

Supporting Information – Computational

Mechanism of Triflimide-Catalyzed [3,3]-Sigmatropic Rearrangements of *N*-Allylhydrazones—Predictions and Experimental Validation

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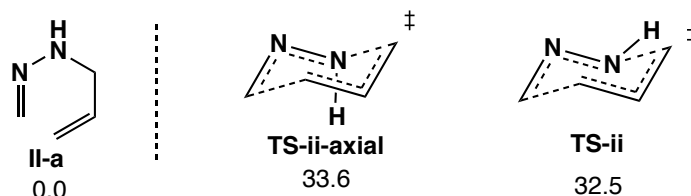
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All energy barriers (Gibbs free energies at 298.15 K) are with respect to the lowest energy conformer (determined by conformational analysis) optimized in diethyl ether solvent (experimental solvent used was diglyme) using B3LYP/6-31G(d,p)¹ with SMD solvation model² (this solvation model has recently been used by Houk and coworkers³ for studying similar systems in the acid-catalyzed Fisher indolizations) as implemented in *GAUSSIAN09*.⁴ For method validation, the parent system gas phase energies were calculated using restricted and unrestricted B3LYP calculations (with guess=(mix, always) keywords) but no difference was observed. For effect of solvent, calculations were performed in diethyl ether and with both CPCM⁵ and SMD solvation models. All methods yield similar energies but CPCM failed to meet convergence criteria for various structures therefore SMD solvation model was used throughout this study.



Appendix-Figure S1. Barriers for the *N*-allylhydrazone thermal [3,3]-sigmatropic rearrangement. All free energies (kcal/mol) were calculated at the B3LYP/6-31G(d,p) in diethyl ether using SMD solvation model with UA0 radii. Selected distances are in Ångstroms

1. (a) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 1372–1377; (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648–5652; (c) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* 1988, **37**, 785–789. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* 1994, **98**, 11623–11627.
2. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*, 2009, **18**, 6378–6396.
3. N. Çelebi-Ölçüm, B. W. Boal, A. D. Hutters, N. K. Garg, K. N. Houk, *J. Am. Chem. Soc.* 2011, **133**, 5752–5755.
4. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.
5. (a) V. Barone, M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995–2001; (b) V. Barone, M. Cossi, J. Tomasi, *J. Comput. Chem.* 1998, **19**, 404–517.

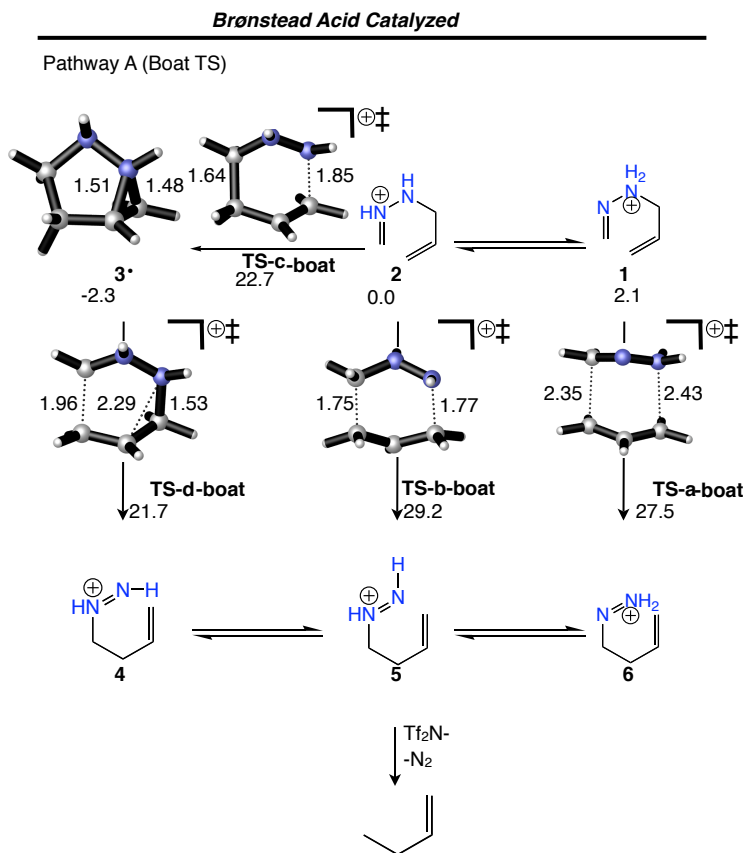


Figure S2. “Boat-like” pathways for the acid-catalyzed [3,3]-sigmatropic rearrangements. All free energies (kcal/mol) were calculated at the B3LYP/6-31G(d,p) in diethyl ether using SMD solvation model with UA0 radii. Selected distances are in Ångstroms.

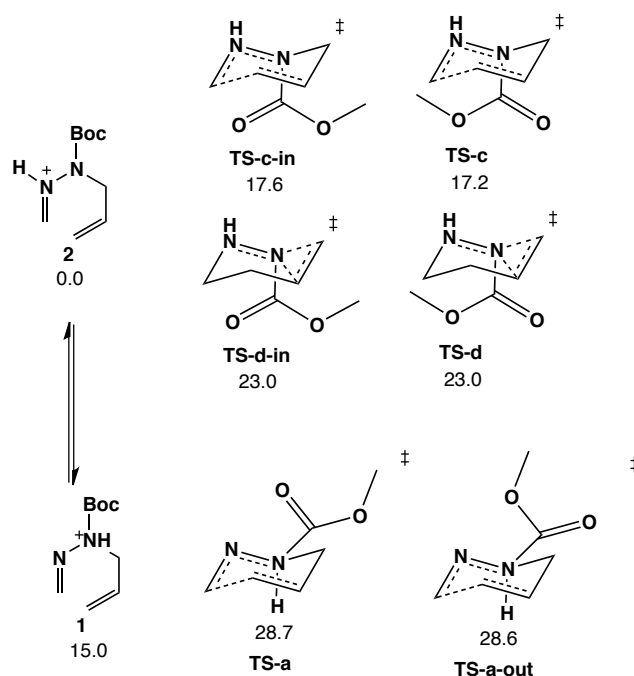


Figure S3. Energetics for the competing pathways in acid-catalyzed [3,3]-sigmatropic rearrangements of parent (unsubstituted) *N*-allyl-hydrazone. All free energies (kcal/mol) were calculated at the B3LYP/6-31G(d,p) in diethyl ether using SMD solvation model with UA0 radii. Selected distances are in Ångstroms.

Coordinates and energies.

See Table 1 in main text for labels.

R'=H			
R1=H R2=H R3=H R4=H			
TS-BF			
Zero-point correction=	0.131450 (Hartree/Particle)		
Thermal correction to Energy=	0.137518		
Thermal correction to Enthalpy=	0.138462		
Thermal correction to Gibbs Free Energy=	0.102214		
Sum of electronic and zero-point Energies=	-266.935240		
Sum of electronic and thermal Energies=	-266.929172		
Sum of electronic and thermal Enthalpies=	-266.928228		
Sum of electronic and thermal Free Energies=	-266.964476		
C	-1.14315700	1.07985100	0.26782100
C	1.20397900	-1.13710700	-0.21241300
C	1.43650800	0.11665800	0.34217300
C	0.98450900	1.26189900	-0.30263400
H	-0.95907900	1.08918600	1.34489200
H	1.00903800	-1.24156200	-1.27565100
H	1.49962300	-2.04193000	0.31254800
H	1.12809200	2.24172300	0.14647000
N	-1.37993600	-0.02740500	-0.40688600
H	0.78495800	1.25231000	-1.36991600
H	1.77676000	0.18627300	1.37368800
N	-0.95797400	-1.14483100	0.16301900
H	-0.93468100	-1.22478600	1.18777200
H	-1.27005600	-1.99245200	-0.31464700
H	-1.50553200	1.99713300	-0.18771000

A			
Zero-point correction=	0.132485 (Hartree/Particle)		
Thermal correction to Energy=	0.139693		
Thermal correction to Enthalpy=	0.140637		
Thermal correction to Gibbs Free Energy=	0.100856		
Sum of electronic and zero-point Energies=	-266.969529		
Sum of electronic and thermal Energies=	-266.962321		
Sum of electronic and thermal Enthalpies=	-266.961377		
Sum of electronic and thermal Free Energies=	-267.001158		
C	-2.45436400	-0.65096900	-0.03334600
C	0.40784800	-0.41436900	0.21885300
C	1.79810900	0.11988300	0.42159800
C	2.82262100	-0.18772500	-0.37038400
H	-2.37366800	1.33855400	-0.20199800
H	-1.91792100	-1.58731800	0.04765500
H	0.39116500	-1.16385500	-0.58091500
H	3.81900000	0.19825000	-0.17730100
N	-1.82685900	0.47336900	-0.10339200
H	2.70945700	-0.84197400	-1.23147300
N	-0.49348900	0.68361700	-0.15592500
H	1.94088500	0.77034800	1.28404400
H	0.03719500	-0.88769400	1.14367000
H	-0.25260200	1.62326900	0.15882400
H	-3.53586000	-0.62114300	-0.07914700

TS-AC			
Zero-point correction=	0.133681 (Hartree/Particle)		
Thermal correction to Energy=	0.139098		
Thermal correction to Enthalpy=	0.140042		
Thermal correction to Gibbs Free Energy=	0.105175		
Sum of electronic and zero-point Energies=	-266.950189		
Sum of electronic and thermal Energies=	-266.944772		
Sum of electronic and thermal Enthalpies=	-266.943827		
Sum of electronic and thermal Free Energies=	-266.978695		
C	1.39039100	-0.53563200	-0.25337700
C	-1.41554300	0.32165900	0.26623200
C	-0.42920200	1.26033400	-0.28433400
C	0.83547500	1.37066000	0.26095700
H	0.41803600	-1.56298700	1.21485300
H	1.42837700	-0.39438700	-1.32919500
H	-1.45308200	0.27733900	1.35583100
H	1.57826200	1.99652700	-0.22913300
N	0.37635300	-1.27018800	0.23657100
H	0.98106400	1.22130200	1.32912800
N	-0.90433300	-1.07035200	-0.21139900
H	-0.60166300	1.63369200	-1.29423800
H	-2.42074300	0.42475400	-0.14244400
H	-0.91274700	-1.10519200	-1.23485800
H	2.34946800	-0.64271100	0.25125300

B			
Zero-point correction=	0.133155 (Hartree/Particle)		
Thermal correction to Energy=	0.140219		
Thermal correction to Enthalpy=	0.141164		
Thermal correction to Gibbs Free Energy=	0.101801		
Sum of electronic and zero-point Energies=	-266.966386		
Sum of electronic and thermal Energies=	-266.959321		
Sum of electronic and thermal Enthalpies=	-266.958377		
Sum of electronic and thermal Free Energies=	-266.997739		
C	2.63124400	0.61373700	-0.02253200
C	-0.53282000	-0.33012900	0.57829900
C	-1.87187500	-0.37785000	-0.08830900
C	-2.74039300	0.63177500	-0.03248200
H	2.36004600	1.49680500	-0.61129100
H	-0.39338500	0.56794700	1.18350100
H	-3.71756800	0.55836300	-0.49999200
N	1.88827700	-0.40026000	0.16288200
H	-2.51890400	1.55685800	0.49500800
H	-2.12825800	-1.30173200	-0.60566600
H	-0.31754800	-1.21388200	1.18487100
H	3.61350200	0.58342100	0.44497200
H	0.46450800	0.53146000	-1.07850000
H	0.49150100	-1.13048300	-1.07917600
N	0.57726200	-0.30066200	-0.47118600

TS-AD			
Zero-point correction=	0.133995 (Hartree/Particle)		
Thermal correction to Energy=	0.139436		
Thermal correction to Enthalpy=	0.140380		
Thermal correction to Gibbs Free Energy=	0.105463		
Sum of electronic and zero-point Energies=	-266.801380		
Sum of electronic and thermal Energies=	-266.795939		
Sum of electronic and thermal Enthalpies=	-266.794995		
Sum of electronic and thermal Free Energies=	-266.829911		
C	1.08231400	-0.89139300	-0.26258800
C	-1.13674800	1.02642000	0.23834300
C	0.13699200	1.34831700	-0.26047700
C	1.28748000	0.72830200	0.29813000
H	-0.21882000	-1.64657300	1.16211700
H	1.13113100	-0.85347400	-1.34815700
H	-1.23721000	0.88721200	1.31407600
H	2.25025000	1.03846200	-0.10716900
N	-0.15556500	-1.31369100	0.19413200
H	1.30015800	0.62379900	1.38282500
N	-1.18808600	-0.68479200	-0.34896100
H	0.21028200	1.79244600	-1.25313700
H	-2.00234800	1.46862900	-0.24775100
H	-2.04443100	-0.98850000	0.13592800
H	1.90823600	-1.44222600	0.18430400

C			
Zero-point correction=	0.137149 (Hartree/Particle)		
Thermal correction to Energy=	0.142247		
Thermal correction to Enthalpy=	0.143191		
Thermal correction to Gibbs Free Energy=	0.108891		
Sum of electronic and zero-point Energies=	-266.976789		
Sum of electronic and thermal Energies=	-266.971692		
Sum of electronic and thermal Enthalpies=	-266.970747		
Sum of electronic and thermal Free Energies=	-267.005048		
C	1.53353200	-0.15344500	-0.01283500
C	-1.57859900	0.11774500	0.50005100
C	-0.63018100	0.84271900	-0.37574200
C	0.75874500	1.17802800	0.15248300
H	0.37936200	-1.57579500	1.01019100
H	2.02177200	-0.19433600	-0.99055600
H	-1.34360900	-0.01433000	1.55262200
H	1.21196900	1.98750400	-0.42293600
N	0.53242000	-1.24303000	0.05583800
H	0.70731000	1.48908100	1.19967200
N	-0.68950600	-0.67169700	-0.41331000
H	-1.01321700	1.32673200	-1.26979300
H	-2.63059400	0.07024700	0.23370200
H	-1.10776800	-1.15217600	-1.21806800
H	2.28916400	-0.31654300	0.75801500

TS-CE

Zero-point correction=	0.134024 (Hartree/Particle)
Thermal correction to Energy=	0.139319
Thermal correction to Enthalpy=	0.140263
Thermal correction to Gibbs Free Energy=	0.105604
Sum of electronic and zero-point Energies=	-266.951642
Sum of electronic and thermal Energies=	-266.946347
Sum of electronic and thermal Enthalpies=	-266.945403
Sum of electronic and thermal Free Energies=	-266.980062

C	1.46885700	0.12083800	-0.17413400
C	-1.64861200	0.01524300	0.31967200
C	-0.86157600	0.97689500	-0.29794400
C	0.46038200	1.33258900	0.22203000
H	0.88231700	-1.35890800	1.20521700
H	1.62931300	0.12993700	-1.25444500
H	-1.55126000	-0.19175200	1.38159800
H	0.87326400	2.23459000	-0.23661900
N	0.79056200	-1.07667600	0.22466500
H	0.48447400	1.42142600	1.31092400
N	-0.38180200	-1.34557600	-0.28038300
H	-1.12451200	1.29604400	-1.30671200
H	-2.59005600	-0.28959500	-0.12869300
H	-0.37425600	-1.14649700	-1.29068000
H	2.41968900	0.22953500	0.35057300

R'=Boc

R1=H R2=H R3=H R4=H

TS-BF

Zero-point correction=	0.172932 (Hartree/Particle)
Thermal correction to Energy=	0.183708
Thermal correction to Enthalpy=	0.184652
Thermal correction to Gibbs Free Energy=	0.136336
Sum of electronic and zero-point Energies=	-494.762973
Sum of electronic and thermal Energies=	-494.752197
Sum of electronic and thermal Enthalpies=	-494.751253
Sum of electronic and thermal Free Energies=	-494.799569

C	1.85621400	-1.55258300	-0.69604200
C	1.03896100	1.52350900	0.41312500
C	2.35982700	1.14877900	0.20284100
C	2.86780600	0.02770100	0.83344900
H	2.34434400	-1.10117200	-1.56350000
H	0.48043000	1.12668100	1.25614600
H	3.87954200	-0.31840200	0.63638400
N	0.64776600	-1.25547400	-0.31042800
H	2.35370900	-0.42236700	1.67758200
N	0.10630900	-0.16425800	-0.85918200
H	2.94046700	1.64085800	-0.57458800
C	-1.31202200	0.08683400	-0.70589900
O	-1.87067500	0.80100100	-1.49925000
O	-1.78900300	-0.50658300	0.36644800
C	-3.20957500	-0.31060700	0.60817800
H	-3.41851600	0.74926700	0.76358900
H	-3.78671700	-0.68928200	-0.23688100
H	-3.42248000	-0.88380200	1.50846800
H	2.29462600	-2.44774100	-0.26379400
H	0.60498400	2.37276600	-0.10847400
H	0.43831200	0.17003800	-1.77678600

B

Zero-point correction=	0.174985 (Hartree/Particle)
Thermal correction to Energy=	0.186368
Thermal correction to Enthalpy=	0.187312
Thermal correction to Gibbs Free Energy=	0.137138
Sum of electronic and zero-point Energies=	-494.783547
Sum of electronic and thermal Energies=	-494.772164
Sum of electronic and thermal Enthalpies=	-494.771220
Sum of electronic and thermal Free Energies=	-494.821394

C	1.22981000	2.13301700	-0.45647700
C	0.92569700	-1.06000200	0.25556800
C	2.37710100	-0.87357400	0.55393300
C	3.31576200	-0.88087200	-0.39364700
H	1.59822100	2.38231300	0.54296300
H	0.72931400	-1.38323600	-0.76647600
H	4.36684300	-0.77080800	-0.14369000
N	0.49129200	1.13880500	-0.74584200
H	3.07360600	-1.01623900	-1.44501700
H	2.64941600	-0.75293500	1.60180600
N	0.16929600	0.28272200	0.39947600
H	0.41280900	0.71956600	1.30943700
C	-1.34266900	0.12465500	0.44527800
O	-1.95252000	0.61064300	1.35148400
O	-1.72494900	-0.56804400	-0.59064000
C	-3.16542700	-0.78708900	-0.71809700
H	-3.66876500	0.17496500	-0.82288000
H	-3.27524500	-1.38660400	-1.61895500
H	-3.53214800	-1.32203300	0.15892500
H	1.50099000	2.78176400	-1.28766000
H	0.43550200	-1.73624500	0.96270100

