

SUPPORTING INFORMATION

Understanding the Mechanism of Stereoselective Synthesis of
Cyclopentenes via N-Heterocyclic Carbene Catalyzed Reactions of enals
with enones.

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- S25** MPWB1K/6-31G** computed total energies, unique frequency imaginary, and cartesian coordinates of the TSs involved in the formation of the bicyclic lactone **22**.

Table S1. B3LYP/6-31G** Enthalpies (H, in au) and free energies (G, in au) computed at 298.15 K and 1 atm in THF of the stationary points involved in the NHC catalyzed addition of the *E*-but-2-enal **12** to *E*-pent-3-en-2-one **13**.

	H	G
<i>i) Formation of the Breslow intermediate 17.</i>		
12	-231.154595	-231.190527
14	-304.682703	-304.721877
TS1	-535.831268	-535.883501
16	-535.839072	-535.893851
17	-535.846990	-535.902672
<i>ii) Formation of the bicyclic lactone 22.</i>		
13	-270.453248	-270.493207
TS2	-806.294859	-806.364755
TS7	-806.290817	-806.359396
18	-806.332212	-806.402256
23	-806.332582	-806.400716
19	-806.340523	-806.410988
TS3	-806.312985	-806.379329
TS4	-806.317794	-806.382251
21	-806.328376	-806.394127
TS5	-806.316922	-806.383274
22+14	-806.331595	-806.397977
<i>iii) Formation of the trans-cyclopentene 15.</i>		
22	-501.648614	-501.697236
TS6	-501.603903	-501.655252
15+CO₂	-501.665518	-501.723415
15	-313.096689	-313.140500

Table S2. MPWB1K/ 6-31G** Total and relative enthalpies (H, in au, and ΔH , in kcal/mol) and total and relative free energies (G, in au, and ΔG , in kcal/mol) computed at 298.15 K and 1 atm in THF of the stationary points involved in the formation of the bicyclic lactone **22**.

	H	ΔH	G	ΔG
13	-270.297740		-270.337201	
14	-304.518189		-304.556996	
17	-535.561702		-535.616406	
TS2	-805.853848	3.5	-805.921845	19.9
TS7	-805.851146	5.2	-805.917988	22.4
18	-805.906739	-29.7	-805.974580	-13.2
23	-805.906379	-29.5	-805.973878	-12.7
19	-805.915132	-34.9	-805.983216	-18.6
TS3	-805.894694	-22.1	-805.958853	-3.3
TS4	-805.900255	-25.6	-805.963068	-5.9
21	-805.917590	-36.5	-805.982892	-18.4
TS5	-805.902244	-26.9	-805.967408	-8.7
22	-501.393244	-32.6	-501.441465	-28.1

Table S3. B3LYP/6-31G** Total energies (E, in au), in gas-phase and THF, of the TSs associated with nucleophilic addition of the Breslow intermediate **26** to the chalcone **10**.

	gas-phase	THF
TS8	-1381.865684	-1381.886985
TS9	-1381.860981	-1381.881644

Table S4. B3LYP/6-31G** Enthalpies (H, in au) and free energies (G, in au) computed at 298.15 K and 1 atm in THF of the stationary points associated with the addition of the Breslow intermediate **29** to the γ -cetoenoate **6**.

	H	G
6	-650.688090	-650.739750
29	-727.549798	-727.612609
TS10	-1378.236398	-1378.328203
TS11	-1378.235338	-1378.324300
TS12	-1378.215438	-1378.308702
30	-1378.257500	-1378.350341
31	-1378.260580	-1378.348595
32	-1378.214881	-1378.310165

Complete citation for reference 22.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.;
Cheeseman, J. R.; Montgomery, J., J. A. ; Vreven, T.; Kudin, K. N.; Burant, J. C.;
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B3LYP/6-31G** computed total energies, unique frequency imaginary, and cartesian coordinates of the stationary points involved in the NHC catalyzed addition of the *E*-but-2-enal **12** to *E*-pent-3-en-2-one **13**, and the TSs **TS8** - **TS12**.

12

E(RB+HF-LYP) = -231.242910251 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.469158940000
C	1.148501698921	0.000000000000	2.163160135555
C	1.272705329250	-0.000423504628	3.652814329763
O	-1.002622400546	-0.000110470529	-0.689869266168
H	-0.970785949353	-0.000023718742	1.960071204626
H	2.084624785189	0.000071709295	1.601185347562
H	0.296389004223	0.002579266175	4.143848816720
H	1.831354178015	-0.880689271314	3.994796313088
H	1.837219162811	0.875921243383	3.995059683488
H	1.014468995842	0.000111775806	-0.462088425902

13

E(RB+HF-LYP) = -270.567923000 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.340908180000
C	1.226944483382	0.000000000000	-0.858300617182
C	-1.206019305198	0.000237630039	2.205226381024
C	-2.586740630745	-0.000737570554	1.565592184722
H	-0.951466734922	0.000187473846	-0.530973397223
H	0.936720521149	-0.000152856749	1.895071138847
H	2.140880592639	-0.000177157104	-0.258808874936
H	1.243369057153	0.878711912345	-1.515255727456
H	1.243229194197	-0.878550508009	-1.515490166752
O	-1.078784782689	0.001010365015	3.421762972793
H	-2.727124966441	-0.884584097822	0.933902836047
H	-3.336555459698	0.000221089087	2.357093980270
H	-2.727628310441	0.881047916935	0.931186256128

14

E(RB+HF-LYP) = -304.803844949 A.U.

C	0.000000000000	0.000000000000	0.000000000000
N	0.000000000000	0.000000000000	1.372387410000
N	1.345186615202	0.000000000000	-0.272549522598
C	1.278842873749	0.000000000000	1.921786506542
C	-1.225106368259	-0.000135565974	2.152173116719
C	2.137472148814	-0.000204901019	0.871678943936
C	1.866098007129	-0.000506528435	-1.628152188880
H	1.467363469440	0.000068378732	2.984898760800
H	-1.287200633829	-0.889673519845	2.788343836198
H	-2.057155186586	-0.001631795009	1.448681401715
H	-1.288721481287	0.890661221263	2.786422973194
H	3.216863083429	0.000277352718	0.845389715311

H	1.011304801693	-0.000850485997	-2.303813783835
H	2.476269391799	-0.890673613928	-1.815513540954
H	2.476052838257	0.889670301435	-1.816298107711

15

E(RB+HF-LYP) = -313.2978995 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.338278110000
C	1.420232458291	0.000000000000	1.869595910160
C	2.279302653812	-0.377239121865	0.636032236028
C	-1.187552426566	0.053200464409	2.249819242197
C	1.392212608355	-0.011410217703	-0.592996540723
C	1.569337110640	-0.954089774665	-1.789680446463
C	3.677887397100	0.239526316642	0.619794527051
H	-0.895708553626	0.039628717400	-0.615962325613
H	1.647249221900	1.008355392017	-0.930207576714
H	2.381528162747	-1.471842366181	0.634056849054
H	1.564138765968	-0.690937214225	2.710798167730
H	1.682343452054	1.000800164476	2.249575205105
H	1.298399579341	-1.981175091436	-1.520330778683
H	0.938147066787	-0.651905252844	-2.632690981376
H	2.607186408267	-0.959421490246	-2.141237813001
H	3.624344822118	1.334652576116	0.627112084325
H	4.261814957995	-0.070122458222	1.493672668418
H	4.238572024293	-0.060079507207	-0.272727289639
H	-2.127431957909	0.070774683244	1.690627834312
H	-1.156726337715	0.945417774138	2.889264299397
H	-1.208456306478	-0.811605578724	2.925817163181

