Supporting Information

for

Stereoselectivity in Oxyallyl–Furan 4+3 Cycloadditions: Control of Intermediate Conformations and Dispersive Stabilisation in Cycloadditions involving Oxazolidinone Auxiliaries

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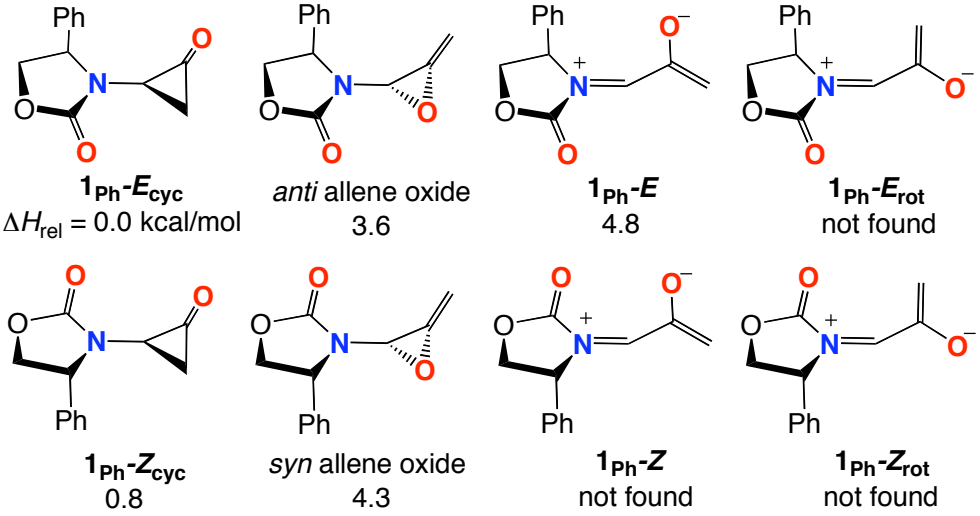
Part 1 – Computational Data

Contents

Isomers of $\mathbf{1}_{Ph}$ and their Cycloadditions with Furan

In addition to the oxyallyls $\mathbf{1}_{Ph}$-***E*** and $\mathbf{1}_{Ph}$-***Z***, several other isomeric species can be drawn. The possibilities are shown in Scheme S1. Five of the species in Scheme S1 were located at the B3LYP/6-31G(d) level. The cyclopropanone $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{cyc}$ is the most stable species, while its rotamer $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{cyc}$ lies 0.8 kcal mol^{-1} higher in energy. The oxyallyl $\mathbf{1}_{Ph}$-***E*** lies 4.8 kcal mol^{-1} above $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{cyc}$. $\mathbf{1}_{Ph}$-***Z*** collapsed to $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{cyc}$ upon attempted optimisation. The "sickle"-conformer oxyallyls $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{rot}$ and $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{rot}$, in which nitrogen is *anti* to the oxyallyl oxygen, collapsed to a cyclopropanone or allene oxide upon attempted optimisation.

Scheme S1



As well as the *endo* (4 + 3) cycloadditions of $\mathbf{1}_{Ph}$-***E*** and $\mathbf{1}_{Ph}$-***Z*** with furan, we also investigated alternative mechanisms:

(1) *Exo* cycloadditions of $\mathbf{1}_{Ph}$-***E***
(2) *Endo* cycloadditions of $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{rot}$ and $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{rot}$, and
(3) *Exo* cycloadditions of $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{rot}$ and $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{rot}$.

Transition structures are shown in Figure S1.

In experiment, only the cycloadducts *I* and *II* have been detected, and are obtained from the *endo* (4 + 3) cycloadditions of $\mathbf{1}_{Ph}$-***E*** and $\mathbf{1}_{Ph}$-***Z*** (**TSA**/**TSB**). In principle, *I* and *II* could also be obtained from the *exo* (4 + 3) cycloadditions of $\mathbf{1}_{Ph}$-$\boldsymbol{E}_{rot}$ and $\mathbf{1}_{Ph}$-$\boldsymbol{Z}_{rot}$, but the corresponding transition states (**TS-S7**–**TS-S10**) lie at least 17.2 kcal mol^{-1} above **TSA**/**TSB**. The activation energies for the other modes of cycloaddition in Figure S1 are also ≥12.9 kcal mol^{-1} higher than those of **TSA**/**TSB**, consistent with the absence of their products in experiment.

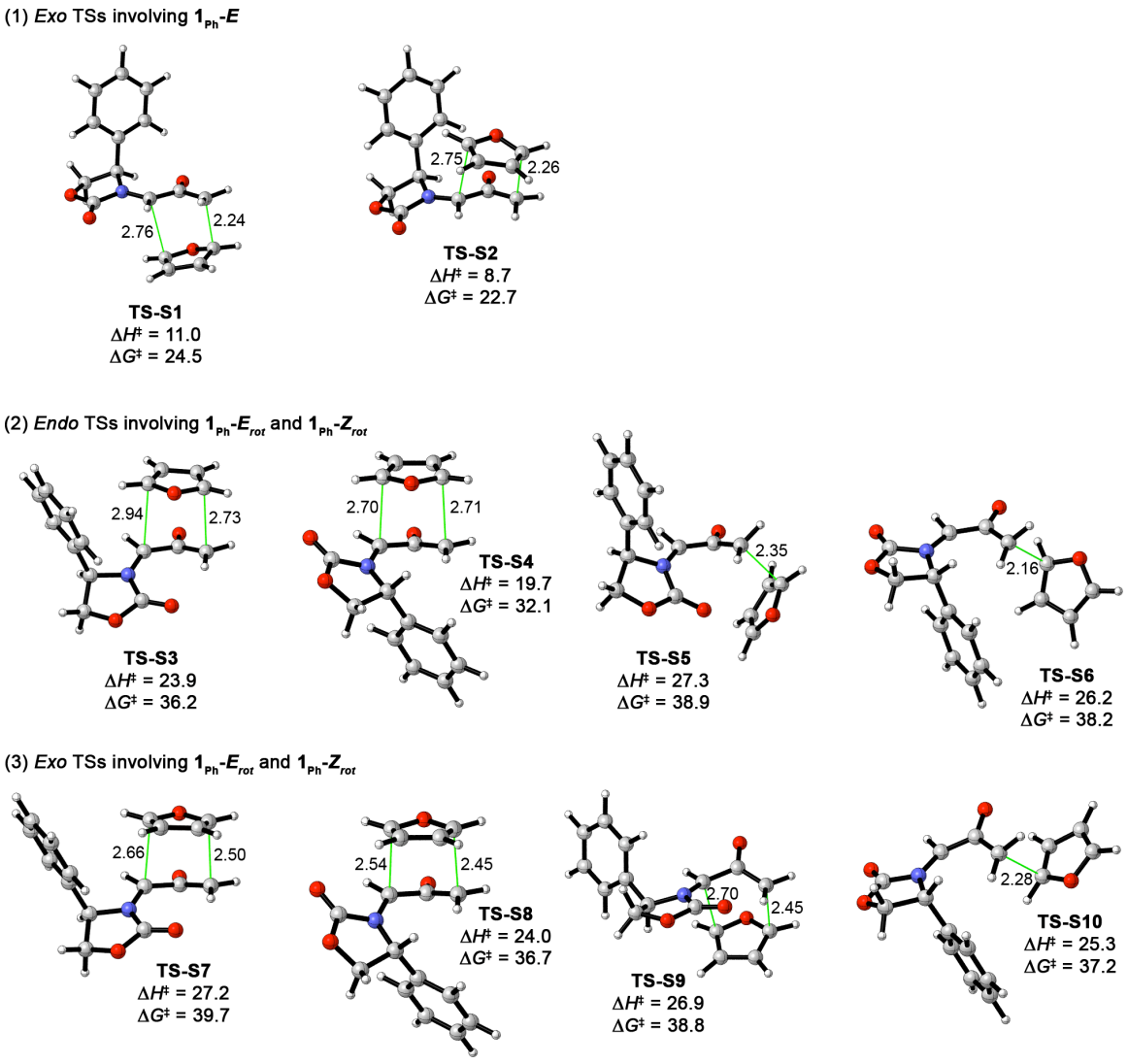


Figure S1. Transition structures for alternative (4 + 3) cycloaddition pathways.

Solvation Effects

The effects of solvation were computed with the Conductorlike Polarizable Continuum Model (CPCM) of Tomasi and Barone, as implemented in Gaussian 03. CPCM calculations with THF as solvent were performed using the UAKS cavity. The four transition states for cycloaddition of $\mathbf{1}_{Ph}$ with furan, **TSA**–**TSD**, were considered. Their B3LYP/6-31G(d) gas-phase geometries are reproduced in Figure S2.

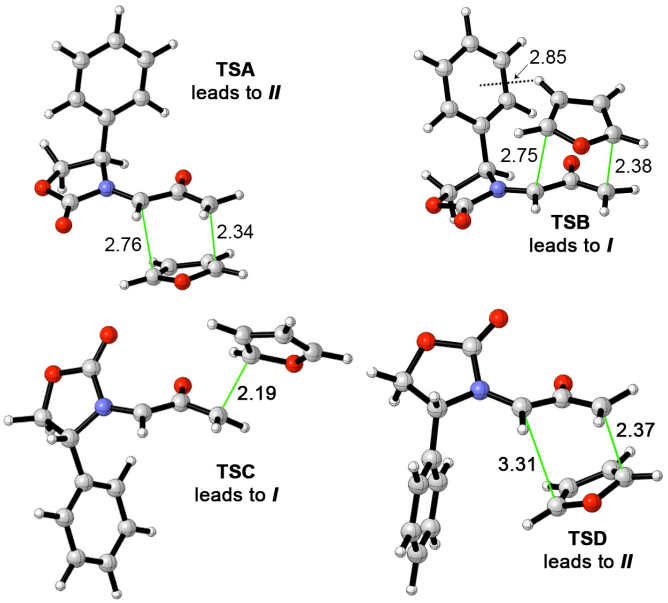


Figure S2. B3LYP/6-31G(d) gas-phase geometries of **TSA**–**TSD**.

Free energies of solvation were calculated at various levels of theory and temperatures, and were added to the gas-phase free energies to obtain free energies in solution. The resulting values are shown in the first five entries of Table S1. Inclusion of solvation in this way raises the activation barriers for the *E* TSs by approximately 3–4 kcal mol^{-1} and lowers those for the *Z* TSs by 0–2 kcal mol^{-1}. There are negligible overall effects on the mechanism and diastereoselectivity. The two *Z* transition states, **TSC** and **TSD**, remain ≥9.5 kcal mol^{-1} higher in energy than the *E* transition states **TSA** and **TSB**, and the diastereoselectivity between **TSA** and **TSB** ranges from 0–0.3 kcal mol^{-1}.

Solution-phase optimisations were also performed. The resulting TS geometries are shown in Figure S3. Optimisation in THF has minimal effect on the TS geometries; the forming bond lengths change by 0–0.03 Å in all but one case. The *Z* transition states are again ≥9.6 kcal mol^{-1} higher in energy than the *E* transition states. Diastereoselectivity between **TSA** and **TSB** is 0.4 kcal mol^{-1}.

Table S1. Effects of solvation on activation energies for **TSA**–**TSD**.

	Temp. (K)	$\Delta G^{\ddagger}$ (kcal mol^{-1})			
		TSA	**TSB**	**TSC**	**TSD**
Gas-phase optimised geometries:					
B3LYP/6-31G(d) gas-phase $\Delta G^{\ddagger}$	298.15	22.2	21.9	37.5	36.6
B3LYP/6-31G(d) gas-phase $\Delta G^{\ddagger}$ + B3LYP/6-31G(d)-CPCM $\Delta G^{\ddagger}_{solv}$	298.15	25.0	24.9	36.6	35.0
B3LYP/6-31G(d) gas-phase $\Delta G^{\ddagger}$ + B3LYP/6-311+G(2df,p)-CPCM $\Delta G^{\ddagger}_{solv}$	298.15	25.3	25.2	36.5	34.8
B3LYP/6-31G(d) gas-phase $\Delta G^{\ddagger}$	195.15	16.7	16.4	32.8	31.4
B3LYP/6-31G(d) gas-phase $\Delta G^{\ddagger}$ + B3LYP/6-31G(d)-CPCM $\Delta G^{\ddagger}_{solv}$	195.15	20.4	20.4	32.5	30.8
Solution-optimised geometries:					
B3LYP/6-31G(d)-CPCM $\Delta G^{\ddagger}$	298.15	20.1	19.7	31.2	29.7

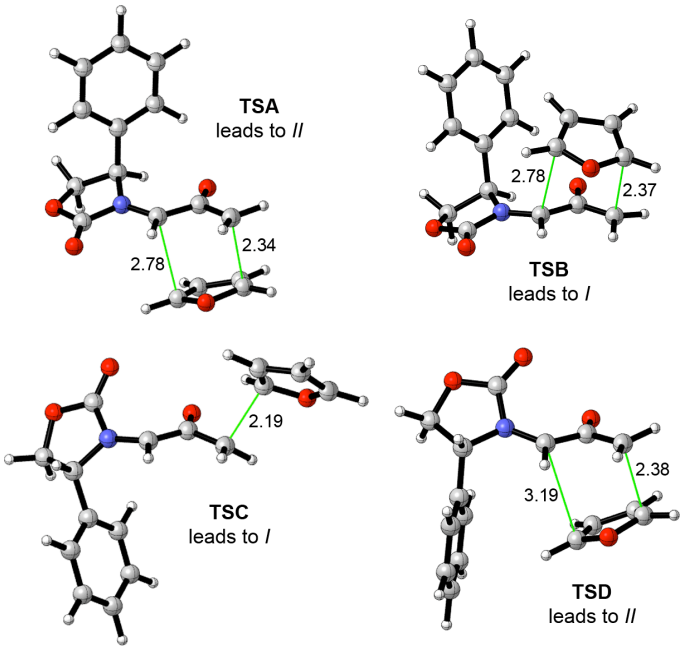


Figure S3. B3LYP/6-31G(d) solution-optimised geometries of **TSA**–**TSD**.

