

Supporting Information

for

The Intramolecular Diels–Alder Reaction of Tryptamine-Derived Zincke Aldehydes is a Stepwise Process

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2025

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*For experimental procedures corresponding to the computational experiments
described herein, please see reference 7 from the text of the main paper.*

Complete Citation for Gaussian 09

All calculations were conducted using the Gaussian 09 package. The complete citation is as follows:

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

List of Different Bases Surveyed for the Anionic Cycloaddition

KOt-Bu*, THF, 80 °C, sealed tube	optimum conditions
KOt-Bu, THF, 50 °C,	partial conversion to product
KOt-Bu, 18-c-6, THF, up to 50 °C	no reaction
KOt-Bu, DMSO, THF, up to 50 °C	no reaction
KOt-Bu, PhH, up to 60 °C	no reaction
KH, THF, up to 50 °C	minimal conversion to product
KH, 18-c-6, THF, up to 50 °C	trace conversion to product
KHMDS, THF, up to 60 °C	minimal conversion to product
NaOt-Bu, THF, up to 50 °C,	no reaction
NaH, THF, up to 50 °C	no reaction
NaHMDS, THF, up to 50 °C	no reaction
MeLi, THF, up to 50 °C	partial decomposition, no product
LiOt-Bu, THF, 80 °C, sealed tube	no reaction
EtMgBr, THF, up to 80 °C (microwave)	no reaction
K ₂ CO ₃ , Cs ₂ CO ₃ , K ₃ PO ₄ , CaH ₂ , or Na ₂ CO ₃ , THF, 65 °C	no reaction
K ₂ CO ₃ , DMF, up to 80 °C	no reaction
DBU, THF, 65 °C	no reaction
P ₂ Et and P ₄ <i>t</i> -Bu phosphazene bases, THF or MeCN, 60 °C	no reaction

*in all cases for KOt-Bu, a commercially available 1 M solution in THF (Sigma–Aldrich) was used. Solid base did not dissolve readily in THF and led to poor results.

Reaction Coordinate Diagram for the IMDA Reaction with Li⁺ counterion

In addition to using a potassium cation as a counterion, Li⁺ was also studied computationally to determine why lithiated bases did not effect the IMDA reaction. The reaction coordinate diagram for Li⁺ is shown below. M06-2X/6-311+G** single point calculations were conducted on B3LYP/6-31G* optimized geometries. Solvent-corrected energies using CPCM for THF are shown in parentheses. The reaction profile is similar to that for the potassiated starting material, and product **8L** is 2.6 kcal/mol lower in energy than the starting material **5L**. These results suggest that the reaction is both kinetically and thermodynamically feasible, although laboratory experiments of this type have never succeeded.

QuickTime™ and a
decompressor
are needed to see this picture.

B3LYP/6-31G(d) Gas-Phase Geometries and M06-2x/6-311+G(d,p) Total Energies
(Hartrees)

5

C	-5.295924	1.190226	0.193969
C	-4.420894	0.124812	-0.082631
C	-3.003278	0.383100	-0.233574
C	-2.517202	1.699067	-0.104012
C	-3.406399	2.734825	0.170581
C	-4.788790	2.480709	0.320656
C	-2.429148	-0.894171	-0.510422
C	-3.522768	-1.778683	-0.493498
N	-4.721453	-1.203287	-0.246222
C	-0.984689	-1.234512	-0.689868
C	-0.222513	-1.206469	0.656540
N	1.213036	-1.527537	0.562522
C	2.135675	-0.554111	0.435792
C	3.473975	-0.697048	0.143238
C	4.347982	0.421894	0.099916
C	5.691267	0.410424	-0.161268
C	1.587359	-2.911503	0.327051
C	6.464883	1.627921	-0.172712
O	7.671078	1.720717	-0.389369
H	-6.361277	0.992148	0.305612
H	-1.453912	1.916886	-0.224889
H	-3.034561	3.754314	0.270028
H	-5.463460	3.308924	0.535953
H	-3.461799	-2.854669	-0.671140
H	-0.881841	-2.236808	-1.132718
H	-0.469953	-0.538674	-1.373602
H	-0.314149	-0.212372	1.104087
H	-0.685172	-1.917036	1.350201
H	1.743565	0.446808	0.608698
H	3.890194	-1.680176	-0.059812
H	3.893723	1.396945	0.298109
H	0.741146	-3.555158	0.575305
H	1.867225	-3.090051	-0.720884
H	2.439108	-3.187937	0.960803
H	5.865406	2.547566	0.042642
H	6.218820	-0.519574	-0.366088

G(B3LYP/6-31G(d)) = -804.426331

G(M06-2X/6-311+G(d,p)) = -804.3061272

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3786408

0 imaginary frequencies

TS_5-6

C	-2.072791	-2.819648	-0.062883
C	-1.294358	-1.791360	0.472654
C	-1.642993	-0.420088	0.282811
C	-2.815444	-0.111866	-0.418579
C	-3.601598	-1.145445	-0.937858
C	-3.229799	-2.488713	-0.770398
C	-0.584431	0.358726	0.950447
C	0.226154	-0.705829	1.539946
N	-0.140245	-1.933641	1.247385
C	-0.883694	1.656602	1.678805
C	-1.162616	2.737769	0.620944
N	-0.264964	2.499824	-0.510689
C	0.588370	1.342588	-0.347437
C	1.893329	1.631296	0.164358
C	3.011134	0.798524	0.104505
C	3.154700	-0.500441	-0.376350
C	4.441657	-1.116354	-0.414633
O	4.740447	-2.239531	-0.842389
C	-0.857961	2.662976	-1.823675
H	-1.774664	-3.854291	0.088042
H	-3.132910	0.917702	-0.563150
H	-4.513261	-0.902936	-1.481102
H	-3.851941	-3.276457	-1.191290
H	1.126332	-0.522572	2.121257
H	-1.733083	1.574022	2.370812
H	-0.003168	1.934422	2.270981
H	-2.213403	2.675361	0.293805
H	-1.028399	3.748870	1.039019
H	0.540263	0.631975	-1.175893
H	2.007314	2.605619	0.634880
H	3.936542	1.247467	0.481231
H	2.304488	-1.077448	-0.731781
H	5.254511	-0.460078	0.003025
H	-1.328237	3.652946	-1.891855
H	-0.073564	2.621159	-2.587280
H	-1.621881	1.904790	-2.074413

G(B3LYP/6-31G(d)) = -804.374724

G(M06-2X/6-311+G(d,p)) = -804.2606726

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3304289

1 imaginary frequency

6

C	-3.413651	-1.586010	0.758549
C	-2.576227	-0.476128	0.708639
C	-1.679689	-0.278056	-0.358845

C	-1.608392	-1.203338	-1.390311
C	-2.447399	-2.326718	-1.347678
C	-3.339604	-2.513853	-0.287043
C	-0.947028	1.009910	-0.089233
C	-1.602871	1.387116	1.221604
N	-2.504945	0.576571	1.663954
C	0.626033	0.917703	0.038919
C	1.174163	0.186598	1.207539
C	2.198626	-0.733020	1.141074
C	2.980799	-1.204197	0.064135
N	0.946713	2.378350	-0.025839
C	0.223868	2.889878	-1.178846
C	-1.126005	2.130990	-1.163794
C	3.977153	-2.187339	0.250881
O	4.742409	-2.696912	-0.593246
C	2.364032	2.679414	-0.041670
H	-4.096835	-1.720682	1.592686
H	-0.906512	-1.075638	-2.211177
H	-2.395991	-3.065044	-2.144323
H	-3.978661	-3.394055	-0.271702
H	0.726874	0.402971	2.176288
H	2.460590	-1.190784	2.102264
H	2.844535	-0.819079	-0.946187
H	-1.330851	2.287565	1.768147
H	0.981264	0.427549	-0.889447
H	0.759911	2.679570	-2.128628
H	0.103529	3.980522	-1.116130
H	-1.334867	1.680857	-2.139172
H	-1.971423	2.785574	-0.924992
H	4.060185	-2.524730	1.324150
H	2.516805	3.763480	0.053437
H	2.839691	2.171761	0.801219
H	2.867258	2.343303	-0.970784

G(B3LYP/6-31G(d)) = -804.389652

G(M06-2X/6-311+G(d,p)) = -804.2837544

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3583501

0 imaginary frequencies

TS_6-7

C	3.396725	-1.261549	-0.057874
C	2.044759	-0.976923	-0.321638
C	1.582399	0.361625	-0.198802
C	2.437190	1.383886	0.172465
C	3.792437	1.096580	0.429799
C	4.252065	-0.219517	0.313363
C	0.100569	0.344689	-0.515760
C	-0.079886	-1.173567	-0.810301

