SUPPORTING INFORMATION

'Concerted' Transition State, Stepwise Mechanism. Dynamics Effects in C^2-C^6 Enyne Allene Cyclizations

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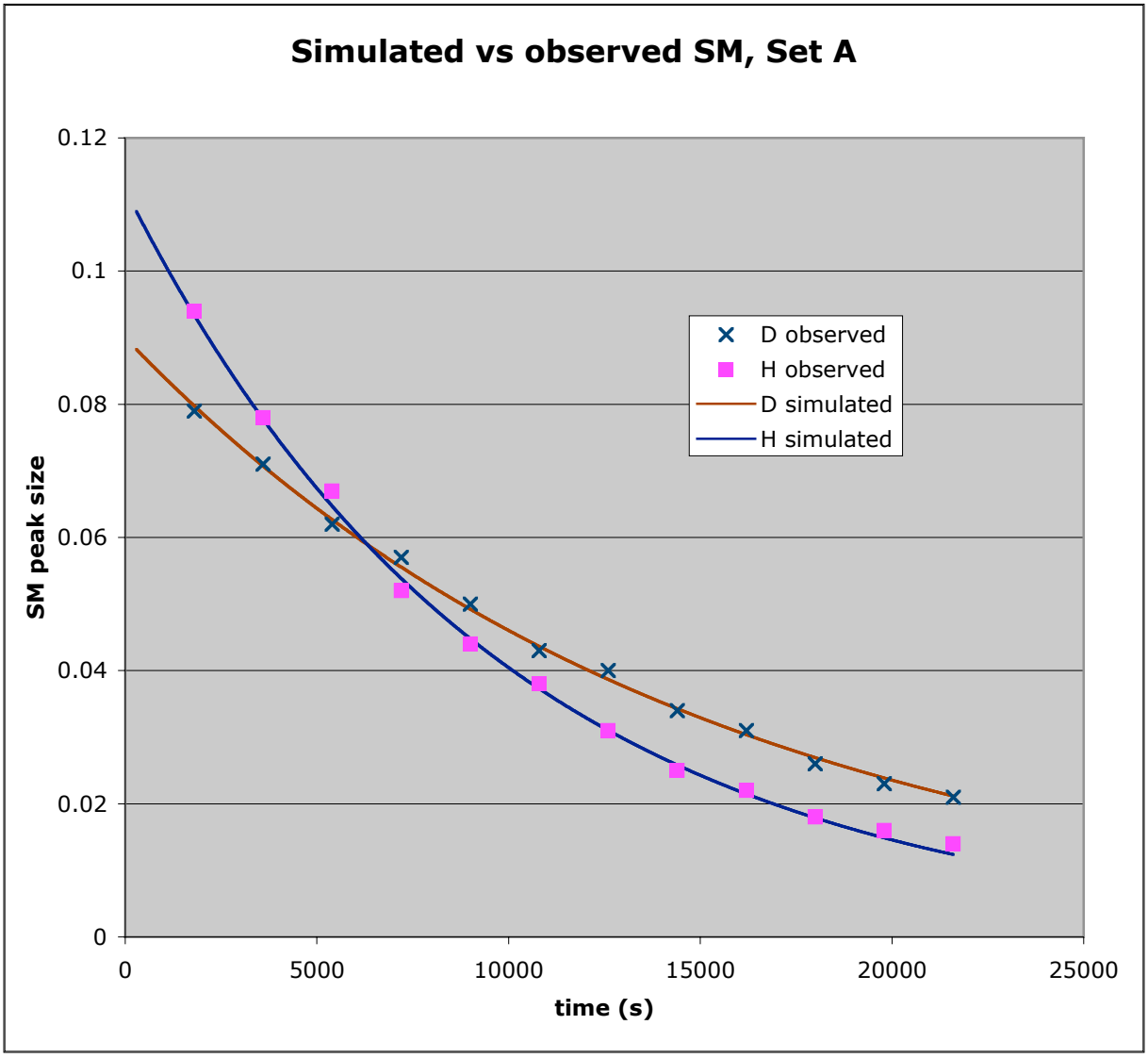
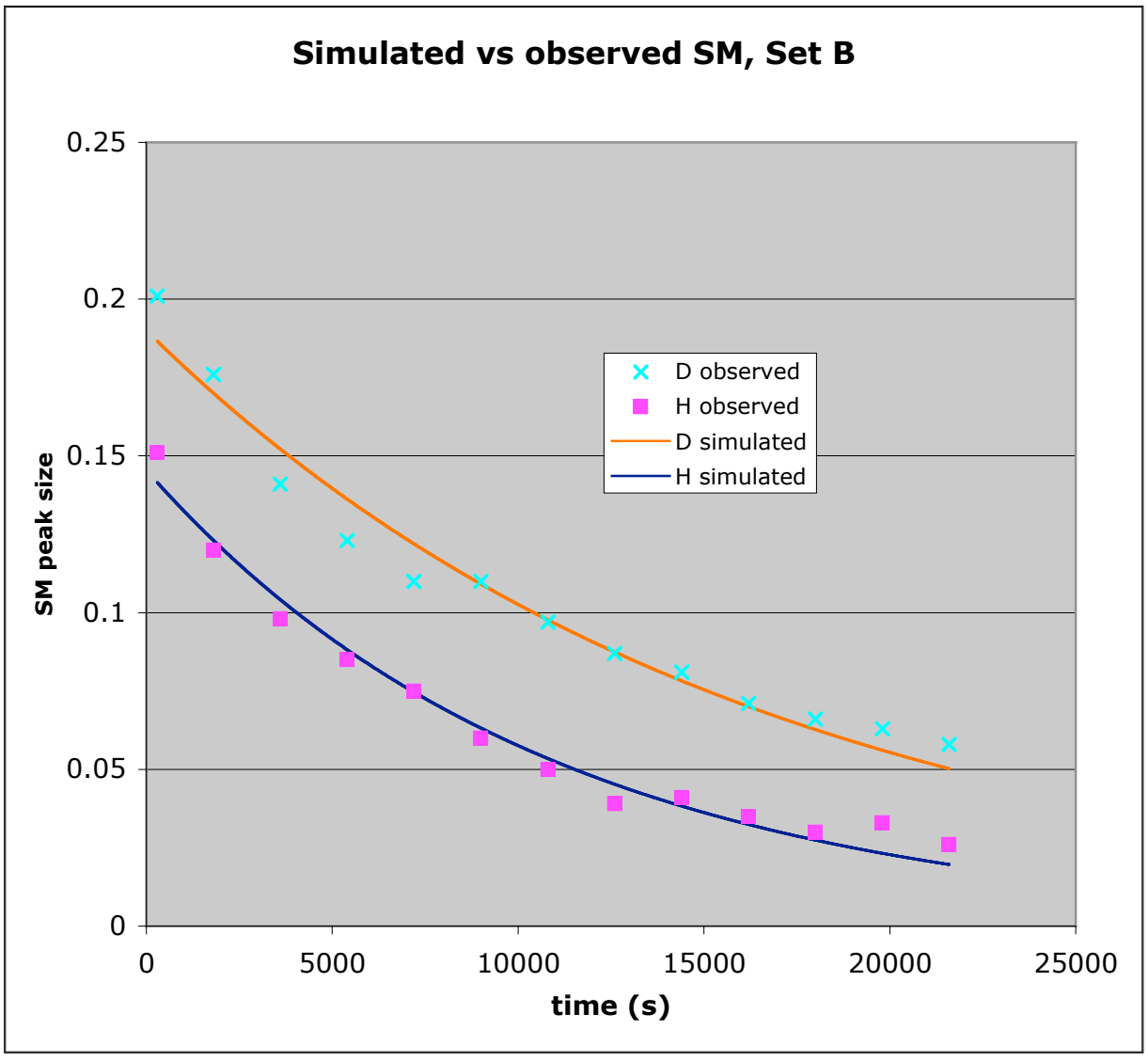
Kinetic Data and Simulations

The graph below shows a plot of experimental starting material peak size observations versus time for paired reactions of **9a** versus **9b**, set A. A k_H of 10.2 x 10^{-5} and a k_D of 6.7 x 10^{-5}, with an overall k_H/k_D of 1.52, were assigned based on a least-squares fit of the data versus the simulation. Approximate error limits of ±1.0 x 10^{-5} for k_H and ±0.8 x 10^{-5} for k_D were assigned visually, that is, rate constants outside of the error range exhibited an obviously worse fit to the curvature of the experimental data (the time=0 peak height was used as a second adjustable parameter in such simulations, but no adjustments with rate constants outside of the error range led to an acceptable fit).

