0.026607
H	1.088052	2.594668	-0.049000
H	-0.297786	-0.328368	2.157956
H	-1.634809	2.067431	-1.187067
H	-3.039531	-0.154731	-1.250697
H	1.094783	-2.330607	-1.221996
H	-2.240143	-1.748845	0.807910
H	3.110342	-1.050018	-0.549069

Spiro-radical mechanism

TS1_16
Sum of electronic and zero-point Energies= -385.301460

C	-0.238283	0.304937	-0.193541
C	0.740672	1.355706	0.148830
C	2.058596	1.051867	0.312718

C	2.521331	-0.279812	0.082863
C	1.675720	-1.306078	-0.321141
C	0.318106	-1.033042	-0.509000
C	-0.863906	-0.387355	1.058937
C	-2.203689	-0.481589	0.938615
C	-2.587560	0.150593	-0.325216
C	-1.498391	0.622320	-0.976542
H	0.366624	2.363317	0.303146
H	2.771326	1.820738	0.591977
H	3.581066	-0.487954	0.207140
H	2.066902	-2.296085	-0.529906
H	-0.359629	-1.781041	-0.907417
H	-2.886678	-0.902872	1.667982
H	-3.611661	0.210697	-0.677476
H	-1.463522	1.087922	-1.954577

TS16_17

Sum of electronic and zero-point Energies= -385.302215

C	0.218130	0.537576	-0.389475
C	-0.144465	-0.869697	-0.618675
C	-1.533512	-1.246795	-0.459220
C	-2.429917	-0.353394	0.064377
C	-2.036769	0.981437	0.389061
C	-0.759224	1.432318	0.151083
C	0.714448	-0.750565	0.810220
C	2.072221	-0.554494	0.824930
C	2.606634	0.247010	-0.270848
C	1.569469	0.879904	-0.832276
H	0.463523	-1.447869	-1.312100
H	-1.849893	-2.229561	-0.793929
H	-3.470011	-0.638519	0.189554
H	-2.778557	1.668394	0.784808
H	-0.476322	2.461511	0.344460
H	0.115232	-1.024816	1.669672
H	2.682236	-0.908140	1.653732
H	3.651703	0.299198	-0.551248

TS6_17

Sum of electronic and zero-point Energies= -385.339696

C	2.484729	0.609140	-0.045957
C	1.330145	1.344447	-0.000507
C	-1.299242	-1.439171	-0.004155
C	0.035070	0.711506	0.043193
C	-1.219671	1.417462	-0.007375
C	-2.405429	0.735188	-0.047424
C	-0.013479	-0.789488	0.048181
C	1.252018	-1.430297	-0.009781
C	-2.445492	-0.693487	-0.045177
C	2.458364	-0.829455	-0.050294
H	3.445684	1.114132	-0.079280
H	1.362241	2.429227	-0.012955
H	-1.320352	-2.523289	-0.023173

H	0.003861	-0.038581	1.121133
H	-1.193571	2.502525	-0.029718
H	-3.338701	1.287868	-0.088426
H	-3.407853	-1.193879	-0.084282
H	3.386624	-1.393072	-0.087518

16
Sum of electronic and zero-point Energies= -385.304766

C	-0.233628	-0.000430	-0.200698
C	0.545941	1.252576	-0.160819
C	1.910064	1.240399	-0.004102
C	2.581759	0.000528	0.067179
C	1.910947	-1.239762	-0.004553
C	0.546815	-1.252886	-0.161421
C	-1.097670	-0.000778	1.136315
C	-2.402650	-0.000252	0.805456
C	-2.590596	0.000525	-0.656841
C	-1.372478	-0.000005	-1.201119
H	-0.009889	2.183507	-0.228921
H	2.473878	2.165576	0.049136
H	3.663585	0.000934	0.180035
H	2.475362	-2.164593	0.048305
H	-0.008276	-2.184185	-0.229976
H	-0.622965	-0.001412	2.108240
H	-3.216780	-0.000384	1.524314
H	-3.545943	0.001069	-1.167522

17
Sum of electronic and zero-point Energies= -385.354222

C	2.490701	0.599678	-0.133045
C	1.352215	1.336358	-0.023887
C	-1.271580	-1.451225	0.027316
C	0.034405	0.687960	0.238443
C	-1.239528	1.411852	-0.019221
C	-2.410106	0.728442	-0.128688
C	-0.016975	-0.810877	0.089941
C	1.221787	-1.441414	0.042884
C	-2.426037	-0.700971	-0.085665
C	2.434505	-0.838589	-0.084242
H	3.451278	1.086552	-0.270595
H	1.384729	2.422212	-0.029890
H	-1.309571	-2.535280	0.011813
H	0.043791	0.766240	1.366890
H	-1.213963	2.498224	-0.028472
H	-3.343694	1.264410	-0.265677
H	-3.381015	-1.212410	-0.166365
H	3.352117	-1.417234	-0.160723

C_2H_2 elimination (Azulene)

TS1_18

Sum of electronic and zero-point Energies= -385.321790

C	1.666138	1.312479	0.212969
C	0.472032	1.778402	-0.283695
C	-0.205481	-0.640119	-0.088546
C	-0.531831	0.782817	-0.271676
C	-1.958351	0.935172	-0.149508
C	-2.512519	-0.301746	0.197307
C	0.902704	-1.481703	-0.623200
C	2.066165	-1.081438	-0.088705
C	-1.490983	-1.254271	0.270802
C	1.547481	-0.008813	0.792072
H	2.636801	1.768360	0.022358
H	0.317643	2.775185	-0.685784
H	-2.486602	1.878435	-0.224949
H	-3.561978	-0.489954	0.387992
H	0.715896	-2.323562	-1.286559
H	3.093562	-1.350941	-0.306045
H	-1.618336	-2.308085	0.490448
H	1.170882	-0.194119	1.795624

TS18_19

Sum of electronic and zero-point Energies= -385.299721

C	-1.859236	0.876148	-0.578751
C	-0.919718	1.606582	0.052286
C	0.110419	-0.476060	-0.432835
C	0.258337	0.753829	0.297182
C	1.699204	0.975733	0.429763
C	2.359944	-0.052650	-0.254716
C	-0.232815	-0.808819	1.194067
C	-1.424260	-1.245120	0.722549
C	1.437302	-0.945852	-0.823853
C	-1.417590	-0.574862	-0.670002
H	-2.846139	1.210382	-0.876619
H	-0.988984	2.644420	0.352788
H	2.163917	1.793923	0.966050
H	3.436035	-0.171456	-0.305768
H	0.420653	-1.085644	2.011426
H	-2.096925	-2.012749	1.096437
H	1.660700	-1.848126	-1.379386
H	-1.818779	-1.184321	-1.479055

TS1_20

Sum of electronic and zero-point Energies= -385.308427

C	-2.083143	0.950771	-0.234092
C	-0.689573	0.835724	0.186514
C	-0.440039	-0.546418	0.452563
C	0.453815	1.612500	0.088388
C	1.752178	1.000924	0.105543
C	-1.605429	-1.283408	0.032621
C	-2.599330	-0.352706	-0.314760
C	0.912953	-0.816590	0.798493

C	2.306820	-0.150042	-0.677175
C	1.769769	-1.320062	-0.302025
H	-2.603022	1.867769	-0.482984
H	0.401708	2.699562	0.041262
H	2.533982	1.671726	0.475922
H	-1.714203	-2.360686	0.053411
H	-3.613613	-0.606236	-0.596775
H	1.333460	-0.549021	1.766550
H	3.132917	0.014063	-1.367766
H	1.860643	-2.321344	-0.706042

TS20_21

Sum of electronic and zero-point Energies= -385.307155

C	-1.486405	0.465733	-0.691306
C	-2.468563	-0.907465	0.992385
C	0.729086	0.793931	0.010297
C	0.578517	-0.625156	-0.348256
C	1.836476	-1.251681	-0.128550
C	2.729888	-0.261847	0.333871
C	-0.447235	1.447198	-0.190286
C	-2.595249	0.208723	0.327193
C	2.083127	0.983749	0.424909
C	-0.698531	-0.850648	-0.781673
H	-1.914493	0.778472	-1.654621
H	-2.854993	-1.630209	1.694707
H	2.079645	-2.297068	-0.278577
H	3.769870	-0.437696	0.581617
H	-0.661817	2.494830	-0.004863
H	-3.418635	0.917486	0.449418
H	2.544434	1.912632	0.738826
H	-1.110677	-1.753672	-1.218009

TS19_21

Sum of electronic and zero-point Energies= -385.275789

C	-1.543317	0.950713	-0.839012
C	-0.589390	1.659557	-0.129754
C	0.246602	-0.484547	-0.611923
C	0.462632	0.769780	0.200418
C	1.816642	0.779548	0.629259
C	2.404225	-0.323849	0.021570
C	-1.135843	-0.587125	1.640964
C	-1.728665	-1.053325	0.580553
C	1.430688	-1.109245	-0.761373
C	-1.243057	-0.531599	-0.814291
H	-2.439741	1.374104	-1.281518
H	-0.636712	2.716634	0.105262
H	2.323657	1.545798	1.199895
H	3.458882	-0.573456	0.086796
H	-0.939366	-0.512717	2.697050
H	-2.500317	-1.825958	0.621399
H	1.659242	-2.025075	-1.290470
H	-1.648749	-1.118783	-1.636870

TS21_P1

Sum of electronic and zero-point Energies= -385.285264

C	-2.031622	0.997886	-0.528095
C	-0.752947	0.795478	-0.014843
C	-0.655314	-0.619389	0.400978
C	0.447347	1.442255	0.306875
C	1.329429	0.466377	0.859905
C	-1.925848	-1.239310	0.099870
C	-2.735152	-0.259432	-0.456828
C	0.566192	-0.832945	0.941910
H	-2.451200	1.921612	-0.909674
H	0.685089	2.490690	0.171204
H	2.087260	0.712397	1.598338
H	-2.203866	-2.271121	0.275670
H	-3.755395	-0.406062	-0.790960
H	0.970648	-1.739826	1.376660
C	2.796260	0.198696	-0.544011
C	2.754990	-0.934666	-1.038696
H	3.321692	1.136802	-0.500404
H	2.585763	-1.934187	-1.383225

18

Sum of electronic and zero-point Energies= -385.344792

C	1.521608	1.303646	0.410731
C	0.425217	1.835096	-0.236814
C	-0.031177	-0.500336	0.089931
C	-0.569002	0.833983	-0.332630
C	-1.976383	0.786200	-0.356902
C	-2.374310	-0.451262	0.209021
C	0.828671	-1.339422	-0.897081
C	1.992295	-1.077992	-0.301323
C	-1.255187	-1.188894	0.592382
C	1.360523	-0.152313	0.749474
H	2.425953	1.860935	0.640298
H	0.320695	2.868226	-0.549252
H	-2.644967	1.588920	-0.647377
H	-3.403561	-0.757652	0.358761
H	0.505338	-1.937490	-1.742281
H	3.024157	-1.350151	-0.488904
H	-1.270829	-2.166412	1.061948
H	1.509685	-0.398605	1.806078

