Supporting Information

Sequential Catalytic Role of Bifunctional Bicyclic Guanidine in Asymmetric Phospha-Michael Reaction

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Table S1. Cartesian coordinates, total energies (E, Hartrees) and number of imaginary frequencies (in parenthesis) of the M06-2X/cc-pVDZ optimized geometries of all calculated structures.

Phosphine Oxide -880.4564346 (0)

P	0.018507	1.129877	-0.82935
O	0.08424	2.561339	-0.344379
H	-0.006743	0.921231	-2.242567
C	-1.473259	0.24453	-0.276363
C	-1.972719	-0.889061	-0.921453
C	-2.1262	0.766799	0.841317
C	-3.112784	-1.518234	-0.427179
H	-1.487384	-1.275253	-1.818518
C	-3.265686	0.134179	1.332356
H	-1.735853	1.675255	1.298948
C	-3.754471	-1.008856	0.701562
H	-3.50736	-2.400751	-0.927772
H	-3.778332	0.537669	2.203877
H	-4.647536	-1.500502	1.084045
C	1.463267	0.159042	-0.281534
C	1.642953	-1.195199	-0.573741
C	2.413761	0.852681	0.467941
C	2.778972	-1.85396	-0.113492
H	0.899431	-1.741776	-1.153406
C	3.548731	0.187678	0.929159
H	2.2421	1.908285	0.675328
C	3.7302	-1.16242	0.638225
H	2.92381	-2.909134	-0.338421
H	4.292531	0.724846	1.515197
H	4.617211	-1.681811	0.997765

PO Tautomer -880.4561922 (0)

H	1.985406	-0.451662	-2.205483
C	2.196517	-0.439709	-1.132937
C	1.405551	0.332247	-0.278095
C	3.260726	-1.186066	-0.623542
P	-0.009554	1.286987	-0.985877
C	1.701158	0.374986	1.089301
C	3.548232	-1.143712	0.738569
H	3.873078	-1.79146	-1.293372
O	-0.140659	2.512769	0.171149
C	-1.38887	0.234998	-0.356655
C	2.771016	-0.358191	1.593553
H	1.087799	0.995386	1.745465
H	4.384537	-1.719854	1.137616
C	-2.309803	0.7169	0.576927
C	-1.542609	-1.057431	-0.872921
H	3.000763	-0.322621	2.659669
C	-3.366969	-0.092552	0.995759
H	-2.187291	1.723696	0.976381
C	-2.597823	-1.861657	-0.452769
H	-0.826489	-1.443359	-1.60357
C	-3.514093	-1.379589	0.483753
H	-4.080202	0.288628	1.728342
H	-2.707125	-2.868617	-0.857959
H	-4.34303	-2.008579	0.810948
H	0.102946	3.350147	-0.244736

Bicyclic Guanidine -674.6397305 (0)

N	-1.182774	1.145301	0.380858
C	0.012007	0.610221	-0.035103
N	-0.158364	-0.758512	-0.270792
N	1.169497	1.122748	-0.194392
C	-2.097781	0.060623	0.771354
H	-1.132237	1.989601	0.936338
C	2.019575	-0.010768	-0.603912
C	-1.20731	-1.205659	0.631979
C	1.201278	-1.28564	-0.247771
H	1.341829	-2.100024	-0.969786
H	-2.405266	0.187032	1.822532
H	-1.759928	-2.063792	0.226989
H	2.14527	0.024102	-1.703674
H	1.451752	-1.660358	0.764865
H	-0.784363	-1.497086	1.613698
C	3.431055	0.070381	0.007814
C	4.218264	-1.184052	-0.380468
H	5.258624	-1.110911	-0.027617
H	3.779706	-2.092384	0.062961
H	4.240844	-1.313227	-1.47468

Nitrostyrene -514.1241428 (0)

N	2.987525	-0.029377	-0.000091
O	3.234233	1.15753	-0.000072
O	3.812815	-0.919238	0.000004
C	1.597776	-0.465194	-0.000036
H	1.517767	-1.54642	0.000015
C	0.620533	0.443051	-0.000051
H	0.933311	1.487942	-0.000102
C	-0.818298	0.172338	-0.000004
C	-1.696107	1.263642	-0.000006
C	-1.350719	-1.125784	0.000043
C	-3.074138	1.067759	0.000041
H	-1.288279	2.273866	-0.000044
C	-2.725203	-1.32055	0.000089
H	-0.68881	-1.989407	0.000042
C	-3.591224	-0.224926	0.000088
H	-3.743501	1.925839	0.000039
H	-3.127035	-2.331922	0.000125
H	-4.668226	-0.382611	0.000124

C	4.118982	1.311357	-0.568954
H	5.123601	1.435954	-0.13602
H	4.225108	1.226689	-1.662198
H	3.521664	2.207768	-0.351618
C	-3.381532	0.052336	-0.090463
C	-3.045176	-0.202083	-1.561843
H	-2.346701	0.560297	-1.935928
H	-2.580132	-1.188266	-1.709131
H	-3.96166	-0.163327	-2.170392
C	-4.333768	-1.026053	0.434532
H	-4.570558	-0.86273	1.498281
H	-5.279403	-1.002286	-0.127629
H	-3.913722	-2.037491	0.328689
C	3.367189	0.202221	1.531734
H	2.777461	1.08632	1.812217
H	2.91163	-0.681662	2.005386
H	4.382377	0.310623	1.943859
C	-4.057274	1.420153	0.045881
H	-4.993257	1.445381	-0.532054
H	-4.304145	1.638176	1.098053
H	-3.400054	2.21662	-0.331527

1 -1555.1216818 (0**)**

N	1.362623	1.030554	-1.509718
C	1.841114	0.006514	-0.766656
N	3.044494	0.381735	-0.171642
N	1.436201	-1.203888	-0.575578
C	2.221532	2.202606	-1.36309
H	0.375371	1.049113	-1.784855
C	2.50176	-1.810401	0.244302
C	3.543077	1.539916	-0.891065
C	3.731711	-0.874642	0.075029
H	4.365924	-0.834621	0.970036
H	2.369041	2.676401	-2.347115
H	4.138565	2.20078	-0.246801
H	2.206324	-1.768754	1.316134
H	4.352813	-1.166782	-0.795702
H	4.159059	1.242195	-1.761377
C	2.728722	-3.29546	-0.091808
C	3.900215	-3.825015	0.73895
H	4.030657	-4.906627	0.579963
H	4.845311	-3.330991	0.462691
H	3.728913	-3.65902	1.815187
C	1.451738	-4.056733	0.278116
H	1.555326	-5.129439	0.052069
H	1.233805	-3.955884	1.354394
H	0.597157	-3.658906	-0.288772
C	1.646198	3.284075	-0.412346
C	1.531671	2.772717	1.026571
H	0.914496	1.862895	1.078433
H	2.516796	2.538512	1.457468
H	1.055775	3.541033	1.657055
C	2.554338	4.51669	-0.458109
H	2.653309	4.899419	-1.486513

TS1 -1555.0948426 (1)

N	-1.843519	-0.670433	-1.165195
C	-1.946747	0.381376	-0.352954
N	-3.243394	0.607453	0.034729
N	-1.0709	1.248768	0.088767
C	-3.162881	-1.291486	-1.319497
H	-0.898645	-1.127264	-1.306931
C	-1.829972	2.225454	0.891299
C	-4.106021	-0.137189	-0.869232
C	-3.304109	2.00345	0.445949
H	-4.019825	2.160679	1.262371
H	-3.336048	-1.520743	-2.382626
H	-5.007865	-0.503607	-0.361739
H	-1.75208	1.954097	1.96221
H	-3.576794	2.655823	-0.405435
H	-4.408726	0.481888	-1.733568
C	-1.278921	3.653873	0.740824
C	-2.137481	4.603095	1.581215
H	-1.735722	5.62663	1.535924
H	-3.176314	4.636803	1.215851
H	-2.154825	4.292228	2.638125
C	0.160058	3.655256	1.269085
H	0.587596	4.668388	1.221313
H	0.196258	3.317083	2.317075
H	0.796435	2.98798	0.66677
C	-3.294961	-2.616357	-0.529991
C	-3.117183	-2.39046	0.973783
H	-2.122351	-1.972297	1.191708
H	-3.875796	-1.704836	1.380446
H	-3.201392	-3.349979	1.506593
C	-4.667363	-3.232412	-0.815776
H	-4.820528	-3.371856	-1.897959

H	2.13145	5.322533	0.161053	H	-4.745493	-4.21985	-0.336719
H	3.56331	4.300652	-0.074121	H	-5.49179	-2.613331	-0.429498
C	3.006737	-3.488652	-1.584479	C	-1.269892	4.105107	-0.722231
H	2.192899	-3.051051	-2.179435	H	-0.714366	3.389555	-1.345113
H	3.950719	-3.011943	-1.890461	H	-2.286536	4.204748	-1.131767
H	3.085924	-4.561579	-1.819749	H	-0.785663	5.08993	-0.806858
C	0.253888	3.673637	-0.922778	C	-2.202986	-3.571278	-1.029792
H	-0.171856	4.469895	-0.292331	H	-2.284906	-4.540232	-0.514091
H	0.305174	4.053382	-1.956559	H	-2.308943	-3.755382	-2.11125
H	-0.437719	2.817322	-0.910123	H	-1.19505	-3.167914	-0.846433
C	-6.353437	-0.983496	-0.656216	C	5.020527	0.941728	-2.765509
C	-5.593857	-1.545058	0.372227	C	4.80318	1.530816	-1.518314
C	-5.737436	-0.229947	-1.653837	C	4.14751	-0.038385	-3.234815
H	-7.433867	-1.13327	-0.675967	H	5.873985	1.249305	-3.3716
C	-4.215509	-1.352959	0.402249	C	3.714615	1.138586	-0.742908
H	-6.079852	-2.12898	1.15483	H	5.486528	2.29715	-1.149331
C	-4.355971	-0.037367	-1.629924	C	3.056082	-0.432521	-2.460411
H	-6.334072	0.210508	-2.453829	H	4.316795	-0.499065	-4.209569
C	-3.598021	-0.601534	-0.602646	C	2.840709	0.151867	-1.210629
H	-3.620601	-1.781113	1.213264	H	3.552211	1.599624	0.235064
H	-3.844559	0.548334	-2.396138	H	2.354569	-1.19697	-2.800193
P	-1.799954	-0.328209	-0.632348	P	1.362879	-0.398544	-0.265209
O	-1.431872	0.663204	-1.73107	O	0.671183	-1.532987	-1.091901
H	-1.215958	-1.615618	-0.733793	H	0.204637	0.753233	0.071513
C	-1.353166	0.189314	1.049197	C	2.098906	-1.133067	1.248431
C	-0.480416	-0.57426	1.828678	C	2.460004	-0.347723	2.347297
C	-1.867116	1.395854	1.541016	C	2.26739	-2.519341	1.299344
C	-0.120452	-0.128129	3.100487	C	3.01515	-0.941989	3.479847
H	-0.064733	-1.498506	1.423967	H	2.295739	0.733366	2.325015
C	-1.503026	1.836985	2.809795	C	2.819153	-3.112176	2.433581
H	-2.545878	1.989736	0.924025	H	1.95377	-3.114058	0.438701
C	-0.627367	1.075993	3.587122	C	3.197339	-2.324246	3.521511
H	0.564729	-0.719977	3.708893	H	3.297881	-0.327431	4.335851
H	-1.897436	2.778836	3.19318	H	2.954049	-4.194396	2.471634
H	-0.336817	1.426337	4.57864	H	3.628606	-2.789636	4.409118

2 -1555.1230864 (0)

N	1.154848	0.927728	-1.399684
C	1.876317	0.108793	-0.714838
N	3.063868	0.587853	-0.194041
N	1.764805	-1.224729	-0.450444
C	1.92768	2.192714	-1.432891
H	-0.508932	0.610469	-1.762909
C	2.875006	-1.629677	0.41603
C	3.360708	1.784147	-0.965403
C	3.926263	-0.54735	0.07981
H	4.604517	-0.356269	0.920992
H	1.962671	2.548928	-2.475043
H	3.854113	2.550766	-0.353843
H	2.594192	-1.508064	1.481215
H	4.523435	-0.828126	-0.809257
H	4.008577	1.544398	-1.829344
C	3.298461	-3.094308	0.210134
C	4.516229	-3.37303	1.095466

R-**3** -2069.2686915 (0)

N	-1.595114	2.176186	-0.095027
C	-2.717778	1.562101	-0.521361
N	-3.834174	2.288766	-0.128609
N	-2.919092	0.45625	-1.153764
C	-1.918258	3.193581	0.907671
H	-0.698067	1.698366	-0.105833
C	-4.383805	0.295469	-1.21635
C	-3.456491	3.020511	1.073894
C	-4.939896	1.341604	-0.204918
H	-5.865379	1.817486	-0.553494
H	-1.404895	2.947955	1.851408
H	-3.980679	3.98275	1.146736
H	-4.728077	0.565613	-2.232996
H	-5.124716	0.886481	0.787074
H	-3.68828	2.427629	1.978682
C	-4.829042	-1.159746	-0.961346
C	-6.353314	-1.235789	-1.086602

H	4.798867	-4.434712	1.033884	H	-6.697786	-2.269372	-0.928806
H	5.386878	-2.776519	0.781239	H	-6.853642	-0.600555	-0.337828
H	4.302449	-3.140992	2.151099	H	-6.686511	-0.916003	-2.087096
C	2.133982	-3.989432	0.651499	C	-4.183726	-2.050642	-2.027677
H	2.412725	-5.050906	0.571173	H	-4.540646	-3.087432	-1.924906
H	1.855845	-3.789034	1.698536	H	-4.436805	-1.69788	-3.040604
H	1.244211	-3.833058	0.021185	H	-3.089712	-2.050989	-1.925085
C	1.270303	3.31778	-0.595915	C	-1.451178	4.601926	0.47698
C	1.207767	2.947674	0.888427	C	-2.143081	5.028969	-0.819157
H	0.608132	2.037761	1.042424	H	-1.923974	4.31517	-1.626561
H	2.21032	2.779723	1.312296	H	-3.236255	5.080608	-0.699465
H	0.73029	3.761362	1.457108	H	-1.788169	6.023539	-1.130686
C	2.068445	4.613078	-0.77995	C	-1.753972	5.598526	1.598989
H	2.149005	4.880303	-1.84606	H	-1.286679	5.282106	2.545426
H	1.562518	5.442748	-0.263296	H	-1.35535	6.591859	1.342198
H	3.086095	4.541167	-0.366672	H	-2.835038	5.711685	1.771807
C	3.632959	-3.391966	-1.254117	C	-4.393998	-1.644601	0.42619
H	2.794073	-3.122329	-1.910895	H	-3.339819	-1.395126	0.615975
H	4.524217	-2.842258	-1.591687	H	-5.003064	-1.201483	1.229735
H	3.841715	-4.465472	-1.377318	H	-4.494851	-2.739096	0.499155
C	-0.150571	3.540486	-1.123512	C	0.0644	4.544772	0.257001
H	-0.645661	4.343263	-0.554453	H	0.44823	5.533197	-0.039129
H	-0.131994	3.837872	-2.184798	H	0.581389	4.236272	1.180421
H	-0.755227	2.627979	-1.034779	H	0.31744	3.824518	-0.53568
C	-6.099259	-1.753348	-0.782467	C	4.099862	-2.327394	-0.20622
C	-5.333848	-2.255472	0.271549	C	3.493133	-2.307778	1.049117
C	-5.503657	-0.942437	-1.74615	C	3.34776	-2.02118	-1.341296
H	-7.160632	-1.996427	-0.850712	H	5.161218	-2.565302	-0.299214
C	-3.979631	-1.946875	0.356416	C	2.13951	-1.989454	1.164824
H	-5.795235	-2.890806	1.029216	H	4.075069	-2.545083	1.941852
C	-4.146058	-0.627878	-1.662348	C	1.992227	-1.707277	-1.228349
H	-6.099479	-0.54884	-2.571518	H	3.821956	-2.031366	-2.32539
C	-3.379706	-1.125924	-0.605837	C	1.376186	-1.703034	0.026438
H	-3.382756	-2.339672	1.184468	H	1.667	-1.974254	2.151714
H	-3.668642	0.00773	-2.40887	H	1.39191	-1.463048	-2.105734
P	-1.581632	-0.765376	-0.476921	P	-0.407427	-1.246882	0.217608
O	-1.482807	0.370199	-1.686394	C	-1.05105	-2.933088	0.650701
H	0.832247	-1.625664	-0.362432	O	-0.807235	-1.158016	-1.3906
C	-1.594483	0.299669	1.038758	C	-1.314565	-3.249144	1.986359
C	-0.827072	-0.071774	2.145457	C	-1.343041	-3.868262	-0.347279
C	-2.305597	1.505641	1.068518	H	-1.610043	-0.542988	-1.450391
C	-0.77893	0.743993	3.279352	H	-1.122212	-2.507586	2.766828
H	-0.254115	-1.003562	2.117808	C	-1.848102	-4.492979	2.32594
C	-2.250089	2.324529	2.191839	C	-1.887784	-5.105194	-0.009931
H	-2.896006	1.795834	0.195993	H	-1.14723	-3.604937	-1.388911
C	-1.487933	1.94222	3.299917	C	-2.139245	-5.420485	1.327058
H	-0.178828	0.448338	4.141275	H	-2.052373	-4.731791	3.371021
H	-2.804168	3.264531	2.209146	H	-2.116296	-5.830238	-0.79324
H	-1.446855	2.585097	4.180526	H	-2.568229	-6.389078	1.589068
				H	5.504457	0.964586	-2.515434
				C	6.061938	0.748607	-1.60191
				C	5.386067	0.743057	-0.375058
				C	7.426492	0.478182	-1.663031
				C	3.947161	1.010231	-0.374016