B3LYP/6-31G(d) Gas-Phase Geometries and Total Energies (Hartrees)

1_{Ph}-*E*

O	-0.911257	-2.592951	0.361290
C	-1.543517	-1.739831	-0.463236
N	-1.267184	-0.408107	-0.013983
C	-0.181898	-0.425604	1.009138
C	-0.343563	-1.874967	1.491252
C	-1.922336	0.642455	-0.490534
H	-0.442554	0.322621	1.757563
O	-2.231443	-2.036041	-1.400314
C	1.174856	-0.097808	0.397775
H	-1.046649	-1.957937	2.325555
H	0.598591	-2.356703	1.748114
C	1.675033	1.205482	0.515987
C	2.919409	1.528699	-0.027110
C	3.669157	0.561998	-0.698771
C	3.168421	-0.734566	-0.830963
C	1.927241	-1.063706	-0.286248
H	1.065820	1.957473	1.009482
H	3.301379	2.540948	0.074511
H	4.637835	0.816894	-1.120267
H	3.742630	-1.491741	-1.357886
H	1.550624	-2.076928	-0.402947
C	-1.803069	1.994509	0.054948
H	-2.611757	0.403084	-1.294512
C	-2.375106	2.891790	-0.855366
O	-1.216616	2.235687	1.146816
H	-2.267213	3.962329	-0.710722
H	-2.971647	2.552447	-1.694575

E = -744.2600707

0 imaginary frequencies

4 (singlet diradical)

C	0.000000	0.000000	0.125057
O	0.000000	0.000000	1.364582
C	0.000000	1.226421	-0.657993
C	0.000000	-1.226421	-0.657993
H	0.000000	-1.220083	-1.743752
H	0.000000	-2.180862	-0.141791
H	0.000000	1.220083	-1.743752
H	0.000000	2.180862	-0.141791

E = -191.833387

0 imaginary frequencies

5a

H	2.327673	1.655178	0.000000
C	2.421606	0.567730	0.000000
N	1.099369	-0.055392	0.000000
C	1.100702	-1.527971	0.000000
H	0.055180	-1.852614	0.000000
C	0.000000	0.669070	0.000000
H	0.167760	1.741985	0.000000
C	-1.395901	0.179854	0.000000
O	-1.690395	-1.048401	0.000000

C	-2.249982	1.284911	0.000000
H	-1.883378	2.305239	0.000000
H	-3.325148	1.137930	0.000000
H	2.979022	0.251535	0.888917
H	2.979022	0.251535	-0.888917
H	1.634448	-1.878698	0.890781
H	1.634448	-1.878698	-0.890781

E = -325.8488836

0 imaginary frequencies

TSA

C	3.826409	-1.106048	0.980828
C	4.037841	-1.167850	-0.393178
O	3.876941	0.081735	-0.940446
C	3.328785	0.854479	0.034984
C	3.341295	0.185681	1.243600
H	4.601862	-1.864719	-0.995142
C	1.959959	-1.928282	-1.148797
C	1.117255	-1.232015	-0.239462
O	0.795380	-1.659740	0.906734
C	0.788733	0.088602	-0.718471
N	-0.112114	0.902309	-0.111081
C	-0.258723	2.244947	-0.492590
O	-1.125474	2.843629	0.361495
C	-1.401579	1.956489	1.471983
C	-1.079759	0.542094	0.957210
O	0.302892	2.796403	-1.406169
C	-2.278178	-0.224735	0.410307
C	-2.343851	-1.612176	0.587160
C	-3.438290	-2.331061	0.102837
C	-4.470947	-1.675434	-0.568605
C	-4.403947	-0.293750	-0.760654
C	-3.313761	0.427622	-0.274755
H	-2.445342	2.087581	1.755581
H	-0.752920	2.246940	2.305402
H	-0.556192	-0.071299	1.688412
H	-1.515340	-2.117867	1.074227
H	-3.480278	-3.407296	0.248637
H	-5.322227	-2.236888	-0.944587
H	-5.200325	0.224050	-1.288604
H	-3.272671	1.502146	-0.436220
H	1.164339	0.470600	-1.659731
H	2.136160	-2.985467	-0.974546
H	2.146273	-1.552149	-2.148833
H	2.988764	0.572126	2.189198
H	3.917177	-1.927011	1.676725
H	3.110155	1.875497	-0.240245

E = -974.2786561

1 imaginary frequency

TSB

O	-3.120530	0.043470	-1.443562
C	-1.830666	0.452813	-1.587763
C	-0.986260	-1.393562	0.273689
C	-1.679355	-0.647721	1.300524
C	-3.086016	-0.836350	1.210731

C	-3.648816	0.795798	-0.427492
C	-2.775449	1.826240	-0.104079
C	-1.597757	1.586149	-0.833380
N	0.362545	-1.536766	0.225150
C	0.963426	-2.461706	-0.649231
O	2.282435	-2.543047	-0.346910
C	2.539381	-1.828876	0.885371
C	1.391250	-0.807384	1.007946
O	0.415315	-3.083404	-1.523709
C	1.727743	0.567175	0.443796
C	2.394147	0.711338	-0.782132
C	2.724287	1.978823	-1.263082
C	2.400467	3.116327	-0.519708
C	1.736750	2.978657	0.701069
C	1.393677	1.711568	1.177463
O	-1.099984	0.107268	2.129384
H	2.531714	-2.553601	1.706505
H	3.523083	-1.367197	0.805206
H	1.025989	-0.699291	2.026497
H	2.664091	-0.165994	-1.364778
H	3.239943	2.076657	-2.214671
H	2.664753	4.103136	-0.890607
H	1.478056	3.859487	1.282959
H	0.827951	1.598481	2.095882
H	-1.260316	-0.048402	-2.355081
H	-0.669942	2.136695	-0.783906
H	-2.945860	2.595278	0.635320
H	-4.710605	0.681000	-0.269865
H	-3.702354	-0.455295	2.019803
H	-1.509944	-2.080232	-0.380181
H	-3.513126	-1.613389	0.586904

E = -974.2791128

1 imaginary frequency

TSC

C	4.275569	0.308990	0.827530
C	3.818331	-0.207742	-0.381675
O	4.687811	-1.205373	-0.781573
C	5.619456	-1.345244	0.188773
C	5.418394	-0.439783	1.198496
H	6.347020	-2.128562	0.034351
C	1.909413	-1.180980	0.047778
C	1.056765	-0.094259	-0.374579
O	1.116239	0.398307	-1.527889
C	0.110819	0.262970	0.634725
N	-0.885929	1.174020	0.376933
C	-0.639224	2.459168	-0.140310
O	-1.847214	3.068569	-0.347634
C	-2.912018	2.135328	-0.139890
C	-2.303469	0.993355	0.712145
O	0.419479	2.998344	-0.298976
C	-2.856343	-0.371863	0.362283
C	-3.800055	-0.976598	1.198483
C	-4.363413	-2.208014	0.858006
C	-3.977159	-2.849024	-0.319344
C	-3.026504	-2.254634	-1.153561
C	-2.467565	-1.021895	-0.818664
H	-3.733728	2.650447	0.361867

H	-3.252850	1.756382	-1.109333
H	-2.464960	1.190912	1.782454
H	-4.096779	-0.482775	2.121590
H	-5.097231	-2.666641	1.515297
H	-4.410078	-3.809951	-0.583990
H	-2.715771	-2.753402	-2.067521
H	-1.717321	-0.568272	-1.462063
H	0.003239	-0.318776	1.544308
H	1.909936	-1.529154	1.077542
H	2.202902	-1.914261	-0.696937
H	6.013344	-0.336797	2.095136
H	3.801075	1.111295	1.375684
H	3.224193	0.243988	-1.179520

E = -974.2498687

1 imaginary frequency

TSD

N	-0.514922	1.494344	0.291321
C	-0.526789	2.841356	-0.162134
O	0.364859	3.636401	-0.152612
O	-1.809098	3.140614	-0.539487
C	-2.640995	1.982935	-0.444892
H	-3.621204	2.284939	-0.070841
H	-2.751966	1.532293	-1.437192
C	-1.897595	1.034639	0.518344
H	-2.183718	1.258639	1.556396
C	-2.148258	-0.431181	0.242064
C	-2.813749	-1.214193	1.190985
C	-3.103701	-2.555327	0.930724
C	-2.725931	-3.126875	-0.284156
C	-2.055507	-2.352926	-1.236363
C	-1.765397	-1.014464	-0.974726
H	-3.109668	-0.771820	2.139666
H	-3.622040	-3.150340	1.677383
H	-2.950897	-4.169643	-0.490073
H	-1.758391	-2.793258	-2.184421
H	-1.229309	-0.421279	-1.710834
C	0.577750	0.846031	0.797027
H	0.354996	0.123689	1.575169
C	1.935391	1.078859	0.371483
O	2.289084	1.605713	-0.701177
C	2.824558	0.626372	1.405898
H	2.463018	0.118951	2.294013
H	3.812222	1.075091	1.463067
C	1.649467	-2.066869	-0.351559
C	2.316513	-1.470111	-1.391463
C	3.574084	-1.071495	-0.884780
O	2.432245	-2.115699	0.759412
C	3.574748	-1.409795	0.457635
H	0.685845	-2.545048	-0.269561
H	1.931621	-1.295903	-2.385889
H	4.345021	-0.524647	-1.406538
H	4.374671	-1.500042	1.176793

E = -974.2531505

1 imaginary frequency

$\mathbf{1}_{Ph}$-*E*•$ZnCl_2$

C	2.918311	1.344115	-0.870563
C	1.827292	1.134185	-0.014055
C	0.774906	2.055811	0.001559
C	0.812712	3.174335	-0.833652
C	1.893721	3.374825	-1.691943
C	2.947388	2.457472	-1.708819
C	1.783376	-0.049125	0.938931
N	1.925047	-1.356702	0.231163
C	3.281661	-1.850218	0.358596
O	3.918062	-1.080090	1.241853
C	3.003075	-0.149941	1.881419
O	3.726476	-2.790429	-0.235345
C	1.050106	-2.038661	-0.482986
C	-0.355767	-1.741083	-0.608883
O	-0.863277	-0.790165	0.118887
C	-0.984795	-2.553205	-1.529122
H	0.841461	-0.052820	1.482482
H	2.743687	-0.561699	2.860816
H	3.527518	0.797041	1.996934
H	-0.074634	1.905483	0.662008
H	-0.009201	3.883978	-0.809972
H	1.918665	4.242752	-2.344904
H	3.794221	2.609237	-2.372132
H	3.753379	0.647549	-0.888808
H	1.472960	-2.911842	-0.972039
H	-2.036802	-2.418959	-1.763839
H	-0.442088	-3.344982	-2.032710
Zn	-2.686217	-0.023511	0.278569
Cl	-2.605743	1.621237	1.793239
Cl	-4.237787	-0.930594	-1.054362

E = -1730.4088735

0 imaginary frequencies

1_{Ph}-*Z*·$ZnCl_2$

O	-0.117220	-2.115212	-1.572834
C	0.398770	-0.899333	-1.423046
N	-0.669519	0.011956	-1.110090
C	-1.975347	-0.715330	-1.228363
C	-1.468718	-2.156843	-1.062809
C	-0.585029	1.304061	-0.815154
H	-2.330932	-0.569177	-2.255449
O	1.551237	-0.601511	-1.615378
C	-3.039454	-0.281805	-0.250587
H	-2.028655	-2.879557	-1.655149
H	-1.422476	-2.460597	-0.014588
C	-4.294898	0.106367	-0.734638
C	-5.308498	0.476280	0.150900
C	-5.067287	0.470125	1.524860
C	-3.812435	0.093515	2.012150
C	-2.798916	-0.284986	1.133345
H	-4.484117	0.113135	-1.805893
H	-6.280376	0.771395	-0.233803
H	-5.853461	0.760918	2.215845
H	-3.619561	0.092310	3.080884
H	-1.821660	-0.566205	1.520537
C	0.563902	2.149951	-0.526242
H	-1.557185	1.781458	-0.756849
C	0.213218	3.464347	-0.810246