A

Zero-point correction=	0.175765 (Hartree/Particle)
Thermal correction to Energy=	0.186878
Thermal correction to Enthalpy=	0.187822
Thermal correction to Gibbs Free Energy=	0.138609
Sum of electronic and zero-point Energies=	-494.808123
Sum of electronic and thermal Energies=	-494.797010
Sum of electronic and thermal Enthalpies=	-494.796065
Sum of electronic and thermal Free Energies=	-494.845278

C	-2.13857200	1.73622400	-0.21605200
C	-0.91662600	-0.77382300	-1.00040000
C	-1.87943600	-1.54177300	-0.12781100
C	-1.98271200	-1.44289500	1.19521700
H	-0.24403800	2.16772200	0.38183700
H	-2.81972900	0.99825200	-0.62079200
H	-0.12956900	-1.42575900	-1.38536000
H	-2.69614100	-2.04925000	1.74361600
N	-0.89447200	1.47558000	-0.03464000
H	-1.36084700	-0.77535100	1.78721200
N	-0.23008000	0.32728400	-0.31789400
H	-2.51348600	-2.23250800	-0.68147000
C	1.13233600	0.38851200	0.05970400
O	1.58651700	1.37992800	0.59397300
O	1.75447700	-0.72954400	-0.25149800
C	3.17008600	-0.77569300	0.07998400
H	3.30110700	-0.67979900	1.15878400
H	3.50641900	-1.75136900	-0.26539700
H	3.69941000	0.02469200	-0.43945500
H	-2.47789900	2.72631900	0.06691900
H	-1.42634100	-0.35447700	-1.87964800

TS-AC

Zero-point correction=	0.133681 (Hartree/Particle)
Thermal correction to Energy=	0.139098
Thermal correction to Enthalpy=	0.140042
Thermal correction to Gibbs Free Energy=	0.105175
Sum of electronic and zero-point Energies=	-266.950189
Sum of electronic and thermal Energies=	-266.944772
Sum of electronic and thermal Enthalpies=	-266.943827
Sum of electronic and thermal Free Energies=	-266.978695

C	1.25420900	-1.51835700	-0.28469400
C	1.22170600	1.29051900	0.58504100
C	1.85645700	0.86089400	-0.67817500
C	2.69648600	-0.24007300	-0.70804500
H	1.08935100	-1.26206100	1.74385600
H	0.66976500	-1.45850100	-1.19784600
H	1.83001500	-2.43450300	-0.15749800
H	1.87450100	1.25101100	1.45868000
H	3.08267500	-0.58770100	-1.66430600
N	0.66727100	-1.03789500	0.84009600
H	3.32167800	-0.45977600	0.15628300
N	0.14208000	0.22714100	0.77896400
H	1.42135300	1.23064900	-1.60733200
C	-1.11288700	0.45019400	0.16315300
O	-1.45466600	1.54757200	-0.21565500
O	-1.82550000	-0.67283100	0.12770800
C	-3.16230300	-0.53495800	-0.41370600
H	-3.75854400	0.12542100	0.21904100
H	-3.12184300	-0.13924200	-1.43030900
H	-3.57433800	-1.54284100	-0.40941200
H	0.70627100	2.24724000	0.52374400

TS-AD

Zero-point correction=	0.175389 (Hartree/Particle)
Thermal correction to Energy=	0.185260
Thermal correction to Enthalpy=	0.186204
Thermal correction to Gibbs Free Energy=	0.140208
Sum of electronic and zero-point Energies=	-494.773383
Sum of electronic and thermal Energies=	-494.763512
Sum of electronic and thermal Enthalpies=	-494.762568
Sum of electronic and thermal Free Energies=	-494.808564

C	2.22462100	-1.03221600	-0.45643000
C	0.63682400	1.37616600	0.32687100
C	2.01038700	1.36805500	-0.01281700
C	2.85529000	0.32708300	0.45716100
H	0.61265900	-1.71976800	0.70055400
H	2.38459300	-0.78633900	-1.50313600
H	0.37386500	1.12988900	1.35521100
H	3.90528900	0.38338700	0.16995100
N	0.89008000	-1.16468100	-0.12107700
H	2.71765100	0.00801200	1.49004100
N	0.08144800	-0.17621400	-0.49586600
H	2.33199100	1.95447100	-0.87341500
C	-1.27347600	-0.42025900	-0.03668800
O	-1.61149900	-1.45014300	0.49913700
O	-2.02779700	0.61692500	-0.35201100
C	-3.43179600	0.50072000	-0.00251900
H	-3.54125600	0.34751000	1.07279100
H	-3.87851900	1.44552200	-0.30641900
H	-3.88155300	-0.33151900	-0.54698800
H	2.81960100	-1.88037000	-0.12055400
H	0.00504800	2.12850100	-0.13306800

C

Zero-point correction=	0.179034 (Hartree/Particle)
Thermal correction to Energy=	0.188557
Thermal correction to Enthalpy=	0.189501
Thermal correction to Gibbs Free Energy=	0.144010
Sum of electronic and zero-point Energies=	-494.799045
Sum of electronic and thermal Energies=	-494.789522
Sum of electronic and thermal Enthalpies=	-494.788578
Sum of electronic and thermal Free Energies=	-494.834069

C	1.83028400	-1.43755300	-0.22669900
C	1.07199700	1.43732900	0.83176500
C	1.36971000	0.91421600	-0.50933500
C	2.47728000	-0.10788500	-0.69440200
H	1.12419800	-1.03269600	1.71434000
H	1.35759800	-1.95063900	-1.06886800
H	2.53763500	-2.12292500	0.24379000
H	1.74469500	1.22317800	1.65778200
H	2.79396600	-0.15619200	-1.73803700
N	0.78323300	-1.08247900	0.75262100
H	3.34434500	0.15536900	-0.08191800
N	0.30780300	0.20400100	0.38003700
H	0.92728600	1.42375200	-1.36156600
C	-1.12691100	0.38867300	0.02884000
O	-1.52216300	1.48330500	-0.26786900
O	-1.75492500	-0.75269900	0.09540100
C	-3.17393900	-0.70607500	-0.24120100
H	-3.29867100	-0.34723400	-1.26391500
H	-3.51585000	-1.73422500	-0.14323300
H	-3.69526600	-0.05210300	0.45945700
H	0.43721500	2.31254700	0.92768900

TS-CE

Zero-point correction=	0.175317 (Hartree/Particle)
Thermal correction to Energy=	0.185286
Thermal correction to Enthalpy=	0.186230
Thermal correction to Gibbs Free Energy=	0.139628
Sum of electronic and zero-point Energies=	-494.772896
Sum of electronic and thermal Energies=	-494.762927
Sum of electronic and thermal Enthalpies=	-494.761983
Sum of electronic and thermal Free Energies=	-494.808585

C	1.05958700	-1.58476600	-0.30659500
C	1.77221900	1.56453400	0.33338700
C	1.74468300	0.77837100	-0.78224400
C	2.24388600	-0.60743800	-0.79593800
H	1.21709600	-1.31749700	1.78289500
H	0.23382300	-1.56661200	-1.01672900
H	1.43619500	-2.60026600	-0.17714600
H	2.36603400	1.30119700	1.20456300
H	2.49542800	-0.95728800	-1.80185500
N	0.65494100	-1.04441900	0.96445000
H	3.09814500	-0.76291900	-0.13229900
N	0.09509900	0.09033000	1.09756300
H	1.19588600	1.12828800	-1.65522700
C	-1.02089800	0.46965600	0.22986100
O	-1.19922500	1.59608000	-0.14412800
O	-1.83241500	-0.57527800	0.11346900
C	-3.12500300	-0.29638100	-0.49629600
H	-2.98688600	0.09131900	-1.50687300
H	-3.63966600	-1.25529600	-0.51202700
H	-3.66971800	0.42657600	0.11332900
H	1.31706000	2.54875200	0.33324400

R²=H

R1=Ph R2=H R3=H R4=H

TS-BF

Zero-point correction=	0.211944 (Hartree/Particle)
Thermal correction to Energy=	0.222687
Thermal correction to Enthalpy=	0.223631
Thermal correction to Gibbs Free Energy=	0.175382
Sum of electronic and zero-point Energies=	-497.929675
Sum of electronic and thermal Energies=	-497.918933
Sum of electronic and thermal Enthalpies=	-497.917988
Sum of electronic and thermal Free Energies=	-497.966238

C	0.50932900	-0.06626100	0.66172700
C	3.68848400	0.22882100	-0.63334600
C	2.76886900	1.23464800	-0.45458600
C	1.45564100	1.09963400	-0.92534200
H	0.81387200	0.61246900	1.46551100
H	3.52101500	-0.56349600	-1.35663000
H	0.74698400	1.91305800	-0.80311600
N	1.24933100	-1.15058400	0.40123700
H	1.23072700	0.39705600	-1.72172000
N	3.00623700	2.06261400	0.21084000
N	2.45380500	-1.18310100	0.89398000
H	2.71015300	-0.63429200	1.72167100
H	2.95329700	-2.06150100	0.76112000
C	-0.91822500	-0.05802900	0.30040600
C	-1.74111500	0.93818800	0.84906900
C	-1.47075300	-1.01293200	-0.57034800
C	-3.09789200	0.97834700	0.53521700
H	-1.31918500	1.67787500	1.52574000
C	-2.82661000	-0.96827000	-0.87729900
H	-0.83845200	-1.78858700	-0.99078700
C	-3.64205300	0.02621000	-0.32798600
H	-3.72889600	1.74999600	0.96622800
H	-3.25119000	-1.71154000	-1.54588600
H	-4.70009300	0.05620000	-0.57230200
H	4.68096100	0.28640500	-0.19443600

A

Zero-point correction=	0.213892 (Hartree/Particle)
Thermal correction to Energy=	0.225608
Thermal correction to Enthalpy=	0.226552
Thermal correction to Gibbs Free Energy=	0.174153
Sum of electronic and zero-point Energies=	-497.970968
Sum of electronic and thermal Energies=	-497.959252
Sum of electronic and thermal Enthalpies=	-497.958308
Sum of electronic and thermal Free Energies=	-498.010706

C	0.20825500	-0.66835200	-0.20413800
C	-3.09971200	0.17284300	0.55325700
C	-4.46738400	-0.34130100	0.20692400
C	-5.50325100	0.44284800	-0.08236900
H	-0.71141200	1.13277700	-0.11472800
H	-0.00937500	-1.73290700	-0.28778300
H	-3.09768000	1.26767100	0.59056500
H	-6.48261400	0.02740500	-0.30032100
N	-0.82714100	0.12034200	-0.21341000
H	-5.41764500	1.52673200	-0.10207800
N	-2.13313300	-0.24290000	-0.49782000
H	-4.59197700	-1.42422200	0.22678100
H	-2.16749900	-1.24732500	-0.68797200
C	1.58394800	-0.25119900	-0.10397800
C	2.55006200	-1.26765900	0.05036600
C	1.99652200	1.09846800	-0.14216900
C	3.89474000	-0.94070400	0.17968200
H	2.23719500	-2.30843500	0.07297500
C	3.34032900	1.41471300	-0.01366800
H	1.27804400	1.90074800	-0.29293700
H	4.29006100	0.39803200	0.14914600
C	4.63372200	-1.72673700	0.29993100
H	3.65528500	2.45308100	-0.04922700
H	5.34149800	0.65422800	0.24390800
H	-2.77870700	-0.20594100	1.53560200

B

Zero-point correction=	0.214622 (Hartree/Particle)
Thermal correction to Energy=	0.226141
Thermal correction to Enthalpy=	0.227085
Thermal correction to Gibbs Free Energy=	0.175439
Sum of electronic and zero-point Energies=	-497.969738
Sum of electronic and thermal Energies=	-497.958218
Sum of electronic and thermal Enthalpies=	-497.957274
Sum of electronic and thermal Free Energies=	-498.008920

C	-0.10795500	0.39248300	0.43310100
C	3.02047800	-0.51616200	-0.43381300
C	4.44247400	-0.22753200	-0.06421600
C	5.15268100	0.74679500	-0.63237100
H	0.21201700	1.42574200	0.62591700
H	2.67233500	0.08468500	-1.27621700
H	6.19063700	0.91794300	-0.36362400
N	0.72933800	-0.58625600	0.45039200
H	4.73222700	1.39588900	-1.39722800
H	4.89457500	-0.87610000	0.68560500
H	2.18831400	0.82449400	0.96682200
H	2.39380800	-0.70928100	1.56092900
N	2.09275000	-0.17931500	0.72891300
C	-1.52237000	0.19329100	0.16166700
C	-2.36149600	1.32117800	0.14852000
C	-2.06168700	-1.08469800	-0.08406700
C	-3.72207600	1.17592000	-0.10720300
H	-1.94442800	2.30715400	0.33900000
C	-3.41959000	-1.22119900	-0.33706700
H	-1.41004600	-1.95250100	-0.07248900
C	-4.25001400	-0.09332200	-0.34907000
H	-4.36839800	2.04822100	-0.11748000
H	-3.83824800	-2.20522800	-0.52587600
H	-5.31193100	-0.20764700	-0.54809400
H	2.83244000	-1.57261300	-0.64208900

TS-AD

Zero-point correction=	0.213569 (Hartree/Particle)
Thermal correction to Energy=	0.223700
Thermal correction to Enthalpy=	0.224644
Thermal correction to Gibbs Free Energy=	0.177760
Sum of electronic and zero-point Energies=	-497.928037
Sum of electronic and thermal Energies=	-497.917906
Sum of electronic and thermal Enthalpies=	-497.916962
Sum of electronic and thermal Free Energies=	-497.963846

C	0.59594600	-0.44672200	-0.31608300
C	3.50857200	0.31079700	0.35074000
C	2.74414200	-0.65441400	1.01860900
C	1.37740400	-0.40600800	1.31356600
H	0.97372400	1.46843300	-1.03990900
H	0.81757100	-1.45428300	-0.66294000
H	3.34481400	1.36152300	0.58238400
H	0.84375800	-1.18381300	1.85727200
N	1.30630100	0.49712800	-1.06001200
H	1.12281800	0.59465200	1.65914800
N	2.57960900	0.23945900	-1.30929800
H	3.09388700	-1.68601000	1.00619700
H	2.98664900	1.08184600	-1.74158500
C	-0.86526900	-0.18110800	-0.13475500
C	-1.34179100	1.06502300	0.29902700
C	-1.77475400	-1.21184400	-0.40764000
C	-2.71157400	1.28351700	0.42788800
H	-0.65278800	1.86999600	0.54906000
C	-3.14408200	-0.99129300	-0.26966000
H	-1.41137600	-2.18169800	-0.73755100
C	-3.61383200	0.25576400	0.14468200
H	-3.07324500	2.25228700	0.75950700
H	-3.84257500	-1.79347600	-0.48851900
H	-4.68108900	0.42618000	0.25296100
H	4.52219200	0.06116000	0.04960600

TS-AC

Zero-point correction= 0.215033 (Hartree/Particle)
Thermal correction to Energy= 0.224740
Thermal correction to Enthalpy= 0.225684
Thermal correction to Gibbs Free Energy= 0.179695
Sum of electronic and zero-point Energies= -497.940398
Sum of electronic and thermal Energies= -497.930691
Sum of electronic and thermal Enthalpies= -497.929747
Sum of electronic and thermal Free Energies= -497.975735

C	0.58269300	-0.52820700	-0.17756400
C	3.42269100	0.56529100	0.06416000
C	2.77840600	-0.27820000	1.05440000
C	1.40375600	-0.09411000	1.35369000
H	1.09408400	1.13407500	-1.32121400
H	0.76490300	-1.60285500	-0.23494700
H	3.17924400	1.62763000	0.08576200
H	0.98187000	-0.77229900	2.09433800
N	1.33747500	0.15664700	-1.15768300
H	1.07906900	0.93698100	1.49279000
N	2.68053200	-0.04148900	-1.17218400
H	3.25161300	-1.23200200	1.28828600
H	2.89926200	-1.03532300	-1.28026500
C	-0.87203100	-0.20848600	-0.09058900
C	-1.79340000	-1.26427800	-0.03313800
C	-1.33781700	1.11616700	-0.05254600
C	-3.15981800	-1.00082600	0.04219400
H	-1.43954900	-2.29203900	-0.05489900
C	-2.70324700	1.37573000	0.01580400
H	-0.64084300	1.95180700	-0.06957300
C	-3.61547000	0.31770700	0.06382000
H	-3.86691000	-1.82408600	0.08157300
H	-3.05664200	2.40228700	0.03873800
H	-4.68042400	0.52359200	0.12267200
H	4.48873700	0.40466400	-0.08809500

C

Zero-point correction= 0.218057 (Hartree/Particle)
Thermal correction to Energy= 0.227564
Thermal correction to Enthalpy= 0.228508
Thermal correction to Gibbs Free Energy= 0.182499
Sum of electronic and zero-point Energies= -497.958574
Sum of electronic and thermal Energies= -497.949067
Sum of electronic and thermal Enthalpies= -497.948123
Sum of electronic and thermal Free Energies= -497.994132