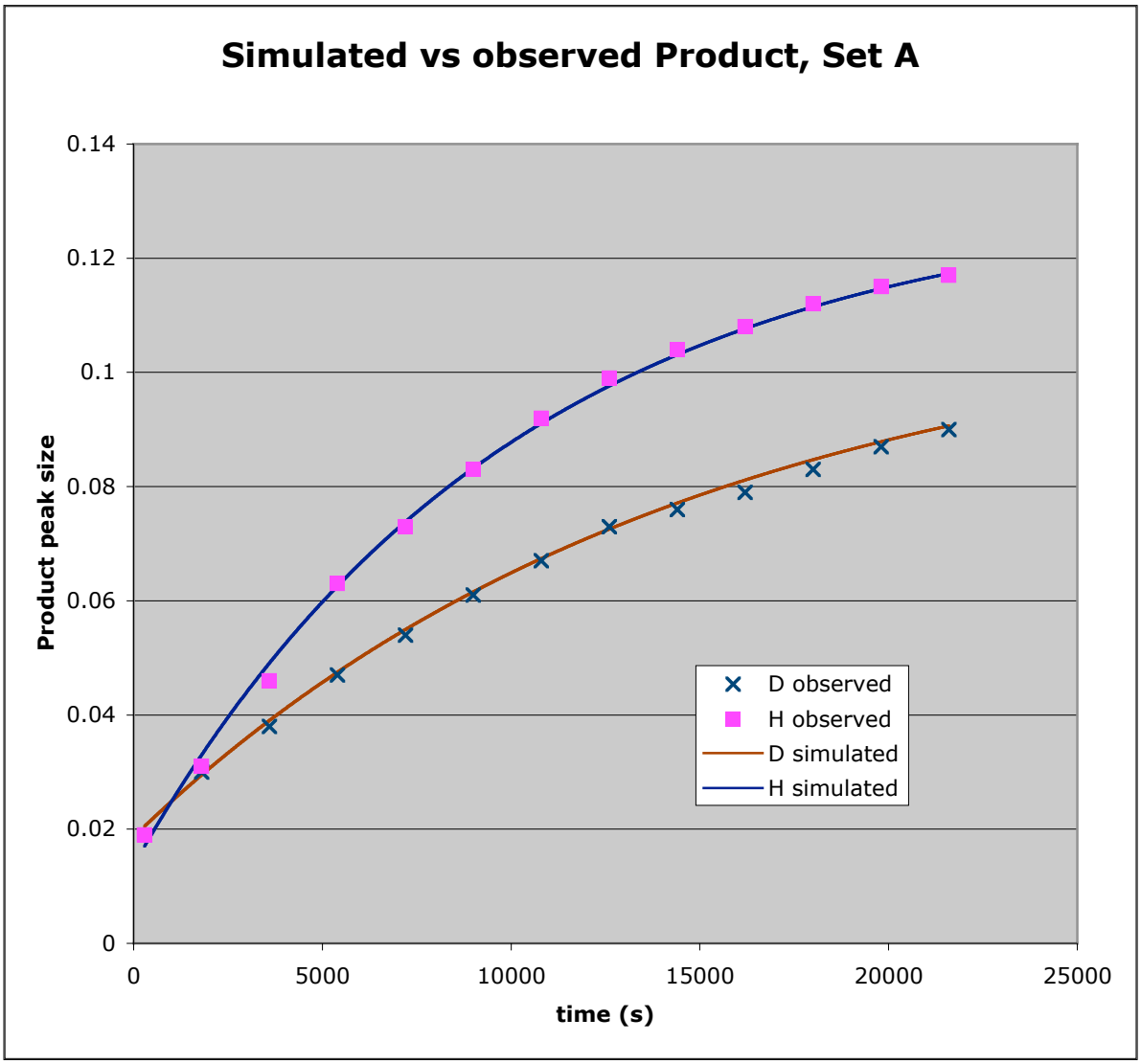
Slightly better fits could be obtained if were assumed that a trace unknown impurity was underneath the observed peaks, contributing 0.002 to the peak height. However, this did not significantly affect the best-fit isotope effect. The absence of a time = infinity observation is a deficiency in this study but the resulting increased uncertainty in the isotope effect does not impact its interpretation in the present context.



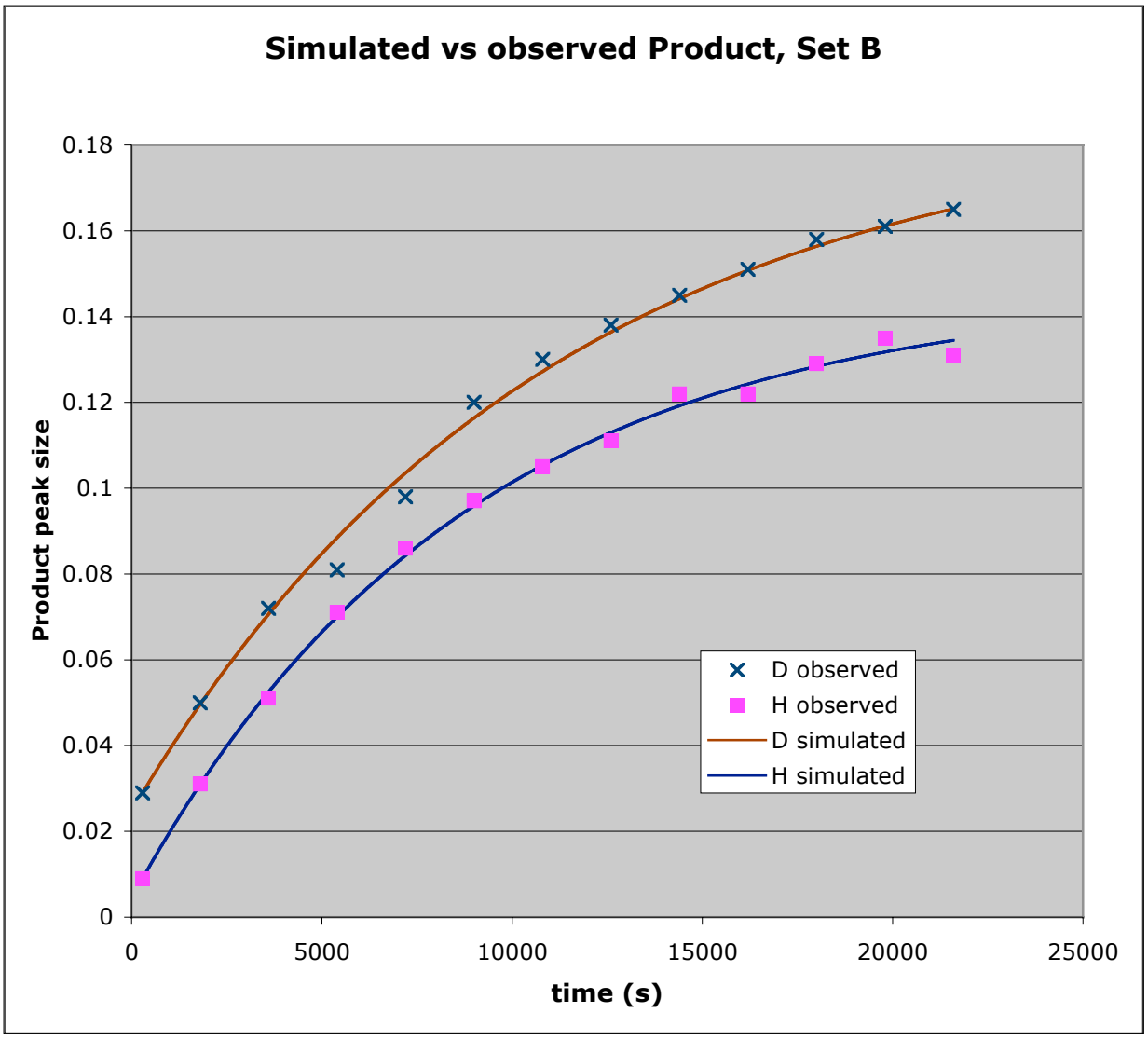
The graph below shows a plot of experimental starting material peak size observations versus time for paired reactions of **9a** versus **9b**, set B. A k_H of 9.3 x 10^{-5} and a k_D of 6.2 x 10^{-5}, with an overall k_H/k_D of 1.50, were assigned based on a least-squares fit of the data versus the simulation. Approximate error limits of ±1.4 x 10^{-5} for k_H and ±0.8 x 10^{-5} for k_D were assigned visually, that is, rate constants outside of the error range exhibited an obviously worse fit to the curvature of the experimental data (the time=0 peak height was used as a second adjustable parameter in such simulations, but no adjustments with rate constants outside of the error range led to an acceptable fit).



The graph below shows a plot of experimental product peak size observations versus time for paired reactions of **9a** versus **9b**, set A. A k_H of 1.0 x 10^{-5} and a k_D of 6.8 x 10^{-5}, with an overall k_H/k_D of 1.46, were assigned based on a least-squares fit of the data versus the simulation. Approximate error limits of ±1.5 x 10^{-5} for k_H and ±1.3 x 10^{-5} for k_D were assigned visually, that is, rate constants outside of the error range exhibited an obviously worse fit to the curvature of the experimental data (the time=0 peak height was used as a second adjustable parameter in such simulations, but no adjustments with rate constants outside of the error range led to an acceptable fit).



The graph below shows a plot of experimental product peak size observations versus time for paired reactions of **9a** versus **9b**, set B. A k_H of 11.5 x 10^{-5} and a k_D of 9.2 x 10^{-5}, with an overall k_H/k_D of 1.25, were assigned based on a least-squares fit of the data versus the simulation. Approximate error limits of ±2.5 x 10^{-5} for k_H and ±1.8 x 10^{-5} for k_D were assigned visually, that is, rate constants outside of the error range exhibited an obviously worse fit to the curvature of the experimental data (the time=0 peak height was used as a second adjustable parameter in such simulations, but no adjustments with rate constants outside of the error range led to an acceptable fit).



Theoretical Results

All structures and energies were obtained using standard procedures in Gaussian98[1] or Gaussian03.[2] Vibrational frequency analyses were carried out on all stationary points.

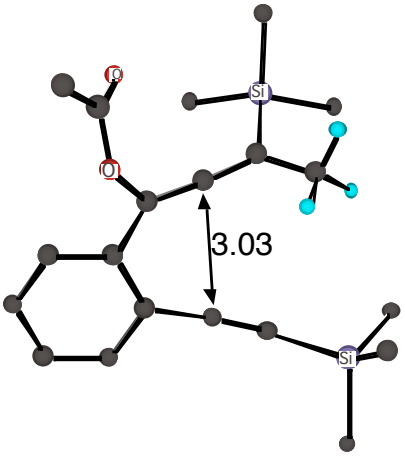
The program used for dynamics was described in Supporting Information for a previous publication.[3] The latest version of this program may be obtained for free by emailing D. Singleton: singleton@mail.chem.tamu.edu

1. Gaussian 98, Revision A.11.3, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, N. Rega, P. Salvador, J. J. Dannenberg, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2002.