N	1.077982	-1.853476	-0.764030
C	-0.748892	0.998611	0.644486
C	-0.951629	0.167231	1.878280
C	-1.152531	-1.168883	1.869204
C	-1.463344	-1.932004	0.674258
N	-1.953882	1.482628	-0.058578
C	-1.436054	2.150093	-1.242791
C	-0.340718	1.198393	-1.759108
C	-2.706944	-1.717430	-0.021192
O	-3.140962	-2.411975	-0.952502
C	-2.820076	2.309837	0.750593
H	3.758989	-2.282672	-0.150048
H	2.074926	2.408205	0.265023
H	4.475255	1.894139	0.715211
H	5.300329	-0.438623	0.516265
H	-0.745155	0.664876	2.825415
H	-1.034964	-1.704147	2.818378
H	-1.102835	-2.958716	0.628602
H	-0.817427	-1.482300	-1.548821
H	-0.168970	1.892588	0.965347
H	-0.995316	3.139798	-0.988662
H	-2.237913	2.327529	-1.971292
H	0.504408	1.745987	-2.187037
H	-0.740975	0.545168	-2.540386
H	-3.267352	-0.810855	0.296140
H	-3.699635	2.610370	0.167130
H	-3.158858	1.738758	1.620913
H	-2.321923	3.235202	1.116190

G(B3LYP/6-31G(d)) = -804.361063

G(M06-2X/6-311+G(d,p)) = -804.2553887

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3259343

1 imaginary frequency

7

C	-2.459359	-2.365388	0.154440
C	-1.290534	-1.583491	0.396510
C	-1.306726	-0.220478	-0.076836
C	-2.382452	0.301274	-0.772400
C	-3.515788	-0.497719	-1.027630
C	-3.531293	-1.815622	-0.543131
H	-2.489093	-3.395545	0.504599
H	-2.363019	1.332553	-1.129949
H	-4.361871	-0.097893	-1.582314
H	-4.409459	-2.436736	-0.729562
C	-0.035781	0.420253	0.458388
C	0.776600	-0.878786	0.802026
N	-0.160311	-1.966022	1.009586

C	0.649131	1.474976	-0.482911
C	2.102914	1.191038	-0.777019
H	2.730856	2.052767	-1.006402
C	2.613034	-0.043420	-0.770162
H	3.666687	-0.224652	-0.974802
C	1.758530	-1.218843	-0.403781
H	1.066732	-1.480251	-1.223065
H	1.415517	-0.702409	1.680440
H	0.090784	1.488103	-1.437691
N	0.504607	2.793149	0.191132
C	-0.556659	2.666573	1.188486
H	-1.567773	2.749643	0.742798
H	-0.463556	3.458798	1.945579
C	-0.334759	1.262609	1.736476
H	-1.189793	0.868381	2.291452
H	0.543070	1.265715	2.396519
C	2.533981	-2.466315	-0.090327
H	1.898461	-3.286443	0.298169
O	3.741606	-2.606928	-0.221579
C	0.341235	3.908155	-0.713940
H	0.305762	4.847909	-0.146870
H	1.193733	3.967803	-1.401756
H	-0.582412	3.848901	-1.328688

G(B3LYP/6-31G(d)) = -804.379609

G(M06-2X/6-311+G(d,p)) = -804.282635

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3503325

0 imaginary frequencies

8

C	-2.567514	-2.298229	-0.568628
C	-1.403322	-1.626173	-0.181522
C	-1.470922	-0.306512	0.315463
C	-2.698950	0.328867	0.442351
C	-3.873643	-0.347845	0.074237
C	-3.798837	-1.644592	-0.439075
C	-0.056773	0.230776	0.477987
C	0.776808	-1.091500	0.514507
N	-0.095685	-2.114804	-0.170114
C	0.247173	1.201937	-0.722556
C	1.686019	1.154744	-1.163632
C	2.513771	0.127481	-0.828989
C	2.173821	-0.988796	-0.008472
N	-0.220464	2.497403	-0.145810
C	0.347147	2.563495	1.196801
C	0.202806	1.122585	1.726009
C	3.146576	-1.941688	0.374709
O	4.345211	-2.019087	0.026933

C	0.009461	3.675724	-0.951860
H	-2.513730	-3.315591	-0.950015
H	-2.739690	1.359242	0.786161
H	-4.839191	0.143200	0.176023
H	-4.710437	-2.163088	-0.732375
H	2.038300	1.947156	-1.822541
H	3.543804	0.132500	-1.187518
H	0.791121	-1.418778	1.568000
H	-0.434683	0.983275	-1.561482
H	-0.197327	3.305160	1.799387
H	1.411811	2.863205	1.184605
H	-0.620556	1.033600	2.443690
H	1.120093	0.799953	2.229614
H	2.746194	-2.717113	1.086142
H	1.078779	3.931551	-1.083488
H	-0.429586	3.534347	-1.947568
H	-0.483774	4.541367	-0.487055
H	0.288504	-2.447133	-1.049553

G(B3LYP/6-31G(d)) = -804.399206

G(M06-2X/6-311+G(d,p)) = -804.3024628

G(M06-2X/6-311+G(d,p),CPCM/THF) = -804.3725469

0 imaginary frequencies

5K

C	-1.079438	2.634625	-0.487553
C	-0.349984	1.854206	0.432663
C	1.028252	1.526050	0.164064
C	1.624262	1.972892	-1.029723
C	0.877749	2.718770	-1.936041
C	-0.466967	3.051268	-1.666310
C	1.463853	0.771322	1.297948
C	0.341347	0.698753	2.127930
N	-0.766614	1.327905	1.634603
C	1.634166	-1.936148	-0.805920
C	0.450792	-2.138684	-0.128592
C	-0.766320	-2.320338	-0.809615
C	-2.003453	-2.273007	-0.199205
N	2.824803	-1.588238	-0.289737
C	3.017024	-1.302163	1.137368
C	2.825144	0.185515	1.537792
C	-3.224307	-2.129934	-0.924196
O	-4.285165	-1.695438	-0.436422
C	3.964245	-1.326843	-1.158922
H	-2.090107	2.978882	-0.251224
H	2.670027	1.753156	-1.245528
H	1.338762	3.068859	-2.856908
H	-1.020468	3.662460	-2.375641

H	0.402049	-1.962559	0.939391
H	-0.737147	-2.410765	-1.898130
H	-2.051285	-2.178244	0.886566
H	0.292477	0.207633	3.098718
H	1.636392	-2.054117	-1.888022
H	4.036364	-1.622833	1.389180
H	2.334119	-1.936348	1.707483
H	3.591018	0.783267	1.023871
H	3.083665	0.232427	2.605922
H	-3.183281	-2.372591	-2.007721
H	4.819512	-1.946293	-0.861965
H	3.704299	-1.559192	-2.193674
H	4.263481	-0.273573	-1.106438
K	-3.117582	0.478840	0.726385

G(B3LYP/6-31G(d)) = -1404.335443

G(M06-2X/6-311+G(d,p)) = -1404.231432

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1404.262572

0 imaginary frequencies

TS_5-6K

C	0.791912	3.157542	-0.168409
C	0.592108	1.880345	0.359789
C	1.605880	0.885084	0.302450
C	2.851860	1.215716	-0.241535
C	3.055473	2.497791	-0.757271
C	2.031685	3.457402	-0.733259
C	1.034469	-0.322516	0.926911
C	-0.254595	0.166150	1.382138
N	-0.549440	1.404219	1.023477
C	0.610151	-1.757832	-0.430405
C	-0.413987	-2.645196	0.081945
C	-1.769697	-2.434845	-0.027255
C	-2.439581	-1.314338	-0.567400
N	1.917173	-2.292883	-0.519853
C	2.664362	-2.209889	0.739383
C	1.872523	-1.308464	1.721287
C	-3.837002	-1.173937	-0.541282
O	-4.495390	-0.149377	-0.885336
C	2.660766	-2.020593	-1.742531
H	0.008630	3.910827	-0.106181
H	3.666774	0.497160	-0.257908
H	4.023399	2.757959	-1.177777
H	2.214153	4.448446	-1.140579
H	-0.061267	-3.552567	0.564525
H	-2.414951	-3.220960	0.371517
H	-1.855584	-0.516743	-1.027567
H	-0.977874	-0.447618	1.910568

H	0.327373	-1.152335	-1.293276
H	3.655794	-1.784119	0.533846
H	2.834272	-3.201463	1.181657
H	2.561360	-0.804053	2.409615
H	1.201676	-1.924776	2.329432
H	-4.397989	-2.045629	-0.139533
H	3.566871	-2.635529	-1.753206
H	2.057989	-2.314946	-2.607063
H	2.953328	-0.966664	-1.865258
K	-3.121733	1.680745	0.199851