16

E(RB+HF-LYP) = -536.042346145 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.539228250000
C	1.093758955017	0.000000000000	2.308887868232
C	1.113860220813	-0.160163857821	3.803471900073
C	-0.710779353117	1.347029684495	-0.424182949130
O	-0.547675518576	-1.064438928743	-0.540990491951
N	-1.944436201346	1.459928602442	-0.955047767593
N	-0.184174135358	2.596564802051	-0.412246294912
C	-2.198637863020	2.782348801050	-1.281031788727
C	-2.884385748611	0.342476390495	-1.142083110273
C	-1.094686619060	3.497334869392	-0.942572330682
C	1.142800671537	2.931305066996	0.096361033873
H	-0.985013686443	-0.132281364862	1.990661221569
H	2.068532950290	0.079028257761	1.821688279276
H	0.101228043151	-0.233281474787	4.211828801914
H	1.661569439840	-1.064738421927	4.098757103304
H	1.617380867020	0.682297928132	4.296126319598
H	-3.132941580654	3.089835235152	-1.722370721892
H	-3.707189860657	0.440614667940	-0.428887203984
H	-2.280708820256	-0.563479279687	-0.958444370322
H	-3.275480276858	0.381246815382	-2.161606732372
H	-0.875603268855	4.549061336072	-1.034528099159
H	1.243308338536	2.569859712783	1.121216798947
H	1.261722466764	4.014930777810	0.068109322601
H	1.913123050773	2.461488682104	-0.520258078008
H	1.070251735724	0.218509484573	-0.301971183915

17

E(RB+HF-LYP) = -536.062943000 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.437519890000
C	1.103624456800	0.000000000000	2.223485729503
C	1.078682652293	-0.130662546929	3.718274533842
C	-1.109110610633	0.107301544955	-0.814839503385
O	1.235514202107	-0.183578723766	-0.638651814109
N	-1.214259769920	-0.257140212952	-2.161091484659
N	-2.354513583564	0.652094218472	-0.475911819614
C	-2.513799551328	0.011975196077	-2.601081383439
C	-0.346004434835	-1.210384511560	-2.831220617866
C	-3.199750536031	0.576035495046	-1.591116268856
C	-2.586002647891	1.565734836332	0.627117173121
H	-0.969643013469	-0.093117727629	1.923082306946
H	2.081681058938	0.126291703998	1.761657819706
H	0.052975448526	-0.202855195602	4.096484996970
H	1.619014689665	-1.022638358885	4.067230510489
H	1.554667365227	0.727642215514	4.213304128283
H	-2.820825326208	-0.226551158641	-3.606925754463
H	-0.459306054250	-2.220470080393	-2.413033545316
H	0.693184745824	-0.905591781622	-2.725217402640
H	-0.617935944256	-1.238043085595	-3.889013266868
H	-4.209832486389	0.950731559096	-1.552741452714
H	-1.657645133752	2.096081106493	0.860016489608
H	-2.927555626282	1.054668165525	1.534190815504
H	-3.348615038295	2.292613102292	0.334466670615
H	1.691580254813	-0.887841197002	-0.149984127932

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E(RB+HF-LYP) = -806.666118758 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.374420480000
C	1.317634882043	0.000000000000	2.102858128906
C	1.182458958332	0.382618782438	3.580890222006
C	2.103122804546	-1.350757587781	1.865619675946
C	3.598550412510	-1.141665943029	1.867676958848
C	1.675727605390	-2.474265308532	2.818953646162
C	4.267491285066	-0.564487732141	0.849844930503
C	5.757406805948	-0.364697093120	0.844759821003
C	-1.320395651859	-0.071462775223	-0.692270018786
O	1.023477745115	0.007707925260	-0.788263849998
N	-1.554753382099	-0.756538291993	-1.839528518019
N	-2.480073882913	0.572879168220	-0.387596618491
C	-2.862945571739	-0.561331181398	-2.240868901747
C	-0.594343120611	-1.634399069692	-2.518722704082
C	-3.443153354318	0.267912241130	-1.337185410549
C	-2.685213552254	1.523993896351	0.702565616572
H	-0.929288816859	-0.092434848406	1.929380595103
H	1.935187233488	0.769425964433	1.622877136535
H	0.521957297506	-0.303140278568	4.123913906889
H	2.158049132392	0.372320921986	4.077943187112
H	0.766138074370	1.391129332908	3.683686807915
H	-3.259790141129	-1.024861916606	-3.129504571880
H	-0.760213377794	-2.671301831678	-2.214109648641
H	0.402012015839	-1.298528736319	-2.225201742098
H	-0.741091128261	-1.540418305335	-3.596334190134
H	-4.438883209380	0.677960973557	-1.291171051213

H	-1.712529284848	1.905936213474	1.012918095700
H	-3.160309121844	1.036407932574	1.557862697549
H	-3.323159879773	2.334678034091	0.344301613982
H	1.821949801470	-1.666504338293	0.853839661053
H	4.172082518110	-1.463842800819	2.732818998311
O	3.716475710424	-0.090492124413	-0.296797255795
H	1.981803922001	-2.272108349155	3.851635187688
H	2.136438070094	-3.422586970935	2.522507048522
H	0.588251426581	-2.611724199172	2.811568900432
H	6.217538602696	-0.756091667082	1.754708699241
H	6.000626195253	0.700631719568	0.753780358391
H	6.204901513878	-0.865958624632	-0.021786653216
H	2.725326983887	-0.125548188186	-0.326034975609

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E(RB+HF-LYP) = -806.675300400 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.521548760000
C	1.366358372019	0.000000000000	2.244046222453
C	2.017307518908	-1.425240793702	2.273966770281
C	1.065945383644	0.808225272018	-0.726347010484
C	1.745037021261	-2.249872985485	1.041824777099
C	3.527163111490	-1.337588143594	2.558060080184
C	0.668677013949	-3.116594218082	1.010394172348
C	0.420578474832	-3.839761815606	-0.290257982600
O	-0.194564412204	-3.351108238725	1.914938358899
N	-0.809313431349	-4.038970761448	-0.816288785794
N	1.296882293480	-4.493464444553	-1.097446126081
C	-0.705788837500	-4.796326852492	-1.965217766475
C	-2.063553344421	-3.503364218900	-0.263985919002
C	0.609394693898	-5.085012757177	-2.145187468933
C	2.734641069556	-4.627556374128	-0.879620616562
H	2.375933755442	-2.121039826283	0.165676498643
H	1.533049594817	-1.960605563858	3.101061817380
H	4.057173564927	-0.873908185695	1.715502615194
H	3.752532101381	-0.745535588036	3.451587623711
H	3.951140250152	-2.336065984939	2.705395811624
H	-0.610848407647	-0.842559048577	1.859832653438
O	-0.892481629561	-0.535420045649	-0.643652119337
H	2.041669802064	0.320886273285	-0.638796831134
H	0.795590552471	0.887862561296	-1.780487389409
H	1.166782688994	1.808841682292	-0.290720787776
H	-1.571329370275	-5.062419147296	-2.549785297487
H	-2.048999382123	-3.688044578106	0.809298548066
H	-2.890693777905	-4.012147759695	-0.761368260458
H	-2.099727965921	-2.426854348136	-0.440468659983
H	1.110552765505	-5.659812310226	-2.906876052313
H	2.946292337724	-4.374474331614	0.159183382339
H	3.287780409762	-3.944164831338	-1.529655703413
H	3.031936025963	-5.656284045209	-1.095470065477
H	-0.539020310390	0.922552918086	1.793985215782
H	2.048064344410	0.674670057423	1.705866437890
C	1.195933904924	0.557643589487	3.667681890905
H	2.136051016330	0.540789610640	4.227194968504
H	0.841215102926	1.594577499026	3.651275067309
H	0.465293221510	-0.036831605345	4.228249694937