C	0.56217000	-0.71356800	0.11460600
C	3.25747600	0.97231000	-0.16153600
C	2.83570800	-0.13624000	0.72503500
C	1.42179000	-0.14352600	1.28352900
H	0.99972600	0.57662300	-1.49596500
H	0.60172900	-1.80620300	0.16912600
H	2.62689100	1.85089100	-0.26294400
H	1.35047800	-0.77467000	2.17141900
N	1.29211600	-0.33530100	-1.13697000
H	1.10838200	0.86639900	1.56011900
N	2.67018900	-0.26056600	-0.77926300
H	3.59924400	-0.78593200	1.14333700
H	3.28574500	-0.88497200	-1.31192900
C	-0.88707400	-0.28328400	0.06217400
C	-1.25280300	1.07109700	0.06991900
C	-1.89041900	-1.25662900	-0.01007900
C	-2.59533700	1.44049100	0.00765400
H	-0.49493500	1.84970200	0.12791400
C	-3.23447600	-0.88748600	-0.06557600
H	-1.61840400	-2.30922200	-0.01977300
C	-3.58882200	0.46149300	-0.05840000
H	-2.86558600	2.49257400	0.01505300
H	-4.00236800	-1.65415000	-0.11527700
H	-4.63508100	0.75062600	-0.10178500
H	4.31111500	1.11111200	-0.38595500

TS-CE

Zero-point correction=	0.215360 (Hartree/Particle)
Thermal correction to Energy=	0.225158
Thermal correction to Enthalpy=	0.226102
Thermal correction to Gibbs Free Energy=	0.179770
Sum of electronic and zero-point Energies=	-497.912330
Sum of electronic and thermal Energies=	-497.902532
Sum of electronic and thermal Enthalpies=	-497.901587
Sum of electronic and thermal Free Energies=	-497.947919

C	0.58254300	-0.57343100	0.02593000
C	3.54260500	0.64483900	0.10261000
C	2.83339000	-0.05891400	1.06203800
C	1.40403200	0.15804800	1.26584900
H	0.99964800	0.74602100	-1.57821300
H	0.74133900	-1.64871000	0.14715700
H	3.21317500	1.62335800	-0.23661100
H	1.01786900	-0.31093700	2.17402600
N	1.29538000	-0.14115200	-1.15780200
H	1.12085700	1.21255100	1.24078900
N	2.56557400	-0.37953900	-1.29315500
H	3.29163100	-0.94574000	1.50102200
H	2.76909800	-1.33129300	-0.95586600
C	-0.88390500	-0.23468900	0.02062900
C	-1.82528900	-1.26855600	0.10228800
C	-1.32549600	1.09441200	-0.06936900
C	-3.18946800	-0.97980800	0.08679500
H	-1.49082400	-2.30112100	0.17407400
C	-2.68941900	1.37936200	-0.09350900
H	-0.61353000	1.91674900	-0.11791200
C	-3.62245700	0.34310400	-0.01301800
H	-3.91240000	-1.78856500	0.14990400
H	-3.02274800	2.41095000	-0.16676900
H	-4.68563500	0.56820600	-0.02507500
H	4.58650600	0.41244200	-0.09142400

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TS-BF

Zero-point correction=	0.253474 (Hartree/Particle)
Thermal correction to Energy=	0.269171
Thermal correction to Enthalpy=	0.270116
Thermal correction to Gibbs Free Energy=	0.209147
Sum of electronic and zero-point Energies=	-725.760464
Sum of electronic and thermal Energies=	-725.744767
Sum of electronic and thermal Enthalpies=	-725.743822
Sum of electronic and thermal Free Energies=	-725.804791

C	-0.65000300	0.51502900	0.64063600
C	2.11153900	2.20774600	-0.92411400
C	0.84986800	2.66821600	-0.66071400
C	-0.28254800	1.94736600	-1.07149300
H	-0.60194200	1.28726300	1.41662400
H	2.27538400	1.37089200	-1.59756400
H	-1.27758900	2.34953200	-0.90894900
N	0.44877600	-0.15838000	0.30628000
H	-0.19871900	1.17618300	-1.83092700
N	1.58975500	0.26362500	0.78550100
C	0.71625300	3.53871300	-0.02153100
C	2.80678900	-0.47185400	0.59065800
C	3.77359000	-0.20621500	1.26144500
O	2.68036300	-1.37003200	-0.36665700
C	3.85901400	-2.18210200	-0.61150800
H	4.70627600	-1.54721000	-0.87654100
H	4.09536100	-2.77160800	0.27621400
H	3.58743400	-2.83138900	-1.44200300
H	1.63845500	0.91821300	1.57827500
H	2.99342800	2.72034700	-0.54938000
C	-1.97286200	-0.03283900	0.32237400
C	-3.10193900	0.57599900	0.89466900
C	-2.13521300	-1.13845700	-0.53208700
C	-4.37630400	0.08664300	0.61901900
H	-2.97939100	1.42814600	1.55928000
C	-3.41073700	-1.62072900	-0.80212200
H	-1.26271900	-1.61490900	-0.96812500
C	-4.53200300	-1.01010800	-0.23015500
H	-5.24511300	0.55902900	1.06758300
H	-3.53455300	-2.47703100	-1.45856300
H	-5.52581000	-1.39200500	-0.44597000

A

Zero-point correction=	0.257061 (Hartree/Particle)
Thermal correction to Energy=	0.272831
Thermal correction to Enthalpy=	0.273775
Thermal correction to Gibbs Free Energy=	0.212580
Sum of electronic and zero-point Energies=	-725.813141
Sum of electronic and thermal Energies=	-725.797372
Sum of electronic and thermal Enthalpies=	-725.796427
Sum of electronic and thermal Free Energies=	-725.857623

C	0.84862100	0.52623400	-0.29044400
C	-1.85784700	1.43355300	-0.90465500
C	-1.73081300	2.61896900	0.02044200
C	-1.52052200	2.56549200	1.33346000
H	-0.15673900	-1.21053100	0.14501600
H	0.68547300	1.57188300	-0.53304500
H	-2.88364700	1.33654800	-1.26712100
H	-1.45655300	3.47325000	1.92469800
N	-0.20469000	-0.22065000	-0.13724300
H	-1.41798400	1.62602100	1.87107500
N	-1.51840600	0.14575000	-0.29771900
H	-1.84134600	3.57890100	-0.48215000
C	-2.39573500	-0.90818900	-0.01040900
O	-1.98321600	-1.99175500	0.36414500
O	-3.65541500	-0.54662600	-0.19472100
C	-4.64374400	-1.57765800	0.06023200
H	-4.58835500	-1.90018000	1.10138700
H	-5.60272300	-1.10546000	-0.14532800
H	-4.48038200	-2.42701900	-0.60528000
C	2.20288200	0.05700400	-0.13962200
C	3.22573300	1.01832000	-0.28008200
C	2.54179500	-1.28704700	0.13217300
C	4.55794200	0.64606500	-0.14472500
H	2.96692400	2.05239000	-0.49280500
C	3.87366400	-1.64741400	0.26620300
H	1.77647700	-2.05335000	0.23107100
C	4.88194400	-0.68389000	0.12882400
H	5.34130700	1.38977600	-0.25245900
H	4.13406600	-2.68062800	0.47408500
H	5.92297300	-0.97640200	0.23298600
H	-1.22703200	1.56202100	-1.79604500

B

Zero-point correction=	0.256469 (Hartree/Particle)
Thermal correction to Energy=	0.272434
Thermal correction to Enthalpy=	0.273378
Thermal correction to Gibbs Free Energy=	0.211003
Sum of electronic and zero-point Energies=	-725.787000
Sum of electronic and thermal Energies=	-725.771035
Sum of electronic and thermal Enthalpies=	-725.770091
Sum of electronic and thermal Free Energies=	-725.832466

C	-0.65066400	0.15575600	0.70981500
C	2.28435400	1.53633500	-0.21747200
C	1.56859200	2.81222000	0.08868600
C	0.78201100	3.42919000	-0.79283500
H	-0.52274100	0.48115500	1.75016800
H	2.24029600	1.25997700	-1.27033400
N	0.35553300	0.02672000	-0.08739800
H	0.60638100	3.02852700	-1.78807700
H	1.73737100	3.24268100	1.07509500
N	1.63385300	0.35535900	0.52910000
C	1.54031200	0.59685700	1.53449800
C	2.48764600	-0.89741300	0.52425000
O	2.73365000	-1.44713600	1.55842000
O	2.82894300	-1.17428900	-0.70504800
C	3.63962100	-2.37506700	-0.88851400
C	3.08390000	-3.24639400	-0.53925100
H	3.81799800	-2.42817200	-1.96032900
H	4.57667200	-2.27084800	-0.33949400
H	3.32544000	1.55129100	0.12125300
C	-2.01067600	-0.12435500	0.28185300
C	-3.04484300	0.02603700	1.22294400
C	-2.31204800	-0.53977500	-1.03058000
C	-4.36255100	-0.23638500	0.85979800
H	-2.81153300	0.34625900	2.23553900
C	-3.62881700	-0.79780500	-1.38486300
H	-1.51160300	-0.65380600	-1.75456900
C	-4.65372300	-0.64746800	-0.44192900
H	-5.15913600	-0.12150600	1.58853300
H	-3.86453100	-1.11698200	-2.39572700
H	-5.68206700	-0.85233000	-0.72659900
H	0.29613600	4.36975200	-0.55093600

TS-AD

Zero-point correction=	0.255409 (Hartree/Particle)
Thermal correction to Energy=	0.270305
Thermal correction to Enthalpy=	0.271249
Thermal correction to Gibbs Free Energy=	0.212436
Sum of electronic and zero-point Energies=	-725.760757
Sum of electronic and thermal Energies=	-725.745862
Sum of electronic and thermal Enthalpies=	-725.744917
Sum of electronic and thermal Free Energies=	-725.803730

C	0.67598200	0.60907800	-0.50760200
C	-2.00729800	1.78295700	0.72623800
C	-0.86449500	2.50813400	0.39626600
C	0.41393700	2.04121300	0.75526400
H	-0.33929100	-1.00287500	0.37557900
H	0.57696200	1.17270400	-1.43193900
H	-2.01458600	1.16558300	1.62207400
H	1.27556100	2.65724700	0.50907700
N	-0.41013900	-0.19978900	-0.27081000
H	0.51887900	1.48566100	1.68458300
N	-1.61375100	0.22190500	-0.57899300
H	-0.94398800	3.27461800	-0.37311600
C	-2.59736900	-0.76348900	-0.16018700
O	-2.31485500	-1.79979500	0.40094600
O	-3.79110000	-0.34087100	-0.52753500
C	-4.89763200	-1.22814100	-0.22284200
H	-4.94260600	-1.42163500	0.85063000
H	-5.78732400	-0.69787100	-0.55756200
H	-4.78025400	-2.16687000	-0.76753600
C	2.02562900	0.05383800	-0.23513600
C	3.04763200	0.31779300	-1.15894800
C	2.30194000	-0.71542000	0.90644500
C	4.32311900	-0.20458000	-0.95686600
H	2.83972200	0.92028300	-2.03962100
C	3.57701500	-1.23948600	1.09965200
H	1.53316900	-0.90290800	1.65387900
C	4.58806900	-0.98546800	0.16907300
H	5.10781700	-0.00315200	-1.67995100
H	3.78446600	-1.83877200	1.98106400
H	5.58329900	-1.39092900	0.32673200
H	-2.97654800	2.10121300	0.35794000

TS-AC

Zero-point correction=	0.257603 (Hartree/Particle)
Thermal correction to Energy=	0.271702
Thermal correction to Enthalpy=	0.272646
Thermal correction to Gibbs Free Energy=	0.215716
Sum of electronic and zero-point Energies=	-725.772095
Sum of electronic and thermal Energies=	-725.757997
Sum of electronic and thermal Enthalpies=	-725.757052
Sum of electronic and thermal Free Energies=	-725.813982

C	0.37214700	-0.17705800	0.36341200
C	-1.91560900	-2.09533300	-0.29931300
C	-1.29515800	-1.92140000	1.01390400
C	0.11677500	-1.71754900	1.10755700
H	-0.02199000	-0.66516200	-1.63172800
H	-0.05852800	0.52483700	1.07993200
H	-1.36541600	-2.68107900	-1.03604800
H	0.50094900	-1.62099500	2.12301300
N	-0.43562900	-0.20441800	-0.81958400
H	0.71447600	-2.40080200	0.50195300
N	-1.71645500	-0.61524000	-0.60364200
H	-1.94981400	-1.64461200	1.84000600
C	-2.74256600	0.29160900	-0.21383300
O	-3.80986200	-0.10239600	0.19713600
O	-2.36108300	1.54574100	-0.40857000
C	-3.37147600	2.54479100	-0.11829900
H	-4.24977700	2.38300600	-0.74558900
H	-3.65333900	2.50306900	0.93566200
H	-2.90133400	3.49811500	-0.35368000
C	1.82841300	0.08299300	0.14981700
C	2.44816200	1.10828300	0.87820100
C	2.58693500	-0.67135000	-0.75960200
C	3.80093600	1.38545100	0.68934100
H	1.86859700	1.69385600	1.58731400
C	3.93602200	-0.38830800	-0.95086300
H	2.13408500	-1.48634300	-1.32125600
C	4.54475200	0.64007200	-0.22606900
H	4.27209200	2.18368900	1.25511700
H	4.51461500	-0.97293800	-1.65986500
H	5.59920200	0.85564600	-0.37312100
H	-2.98032100	-2.31380000	-0.30311100

C

Zero-point correction=	0.259738 (Hartree/Particle)
Thermal correction to Energy=	0.273850
Thermal correction to Enthalpy=	0.274794
Thermal correction to Gibbs Free Energy=	0.217460
Sum of electronic and zero-point Energies=	-725.781227
Sum of electronic and thermal Energies=	-725.767115
Sum of electronic and thermal Enthalpies=	-725.766171
Sum of electronic and thermal Free Energies=	-725.823505

C	0.51690800	-0.12781300	0.63529800
C	-1.68471500	-2.03382100	-0.63764800
C	-1.31835500	-1.71174500	0.74858900
C	0.13953400	-1.55937300	1.12888300
H	-0.00172600	-0.16371000	-1.41533200
H	0.23291900	0.58392600	1.41724200
H	-0.91850500	-2.33066800	-1.34844400
H	0.27720400	-1.65248800	2.20778400
N	-0.38785800	0.14564900	-0.52101100
H	0.74454500	-2.32644300	0.63924300
N	-1.59161200	-0.56262300	-0.27210400
H	-2.09432600	-1.78602300	1.50596200
C	-2.87504700	0.17673500	-0.14697100
O	-3.88571800	-0.43353300	0.07597900
O	-2.67619600	1.45701300	-0.30259700
C	-3.87240600	2.28618300	-0.19956900
H	-4.30647200	2.18340100	0.79622300
H	-3.52182600	3.30196800	-0.36944800
H	-4.59268000	1.98733300	-0.96248000
C	1.96401100	0.10611300	0.26448000
C	2.63983400	1.21087300	0.79603100
C	2.64070200	-0.74552100	-0.62092100
C	3.96913900	1.45939200	0.45477700
H	2.12308000	1.87854800	1.48086200
C	3.96724800	-0.49339800	-0.96724500
H	2.14241100	-1.61466800	-1.04515800
C	4.63408700	0.60868600	-0.42843000
H	4.48278800	2.31778600	0.87796300
H	4.48134400	-1.16035800	-1.65336500
H	5.66920300	0.80160600	-0.69560800
H	-2.70100300	-2.34778200	-0.85309900

TS-CE

Zero-point correction=	0.256264 (Hartree/Particle)
Thermal correction to Energy=	0.270685
Thermal correction to Enthalpy=	0.271630
Thermal correction to Gibbs Free Energy=	0.214546
Sum of electronic and zero-point Energies=	-725.755897
Sum of electronic and thermal Energies=	-725.741476
Sum of electronic and thermal Enthalpies=	-725.740531
Sum of electronic and thermal Free Energies=	-725.797615

C	0.26400500	-0.24808300	0.30175100
C	-2.17254300	-2.55555900	0.06855600
C	-1.49508000	-1.92880500	1.06642200
C	-0.04400600	-1.67902700	1.01680700
H	0.06900000	-0.82764400	-1.73319600
H	-0.21934000	0.53011200	0.89391100
H	-1.65701000	-3.06604900	-0.74080900
H	0.40059500	-1.56764600	2.00985700
N	-0.44515600	-0.36834200	-0.96677400
H	0.50041100	-2.44708600	0.46339400
N	-1.70076800	-0.42540800	-1.10371500
H	-2.05834000	-1.47980200	1.88267600
C	-2.57560000	0.46346600	-0.33788700
O	-3.64516600	0.11903700	0.08282700
O	-2.06462600	1.68949600	-0.38117300
C	-2.94433600	2.74430500	0.10028100
H	-3.19114900	2.57355900	1.14942000
H	-2.37338500	3.66297600	-0.02167700
H	-3.85473200	2.76990600	-0.50105600
C	1.73756000	0.02235100	0.13568500
C	2.28531100	1.16774700	0.72557800
C	2.56781600	-0.85009400	-0.58296100
C	3.64730500	1.43809900	0.59967600
H	1.64801100	1.84768800	1.28541800
C	3.92660700	-0.57016600	-0.71642800
H	2.17037500	-1.75643200	-1.03629500
C	4.46807400	0.57160800	-0.12270100
H	4.06473200	2.32645500	1.06448400
H	4.56304100	-1.24914400	-1.27607500
H	5.52904800	0.78277500	-0.22036600
H	-3.25160300	-2.65962000	0.10151500

R'=H

R1=CH3 R2=H R3=H R4=H

TS-BF

Zero-point correction=	0.159288 (Hartree/Particle)
Thermal correction to Energy=	0.166893
Thermal correction to Enthalpy=	0.167837
Thermal correction to Gibbs Free Energy=	0.128111
Sum of electronic and zero-point Energies=	-306.233777
Sum of electronic and thermal Energies=	-306.226172
Sum of electronic and thermal Enthalpies=	-306.225228
Sum of electronic and thermal Free Energies=	-306.264954