O	1.729940	1.776549	-0.161561
H	0.986017	4.223735	-0.873423
H	-0.814335	3.771768	-0.962285
Zn	2.533074	0.052091	0.428068
Cl	4.736825	-0.180035	0.475552
Cl	0.890095	-1.085982	1.621268

E = -1730.3985083

0 imaginary frequencies

TS: 1_{Ph}-*E*•$ZnCl_2$ + furan (furan opposite Ph)

C	-3.591060	-0.778990	-0.906953
C	-2.537585	-0.993275	-0.006547
C	-1.943198	-2.257632	0.065012
C	-2.395898	-3.294422	-0.754232
C	-3.439963	-3.074761	-1.652802
C	-4.037346	-1.813825	-1.727550
C	-2.062205	0.107968	0.927750
N	-1.728611	1.365475	0.215284
C	-2.728844	2.343369	0.400347
O	-3.629513	1.878441	1.287383
C	-3.158094	0.646193	1.880426
C	-0.702709	1.613092	-0.636876
C	0.444158	0.802332	-0.794463
O	0.691121	-0.160509	0.051086
O	-2.766620	3.422793	-0.134830
C	1.326364	1.197116	-1.824182
C	2.608452	2.733801	-0.893732
C	2.895567	2.181739	0.359099
C	1.900127	2.648097	1.229651
C	1.105521	3.506782	0.489768
O	1.602185	3.664401	-0.757470
H	3.243913	2.864691	-1.757606
H	-4.008546	-0.028815	1.970143
H	-2.762601	0.881230	2.873559
H	-1.188750	-0.235649	1.478241
H	-1.122144	-2.436658	0.754244
H	-1.924894	-4.271129	-0.687756
H	-3.788634	-3.880790	-2.292646
H	-4.852513	-1.635785	-2.423585
H	-4.069737	0.195463	-0.972229
H	-0.861124	2.477662	-1.270038
H	2.135819	0.528423	-2.101620
H	0.982446	1.895485	-2.578747
H	1.749455	2.375875	2.264786
H	3.682445	1.466862	0.555887
H	0.261151	4.130747	0.744276
Zn	2.087347	-1.531743	0.245224
Cl	1.472988	-3.068554	1.745752
Cl	3.981510	-1.153809	-0.917415

E = -1960.4322438

1 imaginary frequency

TS: 1_{Ph}-*E*•$ZnCl_2$ + furan (furan on same side as Ph)

C	2.929423	-0.963620	1.208076
C	1.896680	-1.357199	0.343387
C	0.888392	-2.200572	0.822399

C	0.908096	-2.639627	2.148786
C	1.930757	-2.235283	3.008766
C	2.943317	-1.396587	2.534189
C	1.876929	-0.925181	-1.115250
N	1.984213	0.543298	-1.292667
C	3.310577	0.912579	-1.624484
O	4.016607	-0.208243	-1.873507
C	3.132284	-1.352695	-1.909364
C	1.053807	1.507849	-1.091935
C	-0.338148	1.306820	-0.947213
O	-0.828829	0.101342	-0.849783
Zn	-2.618059	-0.674274	-0.605997
Cl	-2.532371	-2.894585	-0.852208
O	3.741794	2.035388	-1.669956
C	-1.105578	2.487511	-0.855080
C	-1.066982	3.041564	1.299008
C	-1.257993	1.806270	1.924874
C	0.021473	1.275790	2.147431
C	0.918220	2.234558	1.711040
O	0.272264	3.354592	1.313605
Cl	-4.248767	0.765736	-0.018894
H	2.901494	-1.571075	-2.956816
H	3.656750	-2.194308	-1.458505
H	0.962681	-1.277924	-1.587636
H	3.734216	-0.325470	0.851088
H	3.748780	-1.085499	3.193991
H	1.944746	-2.576078	4.040450
H	0.119528	-3.296969	2.504256
H	0.079530	-2.511607	0.166691
H	1.995877	2.293352	1.739090
H	0.277413	0.302154	2.540356
H	-2.219326	1.343753	2.100926
H	-1.737332	3.881865	1.191636
H	-2.186602	2.412715	-0.923794
H	1.449701	2.508517	-1.220209
H	-0.658042	3.434456	-1.134863

E = -1960.4341564

1 imaginary frequency

TS: 1_{Ph}-*Z*·$ZnCl_2$ + furan (furan opposite Ph)

C	-0.519109	1.317342	-0.231577
C	-0.929231	2.649245	-0.546385
C	-2.799307	2.949952	0.742882
C	-3.692300	3.567178	-0.133335
C	-4.560035	2.559219	-0.603462
C	-4.196062	1.402649	0.053083
O	-3.174608	1.635532	0.895429
H	-2.222747	3.359151	1.558508
H	-3.678219	4.611015	-0.417423
H	-5.344835	2.651861	-1.340326
H	-4.507758	0.367851	-0.022198
H	-1.514607	2.778724	-1.447721
H	-0.364172	3.508606	-0.199212
O	-1.117739	0.327779	-0.782716
C	0.587368	1.279530	0.645325
H	1.097641	2.203356	0.895840
N	1.208607	0.150476	1.121405
C	0.566674	-0.989289	1.600797

O	-0.635109	-1.196560	1.605667
Zn	-1.389265	-1.621552	-0.441781
Cl	0.471187	-2.743085	-1.185727
Cl	-3.591278	-2.137744	-0.433075
O	1.466270	-1.817529	2.142749
C	2.796093	-1.390873	1.784611
H	3.454245	-1.580159	2.632787
H	3.112236	-1.974071	0.916418
C	2.654204	0.108962	1.441627
H	2.834839	0.724779	2.333705
C	3.544738	0.576938	0.311890
C	3.373748	0.074716	-0.987475
H	2.579453	-0.638836	-1.200026
C	4.220889	0.497209	-2.010667
H	4.081568	0.106319	-3.014460
C	5.242870	1.414381	-1.749148
H	5.901602	1.738057	-2.550333
C	5.414891	1.915066	-0.458596
H	6.206095	2.629522	-0.248908
C	4.563964	1.500040	0.567769
H	4.697025	1.893775	1.573495

E = -1960.4150888

1 imaginary frequency

TS: 1_{Ph}-*Z*•$ZnCl_2$ + furan (furan on same side as Ph)

C	-0.226693	3.975037	-0.575209
C	0.675929	3.602348	0.398146
C	0.006888	2.667428	1.225744
C	-1.264902	2.556530	0.724135
O	-1.441325	3.385093	-0.340619
C	0.386559	2.227090	-2.296042
C	0.665596	1.111887	-1.481966
O	1.808869	0.973032	-0.919333
C	-0.465581	0.235301	-1.435540
N	-0.552314	-1.077310	-1.095876
C	0.495557	-2.016628	-1.000182
O	-0.017683	-3.231504	-0.787601
C	-1.417640	-3.138878	-0.467010
C	-1.866486	-1.779177	-1.036505
O	1.680531	-1.812240	-1.156734
C	-2.931574	-1.091771	-0.212291
C	-4.177576	-0.817989	-0.787568
C	-5.196141	-0.238650	-0.027821
C	-4.971703	0.072231	1.313185
C	-3.726348	-0.193658	1.891620
C	-2.706274	-0.771753	1.136318
H	-1.929141	-3.985020	-0.926267
H	-1.519813	-3.180344	0.619747
H	-2.223733	-1.901302	-2.066954
H	-4.357430	-1.066060	-1.831520
H	-6.160390	-0.033522	-0.483767
H	-5.763154	0.519570	1.907952
H	-3.547171	0.046920	2.935868
H	-1.732622	-0.953540	1.587277
H	-1.417281	0.644077	-1.753216
H	-0.584871	2.386207	-2.746688
H	1.218745	2.817928	-2.662838
H	-2.132766	1.993931	1.030575

H	0.415836	2.100681	2.050141
H	1.705568	3.922105	0.470734
H	-0.222700	4.756318	-1.319866
Zn	2.579791	-0.382327	0.329503
Cl	4.800267	-0.439438	0.506147
Cl	1.011649	-0.852804	1.987682

E = -1960.4247481

1 imaginary frequency

1_{Ph}-E_{cyc}

C	1.843633	-1.103122	-0.379692
C	1.239537	-0.136500	0.438087
C	1.899639	1.078667	0.654878
C	3.147004	1.321975	0.076100
C	3.745713	0.351392	-0.727358
C	3.089885	-0.861109	-0.955984
C	-0.130640	-0.365198	1.057342
N	-1.237485	-0.255017	0.091460
C	-1.665905	-1.502856	-0.330534
O	-1.122413	-2.450189	0.497180
C	-0.409822	-1.798013	1.564073
O	-2.392646	-1.755341	-1.259165
C	-1.427751	0.896239	-0.731451
C	-1.700270	2.185239	-0.045855
O	-1.269134	3.030923	0.693923
C	-2.837041	1.590937	-0.754897
H	-0.278225	0.360475	1.862918
H	-1.048100	-1.787160	2.454500
H	0.497210	-2.367609	1.771205
H	1.425156	1.843848	1.264801
H	3.648139	2.269706	0.253405
H	4.717766	0.537814	-1.175887
H	3.549336	-1.619647	-1.583931
H	1.339271	-2.047694	-0.568365
H	-0.890083	0.917119	-1.681768
H	-3.632245	1.137923	-0.165578
H	-3.156178	1.991298	-1.715282

E = -744.2678456

0 imaginary frequencies

1_{Ph}-Z_{cyc}

N	0.914886	0.280641	0.016665
C	-0.284015	0.931026	0.554839
C	-0.114191	2.319491	-0.102995
O	1.301003	2.461552	-0.308394
C	1.879030	1.224912	-0.289802
H	-0.459626	3.140939	0.526991
H	-0.204436	1.022578	1.649703
C	-1.588575	0.241865	0.214999
O	3.053315	1.024723	-0.492670
C	1.293475	-1.048955	0.390723
H	-0.621742	2.359528	-1.072872
C	-2.600190	0.154847	1.177792
C	-3.827362	-0.434276	0.868464
C	-4.050124	-0.953347	-0.407274
C	-3.041893	-0.879343	-1.371718

C	-1.819538	-0.283050	-1.064480
H	-2.426282	0.550076	2.176382
H	-4.604045	-0.493492	1.625966
H	-5.002062	-1.418237	-0.648446
H	-3.206884	-1.287923	-2.364907
H	-1.033646	-0.233532	-1.813476
C	2.566269	-1.721698	0.012608
H	0.432096	-1.714184	0.426228
C	2.422660	-1.375375	1.443000
O	3.201978	-2.269644	-0.843611
H	3.033889	-0.541401	1.783380
H	2.224892	-2.138480	2.194860

E = -744.2664018

0 imaginary frequencies

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anti-Allene oxide

N	-1.355067	-0.090094	-0.034065
C	-2.114661	-1.208079	-0.362480
O	-3.002606	-1.271757	-1.174926
O	-1.662927	-2.263470	0.369281
C	-0.757908	-1.799909	1.386750
H	-1.295777	-1.768265	2.340127
H	0.069927	-2.506528	1.453981
C	-0.301514	-0.381569	0.938661
H	-0.371378	0.314876	1.779800
C	1.105350	-0.336327	0.365041
C	1.409872	-0.948900	-0.857853
C	2.716349	-0.940616	-1.345099
C	3.735078	-0.323791	-0.614766
C	3.439563	0.287380	0.604210
C	2.130297	0.282017	1.088474
H	0.624320	-1.428944	-1.435502
H	2.939015	-1.416337	-2.296323
H	4.752420	-0.317425	-0.996270
H	4.224476	0.775509	1.175478
H	1.901246	0.771068	2.032663
C	-1.687973	1.174918	-0.534550
C	-0.965234	2.373645	-0.212198
H	-2.341034	1.114166	-1.399947
O	-2.137785	2.218011	0.465538
C	0.039287	3.231145	-0.295283
H	0.869417	3.034324	-0.962348
H	0.048346	4.136441	0.302218

E = -744.2621979

0 imaginary frequencies

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syn-Allene oxide

N	-1.432020	-0.000544	0.103981
C	-2.201525	-1.098497	-0.265943
O	-3.091262	-1.125520	-1.078598
O	-1.793260	-2.173577	0.463560
C	-0.859134	-1.752814	1.473869
H	-0.061454	-2.494013	1.531439
H	-1.387165	-1.701635	2.432257
C	-0.348254	-0.355763	1.024342
H	-0.346745	0.338394	1.870574