G(B3LYP/6-31G(d)) = -1404.298962

G(M06-2X/6-311+G(d,p)) = -1404.199414

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1404.226853

1 imaginary frequency

6K

C	-1.215493	2.897573	0.159008
C	-0.496589	1.787991	0.594763
C	0.701249	1.382482	-0.024962
C	1.178242	2.091989	-1.121118
C	0.455142	3.205021	-1.577216
C	-0.723445	3.607753	-0.943961
C	1.210030	0.174280	0.736363
C	0.071080	0.012362	1.713756
N	-0.859399	0.910980	1.658504
C	1.556310	-1.109120	-0.165064
C	0.930727	-2.421038	0.229675
C	-0.353812	-2.783147	-0.021397
C	-1.394239	-2.011821	-0.635161
N	3.030949	-1.215081	-0.085016
C	3.595803	0.020630	0.421884
C	2.565700	0.451732	1.462296
C	-2.710296	-2.465858	-0.744306
O	-3.723683	-1.792666	-1.122930
C	3.655245	-1.750086	-1.278021
H	-2.114611	3.221111	0.680293
H	2.088897	1.794197	-1.632373
H	0.819483	3.762073	-2.435836
H	-1.260837	4.479211	-1.307502
H	1.595413	-3.101240	0.755696
H	-0.657180	-3.775263	0.323079
H	0.027701	-0.801369	2.431899
H	1.240576	-0.839611	-1.188837
H	3.719889	0.805278	-0.352892
H	4.586765	-0.157646	0.858898
H	2.661149	1.493802	1.779192
H	2.647761	-0.193913	2.343306

H	-2.879951	-3.513910	-0.409125
H	4.717953	-1.941030	-1.088302
H	3.179241	-2.699548	-1.541486
H	3.579925	-1.073207	-2.153366
K	-3.282467	0.079152	0.480703
H	-1.150598	-1.037266	-1.066210

G(B3LYP/6-31G(d)) = -1404.298962

G(M06-2X/6-311+G(d,p)) = -1404.199414

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1404.226853

0 imaginary frequencies

TS_6-7K

C	-3.372525	-0.312345	-0.012555
C	-1.992784	-0.222620	-0.231778
C	-1.174589	-1.364535	-0.042232
C	-1.718682	-2.571514	0.365939
C	-3.101700	-2.656559	0.596963
C	-3.912343	-1.534697	0.401769
C	0.229453	-0.967213	-0.434840
C	0.041114	0.555855	-0.528618
N	-1.269234	0.891334	-0.655513
C	1.435458	-1.470312	0.397972
C	1.550046	-0.964057	1.808222
C	1.168423	0.253437	2.211621
C	0.694772	1.333877	1.320812
N	2.561232	-1.111424	-0.484631
C	2.183829	-1.591719	-1.818020
C	0.639740	-1.497504	-1.854640
C	1.610536	2.290736	0.793031
O	1.290493	3.400964	0.294489
C	3.865361	-1.569431	-0.047094
H	-4.011527	0.555368	-0.164243
H	-1.089287	-3.448276	0.508699
H	-3.540676	-3.595284	0.923745
H	-4.983062	-1.610992	0.578590
H	1.893511	-1.681400	2.551850
H	1.180831	0.462984	3.285228
H	-0.260443	1.766435	1.630910
H	0.759637	1.108015	-1.130134
H	1.343931	-2.576883	0.460590
H	2.500467	-2.640699	-1.974951
H	2.677805	-0.986927	-2.588641
H	0.195459	-2.485283	-2.008912
H	0.264379	-0.846300	-2.649334
H	2.666786	1.966895	0.727128
H	4.630507	-1.221681	-0.750717
H	4.093583	-1.151317	0.938030

H	3.939348	-2.674573	0.015322
K	-1.079255	3.532865	-0.646704

G(B3LYP/6-31G(d)) = -1404.28135

G(M06-2X/6-311+G(d,p)) = -1404.189495

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1404.21813

1 imaginary frequency

7K

C	-1.850917	2.333704	0.244893
C	-1.037842	1.182545	0.428393
C	0.298315	1.221133	-0.086572
C	0.758549	2.295973	-0.822379
C	-0.081654	3.405845	-1.052339
C	-1.359522	3.418876	-0.493214
C	0.987461	-0.022995	0.446294
C	-0.271142	-0.890353	0.800714
N	-1.376561	0.012414	1.028505
C	2.079542	-0.648413	-0.487718
C	1.888628	-2.123130	-0.731793
C	0.687467	-2.704348	-0.722984
C	-0.558272	-1.906618	-0.438126
N	3.381339	-0.403416	0.173582
C	3.190935	0.637343	1.181617
C	1.806329	0.318327	1.730136
C	-1.719647	-2.771402	-0.112974
O	-2.898971	-2.488875	-0.314824
C	4.484059	-0.171675	-0.736756
H	-2.811189	2.425234	0.758876
H	1.772577	2.302059	-1.219318
H	0.276311	4.252707	-1.630389
H	-1.992162	4.295330	-0.624934
H	2.786610	-2.708295	-0.921144
H	0.595910	-3.775919	-0.897362
H	-0.825592	-1.248986	-1.277711
H	-0.067580	-1.529175	1.667820
H	2.042714	-0.123055	-1.460280
H	3.211739	1.657114	0.750405
H	3.983157	0.583632	1.939168
H	1.358173	1.137618	2.297546
H	1.866152	-0.566002	2.376482
H	-1.478523	-3.731614	0.391246
H	5.415846	-0.067643	-0.168956
H	4.603000	-1.023936	-1.415905
H	4.358254	0.739786	-1.356387
K	-3.776359	-0.074721	0.000615

G(B3LYP/6-31G(d)) = -1404.296142

G(M06-2X/6-311+G(d,p)) = -1404.211389
G(M06-2X/6-311+G(d,p),CPCM/THF) = -1404.240008

0 imaginary frequencies

8K

C	-0.767657	3.028125	-0.795816
C	-0.493680	1.707203	-0.451282
C	0.694989	1.352159	0.201684
C	1.630561	2.334338	0.514059
C	1.363465	3.667729	0.176905
C	0.177917	4.010661	-0.477689
C	0.755646	-0.155484	0.368147
C	-0.741461	-0.538410	0.181620
N	-1.348735	0.571688	-0.671760
C	1.744466	-0.764166	-0.683683
C	1.333128	-2.151277	-1.119633
C	0.081242	-2.632129	-0.946677
C	-1.006020	-1.919948	-0.325154
N	3.020352	-0.670876	0.062424
C	2.747874	-1.197064	1.397922
C	1.336454	-0.662387	1.720977
C	-2.244596	-2.517009	-0.118323
C	4.196085	-1.219100	-0.583190
H	-1.690900	3.289915	-1.309481
H	2.567350	2.059661	0.989393
H	2.087384	4.440767	0.421094
H	-0.016707	5.047921	-0.738449
H	2.081268	-2.760491	-1.621321
H	-0.144577	-3.641282	-1.297021
H	-1.220711	-0.415360	1.168103
H	1.839942	-0.099400	-1.557462
H	3.514244	-0.847405	2.101551
H	2.755347	-2.301991	1.421925
H	1.363863	0.148358	2.456530
H	0.702625	-1.456691	2.128543
H	4.179517	-2.319477	-0.692647
H	4.309338	-0.778227	-1.580513
H	5.086611	-0.958312	0.002404
H	-1.302059	0.271096	-1.648636
K	-3.901657	0.343209	0.349161
H	-2.333280	-3.562957	-0.477716
O	-3.274945	-2.000279	0.438225

G(B3LYP/6-31G(d)) =
G(M06-2X/6-311+G(d,p)) =
G(M06-2X/6-311+G(d,p),CPCM/THF) =

0 imaginary frequencies

5aM

C	-5.683618	1.128574	0.155420
C	-4.784491	0.077868	-0.099280
C	-3.371047	0.363041	-0.240763
C	-2.913121	1.690227	-0.123624
C	-3.825810	2.710992	0.129244
C	-5.204152	2.430705	0.269860
C	-2.768635	-0.905655	-0.496191
C	-3.844300	-1.811914	-0.477942
N	-5.056582	-1.258038	-0.248460
C	-1.316309	-1.219297	-0.660175
C	-0.565454	-1.165596	0.691881
N	0.876328	-1.460751	0.610883
C	1.782753	-0.471686	0.487107
C	3.125415	-0.593738	0.201444
C	3.979817	0.540768	0.161849
C	5.327735	0.558925	-0.097009
C	1.276951	-2.838592	0.383545
C	6.000402	1.843474	-0.082550
O	7.196982	2.042209	-0.286467
H	-6.745714	0.910067	0.259818
H	-1.853355	1.928283	-0.237100
H	-3.475620	3.739023	0.218938
H	-5.897509	3.247681	0.468049
H	-3.759918	-2.888567	-0.641458
H	-1.190750	-2.223122	-1.093711
H	-0.809444	-0.519515	-1.345690
H	-0.678776	-0.169498	1.129938
H	-1.020398	-1.878736	1.388069
H	1.372494	0.522724	0.655689
H	3.551342	-1.571996	0.001198
H	3.507352	1.506300	0.360868
H	0.440783	-3.496439	0.628595
H	1.567316	-3.016159	-0.661756
H	2.129483	-3.096704	1.024002
H	5.327187	2.705692	0.140684
C	6.141470	-0.675239	-0.391663
H	6.106485	-1.398593	0.434783
H	5.785425	-1.196922	-1.290690
H	7.183899	-0.386797	-0.552360