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

3. Singleton, D. A.; Hang, C.; Szymanski, M. J.; Greenwald, E. E. *J. Am. Chem. Soc.* **2003**, *125*, 1176-1177.

Structure 9, starting material, RB3LYP/6-31G(d,p)



(some hydrogens removed for clarity)
E(RB+HF-LYP) = -1508.47276852

Zero-point correction=	0.421576 (Hartree/Particle)
Thermal correction to Energy=	0.453560
Thermal correction to Enthalpy=	0.454504
Thermal correction to Gibbs Free Energy=	0.355897
Sum of electronic and zero-point Energies=	-1508.051192
Sum of electronic and thermal Energies=	-1508.019209
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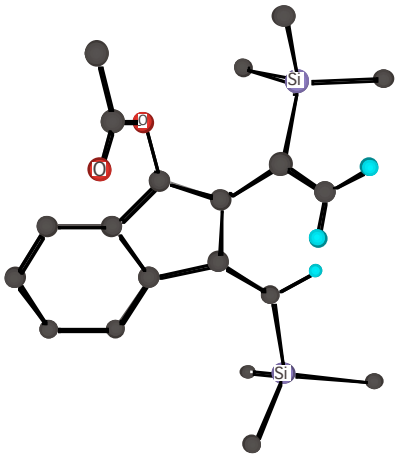
Structure 10 (ene product), RB3LYP/6-31G(d,p)



(most hydrogens removed for clarity)
E(RB+HF-LYP) = -1508.52060319

Zero-point correction=	0.424179 (Hartree/Particle)
Thermal correction to Energy=	0.454476
Thermal correction to Enthalpy=	0.455420
Thermal correction to Gibbs Free Energy=	0.361547
Sum of electronic and zero-point Energies=	-1508.096424
Sum of electronic and thermal Energies=	-1508.066127
Sum of electronic and thermal Enthalpies=	-1508.065183
Sum of electronic and thermal Free Energies=	-1508.159056

E (Thermal)	CV	S

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	285.188	110.412	197.572

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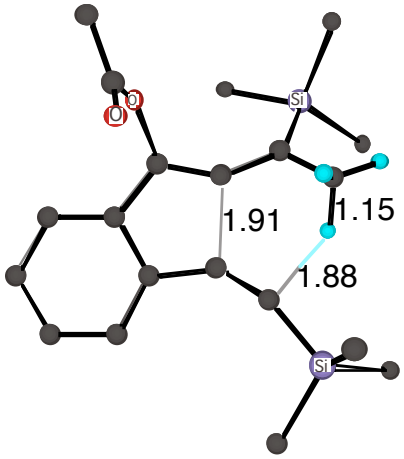
Structure 11 (ene transition structure), RB3LYP/6-31G(d,p)



(most hydrogens removed for clarity)
E(RB+HF-LYP) = -1508.43292752

Zero-point correction=	0.419670 (Hartree/Particle)
Thermal correction to Energy=	0.450177
Thermal correction to Enthalpy=	0.451121
Thermal correction to Gibbs Free Energy=	0.355928
Sum of electronic and zero-point Energies=	-1508.013257
Sum of electronic and thermal Energies=	-1507.982751
Sum of electronic and thermal Enthalpies=	-1507.981806
Sum of electronic and thermal Free Energies=	-1508.077000

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	282.490	110.692	200.351

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Structure 11 (ene transition structure), UBPW91/6-31G(d,p)

```
E(UB-PW91) = -1508.27172091

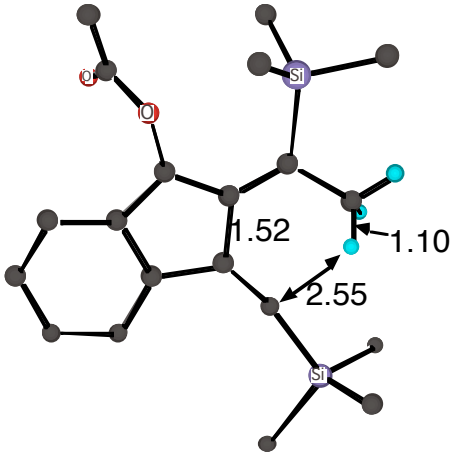
 Zero-point correction=                           0.409826
(Hartree/Particle)
 Thermal correction to Energy=                    0.441225
 Thermal correction to Enthalpy=                  0.442169
 Thermal correction to Gibbs Free Energy=         0.344612
 Sum of electronic and zero-point Energies=          -1507.861895
 Sum of electronic and thermal Energies=             -1507.830496
 Sum of electronic and thermal Enthalpies=           -1507.829552
 Sum of electronic and thermal Free Energies=        -1507.927109

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin   Cal/Mol-
Kelvin
 Total                 276.873            113.630
205.327

 C,0,-0.3270068822,-4.1446238077,-1.6150997404
 C,0,1.0733021562,-4.1789497529,-1.4939698758
 C,0,1.7691378245,-3.0889753432,-0.952124938
 C,0,1.051017852,-1.9606481228,-0.5272126267
 C,0,-0.3644241887,-1.9241989748,-0.6397328276
```

C,0,-1.0493883791,-3.0171007394,-1.1960128902
C,0,1.5702019537,-0.7270931979,0.0367735937
O,0,2.9191603473,-0.6382088025,0.4311292479
C,0,-0.9959336617,-0.7154803648,-0.1280468774
C,0,-2.1131405809,-0.1724081854,0.1545837564
Si,0,-3.8950813428,0.1397830898,0.5139869468
C,0,0.7007594318,0.2969954974,0.1919833194
C,0,0.5360380177,1.6387571904,0.3412538047
C,0,-0.5622963707,2.0944152762,1.2214626282
Si,0,1.3870098403,2.8524253144,-0.8628206703
C,0,2.4490962102,4.040435023,0.1778205994
C,0,0.0562248963,3.8482880696,-1.7889671093
C,0,2.4690911026,1.9180139702,-2.1036786655
C,0,-4.9197154507,-1.3465693279,-0.0868618612
C,0,-4.4692445961,1.7007077548,-0.4023638979
C,0,-4.1157728635,0.3525787509,2.3874866945
C,0,3.2452257265,-1.0999537825,1.7047826452
H,0,-2.1373205391,-2.9870831241,-1.2803337803
H,0,-0.8595733356,-5.0041507853,-2.0288807986
H,0,2.8582709757,-3.1041955715,-0.8750856545
H,0,1.6254869698,-5.0610806606,-1.8274979249
H,0,-0.7365118763,3.1791832576,1.2282745077
H,0,-1.4813972147,1.5480635321,0.7981165909
H,0,-0.4948425811,1.7141335388,2.252202603
H,0,2.9307536369,4.7960657813,-0.4635252592
H,0,1.8405584378,4.5729841436,0.9250591209
H,0,3.2417381784,3.4976648099,0.7148915149
H,0,3.0025984671,2.6277459914,-2.7560618413
H,0,3.2178358055,1.2932840661,-1.5953899175
H,0,1.8634750364,1.2602406856,-2.7452155762
H,0,0.5248792228,4.5709362474,-2.476475443
H,0,-0.587857945,3.1849818777,-2.3861693318
H,0,-0.5892985005,4.4169359761,-1.1022353215
H,0,-5.9909959322,-1.1846447961,0.1162392677
H,0,-4.8035918626,-1.4992624137,-1.1707977154
H,0,-4.6149558384,-2.2728651526,0.4231694424
H,0,-5.1794760726,0.5028470417,2.6324943879
H,0,-3.7648663735,-0.5370921948,2.9316957462
H,0,-3.5570494553,1.2220041125,2.7649066701
H,0,-5.5406683132,1.883895009,-0.2215755302
H,0,-3.9135178335,2.5909543504,-0.0713282373
H,0,-4.3246753465,1.5981154199,-1.4887774127
O,0,2.4360569009,-1.5341927842,2.4968081528
C,0,4.7351959076,-0.9489283036,1.9250519257
H,0,5.0153396078,0.1141878082,1.8811437377
H,0,5.0001669947,-1.3606998804,2.90495316
H,0,5.2965501046,-1.4664238134,1.1336099746

Structure 12 (diradical), UB3LYP/6-31G(d,p)



(most hydrogens removed for clarity)
E(UB+HF-LYP) = -1508.44810618

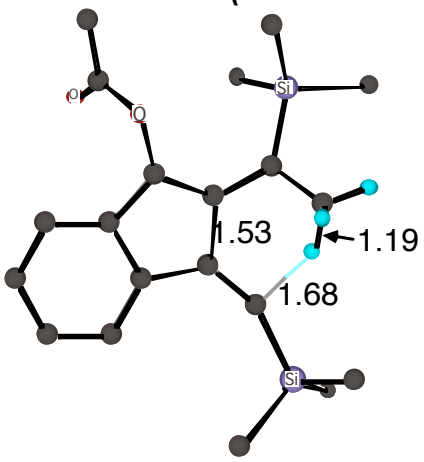
Zero-point correction=	.422109 (Hartree/Particle)
Thermal correction to Energy=	.452698
Thermal correction to Enthalpy=	.453643
Thermal correction to Gibbs Free Energy=	.359205
Sum of electronic and zero-point Energies=	-1508.025997
Sum of electronic and thermal Energies=	-1507.995408
Sum of electronic and thermal Enthalpies=	-1507.994464
Sum of electronic and thermal Free Energies=	-1508.088901