19

Sum of electronic and zero-point Energies= -385.325640

C	1.564937	0.060924	-1.258703
C	0.671859	-0.951054	-1.221746
C	-0.150895	0.785041	-0.028221
C	-0.208589	-0.724392	0.021452
C	-1.680810	-0.987570	0.027727
C	-2.348666	0.233812	-0.010349
C	0.661817	-0.862224	1.285281

C	1.554562	0.150711	1.258398
C	-1.433063	1.327889	-0.044006
C	1.335430	0.971141	-0.032071
H	2.315526	0.246694	-2.018952
H	0.562316	-1.770040	-1.922492
H	-2.155008	-1.962121	0.056612
H	-3.427475	0.348495	-0.014035
H	0.545017	-1.628429	2.042344
H	2.296395	0.392267	2.011567
H	-1.700822	2.377446	-0.076033
H	1.764570	1.970020	-0.065578

20

Sum of electronic and zero-point Energies= -385.349147

C	-2.425279	0.090132	-0.649157
C	-0.979247	-0.774457	0.645484
C	0.691541	0.839187	0.039464
C	0.444917	-0.559895	0.320667
C	1.658920	-1.274973	0.129874
C	2.644864	-0.343031	-0.239664
C	-0.460323	1.563196	0.139983
C	-1.600416	0.670048	0.520954
C	2.090979	0.961190	-0.308479
C	-1.893296	-1.128514	-0.557921
H	-3.186708	0.547801	-1.270695
H	-1.178027	-1.340396	1.561839
H	1.807819	-2.341696	0.244973
H	3.681544	-0.582654	-0.445900
H	-0.571010	2.624182	-0.066922
H	-2.192609	1.039762	1.366227
H	2.628395	1.867415	-0.560821
H	-2.025359	-2.071716	-1.075922

21

Sum of electronic and zero-point Energies= -385.307073

C	2.064182	1.033432	0.418059
C	0.733003	0.776959	-0.016277
C	0.643559	-0.659249	-0.323367
C	-0.464510	1.372380	-0.270537
C	-1.454771	0.322271	-0.750937
C	1.924182	-1.226361	-0.059797
C	2.766969	-0.188298	0.382022
C	-0.611607	-0.951749	-0.758375
H	2.480555	1.988455	0.717554
H	-0.726662	2.417637	-0.141252
H	-1.824388	0.560176	-1.759754
H	2.212848	-2.265254	-0.171355
H	3.807414	-0.311121	0.657783
H	-1.003934	-1.910711	-1.079517
C	-2.644772	0.192221	0.197688
C	-2.653969	-0.710967	1.148512
H	-3.483602	0.878658	0.042836

H	-3.275824	-1.121671	1.931767

C_2H_2 elimination (Naphthalene)

TS2_22
Sum of electronic and zero-point Energies= -385.313245

C	-0.982956	1.618016	0.139545
C	-0.269003	-0.541205	-0.083814
C	0.121277	0.886667	-0.277124
C	1.486666	1.267562	-0.358593
C	2.450298	0.311877	-0.100216
C	0.775422	-1.434013	0.308510
C	2.092677	-1.013184	0.280882
C	-1.679975	0.468797	0.771816
C	-1.562311	-1.088784	-0.679328
C	-2.537439	-0.386704	-0.109002
H	-1.230640	2.672698	0.119951
H	1.749403	2.308323	-0.523614
H	3.501393	0.580797	-0.143136
H	0.543337	-2.477221	0.503241
H	2.883415	-1.721462	0.509170
H	-1.616845	0.323353	1.850743
H	-1.587379	-1.883497	-1.419150
H	-3.610628	-0.337163	-0.253267

TS22_24
Sum of electronic and zero-point Energies= -385.291331

C	0.962754	1.615704	-0.284070
C	0.208064	-0.278375	-0.409995
C	-0.245143	1.011987	0.045584
C	-1.579071	1.237430	0.468076
C	-2.427856	0.150869	0.330554
C	-0.681702	-1.331586	-0.635411
C	-1.995865	-1.092920	-0.216029
C	1.616262	0.306378	-0.726774
C	1.686421	-1.106804	1.045378
C	2.483496	-0.363688	0.328144
H	1.336310	2.635469	-0.255266
H	-1.926737	2.193366	0.845556
H	-3.469301	0.245230	0.622065
H	-0.388970	-2.280428	-1.073403
H	-2.731011	-1.885853	-0.319980
H	2.009602	0.259606	-1.746368
H	1.448114	-1.833185	1.806276
H	3.557833	-0.228176	0.448375

TS2_23
Sum of electronic and zero-point Energies= -385.329329

C	-1.317683	0.998894	0.473975
C	-2.464559	0.667612	-0.431598
C	0.083354	-0.704389	0.080137

C	0.083341	0.704368	0.080121
C	1.261145	1.440607	0.012584
C	2.436457	0.706305	-0.176666
C	1.261144	-1.440622	0.012571
C	-2.464530	-0.667714	-0.431573
C	2.436456	-0.706308	-0.176685
C	-1.317675	-0.998799	0.474106
H	-1.502536	1.631644	1.345178
H	-3.142866	1.390105	-0.876032
H	1.274399	2.523526	0.082827
H	3.378584	1.230632	-0.303051
H	1.274412	-2.523540	0.082832
H	-3.142721	-1.390277	-0.876064
H	3.378582	-1.230632	-0.303095
H	-1.502549	-1.631178	1.345571

TS24_P2

Sum of electronic and zero-point Energies= -385.277340

C	-0.800152	1.646334	0.270718
C	-0.020266	-0.228729	0.513895
C	0.449487	1.003699	-0.044520
C	1.746403	1.158366	-0.532030
C	2.545520	0.010314	-0.446658
C	0.761524	-1.348576	0.620871
C	2.076145	-1.198345	0.110139
C	-1.344414	0.438811	0.820348
H	-1.193610	2.651171	0.163790
H	2.125491	2.088811	-0.940937
H	3.566662	0.046784	-0.813319
H	0.434499	-2.283492	1.064303
H	2.754917	-2.044762	0.153452
H	-1.977546	0.315929	1.694482
C	-2.542938	-1.215757	-0.898022
C	-2.867410	-0.144518	-0.382637
H	-2.124862	-2.124541	-1.280714
H	-3.608933	0.620507	-0.233686

TS17_25

Sum of electronic and zero-point Energies= -385.291457

C	2.535426	0.488700	-0.582246
C	1.572059	1.359561	-0.704186
C	-1.111098	-1.411258	-0.304234
C	-0.266164	0.634814	0.827364
C	-1.473336	1.282763	0.524899
C	-2.471312	0.594794	-0.159529
C	-0.078177	-0.729896	0.397545
C	1.228958	-1.153880	0.483676
C	-2.293968	-0.747870	-0.566757
C	2.452181	-0.747375	0.286946
H	3.481477	0.649831	-1.107335
H	1.243319	2.310338	-1.089434
H	-0.950103	-2.432366	-0.633175

H	0.440794	1.081268	1.519892
H	-1.639227	2.301736	0.860645
H	-3.414410	1.090324	-0.370555
H	-3.092517	-1.254466	-1.099285
H	3.363263	-1.168774	0.698381

TS25_P3a

Sum of electronic and zero-point Energies= -385.290541

C	-3.403332	-0.454038	-0.748123
C	-3.762416	0.711290	-0.842524
C	0.987303	1.204730	0.305021
C	1.096970	-1.252653	0.031762
C	2.414845	-1.138009	-0.364491
C	3.020800	0.130695	-0.427290
C	0.358304	-0.077069	0.371680
C	-0.959976	-0.180384	0.791165
C	2.306696	1.296160	-0.092439
C	-2.156363	-0.273438	1.109836
H	-3.290633	-1.505410	-0.920698
H	-4.023167	1.749863	-0.845003
H	0.418372	2.089084	0.571395
H	0.612217	-2.221129	0.094476
H	2.984995	-2.023844	-0.624265
H	4.058371	0.211416	-0.737903
H	2.794054	2.264063	-0.146107
H	-2.971208	-0.367755	1.800523

22

Sum of electronic and zero-point Energies= -385.315259

C	-0.953180	1.594388	0.322237
C	-0.339392	-0.451313	0.021213
C	0.148136	0.953263	-0.226919
C	1.505070	1.263544	-0.424531
C	2.417034	0.234462	-0.188623
C	0.689057	-1.393759	0.443205
C	2.016653	-1.050407	0.286417
C	-1.593266	0.300840	0.788992
C	-1.492883	-0.981130	-0.871312
C	-2.494327	-0.372692	-0.232942
H	-1.230268	2.634385	0.458478
H	1.841995	2.276132	-0.627902
H	3.478992	0.433641	-0.301911
H	0.412780	-2.402247	0.740090
H	2.789806	-1.779402	0.509165
H	-1.738285	0.156428	1.860959
H	-1.411566	-1.620111	-1.744113
H	-3.560869	-0.282005	-0.401182

23

Sum of electronic and zero-point Energies= -385.336218

C	1.427889	-0.797232	0.642340
C	2.182902	-0.682965	-0.673485

C	-0.050010	0.719811	0.281995
C	-0.050144	-0.719808	0.282047
C	-1.189054	-1.469479	0.021678
C	-2.339269	-0.717787	-0.223102
C	-1.188708	1.469616	0.021565
C	2.183361	0.682940	-0.673093
C	-2.339115	0.718034	-0.223128
C	1.428182	0.796837	0.642532
H	1.784704	-1.417759	1.463104
H	2.507991	-1.431315	-1.389452
H	-1.209960	-2.554239	0.035204
H	-3.281708	-1.225097	-0.407640
H	-1.209682	2.554368	0.035130
H	2.509063	1.431561	-1.388511
H	-3.281479	1.225562	-0.407450
H	1.784873	1.417130	1.463526

24

Sum of electronic and zero-point Energies= -385.294701

C	0.834656	1.590392	-0.207636
C	0.077210	-0.268383	-0.484609
C	-0.400941	0.987921	0.005365
C	-1.730809	1.188186	0.454317
C	-2.540527	0.068871	0.373144
C	-0.726166	-1.382670	-0.554852
C	-2.051384	-1.174134	-0.117697
C	1.488283	0.318339	-0.741528
H	1.233234	2.586735	-0.026519
H	-2.094695	2.140677	0.825464
H	-3.577825	0.125646	0.686674
H	-0.399660	-2.349551	-0.923025
H	-2.746850	-2.008540	-0.157869
H	1.799205	0.372492	-1.790949
C	2.474030	-1.032260	1.118713
C	2.638678	-0.201969	0.123818
H	1.776264	-1.589652	1.723983
H	3.632142	0.156437	-0.151961

25

Sum of electronic and zero-point Energies= -385.314493

C	-3.443596	-0.000182	0.000011
C	-3.388680	0.002562	1.317892
C	1.022484	-1.245069	-0.130747
C	1.020965	1.244229	-0.133647
C	2.365460	1.231690	0.173827
C	3.031449	0.001333	0.326970
C	0.318936	-0.000969	-0.292299
C	-1.008436	-0.002319	-0.590393
C	2.367114	-1.230205	0.176478
C	-2.269689	-0.001822	-0.899492
H	-4.406069	-0.000921	-0.518364
H	-4.085137	0.004424	2.146001