G(B3LYP/6-31G(d)) = -843.719037

G(M06-2X/6-311+G(d,p), CPCM/THF) = -843.6605785

0 imaginary frequencies

TS_5-6aM

C	0.084353	3.242979	0.820794
C	0.821001	2.062039	0.900240
C	1.186004	1.346269	-0.273880
C	0.811048	1.830050	-1.528396
C	0.083519	3.023700	-1.604255
C	-0.280080	3.719765	-0.441794
C	1.881109	0.143152	0.190881
C	1.982943	0.401999	1.624052
N	1.328574	1.449590	2.059788
C	3.022224	-0.538685	-0.555385
C	2.566403	-1.934854	-1.021774
N	1.588401	-2.373385	-0.044888
C	0.555309	-1.354655	0.055425
C	-0.403464	-1.494610	1.096660
C	-1.772440	-1.197997	1.080754
C	-2.680749	-0.820856	0.088619
C	-4.051269	-0.676638	0.486154
O	-5.022768	-0.387835	-0.229913
C	1.058923	-3.699309	-0.333623
H	-0.192839	3.773454	1.728399
H	1.079680	1.296697	-2.439270
H	-0.210315	3.413040	-2.576991
H	-0.857043	4.638422	-0.525763
H	2.487096	-0.268512	2.319627
H	3.359130	0.066168	-1.406000
H	3.882034	-0.650458	0.116434
H	2.124279	-1.874899	-2.039938
H	3.398056	-2.649940	-1.075035
H	0.153833	-1.053219	-0.917842
H	-0.000039	-1.834933	2.050236
H	-2.245741	-1.330693	2.058932
H	-4.222833	-0.862887	1.577652
H	1.875226	-4.433701	-0.304213
H	0.311609	-3.961558	0.418662
H	0.575203	-3.765661	-1.329383
C	-2.352434	-0.601754	-1.363781
H	-1.679626	0.253166	-1.523842
H	-1.864052	-1.479884	-1.815815
H	-3.284730	-0.408921	-1.904998

G(B3LYP/6-31G(d)) = -843.670228

G(M06-2X/6-311+G(d,p),CPCM/THF) = -843.6151183

1 imaginary frequency

6aM

C	3.181771	-2.065367	-0.783028
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C	2.560611	-0.821317	-0.747616
C	1.747121	-0.434555	0.334557
C	1.542114	-1.303650	1.397332
C	2.162432	-2.561499	1.369240
C	2.973250	-2.936136	0.293097
C	1.247984	0.954526	0.039605
C	1.923189	1.171512	-1.297513
N	2.652061	0.200160	-1.734344
C	-0.326950	1.142479	-0.050142
C	-1.026787	0.523133	-1.203764
C	-2.111873	-0.328697	-1.191264
C	-2.922332	-0.923665	-0.193216
N	-0.372822	2.639045	-0.028845
C	0.467448	3.051930	1.082978
C	1.650277	2.052132	1.074696
C	-3.988018	-1.757719	-0.623387
O	-4.824329	-2.371448	0.073277
C	-1.706370	3.203036	0.003230
H	3.803686	-2.344007	-1.629318
H	0.901486	-1.028604	2.231987
H	2.001949	-3.256758	2.189745
H	3.441361	-3.918031	0.289595
H	-0.627155	0.798983	-2.180186
H	-2.429111	-0.620400	-2.199244
H	1.802572	2.089899	-1.868221
H	-0.732017	0.746782	0.895410
H	-0.069338	2.988305	2.053092
H	0.788843	4.096461	0.965462
H	1.786408	1.598670	2.061389
H	2.599600	2.529366	0.807705
H	-4.055913	-1.850306	-1.741162
H	-1.654732	4.291868	-0.136627
H	-2.293309	2.760690	-0.805984
H	-2.238200	3.008197	0.957424
C	-2.748121	-0.744725	1.292934
H	-1.771315	-1.102350	1.660574
H	-2.839149	0.304599	1.622090
H	-3.530191	-1.324723	1.795946

G(B3LYP/6-31G(d)) = -843.677947

G(M06-2X/6-311+G(d,p),CPCM/THF) = -843.6330021

0 imaginary frequencies

TS_6-7αM

C	3.118064	-1.758073	0.001293
C	1.863224	-1.188611	-0.297400
C	1.700761	0.219449	-0.168813
C	2.744722	1.029857	0.239769

C	3.999942	0.457427	0.527277
C	4.165693	-0.927240	0.406077
C	0.259642	0.532642	-0.525412
C	-0.241759	-0.918409	-0.858422
N	0.750332	-1.832132	-0.769417
C	-0.433926	1.348732	0.639794
C	-0.975414	0.531257	1.772170
C	-1.543799	-0.682651	1.621743
C	-1.940004	-1.285818	0.348325
N	-1.373203	2.253215	-0.064209
C	-0.605240	2.748738	-1.198061
C	0.063761	1.484303	-1.757354
C	-2.037889	-2.733980	0.353673
O	-2.688256	-3.425225	-0.434354
C	-1.918591	3.292797	0.780632
H	3.254660	-2.832726	-0.092385
H	2.609183	2.107887	0.335518
H	4.830873	1.087379	0.837680
H	5.135900	-1.369548	0.633322
H	-0.719449	0.870525	2.775148
H	-1.674019	-1.282910	2.528631
H	-0.919645	-1.015783	-1.708110
H	0.365876	1.987218	1.071284
H	0.162320	3.486235	-0.875447
H	-1.258867	3.252548	-1.922502
H	1.013358	1.701385	-2.255259
H	-0.598122	1.012254	-2.491073
H	-1.415341	-3.235342	1.134904
H	-2.610054	3.920265	0.203939
H	-2.472311	2.836352	1.607712
H	-1.137019	3.955299	1.213202
C	-3.017336	-0.600817	-0.484573
H	-4.005068	-0.695925	-0.006651
H	-2.809654	0.462499	-0.622347
H	-3.097584	-1.091010	-1.461645

G(B3LYP/6-31G(d)) = -843.653095

G(M06-2X/6-311+G(d,p),CPCM/THF) = -843.606234

1 imaginary frequency

7aM

C	-1.835802	-2.897578	0.239106
C	-0.905799	-1.833332	0.435600
C	-1.326552	-0.515284	0.025965
C	-2.549169	-0.292831	-0.580621
C	-3.441091	-1.364784	-0.797322
C	-3.064254	-2.646173	-0.366877
H	-1.559924	-3.904713	0.546420

H	-2.833797	0.711066	-0.901226
H	-4.401689	-1.197304	-1.279491
H	-3.752274	-3.479643	-0.521378
C	-0.232267	0.435855	0.481684
C	0.919779	-0.598342	0.795685
N	0.330816	-1.914606	0.948269
C	0.107173	1.619726	-0.485170
C	1.590229	1.817357	-0.697395
H	1.911728	2.836594	-0.914735
C	2.482753	0.827116	-0.619107
H	3.545322	1.019744	-0.758144
C	2.071290	-0.587396	-0.313530
H	1.428236	-0.274547	1.719213
H	-0.377390	1.424130	-1.458098
N	-0.479460	2.844993	0.125686
C	-1.359441	2.441353	1.221804
H	-2.380900	2.192186	0.875830
H	-1.449581	3.254930	1.956732
C	-0.668907	1.197922	1.768566
H	-1.310987	0.583852	2.405694
H	0.218012	1.496104	2.344164
C	3.215787	-1.391269	0.265814
H	2.905047	-2.400992	0.606138
O	4.373247	-1.022026	0.377277
C	-1.071656	3.766190	-0.816965
H	-1.401636	4.674391	-0.294767
H	-0.331512	4.067417	-1.568813
H	-1.949011	3.350754	-1.356684
C	1.617493	-1.334901	-1.593837
H	1.316901	-2.354348	-1.337357
H	0.754697	-0.835479	-2.043582
H	2.425887	-1.362411	-2.336208

G(B3LYP/6-31G(d)) = -843.663429

G(M06-2X/6-311+G(d,p),CPCM/THF) = -843.6276615

0 imaginary frequencies

5aM (with K⁺)

C	5.014339	1.243096	-0.867244
C	4.142152	0.166238	-0.593511
C	2.743096	0.418414	-0.330362
C	2.251038	1.742655	-0.380246
C	3.127229	2.782129	-0.661667
C	4.501632	2.534274	-0.901128
C	2.185884	-0.860734	0.003283
C	3.270478	-1.750168	-0.091750
N	4.459834	-1.160372	-0.413840
C	0.740238	-1.198335	0.234029