C	1.13690800	0.15110500	0.37011500
C	-2.14876800	-0.07188800	-0.26598700
C	-1.39239700	-1.05866200	0.34056200
C	-0.20061000	-1.48919900	-0.23991900
H	0.90771000	0.05409100	1.43732000
H	-2.03467200	0.14460900	-1.32376200
H	-3.03224200	0.33518500	0.21881600
H	0.39761100	-2.25444000	0.24719000
N	0.50619700	1.06246900	-0.36235400
H	-0.03099700	-1.35889800	-1.30436900
H	-1.61584300	-1.34526200	1.36642000
N	-0.60612500	1.55277200	0.14040200
H	-0.74227700	1.60467100	1.15669500
H	-0.99435800	2.33518200	-0.38697600
C	2.49176600	-0.30220100	-0.08915500
H	3.25218200	0.36334000	0.33750700
H	2.71616400	-1.31243800	0.26099200
H	2.57462500	-0.26306400	-1.17719000

A

Zero-point correction=	0.160831 (Hartree/Particle)
Thermal correction to Energy=	0.169434
Thermal correction to Enthalpy=	0.170378
Thermal correction to Gibbs Free Energy=	0.127511
Sum of electronic and zero-point Energies=	-306.273076
Sum of electronic and thermal Energies=	-306.264474
Sum of electronic and thermal Enthalpies=	-306.263530
Sum of electronic and thermal Free Energies=	-306.306397

C	-1.89284100	-0.39395600	0.01376400
C	0.98101200	-0.34734800	0.25041200
C	2.41711600	0.07235500	0.39459000
C	3.39845300	-0.39300200	-0.37460100
H	-1.66854100	1.58084700	-0.23925800
H	-1.36352500	-1.33457700	0.13441200
H	0.88694700	-1.13848700	-0.50193200
H	4.42863300	-0.08597100	-0.22128600
N	-1.18894700	0.68400400	-0.09867700
H	3.21417600	-1.10305500	-1.17727300
N	0.17419400	0.80317700	-0.18317700
H	2.63317700	0.77708700	1.19744100
H	0.59691000	-0.73556700	1.20934000
H	0.45836800	1.70151500	0.21030200
C	-3.37506100	-0.37808400	-0.03865300
H	-3.71988200	-0.98412500	-0.88523000
H	-3.77837300	-0.84302700	0.86823300
H	-3.78415700	0.63112400	-0.13497800

B

Zero-point correction=	0.161352 (Hartree/Particle)
Thermal correction to Energy=	0.169904
Thermal correction to Enthalpy=	0.170848
Thermal correction to Gibbs Free Energy=	0.127905
Sum of electronic and zero-point Energies=	-306.272460
Sum of electronic and thermal Energies=	-306.263908
Sum of electronic and thermal Enthalpies=	-306.262964
Sum of electronic and thermal Free Energies=	-306.305907

C	2.05635200	0.33541800	-0.29172200
C	-1.13539700	-0.26193000	0.59483400
C	-2.51535100	-0.30019100	0.01579000
C	-3.31698200	0.76400700	-0.01193100
H	1.76389500	1.14029400	-0.98050100
H	-0.90381000	0.69202700	1.07261800
H	-4.32409300	0.69933500	-0.41247000
N	1.24192100	-0.58211100	0.06684700
H	-3.00727700	1.73145100	0.37694800
H	-2.85949300	-1.26173500	-0.36393600
H	-0.93975600	-1.07494700	1.29900400
H	-0.17531000	0.32468100	-1.19468400
H	-0.28465800	-1.32138100	-1.00932300
N	-0.09329400	-0.44288700	-0.50368100
C	3.44955500	0.33622100	0.22663000
H	3.62686400	-0.51010500	0.89173500
H	4.15533000	0.30310000	-0.61148700
H	3.63926100	1.27345600	0.76316800

TS-AD

Zero-point correction=	0.160872 (Hartree/Particle)
Thermal correction to Energy=	0.167897
Thermal correction to Enthalpy=	0.168841
Thermal correction to Gibbs Free Energy=	0.130393
Sum of electronic and zero-point Energies=	-306.237095
Sum of electronic and thermal Energies=	-306.230070
Sum of electronic and thermal Enthalpies=	-306.229126
Sum of electronic and thermal Free Energies=	-306.267573

C	0.97788300	-0.07097500	-0.37581400
C	-1.97127800	0.11592400	0.28124800
C	-1.18782500	1.16870800	-0.23617500
C	0.13607400	1.36766900	0.23900400
H	0.47692700	-1.45931800	1.08314500
H	0.85652100	-0.00325600	-1.45627200
H	-1.93468200	-0.06223900	1.35526200
H	0.68221400	2.20433500	-0.19563700
N	0.25711000	-1.15242000	0.12802800
H	0.28805600	1.28313100	1.31508600
N	-0.99096400	-1.29278000	-0.32677900
H	-1.46239500	1.58763000	-1.20379100
H	-2.94582800	-0.06120700	-0.16641200
H	-1.43607100	-2.04608100	0.21629400
C	2.42229200	0.01071500	0.08156100
H	2.86901900	0.95099000	-0.24699600
H	2.51233700	-0.04973500	1.17064800
H	2.99475500	-0.80779800	-0.36503900

TS-AC

Zero-point correction=	0.161930 (Hartree/Particle)
Thermal correction to Energy=	0.168685
Thermal correction to Enthalpy=	0.169629
Thermal correction to Gibbs Free Energy=	0.131740
Sum of electronic and zero-point Energies=	-306.249045
Sum of electronic and thermal Energies=	-306.242290
Sum of electronic and thermal Enthalpies=	-306.241346
Sum of electronic and thermal Free Energies=	-306.279235

C

Zero-point correction=	0.165018 (Hartree/Particle)
Thermal correction to Energy=	0.171511
Thermal correction to Enthalpy=	0.172455
Thermal correction to Gibbs Free Energy=	0.134860
Sum of electronic and zero-point Energies=	-306.270560
Sum of electronic and thermal Energies=	-306.264067
Sum of electronic and thermal Enthalpies=	-306.263123
Sum of electronic and thermal Free Energies=	-306.300718

C	1.02794000	-0.13007200	-0.38358300
C	-1.89911600	-0.03233900	0.38075400
C	-1.21194300	1.10257000	-0.22918100
C	0.07660800	1.45327900	0.17853600
H	0.39753500	-1.39666200	1.10969300
H	0.91624500	-0.01633300	-1.46186100
H	-1.81316700	-0.11695900	1.46470700
H	0.57683600	2.26017800	-0.35385400
N	0.24258500	-1.13446400	0.13423000
H	0.31661600	1.39537400	1.23966000
N	-1.07087400	-1.21106100	-0.22227200
H	-1.56765300	1.43967400	-1.20320700
H	-2.92959800	-0.18366300	0.06165500
H	-1.15528400	-1.21772000	-1.24242600
C	2.44285900	-0.02623300	0.11946800
H	3.03934000	-0.83426000	-0.31859100
H	2.88827300	0.92006100	-0.19370300
H	2.50131700	-0.10035500	1.20930100

C	1.08095000	0.03919200	-0.40394000
C	-1.89247400	-0.05552500	0.72923000
C	-1.21161200	0.80258700	-0.26666500
C	0.21270300	1.26313300	0.00218300
H	0.29380000	-1.52119000	0.76682800
H	1.27030400	0.09109500	-1.48216200
H	-1.44698200	-0.19828600	1.70975600
H	0.45821600	2.14708400	-0.58992700
N	0.21703600	-1.15642500	-0.18617900
H	0.34724600	1.51231100	1.05976300
N	-1.12310700	-0.70955000	-0.37825100
H	-1.80873700	1.27253400	-1.04301200
H	-2.96562900	-0.20996100	0.66370400
H	-1.64067600	-1.20332800	-1.11383700
C	2.40126800	-0.10245500	0.33684700
H	2.93745400	-0.99748900	0.00938800
H	3.03780900	0.76235400	0.13188100
H	2.25010200	-0.16090800	1.42082900

TS-CE

Zero-point correction=	0.161955 (Hartree/Particle)
Thermal correction to Energy=	0.168680
Thermal correction to Enthalpy=	0.169625
Thermal correction to Gibbs Free Energy=	0.131744
Sum of electronic and zero-point Energies=	-306.246433
Sum of electronic and thermal Energies=	-306.239708
Sum of electronic and thermal Enthalpies=	-306.238763
Sum of electronic and thermal Free Energies=	-306.276644

C	1.02243500	-0.00356300	-0.36311600
C	-2.06163900	0.13362200	0.44585800
C	-1.26961300	1.02068600	-0.26469900
C	0.11867800	1.27883700	0.11489500
H	0.44888100	-1.41751600	1.10061100
H	0.99683200	-0.02062000	-1.45733400
H	-1.86960700	-0.07606100	1.49417700
H	0.54485800	2.14657300	-0.39446200
N	0.28226900	-1.14106800	0.12747400
H	0.26018500	1.37120100	1.19503100
N	-0.94511100	-1.33760700	-0.25664800
H	-1.60710100	1.34783400	-1.24826100
H	-3.06190400	-0.10819400	0.09792000
H	-1.02281400	-1.13932500	-1.26428100
C	2.44606900	0.06569000	0.16204300
H	3.03422900	-0.77597500	-0.21323400
H	2.92203700	0.98756200	-0.17986100
H	2.47484300	0.05577200	1.25664100

R'=Boc

R1=Me R2=H R3=H R4=H

TS-BF

Zero-point correction=	0.200616 (Hartree/Particle)
Thermal correction to Energy=	0.213055
Thermal correction to Enthalpy=	0.213999
Thermal correction to Gibbs Free Energy=	0.161980
Sum of electronic and zero-point Energies=	-534.063134
Sum of electronic and thermal Energies=	-534.050695
Sum of electronic and thermal Enthalpies=	-534.049751
Sum of electronic and thermal Free Energies=	-534.101770

C	-1.83241800	-0.92996400	0.50558200
C	-0.36695000	2.11683900	-0.34854100
C	-1.71158800	1.92980500	-0.10485200
C	-2.41645500	0.94973300	-0.79500500
H	-2.13876600	-0.45024200	1.44255500
H	0.10449200	1.69213900	-1.23019800
H	-3.47032700	0.77919900	-0.59302000
N	-0.58692200	-0.85032200	0.08770600
H	-2.01876100	0.51623500	-1.70760100
N	0.20967900	0.00057500	0.71889800
H	-2.18236100	2.43635500	0.73512700
C	1.63166000	-0.02463800	0.48690300
O	2.37096700	0.48285800	1.29299000
O	1.92390200	-0.61041700	-0.65629400
C	3.34143300	-0.70147200	-0.96194900
H	3.77283600	0.29802900	-1.04128000
H	3.85426500	-1.27181500	-0.18557600
H	3.39084800	-1.22096800	-1.91710900
H	0.22290100	2.81750100	0.23671400
H	-0.01485400	0.32527300	1.67014300
C	-2.71000900	-2.00257400	-0.05923000
H	-3.75454700	-1.68472300	-0.10997200
H	-2.36744200	-2.31607000	-1.04728900
H	-2.67529000	-2.87220400	0.60945800

A

Zero-point correction=	0.203543 (Hartree/Particle)
Thermal correction to Energy=	0.216375
Thermal correction to Enthalpy=	0.217319
Thermal correction to Gibbs Free Energy=	0.163661
Sum of electronic and zero-point Energies=	-534.113762
Sum of electronic and thermal Energies=	-534.100930
Sum of electronic and thermal Enthalpies=	-534.099986
Sum of electronic and thermal Free Energies=	-534.153644

C	2.27876000	-0.63891600	-0.26748100
C	0.18740000	1.25579000	-1.00372000
C	0.80137800	2.32010500	-0.12642400
C	0.95077400	2.25411700	1.19447800
H	0.67076800	-1.75659100	0.30569200
H	2.57565500	0.33337100	-0.65156100
H	-0.79072200	1.57254500	-1.37234000
H	1.39049600	3.07837000	1.74649100
N	1.02282900	-0.86520500	-0.08529800
H	0.63296500	1.39386400	1.77896600
N	-0.03019900	-0.03026200	-0.33881200
H	1.12108300	3.20536800	-0.67419400
C	-1.26081000	-0.60452400	0.02787600
O	-1.31317900	-1.71395000	0.52441900
O	-2.26275600	0.21363100	-0.23585400
C	-3.58289700	-0.27538000	0.12310600
H	3.62607400	-0.47761500	1.19443700
H	-4.26278100	0.53113700	-0.14482300
H	-3.81263400	-1.18015300	-0.44206500
H	0.80612200	1.07354400	-1.89397400
C	3.30376600	-1.65993500	0.05023200
H	3.88110400	-1.88758600	-0.85409200
H	4.01193500	-1.24741300	0.77893600
H	2.87439200	-2.58364500	0.44539200

B

Zero-point correction=	0.202667 (Hartree/Particle)
Thermal correction to Energy=	0.215834
Thermal correction to Enthalpy=	0.216779
Thermal correction to Gibbs Free Energy=	0.161693
Sum of electronic and zero-point Energies=	-534.090025
Sum of electronic and thermal Energies=	-534.076857
Sum of electronic and thermal Enthalpies=	-534.075913
Sum of electronic and thermal Free Energies=	-534.130999

C	1.40362600	1.60481300	0.26873300
C	0.42377600	-1.57013800	0.04484700
C	1.84897200	-1.81155900	0.42623600
C	2.84060900	-1.81620200	-0.46485700
H	1.63435700	1.48553900	1.33537100
H	0.25994300	-1.57010600	-1.03255900
H	3.86364500	-2.02681500	-0.16760600
N	0.56631100	0.85219600	-0.33933200
H	2.66570900	-1.62892000	-1.52156400
H	2.04679900	-2.01802100	1.47734200
N	-0.03451100	-0.17560700	0.51656600
C	0.21364000	-0.05270800	1.51724400
C	-1.53872700	0.01345500	0.47484900
O	-2.11030600	0.39208000	1.45524700
O	-1.97193200	-0.29582700	-0.71632700
C	-3.40820800	-0.13743600	-0.93484600
H	-3.69378100	0.89727200	-0.74063900
H	-3.56071900	-0.39570500	-1.98036700
H	-3.95319000	-0.81695300	-0.27806600
H	-0.26116400	-2.27514200	0.52632800
C	2.09804200	2.68689700	-0.47686300
H	1.89677100	3.65087900	0.00497700
H	3.18170300	2.52799300	-0.42678600
H	1.77898600	2.72026600	-1.51944100

TS-AD

Zero-point correction=	0.203105 (Hartree/Particle)
Thermal correction to Energy=	0.214588
Thermal correction to Enthalpy=	0.215532
Thermal correction to Gibbs Free Energy=	0.166066
Sum of electronic and zero-point Energies=	-534.068198
Sum of electronic and thermal Energies=	-534.056715
Sum of electronic and thermal Enthalpies=	-534.055771
Sum of electronic and thermal Free Energies=	-534.105237

C	2.05158800	-0.48081700	-0.45481200
C	0.02486500	1.66936400	0.34610400
C	1.36718600	1.89352700	-0.01430400
C	2.38892100	1.03840200	0.46420300
H	0.55981800	-1.40693400	0.70377900
H	2.12149600	-0.15381400	-1.49108100
H	-0.18849400	1.35132000	1.36546900
H	3.40870500	1.28210700	0.16897100
N	0.75107300	-0.81388000	-0.11792100
H	2.31187100	0.69598700	1.49567900
N	-0.21909600	-0.00565200	-0.52098500
H	1.56830800	2.50695500	-0.89212500
C	-1.50232500	-0.47526500	-0.02587400
O	-1.63612800	-1.49950500	0.60396500
O	-2.44309300	0.36223900	-0.41960400
C	-3.79664100	0.01264900	-0.02969000
H	-3.87670500	-0.02326400	1.05865300
H	-4.42215100	0.80487100	-0.43691900
H	-4.06943000	-0.95365700	-0.45733100
H	-0.74559000	2.27562900	-0.11802100
C	3.09948100	-1.49853400	-0.04923800
H	4.10020300	-1.10048800	-0.22626500
H	3.01809200	-1.77417000	1.00638400
H	2.98312900	-2.40021700	-0.65852100

TS-AC

Zero-point correction=	0.204360 (Hartree/Particle)
Thermal correction to Energy=	0.215555
Thermal correction to Enthalpy=	0.216499
Thermal correction to Gibbs Free Energy=	0.167407
Sum of electronic and zero-point Energies=	-534.081299
Sum of electronic and thermal Energies=	-534.070104
Sum of electronic and thermal Enthalpies=	-534.069160
Sum of electronic and thermal Free Energies=	-534.118252

C	1.45189900	0.87903800	0.25452200
C	0.49812200	-1.85038300	-0.58187700
C	1.18106600	-1.58126800	0.69088100
C	2.28096100	-0.71112900	0.72366200
H	1.16728400	0.54148800	-1.76377400
H	0.83634200	1.05440600	1.13717200
H	1.14514300	-1.99033900	-1.44917900
H	2.72492700	-0.50796100	1.69702000
N	0.68497300	0.55476300	-0.86195000
H	3.00215300	-0.78809600	-0.09079100
N	-0.18041600	-0.48908100	-0.72056000
H	0.62844600	-1.79528600	1.60610100
C	-1.45483800	-0.31666200	-0.12342700
O	-2.10618800	-1.25707000	0.27130700
O	-1.80413200	0.96529000	-0.12701800
C	-3.13674400	1.24297000	0.36973400
H	-3.88296600	0.78618600	-0.28323000
H	-3.25162400	0.86490900	1.38720400
H	-3.22511800	2.32811700	0.34932400
H	-0.28467400	-2.60427700	-0.53899200
C	2.52704800	1.91384300	0.03866400
H	2.05372300	2.89220700	-0.09784900
H	3.17603700	1.97801500	0.91430400
H	3.14060200	1.69532100	-0.84026100