C	6.104416	0.452858	0.795554
C	8.130431	0.194183	-0.494641
H	7.940518	0.485984	-2.624656
C	3.174879	1.12711	0.710276
H	3.45287	1.117965	-1.342575
C	7.465414	0.181859	0.73423
H	5.590868	0.420823	1.757551
H	9.198565	-0.021836	-0.538019
N	1.757724	1.380036	0.553751
H	3.459436	1.063294	1.756303
H	8.014011	-0.046685	1.648445
O	1.276093	1.410836	-0.567731
O	1.116958	1.545155	1.574489

***S*-3** -2069.2675936 (0)

N	-1.736429	2.133675	-0.064637
C	-2.857347	1.463814	-0.397492
N	-3.971342	2.143605	0.079069
N	-3.057849	0.345209	-1.007319
C	-2.026765	3.168337	0.92725
H	-0.814979	1.722385	-0.18209
C	-4.51411	0.11781	-0.948652
C	-3.531617	2.91416	1.234703
C	-5.035954	1.148	0.097371
H	-6.005865	1.579641	-0.181522
H	-1.422104	2.98882	1.831482
H	-4.099461	3.847928	1.342994
H	-4.952966	0.360055	-1.935546
H	-5.124392	0.695541	1.1038
H	-3.646187	2.3246	2.1642
C	-4.86957	-1.353627	-0.647376
C	-6.393797	-1.498903	-0.641991
H	-6.677519	-2.547107	-0.461261
H	-6.85717	-0.887584	0.149355
H	-6.824376	-1.192291	-1.609049
C	-4.275392	-2.225254	-1.758325
H	-4.57291	-3.276434	-1.618489
H	-4.627641	-1.895279	-2.748978
H	-3.177679	-2.174241	-1.746334
C	-1.683031	4.583581	0.410396
C	-2.534641	4.935702	-0.811096
H	-2.383552	4.196343	-1.610984
H	-3.607836	4.959365	-0.567423
H	-2.251564	5.927145	-1.197115
C	-1.912105	5.597373	1.534505
H	-1.31125	5.344263	2.422596
H	-1.617099	6.604977	1.20457
H	-2.968978	5.64502	1.838683
C	-4.29311	-1.802911	0.69937
H	-3.238128	-1.505462	0.786665
H	-4.844655	-1.374997	1.551195
H	-4.339457	-2.899643	0.790537
C	-0.200427	4.593919	0.021382
H	0.100555	5.598011	-0.314908

***R*-TS2a** -2069.252557 (1)q

P	1.577219	-0.223705	-0.557761
O	0.705663	0.452054	-1.748792
C	0.325201	-1.133347	1.158253
H	-0.563336	-0.724835	0.671856
C	0.763965	-0.349602	2.345986
C	1.479886	-0.916841	3.405037
C	0.476114	1.022231	2.379594
C	1.918813	-0.121443	4.463867
H	1.697941	-1.98494	3.409973
C	0.911568	1.813878	3.4362
H	-0.072396	1.462963	1.540826
C	1.643018	1.244752	4.4805
H	2.476815	-0.576822	5.283229
H	0.688093	2.881544	3.441763
H	1.990178	1.864371	5.308212
C	2.400713	-1.645044	-1.327432
C	3.469948	-2.264048	-0.670919
C	1.871972	-2.20494	-2.493739
C	4.019418	-3.434125	-1.190856
H	3.881533	-1.82748	0.243229
C	2.428553	-3.371388	-3.009838
H	1.016718	-1.729688	-2.973042
C	3.497679	-3.987521	-2.359248
H	4.852162	-3.917793	-0.6792
H	2.016092	-3.809807	-3.919079
H	3.921669	-4.908674	-2.761083
C	2.930722	0.973517	-0.236551
C	3.27856	1.87865	-1.247234
C	3.590658	1.019741	0.996633
C	4.287249	2.812439	-1.028795
H	2.741601	1.846493	-2.197332
C	4.604133	1.955501	1.207905
H	3.305682	0.341456	1.804336
C	4.951682	2.850491	0.198504
H	4.557207	3.514113	-1.819522
H	5.113397	1.991246	2.171986
H	5.739028	3.586287	0.368387
C	0.478684	-2.522514	1.091575
H	1.141435	-3.130733	1.696043

H	0.433307	4.312041	0.877767	N	-0.037019	-3.193899	-0.005906
H	-0.006944	3.884017	-0.79719	O	-0.638821	-2.526396	-0.890304
C	4.144948	-2.143965	-0.685973	O	0.121332	-4.400267	-0.113138
C	3.633263	-2.130249	0.613699	H	-0.186336	0.833036	-1.342538
C	3.300976	-1.874245	-1.76146	H	-6.13066	-2.76216	1.664779
H	5.202707	-2.35402	-0.854984	C	-5.895967	-2.236273	0.727445
C	2.286213	-1.849934	0.828965	C	-4.439178	-1.764876	0.735157
H	4.290392	-2.337671	1.460712	H	-6.080448	-2.933281	-0.105252
C	1.946391	-1.59902	-1.548063	H	-6.601212	-1.395692	0.632942
H	3.695874	-1.88431	-2.77973	C	-4.15327	-1.047018	-0.606321
C	1.428859	-1.598176	-0.249855	C	-4.186852	-0.847065	1.934891
H	1.890284	-1.839781	1.848721	C	-3.511311	-2.981293	0.840262
H	1.273354	-1.384164	-2.379851	N	-2.73796	-0.726117	-0.794122
P	-0.346614	-1.203043	0.088946	C	-4.80076	0.355641	-0.762662
C	-0.872093	-2.908054	0.604764	H	-4.484689	-1.71284	-1.418068
O	-0.896998	-1.16611	-1.47661	H	-3.151498	-0.471886	1.937008
C	-1.018409	-3.212014	1.960728	H	-4.863426	0.020866	1.944516
C	-1.190488	-3.874999	-0.354177	H	-4.341123	-1.408503	2.869149
H	-1.727114	-0.588166	-1.463379	H	-3.799521	-3.602687	1.701128
H	-0.806656	-2.44782	2.713894	H	-3.550862	-3.608072	-0.064832
C	-1.459949	-4.475104	2.357894	H	-2.466632	-2.668832	0.988222
C	-1.642888	-5.131767	0.041278	C	-2.530819	0.582616	-0.606243
H	-1.089983	-3.6203	-1.411461	H	-1.983346	-1.423116	-0.856389
C	-1.776091	-5.434717	1.397906	N	-3.720028	1.228586	-0.327683
H	-1.57259	-4.704345	3.418874	H	-5.69886	0.473932	-0.142336
H	-1.892169	-5.881616	-0.711903	H	-5.066772	0.550371	-1.818264
H	-2.132236	-6.4188	1.706574	N	-1.472264	1.336319	-0.687213
H	5.772803	0.549551	2.317636	C	-3.492854	2.618627	-0.696186
C	6.239324	0.543645	1.33034	C	-1.96311	2.713148	-0.455165
C	5.461008	0.844648	0.205156	H	-4.063739	3.31102	-0.06537
C	7.588978	0.227321	1.197143	H	-3.754304	2.794678	-1.758461
C	4.037255	1.124863	0.396086	H	-1.812782	2.966675	0.613978
C	6.065963	0.833936	-1.061342	C	-1.20409	3.768333	-1.276538
C	8.178054	0.215657	-0.065153	C	-1.87532	5.128723	-1.066866
H	8.181473	-0.011186	2.080846	C	0.235333	3.819724	-0.75441
C	3.142076	1.289857	-0.580549	C	-1.182216	3.412805	-2.765993
H	3.662065	1.173584	1.421546	H	-1.296533	5.921624	-1.564164
C	7.413152	0.523178	-1.193627	H	-2.894395	5.148211	-1.484823
H	5.478987	1.069809	-1.949966	H	-1.938034	5.377672	0.004954
H	9.235162	-0.029919	-0.173371	H	0.826244	4.564909	-1.309674
N	1.746949	1.499461	-0.24847	H	0.260671	4.091901	0.313454
H	3.29207	1.228488	-1.653898	H	0.724939	2.843288	-0.874093
H	7.87304	0.518756	-2.18244	H	-0.666546	2.456356	-2.93477
O	1.40996	1.650518	0.909327	H	-2.19663	3.336558	-3.186993
O	0.970693	1.495543	-1.191255	H	-0.648827	4.195616	-3.326827

***R*-TS2b** -2069.2524679 (1)

P	1.428319	-0.34962	-0.690157
O	0.39018	0.41233	-1.669672
C	0.783173	-0.793412	1.544862
H	-0.037496	-0.089788	1.378125
C	1.929728	-0.272786	2.331871
C	2.838404	-1.113138	2.987397
C	2.140174	1.111211	2.378985

***R*-TS2c** -2069.255322 (1)

P	-1.428742	-0.08028	-0.673326
O	-0.168032	0.358631	-1.575291
C	-1.797088	-2.504558	-0.405045
H	-1.615394	-2.633581	-1.472483
C	-3.205707	-2.416996	0.037208
C	-3.537664	-2.156283	1.375462
C	-4.23446	-2.543557	-0.904755

C	3.934995	-0.578326	3.66161	C	-4.870989	-2.032946	1.757526
H	2.695938	-2.193898	2.973167	H	-2.746753	-2.017914	2.115503
C	3.233292	1.646244	3.051594	C	-5.567432	-2.427872	-0.519731
H	1.447898	1.767881	1.846241	H	-3.980701	-2.727386	-1.950652
C	4.139499	0.800679	3.692357	C	-5.889965	-2.170114	0.812655
H	4.633923	-1.24572	4.167722	H	-5.115726	-1.822725	2.799532
H	3.385535	2.726058	3.066255	H	-6.356884	-2.532586	-1.264833
H	5.001711	1.216157	4.215484	H	-6.933567	-2.074222	1.115116
C	1.617721	-2.021664	-1.3791	C	-1.079565	0.36729	1.068595
C	0.690096	-2.49128	-2.31285	C	-1.936203	1.152523	1.851734
C	2.595159	-2.882914	-0.868909	C	0.038875	-0.232091	1.672657
C	0.76181	-3.809767	-2.754674	C	-1.677941	1.336874	3.209451
H	-0.082976	-1.812937	-2.675342	H	-2.799155	1.640156	1.396257
C	2.66086	-4.201902	-1.312731	C	0.290548	-0.04743	3.030764
H	3.312673	-2.524068	-0.126208	H	0.740539	-0.824346	1.084705
C	1.744425	-4.665014	-2.255778	C	-0.569414	0.733282	3.803016
H	0.040674	-4.176399	-3.486171	H	-2.343823	1.962492	3.80564
H	3.424304	-4.872099	-0.915912	H	1.164093	-0.519337	3.483356
H	1.791077	-5.699981	-2.59718	H	-0.372887	0.87706	4.866474
C	3.024172	0.493142	-1.011875	C	-2.797348	1.013952	-1.209092
C	3.107249	1.433229	-2.04643	C	-2.567905	1.926085	-2.245993
C	4.139083	0.263154	-0.195413	C	-4.09451	0.863407	-0.69498
C	4.300491	2.11524	-2.274506	C	-3.615013	2.703886	-2.737328
H	2.226494	1.621601	-2.662783	H	-1.562277	2.010009	-2.661158
C	5.330994	0.945556	-0.431097	C	-5.136256	1.643949	-1.190657
H	4.078288	-0.430947	0.645719	H	-4.295429	0.137202	0.096486
C	5.414149	1.870683	-1.470573	C	-4.898845	2.566211	-2.210484
H	4.362153	2.841742	-3.086308	H	-3.427798	3.419428	-3.539423
H	6.192954	0.760291	0.211495	H	-6.14024	1.523275	-0.78076
H	6.346483	2.407944	-1.650381	H	-5.717524	3.173442	-2.599476
C	0.43411	-2.144202	1.573061	C	-0.813318	-2.963622	0.456084
H	1.002898	-2.966062	1.991025	H	-0.914996	-3.135017	1.521806
N	-0.649834	-2.539348	0.809173	N	0.500449	-3.011982	0.001606
O	-1.190246	-1.660595	0.091917	O	0.739807	-2.699613	-1.179865
O	-1.036169	-3.70124	0.819817	O	1.400241	-3.289719	0.798575
H	-0.436664	0.814987	-1.128505	H	0.639662	0.955189	-1.146673
H	-6.683941	-2.126834	1.697386	H	6.666691	-3.28048	-0.815883
C	-6.469283	-1.375184	0.923253	C	6.018344	-2.736939	-0.112209
C	-4.961478	-1.316714	0.658644	C	4.864911	-2.069431	-0.867091
H	-7.020697	-1.663884	0.013899	H	5.637073	-3.461837	0.624011
H	-6.870621	-0.413836	1.278108	H	6.646715	-2.005269	0.419575
C	-4.698426	-0.339003	-0.512148	C	3.963417	-1.349404	0.159405
C	-4.212536	-0.891683	1.925056	C	5.40841	-1.09427	-1.913854
C	-4.483855	-2.715247	0.240501	C	4.027247	-3.154584	-1.554896
N	-3.278945	-0.242721	-0.880375	N	2.745171	-0.793209	-0.437501
C	-5.042137	1.151929	-0.248656	C	4.578415	-0.08929	0.831216
H	-5.272344	-0.702052	-1.379206	H	3.670543	-2.090109	0.918386
H	-3.128211	-0.850234	1.736611	H	4.586877	-0.579496	-2.434136
H	-4.543799	0.092699	2.289003	H	6.061183	-0.329164	-1.465551
H	-4.386446	-1.629207	2.723424	H	5.996941	-1.640986	-2.666772
H	-4.943488	-3.02138	-0.713549	H	4.675424	-3.801289	-2.165917
H	-3.388969	-2.776343	0.146825	H	3.494947	-3.772885	-0.815438
H	-4.779365	-3.451197	1.003753	H	3.264905	-2.715959	-2.214699
C	-2.768253	0.905863	-0.381876	C	2.763238	0.54414	-0.394142

H	-2.680367	-1.06973	-0.851548	H	2.01311	-1.359813	-0.875504
N	-3.758809	1.679564	0.179133	N	3.98205	1.001283	0.068533
H	-5.812125	1.278595	0.522891	H	5.674288	-0.075579	0.773111
H	-5.385331	1.643365	-1.178288	H	4.279496	-0.027852	1.894805
N	-1.58315	1.43612	-0.418099	N	1.860393	1.449661	-0.621531
C	-3.275317	3.048404	0.112342	C	3.720467	2.351979	0.55385
C	-1.740807	2.798707	0.135109	C	2.502285	2.74379	-0.327631
H	-3.615873	3.652395	0.962472	H	4.582759	3.013992	0.406749
H	-3.600139	3.535439	-0.828481	H	3.453738	2.331439	1.627731
H	-1.414286	2.797199	1.193891	H	2.88644	3.166775	-1.276377
C	-0.890249	3.848618	-0.606271	C	1.531814	3.782994	0.264735
C	-1.295897	5.244818	-0.12383	C	2.249222	5.134265	0.331605
C	0.582893	3.608121	-0.2619	C	0.322159	3.888062	-0.670954
C	-1.073106	3.73595	-2.122425	C	1.041126	3.383746	1.658659
H	-0.618317	6.003727	-0.543314	H	1.579033	5.902186	0.746869
H	-2.319825	5.50421	-0.435115	H	3.140988	5.085795	0.976948
H	-1.241644	5.314736	0.97482	H	2.567703	5.465999	-0.669314
H	1.233512	4.291732	-0.829107	H	-0.335196	4.712454	-0.354534
H	0.767026	3.778452	0.811329	H	0.636639	4.077867	-1.710312
H	0.878705	2.579946	-0.515774	H	-0.265716	2.957915	-0.656894
H	-0.707771	2.765395	-2.487912	H	0.683934	2.344606	1.660689
H	-2.129261	3.836193	-2.417573	H	1.828866	3.485192	2.420924
H	-0.508834	4.535008	-2.627565	H	0.204913	4.032602	1.962248