C	1.038956	-0.374019	0.402554
C	1.297412	-1.083067	-0.778172
C	2.586641	-1.128658	-1.304473
C	3.634569	-0.469053	-0.656573
C	3.384917	0.238109	0.519004
C	2.091670	0.285154	1.043666
H	0.489092	-1.594304	-1.294429
H	2.773426	-1.677302	-2.223510
H	4.638857	-0.504138	-1.069848
H	4.192667	0.758765	1.026220
H	1.898837	0.846357	1.955267
C	-1.656297	1.256567	-0.474147
C	-0.917292	2.433587	-0.110155
H	-2.626436	1.312076	-0.958999
O	-0.555397	1.876792	-1.297998
C	-0.575829	3.442554	0.676527
H	0.218357	4.125253	0.394667
H	-1.100947	3.608192	1.609795

E = -744.2611512

0 imaginary frequencies

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s-*cis* Methyl vinyl ketone

C	-0.602014	-1.925992	0.000000
C	0.346392	-0.984863	0.000000
C	0.000000	0.470395	0.000000
O	-1.157503	0.857205	0.000000
C	1.167640	1.440389	0.000000
H	1.401885	-1.251943	0.000000
H	-0.364051	-2.985688	0.000000
H	-1.650476	-1.640294	0.000000
H	0.798230	2.467368	0.000000
H	1.801165	1.276672	0.881408
H	1.801165	1.276672	-0.881408

E = -231.2351829

0 imaginary frequencies

Acetone enolate

O	-0.952137	1.029895	0.000000
C	0.000000	0.185814	0.000000
C	1.365415	0.412824	0.000000
C	-0.442574	-1.304734	0.000000
H	2.086921	-0.403072	0.000000
H	1.757855	1.429930	0.000000
H	0.386065	-2.028133	0.000000
H	-1.075396	-1.500660	0.879565
H	-1.075396	-1.500660	-0.879565

E = -192.5288677

0 imaginary frequencies

$\mathbf{1}_{Bn}$-*E*

N	-1.859437	-0.283179	0.132676
C	-2.377622	-1.558414	-0.034685
O	-3.446975	-1.854637	-0.508873
O	-1.457902	-2.462139	0.418178

C	-0.358329	-1.755051	1.024239
H	0.566304	-2.281229	0.781763
H	-0.500713	-1.751474	2.110608
C	-0.424831	-0.333688	0.434861
H	-0.166638	0.412407	1.192609
C	0.463140	-0.114907	-0.813116
C	-2.509161	0.829418	-0.479834
H	-2.853575	0.667411	-1.502362
C	-2.121182	2.202986	-0.086908
O	-1.217507	2.995941	-0.009262
C	-3.460020	1.788106	0.342408
H	-3.600615	1.591206	1.404902
H	-4.351265	2.127909	-0.181447
H	0.297557	-0.942405	-1.514194
H	0.126509	0.804425	-1.305521
C	1.929673	0.007237	-0.462229
C	2.816835	-1.062324	-0.638694
C	4.160921	-0.943540	-0.277863
C	4.636313	0.250011	0.265947
C	3.761999	1.325465	0.442300
C	2.420878	1.204668	0.080296
H	2.456797	-1.991475	-1.075853
H	4.835707	-1.782382	-0.426973
H	5.682252	0.344939	0.544878
H	4.126729	2.261904	0.856192
H	1.744394	2.047897	0.205970

E = -783.5834143

0 imaginary frequencies

TS: 1_{Bn}-*E* + furan, analogous to TSA

N	0.574035	1.273178	-0.240848
C	0.653290	2.672544	-0.099615
O	1.543018	3.381258	-0.497747
O	-0.440393	3.098514	0.572846
C	-1.169978	1.963252	1.096004
H	-2.235847	2.177532	1.009909
H	-0.905825	1.849011	2.152675
C	-0.723831	0.764454	0.241964
H	-0.556730	-0.139359	0.823059
C	-1.679641	0.445706	-0.929762
C	1.580592	0.564135	-0.808917
H	2.362220	1.183351	-1.232444
C	1.541206	-0.864255	-1.013360
O	0.670784	-1.622174	-0.497171
C	2.658153	-1.318323	-1.768174
H	3.325159	-0.622932	-2.266163
H	2.637925	-2.338167	-2.140493
C	4.168501	-1.693134	-0.034749
O	4.409050	-0.355845	0.165367
C	3.531693	0.046817	1.123018
C	2.898186	-1.043452	1.686217
C	3.327744	-2.170974	0.966200
H	4.886272	-2.200719	-0.661704
H	3.575158	1.091737	1.391516
H	2.174544	-1.016469	2.488472
H	2.996272	-3.191838	1.086061
C	-2.933253	-0.255430	-0.453124
H	-1.928124	1.376008	-1.456324

H	-1.135189	-0.203027	-1.620465
C	-4.164521	0.407211	-0.379889
C	-5.304791	-0.253258	0.084856
C	-5.224612	-1.587650	0.482988
C	-4.000568	-2.258819	0.410685
C	-2.863081	-1.599879	-0.053610
H	-4.236881	1.443991	-0.703225
H	-6.253994	0.274444	0.130067
H	-6.110722	-2.104331	0.842272
H	-3.933770	-3.301192	0.711810
H	-1.908899	-2.117971	-0.119842

E = -1013.5971742

1 imaginary frequency

TS: 1_{Bn}-*E* + furan, analogous to TSB

N	0.640662	1.425816	0.491672
C	0.720018	2.735911	-0.021253
O	1.723489	3.304040	-0.373165
O	-0.528085	3.254263	-0.068174
C	-1.444673	2.373244	0.624904
H	-1.579324	2.754685	1.642500
H	-2.397941	2.394240	0.096091
C	-0.766592	0.993356	0.598771
H	-0.899369	0.439428	1.525575
C	-1.201671	0.109149	-0.589503
C	1.761748	0.720253	0.784848
H	2.665994	1.315327	0.749715
C	1.750715	-0.618600	1.324574
O	0.724899	-1.355318	1.351505
C	3.051246	-1.024313	1.738202
H	3.864025	-0.311410	1.822827
H	3.134694	-1.940094	2.316243
O	4.091934	-0.582048	-0.795477
C	2.964881	-0.311557	-1.506299
C	2.186423	-1.446878	-1.621162
C	2.811823	-2.441873	-0.850602
C	3.922060	-1.838112	-0.268806
H	2.923239	0.661000	-1.973322
H	1.257162	-1.527392	-2.166781
H	2.459760	-3.445212	-0.660322
H	4.796013	-2.262488	0.202293
C	-2.596733	-0.444079	-0.394260
H	-1.140045	0.691911	-1.517784
H	-0.483320	-0.712008	-0.637676
C	-3.693599	0.052074	-1.109519
C	-4.975641	-0.462156	-0.899239
C	-5.174830	-1.480462	0.032976
C	-4.086146	-1.984326	0.750460
C	-2.806872	-1.471828	0.539196
H	-3.542402	0.837434	-1.847775
H	-5.815168	-0.069165	-1.466922
H	-6.170807	-1.883397	0.196814
H	-4.233944	-2.783143	1.472692
H	-1.954035	-1.866724	1.086883

E = -1013.5970986

1 imaginary frequency

$\mathbf{1}_{i\mathrm{Pr/Ph}}$-*E*

N	-1.632083	-0.643431	0.556088
C	-1.125025	-0.393403	1.809256
O	-1.712894	-0.385436	2.863539
O	0.218071	-0.141382	1.680662
C	0.536916	0.068927	0.278122
C	1.988247	-0.351202	0.048766
C	0.374728	1.577005	-0.015675
C	-0.567511	-0.788091	-0.445576
H	-0.876844	-0.287228	-1.365381
C	-0.221655	-2.257447	-0.802156
C	-3.019471	-0.909497	0.361913
H	-3.389972	-1.875414	0.711892
C	-3.704106	-0.276642	-0.796204
O	-3.781407	-0.215363	-1.995039
C	-4.051480	0.269475	0.517959
H	-3.656244	1.248718	0.783277
H	-5.000861	0.018892	0.987315
H	0.700582	-2.206385	-1.394890
C	0.045909	-3.154306	0.415416
C	-1.305216	-2.877941	-1.703677
C	2.546162	-0.294928	-1.236863
C	3.876621	-0.649737	-1.452691
C	4.678353	-1.054624	-0.383466
C	4.135397	-1.100806	0.899540
C	2.799944	-0.752808	1.116281
H	1.944672	0.036363	-2.078441
H	4.287494	-0.603918	-2.457659
H	5.716924	-1.326707	-0.550584
H	4.749865	-1.408107	1.741596
H	2.384736	-0.790339	2.116492
C	0.118814	2.068439	-1.302776
C	0.025491	3.441192	-1.539172
C	0.190180	4.347623	-0.492462
C	0.452815	3.868600	0.791625
C	0.547859	2.497372	1.027384
H	-0.013795	1.390251	-2.140706
H	-0.181200	3.797615	-2.544715
H	0.114153	5.415933	-0.675654
H	0.584268	4.563196	1.617056
H	0.747472	2.132722	2.028689
H	0.284528	-4.171061	0.083559
H	0.883560	-2.795981	1.018960
H	-0.835879	-3.219788	1.063863
H	-0.953231	-3.833234	-2.109167
H	-2.227864	-3.080668	-1.149108
H	-1.565782	-2.226613	-2.545581

E = -1093.2543888

0 imaginary frequencies

TS: $\mathbf{1}_{i\mathrm{Pr/\ Ph}}$-*E* + furan, analogous to TSA

N	-0.627885	-1.061854	0.652444
C	-0.113139	-0.687881	1.899511
O	-0.672479	-0.757436	2.966071
O	1.134202	-0.188787	1.711072
C	1.347673	0.073718	0.284448
C	2.843674	-0.026089	-0.001252

C	0.868057	1.512630	0.002828
C	0.428172	-1.001016	-0.381770
H	-0.040478	-0.648334	-1.298355
C	1.065531	-2.393448	-0.653999
C	-1.948218	-1.348516	0.496408
H	-2.452661	-1.608724	1.418763
C	-2.608045	-1.428039	-0.785873
O	-2.094307	-1.015437	-1.864217
C	-3.941622	-1.907133	-0.657653
H	-4.302344	-2.333000	0.272137
H	-4.481874	-2.163309	-1.564126
C	-5.049723	0.110102	-0.217614
O	-4.557574	0.199438	1.060885
C	-3.415501	0.934527	0.975703
C	-3.290532	1.489274	-0.283225
C	-4.358277	0.987922	-1.046213
H	-6.035910	-0.321388	-0.302391
H	-2.879117	1.082518	1.900932
H	-2.489909	2.134305	-0.615463
H	-4.551206	1.156193	-2.095688
H	1.926540	-2.184354	-1.301701
C	1.583978	-3.124548	0.594814
C	0.110756	-3.305924	-1.442844
C	3.309764	0.085651	-1.319119
C	4.674403	0.036090	-1.597383
C	5.598075	-0.112425	-0.560557
C	5.142875	-0.210511	0.753237
C	3.775000	-0.167122	1.033763
H	2.606176	0.219329	-2.135932
H	5.015097	0.117910	-2.625933
H	6.662295	-0.147341	-0.776684
H	5.851459	-0.320918	1.569751
H	3.429462	-0.243168	2.058149
C	0.429497	1.912511	-1.266430
C	0.071383	3.240517	-1.509518
C	0.139741	4.188198	-0.487809
C	0.573567	3.797359	0.779820
C	0.939697	2.473373	1.021519
H	0.344604	1.196319	-2.077101
H	-0.266934	3.528316	-2.501370
H	-0.142446	5.220193	-0.677579
H	0.630953	4.524199	1.585664
H	1.277447	2.178954	2.009180
H	2.032088	-4.079564	0.298321
H	2.344836	-2.555372	1.134225
H	0.768496	-3.354364	1.291300
H	0.652749	-4.196311	-1.782271
H	-0.721906	-3.648009	-0.817394
H	-0.321673	-2.798656	-2.308780

E = -1323.266041

1 imaginary frequency

TS: $1_{iPr/Ph}$-*E* + furan, analogous to TSB

N	-0.805847	0.302934	0.651088
C	-0.170729	0.337319	1.906887
O	-0.682045	0.610663	2.963643
O	1.126626	-0.000075	1.730267
C	1.446975	0.051254	0.290298