21

E(RB+HF-LYP) = -806.661577000 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.547304500000
C	1.488558493722	0.000000000000	1.949274980881
C	2.170076971460	-0.878276529082	0.864080322751
C	-0.430562175138	1.322673481573	-0.618016345251
C	1.362080359183	-0.592912307553	-0.411771216118
C	3.677196345249	-0.643401560669	0.737021857641
C	0.543330462177	-1.843997067180	-0.973556792660
C	0.530604442697	-1.924597515707	-2.534060480424
O	0.734390249783	-3.026142978321	-0.531030305666
N	-0.486712932034	-1.882716688478	-3.424937422002
N	1.625671595424	-2.323179593095	-3.226097672702
C	-0.024559106370	-2.253908706966	-4.680964307427
C	-1.893057134399	-1.560509476786	-3.157263720411
C	1.297560744222	-2.527225351727	-4.554534216515
C	2.916019393615	-2.641287056398	-2.612120973420
H	1.918400345445	-0.019304294725	-1.163859682952
H	1.991946841751	-1.936355648312	1.107968002540
H	3.896008728896	0.391687594474	0.444617475353
H	4.195252059169	-0.836417686263	1.682964859187
H	4.125887026966	-1.303144107556	-0.014118586943
H	-0.480511527748	-0.925983658171	1.880677608480
O	-0.742115908036	-1.115595108266	-0.554766127496
H	0.160409706514	2.154580473350	-0.217249419302
H	-0.304481223663	1.308402736595	-1.706311515397
H	-1.485585387289	1.524071317473	-0.399187914762
H	-0.677406493330	-2.293326523988	-5.537836222561
H	-1.969638257407	-1.243708802146	-2.118122057456
H	-2.503216524480	-2.450594330493	-3.330268560938
H	-2.210798005651	-0.762738764029	-3.833483995415
H	2.026441960566	-2.850037832937	-5.280212584468
H	2.700069906369	-3.095282151614	-1.641975149731
H	3.519489467691	-1.739020992688	-2.486934134143
H	3.442338800067	-3.344024979788	-3.259562238040
H	-0.553364790446	0.840931503176	1.981710897562
H	1.873141967984	1.027054735213	1.835189855302
C	1.744021680831	-0.449725446310	3.388814283959
H	2.811153136325	-0.431870987878	3.636245307365
H	1.230258314829	0.199393594071	4.106907743477
H	1.381027316946	-1.472385702169	3.543596571432

22

E(RB+HF-LYP) = -501.859927200 A.U.

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.538232220000
C	1.494174277973	0.000000000000	1.930529160259
C	2.164092193346	-0.918782845283	0.870319621096
C	-0.495105829013	1.262291735793	-0.671243135548
C	1.357664547513	-0.618387985304	-0.418582168022
C	3.672998673124	-0.723336749434	0.713495756331
C	0.490607431781	-1.749005047834	-0.968175801979
O	0.654700664862	-2.793610621757	-1.530045523502
H	1.931340145988	-0.084490560025	-1.181484162451
H	1.981771641768	-1.961677039962	1.165113385155
H	3.906483513394	0.305089543533	0.413086832374
H	4.201262836606	-0.927262878475	1.650329146207
H	4.079948120011	-1.396210092879	-0.047797763576
H	-0.484024353290	-0.917748446583	1.891533516502
O	-0.699827141319	-1.190358418032	-0.568166240587

H	0.054194442094	2.132451472085	-0.296493136319
H	-0.364110236721	1.208999989946	-1.755943978200
H	-1.558382506639	1.414169863013	-0.460749247705
H	-0.548579382048	0.846357958051	1.963460450173
H	1.884319034276	1.018039855550	1.772835146208
C	1.757729786035	-0.401103974872	3.381603496570
H	2.825489847515	-0.372115725378	3.621261297400
H	1.246854818829	0.272582921885	4.077575815946
H	1.396875821279	-1.417992150015	3.575852531993

TS1

E(RB+HF-LYP) = -536.037986769 A.U.

1 imaginary frequencies -203.6544 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.512583530000
C	1.110524742898	0.000000000000	2.256517850303
C	1.163267824634	-0.100837660849	3.754738028937
C	-0.674923935543	1.769312920774	-0.374306292436
O	-0.700740970783	-0.853969628616	-0.610600252751
N	-1.831765212901	1.992072426177	-1.037331929469
N	-0.027113566807	2.961894973762	-0.394277737980
C	-1.912460151274	3.308363244297	-1.471554604526
C	-2.876890602797	0.980836491346	-1.225827798314
C	-0.770000121355	3.922290565462	-1.069979604975
C	1.292344173606	3.181984735845	0.186054662895
H	-0.980206652424	-0.099443147095	1.979328177770
H	2.074484730486	0.047641116631	1.743770810610
H	0.159796621412	-0.148022024875	4.188341513660
H	1.711256219332	-0.996942128909	4.073563589090
H	1.684478918130	0.756724321537	4.200416090989
H	-2.765451512856	3.686595745091	-2.012907726931
H	-3.719496418924	1.189388261302	-0.560158547352
H	-2.426678461037	0.009295719142	-0.998045674652
H	-3.220895506331	1.010073117152	-2.262668355037
H	-0.428649624448	4.937320538796	-1.200444965077
H	1.434480270541	2.474637900760	1.002579009267
H	1.351549922465	4.200725501293	0.575517639094
H	2.077647920740	3.036898728127	-0.562047182539
H	1.025274110235	0.239327458415	-0.384832770366

TS2

E(RB+HF-LYP) = -806.630519054 A.U.

1 imaginary frequencies -311.4344 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.398838930000
C	1.165360536706	0.000000000000	2.176485576241
C	1.123037498376	0.382015414048	3.636233588850

C	1.678004295757	-2.169403099410	2.069719069037
C	3.019748188121	-2.269567799618	1.676130668511
C	1.233478409548	-2.695371672771	3.410325764981
C	3.396784261672	-2.179978353224	0.318932302507
C	4.846554507417	-2.409884668417	-0.071668367081
C	-1.157583091714	-0.231785826316	-0.793011318795
O	1.154262643520	0.170119023484	-0.709981268056
N	-1.155847739818	-0.786664071360	-2.051294013878
N	-2.472716741403	0.080674127856	-0.520476646428
C	-2.453030639638	-0.827851237635	-2.537558102151
C	-0.006719157683	-1.410082750281	-2.709252018639
C	-3.268799468605	-0.298439835896	-1.596935934269
C	-2.943709479726	0.868039432671	0.605821107381
H	-0.945794576234	-0.174704010881	1.909243311776
H	2.070050500593	0.292004308884	1.653164636814
H	0.209978254452	0.028550756736	4.129339579758
H	1.978125179062	-0.021817345784	4.189296621151
H	1.154041279973	1.473818765351	3.761030801478
H	-2.678397377563	-1.237293311447	-3.508818924197
H	0.511773270378	-2.080184626047	-2.018869537522
H	0.704063087710	-0.652597403022	-3.037117200723
H	-0.3827477711421	-1.975569098420	-3.563846556236
H	-4.335470009693	-0.145044039984	-1.594067078650
H	-2.164148693198	1.577211427972	0.893204467031
H	-3.184609400377	0.241269812642	1.470541432653
H	-3.840434429257	1.412997654069	0.303397277423
H	0.963685013553	-2.301144851900	1.262566732941
H	3.795883729630	-2.397443131648	2.427275131958
O	2.580058490845	-1.921895965997	-0.626004169650
H	1.923582780921	-2.412774859756	4.211568152050
H	1.204975427879	-3.793186094120	3.381769878336
H	0.231803481562	-2.350545244212	3.682275769975
H	5.480343732675	-2.676854989900	0.778184924411
H	5.248895137170	-1.506691159084	-0.545139440683
H	4.899407877383	-3.208215734185	-0.820063230525
H	1.765267392530	-0.641971218415	-0.598828107029

TS3

E(RB+HF-LYP) = -806.645428876 A.U.