***R*-TS2d** -2069.2520823 (1)

P	-1.336406	-0.998595	-0.126213
O	-1.045515	0.454172	-0.799118
C	-1.595335	-0.473814	2.199336
H	-1.898212	-1.492965	2.443705
C	-2.681631	0.501314	1.962847
C	-2.401395	1.826289	1.599676
C	-4.015611	0.088322	2.061833
C	-3.438507	2.723195	1.366374
H	-1.363202	2.140541	1.469244
C	-5.053322	0.988886	1.833398
H	-4.237401	-0.951154	2.312869
C	-4.766593	2.308262	1.487037
H	-3.208319	3.750569	1.079900
H	-6.088215	0.654979	1.915747
H	-5.577387	3.014501	1.303353
C	-2.933897	-1.40712	-0.896138
C	-3.359626	-2.738228	-0.982838
C	-3.794636	-0.370915	-1.276010
C	-4.635248	-3.030774	-1.457875
H	-2.685535	-3.547527	-0.690162
C	-5.070313	-0.671324	-1.750068
H	-3.4539	0.663488	-1.193869
C	-5.491962	-1.997491	-1.841078
H	-4.961381	-4.069035	-1.533050
H	-5.739128	0.13734	-2.048753
H	-6.491477	-2.228345	-2.212591
C	-0.142952	-2.145208	-0.924014
C	0.144239	-1.977541	-2.286071
C	0.462311	-3.173056	-0.196818

***R*-TS2e** -2069.2436262 (1)

P	-1.342067	0.279829	-0.647711
O	-0.393382	1.290918	-1.459495
C	-1.242000	0.428168	1.523524
H	-0.155805	0.574681	1.556665
C	-1.712594	-0.926987	1.945300
C	-3.081708	-1.233896	1.961737
C	-0.794444	-1.928821	2.280469
C	-3.515852	-2.515422	2.294444
H	-3.808932	-0.465381	1.691033
C	-1.229571	-3.211411	2.611107
H	0.270606	-1.688534	2.287929
C	-2.591321	-3.511315	2.613022
H	-4.583773	-2.738340	2.301193
H	-0.501391	-3.980556	2.874085
H	-2.931879	-4.514577	2.872054
C	-3.029897	0.783378	-1.043410
C	-4.041915	-0.123657	-1.376087
C	-3.329762	2.140845	-0.856327
C	-5.350548	0.327690	-1.530290
H	-3.810201	-1.178251	-1.534042
C	-4.642671	2.580784	-1.009934
H	-2.533717	2.848467	-0.610461
C	-5.651207	1.677405	-1.342246
H	-6.137395	-0.376434	-1.803770
H	-4.873046	3.635603	-0.858477
H	-6.678316	2.026793	-1.457409
C	-1.035303	-1.355421	-1.431726
C	-0.113472	-1.405226	-2.488445
C	-1.637335	-2.544500	-0.987615

C	1.009917	-2.860832	-2.923086	C	0.170299	-2.618186	-3.115888
H	-0.318497	-1.153239	-2.832836	H	0.359074	-0.478980	-2.820853
C	1.324488	-4.060357	-0.845859	C	-1.354253	-3.750606	-1.626379
H	0.276868	-3.262868	0.876384	H	-2.332829	-2.535628	-0.146891
C	1.591	-3.909126	-2.204348	C	-0.456471	-3.789967	-2.693530
H	1.231275	-2.735707	-3.984042	H	0.878907	-2.643723	-3.945307
H	1.798095	-4.864031	-0.280047	H	-1.835931	-4.665963	-1.279432
H	2.267574	-4.602499	-2.707007	H	-0.239296	-4.736632	-3.190465
C	-0.367386	-0.068416	2.707704	C	-2.026948	1.526250	1.962115
H	-0.013154	0.953261	2.794741	H	-3.000012	1.454073	2.433456
N	0.570641	-1.040562	3.013794	N	-1.626949	2.798476	1.635078
O	0.297756	-2.234808	2.856442	O	-0.608616	2.917777	0.908789
O	1.694715	-0.66732	3.407841	O	-2.289418	3.770265	1.997824
H	-0.21815	0.952178	-0.398953	H	0.521842	1.452265	-0.964711
H	6.272144	-2.378734	0.131708	H	4.440042	-4.750847	0.073954
C	5.99607	-1.344266	0.385366	C	4.339748	-3.827194	0.663145
C	4.471349	-1.200417	0.409235	C	3.234550	-2.947370	0.070657
H	6.431041	-1.113358	1.371066	H	4.105137	-4.114385	1.700619
H	6.466426	-0.685409	-0.360843	H	5.318324	-3.324975	0.658437
C	4.110461	0.229646	0.874350	C	2.997308	-1.739798	1.007568
C	3.888139	-1.489941	-0.975546	C	3.615965	-2.498047	-1.341767
C	3.893894	-2.19296	1.424811	C	1.938960	-3.766497	0.021306
N	2.661941	0.418723	1.006093	N	1.920155	-0.842725	0.556860
C	4.493523	1.370518	-0.107302	C	4.180549	-0.744957	1.152596
H	4.584227	0.391724	1.854877	H	2.734795	-2.144026	1.999153
H	2.7897	-1.411261	-0.963533	H	2.826597	-1.872624	-1.786974
H	4.277559	-0.799568	-1.739862	H	4.552439	-1.921039	-1.347167
H	4.145035	-2.516234	-1.280826	H	3.750264	-3.378384	-1.989592
H	4.148909	-3.223063	1.130457	H	2.076858	-4.660242	-0.606469
H	4.300442	-2.013502	2.432721	H	1.645113	-4.101695	1.029391
H	2.799316	-2.116758	1.498805	H	1.098915	-3.201336	-0.412841
C	2.20715	1.261625	0.067004	C	2.468326	0.306304	0.052672
H	2.186516	0.18743	1.881460	H	1.095709	-1.235765	0.110115
N	3.233231	1.612996	-0.790429	N	3.837130	0.273187	0.177838
H	5.283806	1.072645	-0.808319	H	5.149039	-1.212341	0.932935
H	4.826132	2.272383	0.440450	H	4.213700	-0.325941	2.175267
N	1.04639	1.807789	-0.161386	N	1.945174	1.390982	-0.402500
C	2.805109	2.851342	-1.417899	C	4.266339	1.665529	0.137700
C	1.266128	2.688707	-1.334392	C	3.085935	2.304567	-0.649708
H	3.167012	2.941648	-2.449823	H	5.229049	1.781586	-0.374506
H	3.15664	3.726931	-0.836274	H	4.345493	2.078298	1.160141
H	0.927859	2.150897	-2.242161	H	3.326856	2.264561	-1.729052
C	0.467403	4.004216	-1.261859	C	2.777300	3.773074	-0.306933
C	0.919292	4.918386	-2.405749	C	4.019837	4.604396	-0.644721
C	-1.019049	3.679467	-1.439449	C	1.597023	4.229699	-1.171574
C	0.673961	4.70512	0.082804	C	2.409592	3.951754	1.168655
H	0.288614	5.819471	-2.444944	H	3.823125	5.670100	-0.455256
H	1.962563	5.248039	-2.278978	H	4.886683	4.313576	-0.028963
H	0.835302	4.405687	-3.377682	H	4.298225	4.495065	-1.705706
H	-1.624078	4.597058	-1.364309	H	1.433452	5.310304	-1.040618
H	-1.206016	3.224228	-2.424817	H	1.793346	4.040502	-2.239738
H	-1.365034	2.965335	-0.679319	H	0.672827	3.714245	-0.874493
H	0.336726	4.063711	0.909547	H	1.539639	3.334036	1.429568
H	1.731414	4.955225	0.260713	H	3.251954	3.718971	1.839391

H	0.101091	5.644881	0.108379	H	2.131522	5.001527	1.348993

***R*-TS2f** -2069.2325894 (1)				***S*-TS2g** -2069.2532161 (1)			
P	2.827854	-0.385258	-0.433628	N	-0.137975	-3.147207	0.052392
O	1.640225	-1.391744	-0.983271	O	-0.828384	-3.947168	0.677593
C	1.88957	1.794195	-0.201336	O	-0.64118	-2.227604	-0.63574
H	1.436962	1.709467	-1.191828	C	1.244745	-3.201394	0.143822
C	3.159244	2.553194	-0.117034	H	1.614078	-3.892076	0.893321
C	3.871323	2.651524	1.086720	C	1.977321	-2.283066	-0.586786
C	3.697615	3.122842	-1.277341	H	1.498704	-1.892008	-1.489612
C	5.098771	3.308513	1.122161	C	3.451076	-2.214567	-0.545934
H	3.475237	2.189998	1.993703	C	4.121503	-1.552161	-1.583735
C	4.920552	3.786586	-1.237770	C	4.198549	-2.725054	0.523668
H	3.15226	3.036586	-2.219415	C	5.504531	-1.401483	-1.55632
C	5.626606	3.877542	-0.037953	H	3.540372	-1.133353	-2.408987
H	5.647956	3.374772	2.062155	C	5.582647	-2.58057	0.548325
H	5.326388	4.2293	-2.148020	H	3.692952	-3.223797	1.352036
H	6.587009	4.39341	-0.005353	C	6.239195	-1.916711	-0.489218
C	3.10587	-0.877441	1.290882	H	6.009035	-0.87269	-2.36566
C	4.374109	-0.862567	1.885097	H	6.153126	-2.982551	1.386865
C	1.969335	-1.111933	2.077894	H	7.322982	-1.796861	-0.461994
C	4.501374	-1.097447	3.251926	H	-1.768666	1.812612	4.433573
H	5.264309	-0.686137	1.277780	C	-1.144518	1.489909	3.598861
C	2.104884	-1.347173	3.444675	C	0.01055	2.202256	3.276133
H	0.977694	-1.140771	1.620524	C	-1.496579	0.359474	2.859006
C	3.368883	-1.336865	4.032090	C	0.810465	1.795869	2.207183
H	5.491643	-1.101811	3.709405	H	0.289221	3.084204	3.854831
H	1.21646	-1.540433	4.047088	C	-0.690432	-0.058847	1.80377
H	3.474296	-1.521179	5.101985	H	-2.39525	-0.206773	3.106978
C	4.289519	-0.8966	-1.380856	C	0.456973	0.667493	1.456651
C	4.247927	-2.030277	-2.199611	H	1.705554	2.364695	1.948771
C	5.436402	-0.090661	-1.344141	H	-0.964064	-0.937753	1.21797
C	5.36673	-2.372027	-2.956046	P	1.433942	0.054355	0.022111
H	3.33868	-2.63157	-2.236444	O	0.699511	0.551879	-1.342476
C	6.552039	-0.445395	-2.100155	C	2.970495	1.037739	0.03191
H	5.456137	0.817759	-0.734054	C	3.9263	0.809217	1.032053
C	6.517548	-1.584707	-2.904053	C	3.28692	1.860798	-1.053358
H	5.340418	-3.258728	-3.590555	C	5.176696	1.41487	0.955799
H	7.446191	0.178207	-2.070733	H	3.693162	0.143913	1.868188
H	7.389609	-1.856207	-3.500222	C	4.542622	2.46413	-1.12684
C	1.026053	1.715711	0.882490	H	2.542351	2.006302	-1.837608
H	1.208346	2.084091	1.885851	C	5.487897	2.24039	-0.127296
N	-0.169439	1.022042	0.738626	H	5.917611	1.233177	1.735698
O	-0.379341	0.374942	-0.314773	H	4.785909	3.107266	-1.974094
O	-0.981841	1.029026	1.656386	H	6.472274	2.706406	-0.192691
H	0.799396	-0.886019	-0.936508	H	-0.331092	0.776289	-1.196249
H	-1.708844	-4.84416	-0.403032	H	-6.095371	-3.709644	0.663248
C	-2.132954	-3.953436	-0.891650	C	-5.996949	-2.78201	0.080176
C	-2.520432	-2.90861	0.158942	C	-4.513961	-2.464698	-0.1396
H	-1.371056	-3.555642	-1.582157	H	-6.518139	-2.932033	-0.879473
H	-2.996928	-4.284285	-1.487347	H	-6.518812	-1.988063	0.635071
C	-2.949673	-1.598983	-0.544915	C	-4.39868	-1.274275	-1.11897
C	-3.647633	-3.437402	1.047397	C	-3.829228	-2.155703	1.193311
C	-1.28557	-2.598922	1.012647	C	-3.844704	-3.684934	-0.784122

N	-3.30523	-0.551933	0.414027	N	-3.016502	-0.861937	-1.406612
C	-4.232351	-1.708814	-1.415476	C	-5.03002	0.064692	-0.643717
H	-2.101584	-1.263111	-1.162228	H	-4.879765	-1.586393	-2.060118
H	-3.902174	-2.699529	1.821793	H	-2.742794	-2.064835	1.047266
H	-4.558636	-3.641408	0.464332	H	-4.218041	-1.226205	1.638552
H	-3.337384	-4.371533	1.541376	H	-3.993992	-2.981079	1.902469
H	-1.002044	-3.47493	1.617230	H	-3.949875	-4.561858	-0.127768
H	-0.428766	-2.344509	0.368698	H	-4.311419	-3.922236	-1.753867
H	-1.479302	-1.752349	1.690670	H	-2.766017	-3.52808	-0.921683
C	-4.605393	-0.180809	0.249064	C	-2.76428	0.339275	-0.835736
H	-2.614152	0.117447	0.741764	H	-2.260268	-1.543675	-1.465049
N	-5.253126	-1.130554	-0.557410	N	-3.874845	0.798505	-0.16001
H	-4.467224	-2.7463	-1.689794	H	-5.779657	-0.079236	0.144674
H	-4.121238	-1.120003	-2.347622	H	-5.507244	0.593296	-1.490126
N	-5.278995	0.83198	0.648113	N	-1.750314	1.146133	-0.886975
C	-6.421492	-0.421936	-1.059741	C	-3.720575	2.240841	-0.075995
C	-6.613495	0.645294	0.055214	C	-2.175098	2.372102	-0.176313
H	-7.290535	-1.083034	-1.176313	H	-4.116537	2.64443	0.864306
H	-6.198996	0.049297	-2.039157	H	-4.232551	2.737931	-0.923202
H	-7.291749	0.221688	0.823098	H	-1.75494	2.357379	0.84858
C	-7.238174	1.9799	-0.397176	C	-1.681584	3.666527	-0.855871
C	-8.57577	1.701944	-1.087768	C	-2.348703	4.86287	-0.168619
C	-7.468135	2.832105	0.854408	C	-0.164714	3.769214	-0.668561
C	-6.302555	2.735131	-1.344758	C	-2.003923	3.667095	-2.352001
H	-9.085537	2.645518	-1.338049	H	-1.931548	5.80551	-0.554462
H	-8.437231	1.138298	-2.024482	H	-3.435728	4.884239	-0.344153
H	-9.244066	1.119072	-0.433163	H	-2.174834	4.836403	0.9196
H	-7.880075	3.817686	0.585637	H	0.228608	4.656675	-1.188958
H	-8.177867	2.338785	1.537764	H	0.088376	3.857693	0.399643
H	-6.518945	2.971561	1.390232	H	0.340865	2.87823	-1.067618
H	-5.322811	2.882933	-0.869228	H	-1.511032	2.82232	-2.853341
H	-6.148726	2.193723	-2.291381	H	-3.085914	3.592354	-2.542734
H	-6.730091	3.719521	-1.592784	H	-1.650116	4.603488	-2.810493