C

Zero-point correction=	0.206877 (Hartree/Particle)
Thermal correction to Energy=	0.217872
Thermal correction to Enthalpy=	0.218817
Thermal correction to Gibbs Free Energy=	0.169151
Sum of electronic and zero-point Energies=	-534.093010
Sum of electronic and thermal Energies=	-534.082015
Sum of electronic and thermal Enthalpies=	-534.081071
Sum of electronic and thermal Free Energies=	-534.130736

C	1.80997000	-0.73287200	-0.38280400
C	0.34245200	1.78668500	0.87238900
C	0.75073100	1.44030600	-0.49588000
C	2.08203300	0.75773600	-0.73659700
H	1.09394000	-0.61438000	1.59847600
H	1.38233900	-1.22490400	-1.26423200
H	1.05894900	1.71885400	1.68643300
H	2.40134900	0.87391100	-1.77433300
N	0.73683200	-0.71038600	0.64482100
H	2.85475000	1.18184500	-0.08704600
N	-0.07107400	0.41962300	0.35386500
H	0.17280000	1.85745400	-1.31629700
C	-1.50692200	0.23699300	0.01491000
O	-2.16414500	1.19517400	-0.29043300
O	-1.83576300	-1.02194800	0.11003100
C	-3.22535600	-1.32858900	-0.21346600
H	-3.41774400	-1.09307600	-1.26140300
H	-3.32431500	-2.39622500	-0.02953900
H	-3.88979800	-0.75564500	0.43484500
H	-0.50305300	2.45193100	1.01651500
C	3.01470800	-1.51879700	0.10562600
H	2.73686200	-2.54907100	0.34418300
H	3.77972100	-1.54888100	-0.67458900
H	3.46021700	-1.06130400	0.99649300

TS-CE

Zero-point correction=	0.203287 (Hartree/Particle)
Thermal correction to Energy=	0.214630
Thermal correction to Enthalpy=	0.215574
Thermal correction to Gibbs Free Energy=	0.166468
Sum of electronic and zero-point Energies=	-534.067161
Sum of electronic and thermal Energies=	-534.055818
Sum of electronic and thermal Enthalpies=	-534.054874
Sum of electronic and thermal Free Energies=	-534.103981

C	1.27561400	-0.96231400	-0.25006000
C	0.96595900	2.32040800	0.27576600
C	1.19510100	1.50776500	-0.79317800
C	2.09683800	0.34444100	-0.74061500
H	1.31373700	-0.56901400	1.83268000
H	0.46650000	-1.14551500	-0.95951300
H	1.58967400	2.28823100	1.16503800
H	2.47687900	0.06661000	-1.72864000
N	0.69974800	-0.51569600	1.00616600
H	2.93716100	0.48202800	-0.05448600
N	-0.19322400	0.37909800	1.11264500
H	0.58357300	1.63137100	-1.68571500
C	-1.35952600	0.37169100	0.22974900
O	-1.87751100	1.37852400	-0.16820300
O	-1.80182000	-0.87707800	0.12757800
C	-3.10666400	-1.02472900	-0.50127800
H	-3.07362000	-0.64495500	-1.52374300
H	-3.30415400	-2.09507900	-0.48907800
H	-3.85790800	-0.48447500	0.07725800
H	0.22777700	3.11337600	0.22580900
C	2.16656100	-2.18236400	-0.07957100
H	1.57989500	-3.04966900	0.23388700
H	2.63913200	-2.42107100	-1.03505400
H	2.96064200	-2.00674400	0.65396500

R'=H

R1=H R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.158759 (Hartree/Particle)
Thermal correction to Energy=	0.166558
Thermal correction to Enthalpy=	0.167502
Thermal correction to Gibbs Free Energy=	0.127299
Sum of electronic and zero-point Energies=	-306.235870
Sum of electronic and thermal Energies=	-306.228071
Sum of electronic and thermal Enthalpies=	-306.227126
Sum of electronic and thermal Free Energies=	-306.267330

C	-2.07035500	-0.01275800	0.35358900
C	1.25677600	0.17711000	-0.37877400
C	0.53290500	1.17410900	0.27913800
C	-0.62504300	1.69178400	-0.27083000
H	-1.85702200	0.09806100	1.41977600
H	1.02941000	-0.00071900	-1.42883200
H	-1.19359900	2.45757100	0.25066700
N	-1.48215500	-0.90115700	-0.40664900
H	-0.85357400	1.55554100	-1.32306400
H	0.80176200	1.43422800	1.30197600
N	-0.36258700	-1.43354800	0.06848000
H	-0.22779500	-1.51523100	1.08300300
H	-0.03853200	-2.23923400	-0.46585400
H	-2.98981200	0.41792300	-0.03160900
C	2.52497900	-0.40392400	0.14116000
H	2.66182600	-1.44233800	-0.17412800
H	3.36143900	0.16045100	-0.29692500
H	2.60809700	-0.33212800	1.22845700

A

Zero-point correction=	0.160968 (Hartree/Particle)
Thermal correction to Energy=	0.169278
Thermal correction to Enthalpy=	0.170222
Thermal correction to Gibbs Free Energy=	0.128646
Sum of electronic and zero-point Energies=	-306.258175
Sum of electronic and thermal Energies=	-306.249865
Sum of electronic and thermal Enthalpies=	-306.248921
Sum of electronic and thermal Free Energies=	-306.290497

C	2.58562700	0.26640800	0.45880700
C	-0.35275900	0.15407600	0.29014300
C	-1.61614900	-0.66959700	0.40133800
C	-2.82777100	-0.29203200	-0.00000600
H	2.45921200	-1.30078300	-0.76704500
H	2.08428900	1.06092500	0.99415700
H	-3.68431500	-0.94338200	0.14464400
N	1.92881400	-0.58014900	-0.26047700
H	-3.02591700	0.66721800	-0.46771600
N	0.60749700	-0.62968400	-0.52090900
H	-1.48390700	-1.64008900	0.87989600
H	0.07294500	0.23265100	1.30526600
H	0.32411300	-1.54937800	-0.85446900
H	3.66174500	0.15390800	0.49470900
C	-0.52674700	1.55347000	-0.30408100
H	-0.97255200	1.50074600	-1.30024400
H	-1.16857200	2.15817300	0.34192900
H	0.43094100	2.07347500	-0.39904400

B

Zero-point correction=	0.160707 (Hartree/Particle)
Thermal correction to Energy=	0.168324
Thermal correction to Enthalpy=	0.169268
Thermal correction to Gibbs Free Energy=	0.128735
Sum of electronic and zero-point Energies=	-306.254456
Sum of electronic and thermal Energies=	-306.246839
Sum of electronic and thermal Enthalpies=	-306.245894
Sum of electronic and thermal Free Energies=	-306.286428

C	2.69150900	-0.82852500	-0.34386900
C	-0.54302200	0.34883700	-0.18862600
C	-1.83496000	-0.30932400	0.19943900
C	-2.55152600	-1.05663400	-0.63898100
H	3.14697400	-0.08379100	0.31768600
H	-0.31598000	0.16339300	-1.24133300
H	-3.49839400	-1.49184900	-0.33408000
N	1.45654800	-1.12616400	-0.37480100
H	-2.22900100	-1.25080400	-1.65911300
H	-2.19054000	-0.11529700	1.21218700
H	3.33421700	-1.36934100	-1.03579300
H	0.23654100	-1.06323100	1.21032100
H	1.17909600	0.30320000	1.13016500
N	0.63407900	-0.36735300	0.56094300
C	-0.48324200	1.83769100	0.13410700
H	-0.67264100	2.03272500	1.19498600
H	0.48049900	2.27640100	-0.14587600
H	-1.25907100	2.34999800	-0.44021800

TS-AD

Zero-point correction=	0.160712 (Hartree/Particle)
Thermal correction to Energy=	0.167845
Thermal correction to Enthalpy=	0.168789
Thermal correction to Gibbs Free Energy=	0.130028
Sum of electronic and zero-point Energies=	-306.238124
Sum of electronic and thermal Energies=	-306.230991
Sum of electronic and thermal Enthalpies=	-306.230047
Sum of electronic and thermal Free Energies=	-306.268808

C	1.82028700	-0.17419100	-0.38767800
C	-1.03671300	0.15775400	0.37397300
C	-0.20726000	1.20748000	-0.15181600
C	1.11965600	1.36540200	0.28693500
H	1.33085200	-1.49316900	1.11069100
H	1.71073700	-0.08059000	-1.46407800
H	-0.94767200	0.03725500	1.45758300
H	1.70826200	2.15932800	-0.17109500
N	1.08726700	-1.19581200	0.16003700
H	1.32651900	1.22979400	1.34721500
N	-0.21326800	-1.23088300	-0.21939500
H	-0.49637000	1.65621600	-1.10338300
H	-0.66775300	-1.98347000	0.31262200
H	2.85127300	-0.13518900	-0.04120600
C	-2.45590500	0.03278800	-0.14160200
H	-2.48120700	0.06267500	-1.23385800
H	-2.91223100	-0.90390600	0.19022600
H	-3.06811200	0.85187900	0.24706600

TS-AC

Zero-point correction=	0.161470 (Hartree/Particle)
Thermal correction to Energy=	0.168406
Thermal correction to Enthalpy=	0.169350
Thermal correction to Gibbs Free Energy=	0.131023
Sum of electronic and zero-point Energies=	-306.244808
Sum of electronic and thermal Energies=	-306.237872
Sum of electronic and thermal Enthalpies=	-306.236928
Sum of electronic and thermal Free Energies=	-306.275255

C	-1.91613200	-0.30836900	0.29942300
C	1.00415300	0.08739900	-0.36195100
C	0.20182400	1.16450000	0.23964200
C	-1.04849000	1.50173900	-0.23841600
H	-1.16784800	-1.46804700	-1.19943200
H	-1.88642400	-0.15449600	1.37349800
H	0.89121000	0.02824300	-1.44785900
H	-1.64439000	2.23883600	0.29554100
N	-1.04562800	-1.18522100	-0.22500900
H	-1.27604400	1.39375200	-1.29696100
N	0.26302600	-1.19094100	0.17659500
H	0.48639500	1.49000300	1.24198000
H	0.30100500	-1.20369000	1.20070300
H	-2.89709600	-0.25967300	-0.17015200
C	2.46246600	-0.00721800	0.05292400
H	2.57423400	0.02022200	1.14205300
H	2.89907300	-0.93673800	-0.31888800
H	3.02404700	0.83231700	-0.36491700

C

Zero-point correction=	0.164860 (Hartree/Particle)
Thermal correction to Energy=	0.171551
Thermal correction to Enthalpy=	0.172495
Thermal correction to Gibbs Free Energy=	0.134561
Sum of electronic and zero-point Energies=	-306.274994
Sum of electronic and thermal Energies=	-306.268304
Sum of electronic and thermal Enthalpies=	-306.267360
Sum of electronic and thermal Free Energies=	-306.305294

C	2.01568700	-0.11994700	0.03217200
C	-1.14039600	0.08606300	0.43234200
C	-0.15863500	0.81728300	-0.40722100
C	1.20185000	1.19120400	0.16718600
H	0.85952900	-1.54782100	1.03735500
H	2.53191600	-0.15467900	-0.93134500
H	-0.88389800	-0.03543500	1.48427400
H	1.65290100	2.01241400	-0.39330300
N	1.04007900	-1.23277700	0.08186500
H	1.10801100	1.50056400	1.21191100
N	-0.17716600	-0.69883100	-0.43843500
H	-0.51014700	1.28410600	-1.32422200
H	-0.53829300	-1.18932900	-1.26418100
H	2.75371100	-0.25889400	0.82458700
C	-2.60029900	0.00573500	0.08298400
H	-3.04160800	-0.92544900	0.44851400
H	-3.12076500	0.83960000	0.56419700
H	-2.77037300	0.08312700	-0.99505100

TS-CE

Zero-point correction=	0.162151 (Hartree/Particle)
Thermal correction to Energy=	0.168929
Thermal correction to Enthalpy=	0.169873
Thermal correction to Gibbs Free Energy=	0.131791
Sum of electronic and zero-point Energies=	-306.250209
Sum of electronic and thermal Energies=	-306.243431
Sum of electronic and thermal Enthalpies=	-306.242487
Sum of electronic and thermal Free Energies=	-306.280569

C	-1.94919200	-0.03615900	0.20136900
C	1.16958600	0.20331900	-0.41108400
C	0.28624900	1.05086900	0.26498700
C	-1.08589000	1.27435600	-0.19929800
H	-1.21172400	-1.42506300	-1.19382900
H	-2.09559100	-0.04887900	1.28394800
H	0.97756400	0.01069500	-1.46619300
H	-1.56161700	2.12769900	0.29066400
N	-1.14337100	-1.14889400	-0.21099400
H	-1.15615700	1.38335400	-1.28439300
N	0.08184700	-1.22924100	0.25485100
H	0.55674900	1.38473700	1.26780900
H	0.07844000	-1.05891000	1.27003200
H	-2.91491700	-0.03661600	-0.30731600
C	2.57393200	-0.05205600	0.04593400
H	2.88248400	-1.06856200	-0.21058500
H	3.25051500	0.63935600	-0.46913100
H	2.69263200	0.09801700	1.12267700

R'=Boc

R1=H R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.200165 (Hartree/Particle)
Thermal correction to Energy=	0.212874
Thermal correction to Enthalpy=	0.213819
Thermal correction to Gibbs Free Energy=	0.161096
Sum of electronic and zero-point Energies=	-534.066877
Sum of electronic and thermal Energies=	-534.054167
Sum of electronic and thermal Enthalpies=	-534.053222
Sum of electronic and thermal Free Energies=	-534.105945

C	1.42580400	-2.14298900	-0.64563100
C	1.11561600	1.16728600	0.45592200
C	2.43169900	0.69900500	0.19219000
C	2.97734800	-0.30636600	0.92512400
H	1.91319800	-1.76944000	-1.55093800
H	0.63186600	0.79677400	1.35931100
H	3.98064300	-0.67199800	0.72227200
N	0.39655600	-1.60441100	-0.10037200
H	2.45849900	-0.73697700	1.77700500
N	-0.01944500	-0.41589600	-0.65046500
H	2.98341800	1.13531000	-0.63875600
C	-1.39908800	-0.04601600	-0.46528500
O	-1.93065400	0.69249400	-1.26022300
O	-1.89197000	-0.54599100	0.64964200
C	-3.28024700	-0.21426700	0.91908600
H	-3.40621000	0.86843000	0.97418800
H	-3.91929800	-0.62612700	0.13605900
H	-3.49968400	-0.67817300	1.87886900
H	0.26138200	-0.21275900	-1.62132400
C	0.59879500	2.42977400	-0.12578300
H	-0.49137900	2.47579900	-0.15921700
H	0.92416700	3.23660200	0.55096500
H	1.01515900	2.64187700	-1.11369100
H	1.78184900	-3.07297000	-0.21015800

A

Zero-point correction=	0.204139 (Hartree/Particle)
Thermal correction to Energy=	0.216539
Thermal correction to Enthalpy=	0.217483
Thermal correction to Gibbs Free Energy=	0.166063
Sum of electronic and zero-point Energies=	-534.095401
Sum of electronic and thermal Energies=	-534.083001
Sum of electronic and thermal Enthalpies=	-534.082057
Sum of electronic and thermal Free Energies=	-534.133478

C	1.89221200	1.85309400	0.23021800
C	0.84075800	-0.94088300	0.41939200
C	1.92494300	-1.22058900	-0.60395500
C	1.97652700	-0.74155100	-1.84563700
H	-0.08694700	2.25346800	0.05090300
H	2.67287100	1.10699300	0.27727900
H	0.08194800	-1.72226300	0.32780400
H	2.77766100	-1.02922600	-2.51900600
N	0.65264100	1.53053600	0.13991600
H	1.22715600	-0.06231000	-2.24612800
N	0.07906500	0.29794200	0.10590800
H	2.69008100	-1.91278300	-0.25592300
C	-1.32421700	0.39557700	-0.06690700
O	-1.86073200	1.47625300	-0.21388500
O	-1.89173900	-0.79310000	-0.04977700
C	-3.33466600	-0.80630300	-0.23449700
H	-3.58860900	-0.36856500	-1.20104500
H	-3.61085400	-1.85844200	-0.20136700
H	-3.81702100	-0.25194100	0.57199000
C	1.33285200	-0.94860700	1.87582900
H	1.75902400	-1.93178400	2.09268500
H	2.10845500	-0.20754700	2.08580500
H	0.49893200	-0.78367200	2.56264100
H	2.11685800	2.91416800	0.23431200

B

Zero-point correction=	0.202773 (Hartree/Particle)
Thermal correction to Energy=	0.215595
Thermal correction to Enthalpy=	0.216539
Thermal correction to Gibbs Free Energy=	0.163494
Sum of electronic and zero-point Energies=	-534.075913
Sum of electronic and thermal Energies=	-534.063091
Sum of electronic and thermal Enthalpies=	-534.062147
Sum of electronic and thermal Free Energies=	-534.115191

C	1.10523200	2.41197200	0.19101300
C	0.94735400	-0.85463400	-0.09670500
C	2.39667400	-0.56806600	0.15328600
C	3.25747800	-0.25886200	-0.81700800
H	1.49732800	2.34228100	1.21004300
H	0.71786600	-0.85506600	-1.16470000
H	4.31183800	-0.10853000	-0.60454500
N	0.37331600	1.54330400	-0.38089900
H	2.94800100	-0.16325200	-1.85489400
H	2.74016000	-0.67599600	1.18270000
N	0.10012700	0.36448200	0.43796500
H	0.31893400	0.51178200	1.44187900
C	-1.39555700	0.11246300	0.40685700
O	-2.01380500	0.12778400	1.43067900
O	-1.76636600	-0.10049400	-0.82598000
C	-3.19709600	-0.32107700	-1.03155500
H	-3.74809000	0.56580000	-0.71559300
H	-3.30130200	-0.48618000	-2.10158800
H	-3.51858700	-1.19662400	-0.46550900
C	0.46116300	-2.12593000	0.59128900
H	0.59324700	-2.08136400	1.67717300
H	-0.58409300	-2.35488100	0.36753900
H	1.06266900	-2.95920100	0.21897400
H	1.34356300	3.29649100	-0.39704100