C	1.846066	1.511878	-0.008419
C	2.628392	-0.875350	0.032991
C	2.885418	2.061571	0.760113
C	3.309127	3.371320	0.557853
C	2.703956	4.159757	-0.424796
C	1.671078	3.625729	-1.190773
C	1.239510	2.310952	-0.984893
H	3.358387	1.453204	1.525015
H	4.112971	3.776953	1.166254
H	3.034932	5.181938	-0.587434
H	1.186597	4.229780	-1.953061
H	0.416166	1.941975	-1.587038
C	3.106055	-1.754648	1.010947
C	4.198625	-2.583576	0.742712
C	4.826125	-2.543095	-0.501536
C	4.363311	-1.655813	-1.476510
C	3.280414	-0.821688	-1.207440
H	2.631317	-1.781227	1.984917
H	4.559182	-3.258379	1.514478
H	5.675316	-3.188643	-0.708363
H	4.851805	-1.605467	-2.445804
H	2.941475	-0.120224	-1.964546
C	0.079908	-0.344384	-0.347104
H	-0.080608	0.133989	-1.307808
C	-0.344301	-1.826934	-0.546972
C	-2.046739	0.814138	0.475611
H	-2.455607	1.266864	1.371010
C	-2.663533	0.993190	-0.815791
O	-2.211558	0.491728	-1.884677
C	-3.857217	1.766542	-0.726437
H	-4.110686	2.302794	0.181823
H	-4.274018	2.148927	-1.653946
C	-5.450437	0.170650	-0.328752
O	-5.074026	-0.023617	0.978775
C	-4.200686	-1.064736	0.972155
C	-4.184336	-1.671648	-0.267533
C	-5.013423	-0.902230	-1.101988
H	-6.275324	0.853051	-0.471437
H	-3.782930	-1.336361	1.929763
H	-3.611670	-2.546861	-0.538780
H	-5.199357	-1.044473	-2.156508
H	-1.388685	-1.702262	-0.854590
C	0.362039	-2.502975	-1.733252
C	-0.320652	-2.714868	0.705362
H	0.351695	-1.859574	-2.620510
H	-0.170563	-3.425656	-1.992457
H	1.398200	-2.769817	-1.512325
H	-0.795721	-3.676957	0.478724
H	-0.871531	-2.271089	1.542419
H	0.697930	-2.926748	1.042137

E = -1323.2627097

1 imaginary frequency

Methyl 2-Furoate

O	1.369833	0.561292	0.000000
C	0.000000	0.542359	0.000000
C	-0.486803	1.822525	0.000000
C	0.648316	2.684259	0.000000

C	1.741066	1.863866	0.000000
H	-1.532554	2.093856	0.000000
C	-0.721299	-0.733297	0.000000
H	0.654170	3.765058	0.000000
H	2.805349	2.046585	0.000000
O	0.109064	-1.797253	0.000000
O	-1.935306	-0.808299	0.000000
C	-0.546016	-3.074235	0.000000
H	0.256518	-3.812031	0.000000
H	-1.171902	-3.186130	0.889528
H	-1.171902	-3.186130	-0.889528

E = -457.9008328

0 imaginary frequencies

TSE

N	0.458881	-0.519955	-0.266544
C	0.311670	-1.896991	-0.571701
O	-0.256068	-2.351487	-1.533065
O	0.922214	-2.613408	0.390015
C	1.252763	-1.738801	1.501398
H	0.416962	-1.771186	2.204634
H	2.165664	-2.116354	1.959804
C	1.408716	-0.347811	0.867182
H	1.032570	0.453249	1.499135
C	2.819071	-0.015947	0.389485
C	3.686541	-1.011017	-0.085695
C	4.975531	-0.683569	-0.506288
C	5.413823	0.641001	-0.457445
C	4.552776	1.636187	0.006597
C	3.260834	1.313032	0.424507
H	3.361148	-2.046684	-0.134505
H	5.636660	-1.465152	-0.871084
H	6.419573	0.894698	-0.782035
H	4.884388	2.670613	0.042304
H	2.571634	2.085807	0.749972
C	-0.266246	0.413957	-0.903356
H	-0.825322	0.026435	-1.748237
C	-0.245242	1.830718	-0.602717
O	0.313753	2.317318	0.419929
C	-1.049763	2.579969	-1.506387
H	-1.448584	2.129376	-2.409644
H	-0.942421	3.660333	-1.501252
C	-2.758959	0.536223	0.463152
C	-3.045065	2.532537	-0.370185
O	-3.309208	1.209807	-0.594127
C	-2.377632	1.432792	1.454334
H	-1.953696	1.160959	2.409396
C	-2.599684	2.712774	0.944584
H	-2.367810	3.657197	1.414379
H	-3.543319	3.218246	-1.040308
C	-2.743886	-0.925073	0.490338
O	-2.101672	-1.554965	1.319972
O	-3.477867	-1.473838	-0.490109
C	-3.435614	-2.912492	-0.572827
H	-4.180503	-3.175882	-1.323978
H	-2.440633	-3.236621	-0.886593
H	-3.685494	-3.357692	0.393055

E = -1202.1644995

1 imaginary frequency

TSF

N	-1.313319	1.033859	-0.163326
C	-1.722937	2.200368	-0.822499
O	-1.158266	2.740252	-1.741938
O	-2.859015	2.653195	-0.235630
C	-3.102254	1.910813	0.982738
H	-4.178579	1.776555	1.085945
H	-2.721549	2.504070	1.821089
C	-2.333845	0.586140	0.818887
H	-1.816844	0.280628	1.726520
C	-3.170465	-0.573405	0.292438
C	-2.929364	-1.868152	0.767189
C	-3.696102	-2.940180	0.306440
C	-4.702788	-2.731965	-0.636994
C	-4.938543	-1.444783	-1.125150
C	-4.176649	-0.371838	-0.663902
H	-2.118531	-2.027457	1.471600
H	-3.502058	-3.940390	0.684692
H	-5.299091	-3.567498	-0.994042
H	-5.716288	-1.274605	-1.864857
H	-4.368673	0.624407	-1.055112
C	-0.143580	0.414842	-0.484493
H	0.254828	0.695757	-1.451942
C	0.412868	-0.671120	0.286166
O	0.029865	-0.965443	1.453109
C	1.557734	-1.254015	-0.337520
H	1.800758	-1.046662	-1.374358
H	1.941819	-2.177175	0.086426
C	1.862739	1.899875	0.348051
C	3.149234	0.137784	0.445538
O	2.767224	1.186687	-0.368018
C	1.869627	1.500535	1.680446
C	2.710325	0.392988	1.758219
H	1.280812	1.933672	2.476370
H	2.936822	-0.220290	2.617066
C	4.312931	-0.688686	0.051473
O	4.832386	-1.493246	0.797360
O	4.690378	-0.464216	-1.220496
C	5.807460	-1.250393	-1.671885
H	6.691965	-1.042144	-1.064476
H	5.972065	-0.950410	-2.706703
H	5.575297	-2.316752	-1.610029
H	1.441548	2.760587	-0.150873

E = -1202.1548906

1 imaginary frequency

TSG

N	0.342051	0.993762	-1.311729
C	0.219874	2.373709	-1.035108
O	-0.806472	2.974174	-0.839016
O	1.451605	2.924890	-1.046388
C	2.411366	1.971352	-1.559333
H	2.571693	2.192263	-2.619908
H	3.340532	2.104294	-1.006566
C	1.771201	0.582160	-1.344998

H	1.907871	-0.076416	-2.199563
C	2.253982	-0.124627	-0.086686
C	2.689164	-1.452724	-0.171414
C	3.195512	-2.101394	0.955974
C	3.259647	-1.433916	2.180946
C	2.815000	-0.113255	2.273538
C	2.319874	0.540179	1.145145
H	2.591905	-1.981200	-1.113178
H	3.533871	-3.131255	0.876989
H	3.650125	-1.940374	3.059823
H	2.848144	0.410403	3.224670
H	1.967984	1.563257	1.237906
C	-0.752430	0.233817	-1.531278
H	-1.681253	0.790158	-1.479600
C	-0.704142	-1.119645	-2.045171
O	0.365428	-1.771840	-2.178064
C	-2.006206	-1.627907	-2.312457
H	-2.079069	-2.560470	-2.864502
H	-2.874047	-0.977647	-2.323542
C	-2.573554	-2.488264	-0.214280
C	-1.742020	-0.815406	0.915936
O	-2.875742	-1.258785	0.297611
C	-1.347999	-2.925427	0.291948
C	-0.805196	-1.839711	0.986390
H	-3.413185	-3.042353	-0.607518
H	-0.881138	-3.878680	0.092010
C	-1.714344	0.528062	1.508849
H	0.162226	-1.765946	1.460724
O	-2.872634	1.188280	1.329761
O	-0.736110	0.980703	2.076738
C	-2.881764	2.547929	1.805115
H	-3.902112	2.898368	1.647670
H	-2.620335	2.584141	2.865622
H	-2.173962	3.146163	1.227240

E = -1202.1611719

1 imaginary frequency

TSH

N	1.420960	-1.525988	0.300962
C	2.014468	-2.477268	-0.547130
O	1.452147	-3.155584	-1.369475
O	3.345803	-2.509503	-0.292361
C	3.628526	-1.724929	0.889822
H	3.674698	-2.404998	1.747082
H	4.593784	-1.240007	0.746567
C	2.455163	-0.730637	1.006638
H	2.130519	-0.582745	2.033872
C	2.730396	0.623044	0.364963
C	2.421546	1.793528	1.067749
C	2.704073	3.043974	0.513779
C	3.283072	3.138062	-0.753407
C	3.583915	1.973842	-1.464515
C	3.314000	0.723692	-0.906765
H	1.923437	1.714727	2.027904
H	2.463947	3.945246	1.071644
H	3.499752	4.111661	-1.184897
H	4.035155	2.037557	-2.451050
H	3.567677	-0.173923	-1.465338

C	0.066616	-1.412565	0.381063
H	-0.453770	-2.169262	-0.193690
C	-0.615244	-0.640825	1.397502
O	-0.036806	0.184196	2.153134
C	-2.027353	-0.854216	1.370573
H	-2.608542	-0.438719	2.188863
H	-2.458368	-1.693294	0.835454
C	-2.645962	0.601665	-0.290254
C	-0.834316	0.224764	-1.446987
O	-2.115017	-0.193693	-1.281857
C	-1.791254	1.694559	-0.069713
C	-0.628466	1.435318	-0.791814
C	-4.099161	0.542946	-0.020306
H	-1.999967	2.517311	0.597435
H	-0.265285	-0.292470	-2.205386
H	0.282753	2.014917	-0.804320
O	-4.690108	-0.501252	-0.631512
O	-4.670719	1.341147	0.693948
C	-6.104082	-0.621805	-0.397926
H	-6.416811	-1.498596	-0.964949
H	-6.306134	-0.758266	0.667720
H	-6.627578	0.271410	-0.748301

E = -1202.1557949

1 imaginary frequency

TS-S1

C	-0.212478	2.201867	-0.428066
O	0.404472	2.727222	-1.321453
O	-1.115136	2.832588	0.366406
C	-1.471134	1.968330	1.471794
C	-1.156924	0.540701	0.990878
H	-0.860501	2.253463	2.335501
H	-2.525029	2.128002	1.697631
N	-0.110363	0.866608	-0.012979
C	0.820053	0.029647	-0.547257
C	-2.340740	-0.194220	0.371501
C	-2.465079	-1.576644	0.556615
C	-3.550241	-2.264206	0.010034
C	-4.515167	-1.582754	-0.732708
C	-4.389056	-0.206435	-0.932864
C	-3.308413	0.483906	-0.384513
H	-1.687625	-2.104534	1.100470
H	-3.637956	-3.336633	0.163556
H	-5.359351	-2.120015	-1.157006
H	-5.132244	0.331741	-1.515245
H	-3.222053	1.554772	-0.551605
C	1.077727	-1.301641	-0.046696
C	2.011254	-2.004674	-0.880019
H	2.135783	-3.068120	-0.693583
O	0.629421	-1.736982	1.047246
H	2.201372	-1.671780	-1.893335
H	1.260099	0.393443	-1.466055
C	3.952483	-1.352250	0.034085
O	3.432724	-0.664677	1.099844
C	3.226747	0.601815	0.670019
H	-0.703294	-0.080426	1.760561
C	4.382142	-0.427801	-0.933721
C	3.869733	0.812945	-0.543174

H	4.331121	-2.335392	0.272858
H	2.778577	1.275942	1.384066
H	3.903332	1.748855	-1.083832
H	4.893019	-0.672303	-1.854907

E = -974.2721364

1 imaginary frequency

TS-S2

C	-3.714437	0.313746	-1.254897
C	-3.438006	0.915628	-0.018651
O	-2.169493	1.429547	-0.049647
C	-1.559011	0.879728	-1.127663
C	-2.494581	0.248186	-1.937185
C	-2.979713	-0.940496	1.192933
C	-1.559749	-0.838377	1.369536
O	-0.998911	-0.284142	2.351526
C	-0.847013	-1.395236	0.238046
N	0.508263	-1.508652	0.192396
C	1.146667	-2.336266	-0.745547
O	2.476294	-2.349107	-0.470586
C	2.713136	-1.681116	0.791497
C	1.505329	-0.748840	0.986111
O	0.623647	-2.943493	-1.645771
C	1.704142	0.669884	0.463368
C	2.475461	0.928835	-0.680168
C	2.636748	2.235284	-1.143578
C	2.029236	3.297422	-0.469569
C	1.254455	3.044541	0.663758
C	1.087348	1.737905	1.127459
H	2.768843	-2.443633	1.575480
H	3.664250	-1.154128	0.719273
H	1.152927	-0.711752	2.015389
H	2.950847	0.111415	-1.216579
H	3.238538	2.422216	-2.029047
H	2.157521	4.315112	-0.828807
H	0.771385	3.865038	1.187571
H	0.445826	1.524269	1.977114
H	-1.349818	-2.012221	-0.495436
H	-3.388927	-1.668263	0.502322
H	-3.600761	-0.696107	2.051173
H	-4.099838	1.381437	0.696628
H	-0.530850	1.166614	-1.284613
H	-2.288844	-0.228334	-2.885880
H	-4.661316	-0.118512	-1.548229