***S*-TS2h** -2069.2513585 (1)

N	-2.859475	-0.72964	-0.391049
C	-2.934108	0.581006	-0.076964
N	-4.25611	0.955568	0.105734
N	-2.04393	1.512605	0.058969
C	-4.198006	-1.245581	-0.705896
H	-2.052908	-1.055698	-0.921963
C	-2.79678	2.761413	0.306685
C	-5.079944	0.033896	-0.662772
C	-4.267857	2.40209	-0.042242
H	-4.991003	2.882365	0.629144
H	-4.188659	-1.666458	-1.723687
H	-6.05083	-0.139543	-0.180536
H	-2.738047	3.008649	1.383618
H	-4.51612	2.678097	-1.085663
H	-5.260058	0.427398	-1.681064
C	-2.237438	3.972517	-0.472631
C	-3.225354	5.136935	-0.339758
H	-2.805448	6.045065	-0.798318
H	-4.183288	4.925654	-0.839707

***S*-TS2i** -2069.251236 (1)

N	-3.244388	0.177767	0.927592
C	-2.804096	-0.869107	0.203933
N	-3.861817	-1.623392	-0.241315
N	-1.6102	-1.314615	-0.069957
C	-4.705687	0.250145	0.853803
H	-2.643524	1.00459	0.996592
C	-1.831044	-2.622664	-0.727615
C	-5.058364	-1.214638	0.47058
C	-3.338782	-2.951724	-0.505546
H	-3.804464	-3.410607	-1.38717
H	-5.109819	0.480436	1.852183
H	-5.953338	-1.280285	-0.161954
H	-1.65045	-2.50948	-1.813843
H	-3.493695	-3.618186	0.364296
H	-5.218081	-1.828806	1.376524
C	-0.850879	-3.699694	-0.217989
C	-1.134317	-5.012339	-0.953406
H	-0.425262	-5.79218	-0.635937
H	-2.151139	-5.382725	-0.745981

H	-3.431805	5.359976	0.719808	H	-1.030652	-4.883921	-2.042731
C	-0.898428	4.390784	0.142531	C	0.571889	-3.233766	-0.533067
H	-0.495748	5.267956	-0.387983	H	1.307126	-4.010702	-0.269881
H	-1.025132	4.664286	1.202483	H	0.689196	-2.996756	-1.60175
H	-0.160674	3.579683	0.084579	H	0.817446	-2.327148	0.040671
C	-4.618624	-2.373946	0.261018	C	-5.207717	1.349639	-0.113474
C	-4.673326	-1.852147	1.698533	C	-4.721989	1.102857	-1.544687
H	-3.701201	-1.42565	1.988101	H	-3.622188	1.098126	-1.594763
H	-5.437345	-1.06901	1.821401	H	-5.09016	0.145386	-1.943161
H	-4.91361	-2.672774	2.392316	H	-5.082735	1.908119	-2.20294
C	-5.985245	-2.920958	-0.159772	C	-6.738464	1.3845	-0.073871
H	-5.96775	-3.264008	-1.206630	H	-7.105711	1.531846	0.954548
H	-6.259076	-3.780896	0.469897	H	-7.111665	2.219461	-0.685586
H	-6.783743	-2.170276	-0.058063	H	-7.186628	0.460184	-0.469497
C	-2.023842	3.620369	-1.947225	C	-0.977776	-3.902259	1.294731
H	-1.315546	2.785204	-2.046800	H	-0.90934	-2.935114	1.815267
H	-2.962901	3.326764	-2.442543	H	-1.92988	-4.377358	1.577149
H	-1.62404	4.492824	-2.487061	H	-0.167322	-4.554785	1.65543
C	-3.577005	-3.492462	0.153386	C	-4.670107	2.70059	0.380754
H	-3.828972	-4.317816	0.837631	H	-5.056803	3.511637	-0.254893
H	-3.537665	-3.896079	-0.870889	H	-5.000578	2.899439	1.413299
H	-2.572194	-3.124014	0.404860	H	-3.570668	2.752717	0.351423
C	-0.068091	-3.570248	2.224658	C	2.536765	4.760267	-1.639692
C	1.127595	-3.590226	1.508803	C	3.53322	3.84744	-1.29272
C	-0.778451	-2.377509	2.364710	C	1.212711	4.339305	-1.754408
H	-0.450932	-4.488813	2.671693	H	2.793384	5.805591	-1.817598
C	1.615289	-2.416965	0.936468	C	3.205556	2.514375	-1.056403
H	1.681221	-4.522987	1.393900	H	4.570536	4.174431	-1.208621
C	-0.302412	-1.20366	1.784063	C	0.877326	3.006733	-1.522515
H	-1.712384	-2.364433	2.928809	H	0.430197	5.053576	-2.012791
C	0.907716	-1.217564	1.082207	C	1.876109	2.091078	-1.176236
H	2.554538	-2.434705	0.378085	H	3.988621	1.799739	-0.790938
H	-0.857351	-0.267551	1.879584	H	-0.158859	2.669248	-1.5804
P	1.52534	0.308877	0.287286	P	1.404027	0.421667	-0.646427
C	2.93325	0.828932	1.341675	C	2.735211	-0.660868	-1.301959
O	0.447298	1.462711	0.635589	O	0.097308	0.029906	-1.523777
C	4.121542	0.086496	1.352629	C	3.848438	-1.007094	-0.527872
C	2.85079	2.011574	2.084973	C	2.590532	-1.190256	-2.590765
H	-0.553262	1.384034	0.272239	H	-0.602198	-0.417216	-0.900278
H	4.212225	-0.825438	0.758255	H	3.961551	-0.620024	0.48685
C	5.206589	0.51271	2.113913	C	4.81811	-1.864539	-1.049909
C	3.941609	2.434113	2.843659	C	3.560335	-2.046454	-3.104244
H	1.923933	2.585343	2.066430	H	1.704303	-0.933957	-3.174091
C	5.119474	1.687779	2.860058	C	4.675076	-2.384728	-2.334392
H	6.126125	-0.074222	2.115417	H	5.682798	-2.133294	-0.441676
H	3.870189	3.353269	3.427452	H	3.445929	-2.455545	-4.109183
H	5.971747	2.022443	3.453314	H	5.430445	-3.061001	-2.737137
H	3.86077	1.59097	-1.943040	H	1.181432	-1.777926	2.357267
C	4.388075	0.634773	-1.908178	C	2.07387	-1.187131	2.575342
C	3.644771	-0.552852	-1.932418	C	2.080823	0.178495	2.264554
C	5.775437	0.606803	-1.807020	C	3.192612	-1.793001	3.141064
C	2.169781	-0.469414	-1.975120	C	0.896276	0.778686	1.596357
C	4.328149	-1.775637	-1.862864	C	3.231407	0.92963	2.540531
C	6.444091	-0.614234	-1.727205	C	4.336596	-1.040149	3.40679

H	6.336185	1.541512	-1.778113	H	3.172341	-2.858687	3.372438
C	1.363075	-1.58867	-2.142438	C	0.635579	2.145014	1.746559
H	1.75081	0.482256	-2.301164	H	0.028697	0.119997	1.485302
C	5.716486	-1.804559	-1.760403	C	4.349837	0.32322	3.108793
H	3.775333	-2.71553	-1.889440	H	3.262475	1.990872	2.288346
H	7.531014	-0.639635	-1.640969	H	5.214412	-1.513061	3.848775
N	0.002335	-1.392632	-1.996775	N	-0.511226	2.676289	1.190295
H	1.660365	-2.630784	-2.133296	H	1.29949	2.882995	2.181839
H	6.234306	-2.763085	-1.706770	H	5.239597	0.918755	3.317832
O	-0.395896	-0.233568	-1.750731	O	-1.218894	1.917807	0.471355
O	-0.779372	-2.349412	-2.025501	O	-0.804182	3.850398	1.367262

***S*-TS2j** -2069.2468504 (1)

N	-3.097734	0.72689	0.060182
C	-2.66593	-0.449197	0.549917
N	-3.747488	-1.169374	1.038813
N	-1.494802	-1.002529	0.696938
C	-4.546665	0.870689	0.256926
H	-2.545557	1.405411	-0.478317
C	-1.781594	-2.308094	1.357536
C	-4.813582	-0.224343	1.318042
C	-3.182588	-2.115351	1.980140
H	-3.758359	-3.047792	2.026756
H	-4.754755	1.867742	0.675373
H	-5.803854	-0.684139	1.209913
H	-1.876916	-3.07975	0.566924
H	-3.11999	-1.674677	2.995683
H	-4.719929	0.185556	2.341658
C	-0.707817	-2.809956	2.341725
C	-1.28499	-4.002879	3.115374
H	-0.495727	-4.476262	3.718836
H	-2.089309	-3.696399	3.802175
H	-1.687822	-4.766248	2.429579
C	0.5037	-3.295267	1.539453
H	1.318563	-3.600494	2.214763
H	0.230819	-4.165813	0.920890
H	0.88022	-2.500212	0.883533
C	-5.375787	0.729285	-1.044110
C	-5.209406	-0.65988	-1.666016
H	-4.152583	-0.8629	-1.896885
H	-5.570207	-1.456911	-0.998793
H	-5.778123	-0.716007	-2.606784
C	-6.850391	0.984652	-0.713297
H	-6.985059	1.974851	-0.249545
H	-7.450347	0.963249	-1.635145
H	-7.266376	0.227423	-0.031741
C	-0.285029	-1.717286	3.327815
H	0.202252	-0.882516	2.808406
H	-1.145658	-1.325569	3.892233
H	0.42652	-2.13413	4.057700
C	-4.90753	1.792472	-2.041603
H	-5.528551	1.75703	-2.949555
H	-4.990874	2.803662	-1.611798
H	-3.858285	1.646871	-2.330810

***S*-TS2k** -2069.2341262 (1)

P	1.813201	0.428183	-0.296153
O	0.252337	0.551197	-0.710249
C	1.912625	0.334672	1.901829
H	2.982624	0.551392	1.973075
C	1.027887	1.508492	2.163393
C	-0.368024	1.378798	2.181571
C	1.591402	2.773592	2.35968
C	-1.174767	2.488642	2.417211
H	-0.820107	0.401692	1.993754
C	0.783195	3.885564	2.593279
H	2.677201	2.88566	2.322773
C	-0.60223	3.746178	2.624575
H	-2.260095	2.369379	2.444238
H	1.240571	4.863574	2.748031
H	-1.236858	4.613369	2.813026
C	2.501117	-0.853652	-1.406017
C	1.977241	-0.927279	-2.704858
C	3.471185	-1.76258	-0.978569
C	2.440957	-1.904602	-3.579708
H	1.199655	-0.226502	-3.014767
C	3.932836	-2.735337	-1.86807
H	3.826359	-1.745039	0.056003
C	3.42273	-2.806612	-3.161755
H	2.0353	-1.966032	-4.59067
H	4.683966	-3.451482	-1.532766
H	3.78242	-3.574178	-3.848848
C	2.491268	2.008229	-0.877408
C	1.658463	3.130126	-0.954867
C	3.865465	2.13579	-1.112058
C	2.200776	4.371841	-1.27838
H	0.591633	3.017041	-0.753998
C	4.400733	3.380571	-1.433213
H	4.513295	1.257239	-1.055596
C	3.569385	4.498543	-1.515998
H	1.551565	5.246389	-1.340571
H	5.470292	3.478127	-1.623101
H	3.991362	5.472897	-1.766796
C	1.549834	-0.92165	2.436588
H	0.554166	-1.21832	2.740985
N	2.492937	-1.924099	2.46205
O	3.654885	-1.66861	2.074414

C	6.106898	-1.047133	-0.060665	O	2.171004	-3.050896	2.860181
C	5.968577	0.340746	-0.109650	H	-0.339481	-0.291056	-0.447073
C	4.976431	-1.856785	0.041663	H	-6.731248	2.3872	-1.932819
H	7.10005	-1.496876	-0.102234	C	-6.378463	1.805038	-1.068623
C	4.702417	0.918201	-0.058599	C	-4.864093	1.593802	-1.160284
H	6.85166	0.977016	-0.182633	H	-6.648446	2.359784	-0.156054
C	3.70665	-1.28533	0.093450	H	-6.929086	0.852551	-1.065754
H	5.080614	-2.94215	0.077987	C	-4.391801	0.842461	0.106948
C	3.565595	0.106165	0.048399	C	-4.512568	0.825156	-2.436715
H	4.596191	2.005488	-0.089627	C	-4.17835	2.965282	-1.186917
H	2.817373	-1.914229	0.160222	N	-2.93747	0.671658	0.185338
P	1.903687	0.841564	-0.060410	C	-4.863203	-0.634953	0.228607
C	1.99771	2.29075	1.066695	H	-4.737555	1.416986	0.981095
O	1.018862	-0.256724	0.745957	H	-3.42818	0.653003	-2.511038
C	1.569506	3.55711	0.663795	H	-5.01537	-0.152207	-2.477327
C	2.47706	2.090758	2.370890	H	-4.823766	1.405753	-3.31848
H	0.002615	-0.402229	0.583579	H	-4.559785	3.566049	-2.02592
H	1.165577	3.704886	-0.340304	H	-4.369217	3.524985	-0.256841
C	1.633655	4.625071	1.562132	H	-3.089487	2.87197	-1.320701
C	2.536255	3.159113	3.258731	C	-2.601711	-0.606842	-0.101519
H	2.802456	1.096278	2.683923	H	-2.255243	1.419526	0.130785
C	2.117018	4.42886	2.852322	N	-3.728987	-1.358553	-0.32323
H	1.296595	5.612996	1.246179	H	-5.784114	-0.826445	-0.33701
H	2.911255	3.003832	4.271347	H	-5.033729	-0.903158	1.287553
H	2.16548	5.266159	3.550351	N	-1.465842	-1.221682	-0.129468
H	3.211375	-0.135644	-3.435125	C	-3.320149	-2.742114	-0.093827
C	2.627117	-0.990172	-3.086791	C	-1.791032	-2.644951	-0.37825
C	1.415896	-0.764983	-2.420009	H	-3.833855	-3.435685	-0.770401
C	3.092982	-2.28509	-3.294924	H	-3.519028	-3.03999	0.952486
C	0.968452	0.629685	-2.200711	H	-1.613182	-2.861488	-1.448447
C	0.684932	-1.862348	-1.942335	C	-0.904313	-3.599934	0.442996
C	2.356587	-3.37205	-2.825608	C	-1.258333	-5.042238	0.071616
H	4.038365	-2.444702	-3.814451	C	0.554029	-3.318966	0.071725
C	-0.381655	0.955183	-2.062409	C	-1.099965	-3.381744	1.950462
H	1.591933	1.403827	-2.649122	H	-0.628229	-5.741005	0.641623
C	1.154896	-3.156451	-2.149302	H	-2.310373	-5.276041	0.30354
H	-0.24229	-1.702649	-1.386649	H	-1.089685	-5.229479	-1.000989
H	2.720974	-4.388247	-2.982626	H	1.234812	-3.985689	0.620949
N	-0.696731	2.296935	-1.950194	H	0.72534	-3.432595	-1.012451
H	-1.191217	0.262359	-1.855017	H	0.818941	-2.290644	0.35595
H	0.579708	-4.004302	-1.774467	H	-1.220996	-2.309801	2.170331
O	0.183964	3.147772	-2.117112	H	-1.987647	-3.910808	2.331837
O	-1.864456	2.620506	-1.646879	H	-0.215786	-3.730406	2.504415

***S*-TS2i** -2069.2400136 (1)

P	-2.615465	-0.449177	0.622742
O	-1.175909	-0.383022	1.4186
C	-2.078861	-0.800081	-1.664559
H	-1.542533	-1.720967	-1.424619
C	-3.461182	-0.954149	-2.17691
C	-4.260450	0.160302	-2.465987
C	-4.002558	-2.238513	-2.317798
C	-5.577041	-0.011589	-2.886098
H	-3.859579	1.167497	-2.335616

***R*-4** -2069.2896421 (0)

P	-1.705778	0.401588	0.087629
O	-0.289447	0.970751	0.17429
C	-1.696873	-1.419925	-0.351726
H	-1.074564	-1.44899	-1.257078
C	-3.08467	-1.929742	-0.648393
C	-4.017339	-2.156997	0.37186
C	-3.478543	-2.127671	-1.976195
C	-5.321466	-2.542307	0.064013
H	-3.730109	-2.017786	1.416214