TS-AD

Zero-point correction=	0.202840 (Hartree/Particle)
Thermal correction to Energy=	0.214524
Thermal correction to Enthalpy=	0.215468
Thermal correction to Gibbs Free Energy=	0.165365
Sum of electronic and zero-point Energies=	-534.065868
Sum of electronic and thermal Energies=	-534.054184
Sum of electronic and thermal Enthalpies=	-534.053240
Sum of electronic and thermal Free Energies=	-534.103343

C	2.11789900	-1.36890200	-0.59182000
C	0.74481400	1.13145500	0.40077300
C	2.14593700	0.99978100	0.11235700
C	2.90976500	-0.07305500	0.56698000
H	0.50637200	-1.99881900	0.55555800
H	2.32136700	-0.96785400	-1.57874000
H	0.46672600	0.84025700	1.41665300
H	3.96365000	-0.10974300	0.29627200
N	0.81957100	-1.39753100	-0.21923300
H	2.67382600	-0.53490100	1.52293500
N	0.05983500	-0.31784800	-0.48755800
H	2.54700900	1.61052600	-0.69764500
C	-1.27560900	-0.57655500	0.02651400
O	-1.55143400	-1.54101000	0.70617100
O	-2.10389600	0.35296900	-0.41066800
C	-3.48734600	0.20840800	0.00510400
H	-3.56239300	0.25984000	1.09306200
H	-4.01086700	1.04286400	-0.45797800
H	-3.88415900	-0.74349200	-0.35169000
C	0.06335700	2.37226700	-0.12846100
H	0.16722400	2.44147800	-1.21436600
H	-0.99415600	2.40032700	0.12540600
H	0.54083900	3.25030200	0.32000500
H	2.68275100	-2.25741800	-0.31943000

TS-AC

Zero-point correction=	0.204032 (Hartree/Particle)
Thermal correction to Energy=	0.215331
Thermal correction to Enthalpy=	0.216275
Thermal correction to Gibbs Free Energy=	0.166966
Sum of electronic and zero-point Energies=	-534.071855
Sum of electronic and thermal Energies=	-534.060557
Sum of electronic and thermal Enthalpies=	-534.059613
Sum of electronic and thermal Free Energies=	-534.108921

C	-0.71421200	-2.01420200	0.03773500
C	-1.41773400	0.84114700	-0.38721100
C	-1.80417000	0.13634300	0.85822000
C	-2.38887800	-1.11216400	0.81023100
H	-0.77663100	-1.37750500	-1.90620400
H	-0.10996300	-1.96912200	0.93753200
H	-2.06560700	0.55385900	-1.22066300
H	-2.57637600	-1.65594200	1.73369000
N	-0.35326500	-1.22175700	-0.98863700
H	-3.02653100	-1.37755000	-0.03149200
N	-0.08856300	0.09961800	-0.71783800
H	-1.36840500	0.49901300	1.79018800
C	1.11823500	0.40987400	-0.03918000
O	1.27468700	1.41525800	0.61416000
O	2.03479100	-0.52810800	-0.28296000
C	3.33826300	-0.27825700	0.29737400
H	3.75714600	0.64840100	-0.09919800
H	3.26601100	-0.21674500	1.38503500
H	3.94732300	-1.13124700	0.00154200
H	-1.10839700	-2.99280900	-0.23123600
C	-1.29234200	2.35746400	-0.34622300
H	-0.74519200	2.70657700	0.52709700
H	-0.78605500	2.71418500	-1.24608600
H	-2.30132400	2.77976300	-0.33365400

C

Zero-point correction=	0.206735 (Hartree/Particle)
Thermal correction to Energy=	0.217967
Thermal correction to Enthalpy=	0.218911
Thermal correction to Gibbs Free Energy=	0.169582
Sum of electronic and zero-point Energies=	-534.095495
Sum of electronic and thermal Energies=	-534.084263
Sum of electronic and thermal Enthalpies=	-534.083319
Sum of electronic and thermal Free Energies=	-534.132647

C	-1.83243000	-1.77533600	0.00292300
C	-1.03609300	1.25252200	-0.55950400
C	-1.41519000	0.50687100	0.65690500
C	-2.53039900	-0.52622300	0.59617700
H	-0.93645300	-1.09700000	-1.77564000
H	-1.44493600	-2.41357900	0.80208600
H	-1.63068200	1.05064700	-1.45064900
H	-2.93882800	-0.72144100	1.58961200
N	-0.69270800	-1.28845300	-0.80244500
H	-3.34268400	-0.17382400	-0.04551700
N	-0.27763800	-0.06765400	-0.19344400
H	-1.06598200	0.88879100	1.61310800
C	1.11637200	0.00717500	0.31119100
O	1.38358900	0.67467600	1.27388200
O	1.89636600	-0.70220000	-0.46238800
C	3.30478900	-0.72077100	-0.08543300
H	3.41465100	-1.16947000	0.90313500
H	3.78793400	-1.33160800	-0.84511900
H	3.70123000	0.29573100	-0.08913600
C	-0.29787400	2.55943100	-0.55176800
H	0.29012700	2.70824900	0.35397600
H	0.34598600	2.65340600	-1.43082000
H	-1.05039000	3.35379300	-0.60706300
H	-2.48286500	-2.37745800	-0.63433300

TS-CE

Zero-point correction=	0.203685 (Hartree/Particle)
Thermal correction to Energy=	0.215013
Thermal correction to Enthalpy=	0.215957
Thermal correction to Gibbs Free Energy=	0.166471
Sum of electronic and zero-point Energies=	-534.071481
Sum of electronic and thermal Energies=	-534.060153
Sum of electronic and thermal Enthalpies=	-534.059209
Sum of electronic and thermal Free Energies=	-534.108695

C	-0.32110800	2.11065600	-0.15898900
C	-1.95200700	-0.71593600	0.22578700
C	-1.60974400	0.07625400	-0.86124700
C	-1.67828400	1.54396300	-0.82225500
H	-0.66120900	1.62839900	1.86449300
H	0.51328300	1.96335300	-0.84499100
H	-2.45340200	-0.23231100	1.06427700
H	-1.72747800	1.98160500	-1.82332300
N	-0.14655000	1.32569400	1.03022800
H	-2.51148100	1.91269600	-0.21916600
N	-0.04219200	0.03827400	0.93683600
H	-1.17293500	-0.40249700	-1.73600700
C	1.01769100	-0.52001100	0.11508700
O	0.92102200	-1.56944900	-0.46617500
O	2.10815400	0.23000500	0.25093800
C	3.31596700	-0.32082900	-0.33950800
H	3.18806500	-0.43797600	-1.41716400
H	4.09422200	0.40733700	-0.11744400
H	3.54673300	-1.28489200	0.11691300
C	-1.99119100	-2.20550600	0.22450200
H	-1.59422700	-2.60429100	1.16242600
H	-3.04377600	-2.51528000	0.17202000
H	-1.44686600	-2.64085000	-0.61255400
H	-0.42684400	3.16759600	0.08938800

R'=H

R1=H R2=H R3=CH3 R4=H

TS-BF

Zero-point correction=	0.159483 (Hartree/Particle)
Thermal correction to Energy=	0.167159
Thermal correction to Enthalpy=	0.168103
Thermal correction to Gibbs Free Energy=	0.127825
Sum of electronic and zero-point Energies=	-306.229173
Sum of electronic and thermal Energies=	-306.221497
Sum of electronic and thermal Enthalpies=	-306.220553
Sum of electronic and thermal Free Energies=	-306.260830

C	-1.19808400	0.99398100	0.28133400
C	1.21756400	-1.06234800	-0.23765000
C	1.41526700	0.17455800	0.39112600
C	0.89476700	1.29971800	-0.24943000
H	-1.02520100	0.97557200	1.36098200
H	1.05561800	-1.10987700	-1.30972800
H	1.55313300	-1.98411000	0.23243500
H	0.98439500	2.28400500	0.20551000
N	-1.39283700	-0.10118200	-0.42845500
H	0.71575500	1.29082900	-1.31941900
N	-0.89156800	-1.20904800	0.10269600
H	-0.89016200	-1.33091900	1.12410700
H	-1.15277300	-2.05588400	-0.40685400
H	-1.61452400	1.90597000	-0.13731800
C	1.94105700	0.25314000	1.80253400
H	3.02388400	0.42455300	1.78598400
H	1.49487800	1.08259100	2.35935900
H	1.77134800	-0.67379800	2.35836800

A

Zero-point correction=	0.160782 (Hartree/Particle)
Thermal correction to Energy=	0.169289
Thermal correction to Enthalpy=	0.170233
Thermal correction to Gibbs Free Energy=	0.127493
Sum of electronic and zero-point Energies=	-306.262215
Sum of electronic and thermal Energies=	-306.253708
Sum of electronic and thermal Enthalpies=	-306.252764
Sum of electronic and thermal Free Energies=	-306.295504

C	-2.46255000	-0.59493100	-0.03079400
C	0.39190300	-0.39584600	0.31406300
C	1.80028900	0.13356500	0.50255500
C	2.73202700	-0.11709500	-0.42015400
H	-2.29976400	1.31211400	-0.60559300
H	-1.96623400	-1.50581900	0.27707500
H	0.38764900	-1.27581800	-0.33902500
H	3.74838300	0.25127200	-0.31431500
N	-1.79079500	0.47422800	-0.29532400
H	2.51728800	-0.70210700	-1.31032300
N	-0.45109400	0.63439100	-0.30752400
H	-0.04513900	-0.68632700	1.28314800
H	-0.18570100	1.61275300	-0.20942000
H	-3.53794000	-0.54872500	-0.14756100
C	2.06039500	0.91790600	1.76284200
H	3.07629500	1.31860400	1.77941700
H	1.36675600	1.76181600	1.87545100
H	1.92865500	0.28744600	2.65114100

B

Zero-point correction=	0.161367 (Hartree/Particle)
Thermal correction to Energy=	0.169769
Thermal correction to Enthalpy=	0.170713
Thermal correction to Gibbs Free Energy=	0.128246
Sum of electronic and zero-point Energies=	-306.258917
Sum of electronic and thermal Energies=	-306.250515
Sum of electronic and thermal Enthalpies=	-306.249571
Sum of electronic and thermal Free Energies=	-306.292037

C	2.60023100	0.71226200	-0.00513200
C	-0.48695900	-0.42751200	0.50779300
C	-1.86934400	-0.45731900	-0.09587200
C	-2.63570900	0.63614500	-0.02382600
H	2.26494800	1.67692700	-0.40108000
H	-0.35233400	0.39503900	1.21226200
H	-3.64123200	0.65004800	-0.43391500
N	1.91547200	-0.35824400	-0.00428100
H	-2.29636700	1.54878900	0.45947200
H	-0.20381200	-1.36630700	0.99057700
H	3.59866800	0.64519500	0.42279000
H	0.41783400	0.70216600	-1.03820200
H	0.49807900	-0.93761200	-1.29403100
N	0.57703000	-0.20823000	-0.56986600
C	-2.32151500	-1.75493100	-0.71622900
H	-3.31629800	-1.65578200	-1.15549300
H	-1.64664000	-2.10275900	-1.51049500
H	-2.35712500	-2.55328000	0.03505100

TS-AD

Zero-point correction=	0.160749 (Hartree/Particle)
Thermal correction to Energy=	0.167848
Thermal correction to Enthalpy=	0.168792
Thermal correction to Gibbs Free Energy=	0.129648
Sum of electronic and zero-point Energies=	-306.245533
Sum of electronic and thermal Energies=	-306.238434
Sum of electronic and thermal Enthalpies=	-306.237490
Sum of electronic and thermal Free Energies=	-306.276635

C	1.18630600	-0.82870600	-0.15701400
C	-1.19798100	0.95091000	0.15543800
C	0.06813500	1.36064400	-0.32074900
C	1.23066900	0.76215700	0.31448800
H	-0.17523700	-1.67801900	1.17409400
H	1.32660400	-0.85931300	-1.23804200
H	-1.31805300	0.80906500	1.22778700
H	2.18967000	1.15243300	-0.03275900
N	-0.06651400	-1.36592300	0.20304800
H	1.19043500	0.74844300	1.40482300
N	-1.10375900	-0.79556900	-0.41416500
H	-2.08388200	1.32912100	-0.34949200
H	-1.96673300	-1.14554300	0.02650600
H	1.99889400	-1.34069800	0.35863700
C	0.20605200	2.05122500	-1.62837900
H	-0.71456700	2.02480100	-2.21535500
H	0.45178200	3.10798100	-1.44199500
H	1.03906700	1.64704200	-2.21513800

TS-AC

Zero-point correction=	0.161446 (Hartree/Particle)
Thermal correction to Energy=	0.168419
Thermal correction to Enthalpy=	0.169363
Thermal correction to Gibbs Free Energy=	0.130843
Sum of electronic and zero-point Energies=	-306.248806
Sum of electronic and thermal Energies=	-306.241833
Sum of electronic and thermal Enthalpies=	-306.240889
Sum of electronic and thermal Free Energies=	-306.279409

C

Zero-point correction=	0.164913 (Hartree/Particle)
Thermal correction to Energy=	0.171462
Thermal correction to Enthalpy=	0.172407
Thermal correction to Gibbs Free Energy=	0.134940
Sum of electronic and zero-point Energies=	-306.272377
Sum of electronic and thermal Energies=	-306.265828
Sum of electronic and thermal Enthalpies=	-306.264884
Sum of electronic and thermal Free Energies=	-306.302350

C	1.33229600	-0.67096900	-0.27940600
C	-1.35815200	0.39524400	0.27734100
C	-0.34678900	1.28569900	-0.35629900
C	0.90987200	1.35933200	0.21066900
H	0.39438700	-1.59989200	1.27003200
H	1.31192400	-0.54084600	-1.35693900
H	-1.36477000	0.44513500	1.36757200
H	1.69572600	1.93352700	-0.27551200
N	0.31048100	-1.31248700	0.29330600
H	1.04448000	1.18630100	1.27547300
N	-0.99123600	-1.05090300	-0.09073400
H	-2.37172400	0.54487100	-0.09884300
H	-1.07143800	-1.18591900	-1.10213700
H	2.31016900	-0.79676600	0.18141300
C	-0.63496100	1.83674100	-1.71699200
H	-1.11441500	1.09329300	-2.36668500
H	-1.35335300	2.66262900	-1.62396700
H	0.25898700	2.22298300	-2.21160200

C	1.52690900	-0.16675600	-0.01970700
C	-1.56781200	0.12203300	0.50508800
C	-0.64536700	0.83650700	-0.41214900
C	0.74987400	1.16259500	0.13019000
H	0.38417800	-1.56470600	1.04455700
H	2.00296300	-0.22420300	-1.00309700
H	-1.32029600	0.02186700	1.55837700
H	1.21023800	1.96831200	-0.44604400
N	0.53025400	-1.25649900	0.08099000
H	0.69211600	1.48136500	1.17472100
N	-0.69223400	-0.69840300	-0.39473700
H	-2.62478300	0.05692300	0.25964200
H	-1.12685500	-1.21580300	-1.16729600
H	2.29404500	-0.31319500	0.74306700
C	-1.15950300	1.53871900	-1.64039600
H	-1.36622300	2.58290800	-1.38543700
H	-0.41383500	1.52651100	-2.44048000
H	-2.08943400	1.09772000	-2.01092500

TS-CE

Zero-point correction=	0.161553 (Hartree/Particle)
Thermal correction to Energy=	0.168504
Thermal correction to Enthalpy=	0.169448
Thermal correction to Gibbs Free Energy=	0.130860
Sum of electronic and zero-point Energies=	-306.249909
Sum of electronic and thermal Energies=	-306.242958
Sum of electronic and thermal Enthalpies=	-306.242014
Sum of electronic and thermal Free Energies=	-306.280602

C	1.46419300	0.11802500	-0.16425600
C	-1.66619400	0.02430300	0.29896000
C	-0.88788000	0.95890100	-0.36359700
C	0.43967000	1.30452800	0.19605800
H	0.95588500	-1.36607000	1.25396500
H	1.62646400	0.09041500	-1.24536500
H	-1.53718700	-0.16784800	1.35906700
H	0.86219700	2.21202300	-0.24439800
N	0.83113400	-1.09569500	0.27301500
H	0.42639700	1.40207000	1.28410500
N	-0.30807300	-1.45624800	-0.22362200
H	-2.60753900	-0.31205500	-0.12732900
H	-0.31504300	-1.25511000	-1.23272000
H	2.41524100	0.26370500	0.35058900
C	-1.25171300	1.46582300	-1.72397200
H	-2.08736300	0.91958000	-2.16730200
H	-1.55114300	2.51971900	-1.64035400
H	-0.39774700	1.45003800	-2.41260500

R'=Boc

R1=H R2=H R3=CH3 R4=H

TS-BF

Zero-point correction=	0.200798 (Hartree/Particle)
Thermal correction to Energy=	0.213219
Thermal correction to Enthalpy=	0.214163
Thermal correction to Gibbs Free Energy=	0.161695
Sum of electronic and zero-point Energies=	-534.056717
Sum of electronic and thermal Energies=	-534.044297
Sum of electronic and thermal Enthalpies=	-534.043353
Sum of electronic and thermal Free Energies=	-534.095820