E = -974.2758183

1 imaginary frequency

TS-S3

C	3.351652	-1.939079	-0.059583
C	2.983651	-1.399625	-1.267463
O	1.630708	-1.460940	-1.426394
C	1.126740	-1.949859	-0.255538
C	2.144966	-2.290422	0.597715
C	2.967781	1.181162	-0.363947
C	2.351126	0.858793	0.859805
O	2.940785	0.494394	1.911915

C	0.888446	0.737020	0.915985
N	-0.171023	1.442896	0.410332
C	-0.201204	2.435090	-0.587861
O	-1.468104	2.931879	-0.664931
C	-2.265287	2.449934	0.426013
C	-1.540360	1.182355	0.923010
O	0.693773	2.811978	-1.296879
C	-2.123308	-0.128955	0.430576
C	-2.443063	-1.134659	1.348415
C	-2.975929	-2.350886	0.913772
C	-3.192266	-2.569824	-0.446643
C	-2.878046	-1.568175	-1.370292
C	-2.348213	-0.354676	-0.935720
H	-3.270344	2.249180	0.053397
H	-2.305885	3.224360	1.199524
H	-1.502078	1.169566	2.016037
H	-2.273614	-0.968737	2.410095
H	-3.218400	-3.123639	1.637828
H	-3.603992	-3.515296	-0.788278
H	-3.043871	-1.733583	-2.431020
H	-2.103948	0.415523	-1.662788
H	0.585418	0.120455	1.756423
H	2.429646	1.632518	-1.183133
H	4.051378	1.136549	-0.404398
H	3.541358	-1.064718	-2.127871
H	0.057677	-2.091506	-0.229983
H	2.040976	-2.701989	1.591369
H	4.355441	-2.016598	0.331319

E = -974.2506352

1 imaginary frequency

TS-S4

N	-0.049056	1.108005	0.294973
C	-0.390067	2.480247	0.409267
O	-1.301656	2.932573	1.051445
O	0.450157	3.212081	-0.353834
C	1.502830	2.380742	-0.866647
H	1.683899	2.655927	-1.906798
H	2.405636	2.559669	-0.275715
C	1.009314	0.919155	-0.709117
H	0.549038	0.577713	-1.644786
C	2.144471	-0.011031	-0.324989
C	2.801192	-0.727416	-1.331143
C	3.909942	-1.519145	-1.029104
C	4.367666	-1.605482	0.285770
C	3.714637	-0.893874	1.294659
C	2.613177	-0.095053	0.991320
H	2.440134	-0.672681	-2.356207
H	4.408153	-2.073354	-1.819640
H	5.224745	-2.228476	0.525349
H	4.059549	-0.963860	2.322306
H	2.107328	0.448258	1.784584
C	-0.843015	0.189092	0.920354
H	-1.411480	0.631989	1.730333
C	-0.853770	-1.277540	0.896432
C	-0.542855	-1.901251	-0.329613
O	-1.321065	-1.845722	1.914671
H	-0.686333	-2.973399	-0.410953

H	-0.004280	-1.412505	-1.129320
C	-3.009314	-1.488363	-1.386220
O	-2.810407	-0.141364	-1.454404
C	-3.260984	0.372581	-0.268343
C	-3.855098	-0.614103	0.482495
C	-3.696952	-1.818419	-0.241755
H	-2.737805	-2.048028	-2.267626
H	-3.206100	1.445427	-0.164452
H	-4.300104	-0.493129	1.459492
H	-3.992263	-2.810973	0.065402

E = -974.2572196

1 imaginary frequency

TS-S5

C	-1.296642	-1.445921	-0.466337
O	-1.784616	-2.348231	-1.184836
C	-1.562064	-1.318140	0.938206
H	-1.283679	-0.435678	1.499453
H	-1.703741	-2.248142	1.481331
C	-0.199433	-0.657283	-0.962234
H	0.317551	-1.148536	-1.783670
N	0.387187	0.546781	-0.635269
C	-0.150378	1.619104	0.071673
O	-1.199569	1.669064	0.666061
O	0.728478	2.664892	0.023773
C	1.777024	2.386419	-0.915467
H	1.560135	2.915060	-1.850156
H	2.716847	2.750941	-0.498878
C	1.757154	0.854057	-1.105548
H	1.825873	0.599809	-2.168659
C	2.828365	0.094214	-0.344748
C	3.608742	-0.860451	-1.003548
C	4.593310	-1.571882	-0.314279
C	4.803644	-1.333153	1.043257
C	4.027497	-0.380653	1.709627
C	3.046153	0.328925	1.020692
H	3.446511	-1.050811	-2.062252
H	5.191758	-2.311635	-0.838652
H	5.568135	-1.885968	1.582111
H	4.186719	-0.191130	2.767539
H	2.445510	1.066612	1.547534
C	-3.874143	-0.915057	1.094438
O	-3.878851	0.446013	1.294264
C	-4.148060	1.011192	0.096825
C	-4.412442	0.055373	-0.852188
C	-4.276596	-1.196946	-0.203570
H	-3.919263	-1.503475	1.998129
H	-4.103116	2.088932	0.069077
H	-4.659138	0.234089	-1.889222
H	-4.356734	-2.180238	-0.641678

E = -974.2449924

1 imaginary frequency

TS-S6

O	3.893841	-1.406891	-0.503896
C	2.801334	-1.254609	0.333130

C	2.805529	0.055000	0.812088
C	3.889089	0.725825	0.195211
C	4.511857	-0.206382	-0.593373
C	1.048333	-1.532536	-0.905286
C	0.264564	-2.271702	0.059102
C	-1.084249	-1.912346	0.355401
N	-1.931931	-0.945238	-0.121031
C	-3.293163	-0.966839	0.260197
O	-3.943401	0.030846	-0.390578
C	-3.085719	0.617562	-1.378728
C	-1.644407	0.196330	-0.982167
O	-3.807927	-1.722799	1.040270
C	-0.857456	1.314892	-0.312170
C	-0.933886	1.548787	1.065592
C	-0.260484	2.631990	1.633682
C	0.490288	3.494298	0.831941
C	0.570580	3.265835	-0.542846
C	-0.098336	2.180522	-1.109539
O	0.767094	-3.280121	0.641093
H	-1.607025	-2.618743	0.993070
H	-3.228533	1.698404	-1.358640
H	-3.366693	0.225014	-2.361815
H	-1.101572	-0.152007	-1.869250
H	-1.509990	0.881649	1.700023
H	-0.327184	2.802758	2.704620
H	1.010730	4.338008	1.276553
H	1.156433	3.928032	-1.174320
H	-0.027054	2.003954	-2.181190
H	2.420542	-2.187598	0.770632
H	4.172453	1.762993	0.307646
H	5.367585	-0.164210	-1.251244
H	0.784190	-0.546769	-1.266157
H	1.683747	-2.117578	-1.561501
H	2.075786	0.474713	1.490268

E = -974.2472084

1 imaginary frequency

TS-S7

C	0.960629	0.460212	1.033002
H	0.477343	-0.016515	1.881277
C	2.427218	0.445180	1.216748
O	2.808196	0.121457	2.365768
C	3.267949	0.597460	0.084154
H	2.928585	1.100972	-0.807678
H	4.336613	0.489535	0.248842
N	0.084591	1.317783	0.394951
C	0.289261	2.136949	-0.719034
O	1.262244	2.221983	-1.424589
O	-0.846157	2.866895	-0.937711
C	-1.750602	2.710276	0.165122
H	-1.632789	3.564240	0.841126
H	-2.768844	2.689116	-0.225125
C	-1.329172	1.390562	0.839567
H	-1.342295	1.496678	1.928165
C	-2.148883	0.172606	0.451392
C	-2.570821	-0.723621	1.439204
C	-3.316933	-1.856077	1.102428
C	-3.651315	-2.099325	-0.229384

C	-3.239341	-1.205999	-1.222692
C	-2.492467	-0.078023	-0.885884
H	-2.319124	-0.534072	2.480460
H	-3.637895	-2.542151	1.881266
H	-4.233708	-2.977326	-0.494204
H	-3.503068	-1.387064	-2.261085
H	-2.176996	0.611384	-1.665198
C	3.059292	-1.763584	-0.714008
O	2.276135	-2.197709	0.307884
C	0.987871	-1.964111	-0.064228
C	0.941054	-1.590799	-1.397197
C	2.274644	-1.472748	-1.822080
H	4.116844	-1.941817	-0.598501
H	0.229702	-2.306994	0.622383
H	0.044731	-1.386747	-1.965125
H	2.635110	-1.138475	-2.784731

E = -974.2455103

1 imaginary frequency

TS-S8

O	3.328083	-1.458201	-0.337771
C	2.922017	-1.953217	0.858536
C	2.879156	-0.927578	1.803278
C	3.086686	0.261938	1.093510
C	3.266019	-0.100108	-0.236952
C	0.532672	-1.992223	0.303824
C	0.630733	-1.406895	-0.989631
C	0.863134	0.046094	-1.036880
N	0.200876	1.057286	-0.375075
C	0.695476	2.369531	-0.489631
O	-0.042076	3.195362	0.293775
C	-1.179777	2.482650	0.803537
C	-0.826741	0.979881	0.673247
O	1.643687	2.718632	-1.145991
C	-2.047951	0.137457	0.361184
C	-2.707039	-0.514359	1.408886
C	-3.885771	-1.223312	1.173597
C	-4.411485	-1.292920	-0.116661
C	-3.755515	-0.648199	-1.167652
C	-2.583702	0.068686	-0.930429
O	0.749385	-2.033490	-2.063465
H	0.165296	-1.442008	1.160169
H	0.477245	-3.075210	0.363698
H	1.330055	0.398279	-1.950765
H	-1.348647	2.791562	1.836304
H	-2.054038	2.735952	0.195867
H	-0.366174	0.626932	1.605229
H	-2.294485	-0.471920	2.414949
H	-4.385685	-1.727192	1.996172
H	-5.323383	-1.852611	-0.304765
H	-4.152377	-0.708071	-2.177001
H	-2.074744	0.558044	-1.755932
H	2.984742	-3.025171	0.964648
H	2.648673	-1.044528	2.853332
H	3.070444	1.274921	1.471956
H	3.616844	0.457046	-1.091296

E = -974.250426

1 imaginary frequency

TS-S9

C	-1.549172	-0.736371	1.604565
C	-2.816519	-0.091118	1.587642
O	-1.283449	-1.777214	2.248178
C	-0.520100	-0.320231	0.635891
H	0.205550	-1.113847	0.487775
C	-1.839300	-1.481639	-1.417999
O	-2.756077	-2.057051	-0.595949
C	-3.749161	-1.142922	-0.420904
C	-3.584309	-0.091359	-1.315187
C	-2.347166	-0.306396	-1.945703
H	-0.999788	-2.103975	-1.687660
H	-1.860258	0.330427	-2.672080
H	-4.245346	0.756411	-1.427442
H	-4.608260	-1.490569	0.130961
N	-0.012143	0.896900	0.231151
C	-0.561618	2.180569	0.374103
O	0.241708	3.076413	-0.268945
C	1.458390	2.442803	-0.678989
C	1.131894	0.939254	-0.709385
H	1.747841	2.837590	-1.654560
H	2.242521	2.666931	0.052290
C	2.306184	0.054599	-0.352277
C	2.834574	0.036495	0.946586
C	3.946253	-0.749499	1.242859
C	4.548714	-1.519778	0.244645
C	4.028882	-1.507271	-1.049436
C	2.908791	-0.727335	-1.343369
H	2.362291	0.621673	1.731306
H	4.339303	-0.764772	2.255333
H	5.414980	-2.132284	0.478280
H	4.487632	-2.108697	-1.829212
H	2.501406	-0.725096	-2.352200
H	-2.922982	0.941212	1.292227
H	-3.590357	-0.532146	2.210385
O	-1.568027	2.508628	0.948163
H	0.759194	0.653828	-1.703284

E = -974.2457304

1 imaginary frequency

TS-S10

C	1.370947	-0.654302	-1.002479
C	0.950637	-1.834723	-0.308272
O	1.744721	-2.784954	-0.045207
C	-0.395143	-1.956983	0.181316
H	-0.575667	-2.835967	0.793667
N	-1.559631	-1.312682	-0.124778
C	-2.788570	-1.798565	0.390253
O	-3.800869	-1.094815	-0.172337
O	-2.927360	-2.677005	1.197936
C	-3.296442	-0.270023	-1.234393
H	-3.819916	0.685650	-1.202555
H	-3.493357	-0.771547	-2.187973
C	-1.776845	-0.133316	-0.958100
H	-1.206845	-0.246804	-1.887951