C	-5.316276	-2.407974	-2.746174	C	-4.779262	-2.518679	-2.284864
H	-3.386473	-3.108485	-2.080847	H	-2.755522	-1.956997	-2.776347
C	-6.108349	-1.293953	-3.026914	C	-5.709161	-2.716761	-1.264511
H	-6.192271	0.862550	-3.102731	H	-6.039236	-2.707837	0.868636
H	-5.725052	-3.412814	-2.85805	H	-5.068109	-2.665524	-3.326568
H	-7.139252	-1.425185	-3.357906	H	-6.730692	-3.016161	-1.502824
C	-3.704275	-1.372556	1.747117	C	-2.522937	0.532085	1.71141
C	-3.267533	-1.733383	3.025929	C	-3.854096	0.915081	1.898112
C	-4.959486	-1.790234	1.283669	C	-1.727724	0.204885	2.81925
C	-4.102555	-2.485626	3.849211	C	-4.394647	0.948687	3.182768
H	-2.277253	-1.422642	3.361454	H	-4.47255	1.199553	1.046533
C	-5.790410	-2.535008	2.118213	C	-2.275796	0.233865	4.099652
H	-5.281799	-1.545367	0.266887	H	-0.681977	-0.06969	2.666292
C	-5.362366	-2.881964	3.399437	C	-3.609318	0.601094	4.28104
H	-3.766680	-2.765986	4.848338	H	-5.432634	1.251901	3.325308
H	-6.768850	-2.858021	1.760943	H	-1.657127	-0.028297	4.958574
H	-6.010034	-3.473909	4.047352	H	-4.035679	0.625795	5.285096
C	-3.195592	1.270972	0.626085	C	-2.691646	1.321589	-1.144629
C	-2.228312	2.269882	0.454495	C	-2.025548	2.366694	-1.794978
C	-4.555054	1.609751	0.627891	C	-4.022514	1.031658	-1.48201
C	-2.618417	3.598209	0.291928	C	-2.680103	3.115884	-2.770996
H	-1.169769	2.008164	0.476522	H	-0.990785	2.5771	-1.519463
C	-4.937372	2.938883	0.468236	C	-4.671604	1.786228	-2.456471
H	-5.315568	0.839238	0.767557	H	-4.558014	0.2149	-0.995439
C	-3.971460	3.932840	0.295523	C	-4.002309	2.825899	-3.102735
H	-1.857876	4.370261	0.167934	H	-2.155308	3.928744	-3.274614
H	-5.995769	3.202202	0.484173	H	-5.705638	1.554221	-2.714714
H	-4.276919	4.972652	0.1714	H	-4.514688	3.410239	-3.868453
C	-1.297369	0.288785	-2.029617	C	-0.980845	-2.145681	0.734827
H	-1.618810	1.153538	-2.599341	H	-1.461733	-2.523816	1.631368
N	0.035566	0.331872	-1.63342	N	0.328598	-2.295437	0.704536
O	0.451406	-0.514578	-0.802456	O	0.977163	-1.902412	-0.372567
O	0.772389	1.194331	-2.088872	O	0.985369	-2.793756	1.641213
H	-0.457451	-0.559592	0.770283	H	2.158236	-1.515196	-0.017034
H	2.555663	5.067805	0.98698	H	3.32505	5.669283	0.726793
C	3.069876	4.376286	0.301606	C	3.547022	4.87471	-0.001256
C	2.807227	2.926190	0.717913	C	2.839477	3.579412	0.40997
H	2.693880	4.567702	-0.716484	H	3.201423	5.220301	-0.98894
H	4.141066	4.627070	0.323876	H	4.641005	4.762206	-0.039821
C	3.432463	1.968459	-0.325868	C	3.033976	2.523462	-0.703803
C	3.375947	2.659247	2.113044	C	3.390643	3.078838	1.747605
C	1.293922	2.688018	0.728597	C	1.338168	3.860446	0.543163
N	3.155277	0.562871	-0.016597	N	2.367322	1.248146	-0.416181
C	4.984094	2.001275	-0.390596	C	4.499305	2.057233	-0.937196
H	3.000448	2.220715	-1.306682	H	2.624118	2.945383	-1.635153
H	3.178798	1.620197	2.414451	H	2.869324	2.164943	2.068944
H	4.464236	2.819080	2.145909	H	4.467424	2.858136	1.690509
H	2.907629	3.331282	2.849366	H	3.240129	3.844739	2.523426
H	0.805474	3.326020	1.483232	H	1.162512	4.604977	1.334492
H	0.860620	2.914254	-0.259633	H	0.936668	4.272888	-0.397622
H	1.069699	1.636755	0.971573	H	0.767377	2.952385	0.78768
C	4.321816	-0.104181	0.21413	C	3.274704	0.320773	-0.124593
H	2.370979	0.081227	-0.450291	H	1.350181	1.101745	-0.286207
N	5.357594	0.827735	0.3829	N	4.55664	0.818352	-0.172885

H	5.404449	2.923197	0.033482	H	5.234804	2.78825	-0.57903
H	5.332181	1.910190	-1.438568	H	4.683398	1.863444	-2.010114
N	4.614028	-1.349394	0.268816	N	3.197333	-0.956527	0.116909
C	6.566048	0.053010	0.138631	C	5.411892	-0.336282	-0.436962
C	6.068965	-1.376986	0.494449	C	4.570104	-1.479993	0.19275
H	7.406041	0.383387	0.763774	H	6.39735	-0.2333	0.032673
H	6.864815	0.127055	-0.927003	H	5.54311	-0.480428	-1.527165
H	6.260383	-1.547995	1.573055	H	4.856183	-1.579702	1.255851
C	6.752889	-2.531292	-0.263806	C	4.703717	-2.868089	-0.458464
C	8.266455	-2.447723	-0.049948	C	6.191241	-3.221831	-0.547417
C	6.222028	-3.847275	0.313026	C	3.983325	-3.88222	0.437761
C	6.427061	-2.480126	-1.758516	C	4.064846	-2.891951	-1.8505
H	8.771614	-3.306645	-0.518812	H	6.31375	-4.257628	-0.897981
H	8.688239	-1.530895	-0.492297	H	6.72907	-2.565876	-1.251019
H	8.514442	-2.454285	1.02402	H	6.676472	-3.141455	0.439034
H	6.661828	-4.708929	-0.213676	H	4.006958	-4.879921	-0.027553
H	6.473512	-3.934341	1.382203	H	4.479905	-3.953928	1.418587
H	5.128166	-3.884228	0.215549	H	2.933571	-3.599652	0.612182
H	5.338217	-2.490902	-1.907354	H	2.980658	-2.719798	-1.782228
H	6.831774	-1.575331	-2.238133	H	4.499749	-2.135832	-2.523734
H	6.866161	-3.350256	-2.271497	H	4.226549	-3.8779	-2.312563

***S*-4** -2069.2939256 (0)

N	-0.676597	-2.065388	0.256348
O	-1.61338	-2.217306	1.084821
O	-0.96294	-1.953715	-1.006958
C	0.585351	-2.017601	0.642854
H	0.743322	-2.156997	1.707066
C	1.658215	-1.622678	-0.309031
H	1.335358	-1.874431	-1.329821
C	3.02047	-2.193084	-0.010963
C	3.807158	-2.697129	-1.051963
C	3.5527	-2.169899	1.284675
C	5.102685	-3.149561	-0.812821
H	3.39983	-2.720329	-2.064824
C	4.850847	-2.617535	1.52459
H	2.954129	-1.785023	2.112909
C	5.632682	-3.102786	0.476202
H	5.701896	-3.536864	-1.638123
H	5.252588	-2.587288	2.538465
H	6.64848	-3.452537	0.66547
H	2.13337	1.845549	5.137374
C	2.072239	1.548851	4.089191
C	3.181267	1.691652	3.258301
C	0.878771	1.036348	3.578247
C	3.106068	1.308886	1.91899
H	4.110903	2.105879	3.650452
C	0.794738	0.65784	2.240671
H	0.005345	0.932936	4.223522
C	1.918645	0.779294	1.406619
H	3.975632	1.437917	1.273825
H	-0.145085	0.265386	1.843228
P	1.699569	0.251003	-0.329209
O	0.4031	0.844683	-0.893271

***R*-TS3** -2069.2696542 (1)

P	2.658119	0.3623	-0.145663
O	2.318217	1.564617	-1.011213
C	1.204434	-0.537044	0.542286
H	1.603553	-1.277445	1.25976
C	0.463132	-1.28148	-0.55672
C	0.076301	-0.628089	-1.734282
C	0.108635	-2.623671	-0.382918
C	-0.670052	-1.300551	-2.700953
H	0.368471	0.413243	-1.888182
C	-0.64126	-3.294157	-1.348514
H	0.392266	-3.131298	0.541527
C	-1.038787	-2.631563	-2.509444
H	-0.963306	-0.77751	-3.613049
H	-0.916878	-4.338174	-1.189722
H	-1.625198	-3.153803	-3.266909
C	3.639133	-0.881331	-1.046006
C	3.773385	-2.21016	-0.630607
C	4.271302	-0.446541	-2.213436
C	4.55602	-3.093453	-1.37035
H	3.252687	-2.568978	0.260156
C	5.055684	-1.332887	-2.949596
H	4.12591	0.586728	-2.534536
C	5.200851	-2.653159	-2.526564
H	4.655678	-4.130642	-1.048215
H	5.550032	-0.993582	-3.860963
H	5.812168	-3.346616	-3.105895
C	3.63928	0.862904	1.310588
C	3.86917	2.231668	1.467716
C	4.151875	-0.046293	2.241929
C	4.607882	2.690672	2.557843
H	3.462748	2.917515	0.722006

C	3.122043	0.83146	-1.314508	C	4.888382	0.416041	3.329027
C	4.458176	0.481912	-1.066043	H	3.98745	-1.119326	2.118843
C	2.810469	1.651874	-2.404533	C	5.115961	1.784356	3.486882
C	5.465658	0.959991	-1.900603	H	4.787798	3.7594	2.681621
H	4.720886	-0.167783	-0.229001	H	5.288657	-0.292496	4.055034
C	3.823823	2.122491	-3.237859	H	5.694442	2.142636	4.339738
H	1.764763	1.905605	-2.584911	C	0.339928	0.478747	1.268516
C	5.150489	1.778194	-2.986036	H	-0.71504	1.118627	0.456303
H	6.502642	0.685417	-1.702897	N	-0.54529	-0.098534	2.215649
H	3.574515	2.758894	-4.087887	O	-1.170435	0.638652	2.965705
H	5.943303	2.146191	-3.639051	O	-0.762487	-1.325464	2.16596
H	-1.191761	0.8678	-0.366615	H	-1.954931	-1.255472	0.527445
H	-6.791814	-3.737971	0.061397	H	-2.012072	5.326505	-2.644039
C	-6.517748	-2.856488	-0.536904	C	-2.484214	4.798832	-1.801921
C	-5.064019	-2.466504	-0.251504	C	-1.824818	3.428982	-1.610569
H	-6.660789	-3.113804	-1.599084	H	-2.361929	5.425403	-0.903736
H	-7.225824	-2.05259	-0.280404	H	-3.559709	4.721239	-2.023308
C	-4.683559	-1.28601	-1.17348	C	-2.399272	2.763875	-0.340824
C	-4.885461	-2.099593	1.224572	C	-2.068846	2.549941	-2.839398
C	-4.14733	-3.647578	-0.591826	C	-0.320547	3.630157	-1.399944
N	-3.26633	-0.899999	-1.065907	N	-1.777241	1.4547	-0.067422
C	-5.404079	0.058906	-0.866545	C	-3.923168	2.428098	-0.388108
H	-4.888542	-1.593304	-2.210642	H	-2.189221	3.432557	0.508596
H	-3.835803	-1.844089	1.429852	H	-1.606102	1.560763	-2.706311
H	-5.533606	-1.259023	1.519631	H	-3.143621	2.401286	-3.029882
H	-5.150894	-2.964968	1.85143	H	-1.627913	3.017916	-3.732638
H	-4.450426	-4.533369	-0.012954	H	0.125924	4.113198	-2.282604
H	-4.212581	-3.903779	-1.662281	H	-0.136523	4.284954	-0.532307
H	-3.103848	-3.415714	-0.334892	H	0.22111	2.68753	-1.229261
C	-3.191268	0.237377	-0.420414	C	-2.697203	0.539683	-0.195345
H	-2.34633	-1.508303	-1.115804	H	0.834261	1.340777	1.728031
N	-4.406139	0.759592	-0.06696	N	-3.916101	0.988959	-0.632012
H	-6.340309	-0.081128	-0.312222	H	-4.451977	2.968637	-1.183167
H	-5.616775	0.618358	-1.796055	H	-4.410698	2.649856	0.578393
N	-2.187261	1.043012	-0.107457	N	-2.725448	-0.763045	0.074167
C	-4.226029	2.197659	0.069001	C	-4.926086	0.034677	-0.183756
C	-2.729391	2.285538	0.466688	C	-4.100518	-1.265579	0.041052
H	-4.882091	2.624054	0.837174	H	-5.711979	-0.10604	-0.935674
H	-4.418764	2.708856	-0.893999	H	-5.392268	0.382936	0.755448
H	-2.657538	2.233998	1.568524	H	-4.218244	-1.932913	-0.830739
C	-1.994799	3.559531	0.005756	C	-4.459331	-2.07203	1.306246
C	-2.820894	4.77177	0.449332	C	-5.920263	-2.513477	1.181362
C	-0.622124	3.60732	0.685352	C	-3.552363	-3.308784	1.359548
C	-1.797999	3.568408	-1.513016	C	-4.250717	-1.253834	2.585334
H	-2.271737	5.699757	0.23168	H	-6.203594	-3.133686	2.044419
H	-3.787931	4.826691	-0.074662	H	-6.605458	-1.651109	1.15369
H	-3.015748	4.743317	1.533708	H	-6.079879	-3.109642	0.26835
H	-0.088887	4.526298	0.396656	H	-3.865419	-3.966413	2.184519
H	-0.721396	3.60046	1.782513	H	-3.60595	-3.88491	0.421814
H	-0.009053	2.748328	0.379079	H	-2.504193	-3.02747	1.547588
H	-1.150267	2.735298	-1.82332	H	-3.2114	-0.906205	2.687366
H	-2.752632	3.493411	-2.057223	H	-4.921004	-0.381765	2.636657
H	-1.316793	4.510927	-1.816023	H	-4.477678	-1.885023	3.458067

S-TS3 -2069.2716961 (1)

N	0.713919	-0.183337	2.461082
O	1.361994	0.653162	3.114659
O	0.951172	-1.385187	2.535986
C	-0.23602	0.304078	1.528642
H	0.579406	1.116148	0.602158
C	-1.077474	-0.775689	0.884368
H	-1.627994	-1.37514	1.634302
C	-0.314125	-1.74357	-0.006189
C	-0.303439	-3.109368	0.289125
C	0.356796	-1.300868	-1.15227
C	0.358335	-4.014361	-0.537233
H	-0.804652	-3.461363	1.192739
C	1.013238	-2.206956	-1.984831
H	0.32217	-0.243302	-1.406273
C	1.017098	-3.567191	-1.681894
H	0.359168	-5.075711	-0.28477
H	1.515183	-1.848364	-2.886638
H	1.530614	-4.275807	-2.333412
H	-5.260136	-4.112761	-2.6492
C	-4.719038	-3.304441	-2.155293
C	-4.836759	-3.13004	-0.775618
C	-3.914219	-2.447013	-2.903606
C	-4.145551	-2.099394	-0.143424
H	-5.471214	-3.796828	-0.190505
C	-3.221364	-1.413353	-2.274891
H	-3.825202	-2.583374	-3.982207
C	-3.335378	-1.242124	-0.893774
H	-4.250149	-1.960274	0.935042
H	-2.58688	-0.727046	-2.838491
P	-2.343635	0.089753	-0.145247
O	-1.758144	1.020294	-1.200023
C	-3.421778	0.995474	1.014666
C	-3.784751	0.523242	2.281111
C	-3.880888	2.241665	0.577599
C	-4.619502	1.287353	3.094445
H	-3.405482	-0.432497	2.650086
C	-4.716785	3.001686	1.393403
H	-3.563606	2.602038	-0.402546
C	-5.08816	2.523813	2.648976
H	-4.897865	0.920701	4.083111
H	-5.073767	3.973289	1.04984
H	-5.738333	3.121353	3.289376
H	-0.770797	1.143067	1.987802
H	1.67234	3.758267	-3.726753
C	0.853349	4.049231	-3.050269
H	0.717114	5.137007	-3.148209
C	1.149166	3.68283	-1.593025
H	-0.069924	3.558273	-3.396183
C	1.259204	2.147246	-1.48051
C	2.430755	4.37085	-1.118833
C	-0.032456	4.119693	-0.719106