C	-1.31255800	1.39615200	-0.56631100
C	-0.53268000	-1.57387600	0.77606500
C	-1.86187900	-1.22937000	0.52134900
C	-2.31209600	-0.04046900	1.08067800
H	-1.81021500	0.87533700	-1.38900000
H	0.01296200	-1.10647100	1.58981900
H	-3.31684100	0.32941600	0.88866100
N	-0.09932500	1.13033100	-0.17257400
H	-1.76265000	0.44779300	1.87906900
N	0.42458400	-0.01390200	-0.62150600
C	1.84291000	-0.26385400	-0.46169800
O	2.38126600	-1.06536500	-1.18268600
O	2.34605300	0.43774300	0.52979500
C	3.77271900	0.26176400	0.75162000
H	3.98756000	-0.78095300	0.99192600
H	4.32577700	0.56487100	-0.13906300
H	4.00839000	0.91145900	1.59221800
H	-0.08424200	-2.46260900	0.33736400
H	0.08911000	-0.41861100	-1.50894400
C	-2.69836300	-2.02261400	-0.45366800
C	-3.07023000	-2.93256100	0.03041100
H	-3.56685200	-1.45608500	-0.79814600
H	-2.11846600	-2.33860600	-1.32662700
H	-1.74026500	2.33107500	-0.21590000

A

Zero-point correction=	0.203621 (Hartree/Particle)
Thermal correction to Energy=	0.216321
Thermal correction to Enthalpy=	0.217266
Thermal correction to Gibbs Free Energy=	0.163915
Sum of electronic and zero-point Energies=	-534.102799
Sum of electronic and thermal Energies=	-534.090098
Sum of electronic and thermal Enthalpies=	-534.089154
Sum of electronic and thermal Free Energies=	-534.142505

C	-1.75987900	1.56562400	-0.25442200
C	-0.42480900	-0.95321400	-0.79144800
C	-1.30598700	-1.68871600	0.20372000
C	-1.36158700	-1.36842600	1.49802700
H	0.13450200	2.17370800	0.16224400
H	-2.41622900	0.74433300	-0.51114800
H	0.38383400	-1.59767300	-1.14320400
H	-1.99168300	-1.92594100	2.18364600
N	-0.49458500	1.39728200	-0.11525000
H	-0.77227300	-0.56495300	1.93131800
N	0.22108600	0.25727100	-0.27862200
C	1.59696600	0.44662000	-0.00356900
O	2.01628600	1.52908000	0.35358300
O	2.26723100	-0.67137400	-0.18865200
C	3.69745800	-0.60331000	0.06887300
H	3.87315700	-0.35009300	1.11557400
H	4.06850600	-1.60149100	-0.15510400
H	4.15828500	0.13838600	-0.58514300
H	-0.99899500	-0.66623000	-1.68509100
C	-2.08653600	-2.82093500	-0.40944300
H	-1.41862400	-3.55787500	-0.87325100
H	-2.68772900	-3.33642900	0.34220600
H	-2.76144700	-2.46772300	-1.19976300
H	-2.14182000	2.56659300	-0.08832900

B

Zero-point correction=	0.202832 (Hartree/Particle)
Thermal correction to Energy=	0.215819
Thermal correction to Enthalpy=	0.216764
Thermal correction to Gibbs Free Energy=	0.162053
Sum of electronic and zero-point Energies=	-534.076188
Sum of electronic and thermal Energies=	-534.063200
Sum of electronic and thermal Enthalpies=	-534.062256
Sum of electronic and thermal Free Energies=	-534.116967

C	0.89844000	1.93760800	0.29559800
C	0.50988100	-1.23472400	-0.39843500
C	1.99844000	-1.21718200	-0.17876500
C	2.78970800	-0.65328100	-1.09904600
H	1.38047100	1.71595600	1.25235600
H	0.22084300	-1.07365800	-1.43630300
H	3.86964800	-0.63929600	-0.98251900
N	0.07028100	1.18436200	-0.30856300
H	2.39166200	-0.20592800	-2.00548500
N	-0.18436600	-0.08330900	0.37531400
H	0.13844100	-0.07670200	1.36096700
C	-1.69014500	-0.26678300	0.48731800
O	-2.19230300	-0.28706600	1.57231400
O	-2.19074800	-0.38715100	-0.70955900
C	-3.64231600	-0.54970100	-0.78458200
H	-4.12794700	0.32439900	-0.34865200
H	-3.85711100	-0.62695600	-1.84805600
H	-3.93511900	-1.45848300	-0.25683700
H	0.04101700	-2.14843100	-0.01952800
C	2.51798500	-1.88034600	1.07231600
H	3.60184600	-1.77535100	1.15263600
H	2.07828500	-1.45913500	1.98730600
H	2.27806700	-2.95058300	1.07665000
H	1.12626100	2.88353100	-0.19268900

TS-AD

Zero-point correction=	0.202944 (Hartree/Particle)
Thermal correction to Energy=	0.214594
Thermal correction to Enthalpy=	0.215538
Thermal correction to Gibbs Free Energy=	0.164414
Sum of electronic and zero-point Energies=	-534.076078
Sum of electronic and thermal Energies=	-534.064427
Sum of electronic and thermal Enthalpies=	-534.063483
Sum of electronic and thermal Free Energies=	-534.114607

C	1.82803400	-0.86889200	-0.39656800
C	0.08024500	1.28085500	0.80113600
C	1.43522800	1.41314200	0.42844600
C	2.30622900	0.28956300	0.70851000
H	0.16243100	-1.83957600	0.47848500
H	2.02423700	-0.46710600	-1.39093400
H	-0.15451200	0.76097500	1.72770400
H	3.36370800	0.46399500	0.50256600
N	0.46289400	-1.13115600	-0.20531700
H	2.16605700	-0.16645200	1.68944000
N	-0.35585000	-0.11785900	-0.43752900
C	-1.72486800	-0.47355400	-0.08987500
O	-2.04756400	-1.57427500	0.29170300
O	-2.50443600	0.56843000	-0.31375000
C	-3.91522400	0.36641900	-0.03902200
H	-4.06127000	0.12038600	1.01479200
H	-4.39023400	1.31464600	-0.28355000
H	-4.30577800	-0.43548100	-0.66800600
H	-0.61716900	2.06411400	0.52112300
C	1.82802200	2.46179500	-0.55125300
H	2.85338800	2.34810800	-0.90727500
H	1.13775800	2.45289400	-1.40685100
H	1.72951600	3.45548900	-0.09444400
H	2.42529200	-1.75944200	-0.20133000

TS-AC

Zero-point correction=	0.204172 (Hartree/Particle)
Thermal correction to Energy=	0.215448
Thermal correction to Enthalpy=	0.216392
Thermal correction to Gibbs Free Energy=	0.167242
Sum of electronic and zero-point Energies=	-534.084457
Sum of electronic and thermal Energies=	-534.073181
Sum of electronic and thermal Enthalpies=	-534.072237
Sum of electronic and thermal Free Energies=	-534.121387

C	-1.19148200	1.15283400	-0.35821600
C	-0.56445500	-1.26711300	1.14095900
C	-1.46970600	-1.35478300	-0.05348400
C	-2.54954500	-0.50290700	-0.11652800
H	-0.72348400	1.56271000	1.58861200
H	-0.76461700	0.82491100	-1.29970200
H	-1.10689700	-1.12007300	2.07728900
H	-3.18324600	-0.48068600	-1.00040900
N	-0.42244300	1.09285700	0.73151900
H	-2.98460300	-0.09048000	0.79079700
N	0.31168300	-0.05713800	0.93392700
C	1.57087400	-0.21474000	0.32849700
O	2.10545800	-1.29819100	0.22526100
O	2.06667300	0.96214300	-0.05209400
C	3.39627700	0.91216100	-0.62356800
H	4.10720400	0.51894400	0.10560400
H	3.40317700	0.29058200	-1.52121000
H	3.63615500	1.94502000	-0.87213900
H	0.11251100	-2.11590800	1.23187600
C	-1.02488800	-2.17991600	-1.21482800
H	-1.18303800	-3.23985000	-0.96976300
H	-1.58566500	-1.96094500	-2.12616500
H	0.05073500	-2.07571200	-1.39803500
H	-1.92879500	1.95212900	-0.39457800

C

Zero-point correction=	0.206077 (Hartree/Particle)
Thermal correction to Energy=	0.216679
Thermal correction to Enthalpy=	0.217623
Thermal correction to Gibbs Free Energy=	0.169841
Sum of electronic and zero-point Energies=	-534.090529
Sum of electronic and thermal Energies=	-534.079927
Sum of electronic and thermal Enthalpies=	-534.078983
Sum of electronic and thermal Free Energies=	-534.126765

C	1.76231600	-0.88954500	-0.40972300
C	0.39620500	1.37069600	1.26128300
C	0.79518400	1.33943700	-0.15730200
C	2.10006700	0.62002400	-0.48660500
H	1.07952600	-1.11535600	1.55799600
H	1.37222600	-1.24268900	-1.36879800
H	1.11909200	1.13819700	2.03960400
H	2.45895700	0.89998700	-1.47858100
N	0.70995900	-1.03522000	0.60842500
H	2.86944000	0.88682600	0.24483800
N	-0.08116700	0.13716400	0.53730000
C	-1.52527300	0.01498100	0.26093100
O	-2.24334700	0.97191800	0.38849500
O	-1.80926600	-1.19964500	-0.13258300
C	-3.21077600	-1.44381300	-0.44915800
H	-3.51831900	-0.80882400	-1.28159000
H	-3.25237000	-2.49526900	-0.72593600
H	-3.82759200	-1.24641100	0.42878800
H	-0.42243800	2.02257200	1.55419800
C	0.12121900	2.23324400	-1.17512100
H	0.78772500	2.39225400	-2.02438500
H	-0.80968000	1.80869100	-1.55936900
H	-0.12287600	3.20261200	-0.73432700
H	2.61622200	-1.51057300	-0.13267300

TS-CE

Zero-point correction=	0.203341 (Hartree/Particle)
Thermal correction to Energy=	0.214811
Thermal correction to Enthalpy=	0.215755
Thermal correction to Gibbs Free Energy=	0.166234
Sum of electronic and zero-point Energies=	-534.069003
Sum of electronic and thermal Energies=	-534.057533
Sum of electronic and thermal Enthalpies=	-534.056589
Sum of electronic and thermal Free Energies=	-534.106110

C	1.03083100	1.21316900	0.28144600
C	1.41636000	-1.80381400	-1.08703500
C	1.51770100	-1.28303200	0.16054100
C	2.13012200	0.06696400	0.35599900
H	0.93113700	1.54543900	-1.81147300
H	0.27579000	1.09053700	1.05565800
H	1.88503700	-1.33308800	-1.94680600
H	2.57245000	0.18478800	1.35112900
N	0.42559600	1.09612400	-1.03033000
H	2.89934400	0.28584200	-0.38889700
N	-0.40210400	0.23557900	-1.41415700
C	-1.37932200	-0.34993000	-0.49258300
O	-1.69751600	-1.50309300	-0.56941700
O	-1.92299500	0.61411000	0.23938600
C	-3.10069500	0.22816200	1.00888200
H	-2.83320600	-0.54054100	1.73538500
H	-3.42171600	1.14162300	1.50564900
H	-3.87405500	-0.14201800	0.33404300
H	0.93234100	-2.75893800	-1.26327200
C	0.95726800	-1.97990600	1.36988000
H	1.77477900	-2.32251300	2.01663300
H	0.34460200	-1.30905800	1.98640700
H	0.35286200	-2.84675600	1.09817900
H	1.50169700	2.19463300	0.35552200

R'=H

R1=H R2=H R3=H R4=CH3

TS-BF

Zero-point correction=	0.158557 (Hartree/Particle)
Thermal correction to Energy=	0.166414
Thermal correction to Enthalpy=	0.167358
Thermal correction to Gibbs Free Energy=	0.127013
Sum of electronic and zero-point Energies=	-306.233783
Sum of electronic and thermal Energies=	-306.225926
Sum of electronic and thermal Enthalpies=	-306.224981
Sum of electronic and thermal Free Energies=	-306.265326

C	-1.19494900	1.04954700	0.23780200
C	1.29082000	-1.11495600	-0.15422700
C	1.41031600	0.12303100	0.42958700
C	0.98478200	1.29171700	-0.23032100
H	-1.06841800	1.03336800	1.32316100
H	1.09150800	-1.21908000	-1.21608000
H	1.58715600	-2.01567900	0.37641500
N	-1.40921200	-0.04391600	-0.46633700
H	0.81392300	1.22485200	-1.30359100
H	1.71075800	0.19521500	1.47427100
N	-1.08404200	-1.18075900	0.10139100
H	-1.06895200	-1.28060600	1.12227000
H	-1.34819700	-2.01382500	-0.42292600
H	-1.53089300	1.97395800	-0.22078800
C	1.23866000	2.65977700	0.31886400
H	2.24887700	2.95833600	0.00229600
H	0.55194200	3.40684400	-0.08526000
H	1.21361200	2.68795200	1.41112800

A

Zero-point correction=	0.160775 (Hartree/Particle)
Thermal correction to Energy=	0.169403
Thermal correction to Enthalpy=	0.170348
Thermal correction to Gibbs Free Energy=	0.127320
Sum of electronic and zero-point Energies=	-306.267015
Sum of electronic and thermal Energies=	-306.258387
Sum of electronic and thermal Enthalpies=	-306.257443
Sum of electronic and thermal Free Energies=	-306.300471

C	-2.45820200	-0.64322500	-0.09597200
C	0.41233200	-0.45482100	0.19845100
C	1.79689300	0.05489700	0.47472100
C	2.81722000	-0.09445300	-0.37435400
H	-2.36468200	1.35025700	-0.00481800
H	-1.92652900	-1.58476600	-0.13955100
H	0.40171400	-1.10144000	-0.68671700
N	-1.82302100	0.47663500	-0.02124600
H	2.64110900	-0.60889700	-1.32065600
N	-0.48868300	0.68292300	-0.04983500
H	1.94397700	0.55635200	1.43140300
H	0.02816100	-1.03600600	1.05352300
H	-0.24152000	1.57702000	0.37345400
H	-3.53955900	-0.60154700	-0.13235500
C	4.21371900	0.38409200	-0.13318200
H	4.31407000	0.89517600	0.82836000
H	4.92196000	-0.45333500	-0.15335000
H	4.52842600	1.07424300	-0.92570700

B

Zero-point correction=	0.161392 (Hartree/Particle)
Thermal correction to Energy=	0.169908
Thermal correction to Enthalpy=	0.170852
Thermal correction to Gibbs Free Energy=	0.127956
Sum of electronic and zero-point Energies=	-306.264870
Sum of electronic and thermal Energies=	-306.256354
Sum of electronic and thermal Enthalpies=	-306.255410
Sum of electronic and thermal Free Energies=	-306.298306

C	2.60467800	0.68456100	0.06256400
C	-0.52053400	-0.44619500	0.50455700
C	-1.85508900	-0.46441200	-0.16426500
C	-2.74375100	0.52760000	-0.03068600
H	2.29252900	1.64195200	-0.36856500
H	-0.41369700	0.37001800	1.22194900
N	1.90553300	-0.37642600	0.07274100
H	-2.47878900	1.38956100	0.58507800
H	-2.09620200	-1.34797800	-0.75508800
H	-0.25761700	-1.39058600	0.98788300
H	3.59000600	0.61786500	0.51978300
H	0.44208000	0.68208800	-1.00939700
H	0.51936800	-0.95940500	-1.25586800
N	0.58745400	-0.22632000	-0.53302500
C	-4.10731200	0.55000300	-0.64119200
H	-4.87590400	0.60143900	0.13983400
H	-4.23823100	1.44425000	-1.26259600
H	-4.30001400	-0.33276500	-1.25642400

TS-AD

Zero-point correction=	0.160828 (Hartree/Particle)
Thermal correction to Energy=	0.167909
Thermal correction to Enthalpy=	0.168853
Thermal correction to Gibbs Free Energy=	0.130250
Sum of electronic and zero-point Energies=	-306.235294
Sum of electronic and thermal Energies=	-306.228214
Sum of electronic and thermal Enthalpies=	-306.227269
Sum of electronic and thermal Free Energies=	-306.265873

C	1.06286800	-0.91400100	-0.25588200
C	-1.14560100	1.03101600	0.18199900
C	0.13695300	1.34777300	-0.30555400
C	1.30735300	0.75706100	0.26322000
H	-0.19657600	-1.66014100	1.20899300
H	1.09918900	-0.89934800	-1.34267400
H	-1.27190600	0.94084600	1.25989400
N	-0.16321500	-1.33833200	0.23510100
H	1.27095900	0.64882600	1.35016000
N	-1.23050200	-0.74206000	-0.29343300
H	0.21348900	1.77758900	-1.30529300
H	-2.00351100	1.45184400	-0.33588600
H	-2.05443700	-1.02880500	0.25445500
H	1.89815000	-1.45202600	0.19016300
C	2.67184200	1.19781400	-0.24848000
H	3.45935800	0.51538600	0.08133200
H	2.69575200	1.25256000	-1.34093400
H	2.90873800	2.18994100	0.14665000

TS-AC

Zero-point correction=	0.161867 (Hartree/Particle)
Thermal correction to Energy=	0.168738
Thermal correction to Enthalpy=	0.169682
Thermal correction to Gibbs Free Energy=	0.131449
Sum of electronic and zero-point Energies=	-306.244435
Sum of electronic and thermal Energies=	-306.237564
Sum of electronic and thermal Enthalpies=	-306.236619
Sum of electronic and thermal Free Energies=	-306.274852