1 imaginary frequencies -401.9744 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.551682310000
C	1.445354613901	0.000000000000	2.064248838762
C	2.218577649836	-1.006662810154	1.150558668670
C	0.516065407720	1.341458990816	-0.576146155352
C	1.417717174647	-1.137179308110	-0.146991325200
C	3.683677683346	-0.609849914867	0.933547921636

C	0.721582444380	-2.399302245626	-0.326215835698
C	-0.156916721643	-2.549418415822	-1.565672254116
O	0.620203976114	-3.321394599860	0.484600502804
N	-1.394803056580	-3.083413076522	-1.545270105019
N	0.205191931167	-2.433473337083	-2.862369429249
C	-1.849265673568	-3.226080399275	-2.836720797518
C	-2.232031736828	-3.161196043268	-0.342880639083
C	-0.849130486722	-2.832954817003	-3.667996450573
C	1.472372850752	-1.922111995016	-3.381751291022
H	1.913277310911	-0.771499646958	-1.045841297715
H	2.197797955983	-1.983640679956	1.649496956399
H	3.761850180082	0.335071877008	0.381661063237
H	4.204626521381	-0.475053150615	1.888340195192
H	4.228504248014	-1.374064374912	0.367327814340
H	-0.517754373226	-0.909524665440	1.883436529374
O	-1.062720328588	-0.435105532744	-0.623502907699
H	1.478371351087	1.680049411023	-0.175652628183
H	0.596182087445	1.255765630037	-1.665054074498
H	-0.235637560873	2.111776863190	-0.366332290682
H	-2.839137886090	-3.593279076075	-3.052730521868
H	-1.780296125406	-3.848231398189	0.369795653925
H	-3.221059739374	-3.510229271459	-0.641320909745
H	-2.260310162132	-2.139955666476	0.055542238940
H	-0.784641603855	-2.815541347729	-4.743379056569
H	2.293035805201	-2.242635594029	-2.742150767803
H	1.448705162180	-0.831023761863	-3.429161214221
H	1.622007259239	-2.329307527543	-4.382451895128
H	-0.576633659113	0.855637474506	1.927132424818
H	1.869910012033	1.001329231969	1.901957549326
C	1.574815118564	-0.325419776716	3.555020442745
H	2.623117471679	-0.347005953914	3.875755171195
H	1.057301598349	0.417348002794	4.172422098154
H	1.138659087695	-1.306398076682	3.777285572102

TS4

E(RB+HF-LYP) = -806.652940200 A.U.

1 imaginary frequencies -84.3096 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.557555820000
C	1.480967103586	0.000000000000	1.971045435264
C	2.130471480295	-0.954461307291	0.936756333177
C	-0.222854436692	1.414305642726	-0.553105180440
C	1.361398734068	-0.655990345126	-0.367044793039
C	3.651019857983	-0.835123498787	0.812720373662
C	0.759229340647	-1.916792739480	-1.038676544041
C	0.148274509818	-1.805699079104	-2.414168763509
O	0.938854898586	-3.066625468252	-0.625094075189

N	-0.881276566515	-2.592729858065	-2.802359916472
N	0.544615554487	-1.114768756720	-3.511981125249
C	-1.179964296437	-2.345463337007	-4.127278833896
C	-1.653749886550	-3.447427159135	-1.895302404829
C	-0.294737849973	-1.423928019789	-4.579216209515
C	1.695325551176	-0.222124140213	-3.626477523193
H	1.983329858295	-0.064212265639	-1.049059870373
H	1.886865100223	-1.984639056407	1.226219524348
H	3.947288591514	0.174169365691	0.498377549568
H	4.151721730220	-1.044487879230	1.764361627045
H	4.043716386300	-1.545904071221	0.076861841873
H	-0.477810008145	-0.931559718475	1.882681340791
O	-0.901466569006	-0.917462370165	-0.565571675249
H	0.468649574994	2.149642317586	-0.122183130132
H	-0.107851204299	1.429595600066	-1.643773394290
H	-1.246252495836	1.734882195805	-0.330507950995
H	-1.993771895011	-2.843874545937	-4.628124915458
H	-1.870372512194	-2.862148082480	-1.001468254353
H	-1.065607243037	-4.324106205000	-1.625886210814
H	-2.572630850726	-3.736593761073	-2.407269479362
H	-0.174352564517	-0.968466866874	-5.548152675163
H	1.497096238955	0.737832963559	-3.145334870399
H	1.891342300048	-0.059276949314	-4.686676608060
H	2.575577210526	-0.679804608658	-3.174367666095
H	-0.566491247542	0.833434925860	1.989571449195
H	1.889926561823	1.010437973788	1.804180247115
C	1.729116674687	-0.381479568549	3.431308470501
H	2.796755255445	-0.383125509182	3.678252851597
H	1.235854098402	0.319130151746	4.114325217600
H	1.335717200273	-1.383184378145	3.641508093333

TS5

E(RB+HF-LYP) = -806.653372817 A.U.

1 imaginary frequencies -197.7720 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.544557780000
C	1.490189494837	0.000000000000	1.947355890805
C	2.173766672420	-0.875127600260	0.861808510503
C	-0.493399611519	1.289881194802	-0.633885946585
C	1.378728004961	-0.558410319539	-0.422977810874
C	3.682439562951	-0.653344687601	0.733279026801
C	0.570118269238	-1.750861058812	-1.010957948084
C	0.472925389554	-1.418699820095	-2.975640197139
O	0.806174269313	-2.955056002860	-0.941512335921
N	-0.596609451346	-1.299526838857	-3.802883637200
N	1.465931808427	-1.887200566233	-3.775174508870
C	-0.275027211010	-1.675442105023	-5.101897917537

C	-1.925700173637	-0.855337893388	-3.387403476965
C	1.029760208675	-2.047796963133	-5.082295597208
C	2.790745653984	-2.258246397219	-3.282180753312
H	1.940626607990	0.035055702110	-1.148518501631
H	1.998906047052	-1.931322566038	1.108347738254
H	3.906853486649	0.384659121761	0.457151442795
H	4.203278180669	-0.868141505244	1.672651036177
H	4.114345578849	-1.304448654508	-0.034428433451
H	-0.484209906508	-0.921641991026	1.886275271151
O	-0.684953323970	-1.176266291290	-0.550063748652
H	0.051513758097	2.150579557442	-0.229422368610
H	-0.350494900412	1.274790901960	-1.718262386258
H	-1.558685945527	1.439700581085	-0.424697561073
H	-0.992552615332	-1.654339601106	-5.907058802971
H	-1.961945297761	-0.880837008639	-2.299182764071
H	-2.678418281129	-1.531835970237	-3.800103606259
H	-2.120825413865	0.159478860238	-3.748151953156
H	1.671949029210	-2.413672722315	-5.868012524676
H	2.660799695751	-2.776495587785	-2.330283311643
H	3.419358525074	-1.373143910380	-3.148872383465
H	3.263573796380	-2.924170490166	-4.006149596412
H	-0.551191845694	0.843956374912	1.974503073936
H	1.872512313742	1.027206751619	1.830262606829
C	1.747631461042	-0.447584595845	3.386700366252
H	2.815165806448	-0.429512655313	3.631032886931
H	1.235689912970	0.202766341304	4.104641141950
H	1.384855858279	-1.470004917905	3.544693948462

TS6

E(RB+HF-LYP) = -501.806719855 A.U.

1 imaginary frequencies -716.7096 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.500463720000
C	1.502156011466	0.000000000000	1.884879400074
C	2.230687881472	-0.674457957246	0.678643768722
C	-1.006675689978	0.726766466726	-0.808056351068
C	1.216723065907	-0.580481798412	-0.478947275461
C	3.585338555885	-0.037468480037	0.357513388693
C	0.463923720154	-2.112147322194	-0.750580881420
O	1.222087856233	-3.003379166634	-1.055682249830
H	1.582891126683	-0.262163140744	-1.456125185162
H	2.403118197389	-1.734168924279	0.904174381622
H	3.471704629276	1.015152727272	0.071881463636
H	4.254985324004	-0.079572384006	1.223536901198
H	4.079273199419	-0.560735616114	-0.467317001769
H	-0.505121896807	-0.913921508542	1.837912607449
O	-0.769912364985	-2.017087487765	-0.538219559043

H	-0.776801875207	1.801002165296	-0.724045518206
H	-0.964218833096	0.445294737599	-1.860450849307
H	-2.018121612534	0.574125135452	-0.425265139385
H	-0.567671348306	0.843208220144	1.909388304732
H	1.828845910409	1.049144397456	1.919511111601
C	1.795117235617	-0.643076817414	3.240635353630
H	2.867423048611	-0.626937156425	3.461196628378
H	1.283447428654	-0.117177474984	4.053868944061
H	1.466304219558	-1.688295820197	3.255436950751

TS7

E(RB+HF-LYP) = -806.623828807 A.U.