C	-0.070599	-1.228694	-1.083877
N	-1.492464	-1.526061	-0.909785
C	-2.378950	-0.517530	-0.700199
C	-3.676205	-0.621008	-0.275259
C	-4.512037	0.531858	-0.152418
C	-5.811454	0.565083	0.266875
C	-1.885806	-2.898111	-0.637975
C	-6.463720	1.869297	0.323810
O	-7.616688	2.079238	0.679374
H	6.065938	1.049028	-1.071331
H	1.198368	1.953295	-0.195112
H	2.755597	3.802984	-0.707044
H	5.159939	3.369362	-1.128532
H	3.227724	-2.826149	0.070839
H	0.654506	-2.178613	0.723421
H	0.256944	-0.472289	0.905621
H	0.014757	-0.259183	-1.585108
H	0.362138	-1.975411	-1.759088
H	-1.978616	0.469925	-0.925254
H	-4.091647	-1.590238	-0.017836
H	-4.055521	1.488181	-0.420011
H	-1.098142	-3.571939	-0.982862
H	-2.060929	-3.079089	0.432848
H	-2.809162	-3.137565	-1.177951
H	-5.814293	2.719113	0.006569
K	4.389196	-0.182726	2.124973
C	-6.605494	-0.650108	0.672446
H	-6.686111	-1.377625	-0.145870
H	-6.150861	-1.170044	1.526152
H	-7.614386	-0.340970	0.957579

G(B3LYP/6-31G(d)) = -1443.624096

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1443.543204

0 imaginary frequencies

TS_5-6aM (with K⁺)

C	-0.950017	3.159263	0.169497
C	-0.736533	1.893910	-0.379840
C	-1.738144	0.886230	-0.339745
C	-2.984101	1.189216	0.219377
C	-3.201889	2.460007	0.757341
C	-2.191638	3.433727	0.743628
C	-1.150454	-0.306770	-0.978540
C	0.128849	0.208418	-1.434641
N	0.411230	1.441674	-1.055507
C	-0.723216	-1.721339	0.381528
C	0.350434	-2.559657	-0.116575
C	1.705559	-2.320106	-0.064175

C	2.455571	-1.288322	0.562758
N	-2.012436	-2.318422	0.425649
C	-2.759323	-2.209676	-0.831576
C	-1.965810	-1.295170	-1.794013
C	3.800595	-1.122878	0.161358
O	4.557929	-0.149061	0.446865
C	-2.780843	-2.122472	1.646932
H	-0.175223	3.921990	0.119985
H	-3.788122	0.458579	0.229829
H	-4.170631	2.699777	1.187963
H	-2.385129	4.415368	1.168180
H	0.021286	-3.434437	-0.673182
H	2.315821	-3.020896	-0.640311
H	0.857827	-0.386972	-1.976285
H	-0.508084	-1.104087	1.250201
H	-3.748911	-1.779811	-0.620988
H	-2.936497	-3.192396	-1.290842
H	-2.649703	-0.793668	-2.489384
H	-1.277924	-1.898352	-2.396771
H	4.197901	-1.915027	-0.508680
H	-3.648331	-2.791257	1.635147
H	-2.169041	-2.399557	2.510895
H	-3.140291	-1.091245	1.792116
K	3.030032	1.731162	-0.345897
C	1.914464	-0.403677	1.661810
H	1.180078	0.352374	1.334647
H	1.409325	-1.000366	2.431915
H	2.749011	0.113410	2.150962

G(B3LYP/6-31G(d)) = -1443.581877

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1443.50273

1 imaginary frequency

6aM (with K⁺)

C	0.035573	3.265547	-0.112177
C	-0.209891	1.970153	-0.556628
C	-1.292293	1.205433	-0.078841
C	-2.129371	1.743590	0.892571
C	-1.886898	3.046170	1.354550
C	-0.822349	3.801374	0.855589
C	-1.249885	-0.127942	-0.800641
C	-0.005490	0.085661	-1.625134
N	0.568661	1.240063	-1.501469
C	-1.223861	-1.422988	0.155282
C	-0.252064	-2.507473	-0.243599
C	1.097823	-2.545565	-0.079536
C	2.018969	-1.653295	0.577641
N	-2.608270	-1.947414	0.071786

C	-3.471344	-1.042815	-0.664998
C	-2.516670	-0.396833	-1.666465
C	3.382662	-1.771603	0.272182
O	4.316401	-0.969417	0.608685
C	-3.141560	-2.469306	1.311574
H	0.857728	3.848759	-0.521244
H	-2.956257	1.173410	1.304775
H	-2.538149	3.472563	2.112508
H	-0.658717	4.811190	1.221671
H	-0.719966	-3.303884	-0.817954
H	1.591524	-3.381773	-0.583809
H	0.398253	-0.678857	-2.281657
H	-1.012541	-1.045702	1.165247
H	-3.948229	-0.269249	-0.030511
H	-4.282914	-1.594882	-1.157519
H	-2.909959	0.513413	-2.127460
H	-2.271045	-1.114695	-2.456933
H	3.649940	-2.633117	-0.378312
H	-4.087810	-2.989138	1.119944
H	-2.438686	-3.194382	1.734261
H	-3.332753	-1.688500	2.076283
K	3.175102	1.004790	-0.456518
C	1.598811	-0.681726	1.661112
H	2.496305	-0.305926	2.168001
H	1.005728	0.187267	1.328273
H	0.983705	-1.181008	2.421678

G(B3LYP/6-31G(d)) = -1443.59125

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1443.521562

0 imaginary frequencies

TS_6-7 α M (with K⁺)

C	-3.005679	-1.552644	-0.136191
C	-1.737244	-0.969135	-0.285988
C	-0.580678	-1.752945	-0.027711
C	-0.682530	-3.071898	0.381921
C	-1.954707	-3.645429	0.547369
C	-3.096774	-2.884768	0.279082
C	0.608856	-0.899682	-0.406657
C	-0.077431	0.488461	-0.455643
N	-1.439732	0.322564	-0.691614
C	1.923319	-0.973847	0.396920
C	1.875564	-0.383502	1.774572
C	1.084205	0.634931	2.121473
C	0.175292	1.403354	1.217743
N	2.863881	-0.283168	-0.509506
C	2.628558	-0.854923	-1.839758
C	1.133588	-1.246560	-1.844695

C	0.770403	2.613776	0.652290
O	0.126207	3.545997	0.135612
C	4.254557	-0.314312	-0.100351
H	-3.903360	-0.970762	-0.337029
H	0.209772	-3.666602	0.572604
H	-2.049070	-4.676606	0.876540
H	-4.079706	-3.335386	0.402195
H	2.488862	-0.857724	2.538861
H	1.068665	0.937641	3.171692
H	0.420526	1.180253	-1.138194
H	2.206110	-2.044011	0.496122
H	3.255392	-1.750705	-2.012459
H	2.894362	-0.123149	-2.613212
H	1.016538	-2.320097	-2.018497
H	0.551145	-0.729802	-2.612906
H	1.874469	2.623205	0.585406
H	4.861156	0.244345	-0.822523
H	4.367212	0.163570	0.877904
H	4.665785	-1.342567	-0.036332
K	-2.050572	2.822278	-1.133460
C	-1.193895	1.629008	1.862083
H	-1.106699	1.630888	2.955475
H	-1.610427	2.604488	1.580994
H	-1.900987	0.846668	1.573284

G(B3LYP/6-31G(d)) = -1443.566880

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1443.499972

1 imaginary frequency

7αM (with K⁺)

C	-3.005679	-1.552644	-0.136191
C	-1.737244	-0.969135	-0.285988
C	-0.580678	-1.752945	-0.027711
C	-0.682530	-3.071898	0.381921
C	-1.954707	-3.645429	0.547369
C	-3.096774	-2.884768	0.279082
C	0.608856	-0.899682	-0.406657
C	-0.077431	0.488461	-0.455643
N	-1.439732	0.322564	-0.691614
C	1.923319	-0.973847	0.396920
C	1.875564	-0.383502	1.774572
C	1.084205	0.634931	2.121473
C	0.175292	1.403354	1.217743
N	2.863881	-0.283168	-0.509506
C	2.628558	-0.854923	-1.839758
C	1.133588	-1.246560	-1.844695
C	0.770403	2.613776	0.652290
O	0.126207	3.545997	0.135612

C	4.254557	-0.314312	-0.100351
H	-3.903360	-0.970762	-0.337029
H	0.209772	-3.666602	0.572604
H	-2.049070	-4.676606	0.876540
H	-4.079706	-3.335386	0.402195
H	2.488862	-0.857724	2.538861
H	1.068665	0.937641	3.171692
H	0.420526	1.180253	-1.138194
H	2.206110	-2.044011	0.496122
H	3.255392	-1.750705	-2.012459
H	2.894362	-0.123149	-2.613212
H	1.016538	-2.320097	-2.018497
H	0.551145	-0.729802	-2.612906
H	1.874469	2.623205	0.585406
H	4.861156	0.244345	-0.822523
H	4.367212	0.163570	0.877904
H	4.665785	-1.342567	-0.036332
K	-2.050572	2.822278	-1.133460
C	-1.193895	1.629008	1.862083
H	-1.106699	1.630888	2.955475
H	-1.610427	2.604488	1.580994
H	-1.900987	0.846668	1.573284