H	0.479360	-2.176302	-0.253672
H	0.476652	2.174524	-0.258409
H	2.910146	2.161741	0.297442
H	4.090925	0.002319	0.568785
H	2.913052	-2.159254	0.301972
H	-2.474971	-0.002019	-1.975359

P3a

Sum of electronic and zero-point Energies= -385.312590

C	3.420908	-0.213552	0.153196
C	3.501479	0.680541	1.107130
C	-0.955176	1.169351	-0.382781
C	-1.062054	-1.263372	0.126906
C	-2.406065	-1.131305	0.408969
C	-3.019734	0.129797	0.295110
C	-0.306596	-0.108560	-0.274540
C	1.020820	-0.228048	-0.557448
C	-2.301212	1.273847	-0.098884
C	2.280646	-0.351312	-0.818268
H	4.232572	-0.918340	-0.030243
H	2.986323	1.517802	1.554575
H	-0.373710	2.031824	-0.691713
H	-0.559185	-2.221814	0.202671
H	-2.990264	-1.992702	0.715011
H	-4.079424	0.222916	0.516824
H	-2.806727	2.230495	-0.178068
H	2.552320	-0.614504	-1.845391

H_2 elimination (azulene)

TS1_26

Sum of electronic and zero-point Energies= -385.313153

C	-1.905795	-1.238133	0.276369
C	-0.543524	-1.631470	-0.073587
C	0.484439	0.748154	0.106475
C	0.491758	-0.744367	-0.093546
C	1.882471	-1.123957	-0.182120
C	2.672645	-0.004593	0.008301
C	-0.571820	1.646565	0.015667
C	-1.919189	1.293082	-0.260421
C	1.840157	1.130673	0.185136
C	-2.367245	0.066338	0.115034
H	-0.347271	-2.690491	-0.221586
H	2.229904	-2.139198	-0.331208
H	3.755558	0.011081	0.017366
H	-0.329636	2.706501	0.073293
H	-2.598592	2.034282	-0.673236
H	2.186644	2.148567	0.322870
H	-2.494341	-1.930092	0.883862
H	-2.785643	-0.994395	-0.655208

TS26_P10

Sum of electronic and zero-point Energies= -385.259030

C	1.876419	-1.093480	0.062744
C	0.574405	-1.625509	-0.076102
C	-0.484193	0.730135	0.091232
C	-0.489814	-0.751761	-0.082558
C	-1.872506	-1.143736	-0.156250
C	-2.679720	-0.018659	0.011920
C	0.553127	1.652478	0.047196
C	1.923658	1.364501	-0.215553
C	-1.863874	1.110869	0.168707
C	2.391265	0.107720	0.014517
H	0.409352	-2.696683	-0.172715
H	-2.214047	-2.163467	-0.289308
H	-3.762491	-0.016437	0.017662
H	0.276708	2.702259	0.130788
H	2.569627	2.159432	-0.582850
H	-2.208673	2.129729	0.301575
H	2.807045	-2.102970	0.308157
H	2.549869	-2.007218	1.091564

TS26_27

Sum of electronic and zero-point Energies= -385.306536

C	2.033378	-1.204970	-0.043502
C	0.636691	-1.613383	0.001600
C	-0.531841	0.765581	0.037541
C	-0.498238	-0.758005	-0.007466
C	-1.810144	-1.180799	-0.045017
C	-2.666663	-0.036437	-0.029381
C	0.512414	1.659422	0.026842
C	1.914358	1.363507	-0.035997
C	-1.903935	1.121890	0.029477
C	2.454004	0.123094	-0.061667
H	2.768546	-2.007469	-0.073077
H	1.259777	-1.532408	1.091591
H	-2.144085	-2.210899	-0.083831
H	-3.749042	-0.077065	-0.063203
H	0.254144	2.716149	0.040896
H	2.591364	2.216481	-0.074298
H	-2.279315	2.137282	0.049432
H	0.458464	-2.681468	-0.122089

TS27_P9

Sum of electronic and zero-point Energies= -385.246691

C	2.068708	1.246543	-0.000090
C	0.704328	1.377554	0.000011
C	-0.528309	-0.813396	-0.000025
C	-0.487125	0.721879	0.000013
C	-1.813214	1.167015	0.000010
C	-2.652099	0.040330	-0.000025
C	0.549886	-1.683689	-0.000015
C	1.928115	-1.357649	0.000055
C	-1.890967	-1.138513	-0.000014

C	2.402711	-0.084989	0.000018
H	2.776615	2.070666	-0.000399
H	-2.129557	2.202967	0.000002
H	-3.734754	0.083173	-0.000048
H	0.310237	-2.744651	0.000015
H	2.646052	-2.175869	0.000180
H	-2.279543	-2.149303	0.000018
H	0.359390	2.931373	0.392740
H	0.359364	2.931128	-0.392143

TS1_28

Sum of electronic and zero-point Energies= -385.305913

C	1.739088	1.348438	-0.080709
C	0.389276	1.709132	-0.008249
C	-0.476044	-0.753251	-0.008176
C	-0.621350	0.774341	-0.003333
C	-2.010578	1.051430	0.008676
C	-2.691111	-0.155906	-0.000549
C	0.692630	-1.543741	0.007291
C	2.020378	-1.166606	0.000917
C	-1.762358	-1.249035	-0.005432
C	2.526676	0.181152	-0.053554
H	0.143764	2.768857	0.021299
H	-2.448656	2.041187	0.012607
H	-3.769673	-0.266846	-0.001708
H	0.511372	-2.616790	0.023021
H	2.776542	-1.944317	0.029800
H	-2.034574	-2.297484	-0.004449
H	2.390086	0.826941	1.034146
H	3.591500	0.312725	-0.256002

TS28_P10

Sum of electronic and zero-point Energies= -385.251987

C	1.696495	1.335524	0.080750
C	0.434233	1.685329	-0.309964
C	-0.442896	-0.679650	-0.025460
C	-0.596152	0.756669	-0.051497
C	-2.015478	1.033562	0.070716
C	-2.713906	-0.177943	0.161002
C	0.693134	-1.500029	-0.203117
C	2.032610	-1.138657	-0.129940
C	-1.795091	-1.221228	0.077711
C	2.347938	0.203744	0.190684
H	0.212347	2.659277	-0.743153
H	-2.447550	2.027499	0.078364
H	-3.786855	-0.283636	0.255602
H	0.492169	-2.551345	-0.399199
H	2.803699	-1.882039	-0.317585
H	-2.025327	-2.280588	0.079746
H	3.264443	0.169491	1.307145
H	3.641745	0.357421	0.573780

TS8_P11

Sum of electronic and zero-point Energies= -385.248212

C	1.804999	1.216079	-0.073043
C	0.561175	1.521484	0.197182
C	-0.453886	-0.686781	0.119914
C	-0.598741	0.734240	0.044931
C	-1.990929	1.033002	-0.174539
C	-2.706796	-0.178248	-0.186607
C	0.710865	-1.467650	0.254885
C	2.056384	-1.132774	0.050330
C	-1.812682	-1.228021	-0.002112
C	2.537352	0.128211	-0.409553
H	0.445472	2.372869	1.363963
H	0.363856	2.789791	0.629711
H	-2.411382	2.025429	-0.290415
H	-3.777387	-0.271823	-0.314149
H	0.532887	-2.523908	0.447923
H	2.778770	-1.939546	0.154369
H	-2.055556	-2.283665	0.034351
H	3.476898	0.193596	-0.954081

TS9_P11

Sum of electronic and zero-point Energies= -385.257545

C	1.827353	-1.139134	0.054996
C	0.564883	-1.493915	0.096047
C	-0.590187	0.682317	0.138400
C	-0.590626	-0.786866	-0.054649
C	-1.950869	-1.192854	-0.204867
C	-2.768694	-0.060782	-0.048734
C	0.496524	1.536774	0.065359
C	1.881493	1.264296	-0.151311
C	-1.974011	1.070478	0.168116
C	2.548758	0.052896	-0.151411
H	2.709047	-2.224106	0.230768
H	2.709378	-1.956067	1.011361
H	-2.282751	-2.213344	-0.349812
H	-3.850549	-0.063686	-0.100238
H	0.256373	2.596830	0.123412
H	2.497919	2.140995	-0.331624
H	-2.329917	2.089804	0.263996
H	3.622755	0.030310	-0.319538

TS9_29

Sum of electronic and zero-point Energies= -385.306209

C	1.885425	-1.347678	-0.034876
C	0.509950	-1.564239	-0.034611
C	-0.589032	0.735308	0.011540
C	-0.607458	-0.807344	-0.009268
C	-1.963024	-1.192440	-0.013150
C	-2.743838	-0.035115	0.006838
C	0.531210	1.571279	-0.012717
C	1.887345	1.249362	-0.035610

C	-1.919352	1.123391	0.020718
C	2.514806	-0.027877	-0.026963
H	2.564886	-2.197250	-0.070409
H	2.338514	-0.623747	1.068476
H	-2.320851	-2.213245	-0.030015
H	-3.827831	-0.018883	0.007915
H	0.309353	2.636747	-0.022419
H	2.578857	2.085627	-0.060052
H	-2.274850	2.146847	0.032735
H	3.595730	-0.043977	-0.157639

TS29_P9

Sum of electronic and zero-point Energies= -385.247420

C	1.935226	-1.354383	-0.193315
C	0.580991	-1.488382	-0.058011
C	-0.624274	0.724842	-0.128914
C	-0.568192	-0.781134	0.064418
C	-1.900059	-1.215785	0.197518
C	-2.751636	-0.097735	0.047141
C	0.454447	1.579012	-0.056148
C	1.816558	1.226419	0.162778
C	-2.000016	1.061588	-0.158137
C	2.302791	-0.044862	0.039327
H	2.599085	-2.120294	-0.586662
H	-2.210681	-2.243317	0.335531
H	-3.833266	-0.138006	0.097074
H	0.252326	2.646923	-0.082239
H	2.504236	2.021804	0.430473
H	-2.392501	2.066610	-0.254910
H	3.814972	0.105119	-0.115037
H	3.790804	0.003687	0.675832

TS29_30

Sum of electronic and zero-point Energies= -385.308096

C	1.903053	-1.370600	-0.010300
C	0.555718	-1.567188	-0.008438
C	-0.602067	0.725796	0.005769
C	-0.594341	-0.814991	-0.000831
C	-1.917729	-1.211838	-0.006818
C	-2.743766	-0.045007	0.001736
C	0.485844	1.565360	-0.017375
C	1.869857	1.224044	-0.065086
C	-1.963039	1.105684	0.012327
C	2.514251	-0.073934	-0.031593
H	2.575169	-2.225298	0.002008
H	-2.268429	-2.235692	-0.016467
H	-3.827737	-0.063324	-0.002293
H	0.284171	2.633788	-0.023434
H	2.565279	2.057129	-0.131498
H	-2.325800	2.126078	0.016874
H	3.593002	-0.044514	-0.180321
H	2.357663	0.527875	1.058768