1 imaginary frequencies -353.4576 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.402418600000
C	1.188746662304	0.000000000000	2.157861414891
C	1.168586060484	-0.565292390660	3.557759273491
C	2.045917802511	2.018659417827	2.508531034902
C	-1.325038822043	-0.069931457803	-0.743439554592
C	1.403447245753	2.886593959773	1.606640583180
C	1.951122758746	2.369342728917	3.980840813982
C	1.597760791836	2.902163803333	0.229416033951
C	0.921237276233	3.797163146304	-0.659057037569
O	2.466922333565	2.042843332382	-0.369251594430
N	0.774676307944	3.619514853436	-2.014218947887
N	0.344369103987	5.017473804707	-0.378314777361
C	0.111653903904	4.708400052053	-2.552880822767
C	1.223427973363	2.477345774684	-2.825007255922
C	-0.163687827803	5.570315374907	-1.547635633416
C	0.408962033561	5.743260593313	0.881218392581
H	0.596408231269	3.495690510665	2.006839254041
H	3.014145084078	1.651209775352	2.176440260647
H	0.914997188694	2.565547666153	4.283056155771
H	2.334349686279	1.577295260610	4.627665135982
H	2.532081471388	3.273167562457	4.216937229401
H	2.072579166673	-0.251202551868	1.577437647478
H	-0.957855087086	0.024962408104	1.917815565072
H	0.390381600415	-0.107193566217	4.177263863828
H	2.126670237225	-0.456816062772	4.071518368364
H	0.950208618341	-1.640537498889	3.507214715143
O	1.062013497082	0.008566735184	-0.723074851593
H	-1.467037542228	0.829124093251	-1.355686195304
H	-1.308802527807	-0.921635680296	-1.432329221360
H	-2.182976789582	-0.171924113059	-0.073377138450
H	2.003960118042	1.118777179054	-0.436019735669
H	-0.113783809052	4.764863418988	-3.605220483050
H	2.306216606623	2.507319801306	-2.950440330979

H	0.733202377506	2.563894849374	-3.796807690385
H	0.952857505052	1.533991530681	-2.350011004704
H	-0.670243075897	6.521389610097	-1.550605218787
H	1.363078403406	5.535043885130	1.369359072041
H	-0.403080309706	5.459245819609	1.557085562368
H	0.333790224357	6.811207021893	0.667123196163

TS8

E(RB+HF-LYP) = -1381.86568405 A.U.

1 imaginary frequencies - 365.6214 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.381546300000
C	1.208745078045	0.000000000000	2.144684556368
C	1.743904086903	-2.020816549566	2.114235305379
C	3.091013061050	-2.113070326111	1.651150150529
C	3.381963216851	-2.091942792115	0.287513919297
C	-1.202678919751	-0.205925431831	-0.772080253878
O	1.114490175430	0.130495562856	-0.744904353661
N	-1.248582268371	-0.853648491427	-1.972944682051
N	-2.476137365122	0.225888447616	-0.517508030077
C	-2.545160459646	-0.834839624598	-2.454090140390
C	-0.131232274688	-1.554978801031	-2.616028080873
C	-3.310759580841	-0.171381699257	-1.552886039923
C	-2.887986885449	1.080659490168	0.588879559159
H	-0.944211850513	-0.156868873620	1.895055125316
H	2.069580665492	0.319736032076	1.566178421377
H	-2.807972293763	-1.298679501769	-3.390781352009
H	0.410705089446	-2.159123109237	-1.885473079824
H	0.567913389534	-0.836560181848	-3.041908825414
H	-0.549767562942	-2.193507905476	-3.395458804063
H	-4.362701141887	0.062591642347	-1.556531734526
H	-2.043080216606	1.702900676580	0.887952180185
H	-3.215059385579	0.489807289178	1.449194952398
H	-3.712567328488	1.712584799853	0.253886222262
H	1.025522963837	-2.258384000334	1.334712333396
H	3.901933849632	-2.190163169096	2.365711429855
O	2.477122615083	-1.885355417079	-0.621857712275
H	1.762012303937	-0.715200844922	-0.619436932699
C	4.779939987023	-2.311705931246	-0.199623932740
C	5.779322302991	-2.919032300050	0.579759160595
C	5.107320591774	-1.912724751146	-1.505676770875
C	7.066605031776	-3.098707752817	0.077271918855
H	5.542913810252	-3.277987661291	1.576180519571
C	6.394598932444	-2.089247100648	-2.007776848297
H	4.326751038810	-1.464141587036	-2.109832138724
C	7.382441600328	-2.680689445139	-1.217508444149
H	7.823136302383	-3.575773428582	0.694498638797

H	6.629082288375	-1.765499631869	-3.018485491309
H	8.386152421794	-2.822415148989	-1.608501637489
C	1.355692932367	-2.557705118137	3.439098283250
C	0.090600372959	-3.149881398579	3.596846182620
C	2.201096627932	-2.509028397020	4.561367934148
C	-0.312281115236	-3.685052662713	4.819451909038
H	-0.575867090656	-3.202258065798	2.739107787771
C	1.800416557235	-3.041307848814	5.784577790756
H	3.175771239876	-2.039879973385	4.478566434435
C	0.543342946691	-3.634383214757	5.920876977186
H	-1.291163475092	-4.148446447884	4.910273144604
H	2.471898943912	-2.990435572421	6.637111364042
H	0.234791298952	-4.051848385720	6.875030712012
C	1.237250106436	0.491342666363	3.538085690388
C	0.144352738619	0.398400981976	4.420143068454
C	2.421618680599	1.071507806012	4.030167407074
C	0.229472418311	0.874854629430	5.726117785042
H	-0.779986878082	-0.065631557661	4.089609938495
C	2.508660608691	1.547161546022	5.337129391008
H	3.279468112512	1.153978967188	3.367639117868
C	1.410628355951	1.455021462472	6.194034745594
H	-0.630650881070	0.788345849780	6.384734252831
H	3.435161105374	1.996419569811	5.684666176624
H	1.473992392177	1.827698994970	7.212216225633

TS9

E(RB+HF-LYP) = -1381.86098094 A.U.

1 imaginary frequencies - 399.4748 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.391879150000
C	1.219248498798	0.000000000000	2.129580904299
C	1.935084639674	1.954811431435	2.541570684805
C	1.488664136410	2.851262650450	1.519061033463
C	1.852389968635	2.802092856474	0.190502364475
C	1.417473452342	3.818061718170	-0.748170566953
O	2.617232370373	1.829986713735	-0.338880197463
N	1.267945537301	3.640145625515	-2.093143032419
N	1.140775059267	5.138341052838	-0.505059003847
C	0.888635451059	4.833572015019	-2.676129734444
C	1.450973913123	2.392297778235	-2.850698107854
C	0.800979530225	5.764172164379	-1.694695232956
C	1.313977586329	5.855310108625	0.754848828747
H	0.739862396880	3.584950939749	1.801339821744
H	2.956505570276	1.607359620837	2.403601852810
H	2.080440324191	-0.202318574336	1.498701086445
H	-0.947980986056	-0.048661073634	1.914207789267
O	1.085251755866	-0.024049003920	-0.721530969260