G(B3LYP/6-31G(d)) = -1443.578718

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1443.519746

0 imaginary frequencies

9

C	4.887402	-1.833249	0.671094
C	3.535168	-1.496525	0.676910
C	2.601798	-2.204940	-0.091905
C	3.020845	-3.256928	-0.901675
C	4.379509	-3.598957	-0.926332
C	5.298213	-2.899312	-0.137318
C	1.207816	-1.697689	0.225859
C	1.528978	-0.323403	0.903772
N	2.927180	-0.430637	1.390503
C	0.199588	-1.600725	-0.933984
C	1.037663	0.764715	-1.332744
C	1.460603	0.878389	-0.053248
N	-1.081074	-1.407468	-0.228621
C	-1.053492	-2.317994	0.942163
C	0.437691	-2.620714	1.206046
C	2.003217	2.092942	0.511522
C	-2.273656	-1.600346	-1.067140
C	0.531995	-0.499836	-1.940631
N	1.827147	3.334039	0.167038
C	0.956947	3.871362	-0.910251

C	0.777364	5.344130	-0.531397
C	2.122272	5.704568	0.119348
C	2.468015	4.454534	0.931557
C	-3.574783	-1.281589	-0.337102
C	-4.389913	-2.313924	-0.046191
C	-5.708594	-2.303707	0.675176
Si	-3.969250	0.540967	0.070244
C	-2.696925	1.665692	-0.770221
C	-3.905344	0.847432	1.941577
C	-5.670938	1.042474	-0.606799
H	5.601971	-1.278377	1.272375
H	2.307069	-3.819908	-1.498065
H	4.718791	-4.415795	-1.556702
H	6.348442	-3.177234	-0.159025
H	1.119501	1.606793	-2.011405
H	0.860636	-0.137195	1.748723
H	0.204419	-2.565754	-1.477340
H	-1.595545	-3.252498	0.730658
H	-1.551204	-1.846482	1.795357
H	0.665383	-3.664221	0.968301
H	0.735233	-2.453459	2.245988
H	2.642803	1.950235	1.379885
H	-2.310844	-2.641474	-1.445905
H	-2.174118	-0.950624	-1.944256
H	3.008356	-0.506785	2.400581
H	1.300578	-0.864545	-2.639572
H	-0.329350	-0.266549	-2.577806
H	1.484188	3.770776	-1.864695
H	0.030263	3.294236	-0.950864
H	0.546283	5.955449	-1.406400
H	-0.041760	5.450603	0.187623
H	2.883644	5.882025	-0.647339
H	2.065542	6.590421	0.755565
H	3.537723	4.260297	1.026391
H	2.016946	4.477117	1.928093
H	-4.075891	-3.314881	-0.359418
H	-6.521681	-2.617807	0.006088
H	-5.692235	-3.027126	1.501026
H	-5.970845	-1.328025	1.089826
H	-2.883050	2.711934	-0.497105
H	-1.680074	1.402963	-0.462447
H	-2.751555	1.595339	-1.863477
H	-4.135040	1.896300	2.168279
H	-4.624580	0.225291	2.486378
H	-2.908356	0.630463	2.343834
H	-5.725826	0.866395	-1.688068
H	-6.502337	0.504042	-0.140538
H	-5.835391	2.114601	-0.438911

G(B3LYP/6-31G(d),CPCM/THF) = -1466.70441

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.478814

0 imaginary frequencies

11

C	-3.303961	3.071157	0.458798
C	-2.525119	1.944627	0.720295
C	-1.212143	1.826597	0.228065
C	-0.666824	2.847561	-0.539399
C	-1.438598	3.988020	-0.814293
C	-2.738791	4.093356	-0.315470
C	-0.618642	0.526122	0.761223
C	-1.921531	-0.257713	1.117993
N	-2.844548	0.811842	1.478724
C	0.384161	-0.200243	-0.198570
C	-1.272630	-2.047428	-0.531045
C	-2.400162	-1.112002	-0.133778
N	1.696151	-0.180651	0.485779
C	1.658547	0.900612	1.472522
C	0.246338	0.795594	2.033251
C	-3.615189	-1.877131	0.230309
C	2.840488	-0.137561	-0.422290
C	-0.011546	-1.613389	-0.539003
N	-4.812729	-1.630635	-0.175178
C	-6.008780	-2.421362	0.256906
C	-7.047722	-2.117144	-0.821991
C	-6.742618	-0.657153	-1.195602
C	-5.211261	-0.584107	-1.173534
C	4.167295	-0.622022	0.169161
C	4.161028	-1.330494	1.313124
C	5.327404	-1.923099	2.054721
Si	5.739572	-0.210229	-0.830683
C	6.923404	0.879314	0.174646
C	5.257371	0.754320	-2.392362
C	6.625666	-1.791980	-1.391231
H	-4.317806	3.155046	0.840496
H	0.343441	2.770680	-0.932415
H	-1.021646	4.788574	-1.417936
H	-3.330285	4.978019	-0.535501
H	-1.513059	-3.070253	-0.807543
H	-1.762644	-0.941639	1.954755
H	0.430411	0.375637	-1.140901
H	1.824796	1.891661	1.008353
H	2.432431	0.759848	2.232439
H	-0.075515	1.689280	2.573050
H	0.185228	-0.061416	2.713416
H	-3.508279	-2.712528	0.921661
H	2.963479	0.885360	-0.826575
H	2.603141	-0.763332	-1.294447
H	-3.818668	0.589607	1.643652
H	0.791146	-2.288042	-0.828388

H	-5.731722	-3.471938	0.351016
H	-6.316173	-2.037399	1.234448
H	-6.903960	-2.777353	-1.683537
H	-8.063807	-2.257602	-0.447572
H	-7.136143	-0.375277	-2.174328
H	-7.162849	0.024784	-0.449502
H	-4.771475	-0.868440	-2.133942
H	-4.817052	0.387548	-0.874676
H	3.192095	-1.518523	1.780597
H	6.293601	-1.723479	1.585367
H	5.367488	-1.537005	3.082614
H	5.215261	-3.012873	2.141148
H	7.801871	1.141943	-0.428359
H	6.435396	1.814865	0.473813
H	7.281134	0.386070	1.085039
H	6.152834	0.939433	-2.998843
H	4.545458	0.203727	-3.018880
H	4.813167	1.729000	-2.158922
H	6.975681	-2.402656	-0.552035
H	5.962727	-2.416437	-2.002497
H	7.499216	-1.537504	-2.004808
H	-2.622159	-0.404773	-0.940639

G(B3LYP/6-31G(d),CPCM/THF) = -1466.69301

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.468364

0 imaginary frequencies

12

C	2.766083	3.518890	1.152296
C	1.428308	3.112001	1.088226
C	0.704757	3.058600	-0.138145
C	1.359842	3.440488	-1.325313
C	2.689286	3.844380	-1.265898
C	3.385947	3.880659	-0.039340
C	-0.629816	2.598151	0.173470
C	-0.660805	2.410792	1.535663
N	0.567041	2.711916	2.087206
C	-0.702807	-0.886180	-0.988106
C	1.582295	-1.558670	-0.610606
C	2.962017	-1.375848	-0.517031
N	-1.727920	-0.101207	-1.320393
C	-1.559873	1.269872	-1.830763
C	-1.761825	2.399242	-0.793123
C	3.789925	-2.439876	-0.159846
C	-3.093730	-0.666309	-1.281235
C	0.653496	-0.572653	-0.947870
N	5.105674	-2.398982	-0.021449
C	5.929736	-1.187686	-0.212388