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	284.073	111.608	198.761

C,0,1.6539169668,4.0971440398,-0.2658661267
C,0,0.3005816138,4.4561239005,-0.3263347307
C,0,-0.700814282,3.4874748172,-0.2984413978
C,0,-0.3276582525,2.137984796,-0.2083248019
C,0,1.0406100451,1.7781471122,-0.1548378762
C,0,2.0300858947,2.7513682577,-0.1808783841
C,0,-1.0944348903,0.9250526066,-0.1838564258
O,0,-2.4626198098,0.8782265636,-0.3587485322
C,0,1.1446268754,0.2934528202,-0.0950522578
C,0,2.2826554862,-0.3803431275,-0.0048539529
Si,0,4.0239637534,-0.9398645995,0.1332153692
C,0,-0.2754454185,-0.2379714769,-0.1379875518
C,0,-0.6461627289,-1.5834926435,-0.1400312942
C,0,0.4555990361,-2.6216209569,-0.1368893005
Si,0,-2.4327964278,-2.2512972558,-0.109670261
C,0,-3.3417078912,-1.7240299676,1.4742084938
C,0,-2.3861469507,-4.1494199587,-0.0436878843
C,0,-3.392582544,-1.8330980914,-1.6923532202
C,0,5.2236578095,0.5280322355,0.1737132174
C,0,4.4287736759,-2.0241500606,-1.3636041505
C,0,4.2096944189,-1.9338185033,1.7322443374
C,0,-3.2939403044,1.5820793165,0.4906602449
O,0,-2.9132658541,2.1263296798,1.4947642936
C,0,-4.7063752377,1.5523289963,-0.0323422951
H,0,2.4171782207,4.8691506832,-0.2873075001

```
H,0,0.0270897799,5.5050843529,-0.3926046416
H,0,-1.7440700362,3.779210062,-0.3324369625
H,0,3.0782770004,2.473489747,-0.1420588332
H,0,0.0743619149,-3.6399023288,-0.2192088603
H,0,1.1579610077,-2.4596156962,-0.9647861138
H,0,1.0511760775,-2.5663334921,0.7852674222
H,0,-4.418741771,-1.9105231532,1.3866451576
H,0,-2.978284056,-2.3297126865,2.3120628469
H,0,-3.1968778932,-0.678601915,1.753097609
H,0,-3.4155621051,-4.5230965229,0.0139708353
H,0,-1.9321592955,-4.5944073878,-0.9354479584
H,0,-1.8542673391,-4.5319273836,0.8337836759
H,0,-4.4155424695,-2.2239950783,-1.630519031
H,0,-3.4409811467,-0.7614772116,-1.8902358603
H,0,-2.9138824707,-2.3127088381,-2.5536040109
H,0,6.2547632784,0.1677674097,0.2708746513
H,0,5.1653894972,1.1219915529,-0.7441604976
H,0,5.0224672289,1.1910672346,1.0212911033
H,0,5.4707007907,-2.3617654923,-1.3213464175
H,0,3.7905498586,-2.9126193635,-1.4001619439
H,0,4.2934459978,-1.4755098799,-2.3012591177
H,0,5.244384507,-2.273761817,1.8558958454
H,0,3.9489026127,-1.3308674344,2.6079337021
H,0,3.5645818978,-2.8181158947,1.7304218596
H,0,-4.7524170736,2.0455001385,-1.0080099582
H,0,-5.0374265317,0.5200797958,-0.1718618633
H,0,-5.359874662,2.0639519537,0.6730993973
```

Structure 13 (ts from diradical to product), UB3LYP/6-31G(d,p)



(most hydrogens removed for clarity)
E(UB+HF-LYP) = -1508.44206941

Zero-point correction=	0.419118 (Hartree/Particle)
Thermal correction to Energy=	0.448695
Thermal correction to Enthalpy=	0.449640
Thermal correction to Gibbs Free Energy=	0.359101
Sum of electronic and zero-point Energies=	-1508.022952
Sum of electronic and thermal Energies=	-1507.993374
Sum of electronic and thermal Enthalpies=	-1507.992430
Sum of electronic and thermal Free Energies=	-1508.082968

E (Thermal)	CV	S

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	281.561	109.541	190.554

```
C,0,-0.3603628844,-0.1757387289,-0.3808474133
C,0,-1.0924849276,1.0051729517,-0.3544794447
C,0,-0.258193296,2.1588671423,-0.0955360613
C,0,1.0765534863,1.6977957342,0.0380192017
C,0,1.1023403682,0.2253274449,-0.1429044376
C,0,2.1112621468,2.5936936283,0.2804608763
C,0,1.8211285416,3.9587836298,0.3694260491
C,0,0.5049313664,4.4154721985,0.232919485
C,0,-0.5445177142,3.5258046211,0.0031760183
O,0,-2.407668887,1.0623279916,-0.7917758086
C,0,-3.3541591698,1.7465212113,-0.0690768403
C,0,-4.6562565448,1.7867220017,-0.8274091608
C,0,2.1222118506,-0.6159440102,-0.0437987884
Si,0,3.905754453,-1.0751828527,0.0845564319
C,0,4.1686485624,-1.9379850067,1.7471813237
C,0,-0.7456990384,-1.5278776081,-0.4831952089
Si,0,-2.3819299574,-2.2446162639,0.159277691
C,0,-3.7091151965,-2.1345472333,-1.1921633469
C,0,5.1010821799,0.3928423766,-0.046447881
C,0,4.2787113316,-2.270614033,-1.3357622663
C,0,0.3243052018,-2.4297659491,-0.9134561725
C,0,-2.9370562707,-1.3919387362,1.7549600208
C,0,-2.1242325782,-4.0805088551,0.5604133412
O,0,-3.153317787,2.2220100946,1.0213884916
H,0,2.6243214969,4.6695661288,0.5390532308
H,0,0.2946427608,5.4780184363,0.3128804029
H,0,-1.562342767,3.8893242249,-0.0637565764
H,0,3.1311655461,2.2415677277,0.3810555282
H,0,0.1518146355,-3.4950241026,-0.7544809883
H,0,0.6893150365,-2.256141302,-1.9321839964
H,0,1.273718043,-2.0441943389,-0.3055357493
H,0,-3.9312068494,-1.747440661,2.050158514
H,0,-2.2461611725,-1.6436197446,2.5673247582
H,0,-2.9744373069,-0.3018508934,1.6921842809
H,0,-3.0459295014,-4.4930875741,0.9867533544
H,0,-1.881474273,-4.6761209059,-0.3255992173
H,0,-1.328213697,-4.2321270098,1.2972739421
H,0,-4.6825590638,-2.4691471788,-0.8147128003
H,0,-3.8143210534,-1.1143549841,-1.5695458487
H,0,-3.4453486763,-2.7738138857,-2.0416980821
H,0,6.1328054422,0.0243640478,-0.0979555882
H,0,4.9173772826,0.9895267596,-0.9455654722
H,0,5.033759884,1.0553872653,0.8224250411
H,0,5.3212105443,-2.605594621,-1.2901245537
H,0,3.6404040941,-3.1588495225,-1.2935979444
H,0,4.1255252669,-1.7932249463,-2.3092037726
H,0,5.2112084067,-2.2590564999,1.8530119115
H,0,3.9388917657,-1.2693319844,2.5830990997
H,0,3.5329710425,-2.823718636,1.8436669056
H,0,-4.4951463778,2.1419457395,-1.8483785116
H,0,-5.0775418113,0.7788694994,-0.8926036699
H,0,-5.3546827338,2.4381152274,-0.3033991467
```

Structure 14 (ts for reversed diradical formation), UB3LYP/6-31G(d,p)

4threversedTSBetter
E(UB+HF-LYP) = -1508.41856655

Zero-point correction=	0.419274 (Hartree/Particle)
Thermal correction to Energy=	0.450519
Thermal correction to Enthalpy=	0.451463
Thermal correction to Gibbs Free Energy=	0.355038
Sum of electronic and zero-point Energies=	-1507.999293
Sum of electronic and thermal Energies=	-1507.968047
Sum of electronic and thermal Enthalpies=	-1507.967103
Sum of electronic and thermal Free Energies=	-1508.063529

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	282.705	111.880	202.945

C,0,0.1178667812,2.3322152879,-0.1129367517
C,0,-0.3393228295,3.6034127871,-0.4606013578
C,0,0.5750327146,4.6569735784,-0.544855309
C,0,1.9305960623,4.4451371565,-0.270583048
C,0,2.3937740782,3.1766634968,0.0858416157
C,0,1.4816764709,2.1241392313,0.1587865683
C,0,1.7140023493,0.7330606142,0.491608408
O,0,3.0200641035,0.3171327101,0.7768255638
C,0,3.6984612613,-0.4597513159,-0.1238902457
O,0,3.2437448117,-0.8420483464,-1.1742310924
C,0,-0.7069191323,1.1291945894,0.0347757616
C,0,-1.9490674263,0.8598143405,0.0126514836
Si,0,-3.7094018767,0.3537598776,0.1265953975
C,0,-3.9739460209,-0.6976104503,1.6784723972
C,0,0.6628457239,-0.10517181,0.506946866
C,0,0.5208084427,-1.4399360721,0.8326402953
C,0,0.7187278506,-1.83852592,2.2784093263
Si,0,0.0957699326,-2.7522494976,-0.470109453
C,0,1.544686673,-3.9730565939,-0.5465505436
C,0,-0.1450350535,-1.9439575152,-2.1548173509
C,0,-1.4584330733,-3.7044269096,0.0635272434
C,0,-4.1915440721,-0.6060469971,-1.4287737662
C,0,-4.7670237493,1.9186462865,0.2575770255
C,0,5.0759485314,-0.7718376205,0.4070043184
H,0,-1.3923645173,3.7598211814,-0.6714501879
H,0,0.2293596957,5.6463334993,-0.8291061607
H,0,3.4422046271,3.0080838621,0.309685235
H,0,2.6292931893,5.2741583507,-0.3353145033
H,0,1.1069238347,-2.8593927583,2.3705863982
H,0,1.3989075057,-1.1551874353,2.796823683
H,0,-0.2378730834,-1.8187405353,2.8238242097
H,0,-1.6572042162,-4.5298409926,-0.6298380336
H,0,-1.3404462842,-4.1370272142,1.0631335642
H,0,-2.3469832997,-3.0657132606,0.0791606821
H,0,-0.3379790357,-2.6984457709,-2.9257051975
H,0,-0.9796785129,-1.2368825595,-2.1543615101
H,0,0.7595592369,-1.3946737689,-2.4331340212
H,0,1.3228659079,-4.7819198991,-1.2524441302
H,0,2.4502373228,-3.4635249971,-0.8888223101
H,0,1.7537029986,-4.4334496004,0.4251696108
H,0,-5.8273573941,1.6573253284,0.3540541255