H	2.017463477585	0.936805815349	-0.435803938902
H	0.704951520673	4.911037074106	-3.735223751271
H	2.514272578771	2.205727374002	-3.005390743462
H	0.946573070328	2.520580167967	-3.809691692275
H	1.023723535742	1.547781311358	-2.310444916290
H	0.533526439849	6.807407063096	-1.731490609253
H	2.115329153835	5.385769432598	1.326127549540
H	0.399006205567	5.841346103156	1.352661080739
H	1.577781748193	6.889789564629	0.527079644672
C	-1.293207423147	-0.056494402163	-0.754107707511
C	-1.293961955413	-0.586360997254	-2.055643339030
C	-2.510799300731	0.404934604574	-0.225621855911
C	-2.471451180670	-0.667677954134	-2.796207904639
H	-0.352607549403	-0.940235715627	-2.461858598255
C	-3.688110849145	0.329464032649	-0.968156869753
H	-2.533003387394	0.847475125483	0.765244578520
C	-3.675511605744	-0.209898224409	-2.256416956053
H	-2.451613667857	-1.093145566580	-3.796217447907
H	-4.617288780152	0.698919950067	-0.542453681058
H	-4.593984999772	-0.270238639825	-2.833543316242
C	1.318413541791	-0.649547839748	3.455774304753
C	0.243698653102	-0.723096798923	4.359695068089
C	2.536818109278	-1.238839681160	3.837202732195
C	0.382994768394	-1.365012382524	5.587726446935
H	-0.707736970721	-0.269616569651	4.102776214051
C	2.677144583741	-1.885650356100	5.063622419135
H	3.378775157448	-1.198412762785	3.150282847769
C	1.598411664542	-1.952077334046	5.946506298073
H	-0.462354039260	-1.408433523272	6.268933244881
H	3.627369486306	-2.342105248890	5.327191404962
H	1.702225734478	-2.455782463333	6.903257991603
C	1.594315780044	2.309573655088	3.935793975442
C	0.320266201047	2.794618473795	4.291756449315
C	2.540825672641	2.156912885598	4.965277477698
C	0.017969245516	3.135359636959	5.608782611482
H	-0.450091521535	2.883792106529	3.529871381472
C	2.238063556984	2.491832751314	6.283217086305
H	3.527461249018	1.773327220972	4.721002726639
C	0.976058064886	2.989397877117	6.613975234646
H	-0.974182772789	3.506089845411	5.853463176087
H	2.992374205944	2.365957361254	7.055232744139
H	0.739853625704	3.251901284021	7.641046636118

TS10

E(RB+HF-LYP) = -1378.68763425A.U.

1 imaginary frequencies -311.1710 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
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C	0.000000000000	0.000000000000	1.381523950000
C	1.202987614770	0.000000000000	2.148169994845
C	1.741896587630	-2.056960660667	2.022127078185
C	3.068231551908	-2.209443390768	1.554334590063
C	1.340446030972	-2.495512197299	3.380594560619
C	3.339258826827	-2.206979804162	0.179371935437
O	2.369493968676	-2.501783846034	4.259918566619
C	2.026656711649	-2.870321177881	5.602779379448
C	-1.206393883830	-0.186514302934	-0.771247286701
O	1.120291499964	0.116091372527	-0.742728356733
N	-1.264801705975	-0.819848918999	-1.979294539485
N	-2.476061948539	0.246195714259	-0.500703400389
C	-2.565658476612	-0.792288958454	-2.448024619136
C	-0.158626003933	-1.520969574906	-2.641581349270
C	-3.320834198967	-0.137175353074	-1.532268699817
C	-2.881170508496	1.084616009768	0.621190746088
H	-0.942514364811	-0.156072303244	1.896297117018
H	2.077339219675	0.312043533331	1.586196987391
H	0.968303650878	-2.274002883276	1.295637578614
H	3.873981204131	-2.288761520567	2.272545514612
O	0.201430541242	-2.798860910175	3.692288813786
O	2.428741355503	-1.959687334493	-0.706084604152
H	1.731994174636	-0.745157693314	-0.651263624126
H	-2.838408938620	-1.245355616817	-3.387081268493
H	0.550875358406	-0.802212723751	-3.049208794981
H	0.373379492948	-2.154243722646	-1.928637372973
H	-0.587473310307	-2.131061180785	-3.437810643152
H	-4.372250697798	0.098852117325	-1.522879007895
H	-2.038012405704	1.709286819791	0.919450259382
H	-3.712731610006	1.715276740223	0.301563525812
H	-3.196111940749	0.480171361441	1.476342786570
H	2.962094712577	-2.845427812524	6.162228043999
H	1.591261363025	-3.872687219137	5.629812340132
H	1.311875550382	-2.159892251731	6.023962921472
C	1.220351526706	0.441891229970	3.557896794549
C	0.120207887375	0.307130679957	4.427341403858
C	2.394712239657	1.020596953160	4.076187903545
C	0.189836014340	0.750132672349	5.747125557421
H	-0.789474813944	-0.170049321049	4.078683253349
C	2.464682899900	1.460921729472	5.395398917508
H	3.258469218530	1.127626762893	3.425454382675
C	1.359966969220	1.332375053965	6.240139793204
H	-0.675471042979	0.637367435253	6.395019680443
H	3.383207816944	1.909423691514	5.763968109020
H	1.409844719336	1.679900030769	7.267943765316
C	4.716897855541	-2.489395092927	-0.329257058324
C	5.720411503787	-3.079426312479	0.458322433654
C	5.019811052147	-2.167612928738	-1.662356061463

C	6.988723718701	-3.320054018572	-0.065841859801
H	5.503716051080	-3.373137950348	1.480031848161
C	6.287959303762	-2.406403133635	-2.186208013444
H	4.235717279355	-1.728150271027	-2.268573176668
C	7.280180535496	-2.981536995031	-1.389317529625
H	7.749831573115	-3.780897788803	0.557846952477
H	6.504500297985	-2.143603153795	-3.218276218692
H	8.269456245689	-3.170606852173	-1.796637191125

TS11

E(RB+HF-LYP) = -1378.68368073 A.U.

1 imaginary frequencies -366.8980 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.392500730000
C	1.199129135862	0.000000000000	2.150087915669
C	2.053021903907	1.910767431941	2.547843881503
C	1.292286842344	2.847874201265	1.786663909533
C	1.384711532668	2.962279548051	0.415014584088
C	0.633363024369	3.960002912969	-0.327919965047
O	2.202490135046	2.207248927881	-0.333939327840
N	0.324497697558	3.884162862899	-1.654684105242
N	0.158200842718	5.169237676915	0.105716336892
C	-0.348616923579	5.028211746808	-2.036899171151
C	0.642564408024	2.793308751697	-2.590230125565
C	-0.460173635377	5.825522250717	-0.946976339739
C	0.366821668860	5.782405873000	1.414295302792
H	0.533644923073	3.422489722649	2.305997303323
H	2.984708400445	1.626647946415	2.065350066807
H	2.090003914323	-0.318079896800	1.619142959104
H	-0.933420431297	-0.048133591179	1.940249828349
O	1.088594367674	0.085838943970	-0.709114714891
H	1.803747690082	1.200071286290	-0.433106238882
H	-0.695770893169	5.167583936059	-3.047523948460
H	1.678242092946	2.880342888390	-2.921185038929
H	-0.035181352218	2.890535302752	-3.439651079745
H	0.508307659920	1.824382996199	-2.115511987279
H	-0.916911793776	6.793566292275	-0.822487426237
H	1.337948604762	5.476862727057	1.805172741849
H	-0.411373792163	5.485859182404	2.122246041210
H	0.343546733069	6.866240956043	1.290060257996
C	1.088738778713	-0.508956476361	3.539511654026
O	0.091666841590	-0.467457898787	4.236833280774
O	2.264953854719	-1.035577695410	3.965097321528
C	2.262830818081	-1.514786852309	5.317340489926
H	1.498370790816	-2.284081403999	5.453367354221
H	3.256666249528	-1.931569805800	5.483417410855
H	2.071636662468	-0.696741464730	6.015848327622

C	2.181781130661	2.136548964600	4.006685538805
C	1.092156783722	2.512900350933	4.814663944123
C	3.434089513575	1.980267230543	4.628898895614
C	1.256544008219	2.753642141640	6.176967495010
H	0.100310841316	2.582897013155	4.378272755767
C	3.599103190397	2.218653605298	5.991944987781
H	4.286397259892	1.676650501608	4.027086103414
C	2.511378398527	2.613260754873	6.774346382542
H	0.397273452433	3.037687722335	6.778331260296
H	4.580397858990	2.099577855633	6.443404956585
H	2.637694081874	2.800654921737	7.836707460791
C	-1.280155878330	-0.162440308860	-0.761420096909
C	-2.545346503716	0.115925096186	-0.215633789316
C	-1.216242089356	-0.616436230881	-2.090149138273
C	-3.703376244687	-0.056505808155	-0.971716114467
H	-2.626086629188	0.485752973448	0.801263283933
C	-2.374691529805	-0.796500829553	-2.843374259812
H	-0.238627287622	-0.831739427911	-2.507605534921
C	-3.625097189967	-0.515922795131	-2.288576735830
H	-4.670692197521	0.170873916308	-0.531840084723
H	-2.302657464581	-1.161056785085	-3.864768759883
H	-4.529340320754	-0.653814123908	-2.874729786755

TS12

E(RB+HF-LYP) = -1378.66835960 A.U.