***R*-5** -1394.6336391 (0)

P	-0.678539	0.264616	-0.76389
O	-0.594087	0.166498	-2.274952
C	0.433005	-0.926884	0.114349
H	0.115544	-0.959104	1.167969
C	1.892929	-0.534368	0.02695
C	2.455834	-0.126764	-1.189678
C	2.700826	-0.606758	1.165758
C	3.804925	0.213059	-1.2554
H	1.82479	-0.063783	-2.079692
C	4.050845	-0.26745	1.094771
H	2.269102	-0.94967	2.108458
C	4.605127	0.144945	-0.115252
H	4.232563	0.536245	-2.205421
H	4.671828	-0.328318	1.989442
H	5.661372	0.411589	-0.17021
C	-0.251737	1.905746	-0.112647
C	0.106532	2.136676	1.219872
C	-0.282481	2.962124	-1.025999
C	0.409418	3.429028	1.640218
H	0.17536	1.310046	1.930928
C	0.021051	4.254094	-0.599918
H	-0.532142	2.750447	-2.06749
C	0.361875	4.486934	0.731514
H	0.693149	3.610448	2.677479
H	-0.001928	5.080607	-1.311105
H	0.603145	5.497802	1.063054
C	-2.348899	-0.161421	-0.165952
C	-3.256853	-0.612619	-1.127748
C	-2.732907	-0.068953	1.175921
C	-4.547094	-0.977966	-0.743863
H	-2.932051	-0.662626	-2.169051
C	-4.022045	-0.43458	1.554216
H	-2.033576	0.300551	1.929464
C	-4.927502	-0.889933	0.593949
H	-5.257699	-1.330998	-1.492265
H	-4.323256	-0.362559	2.59985
H	-5.937073	-1.175349	0.89274
C	0.173416	-2.301176	-0.487956
H	0.538592	-2.388944	-1.515966
N	0.881028	-3.364499	0.308289
O	0.886784	-3.242904	1.515898
O	1.364404	-4.280945	-0.31113
H	-0.891229	-2.577738	-0.445025

***S* 5** -1394.6336391 (0)

N	-0.881052	-3.36449	0.308295
O	-0.886793	-3.242898	1.515904
O	-1.364452	-4.280926	-0.31112
C	-0.173431	-2.301176	-0.487955
H	-0.538608	-2.388946	-1.515965
C	-0.433012	-0.92688	0.114346

N	1.415986	1.715223	-0.073377
C	2.488299	1.504494	-2.19908
H	0.312173	1.732594	-1.857534
H	2.649354	4.108176	-0.072807
H	3.300628	4.090601	-1.733651
H	2.317406	5.464517	-1.175864
H	-0.227583	5.195565	-0.84739
H	-0.937612	3.553253	-0.989276
H	0.180809	3.927807	0.342392
C	2.607922	1.188482	0.034494
N	3.394824	1.240998	-1.083044
H	2.945988	2.174292	-2.938205
H	2.213969	0.558239	-2.70036
N	3.182341	0.495111	1.013026
C	4.357002	0.143335	-0.97665
H	2.85199	0.544823	1.981724
C	4.456818	-0.062911	0.560249
H	5.325076	0.403297	-1.421698
H	3.956387	-0.759061	-1.474766
H	5.288429	0.549813	0.954497
C	4.659755	-1.509099	1.054025
C	6.041966	-1.975473	0.590815
C	4.594555	-1.492494	2.58738
C	3.573379	-2.452129	0.529003
H	6.235031	-2.999881	0.942295
H	6.116308	-1.980752	-0.508803
H	6.837981	-1.324609	0.986768
H	4.864647	-2.482655	2.984262
H	5.295791	-0.755265	3.011304
H	3.574917	-1.265047	2.938829
H	2.565171	-2.072017	0.758084
H	3.651232	-2.61785	-0.556007
H	3.677054	-3.433917	1.016035

TS4 -880.3581071 (1)

P	-0.000012	1.094796	-0.942352
O	-0.000047	2.561485	-0.277744
H	-0.000039	2.321068	-1.742618
C	-1.453663	0.17184	-0.338507
C	-1.825181	-1.097344	-0.793108
C	-2.204476	0.823268	0.641876
C	-2.946421	-1.719056	-0.250371
H	-1.249426	-1.599608	-1.573662
C	-3.319953	0.189573	1.188292
H	-1.893138	1.821498	0.958729
C	-3.690897	-1.077523	0.742063
H	-3.244238	-2.707367	-0.602911
H	-3.904362	0.69042	1.961452
H	-4.568697	-1.568672	1.164341
C	1.453678	0.171893	-0.338516
C	1.825412	-1.097154	-0.793318
C	2.204283	0.823224	0.64209
C	2.946646	-1.718843	-0.250538
H	1.249856	-1.599311	-1.574089
H	-0.11555	-0.959099	1.167965
C	-1.892934	-0.534357	0.026946
C	-2.700833	-0.606746	1.165753
C	-2.455835	-0.126746	-1.189681
C	-4.05085	-0.267431	1.094765
H	-2.269111	-0.949663	2.108453
C	-3.804925	0.213084	-1.255404
H	-1.824791	-0.063766	-2.079695
C	-4.605129	0.144971	-0.115257
H	-4.671834	-0.3283	1.989436
H	-4.23256	0.536275	-2.205424
H	-5.661372	0.411619	-0.170215
H	2.033578	0.300542	1.929459
C	2.732906	-0.068968	1.175918
C	2.348897	-0.161437	-0.165955
C	4.022042	-0.434603	1.554213
P	0.67854	0.264612	-0.763893
C	3.256847	-0.612643	-1.12775
C	4.927495	-0.889965	0.593948
H	4.323253	-0.362582	2.599847
O	0.594088	0.166499	-2.274955
C	0.251751	1.905743	-0.112645
C	4.547086	-0.977999	-0.743864
H	2.932046	-0.66265	-2.169053
H	5.937064	-1.175387	0.892739
C	0.282512	2.962125	-1.025993
C	-0.106523	2.136672	1.219873
H	5.257689	-1.331037	-1.492266
C	-0.021008	4.254097	-0.599909
H	0.532175	2.75045	-2.067484
C	-0.409396	3.429027	1.640222
H	-0.175363	1.310042	1.930926
C	-0.361836	4.486935	0.731522
H	0.001984	5.080612	-1.311093
H	-0.69313	3.610447	2.677482
H	-0.603096	5.497806	1.063065
H	0.891211	-2.577745	-0.445021

POH Dimer -1760.9356664 (0)

P	1.794213	-0.913694	0.164613
O	1.052256	-1.223639	-1.129437
H	1.366739	-1.620943	1.312973
C	1.733208	0.834507	0.672272
C	0.731251	1.286902	1.538819
C	2.612757	1.747964	0.078727
C	0.614676	2.650546	1.804484
H	0.023364	0.569185	1.95935
C	2.490563	3.108808	0.349024
H	3.395683	1.39251	-0.595742
C	1.489484	3.559359	1.209841
H	-0.17194	3.005843	2.471673
H	3.178223	3.819469	-0.111645
H	1.390088	4.626209	1.416809
C	3.566124	-1.306462	0.000131

C	3.319753	0.189552	1.188545
H	1.892794	1.821367	0.959074
C	3.690901	-1.077419	0.74213
H	3.244637	-2.707044	-0.603237
H	3.903992	0.690314	1.961888
H	4.568696	-1.568549	1.16444

TS5 -1760.8868945 (1)

P	1.54475	-0.319266	0.232808
O	0.767786	-0.054975	-1.129048
H	-0.114559	-0.499748	1.354093
C	2.771191	1.059517	0.387445
C	3.389867	1.36333	1.602849
C	3.066273	1.822739	-0.746084
C	4.314227	2.40482	1.681194
H	3.139987	0.787591	2.498286
C	3.986235	2.866751	-0.667048
H	2.559281	1.573097	-1.681525
C	4.613798	3.157103	0.545474
H	4.796824	2.635637	2.632541
H	4.220639	3.456905	-1.555113
H	5.333759	3.97477	0.607299
C	2.716676	-1.707528	-0.13354
C	3.567236	-2.246258	0.837415
C	2.711745	-2.24846	-1.420941
C	4.413046	-3.30664	0.519971
H	3.571318	-1.833686	1.850269
C	3.557222	-3.31216	-1.737685
H	2.035483	-1.812276	-2.159214
C	4.40819	-3.842678	-0.769179
H	5.0784	-3.719917	1.280027
H	3.552761	-3.729242	-2.746655
H	5.067234	-4.676574	-1.016129
H	-2.816905	5.283335	-0.693903
C	-2.644457	4.215434	-0.551388
C	-1.495616	3.622739	-1.072607
C	-3.576916	3.452779	0.154941
C	-1.265216	2.259038	-0.89584
H	-0.767781	4.22374	-1.618514
C	-3.362454	2.090646	0.338362
H	-4.472364	3.92146	0.564145
C	-2.208157	1.498098	-0.190891
H	-0.36269	1.767698	-1.275037
H	-4.089902	1.490031	0.888546
P	-1.867784	-0.252725	0.064902
O	-1.155358	-0.548127	1.471539
H	-0.948188	-0.634745	-0.960338
C	-3.436846	-1.140146	0.142299
C	-4.404904	-0.944037	-0.850551
C	-3.651375	-2.057029	1.17459
C	-5.588931	-1.67372	-0.808081
H	-4.23649	-0.218798	-1.649908
C	-4.843487	-2.778966	1.211644
H	-2.885637	-2.193035	1.938701
C	4.47844	-1.093879	1.038863
C	3.994947	-1.842805	-1.214962
C	5.819552	-1.420979	0.859089
H	4.141126	-0.665942	1.98663
C	5.340583	-2.165688	-1.392874
H	3.256328	-1.997495	-2.003653
C	6.249513	-1.95585	-0.357632
H	6.534381	-1.257613	1.666541
H	5.680456	-2.582767	-2.341928
H	7.301671	-2.208725	-0.497084
H	-1.390101	4.626208	-1.416851
C	-1.489493	3.559361	-1.209867
C	-2.490579	3.108817	-0.349054
C	-0.614673	2.650544	-1.804487
C	-2.612769	1.747977	-0.078738
H	-3.178248	3.819482	0.111596
C	-0.731244	1.286903	-1.538801
H	0.171949	3.005835	-2.471672
C	-1.733209	0.834516	-0.672259
H	-3.395701	1.392528	0.595728
H	-0.023348	0.569184	-1.959312
P	-1.794208	-0.913679	-0.164576
O	-1.052273	-1.223592	1.129494
H	-1.366694	-1.620932	-1.312917
C	-3.566117	-1.306463	-0.000126
C	-4.478411	-1.093909	-1.038883
C	-3.994963	-1.842783	1.21497
C	-5.819525	-1.421017	-0.859131
H	-4.141079	-0.665991	-1.986651
C	-5.340601	-2.165673	1.392858
H	-3.25636	-1.997451	2.00368
C	-6.24951	-1.955864	0.357592
H	-6.534337	-1.257673	-1.666602
H	-5.680492	-2.582733	2.341914
H	-7.301668	-2.208744	0.497025

Tautomer dimer -1760.928388 (1)

P	-1.795248	-0.363023	-0.122515
O	-1.283516	-0.646608	1.445189
H	0.307885	-0.608961	-1.44167
C	-2.593927	1.28773	0.039445
C	-2.609087	2.148894	-1.06005
C	-3.17725	1.690908	1.246393
C	-3.22722	3.397366	-0.966335
H	-2.127578	1.846328	-1.993698
C	-3.780866	2.940968	1.342068
H	-3.143323	1.018088	2.105506
C	-3.811286	3.792377	0.234464
H	-3.239533	4.064895	-1.828876
H	-4.233251	3.256379	2.28369
H	-4.287096	4.770992	0.314003
C	-3.287407	-1.437861	-0.109629
C	-4.266548	-1.269243	-1.096072
C	-3.422994	-2.462214	0.830762

C	-5.806829	-2.590346	0.222283
H	-6.345028	-1.526362	-1.579508
H	-5.017347	-3.494293	2.015908
H	-6.735806	-3.161035	0.252668

TS6 -1394.573696 (1)

N	1.41837	3.312503	0.486998
O	2.289823	2.70849	-0.162087
O	1.650474	4.305946	1.159086
C	0.117161	2.784299	0.465901
H	-0.615414	3.329189	1.05278
C	-0.16451	1.804706	-0.510073
H	0.504002	1.806523	-1.374494
C	-1.57518	1.427828	-0.796222
C	-1.944235	1.076245	-2.098613
C	-2.532846	1.351868	0.223626
C	-3.243357	0.656841	-2.37935
H	-1.202177	1.133127	-2.898356
C	-3.827849	0.925633	-0.054232
H	-2.251181	1.598713	1.249957
C	-4.186541	0.574578	-1.356428
H	-3.518322	0.392539	-3.401381
H	-4.559934	0.858204	0.75139
H	-5.201542	0.238603	-1.57226
H	-3.769936	-3.569858	1.27148
C	-2.897726	-2.936199	1.104318
C	-2.450938	-2.695135	-0.196017
C	-2.23425	-2.36611	2.189498
C	-1.344286	-1.879611	-0.410353
H	-2.974053	-3.133994	-1.046444
C	-1.125288	-1.546965	1.981682
H	-2.583698	-2.5556	3.205356
C	-0.675434	-1.306841	0.680033
H	-1.013023	-1.670303	-1.430669
H	-0.606741	-1.080101	2.819976
P	0.639356	-0.093194	0.377354
O	1.000677	0.502136	1.851753
C	2.122946	-0.990409	-0.160062
C	3.306044	-0.255353	-0.321026
C	2.096551	-2.36121	-0.444204
C	4.460407	-0.905031	-0.749865
H	3.311647	0.816135	-0.108907
C	3.255443	-2.995583	-0.886414
H	1.180179	-2.93668	-0.305183
C	4.436008	-2.269983	-1.037971
H	5.383899	-0.336794	-0.866501
H	3.236854	-4.064346	-1.102805
H	5.342144	-2.771099	-1.381635
H	0.737847	1.462154	1.81302

6 -1394.6171369 (0)

N	2.760275	0.039313	-2.208004
O	2.166924	-0.967196	-2.93588
O	3.958226	0.203077	-2.39793
C	-5.371789	-2.114044	-1.137914
H	-4.169978	-0.46437	-1.829548
C	-4.53438	-3.3051	0.786863
H	-2.659065	-2.584603	1.598719
C	-5.507468	-3.135041	-0.195655
H	-6.13327	-1.973583	-1.906162
H	-4.639813	-4.09841	1.528398
H	-6.374847	-3.795608	-0.227303
H	4.288876	4.770228	-0.31343
C	3.812669	3.79179	-0.234097
C	3.78246	2.94037	-1.3417
C	3.227898	3.39701	0.966435
C	3.178365	1.690523	-1.246278
H	4.235395	3.255602	-2.283116
C	2.609279	2.148762	1.059883
H	3.24006	4.064542	1.828975
C	2.594334	1.287572	-0.0396
H	3.144636	1.017724	-2.105415
H	2.127216	1.846379	1.993304
P	1.795066	-0.3629	0.12208
O	1.28357	-0.646225	-1.445746
H	-0.307829	-0.609195	1.440967
C	3.286861	-1.438239	0.109518
C	4.265933	-1.269822	1.096063
C	3.422215	-2.462774	-0.830708
C	5.370869	-2.115006	1.138177
H	4.169549	-0.464799	1.8294
C	4.533296	-3.306047	-0.786537
H	2.658349	-2.585006	-1.598754
C	5.506312	-3.136188	0.196087
H	6.132302	-1.974694	1.9065
H	4.638548	-4.099502	-1.527945
H	6.373453	-3.797058	0.227948

TS7 -1394.5799363 (1)

N	3.086958	0.639177	-1.592557
O	2.619585	-0.07177	-2.520322
O	4.283244	0.681223	-1.359789
C	2.206989	1.359671	-0.793315
H	2.658486	1.778842	0.09884
C	0.853984	1.40393	-1.125887
H	0.610178	1.31284	-2.188338
C	-0.088571	2.206862	-0.303327
C	-1.218979	2.778687	-0.89858
C	0.089212	2.33272	1.081503
C	-2.152747	3.467663	-0.128509
H	-1.36894	2.672599	-1.975072
C	-0.848844	3.016485	1.851134
H	0.952944	1.868524	1.561842
C	-1.972669	3.585012	1.249631
H	-3.026979	3.911459	-0.606286
H	-0.702696	3.103366	2.928634
H	-2.705558	4.120847	1.853991
H	3.033755	-1.894687	3.939036