TS30_P13

Sum of electronic and zero-point Energies= -385.236622

C	-1.833643	-1.470604	-0.002374
C	-0.455730	-1.585135	0.050134
C	0.588838	0.738991	-0.083944
C	0.641917	-0.786268	0.005475
C	2.012826	-1.122682	0.067335
C	2.762243	0.055106	0.012232
C	-0.580156	1.504579	0.035854
C	-1.769992	0.870180	-0.099490
C	1.910175	1.183246	-0.070600
C	-2.535932	-0.238698	-0.004141
H	-2.435726	-2.358668	-0.189939
H	2.400123	-2.130173	0.141037
H	3.844801	0.104381	0.027270
H	-0.533682	2.579454	0.199995
H	2.227307	2.218660	-0.098014
H	-3.612416	-0.228102	-0.153057
H	-3.190470	2.474311	0.680635
H	-3.143215	2.447842	-0.070818

TS30_31

Sum of electronic and zero-point Energies= -385.307912

C	1.893427	-1.377833	-0.016098
C	0.506568	-1.562218	0.023077
C	-0.590105	0.721007	-0.001915
C	-0.610773	-0.806081	0.031214
C	-1.975201	-1.186167	0.016825
C	-2.744282	-0.029661	-0.028141
C	0.574972	1.538925	0.001551
C	1.967369	1.140916	-0.060529
C	-1.902678	1.129894	-0.033078
C	2.547938	-0.159594	-0.045323
H	2.513750	-2.273004	-0.021716
H	-2.335992	-2.205904	0.026816
H	-3.827205	-0.000389	-0.061467
H	0.411995	2.609429	-0.120320
H	2.659363	1.978430	-0.102431
H	-2.252322	2.155224	-0.064441
H	3.633782	-0.178351	-0.071773
H	1.193218	1.459446	1.089839

TS31_P12

Sum of electronic and zero-point Energies= -385.242786

C	-1.947874	-1.359826	0.000120
C	-0.582309	-1.555639	-0.000100
C	0.618785	0.728275	-0.000067
C	0.574751	-0.853260	-0.000202
C	1.926204	-1.226113	-0.000038
C	2.738045	-0.085385	0.000064
C	-0.597197	1.288806	-0.000022

C	-1.953549	1.168722	-0.000102
C	1.961803	1.087473	0.000109
C	-2.564564	-0.105735	0.000138
H	-2.593822	-2.235458	0.000182
H	2.257515	-2.256735	0.000172
H	3.821423	-0.097982	0.000110
H	-2.578392	2.054765	-0.000428
H	2.327372	2.107212	0.000079
H	-3.650932	-0.087230	0.000156
H	-0.313866	2.995607	0.385432
H	-0.313875	2.995912	-0.385107

26

Sum of electronic and zero-point Energies= -385.353797

C	2.392720	-0.055083	0.000000
C	1.347951	1.023555	0.000000
C	-0.847594	-0.342568	0.000000
C	0.000000	0.885231	0.000000
C	-0.922605	1.994234	0.000000
C	-2.225795	1.518843	0.000000
C	-0.481946	-1.672641	0.000000
C	0.850562	-2.207470	0.000000
C	-2.187884	0.107620	0.000000
C	1.951870	-1.448040	0.000000
H	1.753200	2.034900	0.000000
H	-0.623963	3.036643	0.000000
H	-3.123856	2.123478	0.000000
H	-1.290300	-2.402381	0.000000
H	0.952020	-3.291770	0.000000
H	-3.055095	-0.544042	0.000000
H	3.062164	0.110546	0.863782
H	3.062164	0.110546	-0.863782

27

Sum of electronic and zero-point Energies= -385.341289

C	-1.827862	-1.214866	-0.474573
C	-0.644811	-1.676359	0.383289
C	0.419512	0.765301	-0.017022
C	0.489698	-0.717417	0.120859
C	1.857635	-1.080010	0.048863
C	2.635192	0.067361	-0.110085
C	-0.659053	1.645187	0.059150
C	-2.031613	1.246661	0.173889
C	1.768527	1.198850	-0.135994
C	-2.259585	-0.028561	-0.157042
H	-2.080941	-1.731183	-1.397371
H	-0.351821	-2.702287	0.142586
H	2.231181	-2.094851	0.116075
H	3.714029	0.102409	-0.199062
H	-0.426294	2.704881	0.158542
H	-2.766713	1.915938	0.611439
H	2.085012	2.231264	-0.236196

H	-0.890293	-1.663041	1.455983

28
Sum of electronic and zero-point Energies= -385.320916

C	1.696245	1.335537	0.053402
C	0.458107	1.682737	-0.304522
C	-0.472220	-0.697828	-0.047538
C	-0.599566	0.739351	-0.101595
C	-1.996321	1.051462	0.058463
C	-2.721570	-0.146047	0.163924
C	0.678191	-1.509274	-0.199659
C	1.998038	-1.140245	-0.122340
C	-1.820725	-1.215119	0.077635
C	2.539405	0.179462	0.356439
H	0.224102	2.703990	-0.602224
H	-2.407704	2.054053	0.067823
H	-3.796242	-0.228106	0.265277
H	0.486348	-2.561188	-0.403807
H	2.743259	-1.881410	-0.402502
H	-2.074215	-2.268882	0.099349
H	2.727554	0.152083	1.445137
H	3.539392	0.349248	-0.074309

29
Sum of electronic and zero-point Energies= -385.343173

C	1.855987	-1.249235	-0.371134
C	0.574573	-1.424128	-0.202858
C	-0.583335	0.664753	-0.246857
C	-0.605655	-0.804545	-0.090398
C	-1.955399	-1.178441	0.216309
C	-2.745997	-0.013798	0.181865
C	0.569071	1.498385	-0.231314
C	1.868085	1.173158	0.121836
C	-1.929217	1.098282	-0.073767
C	2.477817	-0.165208	0.504658
H	2.401398	-1.649569	-1.223424
H	2.317863	-0.344442	1.578296
H	-2.306859	-2.190247	0.379251
H	-3.815485	0.018374	0.349360
H	0.381620	2.554401	-0.413411
H	2.556188	2.014301	0.184792
H	-2.251283	2.133566	-0.062565
H	3.560981	-0.131718	0.357670

30
Sum of electronic and zero-point Energies= -385.352121

C	-0.588885	-2.290252	0.000000
C	0.594777	-1.534360	0.000000
C	0.000000	0.915331	0.000000
C	0.960451	-0.231305	0.000000
C	2.257256	0.328875	0.000000
C	2.156984	1.737985	0.000000

C	-1.354215	0.867467	0.000000
C	-2.274462	-0.309893	0.000000
C	0.814471	2.098966	0.000000
C	-1.835999	-1.739157	0.000000
H	-0.500715	-3.374412	0.000000
H	3.177222	-0.243945	0.000000
H	2.996040	2.422426	0.000000
H	-1.881100	1.821104	0.000000
H	-2.963905	-0.181543	0.855000
H	0.427325	3.111977	0.000000
H	-2.673227	-2.436010	0.000000
H	-2.963905	-0.181543	-0.855000

31
Sum of electronic and zero-point Energies= -385.332079

C	1.942295	-1.243585	0.273226
C	0.641485	-1.375192	0.267015
C	-0.592990	0.640461	0.346802
C	-0.576245	-0.809512	0.239015
C	-1.889777	-1.212473	-0.212674
C	-2.689322	-0.045715	-0.311943
C	0.661726	1.428973	0.542605
C	1.790206	1.085340	-0.457447
C	-1.906217	1.072643	-0.025865
C	2.392245	-0.109389	-0.583152
H	2.633885	-1.814055	0.890310
H	-2.204087	-2.229825	-0.412711
H	-3.734517	-0.031286	-0.595493
H	0.450369	2.499351	0.502490
H	2.154754	1.922102	-1.048049
H	-2.219217	2.107520	-0.102222
H	3.235469	-0.253163	-1.253911
H	1.042912	1.210035	1.554094

H_2 elimination (naphthalene)

TS17_32
Sum of electronic and zero-point Energies= -385.346302

C	-2.445344	-0.847282	-0.039466
C	-1.203564	-1.425209	0.015671
C	-0.011366	0.676532	0.057972
C	0.032405	-0.795629	0.036299
C	2.448801	-0.699644	-0.032149
C	2.415143	0.726982	-0.055906
C	-1.341201	1.322982	-0.037461
C	-2.508714	0.561866	-0.064351
C	1.232393	1.411071	-0.012277
C	1.293758	-1.444699	0.016056
H	-3.354947	-1.441169	-0.062304
H	3.410588	-1.202179	-0.057430
H	3.349301	1.276375	-0.115411

H	-1.369350	2.408347	-0.058131
H	-3.467849	1.066929	-0.124398
H	1.205349	2.496852	-0.022016
H	1.322435	-2.528892	0.023144
H	-0.569389	1.001924	1.110215

TS32_33

Sum of electronic and zero-point Energies= -385.361017

C	-2.431734	-0.882594	-0.016217
C	-1.192228	-1.425571	-0.007102
C	0.016324	0.672422	-0.005197
C	0.055470	-0.771792	-0.002032
C	2.468628	-0.685057	0.002697
C	2.430909	0.727243	-0.005383
C	-1.261506	1.316131	-0.048278
C	-2.482366	0.555580	-0.043703
C	1.224020	1.402200	-0.003646
C	1.303035	-1.431083	0.006997
H	-3.348570	-1.462962	-0.011502
H	3.429098	-1.190928	0.006195
H	3.360965	1.286571	-0.010687
H	-1.327332	2.397882	-0.139297
H	-3.426304	1.081239	-0.172638
H	1.197356	2.488194	-0.008870
H	1.330899	-2.515312	0.016160
H	-1.999427	1.050445	1.051829

TS33_34

Sum of electronic and zero-point Energies= -385.351581

C	-2.423009	-0.846807	-0.028522
C	-1.167852	-1.423460	-0.036854
C	0.002552	0.689937	-0.012211
C	0.053477	-0.772900	-0.014993
C	2.469126	-0.690470	0.008305
C	2.426991	0.732173	0.010907
C	-1.244084	1.344393	-0.029636
C	-2.454351	0.637102	-0.033118
C	1.229750	1.407867	0.004249
C	1.313339	-1.433844	-0.001796
H	-3.351026	-1.405626	-0.110050
H	3.432281	-1.191056	0.014593
H	3.359297	1.288167	0.019049
H	-1.275936	2.429420	-0.053070
H	-3.414827	1.136601	-0.119639
H	1.205002	2.493555	0.008484
H	1.338713	-2.518054	-0.002122
H	-2.529127	-0.096948	1.044774