1 imaginary frequencies -112.0045 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	1.384092300000
C	1.352640431560	0.000000000000	-0.577323335557
C	2.485423438830	-0.305330395387	0.088382432104
H	1.438710800258	0.257133229980	-1.628944843424
H	2.464372045662	-0.510896834757	1.151990979256
C	-1.389288168693	-1.751655391731	-1.619996047500
N	-2.655295812392	-1.434507888622	-1.986770269729
N	-0.748467774394	-2.125227464126	-2.766570237232
C	-2.807821889210	-1.601450360051	-3.348966154533
C	-1.621569092787	-2.034467881240	-3.837274778931
H	-3.743341502696	-1.393790019150	-3.841896054046
H	-1.319495508274	-2.293010239924	-4.838881764385
C	-3.748686734243	-0.925884744824	-1.140594968795
H	-4.653383397146	-1.486982283776	-1.386570198005
H	-3.444925933257	-1.076350758546	-0.105439431076
H	-3.892602323053	0.135126071331	-1.353945332190
C	0.626044177567	-2.610271865030	-2.933511038492
H	0.803393772403	-2.723473084750	-4.003366725823
H	1.345707667964	-1.897045134104	-2.532080907500
H	0.750858520431	-3.574999808439	-2.441529894559

C	-0.848041073651	-1.691796034277	-0.198917135951
O	-1.778212374474	-1.645245206575	0.724145933426
H	-0.773161373597	-0.605290489741	1.592812141316
C	0.232236839421	-2.726841127681	0.064309300864
C	0.028173967766	-3.704681002243	0.960067198325
H	1.195938989038	-2.628972918186	-0.418741527232
H	-0.956229828209	-3.745746372942	1.422273613102
C	-0.921494641542	1.052190856415	-0.588376042812
C	-0.974243957260	1.348730606663	-1.962193416021
C	-1.793818167551	1.746246368000	0.264188746776
C	-1.870405416266	2.291792100824	-2.464040373601
H	-0.314550210872	0.840341843654	-2.659726877286
C	-2.688803917004	2.692742388999	-0.235031488623
H	-1.741065522312	1.544378795978	1.326567346686
C	-2.737526726816	2.968607027144	-1.602368233025
H	-1.884783141963	2.504740596108	-3.529724350298
H	-3.347689924408	3.220124158254	0.449545041623
H	-3.430762444337	3.708889655001	-1.991440428724
C	0.998132687396	-4.730244758710	1.366242463668
C	2.387333296806	-4.583016539796	1.188425807440
C	0.531071771011	-5.913861290411	1.965470435765
C	3.266279223034	-5.593273947746	1.568656998311
H	2.782545431996	-3.657869788250	0.779569757280
C	1.410594317081	-6.926417257387	2.344072049411
H	-0.536942055959	-6.036563103964	2.126348302029
C	2.782973130518	-6.772214556909	2.143356466891
H	4.334809002851	-5.454324044057	1.430544342123
H	1.024841814470	-7.833572524262	2.800760423305
H	3.471961662269	-7.555992108642	2.444385875680
C	3.807248902150	-0.382593769343	-0.543533943137
O	4.850917473243	-0.588822231546	0.048299665431
O	3.764728300131	-0.224709637851	-1.905548308311
C	5.042847342596	-0.257491540439	-2.551296532268
H	4.843364390882	-0.111820410736	-3.613801172541
H	5.690842094283	0.538377852801	-2.174863647324
H	5.541230672567	-1.216201290256	-2.383971382386

MPWB1K/6-31G** computed total energies, unique frequency imaginary, and cartesian coordinates of the TSs involved in the formation of the lactone **22**.

TS2

E(RmPW+HF-B95) = -806.199031239 A.U.

1 imaginary frequencies -363.3598 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.390079130000
C	1.166371295252	0.000000000000	2.128739372701
C	1.194992621380	0.267523890231	3.595429406696
C	1.564791723423	-2.173940030339	1.924555870866
C	2.919784505020	-2.317534800893	1.696490686443
C	0.916768473068	-2.707871439716	3.155572458699
C	3.418685965106	-2.160298599365	0.389979379587
C	4.873755724809	-2.416623528280	0.120545040260
C	-1.122601939160	-0.291682018550	-0.791251221558
O	1.145806957270	0.218471281853	-0.690365970789
N	-1.075763303017	-0.839963430179	-2.030630778222
N	-2.436319595362	-0.060205370854	-0.529959751618
C	-2.350564142333	-0.957909775229	-2.524242441985
C	0.100833275766	-1.410419032806	-2.645625233428
C	-3.194774522913	-0.481965445680	-1.599850138413
C	-2.940939760548	0.706692112287	0.573080445692
H	-0.930855942444	-0.195819648403	1.907621558293
H	2.059542307048	0.268451543502	1.585030968600
H	0.289603654432	-0.079930984645	4.090654899892
H	2.044583088894	-0.222895665079	4.069041348739
H	1.289318061846	1.334008806545	3.804942381456
H	-2.541619512315	-1.379231640686	-3.490686172553
H	0.652171105197	-2.004741473375	-1.921670977317
H	0.761425131257	-0.633381132440	-3.008994828546
H	-0.227111696756	-2.040352292814	-3.464915925408
H	-4.262187256316	-0.392126284888	-1.604201109071
H	-2.198463795175	1.450254788075	0.848581961830
H	-3.151160822191	0.084420270779	1.439797353423
H	-3.855252062269	1.203127473864	0.266682502421
H	0.956956206986	-2.188402007488	1.030218682234
H	3.600755694958	-2.529868624044	2.507258626607
O	2.704540342461	-1.825217378147	-0.582241438032
H	1.506823983258	-2.508566458190	4.046477530384
H	0.818582871254	-3.790064385107	3.067492807961
H	-0.079120801861	-2.297358331247	3.302050503460
H	5.412680262272	-2.753886619860	1.000111862175
H	5.336374995153	-1.505892204034	-0.253822880689
H	4.965305339727	-3.163431470013	-0.664323448263
H	1.779207384993	-0.537256553327	-0.564958131446

TS3

E(RmPW+HF-B95) = -806.235301666 A.U.

1 imaginary frequencies -355.8798 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.528822470000
C	1.428388714527	0.000000000000	2.029635143831
C	2.179688412700	-1.008328596615	1.135161579831
C	0.624853700316	1.264700721969	-0.586640514684
C	1.367619368672	-1.190661075935	-0.126867738308
C	3.614856827932	-0.595304991346	0.879543774642
C	0.594713402447	-2.391999816785	-0.182904475183
C	-0.226111790907	-2.632613843877	-1.422223308845
O	0.370188521628	-3.167230542866	0.731074210642
N	-1.497019730713	-3.013673998283	-1.391326854138
N	0.165684943068	-2.637110392445	-2.694593563685
C	-1.936154320400	-3.205718571697	-2.664175929032
C	-2.340870118841	-2.959510044480	-0.210990999793
C	-0.894499312288	-2.981676235970	-3.488027049902
C	1.482273762999	-2.319885145396	-3.198998376360
H	1.838459995132	-0.897495832585	-1.056515259155
H	2.177571439837	-1.964210488654	1.661679920013
H	3.656845720590	0.321180916642	0.291290872065
H	4.137516901448	-0.406904365536	1.815864127155
H	4.166900121804	-1.363390179771	0.341253210842
H	-0.509228329403	-0.908500766866	1.856517044053
O	-1.069916619430	-0.370717106774	-0.607864445832
H	1.625611586076	1.490777176276	-0.223310828041
H	0.653162570515	1.161529356742	-1.668703212632
H	-0.027676707680	2.105391615733	-0.354175059539
H	-2.948601865955	-3.483331943849	-2.877039877048
H	-1.965299466364	-3.649271483826	0.531824503330
H	-3.347682207636	-3.223080132374	-0.511016195722
H	-2.278952725288	-1.928501948491	0.137932873232
H	-0.809032731779	-3.048333672879	-4.553582836733
H	2.231800323764	-2.628981292602	-2.482601924194
H	1.568882732623	-1.253218593803	-3.377795836071
H	1.632974795085	-2.859535822574	-4.126223024845
H	-0.577410598734	0.848641633826	1.896257901244
H	1.856004846952	0.991901089155	1.863018666151
C	1.568400703077	-0.328362562793	3.500679582890
H	2.614958104522	-0.368045610933	3.800862515527
H	1.074228419058	0.412268069805	4.126068344499
H	1.124101102421	-1.299024832217	3.715398224978

TS4

E(RmPW+HF-B95) = -806.24473627 A.U.