C	1.993047	0.754201	-1.414849
H	2.519371	1.530226	-0.866062
C	0.514364	0.549473	-1.312828
H	0.11694	0.266623	-2.301616
C	-0.228861	1.748348	-0.782801
C	-1.373151	2.200389	-1.448308
C	0.161332	2.38529	0.402036
C	-2.127574	3.25181	-0.933213
H	-1.681942	1.710551	-2.374194
C	-0.596027	3.435074	0.919764
H	1.05469	2.051005	0.934486
C	-1.745484	3.866933	0.258315
H	-3.017739	3.589975	-1.465305
H	-0.283374	3.918733	1.846267
H	-2.336098	4.688213	0.666194
H	2.778683	-0.170124	4.700574
C	2.262014	-0.33271	3.753696
C	0.88649	-0.118964	3.667392
C	2.975428	-0.767322	2.636815
C	0.221417	-0.324412	2.46023
H	0.325555	0.202584	4.545596
C	2.31612	-0.979963	1.428256
H	4.048334	-0.94888	2.706488
C	0.938012	-0.744221	1.335255
H	-0.856149	-0.167123	2.405339
H	2.860368	-1.34089	0.553477
P	0.206024	-0.996447	-0.308096
O	0.899859	-2.151315	-1.04558
C	-1.580841	-1.276891	-0.153703
C	-2.041423	-2.512331	-0.622648
C	-2.485296	-0.340626	0.370094
C	-3.400181	-2.815911	-0.558499
H	-1.320034	-3.21985	-1.034792
C	-3.841297	-0.652837	0.428449
H	-2.142599	0.633927	0.722857
C	-4.298029	-1.887978	-0.033475
H	-3.758217	-3.779474	-0.922452
H	-4.544986	0.075256	0.833179
H	-5.361746	-2.125499	0.01379
H	1.686231	-1.544364	-2.251096

TS8 **-**1394.5724154 (1)

N	-0.010981	1.353068	2.468227
O	-0.947424	0.510733	2.354574
O	-0.199817	2.481646	2.913194
C	1.208886	0.971136	1.967421
H	1.934802	1.76534	1.834305
C	1.288807	-0.333828	1.448033
H	0.799401	-1.11765	2.031322
C	2.506077	-0.747837	0.705427
C	2.950628	-2.075877	0.764802
C	3.182388	0.157432	-0.128522
C	4.064101	-2.484591	0.032049
H	2.418262	-2.789048	1.397664
C	2.427912	-1.704435	3.051999
C	1.069609	-1.410896	3.1864
C	3.009478	-1.760123	1.786765
C	0.292221	-1.164471	2.057865
H	0.612259	-1.378172	4.176199
C	2.237698	-1.51748	0.651953
H	4.069912	-1.988926	1.676606
C	0.873236	-1.225005	0.784924
H	-0.771296	-0.94182	2.167336
H	2.691583	-1.57953	-0.340511
P	-0.008565	-0.700356	-0.711036
O	0.546675	-1.658814	-1.920195
C	-1.742665	-1.200752	-0.531789
C	-2.231592	-2.322741	-1.209694
C	-2.606648	-0.402322	0.230624
C	-3.577518	-2.661714	-1.094669
H	-1.552521	-2.916602	-1.822885
C	-3.950082	-0.75437	0.344265
H	-2.234909	0.500995	0.724419
C	-4.434784	-1.882966	-0.316018
H	-3.960376	-3.539409	-1.617332
H	-4.621344	-0.135869	0.941099
H	-5.488548	-2.152137	-0.232016
H	1.316343	-1.178891	-2.32134

TS9 **-**1394.5287546 (1)

N	1.189471	-3.219947	-0.478379
O	1.283469	-3.312469	-1.667388
O	1.861873	-3.839034	0.358553
C	0.273628	-2.295879	0.279072
H	1.10467	-2.975078	1.258027
C	0.475962	-0.869632	-0.183885
H	0.176135	-0.806611	-1.247093
C	1.909168	-0.40759	-0.036042
C	2.70082	-0.207335	-1.169172
C	2.463011	-0.208688	1.235487
C	4.031194	0.189408	-1.039792
H	2.274454	-0.375664	-2.16114
C	3.791115	0.190318	1.360412
H	1.834878	-0.352889	2.117301
C	4.57806	0.389003	0.225676
H	4.641485	0.338936	-1.931518
H	4.215397	0.347189	2.352974
H	5.618858	0.698797	0.328318
H	-2.113816	0.128692	-1.911229
C	-2.766805	-0.282654	-1.13796
C	-2.346395	-0.33248	0.195495
C	-4.033907	-0.745378	-1.482843
P	-0.697515	0.215522	0.753815
C	-3.19687	-0.839331	1.181636
C	-4.882197	-1.254375	-0.497747
H	-4.363358	-0.705761	-2.521757
O	-0.570149	0.139661	2.260334
C	-0.414773	1.889486	0.098091

C	4.29293	-0.253475	-0.860844
H	2.817036	1.18311	-0.214644
C	4.738377	-1.573932	-0.780368
H	4.403869	-3.519032	0.094228
H	4.809389	0.459223	-1.50485
H	5.606543	-1.893297	-1.357927
H	-5.424772	-3.002342	-0.299962
C	-4.451013	-2.511436	-0.266663
C	-4.21038	-1.497582	0.659774
C	-3.44314	-2.901424	-1.146918
C	-2.968123	-0.868595	0.713336
H	-4.993016	-1.195594	1.356768
C	-2.198523	-2.277399	-1.109001
H	-3.624785	-3.694833	-1.873174
C	-1.963004	-1.251885	-0.18412
H	-2.77178	-0.098248	1.459096
H	-1.410747	-2.574646	-1.799846
P	-0.327655	-0.433583	-0.153885
O	0.408014	-1.230829	-1.418042
C	-0.53097	1.252624	-0.833337
C	-1.216115	2.253482	-0.131801
C	0.083378	1.553512	-2.056237
C	-1.290776	3.538914	-0.663599
H	-1.676475	2.045577	0.83532
C	0.001421	2.842596	-2.578739
H	0.608222	0.770192	-2.602911
C	-0.684789	3.836582	-1.88317
H	-1.819271	4.314734	-0.108989
H	0.47448	3.067384	-3.53571
H	-0.744996	4.846839	-2.290499
H	1.338384	-1.398335	-1.192469

TS10 -1394.5845755 (1)

N	-1.775951	3.162734	-0.618294
O	-2.699988	2.561138	-0.068248
O	-1.880656	4.288372	-1.060241
C	-0.524592	2.469619	-0.810617
H	0.264915	3.202606	-0.979895
C	-0.260341	1.402698	0.224813
H	-1.032149	1.423705	1.006771
C	1.113425	1.387632	0.841254
C	1.264668	1.107231	2.202136
C	2.260377	1.572063	0.058933
C	2.534452	0.998775	2.769576
H	0.376228	0.968539	2.823102
C	3.527785	1.461464	0.622767
H	2.160274	1.780444	-1.009036
C	3.669302	1.16919	1.980054
H	2.634751	0.783661	3.834368
H	4.411057	1.59892	-0.002492
H	4.662795	1.079991	2.421105
H	4.371932	-2.965446	-1.209692
C	3.4045	-2.471247	-1.109901
C	2.798474	-2.377543	0.145148
C	-4.465823	-1.300121	0.831561
H	-2.844344	-0.859119	2.214774
H	-5.875266	-1.613946	-0.770937
C	-0.482237	2.92929	1.028803
C	-0.132807	2.16684	-1.244057
H	-5.132608	-1.694383	1.599416
C	-0.293762	4.246207	0.612883
H	-0.671743	2.684821	2.075674
C	0.056273	3.483975	-1.654741
H	-0.038373	1.359969	-1.974267
C	-0.029012	4.523061	-0.727322
H	-0.34783	5.0581	1.339192
H	0.279975	3.7001	-2.700015
H	0.12182	5.553615	-1.051891
H	-0.753309	-2.669973	0.160292

7 -1394.6037613 (0)

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O	-0.296008	1.354425	3.483778
C	0.813435	-0.319505	2.38456
H	1.632458	-0.318817	3.09613
C	0.726034	-1.12716	1.140172
H	0.243675	-2.109135	1.301745
C	2.072261	-1.338697	0.485839
C	2.446644	-2.600243	0.010695
C	2.952122	-0.261232	0.31628
C	3.676812	-2.785056	-0.619238
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C	4.179575	-0.44578	-0.316115
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C	4.54567	-1.707725	-0.784311
H	3.957976	-3.775781	-0.978441
H	4.854358	0.401644	-0.442711
H	5.509116	-1.851377	-1.274739
H	-5.96208	-1.65584	-0.919256
C	-4.919906	-1.388136	-0.738933
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C	-3.277745	0.18268	0.083938
H	-5.397898	0.538643	0.109944
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H	-4.139862	-3.233143	-1.543804
C	-2.252006	-0.700598	-0.275673
H	-3.036723	1.132025	0.559543
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C	0.380322	1.600313	-1.909594
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H	-0.191598	2.471916	1.346675
C	0.810509	2.836876	-2.385448

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H	1.104458	-1.652955	1.262308
H	1.048186	-0.852133	-2.972537
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C	-1.698349	-2.592873	0.277191
C	-3.040837	-0.573307	0.459132
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H	-4.985695	-0.81898	1.341225
H	-4.705276	-3.261538	1.721815
H	-0.818654	1.517911	-1.914135
H	0.297616	0.757487	-2.592877
C	0.908793	3.92389	-1.52033
H	0.618548	4.618776	0.502712
H	1.06848	2.94688	-3.439499
H	1.253226	4.890647	-1.890482
H	0.933591	-1.162908	-1.454867

α,α',β-triphenyl {5,5}-bicyclic guanidine

-1053.02800 (0)

N	24.91486119	2.33323694	4.09077019
N	26.70336258	1.74610027	2.77371095
N	27.01188676	1.5047167	4.99718192
C	24.52652667	2.48531127	2.67780384
C	25.56533432	1.6155819	1.87373115
C	27.79625499	0.80340782	2.93194262
C	28.28524492	1.1830512	4.35052215
C	26.12221187	1.92090487	4.03229928
C	23.10210786	2.08390202	2.38875304
C	22.43193973	1.17657015	3.21257689
C	21.13658518	0.7669069	2.90045212
C	20.49897546	1.25776467	1.76135794
C	21.16020781	2.16915297	0.93889886
C	22.45318536	2.58287633	1.25435221
C	25.82317494	2.08484218	0.46706147
C	25.11245266	1.52825638	-0.60051431
C	25.30357148	1.9985781	-1.89887052
C	26.21439037	3.02523984	-2.14437814
C	26.93062211	3.58076233	-1.08415125
C	26.73400567	3.11545612	0.21397351
C	29.0581081	0.0826781	5.03606874
C	28.40318848	-0.9339669	5.7366924
C	29.13335361	-1.96742759	6.32038036
C	30.52281964	-1.99836981	6.20561554
C	31.18099876	-0.98713509	5.50761486
C	30.45066017	0.04995345	4.93041333
H	22.9358517	0.81543253	4.10978124
H	20.61799491	0.06376738	3.55444416
H	19.48481433	0.93686316	1.51890229
H	20.66437739	2.56542059	0.05141748
H	22.96913912	3.30357269	0.61497899
H	24.39757075	0.72494407	-0.40767844
H	24.74219327	1.5574995	-2.72371954
H	26.36899067	3.38991023	-3.16078172
H	27.64746731	4.38205832	-1.26956136
H	27.2903046	3.54260692	1.05001112
H	27.31621853	-0.89981594	5.82699151
H	28.61339501	-2.75258136	6.87103785
H	31.09343532	-2.80644522	6.66497023
H	32.26826999	-1.00005821	5.41921776
H	30.96861168	0.84816637	4.39297883
H	24.66647837	3.53803991	2.36906103
H	25.20324902	0.56737851	1.85925351
H	28.92952931	2.07713306	4.26682021
H	27.4448198	-0.24686073	2.9237217
H	28.57983881	0.93239174	2.17429055

H 27.00401944 1.97422534 5.89540344

Table S2. Comparison of calculated (M06-2X/cc-pVDZ) and experimental structural parameters of α,α',β-triphenyl {5,5}-bicyclic guanidine.

	X ray structure[a]	M06-2X/cc-pVDZ
Bond Length		
N1-C5	1.343	1.352
N2-C5	1.333	1.306
N4-C5	1.320	1.323
N2-C9	1.488	1.490
N4-C27	1.493	1.493
N1-C6	1.463	1.467
N1-C24	1.463	1.464
C6-C9	1.549	1.532
C24-C27	1.556	1.544
C9-C11	1.537	1.543
C27-C29	1.545	1.536
N4-C42	1.455	1.459
N2-H3	1.014	0.863
Mean Unsigned Error	0.018	
Bond angle		
N2-C5-N4	133.1	133.9
N1-C5-N2	112.9	113.0
N1-C5-N4	113.8	113.08409
C5-N2-C9	108.5	108.56169
C5-N4-C27	108.5	109.04936
C5-N1-C6	108.5	106.70473
C5-N1-C24	107.8	107.47518
N4-C27-C24	101.5	102.32127
N2-C9-C6	101.3	101.10669
N1-C6-C9	101.7	101.00483
N1-C24-C27	101.9	103.15196
N4-C27-C29	113.7	114.7016
N2-C9-C11	113.3	114.60247
C5-N4-C42	124.0	122.27774
C5-N2-H3	122.6	125.02154
Mean Unsigned Error	0.92	

[a] T. Isobe, K. Fukuda, K. Yamaguchi, H. Seki, T. Tokunaga, T. Ishikawa, *J. Org. Chem*. **2000**, *65*, 7779–7785.

Table S3. Morokuma-Kitaura energy decomposition analysis of reactants-catalyst intermolecular interaction in **TS2** transition states (HF/cc-pVDZ level)

TS2	***R*-TS2a**	***R*-TS2d**	***S*-TS2h**	***S*-TS2i**
Alignment	**A**	**B**	**A**	**B**
NO_2 hydrogen bonding	**cis**	**trans**	**bidentate**	**cis**
Electrostatic Energy	-211.1	-173.9	-180.0	-174.8
Exchange Repulsion Energy	257.5	232.8	229.5	213.4
Polarization Energy	-63.8	-55.9	-53.4	-51.6
Charge Transfer Energy	-103.8	-92.6	-98.7	-83.1
High Order Coupling Energy	16.9	11.3	10.4	7.0
KM Interaction Energy	-104.2	-78.5	-92.2	-89.1
Dispersion Interaction Energy	-91.9	-103.5	-86.9	-84.9
Total Interaction Energy,	-196.1	-181.9	-179.1	-174.0

Table S4. Morokuma-Kitaura energy decomposition analysis of phosphinic acid-catalyst intermolecular interaction in **TS2** transition states (HF/cc-pVDZ level)

TS2	***R*-TS2a**	***R*-TS2d**	***S*-TS2h**	***S*-TS2i**
Alignment	**A**	**B**	**A**	**B**
NO_2 hydrogen bonding	**cis**	**trans**	**bidentate**	**cis**
Electrostatic Energy	-131.4	-115.6	-145.2	104.3
Exchange Repulsion Energy	174.8	167.1	196.6	-144.9
Polarization Energy	-38.1	-33.9	-41.3	30.3
Charge Transfer Energy	-76.7	-68.0	-81.4	56.5
High Order Coupling Energy	18.0	14.5	17.9	-9.6
KM Interaction Energy	-53.4	-35.9	-53.3	-36.6
Dispersion Interaction Energy	-47.4	-61.8	-57.6	-49.8
Total Interaction Energy,	-100.8	-97.7	-111.0	-86.3

Table S5. Morokuma-Kitaura energy decomposition analysis of nitrostyrene-catalyst intermolecular interaction in **TS2** transition states (HF/cc-pVDZ level).

TS2	***R*-TS2a**	***R*-TS2d**	***S*-TS2h**	***S*-TS2i**
Alignment	**A**	**B**	**A**	**B**
NO_2 hydrogen bonding	**cis**	**trans**	**bidentate**	**cis**
Electrostatic Energy	-59.7	-44.8	-22.0	-51.8
Exchange Repulsion Energy	79.5	67.5	41.7	68.7
Polarization Energy	-13.3	-11.3	-6.5	-11.8
Charge Transfer Energy	-26.9	-24.4	-15.2	-26.1
High Order Coupling Energy	1.1	1.2	-2.7	0.0
KM Interaction Energy	-19.3	-11.8	-4.7	-21.0
Dispersion Interaction Energy	-40.3	-37.4	-21.6	-35.4
Total Interaction Energy,	-59.6	-49.3	-26.3	-56.4

Table S6. Calculated hydrogen bonding properties (M06-2X/cc-pVTZ) of various **TS2** transition states.