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H,0,-4.4883312276,2.5149548465,1.1321976731
H,0,-4.656811364,2.5505525715,-0.6294137938
H,0,-5.2500819205,-0.887593785,-1.3914258413
H,0,-4.0386002471,0.0001504097,-2.3274042536
H,0,-3.6047233013,-1.5227705864,-1.5411948136
H,0,-5.025174409,-0.9958693505,1.7660796788
H,0,-3.3678925907,-1.6083268722,1.6635521436
H,0,-3.7101596065,-0.1347830174,2.5797849308
H,0,4.9921197317,-1.3638004536,1.3234124358
H,0,5.6346868463,-1.3300562207,-0.3431187472
H,0,5.6033625151,0.1511818143,0.6623125205
```

Restricted Analog of Structure 14 (ts for reversed diradical formation), RB3LYP/6-31G(d,p)

```
E(RB+HF-LYP) = -1508.41271658

 Zero-point correction=                           0.420091 (Hartree/Particle)
 Thermal correction to Energy=                    0.450884
 Thermal correction to Enthalpy=                  0.451828
 Thermal correction to Gibbs Free Energy=         0.357271
 Sum of electronic and zero-point Energies=          -1507.992626
 Sum of electronic and thermal Energies=             -1507.961833
 Sum of electronic and thermal Enthalpies=           -1507.960889
 Sum of electronic and thermal Free Energies=        -1508.055445

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 282.934            111.360           199.011

 C,0,0.1457756672,2.1531623571,-0.3157120388
 C,0,0.9108768316,3.3191999283,-0.2824299722
 C,0,0.2686744519,4.5561989452,-0.3643054285
 C,0,-1.1247500913,4.6349528551,-0.5104295125
 C,0,-1.897369687,3.4783157207,-0.5607579212
 C,0,-1.2554296258,2.2367505358,-0.4652568639
 C,0,-1.8066824825,0.9160365398,-0.4762425268
 O,0,-3.1828915284,0.7598397028,-0.3537178356
 C,0,-3.7293536601,0.1528679319,0.7550274128
 O,0,-3.0870724746,-0.2775767936,1.6780904865
 C,0,0.6331783966,0.7646216339,-0.205454659
 C,0,1.8123158156,0.2820440218,-0.1034961844
 Si,0,3.6097498271,0.0210237725,0.1205823577
 C,0,4.3615570971,-0.596297966,-1.5040791223
 C,0,-0.9007758679,-0.1180766513,-0.4741280165
 C,0,-1.065258479,-1.4493706232,-0.71856038
 C,0,-2.0415502439,-1.8801377331,-1.7950491354
 Si,0,-0.1642806891,-2.823857594,0.2355141534
 C,0,-1.3360163721,-4.3115681076,0.3346383046
 C,0,0.2438898303,-2.2616805848,1.9873421322
 C,0,1.3676185785,-3.3305775852,-0.7606741918
 C,0,3.9307141224,-1.2245077706,1.5089023972
 C,0,4.4657912687,1.6522345668,0.586002008
 C,0,-5.2307367068,0.1108679177,0.6161115796
 H,0,1.9867377375,3.2593717855,-0.1602383972
 H,0,0.8540363292,5.4685012699,-0.2979164058
 H,0,-2.9729710578,3.5269228752,-0.6963460578
 H,0,-1.6033222844,5.6071553158,-0.5834747299
```

```
H,0,-2.8518660115,-2.4884381107,-1.370972276
H,0,-2.4859277913,-1.0292023319,-2.3166590396
H,0,-1.5483488571,-2.5177790405,-2.542456759
H,0,1.9936576208,-4.0309809914,-0.1965523577
H,0,1.0731537482,-3.8230189436,-1.6938079242
H,0,1.976078662,-2.4598567816,-1.0169659446
H,0,0.6582460393,-3.0841153197,2.5816003466
H,0,0.9638744554,-1.4401233418,1.9881693714
H,0,-0.6655423651,-1.904216956,2.481617718
H,0,-0.8534320948,-5.1290799643,0.882693246
H,0,-2.2586633016,-4.0598735757,0.8683425797
H,0,-1.6089063106,-4.6961039794,-0.6534478632
H,0,5.536480375,1.4857050446,0.7569343694
H,0,4.3700566578,2.3973225646,-0.2107499902
H,0,4.0430489963,2.079444565,1.5010264722
H,0,5.0099805061,-1.3419238928,1.6606244722
H,0,3.4968771068,-0.8884111555,2.4560424674
H,0,3.5134637108,-2.2086584398,1.27883493
H,0,5.452667712,-0.6575671883,-1.4174605519
H,0,3.9925510236,-1.589685061,-1.7764341448
H,0,4.1319617584,0.0838845714,-2.330820984
H,0,-5.507511601,-0.4536813128,-0.2790586418
H,0,-5.6613834129,-0.3577511588,1.5000693243
H,0,-5.6266663204,1.1235141869,0.4983871211
```

Structure 15 (reversed diradical), UB3LYP/6-31G(d,p)

```
E(UB+HF-LYP) = -1508.44236212

 Zero-point correction=                           0.421634 (Hartree/Particle)
 Thermal correction to Energy=                    0.452512
 Thermal correction to Enthalpy=                  0.453456
 Thermal correction to Gibbs Free Energy=         0.358080
 Sum of electronic and zero-point Energies=          -1508.020728
 Sum of electronic and thermal Energies=             -1507.989850
 Sum of electronic and thermal Enthalpies=           -1507.988906
 Sum of electronic and thermal Free Energies=        -1508.084282

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  283.955            111.902           200.736

 C,0,0.6706497456,0.5617933614,-0.0508663259
 C,0,1.9803394816,0.0265118707,-0.1113639943
 C,0,1.9850392522,-1.3911207182,-0.3457983778
 C,0,0.6375954811,-1.8206566576,-0.402507794
 C,0,-0.2440014597,-0.6423948226,-0.1527132665
 C,0,0.3353221416,-3.1507743865,-0.6604026012
 C,0,1.3839490877,-4.0579736271,-0.8596794949
 C,0,2.7172510929,-3.6334207208,-0.800160533
 C,0,3.0323885715,-2.2992351416,-0.5450273149
 O,0,3.1211772299,0.8044525861,-0.1956163543
 C,0,4.1177469375,0.6495545411,0.7407613312
 C,0,5.2799258674,1.5467682833,0.3990673875
 C,0,-1.5453879788,-0.7072107313,0.0957379306
 Si,0,-3.2006760092,-1.4151101304,0.5019882209
 C,0,-3.489591505,-1.1876506869,2.3577929036
 C,0,0.3045953212,1.908367418,0.0796644973
```

```
Si,0,-1.347875112,2.679703107,-0.4518459864
C,0,-2.6091258022,2.6959027414,0.9655396672
C,0,-3.3002368474,-3.2658784408,0.0966756116
C,0,-4.5387334731,-0.523733898,-0.4924388157
C,0,1.3436317421,2.9057452153,0.5675490151
C,0,-2.0431046654,1.8960656344,-2.0300726846
C,0,-1.0142158735,4.4978027702,-0.8986657513
O,0,4.0373896851,-0.0905759007,1.6874928045
H,0,1.1596077103,-5.0999296867,-1.0672224704
H,0,3.5163783949,-4.3521977677,-0.9559379219
H,0,4.0667055807,-1.9774606162,-0.4937111955
H,0,-0.6945190032,-3.4829574467,-0.7231028292
H,0,0.8684420833,3.8001756595,0.9796718371
H,0,1.9739561347,2.4809794809,1.3536842587
H,0,2.008737457,3.2451651743,-0.2380463079
H,0,-2.9969177255,2.3676823587,-2.2942448412
H,0,-1.351400968,2.066311951,-2.862679449
H,0,-2.2075348853,0.8209087717,-1.9476635503
H,0,-1.9213191725,4.9309539729,-1.336244688
H,0,-0.7466572528,5.1134237061,-0.0342342966
H,0,-0.214965458,4.5979884088,-1.6408872546
H,0,-3.5436136602,3.1737588252,0.6486112791
H,0,-2.8437971133,1.6908534271,1.3227003028
H,0,-2.2191241508,3.2665553287,1.8157153801
H,0,-4.3037199126,-3.6367700794,0.3380145686
H,0,-3.1240482786,-3.4613348244,-0.9660412297
H,0,-2.5818279498,-3.8521045614,0.6776119128
H,0,-5.522636589,-0.9402171255,-0.2475884216
H,0,-4.5641984964,0.5478143777,-0.2763626886
H,0,-4.3855676423,-0.6450062619,-1.5695667252
H,0,-4.4573122824,-1.6143101303,2.6460495669
H,0,-2.7133901552,-1.6929800562,2.9412698068
H,0,-3.4906754305,-0.1326040532,2.6470999739
H,0,5.6358061295,1.3361851442,-0.6132486579
H,0,4.959459984,2.5927275158,0.420593062
H,0,6.081090325,1.3903013253,1.1202093536
```

Structure 16, model starting material, RB3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) = -348.944978128

 Zero-point correction=                           0.155074 (Hartree/Particle)
 Thermal correction to Energy=                    0.166020
 Thermal correction to Enthalpy=                  0.166964
 Thermal correction to Gibbs Free Energy=         0.116662
 Sum of electronic and zero-point Energies=           -348.789904
 Sum of electronic and thermal Energies=              -348.778958
 Sum of electronic and thermal Enthalpies=            -348.778014
 Sum of electronic and thermal Free Energies=         -348.828316

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  104.179             36.973           105.870

 C,0,0.9724769804,1.8574408216,0.0663047322
 C,0,1.4606692184,0.7621228502,-0.0885879885
 C,0,2.1126855815,-0.4781806113,-0.280576767
 C,0,1.5634721155,-1.7121920012,-0.2180233862
```

```
 C,0,0.1840595985,-2.1052134827,0.0530230912
 C,0,-0.8624881572,-1.3419548866,0.2941332517
 C,0,-1.9429571181,-0.6551548821,0.5327783133
 C,0,-2.8992987335,-0.1451831571,-0.5185665695
 C,0,0.353376512,3.1585512663,0.2685836196
 H,0,0.0072098918,-3.1803928289,0.0523935508
 H,0,2.2367453353,-2.5455545474,-0.393487815
 H,0,3.1755473921,-0.4184126759,-0.5007938623
 H,0,-2.1762570835,-0.4061133255,1.5684727758
 H,0,-3.9110231609,-0.5216409748,-0.335290812
 H,0,-2.590462605,-0.4524985236,-1.5183364814
 H,0,-2.9505157027,0.9484704127,-0.4948336243
 H,0,1.003614609,3.8199232239,0.8493034772
 H,0,0.1487161783,3.6514338557,-0.6872673429
 H,0,-0.5955508391,3.0633698807,0.8054303528
```