1 imaginary frequencies $-113.4464 \text{ cm}^{-1}$

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.535895920000
C	1.464487332787	0.000000000000	1.932621179249
C	2.069570364931	-1.001963906372	0.948614169116
C	-0.113228711778	1.413489468419	-0.538801998071
C	1.317141748555	-0.719488666632	-0.345304780974
C	3.575035618423	-0.938117910750	0.816031623126
C	0.660682574258	-1.951283916235	-0.955749474222
C	-0.001015664268	-1.837510409354	-2.290190322268
O	0.761780723148	-3.077241003306	-0.504156301427
N	-1.054438759123	-2.593205655252	-2.605484294603
N	0.356508928421	-1.178945963946	-3.397197387989
C	-1.420881417369	-2.344757776738	-3.898164415103
C	-1.790487630235	-3.394627261840	-1.650609262011
C	-0.543666738885	-1.463039129550	-4.401322888736
C	1.526775142224	-0.356277022507	-3.589816608462
H	1.953682822397	-0.185182791605	-1.049679053321
H	1.786401326385	-2.004483427323	1.273407901365
H	3.894153064031	0.045657619119	0.471151787047
H	4.069745331634	-1.131808673617	1.765418038465
H	3.937385524987	-1.677513530466	0.104761157981
H	-0.466709321662	-0.930789068274	1.857920067763
O	-0.942172789086	-0.837582963266	-0.562131835882
H	0.640217747101	2.079642679231	-0.118383588437
H	-0.014921365312	1.416544299599	-1.623729060056
H	-1.097429144005	1.811219415233	-0.302309810020
H	-2.272535027814	-2.817116666133	-4.344478578692
H	-1.861834508690	-2.816498317299	-0.737053047284
H	-1.266110891343	-4.322112579938	-1.459343742790
H	-2.774425158422	-3.585660227560	-2.062643127002
H	-0.464082229748	-1.020386823635	-5.373243102048
H	1.403114477867	0.617297466512	-3.128567268404
H	1.673072893176	-0.229253350634	-4.655576629078
H	2.401942770364	-0.844941006001	-3.179023048180
H	-0.567277622802	0.825402322781	1.963625509767
H	1.885425204733	0.986947810229	1.710248532102
C	1.722087993473	-0.323597607464	3.386823083226
H	2.785071212586	-0.329303734977	3.620328724723
H	1.246607397287	0.401566566394	4.043766537112
H	1.321279704792	-1.306351437854	3.631466839792

TS5

E(RmPW+HF-B95) = -806.246823651 A.U.

1 imaginary frequencies $-226.1958 \text{ cm}^{-1}$

C	0.000000000000	0.000000000000	0.000000000000
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C	0.000000000000	0.000000000000	1.524935690000
C	1.473497504794	0.000000000000	1.911414417595
C	2.109653099635	-0.912327282200	0.860597439674
C	-0.495664260774	1.267728877873	-0.637385884486
C	1.369145789776	-0.536999895169	-0.418083546280
C	3.613839892632	-0.799659065543	0.752898822596
C	0.561223233430	-1.676402536614	-1.044592935765
C	0.442307788383	-1.117441031946	-2.968958667750
O	0.808589507046	-2.863054283048	-1.116729994465
N	-0.592604103702	-0.889087905508	-3.789687180520
N	1.449824188827	-1.449112377711	-3.789919733473
C	-0.238629292598	-1.065024305154	-5.105633319971
C	-1.918952215762	-0.536511633136	-3.343739118380
C	1.057779990081	-1.420252405541	-5.103656181965
C	2.754645543927	-1.850295954453	-3.318845468753
H	1.955788943633	0.073685594055	-1.098469430049
H	1.851744447961	-1.945785532601	1.103866609923
H	3.908099650615	0.217846423637	0.496307569435
H	4.104331128177	-1.063061532559	1.687363629854
H	4.001428209258	-1.464321554956	-0.015987324684
H	-0.473350151047	-0.920294320865	1.864241964862
O	-0.653737721601	-1.167272728166	-0.541236065439
H	0.036418762788	2.126454228909	-0.232857846715
H	-0.337637083523	1.241928641011	-1.712926088679
H	-1.557304899711	1.405380124783	-0.440643414405
H	-0.930900473299	-0.935195426409	-5.914032165661
H	-1.960395835431	-0.690025782599	-2.272981919873
H	-2.648748237165	-1.175040039931	-3.831471877701
H	-2.138719118112	0.501598579407	-3.579158584878
H	1.721491704725	-1.660028391384	-5.910961938841
H	2.617509972631	-2.454831260737	-2.428085467301
H	3.371030259814	-0.983498298278	-3.096236360848
H	3.241117176143	-2.440851647005	-4.087065203497
H	-0.550344521488	0.836118405215	1.952711934234
H	1.867813661147	1.009070517678	1.749783572477
C	1.736345285075	-0.404440335780	3.343912974209
H	2.798094246757	-0.385382455786	3.579304475447
H	1.234406395910	0.261086474513	4.042868256543
H	1.371367696119	-1.414310172469	3.525192869846

TS7

E(RmPW+HF-B95) = -806.19340654 A.U.

1 imaginary frequencies -399.7529 cm⁻¹

C	0.000000000000	0.000000000000	0.000000000000
C	0.000000000000	0.000000000000	1.396896700000
C	1.188364477353	0.000000000000	2.114865613859
C	1.224715967519	-0.526567210848	3.511610288174

C	1.984877107101	2.050468222034	2.482835092225
C	-1.314334891410	-0.019360115072	-0.732243605493
C	1.146729328293	2.800668919115	1.674519405540
C	1.993127101827	2.338131024937	3.953868857265
C	1.217737322106	2.814312981208	0.296639365704
C	0.317284156676	3.504209411443	-0.550929702818
O	2.212101185603	2.151893503014	-0.334392844284
N	0.182739384254	3.302483152395	-1.885598094628
N	-0.536384075409	4.515091997684	-0.240981026072
C	-0.750787383847	4.171757920276	-2.386738816646
C	0.892563654814	2.351327026409	-2.725055811704
C	-1.204660049530	4.918425759957	-1.373497849094
C	-0.612022939122	5.222103691366	1.007989672546
H	0.293933397238	3.259636653087	2.151762295951
H	2.930629290489	1.771742346750	2.039776803362
H	0.981275386823	2.413241565377	4.351354726866
H	2.510644299961	1.575549737348	4.527060547140
H	2.495246491382	3.282871546149	4.171182817203
H	2.060136051677	-0.205219287852	1.509086549289
H	-0.946519308228	0.040182414740	1.917045106178
H	0.489876002141	-0.041603772239	4.150495848859
H	2.201908796486	-0.421073752538	3.970500047853
H	0.987983062550	-1.590633948123	3.493919585708
O	1.047864083397	-0.041966718414	-0.703376611354
H	-1.404399813974	0.868553805664	-1.356794278314
H	-1.337161519194	-0.878575500564	-1.398589033621
H	-2.168964061727	-0.062803024266	-0.064339086735
H	1.925994033317	1.193228160126	-0.426342382885
H	-1.014430278878	4.170112477381	-3.425078646497
H	1.934438941602	2.633540544552	-2.811133493026
H	0.419755218730	2.381496515881	-3.700500736772
H	0.830955662856	1.350017157704	-2.312377984782
H	-1.937695955269	5.698924791462	-1.346383729725
H	0.385316860653	5.325503843763	1.424138566331
H	-1.244164026582	4.707723945274	1.726636019299
H	-1.025529735632	6.205868751429	0.817230218784