C	7.372651	-1.694542	-0.063640
C	7.235811	-2.925311	0.850061
C	5.926623	-3.563798	0.375880
C	-3.769655	-0.787362	0.084750
C	-3.104624	-0.499156	1.216809
C	-3.601978	-0.591153	2.633221
Si	-5.579641	-1.417345	0.024204
C	-5.734815	-3.082430	0.915473
C	-6.077983	-1.677071	-1.786521
C	-6.757172	-0.136805	0.774333
H	3.298759	3.553984	2.098637
H	0.835165	3.432118	-2.277475
H	3.200918	4.142376	-2.176996
H	4.423547	4.202630	-0.024152
H	1.197020	-2.557091	-0.397830
H	-1.478965	2.096022	2.168475
H	-0.994653	-1.900150	-0.720872
H	-2.292229	1.393693	-2.633898
H	-0.571414	1.341184	-2.288515
H	-2.697228	2.222610	-0.251258
H	-1.913996	3.316752	-1.378766
H	3.338720	-3.410807	0.035509
H	-3.050369	-1.655467	-1.754941
H	-3.701826	-0.046556	-1.945801
H	0.788455	2.665705	3.070812
H	1.001074	0.435004	-1.147830
H	5.727270	-0.743409	-1.191685
H	5.667906	-0.453334	0.558924
H	7.768292	-1.990742	-1.041220
H	8.031585	-0.926332	0.347957
H	8.079658	-3.614711	0.768838
H	7.145162	-2.617015	1.897552
H	6.089400	-4.208253	-0.496810
H	5.409334	-4.141932	1.145506
H	-2.072325	-0.152722	1.145661
H	-3.545993	0.388933	3.126299
H	-4.631085	-0.946719	2.713192
H	-2.964447	-1.267663	3.218101
H	-6.761880	-3.458927	0.829615
H	-5.069721	-3.829158	0.465257
H	-5.491828	-3.020031	1.981581
H	-7.109855	-2.047420	-1.826247
H	-6.044338	-0.748199	-2.368108
H	-5.447617	-2.416069	-2.295022
H	-6.561545	0.052464	1.835078
H	-6.681328	0.820697	0.245252
H	-7.794199	-0.483766	0.683969
H	3.385827	-0.396305	-0.717342

G(B3LYP/6-31G(d),CPCM/THF) = -1466.745834

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.498548

0 imaginary frequencies

13

C	-3.586493	-3.691949	-0.596811
C	-2.250698	-3.324776	-0.520078
C	-1.707399	-2.537336	0.501387
C	-2.543390	-2.087303	1.517074
C	-3.898581	-2.439327	1.468884
C	-4.412846	-3.226672	0.430032
C	-0.232549	-2.348226	0.238674
C	-0.058801	-3.132592	-1.015207
N	-1.184102	-3.654144	-1.403369
C	0.223781	-0.839244	-0.019469
C	-1.138118	0.583983	-1.639297
C	-2.102496	1.177911	-0.751504
N	1.669762	-0.952057	0.196408
C	1.831872	-1.713296	1.435834
C	0.759879	-2.819608	1.362111
C	-3.049115	2.044994	-1.227002
C	2.391997	0.322469	0.177870
C	-0.130007	-0.280954	-1.364492
N	-4.004934	2.679507	-0.513125
C	-4.988552	3.598221	-1.100488
C	-5.513527	4.370430	0.116179
C	-5.453720	3.323707	1.243156
C	-4.172751	2.529140	0.934330
C	3.894647	0.216450	-0.092872
C	4.400205	-0.924920	-0.594756
C	5.825092	-1.238468	-0.959598
Si	4.925483	1.785444	0.256992
C	6.246124	1.458637	1.579058
C	3.785205	3.152861	0.911861
C	5.734300	2.431463	-1.332795
H	-3.970104	-4.305174	-1.405257
H	-2.162625	-1.480233	2.332750
H	-4.564029	-2.097290	2.255420
H	-5.467107	-3.483566	0.421574
H	-1.239148	0.878396	-2.685714
H	0.857894	-3.272233	-1.573826
H	-0.267900	-0.260689	0.783624
H	1.652515	-1.077280	2.321671
H	2.846222	-2.111579	1.513854
H	0.216552	-2.924959	2.303219
H	1.188627	-3.796480	1.123964
H	-3.065129	2.276621	-2.291229
H	2.219537	0.861605	1.127240
H	1.932952	0.944776	-0.601547
H	-1.293752	-4.220705	-2.241951

H	0.503662	-0.617411	-2.183684
H	-4.515514	4.241789	-1.849405
H	-5.798457	3.040664	-1.594206
H	-4.845985	5.210160	0.341494
H	-6.518613	4.769221	-0.046152
H	-5.432725	3.768129	2.241831
H	-6.325936	2.662142	1.188695
H	-3.296509	2.937024	1.459630
H	-4.256366	1.469363	1.207530
H	3.703192	-1.746048	-0.776571
H	6.517637	-0.415033	-0.770402
H	6.183548	-2.113414	-0.399961
H	5.901118	-1.502804	-2.023516
H	6.793817	2.383252	1.801443
H	5.786863	1.113110	2.513166
H	6.979347	0.705307	1.271184
H	4.365810	4.071967	1.060432
H	2.973148	3.387632	0.213412
H	3.332700	2.892775	1.875969
H	6.421745	1.708406	-1.784644
H	4.974350	2.680513	-2.083487
H	6.303828	3.345643	-1.122600
H	-2.081353	0.933482	0.306274

G(B3LYP/6-31G(d),CPCM/THF) = -1466.688396

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.450669

0 imaginary frequencies

14

C	4.177578	2.052774	-0.265549
C	2.876916	1.594387	-0.421356
C	1.744996	2.409370	-0.286798
C	1.910394	3.754052	0.022507
C	3.213223	4.243949	0.187105
C	4.327716	3.407991	0.046579
C	0.513244	1.560344	-0.509300
C	1.135096	0.239707	-0.819035
N	2.431561	0.282490	-0.750578
C	-0.434602	1.413650	0.751395
C	0.386732	-0.833139	1.783550
C	1.576653	-1.380557	1.710422
N	-1.652824	0.871300	0.146373
C	-1.898576	1.752096	-1.006839
C	-0.502876	2.021438	-1.608857
C	2.775744	-1.903597	1.603121
C	-2.794886	0.792996	1.079823
C	0.141979	0.653533	1.964075
N	3.458051	-2.084349	0.342731

C	3.113767	-3.353171	-0.361188
C	4.192190	-3.461088	-1.448495
C	5.423126	-2.712257	-0.859187
C	4.934430	-2.141547	0.484981
C	-4.097843	0.362303	0.412951
C	-5.071805	1.290105	0.328875
C	-6.444830	1.170311	-0.270103
Si	-4.295925	-1.437599	-0.199387
C	-5.821456	-2.253723	0.581261
C	-2.799420	-2.470722	0.329013
C	-4.426626	-1.492143	-2.090871
H	5.034990	1.399152	-0.385401
H	1.056531	4.415717	0.133603
H	3.360717	5.292571	0.426128
H	5.324877	3.816001	0.177507
H	-0.492693	-1.472789	1.713923
H	0.606835	-0.675501	-1.046395
H	-0.599027	2.454366	1.096510
H	-2.356218	2.705017	-0.688284
H	-2.581402	1.279392	-1.714744
H	-0.353324	3.082571	-1.818131
H	-0.341457	1.479826	-2.544167
H	3.313357	-2.237864	2.494137
H	-2.946303	1.774280	1.569911
H	-2.523007	0.081373	1.867992
H	3.000545	-0.606308	-0.634550
H	-0.547926	0.796970	2.804408
H	3.173794	-4.198253	0.341514
H	2.093095	-3.305882	-0.748421
H	4.409660	-4.505630	-1.686386
H	3.854255	-2.977083	-2.370019
H	6.279247	-3.375153	-0.708313
H	5.746451	-1.910890	-1.529906
H	5.202417	-2.812087	1.317130
H	5.331655	-1.148727	0.715129
H	-4.867068	2.283396	0.740993
H	-6.624320	0.214592	-0.766532
H	-7.216578	1.302908	0.500563
H	-6.604790	1.968621	-1.006866
H	-5.869422	-3.309025	0.283631
H	-5.760446	-2.222582	1.675964
H	-6.766211	-1.784712	0.288201
H	-2.711146	-2.524122	1.421144
H	-2.907213	-3.498035	-0.040366
H	-1.866004	-2.062591	-0.070603
H	-5.289206	-0.929558	-2.465396
H	-3.528569	-1.074583	-2.561983
H	-4.531014	-2.528369	-2.436335
H	1.075162	1.150914	2.247655