Structure 17 (model ene transition structure), RB3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) =  -348.891441144

Zero-point correction=                           0.152374 (Hartree/Particle)
 Thermal correction to Energy=                    0.161449
 Thermal correction to Enthalpy=                  0.162393
 Thermal correction to Gibbs Free Energy=         0.118572
 Sum of electronic and zero-point Energies=           -348.739067
 Sum of electronic and thermal Energies=              -348.729992
 Sum of electronic and thermal Enthalpies=            -348.729048
 Sum of electronic and thermal Free Energies=         -348.772870

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 101.311             33.963             92.230

C,0,0.4688658684,1.4746868646,-0.0637473392
 C,0,-0.467956475,0.6315875453,-0.0707044631
 C,0,-1.8913641618,0.4424797564,-0.1836971402
 C,0,-2.321076316,-0.8383257827,-0.0910151472
 C,0,-1.2528221603,-1.7913689582,0.1109636974
 C,0,-0.0151445756,-1.2811476261,-0.0139111032
 C,0,1.2974210572,-1.5031152374,-0.2610784314
 C,0,2.3061524307,-0.6147618687,0.2873755993
 C,0,1.0073360946,2.8230537545,0.1566638756
 H,0,-1.4340744336,-2.8069119179,0.4439383532
 H,0,-3.3641196875,-1.125989407,-0.1232518994
 H,0,-2.537194559,1.2962030258,-0.3468443676
 H,0,1.5533111138,-2.1107697129,-1.1282227243
 H,0,3.3131736806,-0.7628075343,-0.1008677456
 H,0,2.3140499267,-0.5363835203,1.3761034023
 H,0,1.8867572824,0.4370272401,-0.028939308
 H,0,1.6879977599,3.125605357,-0.6451500869
 H,0,0.2102394873,3.5726521234,0.2388730498
 H,0,1.581388856,2.8528436595,1.0892640385
```

Structure 17 (model ene transition structure), MP2/6-31G(d,p)

```
MP2=-347.6769264

 Zero-point correction=                           0.157005 (Hartree/Particle)
```

```
 Thermal correction to Energy=                    0.165993
 Thermal correction to Enthalpy=                  0.166937
 Thermal correction to Gibbs Free Energy=         0.123490
 Sum of electronic and zero-point Energies=           -347.519921
 Sum of electronic and thermal Energies=              -347.510933
 Sum of electronic and thermal Enthalpies=            -347.509989
 Sum of electronic and thermal Free Energies=         -347.553436

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  104.162             33.750             91.442

 C,0,0.4452266038,1.492822413,-0.0331550038
 C,0,-0.4980964457,0.6495573843,-0.1174956174
 C,0,-1.9166999752,0.4239621192,-0.1968212378
 C,0,-2.3247168808,-0.8643232423,-0.069804672
 C,0,-1.244213877,-1.8097807352,0.1327651722
 C,0,-0.0072759242,-1.3147136489,-0.041356437
 C,0,1.3153845687,-1.484043001,-0.2972890983
 C,0,2.2653995115,-0.5712831194,0.3167849944
 C,0,1.0784823471,2.8067523645,0.160768171
 H,0,-1.4153149886,-2.8168727477,0.4918824238
 H,0,-3.3646161327,-1.1608614367,-0.0671329129
 H,0,-2.587503112,1.2586271377,-0.3526833221
 H,0,1.5931481895,-1.96734208,-1.2312528028
 H,0,3.290870494,-0.6758882698,-0.0275887337
 H,0,2.2177211319,-0.5349330809,1.4034923695
 H,0,1.8361328361,0.4647772167,0.0086767549
 H,0,1.7564535247,3.0427530254,-0.6600803332
 H,0,0.3281644728,3.5971394434,0.2269398934
 H,0,1.6640040151,2.8188975867,1.0813690352
```

Structure 18 (model ene product), RB3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) = -349.005755530

 Zero-point correction=                           0.158554 (Hartree/Particle)
 Thermal correction to Energy=                    0.167380
 Thermal correction to Enthalpy=                  0.168325
 Thermal correction to Gibbs Free Energy=         0.125036
 Sum of electronic and zero-point Energies=           -348.847202
 Sum of electronic and thermal Energies=              -348.838375
 Sum of electronic and thermal Enthalpies=            -348.837431
 Sum of electronic and thermal Free Energies=         -348.880719

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  105.033             33.306             91.108

 C,0,0.2713555833,-0.9489497727,-0.1109982059
 C,0,-0.3503880678,0.3958836069,0.0436828193
 C,0,-1.7807334168,0.159374758,0.282181425
 C,0,-2.0051490812,-1.177053217,0.2172019431
 C,0,-0.7441915116,-1.8605960054,-0.0356295849
 C,0,0.2505303631,1.5865197035,-0.1550396142
 C,0,1.6740118868,-1.2990149634,-0.2749663492
 C,0,2.7581063691,-0.6052639999,0.1027670419
 C,0,-0.3855123669,2.9349498494,-0.0547552162
```

```
H,0,-0.6288518549,-2.9336379147,-0.1200942938
H,0,-2.9622464453,-1.669659075,0.3252666778
H,0,-2.5243634795,0.9283808474,0.4280364547
H,0,1.8375683291,-2.2751095688,-0.7288657412
H,0,3.7521833493,-0.9999319749,-0.0709928075
H,0,2.6973199501,0.3433088583,0.6215102636
H,0,1.2986206173,1.5854844746,-0.4387660876
H,0,0.1595344217,3.5580976492,0.6635827155
H,0,-0.3276738026,3.4552571584,-1.0180047786
H,0,-1.4302696329,2.8927097895,0.2516620435
```

Structure 19 (model diradical), UB3LYP/6-311+G(d,p)

```
E(UB+HF-LYP) = -348.924583642

Zero-point correction=                           0.154228 (Hartree/Particle)
 Thermal correction to Energy=                    0.164021
 Thermal correction to Enthalpy=                  0.164965
 Thermal correction to Gibbs Free Energy=         0.119146
 Sum of electronic and zero-point Energies=           -348.770356
 Sum of electronic and thermal Energies=              -348.760563
 Sum of electronic and thermal Enthalpies=            -348.759619
 Sum of electronic and thermal Free Energies=         -348.805438

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 102.924             35.239             96.435

 C,0,-0.9838679972,0.1864479313,0.0124939581
 C,0,0.407279859,-0.3844918799,-0.0069972368
 C,0,0.2389537152,-1.8446462135,-0.0241728365
 C,0,-1.1134969256,-2.1345334527,-0.0060651637
 C,0,-1.8661762607,-0.9452615285,0.0255167039
 C,0,1.562332488,0.2696810493,-0.020892774
 C,0,-1.3692057196,1.494634753,0.0005660547
 C,0,-0.4771313606,2.6927074949,-0.0159814009
 C,0,3.0028264131,0.0041995194,0.0219593358
 H,0,-2.9450864244,-0.8773344481,0.0526431211
 H,0,-1.5328538669,-3.1324877564,-0.0111392828
 H,0,1.052222116,-2.5549755112,-0.0519946768
 H,0,-2.4401484462,1.6856165357,0.0110280935
 H,0,-0.9084446675,3.4946900783,-0.6231700283
 H,0,0.5163312806,2.4508166334,-0.40319193
 H,0,-0.3385091745,3.1007527773,0.9947061167
 H,0,3.4629570605,0.473234033,0.8990262324
 H,0,3.2120405561,-1.0751317183,0.0756453898
 H,0,3.5124062968,0.4023933364,-0.8621128791
```

Restricted Analog of Structure 19 (model diradical), B3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) = -348.918046261

Zero-point correction=                           0.155646 (Hartree/Particle)
 Thermal correction to Energy=                    0.164725
 Thermal correction to Enthalpy=                  0.165669
 Thermal correction to Gibbs Free Energy=         0.122037
```

```
Sum of electronic and zero-point Energies=           -348.762400
Sum of electronic and thermal Energies=              -348.753322
Sum of electronic and thermal Enthalpies=            -348.752377
Sum of electronic and thermal Free Energies=         -348.796009

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  103.366             34.040             91.830

C,0,0.9544309432,0.2356059514,0.0593483964
C,0,-0.5367003219,0.1132960834,0.0108856165
C,0,-1.0204979315,1.436819015,0.0234421576
C,0,0.0681036866,2.3556733321,0.0723508476
C,0,1.2464378881,1.6502173622,0.1332850827
C,0,-1.2687679495,-1.0147070325,-0.3458603572
C,0,1.8894252018,-0.7441905741,-0.0099999221
C,0,1.6234369716,-2.2054298462,-0.050993459
C,0,-2.7022666526,-1.0846276221,0.0225550029
H,0,2.2385924209,2.0656583373,0.2510567941
H,0,-0.0286276639,3.4330294264,0.0868432952
H,0,-2.0593357602,1.716699715,-0.083183002
H,0,2.9291025657,-0.4244493305,-0.0661548644
H,0,2.3911303007,-2.7342721076,-0.6221864578
H,0,0.6180028274,-2.3865109306,-0.458560644
H,0,1.6296833368,-2.6243494802,0.9634617597
H,0,-2.7720120071,-1.8663105114,0.7946156041
H,0,-3.1577230435,-0.1742245154,0.4503465695
H,0,-3.3104239915,-1.4612106192,-0.806319247
```

Structure 20 (model ts from diradical to product), UB3LYP/6-311+G(d,p)

E(UB+HF-LYP) = -348.915179034