C	-1.409235	1.187175	-0.291897
C	-1.382568	1.336375	1.099084
C	-1.097806	2.579707	1.667781
C	-0.842840	3.685018	0.854572
C	-0.870402	3.542775	-0.533968
C	-1.150034	2.300204	-1.102373
H	-1.572009	0.482684	1.743073
H	-1.076616	2.681968	2.749207
H	-0.619359	4.650284	1.299909
H	-0.665406	4.395474	-1.175151
H	-1.158592	2.193269	-2.185514
C	2.759063	0.288713	0.536542
O	3.501454	1.126139	-0.272152
C	4.665598	0.475455	-0.537298
C	4.732576	-0.710299	0.139897
C	3.522813	-0.825475	0.875855
H	1.939372	0.771595	1.045532
H	5.336474	0.976495	-1.219577
H	5.544909	-1.422532	0.105349
H	3.214623	-1.642962	1.506437
H	0.720684	0.184934	-1.210371
H	2.255068	-0.739103	-1.625664

E = -974.2486779

1 imaginary frequency

B3LYP/6-311G(2d,p) Geometries and Total Energies (Hartrees)

4 (Closed-shell singlet)

C	0.000000	0.000000	0.167930
O	0.000000	0.000000	1.400375
C	0.000000	1.158320	-0.682871
C	0.000000	-1.158320	-0.682871
H	0.000000	-1.076371	-1.760851
H	0.000000	-2.152358	-0.247215
H	0.000000	1.076371	-1.760851
H	0.000000	2.152358	-0.247215

E = -191.8772354

1 imaginary frequency

4 (Open-shell singlet)

C	0.000000	0.000000	0.125430
O	0.000000	0.000000	1.358737
C	0.000000	1.221933	-0.655703
C	0.000000	-1.221933	-0.655703
H	0.000000	-1.210528	-1.738167
H	0.000000	-2.172816	-0.138851
H	0.000000	1.210528	-1.738167
H	0.000000	2.172816	-0.138851

E = -191.893491

0 imaginary frequencies

S**2 before annihilation 0.8165, after 0.0264

4 (Triplet)

C	0.000000	0.000000	0.066100
O	0.000000	0.000000	1.331864
C	0.000000	1.253306	-0.628809
C	0.000000	-1.253306	-0.628809
H	0.000000	-1.314879	-1.709444
H	0.000000	-2.161775	-0.043458
H	0.000000	1.314879	-1.709444
H	0.000000	2.161775	-0.043458

E = -191.8948289

0 imaginary frequencies

S**2 before annihilation 2.0284, after 2.0002

5a (Closed-shell singlet)

H	2.311843	1.661450	0.000000
C	2.411855	0.578207	0.000000
N	1.094543	-0.051505	0.000000
C	1.104681	-1.522520	0.000000
H	0.065647	-1.855978	0.000000
C	0.000000	0.665602	0.000000
H	0.157729	1.737074	0.000000
C	-1.392956	0.175896	0.000000
O	-1.680068	-1.048435	0.000000
C	-2.251169	1.270854	0.000000
H	-1.883146	2.286820	0.000000

```
H    -3.322340    1.116394    0.000000
H     2.968877    0.265254    0.886014
H     2.968877    0.265254   -0.886014
H     1.638395   -1.868244    0.888475
H     1.638395   -1.868244   -0.888475

E = -325.9501903

0 imaginary frequencies
```

5a (Triplet)

```
C    -2.311308   -0.949475    0.012378
N    -1.144581   -0.097652   -0.117130
C    -1.392701    1.322737    0.080067
C     0.093845   -0.667366   -0.038659
C     1.365385   -0.011082   -0.016730
O     1.520622    1.240042   -0.061765
C     2.569832   -0.827730    0.067482
H    -2.674059   -0.985521    1.048668
H    -0.495222    1.883733   -0.154492
H     0.087327   -1.749040   -0.053247
H     2.545869   -1.903613    0.187841
H     3.519929   -0.315804    0.026033
H    -2.074267   -1.962959   -0.308746
H    -3.118733   -0.566519   -0.615893
H    -1.676075    1.526596    1.121638
H    -2.217996    1.633851   -0.564996

E = -325.9193393

0 imaginary frequencies

S**2 before annihilation     2.0172,   after     2.0001
```

5b (Closed-shell singlet)

```
C    -2.183020   -0.369449    0.181201
C    -0.936369    0.210046   -0.083829
C     0.026044   -0.886354   -0.137650
O     1.310041   -0.832974   -0.051292
C     2.026578    0.432809    0.158157
O    -0.622860    1.419482   -0.153470
H    -3.019063    0.254511    0.471643
H    -2.352648   -1.431043    0.076618
H    -0.318843   -1.907847   -0.260738
H     1.362986    1.261612   -0.074381
H     2.900075    0.367809   -0.485704
H     2.330646    0.440580    1.203385

E = -306.4751001

0 imaginary frequencies
```

5b (Triplet)

```
C     2.321473   -0.273328    0.000682
C     0.920499    0.096115   -0.000040
C    -0.070567   -0.936954    0.000357
O    -1.399456   -0.805922   -0.001419
C    -2.027390    0.486914    0.001176
O     0.623974    1.322864   -0.001150
H     3.046837    0.526939    0.002455
H     2.658232   -1.302030   -0.000970
```

```
H     0.220929   -1.979545    0.000752
H    -1.743954    1.052809    0.886863
H    -3.094738    0.275251    0.002976
H    -1.747531    1.054564   -0.884575

E = -306.4583754

0 imaginary frequencies

S**2 before annihilation     2.0203,   after     2.0001
```

5c (Closed-shell singlet)

```
H    -1.682612    2.450604    0.000000
C    -2.169528    1.485560    0.000000
H    -3.252080    1.454630    0.000000
C    -1.425650    0.295313    0.000000
O    -1.819701   -0.887929    0.000000
C     0.000000    0.579419    0.000000
H     0.430499    1.573165    0.000000
S     0.980898   -0.779987    0.000000
C     2.659117   -0.046627    0.000000
H     2.812876    0.552006    0.895663
H     2.812876    0.552006   -0.895663
H     3.358051   -0.881172    0.000000

E = -629.4572191

0 imaginary frequencies
```

5c (Open-shell singlet)

```
H     3.378067    0.701233    0.000000
C     2.373040    1.102835    0.000000
H     2.240279    2.176012    0.000000
C     1.264761    0.202896    0.000000
O     1.349862   -1.037125    0.000000
C     0.000000    0.920512    0.000000
H    -0.000083    2.003914    0.000000
S    -1.571473    0.300586    0.000000
C    -1.456445   -1.526129    0.000000
H    -2.494895   -1.857288    0.000000
H    -0.933418   -1.868459    0.885655
H    -0.933418   -1.868459   -0.885655

E = -629.4619144

0 imaginary frequencies

S**2 before annihilation     0.5123,   after     0.0086
```

5c (Triplet)

```
H     3.415868    0.449172    0.000000
C     2.485551    0.998697    0.000000
H     2.502647    2.080986    0.000000
C     1.256464    0.235082    0.000000
O     1.334904   -1.018917    0.000000
C     0.000000    0.934581    0.000000
H     0.002638    2.017959    0.000000
S    -1.602385    0.320638    0.000000
C    -1.490417   -1.499571    0.000000
H    -2.526799   -1.836867    0.000000
H    -0.972505   -1.851427    0.887067
```

```
H    -0.972505   -1.851427   -0.887067
```

E = -629.451185

0 imaginary frequencies

S**2 before annihilation   2.0209,   after   2.0002

1_{Ph}-*E* (Closed-shell singlet)

```
O    -0.915510   -2.589101    0.382651
C    -1.542271   -1.743700   -0.447333
N    -1.253027   -0.407518   -0.017421
C    -0.167512   -0.420142    1.002931
C    -0.321679   -1.863708    1.494187
C    -1.913692    0.629146   -0.496778
H    -0.423133    0.327371    1.749320
O    -2.230168   -2.043894   -1.371802
C     1.185071   -0.090701    0.390274
H    -1.003673   -1.940831    2.341646
H     0.623434   -2.342630    1.730544
C     1.696458    1.199384    0.535200
C     2.934955    1.523935   -0.007186
C     3.668406    0.571030   -0.704273
C     3.158584   -0.713367   -0.860819
C     1.924012   -1.043680   -0.315818
H     1.098167    1.944048    1.046404
H     3.325008    2.527486    0.114461
H     4.632923    0.827199   -1.126455
H     3.722119   -1.460542   -1.406748
H     1.542735   -2.049969   -0.449511
C    -1.812081    1.984475    0.036513
H    -2.606082    0.380947   -1.291892
C    -2.458090    2.864706   -0.830577
O    -1.203819    2.235344    1.108803
H    -2.410723    3.932621   -0.659112
H    -3.046581    2.503870   -1.661858
```

E = -744.4743293

0 imaginary frequencies

1_{Ph}-*E* (Open-shell singlet)

```
O    -0.898436   -2.595783    0.390222
C    -1.536146   -1.751242   -0.435462
N    -1.248540   -0.417208   -0.012339
C    -0.160514   -0.422061    1.003805
C    -0.302636   -1.867175    1.496571
C    -1.907887    0.619974   -0.507049
H    -0.415464    0.319613    1.755298
O    -2.230291   -2.058419   -1.353933
C     1.189262   -0.084676    0.389080
H    -0.978140   -1.947218    2.349132
H     0.647400   -2.339123    1.727671
C     1.707619    1.199987    0.553895
C     2.944024    1.529629    0.009562
C     3.668944    0.586601   -0.709319
C     3.152602   -0.692743   -0.885400
C     1.920221   -1.027712   -0.338531
H     1.117228    1.938826    1.081723
H     3.338867    2.529311    0.146697
H     4.631768    0.846394   -1.133139
```

```
H     3.709561   -1.432402   -1.448078
H     1.533784   -2.029951   -0.487007
C    -1.821791    1.974523    0.021443
H    -2.591915    0.364777   -1.306693
C    -2.519115    2.859114   -0.813040
O    -1.202397    2.241907    1.081490
H    -2.510399    3.921092   -0.604137
H    -3.101415    2.502194   -1.650660
```

E = -744.4745642

0 imaginary frequencies

S**2 before annihilation   0.1754,   after   0.0007

1_{Ph}-*E* (Triplet)

```
O    -1.358514   -2.487047    0.372002
C    -1.922727   -1.476394   -0.334316
N    -1.348226   -0.267988    0.072150
C    -0.225850   -0.488708    1.000080
C    -0.516886   -1.948572    1.409429
C    -1.756363    0.911927   -0.487451
H    -0.322983    0.185159    1.846452
O    -2.766421   -1.621447   -1.171638
C     1.133501   -0.280043    0.356053
H    -1.061847   -2.002881    2.353814
H     0.381374   -2.557769    1.465628
C     2.031817    0.627245    0.913028
C     3.295776    0.801047    0.358591
C     3.670597    0.073185   -0.763570
C     2.776690   -0.830752   -1.329993
C     1.516866   -1.007163   -0.773753
H     1.730220    1.215045    1.771159
H     3.983342    1.512278    0.800710
H     4.653432    0.210280   -1.198650
H     3.061870   -1.400272   -2.206580
H     0.832737   -1.718492   -1.223135
C    -1.373027    2.212471   -0.020829
H    -2.474831    0.788006   -1.285246
C    -1.812296    3.383103   -0.745276
O    -0.667407    2.372375    1.011421
H    -1.560676    4.350514   -0.336073
H    -2.354919    3.318936   -1.679376
```

E = -744.4564398

0 imaginary frequencies

S**2 before annihilation   2.0194,   after   2.0001

M06-2X/6-31G(d) Geometries and Total Energies (Hartrees)

1_{Ph}-E_{cyc}

C	1.825138	-1.137406	-0.293841
C	1.199517	-0.153187	0.476514
C	1.790492	1.105450	0.593570
C	3.005275	1.372378	-0.033735
C	3.633310	0.383517	-0.785333
C	3.039446	-0.870462	-0.917862
C	-0.152983	-0.398334	1.112330
N	-1.246388	-0.257094	0.146627
C	-1.606128	-1.494083	-0.360508
O	-1.079803	-2.457495	0.443261
C	-0.428953	-1.842838	1.558535
O	-2.265802	-1.713541	-1.337387
C	-1.339705	0.893503	-0.688848
C	-1.587495	2.169164	0.015029
O	-1.152957	2.970671	0.791914
C	-2.710563	1.636020	-0.754428
H	-0.300286	0.304972	1.937766
H	-1.106059	-1.868700	2.417557
H	0.478098	-2.404820	1.783947
H	1.283844	1.882667	1.161847
H	3.458984	2.353644	0.065495
H	4.582142	0.588540	-1.271453
H	3.522509	-1.642151	-1.509233
H	1.360343	-2.114003	-0.411364
H	-0.753418	0.892272	-1.608528
H	-3.539773	1.186447	-0.214419
H	-2.964435	2.078970	-1.713330