TS2_34

Sum of electronic and zero-point Energies= -385.360847

C	2.462124	0.676930	-0.003385
C	1.271678	1.351254	-0.000051

C	-0.063237	-0.753890	-0.009311
C	-0.002861	0.691574	-0.006941
C	-1.219226	1.404063	0.004330
C	-2.427313	0.726490	0.001817
C	-1.305082	-1.425066	-0.002856
C	1.188915	-1.393396	-0.066981
C	-2.472469	-0.684368	-0.002440
C	2.449524	-0.769803	-0.055933
H	3.417550	1.189432	0.020107
H	1.278480	2.437921	0.010690
H	-1.197359	2.489819	0.020855
H	-3.356133	1.288437	0.006522
H	-1.327273	-2.509614	-0.012306
H	-3.432567	-1.190212	-0.003780
H	1.967395	-1.301486	1.030756
H	3.357586	-1.347029	-0.222347

TS13_35

Sum of electronic and zero-point Energies= -385.360454

C	-2.481823	-0.821623	-0.009570
C	-1.256749	-1.418917	-0.006538
C	-0.073802	0.692151	0.000610
C	-0.034558	-0.751627	-0.005706
C	2.442599	-0.637465	-0.043619
C	2.379928	0.792457	-0.019146
C	-1.331112	1.335535	0.011220
C	-2.504735	0.599438	0.003388
C	1.158718	1.417848	-0.008331
C	1.233070	-1.410308	-0.045798
H	-3.407403	-1.389834	-0.017747
H	3.391746	-1.154811	-0.160466
H	3.304159	1.358658	-0.022141
H	-1.369952	2.420445	0.022951
H	-3.463469	1.110088	0.007567
H	1.114176	2.503856	-0.004353
H	1.290230	-2.492002	-0.137615
H	1.951299	-1.141330	1.052747

TS35_36

Sum of electronic and zero-point Energies= -385.352134

C	-2.478360	-0.825687	0.007966
C	-1.264077	-1.425682	0.002718
C	-0.070429	0.691865	-0.009032
C	-0.021998	-0.770380	-0.009003
C	2.414124	-0.715312	-0.034673
C	2.373710	0.752718	-0.033828
C	-1.339606	1.338836	0.002290
C	-2.504101	0.607484	0.007020
C	1.134344	1.412164	-0.029518
C	1.211974	-1.438794	-0.029223
H	-3.407050	-1.389500	0.013279
H	3.377513	-1.210388	-0.104964

H	3.308600	1.299432	-0.107311
H	-1.373930	2.423909	0.004593
H	-3.464947	1.113906	0.011250
H	1.115615	2.497579	-0.056166
H	1.237868	-2.523053	-0.054653
H	2.472845	0.024841	1.045669

TS36_37

Sum of electronic and zero-point Energies= -385.359984

C	-2.480479	-0.816977	0.005830
C	-1.257721	-1.421027	0.011562
C	-0.081989	0.672424	-0.005226
C	-0.025352	-0.770770	0.001515
C	2.422379	-0.754333	-0.019502
C	2.406357	0.676570	-0.042573
C	-1.330515	1.332993	-0.008014
C	-2.506973	0.603889	-0.008469
C	1.156578	1.385255	-0.045218
C	1.236112	-1.443475	-0.008070
H	-3.406698	-1.384796	0.012315
H	3.375776	-1.269828	-0.023581
H	3.326024	1.244411	-0.161175
H	-1.361069	2.418506	-0.016309
H	-3.464212	1.116594	-0.016314
H	1.170055	2.469302	-0.135352
H	1.236672	-2.529276	-0.004237
H	1.893072	1.147790	1.053640

TS17_37

Sum of electronic and zero-point Energies= -385.345675

C	-2.460129	-0.833978	-0.030030
C	-1.246370	-1.434899	0.017432
C	-0.055193	0.675935	0.055740
C	-0.001343	-0.794897	0.035250
C	2.435373	-0.715515	-0.036633
C	2.431713	0.687367	-0.063725
C	-1.341241	1.338554	-0.011639
C	-2.493114	0.602034	-0.055290
C	1.232030	1.395890	-0.037779
C	1.248407	-1.440201	0.012203
H	-3.387327	-1.400022	-0.049868
H	3.382776	-1.244478	-0.060113
H	3.364211	1.238423	-0.126855
H	-1.371141	2.423925	-0.019523
H	-3.454190	1.104262	-0.113175
H	1.204839	2.481551	-0.066218
H	1.270947	-2.525427	0.015694
H	0.489085	1.040028	1.106895

TS33_P4

Sum of electronic and zero-point Energies= -385.286697

C	-2.294288	0.287319	0.000000

C	-1.333443	1.229035	0.000000
C	0.129407	-0.751808	0.000000
C	0.000000	0.693366	0.000000
C	1.168613	1.488400	0.000000
C	2.405411	0.876566	0.000000
C	1.416988	-1.347220	0.000000
C	-1.088605	-1.417409	0.000000
C	2.529331	-0.534843	0.000000
C	-2.402509	-1.093966	0.000000
H	-3.892335	1.103101	0.384000
H	-3.892335	1.103101	-0.384000
H	-1.527324	2.294875	0.000000
H	1.080689	2.570503	0.000000
H	3.302608	1.487663	0.000000
H	1.507059	-2.427706	0.000000
H	3.518521	-0.981123	0.000000
H	-3.282307	-1.727051	0.000000

TS34_P15

Sum of electronic and zero-point Energies= -385.281595

C	2.460281	0.712332	-0.025251
C	1.228129	1.372292	-0.003273
C	-0.063672	-0.767099	-0.059306
C	-0.020761	0.683003	-0.003693
C	-1.251573	1.380982	0.018470
C	-2.461166	0.692620	0.053373
C	-1.305920	-1.441481	-0.042565
C	1.198789	-1.383778	-0.034360
C	-2.488851	-0.710349	0.022717
C	2.286213	-0.663063	-0.011568
H	3.404988	1.230588	-0.146554
H	1.226187	2.458356	-0.041564
H	-1.246730	2.466496	-0.025864
H	-3.392719	1.248797	0.080391
H	-1.320286	-2.526020	-0.060984
H	-3.441038	-1.231307	0.022653
H	3.650086	-1.434605	0.735903
H	3.630699	-1.465058	-0.051247

TS37_P19

Sum of electronic and zero-point Energies= -385.283159

C	2.522741	0.580121	-0.000001
C	1.360056	1.315978	-0.000043
C	-0.013196	-0.826286	-0.000020
C	0.100902	0.672374	-0.000078
C	-1.180618	1.116025	0.000050
C	-2.436755	0.667928	-0.000066
C	-1.272702	-1.478971	0.000037
C	1.248227	-1.388006	0.000038
C	-2.450433	-0.768867	0.000040
C	2.483669	-0.847307	0.000019
H	3.485243	1.082067	0.000010

H	-1.197849	3.126746	-0.378508
H	1.385780	2.400363	-0.000096
H	-3.338373	1.268489	-0.000286
H	-1.286378	-2.563185	0.000049
H	-3.416558	-1.263634	0.000054
H	3.394664	-1.437913	0.000002
H	-1.197870	3.129135	0.378920

TS38_39

Sum of electronic and zero-point Energies= -385.360863

C	0.057227	0.758880	0.000483
C	1.263869	1.506211	0.012564
C	0.134729	-0.678207	-0.005526
C	1.386328	-1.337683	-0.007474
C	2.425744	0.791678	0.004315
C	2.558157	-0.594410	-0.008863
C	-1.222435	1.398072	-0.009367
C	-1.089153	-1.417407	-0.041762
C	-2.397403	0.689752	-0.020509
C	-2.354879	-0.738809	-0.044633
H	1.241479	2.592519	0.025292
H	1.423956	-2.423818	-0.014875
H	3.530418	-1.078041	-0.017732
H	-1.252173	2.484326	-0.004502
H	-1.077143	-2.500899	-0.136179
H	-3.359324	1.189409	-0.024032
H	-3.262371	-1.326895	-0.156862
H	-1.817944	-1.205065	1.053523

TS39_40

Sum of electronic and zero-point Energies= -385.346439

C	0.031389	0.782750	0.030728
C	1.252132	1.522046	0.010741
C	0.110553	-0.680624	0.052590
C	1.398222	-1.342638	-0.009443
C	2.403487	0.807846	-0.034376
C	2.544221	-0.590978	-0.056954
C	-1.236586	1.393892	0.011898
C	-1.161992	-1.430979	-0.034391
C	-2.409954	0.649075	-0.035917
C	-2.378336	-0.753225	-0.062568
H	1.229864	2.608469	0.016416
H	1.435063	-2.428615	-0.012442
H	3.520976	-1.062245	-0.114228
H	-1.288829	2.478916	0.017504
H	-1.107571	-2.515367	-0.061688
H	-3.367105	1.160458	-0.057420
H	-3.298083	-1.325342	-0.123805
H	-0.443133	-1.059262	1.101812

TS40_41

Sum of electronic and zero-point Energies= -385.345648

C	-0.003934	0.781433	0.030524
C	1.203581	1.517192	0.005912
C	0.066332	-0.683191	0.049431
C	1.398145	-1.324612	-0.034026
C	2.387667	0.827649	-0.041054
C	2.560082	-0.543335	-0.065156
C	-1.283454	1.396036	0.015626
C	-1.159481	-1.448161	-0.010075
C	-2.423510	0.630153	-0.028511
C	-2.358762	-0.795635	-0.051394
H	1.173410	2.604295	0.008339
H	1.436128	-2.410461	-0.062405
H	3.536867	-1.014354	-0.121947
H	-1.342100	2.479976	0.023529
H	-1.104678	-2.532655	-0.018200
H	-3.395464	1.113060	-0.050313
H	-3.279645	-1.367258	-0.107166
H	0.655493	-1.017765	1.100503

TS41_42
Sum of electronic and zero-point Energies= -385.357418

C	-0.024899	0.756445	-0.000548
C	1.194931	1.519452	-0.009714
C	0.040022	-0.682775	-0.006679
C	1.318470	-1.322375	-0.040824
C	2.378296	0.864325	-0.029559
C	2.532703	-0.535319	-0.039299
C	-1.289337	1.383135	0.012380
C	-1.153852	-1.439301	-0.008973
C	-2.440932	0.617240	0.005628
C	-2.375141	-0.794312	-0.008686
H	1.141738	2.606042	-0.000511
H	1.397792	-2.403347	-0.138306
H	3.495649	-1.027257	-0.158612
H	-1.346738	2.467207	0.023968
H	-1.101963	-2.524113	-0.017077
H	-3.410666	1.105348	0.010467
H	-3.292801	-1.373606	-0.017031
H	2.035421	-1.049370	1.054747

TS2_42
Sum of electronic and zero-point Energies= -385.350146

C	2.434859	0.633997	0.005406
C	1.289049	1.390829	0.001546
C	-1.287673	-1.354928	-0.023186
C	0.016639	0.755018	-0.009478
C	-1.179719	1.506727	-0.028137
C	-2.372839	0.811646	-0.052290
C	-0.048478	-0.703260	-0.005787
C	1.171584	-1.443848	0.005858
C	-2.499411	-0.619137	-0.043137
C	2.376760	-0.790052	0.007373

H	3.403893	1.123622	0.009003
H	1.337826	2.475237	0.003273
H	-1.337309	-2.440065	-0.030543
H	-1.156652	2.592871	-0.038190
H	-2.611589	0.107522	1.038426
H	1.127559	-2.528613	0.010129
H	-3.470221	-1.094794	-0.153385
H	3.301865	-1.357734	0.012280