```
Zero-point correction=                           0.151613 (Hartree/Particle)
Thermal correction to Energy=                    0.160009
Thermal correction to Enthalpy=                  0.160953
Thermal correction to Gibbs Free Energy=         0.118876
Sum of electronic and zero-point Energies=           -348.763566
Sum of electronic and thermal Energies=              -348.755170
Sum of electronic and thermal Enthalpies=            -348.754226
Sum of electronic and thermal Free Energies=         -348.796303

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  100.407             32.649             88.560

C,0,-1.1348927375,-1.7913598576,-0.1784865552
C,0,0.0636097596,-1.0452668253,-0.2031591674
C,0,-0.3188713427,0.3891250253,0.0403865999
C,0,-1.7550469327,0.3910142037,0.1803503704
C,0,-2.2131063211,-0.9182549178,0.0713738713
C,0,1.3813535114,-1.4373233191,-0.2911917644
C,0,2.4218779268,-0.4374327492,-0.4553424893
C,0,0.5606936156,1.348153433,0.3983719213
C,0,0.3712195966,2.8138586902,0.4358556783
H,0,-1.2156014893,-2.8510705337,-0.3794977116
H,0,-3.2487638937,-1.2221972197,0.1516818975
```

H,0,-2.3511184433,1.2548498236,0.4379336471
H,0,1.6427920638,-2.4720042277,-0.082635587
H,0,3.4263530511,-0.7593750121,-0.1790859228
H,0,1.9978119586,0.4897157776,0.2006012588
H,0,2.4364810852,0.0445421059,-1.4360923621
H,0,0.6655185094,3.2282686334,1.4055322498
H,0,1.0383360841,3.2765654677,-0.3031141552
H,0,-0.6528313811,3.135623086,0.1957258961

Restricted Analog of Structure 20 (model ts from diradical to product), B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -348.914503722

Zero-point correction=	0.153204 (Hartree/Particle)
Thermal correction to Energy=	0.161316
Thermal correction to Enthalpy=	0.162260
Thermal correction to Gibbs Free Energy=	0.120767
Sum of electronic and zero-point Energies=	-348.761300
Sum of electronic and thermal Energies=	-348.753188
Sum of electronic and thermal Enthalpies=	-348.752244
Sum of electronic and thermal Free Energies=	-348.793737

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.227	31.833	87.330

C,0,-1.1380842213,-1.7784866941,-0.1905742946
C,0,0.0680961632,-1.0372684624,-0.2102275845
C,0,-0.3050418237,0.3992047482,0.0404868786
C,0,-1.7263759363,0.4071798405,0.1865881847
C,0,-2.2011967589,-0.9067265079,0.0714193864
C,0,1.3759563193,-1.4453996718,-0.3047458609
C,0,2.4384695876,-0.4660893621,-0.4648970269
C,0,0.5713614606,1.3514559213,0.4648249036
C,0,0.3106044134,2.8082866834,0.4304615209
H,0,-1.2257081945,-2.8334966282,-0.4129620748
H,0,-3.2397997686,-1.1997077416,0.1532658249
H,0,-2.3149389083,1.2681520089,0.4703800508
H,0,1.6179854489,-2.4885393444,-0.1134350915
H,0,3.4370089904,-0.825445189,-0.2148096234
H,0,2.062463577,0.4430463497,0.2080168172
H,0,2.45039544,0.0195633005,-1.443786966
H,0,0.5573117211,3.2783134604,1.387874045
H,0,1.0013611683,3.2543741028,-0.2984829863
H,0,-0.7088146983,3.09080071,0.1239233599

Structure 16, model starting material, RB3LYP/6-31G(d,p)

E(RB+HF-LYP) = -348.861795569

Zero-point correction=	0.156101 (Hartree/Particle)
Thermal correction to Energy=	0.166967
Thermal correction to Enthalpy=	0.167911
Thermal correction to Gibbs Free Energy=	0.118081
Sum of electronic and zero-point Energies=	-348.705694

```
 Sum of electronic and thermal Energies=             -348.694829
 Sum of electronic and thermal Enthalpies=           -348.693885
 Sum of electronic and thermal Free Energies=        -348.743715

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  104.773             36.822           104.876

 C,0,0.9661510184,1.8546017229,0.0570704995
 C,0,1.4590101121,0.7554552784,-0.0982281019
 C,0,2.1178400908,-0.4834450762,-0.2897890846
 C,0,1.5684315816,-1.7198808576,-0.2212882687
 C,0,0.1877843851,-2.1086979062,0.0549435574
 C,0,-0.8550537921,-1.3361583835,0.3001033955
 C,0,-1.9363203435,-0.6456745414,0.5464162988
 C,0,-2.8961624079,-0.13276704,-0.5017216913
 C,0,0.3367796297,3.1533788481,0.258061757
 H,0,0.0063421084,-3.1848160398,0.0545775224
 H,0,2.2410485342,-2.5561127621,-0.3962846709
 H,0,3.1818424553,-0.4229663003,-0.5140390799
 H,0,-2.1675467075,-0.3960204545,1.5841577628
 H,0,-3.9096141615,-0.5095818264,-0.318675363
 H,0,-2.5886088057,-0.4379228056,-1.504127474
 H,0,-2.9495918981,0.9622800847,-0.47676273
 H,0,0.920512571,3.7775548978,0.944671954
 H,0,0.2439277453,3.7024005398,-0.6865196952
 H,0,-0.6690734864,3.0443123992,0.6795916041
```

Structure 17 (model ene transition structure), RB3LYP/6-31G(d,p)

```
E(RB+HF-LYP) = -348.812684887

 Zero-point correction=                           0.153791 (Hartree/Particle)
 Thermal correction to Energy=                    0.162837
 Thermal correction to Enthalpy=                  0.163781
 Thermal correction to Gibbs Free Energy=         0.120042
 Sum of electronic and zero-point Energies=           -348.658894
 Sum of electronic and thermal Energies=              -348.649848
 Sum of electronic and thermal Enthalpies=            -348.648904
 Sum of electronic and thermal Free Energies=         -348.692643

                     E (Thermal)             CV                S
                      KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  102.182             33.827            92.056

 C,0,0.4539496138,1.4937090858,-0.0693590327
 C,0,-0.4766072033,0.6383713208,-0.0608461424
 C,0,-1.8989033147,0.4386430987,-0.1786087458
 C,0,-2.3226402213,-0.8478280246,-0.0971657478
 C,0,-1.2524416472,-1.7966146943,0.10399546
 C,0,-0.012545594,-1.2796184474,-0.0155559871
 C,0,1.2996207544,-1.5113845319,-0.2557799979
 C,0,2.3191520257,-0.617296787,0.2815178674
 C,0,1.0079045446,2.8354327688,0.1594650208
 H,0,-1.4316731297,-2.8112593931,0.4471085725
 H,0,-3.3663093723,-1.1397673272,-0.1336212421
 H,0,-2.5497658398,1.2902459635,-0.3450349491
 H,0,1.5587302972,-2.1462950955,-1.1044843055
```

```
H,0,3.326080259,-0.7906214259,-0.1013349977
H,0,2.3323476215,-0.5384508791,1.3722883984
H,0,1.9268851637,0.427344814,-0.0436335025
H,0,1.6901100908,3.1411363625,-0.6420402909
H,0,0.2211659171,3.5970225923,0.2538240639
H,0,1.5874952447,2.8501616553,1.0909520859
```

Structure 18 (model ene product), RB3LYP/6-31G(d,p)

```
E(RB+HF-LYP) = -348.927950138

 Zero-point correction=                           0.159698 (Hartree/Particle)
 Thermal correction to Energy=                    0.168459
 Thermal correction to Enthalpy=                  0.169403
 Thermal correction to Gibbs Free Energy=         0.126294
 Sum of electronic and zero-point Energies=           -348.768252
 Sum of electronic and thermal Energies=              -348.759491
 Sum of electronic and thermal Enthalpies=            -348.758547
 Sum of electronic and thermal Free Energies=         -348.801656

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  105.710             33.116            90.732

 C,0,0.2701615542,-0.9534167569,-0.1078577717
 C,0,-0.352342424,0.3930029269,0.0422734119
 C,0,-1.7832053736,0.1590236053,0.2811809745
 C,0,-2.0087408506,-1.1786099252,0.2182411
 C,0,-0.747273105,-1.8645555023,-0.0306560251
 C,0,0.2541507156,1.5831189333,-0.1581296703
 C,0,1.6747206917,-1.2960542882,-0.2788368002
 C,0,2.7552817948,-0.59608239,0.1038077444
 C,0,-0.3773893074,2.9351515796,-0.05547329
 H,0,-0.6326536184,-2.9398494947,-0.1104616209
 H,0,-2.9672822669,-1.6723250243,0.3273966526
 H,0,-2.5252898079,0.9327193281,0.4241903306
 H,0,1.8435594641,-2.2684560039,-0.7426599309
 H,0,3.7550705652,-0.9767946673,-0.0779816091
 H,0,2.684963759,0.3464126204,0.6355608163
 H,0,1.3035113893,1.5766670307,-0.4431480303
 H,0,0.1669416417,3.5556625889,0.6679338178
 H,0,-0.3163913809,3.461285602,-1.0168998848
 H,0,-1.4246119192,2.8952089254,0.2487714181
```

Structure 19 (model diradical), UB3LYP/6-31G(d,p)