E = -743.9746534

0 imaginary frequencies

Furan

C	0.000000	0.717088	-0.957900
H	0.000000	1.374100	-1.814730
C	0.000000	1.088940	0.346133
H	0.000000	2.043116	0.849495
C	0.000000	-0.717088	-0.957900
H	0.000000	-1.374100	-1.814730
C	0.000000	-1.088940	0.346133
H	0.000000	-2.043116	0.849495
O	0.000000	0.000000	1.151771

E = -229.9225777

0 imaginary frequencies

TSA

C	3.731282	-1.027693	0.991246
C	4.039655	-1.073977	-0.350621
O	3.760258	0.114861	-0.940288
C	3.099853	0.856174	-0.018800
C	3.111930	0.218015	1.201155
H	4.613311	-1.770112	-0.942897
C	1.859775	-2.002580	-1.183792
C	1.082367	-1.304128	-0.249395

O	0.782557	-1.688928	0.913178
C	0.796861	0.034974	-0.720342
N	-0.052354	0.863219	-0.077851
C	-0.192486	2.201077	-0.469337
O	-1.050362	2.804913	0.373001
C	-1.323770	1.941074	1.488792
C	-1.004446	0.521881	0.997135
O	0.376171	2.731709	-1.382179
C	-2.199786	-0.230969	0.442332
C	-2.273578	-1.615754	0.593545
C	-3.366375	-2.311902	0.081553
C	-4.379963	-1.634897	-0.590397
C	-4.299294	-0.253956	-0.757667
C	-3.212745	0.445539	-0.243991
H	-2.368254	2.071492	1.769895
H	-0.673927	2.241981	2.315791
H	-0.487355	-0.085123	1.738106
H	-1.452990	-2.133065	1.083044
H	-3.422240	-3.389130	0.205763
H	-5.230310	-2.180789	-0.988034
H	-5.083272	0.278756	-1.287021
H	-3.154756	1.523428	-0.382743
H	1.136229	0.398240	-1.684865
H	2.093949	-3.046105	-0.998218
H	2.071380	-1.596221	-2.166088
H	2.668112	0.581480	2.116188
H	3.855383	-1.826945	1.705504
H	2.817493	1.852605	-0.328500

E = -973.8852502

1 imaginary frequency

TSB

O	-2.907543	0.014295	-1.469481
C	-1.584882	0.312146	-1.527791
C	-1.010053	-1.383666	0.321817
C	-1.670640	-0.596539	1.343630
C	-3.055735	-0.802213	1.285277
C	-3.461364	0.886971	-0.595682
C	-2.543164	1.839421	-0.220706
C	-1.325985	1.465299	-0.823849
N	0.325758	-1.545324	0.273600
C	0.911833	-2.396639	-0.679308
O	2.228895	-2.475591	-0.423729
C	2.523743	-1.821248	0.821638
C	1.363062	-0.835453	1.044544
O	0.341369	-2.949703	-1.576072
C	1.639218	0.550995	0.498587
C	2.151757	0.716407	-0.791524
C	2.403152	1.991964	-1.289202
C	2.158093	3.109925	-0.494169
C	1.656185	2.946256	0.795456
C	1.386738	1.671832	1.288544
O	-1.041918	0.184570	2.102942
H	2.568977	-2.583739	1.604577
H	3.488927	-1.326380	0.719078
H	1.048626	-0.772134	2.083732
H	2.362885	-0.150790	-1.414232
H	2.794991	2.111846	-2.294478

H	2.355386	4.105139	-0.880900
H	1.455444	3.815084	1.414831
H	0.932344	1.536183	2.263680
H	-0.996494	-0.279431	-2.214939
H	-0.368447	1.957168	-0.734621
H	-2.715725	2.661693	0.456840
H	-4.528712	0.805942	-0.458925
H	-3.689089	-0.354329	2.044659
H	-1.553500	-2.067286	-0.322536
H	-3.494108	-1.538527	0.622769

E = -973.8887567

1 imaginary frequency

Solution-Phase Geometries [B3LYP/6-31G(d), CPCM(THF,UAKS)] and Total Energies (Hartrees)

1_{Ph}-E_{cyc}

C	1.843867	-1.108162	-0.385557
C	1.242511	-0.140429	0.432909
C	1.910810	1.069028	0.656520
C	3.161700	1.306671	0.082211
C	3.756328	0.335262	-0.723831
C	3.093381	-0.872705	-0.957971
C	-0.130330	-0.363417	1.049001
N	-1.230268	-0.256649	0.070465
C	-1.677197	-1.496486	-0.326714
O	-1.142983	-2.444700	0.500384
C	-0.414128	-1.792135	1.563973
O	-2.419683	-1.758520	-1.247843
C	-1.447839	0.900763	-0.739409
C	-1.685969	2.193834	-0.052262
O	-1.223530	3.042445	0.668008
C	-2.853259	1.608108	-0.712549
H	-0.285984	0.363183	1.853515
H	-1.048395	-1.774538	2.456219
H	0.489019	-2.369970	1.764681
H	1.441315	1.832926	1.271685
H	3.669542	2.249883	0.265641
H	4.731037	0.516886	-1.168899
H	3.550491	-1.632840	-1.585967
H	1.336859	-2.051088	-0.576148
H	-0.947934	0.925568	-1.713288
H	-3.627958	1.176694	-0.079247
H	-3.205809	2.004056	-1.663771

E = -744.2777974

0 imaginary frequencies

Furan

C	0.000000	0.718275	-0.959982
H	0.000000	1.374400	-1.819896
C	0.000000	1.096683	0.347236
H	0.000000	2.053013	0.849188
C	0.000000	-0.718275	-0.959982
H	0.000000	-1.374400	-1.819896
C	0.000000	-1.096683	0.347236
H	0.000000	-2.053013	0.849188
O	0.000000	0.000000	1.161796

E = -230.022521

0 imaginary frequencies

TSA

C	3.879020	-1.093946	0.961035
C	4.068603	-1.127872	-0.416951
O	3.872912	0.128154	-0.937879
C	3.333629	0.874880	0.062374
C	3.377364	0.184668	1.257889
H	4.628738	-1.806895	-1.043309
C	1.990099	-1.913160	-1.146312

C	1.132623	-1.238289	-0.234632
O	0.805077	-1.688430	0.904977
C	0.788756	0.077459	-0.708722
N	-0.120833	0.889010	-0.107546
C	-0.286258	2.220963	-0.505459
O	-1.142300	2.828014	0.347863
C	-1.400034	1.952562	1.478576
C	-1.087477	0.536378	0.966913
O	0.251553	2.766364	-1.441436
C	-2.289319	-0.226594	0.419388
C	-2.343587	-1.618430	0.564229
C	-3.437649	-2.336076	0.076725
C	-4.483841	-1.673803	-0.567550
C	-4.429749	-0.287298	-0.727503
C	-3.339265	0.431909	-0.237744
H	-2.437845	2.091320	1.779782
H	-0.732249	2.251053	2.292991
H	-0.565830	-0.073287	1.702265
H	-1.506135	-2.127577	1.031853
H	-3.470296	-3.415768	0.199209
H	-5.335484	-2.233357	-0.945770
H	-5.237260	0.236720	-1.232085
H	-3.312859	1.510409	-0.372201
H	1.164554	0.458761	-1.650252
H	2.192402	-2.966956	-0.978559
H	2.171196	-1.528668	-2.144007
H	3.042452	0.553160	2.217566
H	4.009356	-1.924464	1.640164
H	3.099658	1.899560	-0.186553

E = -974.2880582

1 imaginary frequency

TSB

O	-3.074168	0.013209	-1.465570
C	-1.802996	0.487111	-1.569586
C	-0.939558	-1.420591	0.258853
C	-1.664583	-0.722636	1.293258
C	-3.065868	-0.929436	1.160561
C	-3.661201	0.709341	-0.440847
C	-2.842650	1.768044	-0.066848
C	-1.639046	1.604865	-0.774912
N	0.413259	-1.539906	0.217796
C	1.032471	-2.447503	-0.655615
O	2.352312	-2.495561	-0.369046
C	2.607614	-1.769968	0.862329
C	1.427506	-0.787584	1.000297
O	0.495882	-3.090367	-1.527179
C	1.709998	0.601770	0.444329
C	2.330143	0.779597	-0.801447
C	2.608867	2.061444	-1.276862
C	2.279975	3.180984	-0.508077
C	1.663290	3.010495	0.733188
C	1.371858	1.727862	1.203035
O	-1.120499	0.007009	2.172847
H	2.634486	-2.495572	1.681425
H	3.574930	-1.277921	0.764521
H	1.073746	-0.704807	2.025609
H	2.606467	-0.081987	-1.404378

```
H     3.088584    2.184838   -2.244182
H     2.503785    4.179175   -0.875210
H     1.401324    3.876947    1.335045
H     0.846125    1.589317    2.141538
H    -1.193144    0.038685   -2.339886
H    -0.739498    2.196609   -0.690379
H    -3.070609    2.511075    0.684439
H    -4.720459    0.541766   -0.311397
H    -3.712255   -0.580905    1.961220
H    -1.445783   -2.096248   -0.419761
H    -3.463649   -1.698710    0.508481
```

E = -974.2886993

1 imaginary frequency

TSC

```
C     4.307485    0.132072    1.046436
C     3.915460   -0.022131   -0.280110
O     4.748612   -0.951703   -0.873488
C     5.586771   -1.414085    0.083855
C     5.363570   -0.781914    1.279593
H     6.270487   -2.193073   -0.222714
C     1.934476   -0.939440   -0.185169
C     1.127168    0.222912   -0.478120
O     1.280816    0.904352   -1.526350
C     0.103344    0.372874    0.500757
N    -0.978714    1.206866    0.326994
C    -0.898251    2.552362   -0.045967
O    -2.167441    3.047190   -0.145723
C    -3.125732    1.989430    0.031720
C    -2.350763    0.861311    0.748322
O     0.085039    3.232506   -0.191919
C    -2.795145   -0.528025    0.345449
C    -3.550432   -1.300349    1.233961
C    -4.013710   -2.563424    0.858722
C    -3.714810   -3.068777   -0.407041
C    -2.951992   -2.306346   -1.296212
C    -2.495528   -1.042610   -0.924342
H    -3.961261    2.373805    0.619427
H    -3.481666    1.665267   -0.951997
H    -2.436536    0.977607    1.839826
H    -3.777822   -0.911755    2.224274
H    -4.601269   -3.152078    1.558150
H    -4.069499   -4.053633   -0.698990
H    -2.709723   -2.697882   -2.280606
H    -1.893302   -0.457238   -1.614571
H     0.019227   -0.323465    1.327491
H     1.858718   -1.456254    0.767290
H     2.262184   -1.548167   -1.022755
H     5.886104   -0.963843    2.208598
H     3.845781    0.801063    1.760431
H     3.411909    0.649674   -0.974086
```

E = -974.2659821

1 imaginary frequency

TSD

```
N     0.538598    1.503865   -0.299702
```

C	0.653261	2.832776	0.158551
O	-0.201846	3.673808	0.234954
O	1.963566	3.078811	0.435233
C	2.754486	1.893558	0.252261
H	3.685630	2.172006	-0.244341
H	2.976661	1.464668	1.233865
C	1.881289	0.953090	-0.604138
H	2.090604	1.111790	-1.672802
C	2.051634	-0.513189	-0.268016
C	2.441204	-1.414574	-1.264385
C	2.634457	-2.765873	-0.964975
C	2.438761	-3.227275	0.337163
C	2.045278	-2.333464	1.338674
C	1.849974	-0.986389	1.037470
H	2.598053	-1.057167	-2.279608
H	2.938444	-3.453742	-1.749133
H	2.591327	-4.276925	0.573083
H	1.888654	-2.687129	2.354176
H	1.528369	-0.303034	1.819440
C	-0.609785	0.929182	-0.771748
H	-0.456236	0.229722	-1.586411
C	-1.940254	1.204041	-0.290265
O	-2.234273	1.739182	0.804520
C	-2.888693	0.765950	-1.271240
H	-2.579743	0.302655	-2.201605
H	-3.894734	1.175161	-1.236402
C	-1.503298	-1.953981	0.253698
C	-2.153732	-1.469713	1.362840
C	-3.455946	-1.120816	0.941602
O	-2.337880	-1.979154	-0.819029
C	-3.503782	-1.369273	-0.419487
H	-0.522533	-2.376113	0.100103
H	-1.729250	-1.350023	2.349700
H	-4.240873	-0.673579	1.534368
H	-4.330229	-1.450815	-1.109957

E = -974.2706282

1 imaginary frequency

Complete Citation for Ref. 39

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

Complete Citation for Ref. 40

Gaussian 09, Revision A.02, Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery, Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C. Iyengar, S. S. Tomasi, J. Cossi, M. Rega, Millam, N. J., Klene, M. Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, O., Foresman, J. B., Ortiz, J. V., Cioslowski, J., and Fox, D. J., Gaussian, Inc., Wallingford CT, 2009.