TS2_43

Sum of electronic and zero-point Energies= -385.360746

C	2.439676	0.630081	0.000741
C	1.278111	1.385219	0.001334
C	-0.041558	-0.700488	-0.002460
C	0.031715	0.733355	-0.004367
C	-1.213298	1.471559	-0.060547
C	-2.406129	0.728009	-0.062830
C	-1.314174	-1.357421	-0.010927
C	1.163545	-1.437240	0.005480
C	-2.512372	-0.671863	-0.013425
C	2.381188	-0.778918	0.005196
H	3.404447	1.127506	-0.000117
H	1.323025	2.470226	-0.001752
H	-1.228333	2.549111	-0.218260
H	-1.961374	1.330814	1.027562
H	-1.332023	-2.444968	0.004729
H	1.124524	-2.522323	0.011496
H	-3.473692	-1.172480	0.017124
H	3.303203	-1.351655	0.010046

TS43_44

Sum of electronic and zero-point Energies= -385.345256

C	-2.427956	0.620971	-0.055627
C	-1.294749	1.386946	-0.012929
C	0.070783	-0.721312	0.036390
C	-0.007806	0.740018	0.054591
C	1.281382	1.495139	-0.037591
C	2.430866	0.749815	-0.078381
C	1.333096	-1.352935	0.012366
C	-1.144958	-1.453319	0.020728
C	2.526032	-0.629187	-0.046884
C	-2.355593	-0.801719	-0.029209
H	-3.398905	1.102681	-0.113825
H	-1.342983	2.471678	-0.021434
H	0.545905	1.130368	1.097611
H	1.250453	2.580889	-0.074929
H	1.370595	-2.439296	0.025468
H	-1.101290	-2.538060	0.030347
H	3.485436	-1.137931	-0.070837
H	-3.275791	-1.376829	-0.053122

TS44_45

Sum of electronic and zero-point Energies= -385.346344

C	0.037100	0.746183	0.054283
C	1.272596	1.514172	-0.020622
C	0.105713	-0.719479	0.033983
C	1.380617	-1.353322	0.013199
C	2.410446	0.794140	-0.059124
C	2.538722	-0.605970	-0.037922
C	-1.299001	1.369206	-0.037544
C	-1.097071	-1.448134	0.016126
C	-2.444223	0.575907	-0.063298
C	-2.339164	-0.821415	-0.035073
H	1.243633	2.600524	-0.038193
H	1.424892	-2.438683	0.022846
H	3.513759	-1.083724	-0.063139
H	-1.349760	2.453927	-0.058396
H	-1.045710	-2.533234	0.023795
H	-3.415326	1.056129	-0.123638
H	-3.241497	-1.424153	-0.056248
H	-0.524399	1.061485	1.108926

TS45_46

Sum of electronic and zero-point Energies= -385.360400

C	0.065771	0.741781	-0.006210
C	1.262611	1.504923	-0.009096
C	0.127038	-0.696128	0.000150
C	1.388443	-1.338991	0.010887
C	2.427349	0.796982	-0.009457
C	2.557271	-0.589497	0.004065
C	-1.219426	1.365460	-0.044469
C	-1.087672	-1.450055	-0.008932
C	-2.416645	0.570884	-0.041003
C	-2.324723	-0.856093	-0.020625
H	1.233328	2.591356	-0.017981
H	1.433783	-2.424416	0.021982
H	3.530761	-1.071316	0.008968
H	-1.307870	2.446141	-0.128656
H	-1.016844	-2.534403	-0.004434
H	-3.374765	1.070761	-0.161636
H	-3.235289	-1.443897	-0.024839
H	-1.943215	1.070181	1.054736

TS38_46

Sum of electronic and zero-point Energies= -385.352884

C	0.052667	0.760168	-0.008310
C	1.271162	1.511188	0.003565
C	0.123548	-0.695961	-0.008784
C	1.396073	-1.343003	0.002670
C	2.423398	0.798894	0.007148
C	2.555786	-0.598056	0.007587
C	-1.199719	1.394254	-0.028587
C	-1.064227	-1.443910	-0.028218
C	-2.389141	0.648515	-0.034408

C	-2.319151	-0.816904	-0.036638
H	1.245569	2.597477	0.006376
H	1.436582	-2.428622	0.004562
H	3.531410	-1.075304	0.011658
H	-1.256668	2.478085	-0.052951
H	-1.018987	-2.528349	-0.051884
H	-3.360790	1.126363	-0.113046
H	-3.241569	-1.384756	-0.105559
H	-2.437917	-0.076000	1.044697

TS41_P4

Sum of electronic and zero-point Energies= -385.285520

C	0.028872	-0.813133	0.000000
C	1.312138	-1.451856	0.000000
C	0.000000	0.642971	0.000000
C	1.282023	1.164060	0.000000
C	2.384252	-0.634805	0.000000
C	2.560976	0.751302	0.000000
C	-1.206267	-1.504555	0.000000
C	-1.238610	1.332154	0.000000
C	-2.394207	-0.807146	0.000000
C	-2.409043	0.610218	0.000000
H	1.400437	-2.534179	0.000000
H	1.164966	2.937856	0.384480
H	1.164966	2.937856	-0.384480
H	3.489732	1.310229	0.000000
H	-1.196299	-2.590311	0.000000
H	-1.250439	2.417367	0.000000
H	-3.334925	-1.348395	0.000000
H	-3.359238	1.134312	0.000000

TS42_P20

Sum of electronic and zero-point Energies= -385.281939

C	2.471857	0.573757	0.035435
C	1.324336	1.359300	0.035060
C	-0.044423	-0.682963	-0.030836
C	0.047216	0.758962	0.010620
C	-1.151272	1.549416	-0.047511
C	-2.352678	0.889668	0.065733
C	-1.325538	-1.310611	-0.024498
C	1.144254	-1.454366	-0.029620
C	-2.368932	-0.417643	-0.098797
C	2.382207	-0.829549	0.006404
H	3.446961	1.049666	0.066015
H	1.403535	2.441943	0.063884
H	-1.090587	2.618568	-0.241595
H	-1.439085	-2.385975	0.074870
H	1.077357	-2.537658	-0.066095
H	3.287496	-1.428062	0.002834
H	-3.726193	-1.107401	-0.103849
H	-3.721651	-1.266899	0.672000

TS43_P15

Sum of electronic and zero-point Energies= -385.281077

C	2.437478	0.617098	-0.009092
C	1.271443	1.376081	-0.060020
C	-0.055910	-0.716532	0.007526
C	0.025739	0.732636	-0.063677
C	-1.267094	1.297912	-0.094330
C	-2.413201	0.692512	0.026347
C	-1.314756	-1.376437	0.042275
C	1.163614	-1.442258	0.028011
C	-2.539009	-0.684988	-0.024250
C	2.384828	-0.786493	0.033716
H	3.399091	1.120460	-0.021605
H	1.322525	2.461001	-0.074094
H	-1.330975	-2.463337	0.055689
H	1.126255	-2.527735	0.018246
H	-3.481092	-1.204305	-0.172316
H	3.305771	-1.359635	0.055029
H	-1.222171	2.897616	0.802718
H	-1.278195	2.818753	0.017295

32

Sum of electronic and zero-point Energies= -385.389398

C	2.435143	-0.922784	0.000000
C	1.134175	-1.424633	0.000000
C	0.000000	0.677731	0.000000
C	-0.082112	-0.761561	0.000000
C	-2.497365	-0.665246	0.000000
C	-2.414140	0.741718	0.000000
C	1.351199	1.332754	0.000000
C	2.539415	0.445471	0.000000
C	-1.185124	1.406038	0.000000
C	-1.343297	-1.420509	0.000000
H	3.303792	-1.574012	0.000000
H	-3.468806	-1.148139	0.000000
H	-3.329316	1.326633	0.000000
H	1.439851	2.017441	0.863000
H	3.518985	0.919411	0.000000
H	-1.158251	2.492287	0.000000
H	-1.373468	-2.504936	0.000000
H	1.439851	2.017441	-0.863000

33

Sum of electronic and zero-point Energies= -385.382044

C	2.386147	-0.963623	0.000000
C	1.156399	-1.483831	0.000000
C	0.000000	0.680665	0.000000
C	-0.074660	-0.781535	0.000000
C	-2.482551	-0.608741	0.000000
C	-2.429149	0.809837	0.000000
C	1.239989	1.283869	0.000000
C	2.507562	0.529885	0.000000

C	-1.214519	1.446930	0.000000
C	-1.334703	-1.393628	0.000000
H	3.293280	-1.562144	0.000000
H	-3.453515	-1.096149	0.000000
H	-3.351745	1.380434	0.000000
H	1.306147	2.370231	0.000000
H	3.116946	0.866567	0.860959
H	-1.150501	2.531415	0.000000
H	-1.404652	-2.475895	0.000000
H	3.116946	0.866567	-0.860959

34

Sum of electronic and zero-point Energies= -385.384481

C	2.446751	0.663355	0.000000
C	1.287497	1.359485	0.000000
C	-0.074267	-0.756852	0.000000
C	0.000000	0.705764	0.000000
C	-1.206189	1.415941	0.000000
C	-2.421597	0.738108	0.000000
C	-1.346445	-1.422647	0.000000
C	1.121846	-1.402467	0.000000
C	-2.498755	-0.678056	0.000000
C	2.458584	-0.839364	0.000000
H	3.409950	1.165611	0.000000
H	1.302278	2.445449	0.000000
H	-1.189704	2.501639	0.000000
H	-3.343618	1.312821	0.000000
H	-1.368066	-2.507389	0.000000
H	-3.469184	-1.162756	0.000000
H	3.026891	-1.227489	0.865673
H	3.026891	-1.227489	-0.865673

35

Sum of electronic and zero-point Energies= -385.381682

C	2.574576	-0.578456	0.000000
C	1.424228	-1.290600	0.000000
C	0.000000	0.708877	0.000000
C	0.113286	-0.751369	0.000000
C	-2.369100	-0.924933	0.000000
C	-2.428729	0.558545	0.000000
C	1.182991	1.462085	0.000000
C	2.429142	0.841887	0.000000
C	-1.304159	1.314543	0.000000
C	-1.025459	-1.524752	0.000000
H	3.559032	-1.036084	0.000000
H	-2.937197	-1.336489	0.857159
H	-3.410210	1.022883	0.000000
H	1.124367	2.545960	0.000000
H	3.326891	1.455199	0.000000
H	-1.365548	2.398935	0.000000
H	-0.940781	-2.608878	0.000000
H	-2.937197	-1.336489	-0.857159

36
Sum of electronic and zero-point Energies= -385.380892

C	2.557589	-0.497026	0.000000
C	1.417192	-1.254162	0.000000
C	0.000000	0.684086	0.000000
C	0.118778	-0.775730	0.000000
C	-2.290638	-1.055626	0.000000
C	-2.482167	0.416146	0.000000
C	1.185852	1.498615	0.000000
C	2.432941	0.926076	0.000000
C	-1.260853	1.237825	0.000000
C	-1.053332	-1.608215	0.000000
H	3.543355	-0.956211	0.000000
H	-3.178945	-1.679908	0.000000
H	-3.112234	0.725034	0.858000
H	1.073015	2.578784	0.000000
H	3.328146	1.539625	0.000000
H	-1.376753	2.320163	0.000000
H	-0.916522	-2.684453	0.000000
H	-3.112234	0.725034	-0.858000