```
E(UB+HF-LYP) = -348.848502980

 Zero-point correction=                           0.155361 (Hartree/Particle)
 Thermal correction to Energy=                    0.165133
 Thermal correction to Enthalpy=                  0.166077
 Thermal correction to Gibbs Free Energy=         0.119877
 Sum of electronic and zero-point Energies=           -348.693142
 Sum of electronic and thermal Energies=              -348.683370
 Sum of electronic and thermal Enthalpies=            -348.682426
 Sum of electronic and thermal Free Energies=         -348.728626

                     E (Thermal)             CV                S
```

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	103.623	35.016	97.237

C,0,-0.9839280925,0.187032233,0.0133701387
C,0,0.408509799,-0.3857545424,-0.0074348178
C,0,0.2391546425,-1.8459343302,-0.0226072815
C,0,-1.114202411,-2.1361613716,-0.0063751248
C,0,-1.8668907767,-0.9451465068,0.021711305
C,0,1.5658448717,0.2702165938,-0.0246175467
C,0,-1.3708481904,1.4965563808,0.0117053482
C,0,-0.4827080916,2.6987041198,0.0046152179
C,0,3.0084099147,-0.0018178809,-0.0009335658
H,0,-2.9475658179,-0.8755322113,0.0453562633
H,0,-1.5351534425,-3.1354843146,-0.0110033136
H,0,1.0557477557,-2.5554001661,-0.0469606608
H,0,-2.4436829076,1.6876483305,0.023003125
H,0,-0.8271755619,3.4383568807,-0.728953667
H,0,0.5534009951,2.4329048967,-0.2246460448
H,0,-0.4871948635,3.2040170938,0.9814417043
H,0,3.4842467289,0.4570017086,0.8752085266
H,0,3.216659228,-1.0830495228,0.0382119332
H,0,3.510667891,0.4033691316,-0.8882599058

Restricted Analog of Structure 19 (model diradical), B3LYP/6-31G(d,p)

E(RB+HF-LYP) = -348.840668506

Zero-point correction=	0.156793 (Hartree/Particle)
Thermal correction to Energy=	0.165719
Thermal correction to Enthalpy=	0.166663
Thermal correction to Gibbs Free Energy=	0.123430
Sum of electronic and zero-point Energies=	-348.683875
Sum of electronic and thermal Energies=	-348.674950
Sum of electronic and thermal Enthalpies=	-348.674005
Sum of electronic and thermal Free Energies=	-348.717238

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	103.990	33.748	90.992

C,0,0.9622377549,0.2454895298,0.0647129575
C,0,-0.5306636057,0.116813131,0.0153603049
C,0,-1.0197313265,1.4406165284,0.0224928453
C,0,0.0664379085,2.3619187505,0.072335282
C,0,1.2497667135,1.6596102576,0.1370155236
C,0,-1.247932183,-1.0189648961,-0.3457753326
C,0,1.8891122279,-0.7445315477,-0.0173577829
C,0,1.5871956705,-2.199789585,-0.0488161542
C,0,-2.6846341017,-1.109478499,0.0190407695
H,0,2.2415662327,2.0791737088,0.2594405772
H,0,-0.0334942251,3.4408861896,0.0880107717
H,0,-2.0615577033,1.7152458113,-0.0879785532
H,0,2.9338257698,-0.4410778295,-0.0955715152
H,0,2.3362933273,-2.7563618342,-0.620748273
H,0,0.5670374184,-2.3418938618,-0.4508015185
H,0,1.5787799882,-2.6172782861,0.9676331322
H,0,-2.7468036084,-1.8883703479,0.7961431053
H,0,-3.1591385369,-0.2048641091,0.441665882

H,0,-3.2872430141,-1.4955614589,-0.8118440863

Structure 20 (model ts from diradical to product), UB3LYP/6-31G(d,p)

E(UB+HF-LYP) = -348.839347701

Zero-point correction=	0.152779 (Hartree/Particle)
Thermal correction to Energy=	0.161096
Thermal correction to Enthalpy=	0.162040
Thermal correction to Gibbs Free Energy=	0.120140
Sum of electronic and zero-point Energies=	-348.686569
Sum of electronic and thermal Energies=	-348.678252
Sum of electronic and thermal Enthalpies=	-348.677308
Sum of electronic and thermal Free Energies=	-348.719207

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	101.089	32.402	88.186

C,0,-1.1368637199,-1.7928053866,-0.180862345
C,0,0.0625177131,-1.0458465035,-0.2036667658
C,0,-0.3207285332,0.3881362826,0.0417856386
C,0,-1.7580999929,0.3895662408,0.1837879081
C,0,-2.2168265405,-0.9194408291,0.0710116279
C,0,1.3823498144,-1.4384360198,-0.2895368141
C,0,2.4245238856,-0.4359756494,-0.4481301859
C,0,0.5658130437,1.3488216903,0.387505896
C,0,0.3738409908,2.8165785856,0.4344806493
H,0,-1.216651969,-2.8543929907,-0.3822181046
H,0,-3.2543177389,-1.2246712238,0.1478765452
H,0,-2.3537642667,1.2565251045,0.4397118259
H,0,1.6436967434,-2.4764573839,-0.0877376192
H,0,3.4290854404,-0.7583474308,-0.166456207
H,0,1.9914955106,0.4953813284,0.2011080923
H,0,2.4473593134,0.0419122482,-1.4328792675
H,0,0.6909930058,3.2307321681,1.3989861349
H,0,1.0202712925,3.2855100115,-0.3207269586
H,0,-0.657327298,3.1402177027,0.2240819036

Restricted Analog of Structure 20 (model ts from diradical to product), B3LYP/6-31G(d,p)

E(RB+HF-LYP) = -348.838360073

Zero-point correction=	0.154578 (Hartree/Particle)
Thermal correction to Energy=	0.162610
Thermal correction to Enthalpy=	0.163554
Thermal correction to Gibbs Free Energy=	0.122229
Sum of electronic and zero-point Energies=	-348.683782
Sum of electronic and thermal Energies=	-348.675750
Sum of electronic and thermal Enthalpies=	-348.674806
Sum of electronic and thermal Free Energies=	-348.716131

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	102.039	31.541	86.974

1	6	0	-2.120511	0.030200	0.010859
2	6	0	-0.841658	0.642117	0.028061
3	6	0	0.169340	-0.473276	0.057874
4	6	0	-0.592383	-1.681706	0.055563
5	6	0	-1.957562	-1.360037	0.002574
6	6	0	-0.475460	1.962073	-0.085896
7	6	0	0.911796	2.361246	0.114926
8	6	0	1.483434	-0.320525	-0.282004
9	6	0	2.540863	-1.314674	0.024307
10	1	0	-3.065475	0.557708	0.065565
11	1	0	-2.765995	-2.082000	-0.018037
12	1	0	-0.173183	-2.677096	-0.020655
13	1	0	-1.203143	2.681009	-0.461547
14	1	0	1.172212	3.336310	-0.301942
15	1	0	1.520422	1.449167	-0.343049
16	1	0	1.238850	2.307616	1.158454
17	1	0	3.164282	-1.517432	-0.854601
18	1	0	3.219241	-0.862250	0.762986
19	1	0	2.185635	-2.265545	0.455243

*Full System Energies, (U)B3LYP/6-31G***

	Potential E	zpe	E + zpe	Erel	Free Energy estimate 25 °C	Grel
Starting Material	-1508.472769	0.421576	-1508.051192	0.0	-1508.116872	0.0
Ene TS	-1508.432928	0.419670	-1508.013257	23.8	-1508.077000	25.0
Product	-1508.520603	0.424179	-1508.096424	-28.4	-1508.159056	-26.5
diradical	-1508.448106	0.422109	-1508.025997	15.8	-1508.088901	17.6
TS from diradical to product	-1508.442069	0.419118	-1508.022952	17.7	-1508.082968	21.3
reversed diradical	-1508.442362	0.421634	-1508.02073	19.1	-1508.08428	20.5
ts to reversed diradical	-1508.418567	0.419274	-1507.99929	32.6	-1508.06353	33.5

Model System Energies

	Potential E	zpe	E + zpe	Erel	Free En estimate 298	Grel
B3LYP / 6-31G**						
Starting Material	-348.8617956	0.156101	-348.706	0.0	-348.74372	0.0
Transition State	-348.8126849	0.153791	-348.659	29.4	-348.69264	32.0
Product	-348.9279501	0.159698	-348.768	-39.3	-348.80166	-36.4
Biradical	-348.848503	0.155361	-348.693	7.9	-348.72863	9.5
TS from Birad to prod	-348.8393477	0.152779	-348.687	12.0	-348.71921	15.4
carbene (restricted)	-348.8406685	0.156793	-348.684	13.7	-348.71724	16.6
carbene ts	-348.8383601	0.154578	-348.684	13.7	-348.71613	17.3
B3LYP / 6-311+G**						
Starting Material	-348.9449781	0.155074	-348.79	0.0	-348.82832	0.0
Transition State	-348.8914411	0.152374	-348.739	31.9	-348.77287	34.8
Product	-349.0057555	0.158554	-348.847	-36.0	-348.88072	-32.9
Biradical	-348.9245836	0.154228	-348.77	12.3	-348.80544	14.4
TS from Birad to prod	-348.915179	0.151613	-348.764	16.5	-348.7963	20.1
carbene (restricted)	-348.9180463	0.155646	-348.762	17.3	-348.79601	20.3
carbene ts	-348.9145037	0.153204	-348.761	17.9	-348.79374	21.7
BD(T)/6-31+G**			BD(T) + zpe			
Starting Material	-347.85666	0.155074	-347.70159	0.0		
Transition State	-347.80729	0.152374	-347.65491	29.3		
Product	-347.93029	0.158554	-347.77173	-44.0		
Biradical	-347.82238	0.154228	-347.66816	21.0		
carbene (restricted)	-347.83613	0.155646	-347.68049	13.2		
carbene ts	-347.83112	0.153204	-347.67792	14.9		
Biradical for Ubrk	-347.84019	0.154228	-347.68596	9.8		
TS from Birad to prod	-347.8313	0.151613	-347.67969	13.7		