Hydrogen bonding interactions	X-H Bd length (X= H acceptor)	Y-H-X Bd Angle (Y-H= H donor)	AIMs ρ	AIMs ∇^2 ρ
***R*-TS2a**				
GuaN-H—O_2N	1.74	176	0.039	0.118
P-Ar-H- O_2N	2.78	91	0.009	0.036
Vinylic nitrostyrene C-H-Ngua	2.64	143	0.009	0.028
Aromatic nitrostyrene C-H-Ngua	2.64	154	0.008	0.024
tBu-CH- O2N	2.62	125	0.008	0.029
GuaN--H-O=P	1.53	177	0.081	
***R*-TS2b**				
GuaN-H—O_2N	1.86	138	0.029	0.123
Vinylic nitrostyrene C-H-Ngua	2.82	149	0.006	
tBu-CH- O_2N	2.47	150	0.010	0.035
tBu-CH- O_2N	2.67	144	0.007	0.022
tBu-CH- O_2N	2.62	153	0.007	0.025
GuaN--H-O=P	1.49	177	0.090	
***R*-TS2c**				
GuaN-H—O_2N	1.87	162	0.030	0.099
P-Ar-H- Gua-N	2.52	146	0.010	0.034
Gua-α CH- O_2N	2.57	121	0.008	0.030
tBu-CH- O_2N	2.69	133	0.007	0.021
GuaN--H-O=P	1.42	167	0.106	
***R*-TS2d**				
GuaN-H—O_2N	1.82	162	0.035	0.106
P-Ar-H- O_2N	2.23	146	0.014	0.056
tBu-CH- O_2N	2.64	120	0.008	0.027
GuaN--H-O=P	1.55	166	0.078	
***R*-TS2e**				
Vinylic nitrostyrene C-H-Ngua	2.71	133	0.018	0.070
tBu-CH- O_2N	2.25	144	0.031	0.103
tBu-CH- O_2N	2.34	146	0.009	0.033
GuaN--H-O=P	1.53	167	0.006	0.021
			0.005	0.016
***R*-TS2f**				
GuaN-H—O_2N	2.55	123		

P-OH- O_2N	1.82	159		
Gua-α-CH- O_2N	2.49	122	0.007	0.023
tBu-CH- O_2N	2.8	112	0.013	0.055
tBu-CH- O_2N	2.83	136	0.010	0.044
			0.081	0.033
***S*-TS2g**				
GuaN-H—O_2N	1.94	146		
P-Ar-H- O_2N	2.28	149	0.023	0.099
tBu-CH- O_2N	2.7	148	0.014	0.051
tBu-CH- O_2N	2.51	153	0.007	0.021
tBu-CH- O_2N	2.55	130	0.010	0.032
tBu-CH- O_2N	2.71	131	0.009	0.030
GuaN--H-O=P	1.5	175	0.006	0.021
			0.088	
***S*-TS2h**				
GuaN-H—O_2N	2.02	137		
GuaN-H—O_2N	2.13	160	0.022	0.091
Aromatic POH C-H-Ngua	3.06	98	0.017	0.067
P=O-H - O_2N	2.6	105	0.006	0.018
tBu CH-O=P	2.27	149	0.008	0.034
GuaN--H-O=P	1.51	165	0.013	0.054
			0.085	0.020
***S*-TS2i**				
GuaN-H—O_2N	1.77	150		
Vinylic nitrostyrene C-H-Ngua	2.67	150	0.037	0.125
P-Ar-H- O_2N	2.43	117	0.008	0.023
GuaN--H-O=P	1.59	170	0.011	0.044
			0.071	
***S*-TS2j**				
GuaN-H—O_2N	1.82	168		
Vinylic nitrostyrene C-H-Ngua	2.86	122	0.035	0.103
Aromatic nitrostyrene C-H-Ngua	2.53	152	0.006	0.020
P-Ar-H- O_2N	2.1	156	0.010	0.032
tBu-CH- O_2N	2.32	133	0.018	0.073
tBu-CH- O=P	2.25	141	0.013	0.050
tBu-CH- O=P	2.3	142	0.014	0.058
GuaN--H-O=P	1.62	161	0.013	0.050
			0.066	
***S*-TS2k**				
GuaN-H—O_2N				
Aromatic nitrostyrene C-H-Ngua	2.75	139	0.007	0.022

P-Ar-H- O_2N	2.03	156	0.022	0.086
tBu-CH- O_2N	2.6	116	0.008	0.030
tBu-CH- O_2N	2.51	139	0.009	0.031
GuaN--H-O=P	1.5	165	0.088	0.025
***S*-TS2l**				
GuaN-H—O_2N	2.04	160	0.020	0.075
P-OH- O_2N	1.82	159	0.029	0.100
Gua-α-CH- O_2N	2.58	122	0.009	0.032
tBu-CH- O_2N	2.86	129	0.005	0.017

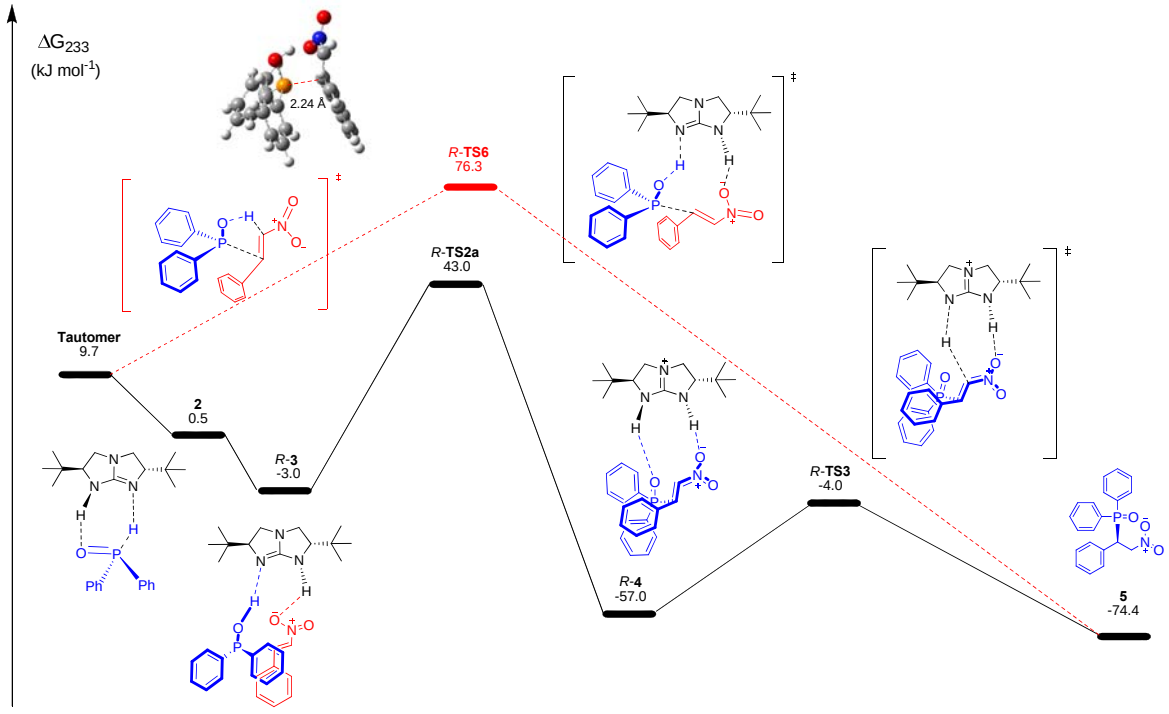

Figure S1. Concerted transition state (*R*-**TS6**) of uncatalyzed-phospha-Michael reaction.

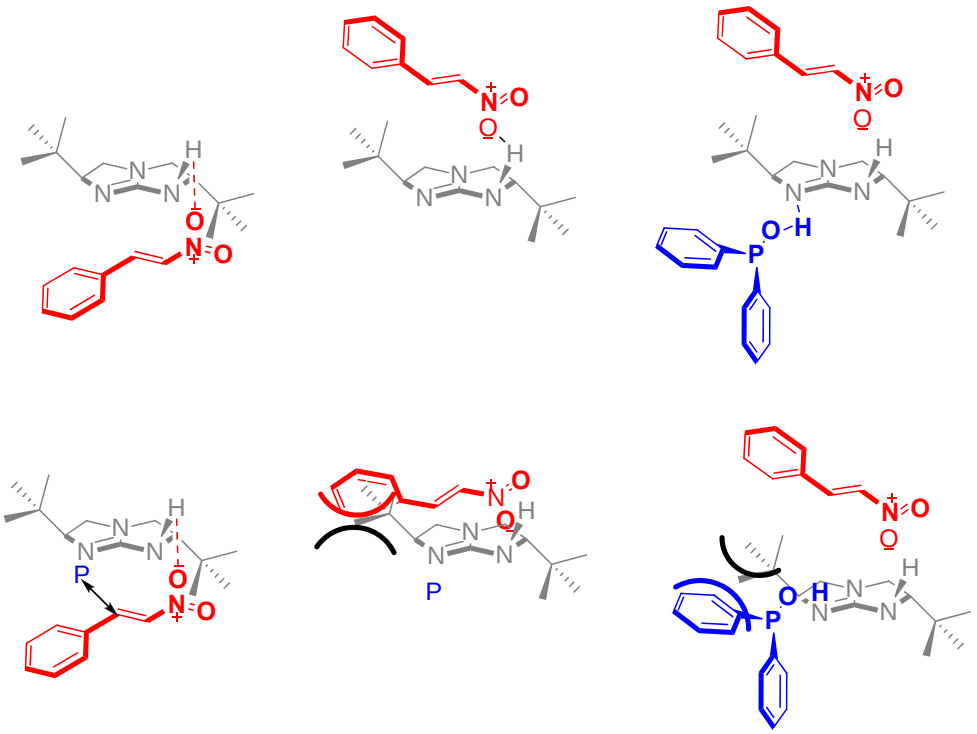

Figure S2. Steric constraints of transition state **TS2** with alignment B. Phosphinic acid represented by P atom.

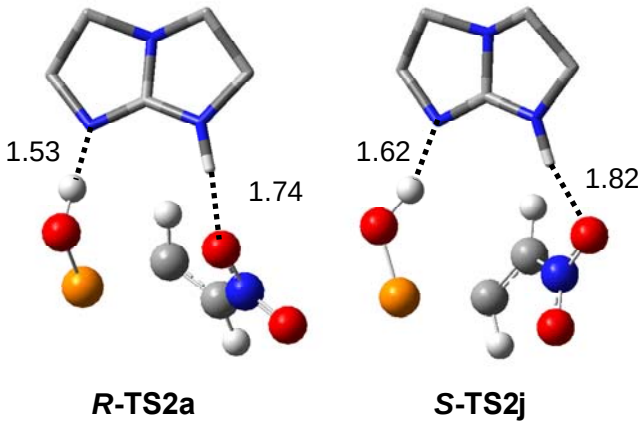

Figure S3. Comparison of s-*cis* (*R*-**TS2a**) and s-*trans* (*S*-**TS2j**) nitrostyrene hydrogen bonding in transition states **TS2**. Hydrogen bonding is represented by dotted line while bond distance is given by dashed line. The aromatic and t-butyl groups are removed for clarity. e.

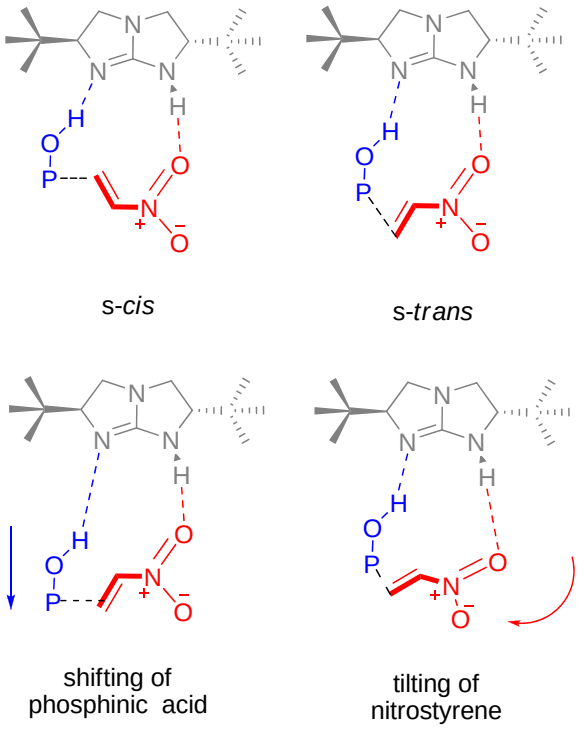

Figure S4. The accessibility of β carbon in s-*cis* and s-*trans* hydrogen bonding of nitrostyrene and the compromise of hydrogen bonding due to s-*trans* hydrogen bonded nitrostyrene.

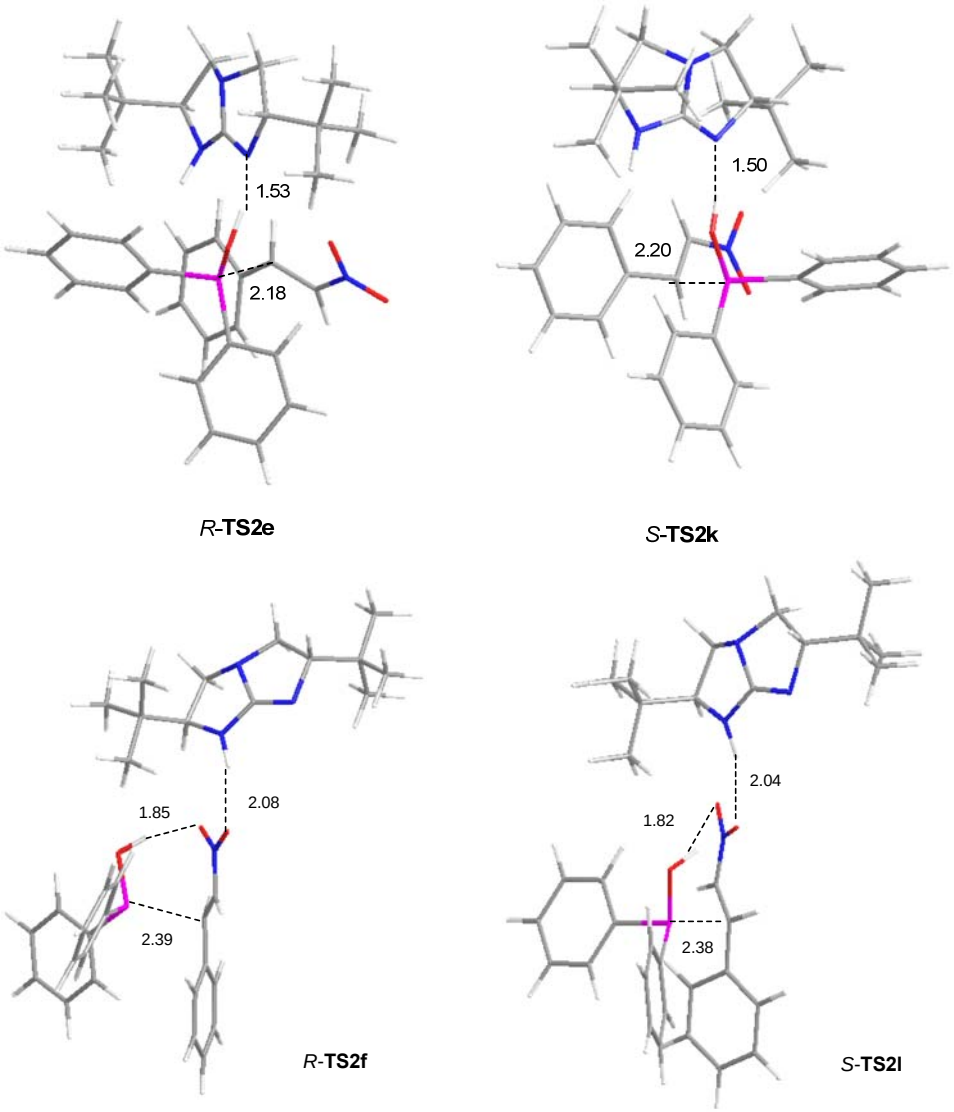

Figure S5. **TS2** transition states with monodentate hydrogen bond.