37
Sum of electronic and zero-point Energies= -385.386459

C	2.573958	-0.559918	0.000000
C	1.421977	-1.284409	0.000000
C	0.000000	0.682797	0.000000
C	0.121719	-0.753081	0.000000
C	-2.341209	-1.018336	0.000000
C	-2.510714	0.339494	0.000000
C	1.158508	1.453600	0.000000
C	2.420451	0.848415	0.000000
C	-1.372148	1.284514	0.000000
C	-1.033369	-1.554813	0.000000
H	3.559669	-1.014790	0.000000
H	-3.194454	-1.688060	0.000000
H	-3.510873	0.765992	0.000000
H	1.089146	2.537592	0.000000
H	3.309572	1.473611	0.000000
H	-1.491683	1.965421	0.863000
H	-0.904735	-2.634764	0.000000
H	-1.491683	1.965421	-0.863000

38
Sum of electronic and zero-point Energies= -385.383185

C	0.204293	-0.746607	0.000000
C	1.527478	-1.229339	0.000000
C	0.000000	0.698821	0.000000
C	1.126377	1.597615	0.000000
C	2.525522	-0.291101	0.000000
C	2.410105	1.103081	0.000000
C	-0.927330	-1.635015	0.000000

C	-1.287529	1.185245	0.000000
C	-2.193532	-1.154699	0.000000
C	-2.466705	0.303804	0.000000
H	1.732944	-2.296218	0.000000
H	0.941933	2.668843	0.000000
H	3.279082	1.753470	0.000000
H	-0.738700	-2.704323	0.000000
H	-1.459113	2.259865	0.000000
H	-3.044715	-1.828930	0.000000
H	-3.111756	0.578235	0.858000
H	-3.111756	0.578235	-0.858000

39

Sum of electronic and zero-point Energies= -385.385760

C	0.207950	-0.725266	0.000000
C	1.537608	-1.255834	0.000000
C	0.000000	0.694621	0.000000
C	1.099052	1.553334	0.000000
C	2.551561	-0.349057	0.000000
C	2.400746	1.031806	0.000000
C	-0.908624	-1.582430	0.000000
C	-1.402429	1.221138	0.000000
C	-2.245100	-1.124419	0.000000
C	-2.490743	0.221838	0.000000
H	1.701480	-2.330248	0.000000
H	0.952643	2.630310	0.000000
H	3.259816	1.697472	0.000000
H	-0.728724	-2.655885	0.000000
H	-1.557496	1.896133	0.862000
H	-3.058125	-1.842562	0.000000
H	-3.512211	0.594267	0.000000
H	-1.557496	1.896133	-0.862000

40

Sum of electronic and zero-point Energies= -385.355524

C	0.011578	0.797118	0.083901
C	1.223070	1.531744	0.020433
C	0.090785	-0.691997	0.241644
C	1.411609	-1.338838	-0.018777
C	2.373048	0.813221	-0.094163
C	2.540814	-0.585501	-0.143249
C	-1.261488	1.403735	0.029794
C	-1.167413	-1.449318	-0.016010
C	-2.400062	0.632111	-0.082985
C	-2.353550	-0.797343	-0.127315
H	1.207755	2.618393	-0.000085
H	1.454076	-2.425295	-0.014685
H	3.517843	-1.037673	-0.284360
H	-1.329447	2.487222	0.013613
H	-1.113808	-2.534414	-0.018673
H	-3.365502	1.124052	-0.162228
H	-3.274509	-1.354855	-0.263252

H	0.093250	-0.767022	1.370030

41
Sum of electronic and zero-point Energies= -385.355524

C	0.013245	-0.751270	0.000000
C	1.256016	-1.421056	0.000000
C	0.000000	0.686511	0.000000
C	1.290680	1.454007	0.000000
C	2.446181	-0.696230	0.000000
C	2.546671	0.647215	0.000000
C	-1.208460	-1.482265	0.000000
C	-1.229172	1.338921	0.000000
C	-2.410366	-0.807007	0.000000
C	-2.416227	0.602210	0.000000
H	1.274533	-2.510283	0.000000
H	1.326915	2.140006	0.866000
H	3.500963	1.169905	0.000000
H	-1.176799	-2.567853	0.000000
H	-1.270089	2.424475	0.000000
H	-3.348255	-1.352290	0.000000
H	-3.365586	1.129826	0.000000
H	1.326915	2.140006	-0.866000

42
Sum of electronic and zero-point Energies= -385.381904

C	2.436703	0.676284	0.000000
C	1.262681	1.381775	0.000000
C	-0.018730	-0.770926	0.000000
C	0.000000	0.690084	0.000000
C	-1.184003	1.391768	0.000000
C	-2.401416	-0.739155	0.000000
C	1.205476	-1.452166	0.000000
C	2.400893	-0.743223	0.000000
C	-1.284523	-1.473038	0.000000
C	-2.509232	0.719860	0.000000
H	3.392180	1.189743	0.000000
H	1.262074	2.467866	0.000000
H	-1.172853	2.480404	0.000000
H	1.216125	-2.537521	0.000000
H	3.338751	-1.291916	0.000000
H	-1.290102	-2.560150	0.000000
H	-3.096632	1.082000	0.864600
H	-3.096632	1.082000	-0.864600

43
Sum of electronic and zero-point Energies= -385.388550

C	2.398813	-0.721316	0.000000
C	1.191019	-1.427696	0.000000
C	0.000000	0.696874	0.000000
C	-0.014082	-0.737492	0.000000
C	-1.345807	-1.460678	0.000000
C	-2.485280	-0.554939	0.000000

C	-1.213950	1.413896	0.000000
C	1.242291	1.391497	0.000000
C	-2.492517	0.795684	0.000000
C	2.428276	0.685176	0.000000
H	3.333723	-1.274240	0.000000
H	1.201063	-2.513905	0.000000
H	-1.419579	-2.137622	0.869000
H	-1.419579	-2.137622	-0.869000
H	-1.168619	2.502160	0.000000
H	1.242237	2.477618	0.000000
H	-3.401014	1.390340	0.000000
H	3.379189	1.207235	0.000000

44

Sum of electronic and zero-point Energies= -385.354430

C	-2.426515	0.614377	-0.129596
C	-1.309281	1.382958	-0.022367
C	0.090077	-0.732879	0.091579
C	0.014370	0.755948	0.230760
C	1.285690	1.516540	-0.042295
C	2.405764	0.791509	-0.142508
C	1.357483	-1.362800	0.033614
C	-1.116352	-1.461059	0.040878
C	2.513103	-0.613031	-0.103759
C	-2.329414	-0.809617	-0.077975
H	-3.398668	1.077543	-0.264222
H	-1.363842	2.467986	-0.026101
H	0.026161	0.852389	1.357358
H	1.256313	2.603257	-0.049198
H	1.408041	-2.448029	0.030126
H	-1.077600	-2.546163	0.033225
H	3.479764	-1.101117	-0.197261
H	-3.239721	-1.397541	-0.153920

45

Sum of electronic and zero-point Energies= -385.387739

C	0.205446	-0.718561	0.000000
C	1.513332	-1.211438	0.000000
C	0.000000	0.703446	0.000000
C	1.108953	1.602032	0.000000
C	2.523110	-0.275108	0.000000
C	2.402528	1.108710	0.000000
C	-0.983702	-1.630372	0.000000
C	-1.315490	1.198870	0.000000
C	-2.314201	-0.984300	0.000000
C	-2.464889	0.374306	0.000000
H	1.718128	-2.279046	0.000000
H	0.924678	2.673239	0.000000
H	3.266270	1.766180	0.000000
H	-0.934577	-2.319259	0.862000
H	-1.455137	2.278272	0.000000
H	-3.185583	-1.634547	0.000000

H	-3.449717	0.828914	0.000000
H	-0.934577	-2.319259	-0.862000

46
Sum of electronic and zero-point Energies= -385.380709

C	0.197448	-0.725786	0.000000
C	1.538645	-1.266036	0.000000
C	0.000000	0.719141	0.000000
C	1.126723	1.560999	0.000000
C	2.552309	-0.371395	0.000000
C	2.411815	1.020741	0.000000
C	-0.905342	-1.551242	0.000000
C	-1.333279	1.258376	0.000000
C	-2.279904	-1.027078	0.000000
C	-2.420203	0.448879	0.000000
H	1.691159	-2.342206	0.000000
H	0.992671	2.638728	0.000000
H	3.281921	1.672468	0.000000
H	-0.772783	-2.631304	0.000000
H	-1.448331	2.338078	0.000000
H	-2.824958	-1.468964	0.857000
H	-3.423990	0.862566	0.000000
H	-2.824958	-1.468964	-0.857000

C4H2 Elimination

TS2_47
Sum of electronic and zero-point Energies= -385.344795

C	-2.481695	-0.780760	-0.058843
C	-1.256886	-1.407533	-0.041257
C	-0.021618	0.719674	0.030402
C	0.031383	-0.756803	0.051034
C	2.452148	-0.684593	-0.055927
C	2.405949	0.742624	-0.024314
C	-1.279704	1.346523	0.005859
C	-2.473787	0.629031	-0.038666
C	1.211870	1.421694	0.021104
C	1.310354	-1.432572	-0.020413
H	-3.408067	-1.344787	-0.109894
H	-0.520571	-1.138069	1.108994
H	3.415482	-1.181058	-0.114977
H	3.338523	1.297765	-0.040965
H	-1.314543	2.432266	0.006568
H	-3.421164	1.159813	-0.060902
H	1.191814	2.507382	0.035360
H	1.330445	-2.517023	-0.038067

TS47_48
Sum of electronic and zero-point Energies= -385.293581

C	-0.124917	-0.610814	0.209935
C	-0.245122	0.788771	0.482623
C	-1.453464	1.436268	0.297366

C	-2.578582	0.706454	-0.127376
C	-2.500467	-0.683395	-0.338208
C	-1.300177	-1.341063	-0.149104
C	1.108085	-1.314375	0.240182
C	2.406010	-0.812776	0.114431
C	2.777850	0.515756	-0.234063
C	2.077268	1.611767	-0.563050
H	0.572402	1.327883	0.954514
H	-1.543209	2.494919	0.517016
H	-3.527764	1.216731	-0.262164
H	-3.382330	-1.234652	-0.647770
H	-1.224854	-2.410175	-0.324867
H	1.039095	-2.399017	0.299715
H	3.218735	-1.525333	0.221873
H	3.849017	0.750081	-0.354723