G(B3LYP/6-31G(d),CPCM/THF) = -1466.649633

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.420276

0 imaginary frequencies

TS_9-14

C	-2.701870	4.149354	-0.064818
C	-2.138634	2.949787	0.348439
C	-0.820215	2.568708	0.070153
C	-0.018634	3.424967	-0.677075
C	-0.559167	4.643553	-1.109631
C	-1.877685	5.001993	-0.805517
C	-0.550799	1.226280	0.730787
C	-1.931870	0.863659	1.212245
N	-2.735387	1.899588	1.086264
C	0.278159	0.205741	-0.135153
C	-1.673711	-1.053896	-1.138846
C	-2.861542	-0.816824	-0.619237
N	1.571153	0.052006	0.560186
C	1.749650	1.177572	1.472100
C	0.346688	1.392658	2.024333
C	-4.193815	-0.670703	-0.521736
C	2.706506	-0.200143	-0.328279
C	-0.406157	-1.159298	-0.322788
N	-5.112272	-1.666437	-0.472077
C	-6.513643	-1.465048	-0.070614
C	-6.942554	-2.855811	0.417428
C	-6.106557	-3.808056	-0.456587
C	-4.757724	-3.084390	-0.587720
C	3.893250	-0.926471	0.310514
C	3.740104	-1.525172	1.505611
C	4.753348	-2.303932	2.298227
Si	5.506709	-0.962781	-0.710223
C	6.920073	-0.096616	0.212266
C	5.233462	-0.040779	-2.345631
C	5.997050	-2.744929	-1.137445
H	-3.729010	4.411308	0.167419
H	1.004142	3.163904	-0.928776
H	0.057199	5.320790	-1.692629
H	-2.271755	5.951107	-1.154786
H	-1.550731	-1.125043	-2.224834
H	-2.190744	0.035848	1.854326
H	0.412220	0.662912	-1.128524
H	2.115072	2.086740	0.958973
H	2.468429	0.933998	2.259945
H	0.195710	2.363662	2.499987
H	0.108984	0.604782	2.745315
H	-4.611188	0.328483	-0.396130
H	3.051267	0.750511	-0.776469
H	2.345018	-0.802452	-1.172842

H	-3.675459	1.936003	1.467945
H	-0.606579	-1.596917	0.660934
H	-6.588956	-0.694557	0.703479
H	-7.116482	-1.143243	-0.931541
H	-6.675938	-2.978860	1.473463
H	-8.019596	-3.015667	0.318104
H	-5.998590	-4.805403	-0.022239
H	-6.569279	-3.918879	-1.443884
H	-4.059925	-3.358388	0.218444
H	-4.255504	-3.283162	-1.540379
H	2.758968	-1.457318	1.980321
H	5.731976	-2.366584	1.816740
H	4.895390	-1.854131	3.290547
H	4.399306	-3.329153	2.474176
H	7.828349	-0.092328	-0.403638
H	6.662883	0.947124	0.430006
H	7.165809	-0.583006	1.162610
H	6.141349	-0.107418	-2.957995
H	4.411132	-0.469046	-2.931127
H	5.017705	1.023270	-2.193762
H	6.214512	-3.350686	-0.251211
H	5.196901	-3.247314	-1.694548
H	6.893458	-2.748632	-1.770471
H	0.303304	-1.822653	-0.830592

G(B3LYP/6-31G(d),CPCM/THF) = -1466.648734

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.442218

1 imaginary frequency

TS_11-13

C	3.044461	3.165676	-0.352902
C	2.364239	2.051683	-0.826953
C	1.035472	1.747064	-0.493130
C	0.354963	2.594216	0.375718
C	1.016377	3.726975	0.869989
C	2.337898	4.011348	0.508250
C	0.629762	0.482976	-1.234065
C	1.951049	0.051174	-1.796449
N	2.838356	1.021218	-1.669918
C	-0.248184	-0.562989	-0.410964
C	1.338398	-2.506521	-0.510438
C	2.439962	-1.730944	0.024671
N	-1.645244	-0.274166	-0.796665
C	-1.702616	0.842323	-1.736349
C	-0.345251	0.802675	-2.427814
C	3.752799	-2.139220	-0.114543
C	-2.611857	-0.231364	0.296376
C	0.103156	-2.000355	-0.699480

N	4.830846	-1.571587	0.441265
C	6.206051	-2.063937	0.238299
C	6.943098	-1.577871	1.490714
C	6.247833	-0.240617	1.802492
C	4.773328	-0.505476	1.456852
C	-4.051334	-0.592447	-0.084435
C	-4.293886	-1.199407	-1.260566
C	-5.610286	-1.657603	-1.825194
Si	-5.395386	-0.178028	1.207005
C	-6.635008	1.078535	0.513272
C	-4.584237	0.596513	2.738083
C	-6.291733	-1.748651	1.779682
H	4.073080	3.369307	-0.632354
H	-0.666044	2.388502	0.679305
H	0.492985	4.393353	1.548601
H	2.827418	4.894628	0.906146
H	1.546956	-3.528513	-0.825653
H	2.113338	-0.771780	-2.475577
H	-0.081129	-0.333894	0.652177
H	-1.856740	1.812242	-1.230113
H	-2.523192	0.718967	-2.450889
H	-0.083177	1.731613	-2.938974
H	-0.310765	-0.021256	-3.147461
H	3.972313	-2.999336	-0.745178
H	-2.604155	0.765306	0.777968
H	-2.270715	-0.932814	1.069625
H	3.777058	0.982699	-2.053215
H	-0.691381	-2.605905	-1.124383
H	6.205086	-3.151258	0.121266
H	6.634132	-1.620224	-0.670700
H	6.792334	-2.287233	2.312208
H	8.018019	-1.472918	1.322999
H	6.371865	0.075854	2.841139
H	6.647505	0.551626	1.159594
H	4.203009	-0.866533	2.323274
H	4.264167	0.382943	1.069367
H	-3.437286	-1.402789	-1.906535
H	-6.465193	-1.437845	-1.181474
H	-5.795370	-1.187336	-2.800783
H	-5.595710	-2.741485	-2.005437
H	-7.372558	1.351358	1.278684
H	-6.123765	1.998067	0.203315
H	-7.183010	0.695410	-0.354428
H	-5.351136	0.779541	3.501187
H	-3.828106	-0.059926	3.185198
H	-4.105443	1.557859	2.518262
H	-6.822035	-2.257361	0.967698
H	-5.581615	-2.464447	2.211574
H	-7.027845	-1.504088	2.555927
H	2.218082	-0.900721	0.690105

G(B3LYP/6-31G(d),CPCM/THF) = -1466.676032
G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.442218

1 imaginary frequency

TS_13-12

C	-3.620108	-2.955760	-0.813703
C	-2.240550	-2.862455	-0.672919
C	-1.602909	-2.468556	0.515886
C	-2.381740	-2.164902	1.632259
C	-3.771779	-2.264493	1.520177
C	-4.382361	-2.645776	0.314377
C	-0.140251	-2.412773	0.253675
C	-0.030551	-2.970436	-1.076945
N	-1.222456	-3.148194	-1.609806
C	0.315602	-0.647798	-0.007509
C	-1.134423	0.717763	-1.550169
C	-2.203631	1.098578	-0.685595
N	1.712022	-0.785007	0.288358
C	1.820380	-1.547183	1.526273
C	0.920177	-2.780275	1.308930
C	-3.226118	1.890872	-1.153631
C	2.517046	0.445220	0.246746
C	-0.026757	-0.042726	-1.289515
N	-4.289282	2.330580	-0.459689
C	-5.340900	3.189093	-1.028524
C	-6.037242	3.758045	0.213438
C	-5.921124	2.610243	1.232299
C	-4.529829	2.018081	0.954918
C	3.999652	0.234079	-0.066648
C	4.416198	-0.945549	-0.560954
C	5.806655	-1.354933	-0.961896
Si	5.141836	1.737032	0.227467
C	6.490155	1.331428	1.498839
C	4.118770	3.181568	0.909526
C	5.926460	2.310937	-1.401411
H	-4.081893	-3.258752	-1.747674
H	-1.924951	-1.866053	2.571133
H	-4.392891	-2.046014	2.383597
H	-5.464400	-2.710868	0.258835
H	-1.213563	1.094374	-2.571374
H	0.872763	-3.139624	-1.648130
H	-0.281612	-0.254155	0.828213
H	1.461794	-0.959014	2.390346
H	2.861373	-1.817780	1.715250
H	0.434079	-3.092798	2.236515
H	1.512364	-3.627522	0.953557
H	-3.203070	2.220383	-2.191342
H	2.408183	0.988115	1.201269

H	2.077854	1.100525	-0.514724
H	-1.385981	-3.447837	-2.566058
H	0.664424	-0.237069	-2.106908
H	-4.901837	3.958329	-1.671174
H	-6.036759	2.591970	-1.634792
H	-5.496948	4.641456	0.572325
H	-7.071221	4.049799	0.011385
H	-6.027248	2.942924	2.268130
H	-6.693300	1.856709	1.040093
H	-3.751929	2.483717	1.576391
H	-4.487008	0.935443	1.122118
H	3.664055	-1.724624	-0.705095
H	6.553762	-0.571589	-0.815213
H	6.128822	-2.237309	-0.392060
H	5.830743	-1.647977	-2.020618
H	7.116627	2.214161	1.679253
H	6.047708	1.037604	2.458394
H	7.148095	0.518323	1.173459
H	4.761874	4.063840	1.018490
H	3.293990	3.458052	0.242071
H	3.693591	2.963383	1.896098
H	6.548063	1.538956	-1.867586
H	5.155216	2.598276	-2.126427
H	6.561024	3.189152	-1.227393
H	-2.214414	0.759638	0.345529

G(B3LYP/6-31G(d),CPCM/THF) = -1466.683541

G(M06-2X/6-311+G(d,p),CPCM/THF) = -1466.444374

1 imaginary frequency