TS48_49

Sum of electronic and zero-point Energies= -385.292081

C	-0.253836	-0.556307	-0.000713
C	-0.276837	0.876681	-0.001944
C	-1.479590	1.548586	-0.001292
C	-2.694876	0.829301	0.000551
C	-2.702928	-0.578366	0.001571
C	-1.505715	-1.261406	0.000831
C	0.918899	-1.352934	-0.000994
C	2.273864	-1.003861	-0.000893
C	2.826001	0.279342	0.000791
C	3.199130	1.511750	0.002650
H	0.643812	1.444802	-0.003873
H	-1.496503	2.633437	-0.002312
H	-3.636043	1.371632	0.001051
H	-3.644278	-1.117562	0.002895
H	-1.495519	-2.347452	0.001616
H	0.749191	-2.426916	-0.001209
H	2.987059	-1.824507	-0.002211
H	4.067605	0.509852	0.000696

TS44_49

Sum of electronic and zero-point Energies= -385.360746

C	2.439676	0.630081	0.000741
C	1.278111	1.385219	0.001334
C	-0.041558	-0.700488	-0.002460
C	0.031715	0.733355	-0.004367
C	-1.213298	1.471559	-0.060547
C	-2.406129	0.728009	-0.062830
C	-1.314174	-1.357421	-0.010927
C	1.163545	-1.437240	0.005480
C	-2.512372	-0.671863	-0.013425
C	2.381188	-0.778918	0.005196
H	3.404447	1.127506	-0.000117
H	1.323025	2.470226	-0.001752
H	-1.228333	2.549111	-0.218260

H	-1.961374	1.330814	1.027562
H	-1.332023	-2.444968	0.004729
H	1.124524	-2.522323	0.011496
H	-3.473692	-1.172480	0.017124
H	3.303203	-1.351655	0.010046

TS49_50

Sum of electronic and zero-point Energies= -385.289778

C	2.856890	0.829248	0.008803
C	1.667186	1.571712	-0.002177
C	0.404117	-0.486847	-0.015410
C	0.441690	0.920982	-0.011974
C	-4.153911	0.834824	0.016007
C	-3.148927	0.112954	-0.014192
C	-0.857239	-1.241573	-0.043928
C	1.600942	-1.229863	0.001393
C	-2.145751	-0.738718	-0.092904
C	2.823911	-0.568088	0.008682
H	3.812023	1.345593	0.016074
H	1.703730	2.656297	-0.007472
H	-0.479451	1.496194	-0.028418
H	-5.018432	1.468788	0.044733
H	-0.770758	-2.318483	-0.220970
H	1.567953	-2.316167	0.002057
H	-1.495905	-1.222206	1.053891
H	3.747396	-1.137800	0.014298

TS50_51

Sum of electronic and zero-point Energies= -385.273550

C	2.965843	0.707009	-0.101658
C	1.842669	1.541731	0.017271
C	0.430326	-0.421109	0.097067
C	0.576928	0.993936	0.124462
C	-4.461779	0.602920	-0.090801
C	-3.332513	0.087441	-0.053267
C	-0.975813	-1.092794	0.005183
C	1.574536	-1.261945	0.004793
C	-2.136882	-0.434537	-0.013849
C	2.830142	-0.688245	-0.105855
H	3.954196	1.148921	-0.183958
H	1.965266	2.619822	0.022617
H	-0.300843	1.626351	0.214921
H	-5.444228	1.027807	-0.124441
H	-0.928534	-2.173689	-0.133350
H	-0.288050	-0.792473	1.085294
H	1.454609	-2.341557	0.010579
H	3.706837	-1.321618	-0.191731

47

Sum of electronic and zero-point Energies= -385.354921

C	-2.461511	-0.822691	-0.133935
C	-1.267904	-1.425922	-0.024432

C	-0.037773	0.730382	0.091491
C	0.013669	-0.768460	0.251402
C	2.448715	-0.681283	-0.135361
C	2.381027	0.747466	-0.084959
C	-1.301437	1.355179	0.032321
C	-2.464045	0.615836	-0.087379
C	1.185973	1.429396	0.032229
C	1.321135	-1.430384	-0.024058
H	-3.389573	-1.370129	-0.271255
H	3.411150	-1.161432	-0.279459
H	3.304725	1.313477	-0.165851
H	-1.349225	2.439877	0.019729
H	-3.417429	1.131940	-0.167513
H	1.172395	2.515307	0.016861
H	0.016334	-0.850602	1.377491
H	1.344517	-2.515551	-0.033920

48
Sum of electronic and zero-point Energies= -385.294134

C	0.000000	0.580707	0.000000
C	-0.520484	-0.748065	0.000000
C	-1.879739	-0.972318	0.000000
C	-2.773861	0.121733	0.000000
C	-2.296016	1.443080	0.000000
C	-0.935177	1.671562	0.000000
C	1.375047	0.927116	0.000000
C	2.544652	0.155900	0.000000
C	2.710702	-1.256972	0.000000
C	1.898228	-2.313890	0.000000
H	0.135215	-1.624013	0.000000
H	-2.265913	-1.986241	0.000000
H	-3.843917	-0.065002	0.000000
H	-2.992627	2.274711	0.000000
H	-0.551478	2.687775	0.000000
H	1.569329	1.997537	0.000000
H	3.470208	0.724162	0.000000
H	3.739083	-1.662044	0.000000

49
Sum of electronic and zero-point Energies= -385.373134

C	-2.798939	0.454704	0.000000
C	-2.020723	-0.722334	0.000000
C	0.000000	0.636509	0.000000
C	-0.644816	-0.642309	0.000000
C	2.494975	-2.696458	0.000000
C	2.416423	-1.477438	0.000000
C	1.404820	0.830061	0.000000
C	-0.815636	1.816855	0.000000
C	2.460692	-0.089381	0.000000
C	-2.191586	1.724279	0.000000
H	-3.882516	0.378608	0.000000
H	-2.510746	-1.690411	0.000000

H	-0.048921	-1.545774	0.000000
H	2.555058	-3.765824	0.000000
H	1.728275	1.868483	0.000000
H	-0.332002	2.789356	0.000000
H	3.463025	0.338479	0.000000
H	-2.803435	2.620156	0.000000

50
Sum of electronic and zero-point Energies= -385.300252

C	2.954602	0.753046	-0.000037
C	1.796461	1.550209	0.000034
C	0.428598	-0.435453	0.000039
C	0.536665	0.958744	0.000071
C	-4.409974	0.669261	-0.000213
C	-3.283524	0.109255	0.000120
C	-0.900063	-1.158596	0.000061
C	1.589790	-1.235428	-0.000060
C	-2.130754	-0.449063	0.000098
C	2.848055	-0.638748	-0.000073
H	3.932726	1.223841	-0.000079
H	1.884647	2.632136	0.000048
H	-0.353547	1.581228	0.000161
H	-5.384728	1.118965	-0.000197
H	-0.950779	-1.859467	-0.861031
H	1.503640	-2.319284	-0.000108
H	-0.950823	-1.859549	0.861092
H	3.739731	-1.257234	-0.000122

51
Sum of electronic and zero-point Energies= -385.293726

C	-2.032725	-1.227399	-0.509691
C	-1.340607	-1.421298	0.711870
C	-0.682207	0.966365	0.673945
C	-0.703128	-0.365445	1.303220
C	3.660893	-1.014859	-0.498054
C	2.760304	-0.206358	-0.272893
C	0.808674	1.457221	0.236747
C	-1.505677	1.116745	-0.537384
C	1.807712	0.683107	-0.035279
C	-2.123739	0.035725	-1.122700
H	-2.521078	-2.078094	-0.977863
H	-1.332895	-2.403607	1.172945
H	-0.164237	-0.490487	2.238420
H	4.457330	-1.701624	-0.695920
H	0.857725	2.541731	0.171787
H	-0.931898	1.734057	1.422000
H	-1.573153	2.103143	-0.988374
H	-2.688804	0.152062	-2.041691

C3H3 elimination

TS25_52

Sum of electronic and zero-point Energies= -385.276661

C	-3.082525	0.000009	0.186832
C	-3.441333	0.000679	1.385073
C	0.993376	-1.236498	-0.201048
C	0.993073	1.236272	-0.201825
C	2.302339	1.219172	0.241557
C	2.962543	0.000344	0.466182
C	0.304276	-0.000269	-0.426004
C	-0.983547	-0.000585	-0.902485
C	2.302625	-1.218786	0.242366
C	-2.289526	-0.000542	-1.036489
H	-4.277381	0.001500	0.218301
H	-3.861360	-0.000039	2.375773
H	0.479418	-2.173791	-0.385998
H	0.478873	2.173317	-0.387361
H	2.822116	2.156533	0.413163
H	3.991941	0.000577	0.810585
H	2.822627	-2.155908	0.414600
H	-2.824042	-0.000967	-1.984018

TS25_53

Sum of electronic and zero-point Energies= -385.245941

C	-3.063918	0.129721	0.195675
C	-3.750374	0.791642	0.964101
C	1.333736	-1.273548	0.291680
C	0.695678	0.963141	-0.546843
C	1.977352	1.409814	-0.289365
C	2.925368	0.537658	0.272723
C	0.344846	-0.394817	-0.253547
C	-0.917953	-0.884501	-0.515632
C	2.602084	-0.795627	0.566985
C	-2.258340	-0.760724	-0.657663
H	-2.698006	0.506045	-0.959079
H	-4.349844	1.396951	1.613427
H	1.067492	-2.305710	0.493172
H	-0.043222	1.626069	-0.985737
H	2.252069	2.434360	-0.518669
H	3.928714	0.901133	0.474764
H	3.350251	-1.454562	0.995129
H	-2.838330	-1.440835	-1.281693

52

Sum of electronic and zero-point Energies= -385.337323

C	-2.904569	0.055289	0.067797
C	-3.547377	0.986424	0.694197
C	1.448097	-1.270594	0.298612
C	0.531713	0.887930	-0.500724
C	1.774950	1.462971	-0.329157
C	2.841757	0.689979	0.163948
C	0.342161	-0.497980	-0.181373
C	-0.880623	-1.110793	-0.358128
C	2.679041	-0.668430	0.479907

C	-2.248768	-0.966236	-0.520562
H	-3.821847	1.917830	0.198354
H	-3.848958	0.865524	1.735474
H	1.298105	-2.321595	0.522445
H	-0.301763	1.463116	-0.889476
H	1.932152	2.507875	-0.576248
H	3.815584	1.153279	0.295092
H	3.519353	-1.243789	0.853879
H	-2.810918	-1.753603	-1.026622

53

Sum of electronic and zero-point Energies= -385.303817

C	-2.394982	-1.625863	0.000000
C	-2.269431	-2.825877	0.000000
C	0.691261	1.893322	0.000000
C	0.759876	-0.598028	0.000000
C	2.136935	-0.539347	0.000000
C	2.786367	0.710179	0.000000
C	0.000000	0.629128	0.000000
C	-1.365805	0.637564	0.000000
C	2.069645	1.920938	0.000000
C	-2.578018	-0.173849	0.000000
H	-3.181417	0.151783	0.867727
H	-2.186856	-3.891990	0.000000
H	0.108842	2.808860	0.000000
H	0.229308	-1.543072	0.000000
H	2.722723	-1.452766	0.000000
H	3.872688	0.739702	0.000000
H	2.601040	2.866689	0.000000
H	-3.181417	0.151783	-0.867727