C	1.36975600	-0.47478100	-0.22575600
C	-1.42440300	0.31556400	0.25338900
C	-0.43481300	1.22096000	-0.32736500
C	0.85613500	1.33379500	0.20307800
H	0.41064900	-1.51071600	1.25647900
H	1.43964700	-0.41917400	-1.31001700
H	-1.46097400	0.29603700	1.34332200
N	0.37767500	-1.27407600	0.26348900
H	0.93688500	1.22692300	1.28747300
N	-0.90034900	-1.09013000	-0.18928600
H	-0.61173000	1.56658700	-1.34781000
H	-2.42752400	0.40963900	-0.16218000
H	-0.91186100	-1.15205200	-1.21141700
H	2.32974800	-0.57267200	0.28163300
C	1.89282800	2.23994900	-0.42738100
H	1.77464800	3.25705200	-0.03973500
H	2.90833900	1.91836200	-0.17992700
H	1.79531600	2.27888700	-1.51609300

C

Zero-point correction=	0.165217 (Hartree/Particle)
Thermal correction to Energy=	0.171719
Thermal correction to Enthalpy=	0.172663
Thermal correction to Gibbs Free Energy=	0.135125
Sum of electronic and zero-point Energies=	-306.267185
Sum of electronic and thermal Energies=	-306.260683
Sum of electronic and thermal Enthalpies=	-306.259739
Sum of electronic and thermal Free Energies=	-306.297277

C	1.52293400	-0.16427700	-0.02971100
C	-1.58397200	0.11781600	0.50080000
C	-0.63799000	0.81988100	-0.39533900
C	0.76034200	1.18179200	0.11833100
H	0.38153800	-1.56112100	1.03992200
H	1.99536200	-0.22197300	-1.01625300
H	-1.34426200	0.01147400	1.55524800
N	0.52749600	-1.25213900	0.07670800
H	0.68430200	1.44133300	1.18074500
N	-0.69902700	-0.69222700	-0.39758500
H	-1.02356200	1.28536200	-1.29914300
H	-2.63718100	0.06303000	0.24048600
H	-1.12291400	-1.19356000	-1.18635300
H	2.29328600	-0.31082200	0.73030100
C	1.40826300	2.33998700	-0.64221100
H	0.84397800	3.26742100	-0.50922000
H	2.42185500	2.51554700	-0.27073900
H	1.47497900	2.12879100	-1.71467200

TS-CE

Zero-point correction=	0.161983 (Hartree/Particle)
Thermal correction to Energy=	0.168803
Thermal correction to Enthalpy=	0.169747
Thermal correction to Gibbs Free Energy=	0.131582
Sum of electronic and zero-point Energies=	-306.242001
Sum of electronic and thermal Energies=	-306.235180
Sum of electronic and thermal Enthalpies=	-306.234236
Sum of electronic and thermal Free Energies=	-306.272401

C	1.05766300	-1.58052500	-0.25474500
C	1.61669100	1.42602300	0.45601600
C	1.72697000	0.75066700	-0.75008300
C	2.25511400	-0.61512200	-0.83617900
H	1.17880600	-1.22509300	1.81417600
H	0.24129000	-1.59095200	-0.98099600
H	1.44374100	-2.59025200	-0.10261200
H	2.26806000	1.18982100	1.29238600
N	0.63414500	-0.99698900	0.97711200
H	3.09003700	-0.76192800	-0.14257900
N	0.16466000	0.21956200	0.98493100
H	1.20317600	1.15209800	-1.61941900
H	1.15728200	2.40998700	0.48931000
C	2.61594300	-1.09943200	-2.24536500
H	3.48535000	-0.55363800	-2.62005900
H	2.86835600	-2.16296800	-2.23776300
H	1.78886400	-0.94737200	-2.94591800
H	-0.46182500	0.34992100	0.17835400

R'=Boc

R1=H R2=H R3=H R4=CH3

TS-BF

Zero-point correction=	0.200193 (Hartree/Particle)
Thermal correction to Energy=	0.212753
Thermal correction to Enthalpy=	0.213697
Thermal correction to Gibbs Free Energy=	0.161289
Sum of electronic and zero-point Energies=	-534.064869
Sum of electronic and thermal Energies=	-534.052308
Sum of electronic and thermal Enthalpies=	-534.051364
Sum of electronic and thermal Free Energies=	-534.103772

C	1.85074100	-1.53227400	-0.67994100
C	1.17710700	1.68925700	0.38065800
C	2.40281400	1.16484300	0.08979000
C	2.86950900	-0.01043500	0.72587500
H	2.29907200	-1.13813000	-1.59564400
H	0.56696400	1.28620700	1.18414700
N	0.61542500	-1.27256100	-0.32378300
H	2.30165000	-0.37422900	1.58105400
N	0.00239600	-0.29464700	-0.95281200
H	3.01544800	1.61402900	-0.69052400
C	-1.37745700	0.00986200	-0.71882900
O	-1.95473600	0.75610800	-1.47157200
O	-1.83308000	-0.59075000	0.36366800
C	-3.23376300	-0.34978700	0.66112700
H	-3.40375400	0.71426300	0.83569800
H	-3.85717200	-0.69752700	-0.16448000
H	-3.43320800	-0.92581600	1.56286500
H	2.29940900	-2.40544300	-0.21769600
H	0.81317900	2.58471700	-0.11582000
H	3.04867600	0.07889700	-1.84703700
C	4.27894200	-0.47538800	0.60711400
H	4.85541100	0.08270200	1.36276700
H	4.39810400	-1.53339900	0.84937800
H	4.72182000	-0.25753200	-0.36758100

A

Zero-point correction=	0.204168 (Hartree/Particle)
Thermal correction to Energy=	0.216710
Thermal correction to Enthalpy=	0.217654
Thermal correction to Gibbs Free Energy=	0.165147
Sum of electronic and zero-point Energies=	-534.104422
Sum of electronic and thermal Energies=	-534.091880
Sum of electronic and thermal Enthalpies=	-534.090936
Sum of electronic and thermal Free Energies=	-534.143443

C	-2.11958200	1.76218500	-0.14347100
C	-0.93555000	-0.73105600	-1.01326200
C	-1.92268500	-1.50345400	-0.17141900
C	-2.00314800	-1.49174800	1.16092300
H	-0.21704500	2.15700700	0.45736700
H	-2.80757000	1.04238800	-0.56844200
H	-0.15708700	-1.38385000	-1.41398400
N	-0.87700000	1.48455200	0.02431500
H	-1.31778300	-0.86404200	1.73375000
N	-0.22843400	0.33806200	-0.29873200
H	-2.59257100	-2.13249700	-0.75687600
C	1.14042000	0.37694900	0.05481200
O	1.61668400	1.35192100	0.60044200
O	1.74458600	-0.74320500	-0.28512000
C	3.16198300	-0.81483800	0.03269500
H	3.30264300	-0.75256100	1.11291300
H	3.48423700	-1.78375700	-0.34371800
H	3.69710600	-0.00565900	-0.46665700
H	-2.44900900	2.74528300	0.17344300
H	-1.42970500	-0.27286600	-1.88243000
C	-2.97232000	-2.30373600	1.96431700
H	-2.43947400	-2.97727700	2.64672900
H	-3.60108200	-1.65995400	2.59141600
H	-3.62559000	-2.90812700	1.32912300

B

Zero-point correction=	0.203002 (Hartree/Particle)
Thermal correction to Energy=	0.215960
Thermal correction to Enthalpy=	0.216904
Thermal correction to Gibbs Free Energy=	0.162836
Sum of electronic and zero-point Energies=	-534.082222
Sum of electronic and thermal Energies=	-534.069264
Sum of electronic and thermal Enthalpies=	-534.068320
Sum of electronic and thermal Free Energies=	-534.122388

C	1.22632800	2.11488000	-0.56066000
C	0.93104500	-1.03140200	0.34476000
C	2.37491700	-0.82681800	0.64369200
C	3.32451900	-0.89880100	-0.29877100
H	1.58039300	2.42236200	0.42781000
H	0.74135100	-1.42011200	-0.65570000
N	0.49176500	-1.10474100	-0.80000500
H	3.02463200	-1.09377200	-1.32997300
H	2.64294700	-0.65199500	1.68551500
N	0.15798500	0.32090400	0.38770200
H	0.38642500	0.81298900	1.27265000
C	-1.34881400	0.14380200	0.42944200
O	-1.96896100	0.62050700	1.33435300
O	-1.72100900	-0.55873200	-0.60432300
C	-3.15736700	-0.79950900	-0.73005800
H	-3.67774900	0.15483000	-0.82184600
H	-3.26073900	-1.38986500	-1.63776100
H	-3.51315700	-1.35089300	-0.14132700
H	1.50940400	2.71491000	-1.42367300
H	0.42732200	-1.65453400	1.09017200
C	4.79122500	-0.75966100	-0.05247300
H	5.31714300	-1.67535100	-0.34954700
H	5.21077500	0.04803700	-0.66459900
H	5.01738300	-0.55567300	0.99736000

TS-AD

Zero-point correction=	0.202786 (Hartree/Particle)
Thermal correction to Energy=	0.214506
Thermal correction to Enthalpy=	0.215450
Thermal correction to Gibbs Free Energy=	0.164949
Sum of electronic and zero-point Energies=	-534.066831
Sum of electronic and thermal Energies=	-534.055111
Sum of electronic and thermal Enthalpies=	-534.054167
Sum of electronic and thermal Free Energies=	-534.104668

C	2.19723600	-1.04856900	-0.47356800
C	0.65516100	1.41079400	0.30535200
C	2.01037800	1.36460500	-0.06325100
C	2.88209900	0.35612600	0.43503200
H	0.59021400	-1.71228900	0.69879100
H	2.35967000	-0.80391700	-1.51991500
H	0.38642900	1.14854300	1.32712700
N	0.87088600	-1.16638200	-0.12920000
H	2.68218100	0.04305100	1.46220700
N	0.05550800	-0.20856200	-0.53770800
C	2.31613000	1.91376200	-0.95475900
C	-1.28447900	-0.42875100	-0.02135500
O	-1.59853400	-1.41345200	0.60756700
O	-2.05419100	0.57539200	-0.39635300
C	-3.44596800	0.48431400	0.00484500
H	-3.52192700	0.43324000	1.09271300
H	-3.91009800	1.39402600	-0.37151100
H	-3.90525500	-0.39785600	-0.44472700
H	2.79532900	-1.88542200	-0.11781600
H	0.01573400	2.14964400	-0.16556100
C	4.36073900	0.41135900	0.08855200
H	4.85662900	-0.53987500	0.29738500
H	4.52398800	0.66721600	-0.96237600
H	4.84596600	1.17613800	0.70292500

TS-AC

Zero-point correction=	0.204516 (Hartree/Particle)
Thermal correction to Energy=	0.215644
Thermal correction to Enthalpy=	0.216589
Thermal correction to Gibbs Free Energy=	0.167701
Sum of electronic and zero-point Energies=	-534.076971
Sum of electronic and thermal Energies=	-534.065843
Sum of electronic and thermal Enthalpies=	-534.064898
Sum of electronic and thermal Free Energies=	-534.113786

C	1.33022500	-1.49406600	-0.26493200
C	1.22939300	1.31103100	0.62060100
C	1.78833700	0.86075300	-0.65902300
C	2.59301600	-0.30146500	-0.72818100
H	1.16276900	-1.18587900	1.76849300
H	0.68494400	-1.54874600	-1.14089500
H	1.89140100	-2.41550400	-0.10081400
H	1.89625600	1.24265200	1.48086900
N	0.68470100	-1.03473500	0.87818300
H	3.27570700	-0.42398200	0.11878300
N	0.16143100	0.22330800	0.77946600
H	1.32240800	1.24795500	-1.56741800
C	-1.08826800	0.44390900	0.14371900
O	-1.41512200	1.53788000	-0.25787400
O	-1.80566300	-0.67357800	0.11822200
C	-3.13298600	-0.53847300	-0.44784400
H	-3.73728000	0.13113400	0.16730500
H	-3.07398900	-0.15457300	-1.46809400
H	-3.54777700	-1.54510000	-0.43821300
H	0.71553500	2.26913000	0.58294200
C	3.17010600	-0.74129800	-2.06474900
H	4.06125700	-0.15010800	-2.29450700
H	3.47275400	-1.79143400	-2.03649800
H	2.45342800	-0.60890600	-2.88057300

C

Zero-point correction=	0.206876 (Hartree/Particle)
Thermal correction to Energy=	0.217902
Thermal correction to Enthalpy=	0.218846
Thermal correction to Gibbs Free Energy=	0.169972
Sum of electronic and zero-point Energies=	-534.089624
Sum of electronic and thermal Energies=	-534.078599
Sum of electronic and thermal Enthalpies=	-534.077654
Sum of electronic and thermal Free Energies=	-534.126528

C	1.81732400	-1.43091600	-0.23609300
C	1.05912100	1.44067500	0.82110500
C	1.34919900	0.91296800	-0.51936500
C	2.46999900	-0.10451200	-0.72180000
H	1.12091500	-1.02921000	1.70893700
H	1.34073100	-1.94428400	-1.07811900
H	2.52923400	-2.11647100	0.22798600
H	1.73749500	1.22960700	1.64322300
N	0.77711100	-1.08041100	0.74842400
H	3.29758100	0.15796300	-0.05212800
N	0.29555300	0.20513300	0.37659800
H	0.90139000	1.42050600	-1.37111200
C	-1.14265400	0.38599500	0.03857500
O	-1.54353700	1.47918100	-0.25624400
O	-1.76773400	-0.75670100	0.11216100
C	-3.18975100	-0.71286800	-0.21198700
H	-3.32426300	-0.35159100	-1.23260500
H	-3.52835400	-1.74208000	-0.11363200
H	-3.70642700	-0.06198900	0.49498200
H	0.42289800	2.31460800	0.91958200
C	2.97702300	-0.17091000	-2.16362500
H	3.42957500	0.77581500	-2.47152700
H	3.74167000	-0.94704700	-2.25781500
H	2.16790400	-0.40906700	-2.86212600

TS-CE

Zero-point correction=	0.203278 (Hartree/Particle)
Thermal correction to Energy=	0.214786
Thermal correction to Enthalpy=	0.215730
Thermal correction to Gibbs Free Energy=	0.165656
Sum of electronic and zero-point Energies=	-534.063382
Sum of electronic and thermal Energies=	-534.051873
Sum of electronic and thermal Enthalpies=	-534.050929
Sum of electronic and thermal Free Energies=	-534.101004

C	1.03925300	-1.57217400	-0.30402100
C	1.75291300	1.55312800	0.32760400
C	1.72853400	0.77337600	-0.79259000
C	2.24360500	-0.60914600	-0.83239400
H	1.21906100	-1.30957800	1.77891800
H	0.21056600	-1.54902600	-1.01110100
H	1.41499200	-2.58888000	-0.17917400
H	2.35387700	1.29195000	1.19427800
N	0.64969900	-1.03536500	0.96640400
H	3.06276700	-0.74582400	-0.11826800
N	0.08751000	0.09857600	1.10971100
H	1.17525300	1.12754900	-1.66261900
C	-1.03478900	0.47702500	0.25325800
O	-1.22055800	1.60496500	-0.11380000
O	-1.84389200	-0.57015400	0.13316300
C	-3.13720000	-0.29268700	-0.47465900
H	-3.00105800	0.09659900	-1.48496800
H	-3.65030400	-1.25247000	-0.49159300
H	-3.68316600	0.42847700	0.13594800
H	1.29334000	2.53530200	0.33204700
C	2.65082600	-1.11250100	-2.22450200
H	3.51815500	-0.55000000	-2.57922300
H	2.92687400	-2.16974000	-2.19400100
H	1.84202800	-0.98632600	-2.95084300

R'=H

R1=Ph R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.239423 (Hartree/Particle)
Thermal correction to Energy=	0.251931
Thermal correction to Enthalpy=	0.252875
Thermal correction to Gibbs Free Energy=	0.200552
Sum of electronic and zero-point Energies=	-537.230589
Sum of electronic and thermal Energies=	-537.218082
Sum of electronic and thermal Enthalpies=	-537.217137
Sum of electronic and thermal Free Energies=	-537.269460

C	-0.02559200	0.10284900	0.71267200
C	-3.31156300	-0.16932700	-0.65459600
C	-2.37200600	-1.15132700	-0.42141400
C	-1.05413700	-1.02533300	-0.87665300
H	-0.33405900	-0.58016900	1.51151100
H	-3.05214100	0.63233500	-1.34545300
H	-0.35824500	-1.84944600	-0.75524600
N	-0.74681500	1.19820300	0.46861100
H	-0.81254200	-0.31964700	-1.66488200
H	-2.62550000	-1.98471700	0.23249600
N	-1.94209100	1.26300600	0.98207200
H	-2.20575700	0.70268000	1.79833600
H	-2.41632700	2.15578800	0.86541400
C	-4.72304900	-0.21944600	-0.18813600
H	-5.05713000	0.75387600	0.18768700
H	-5.37288100	-0.44639400	-1.04580500
H	-4.88934800	-0.98163300	0.57687100
C	1.39256700	0.06199100	0.31771100
C	2.20490900	-0.95787600	0.83774200
C	1.94831700	1.01009400	-0.55858800
C	3.55267300	-1.02799900	0.49096800
H	1.78193300	-1.69256600	1.51919900
C	3.29485500	0.93534100	-0.89918400
H	1.32530200	1.80495000	-0.95650800
C	4.09948100	-0.08255200	-0.37771800
H	4.17488700	-1.81799300	0.90118500
H	3.72076300	1.67404600	-1.57209700
H	5.15049100	-0.13547300	-0.64719200

A

Zero-point correction=	0.241903 (Hartree/Particle)
Thermal correction to Energy=	0.254903
Thermal correction to Enthalpy=	0.255847
Thermal correction to Gibbs Free Energy=	0.201196
Sum of electronic and zero-point Energies=	-537.263063
Sum of electronic and thermal Energies=	-537.250063
Sum of electronic and thermal Enthalpies=	-537.249118
Sum of electronic and thermal Free Energies=	-537.303770

C	0.48235400	-0.61341300	-0.47120200
C	-2.90719800	0.09608100	0.33705000
C	-4.24603000	-0.11280700	-0.32377600
C	-5.16352800	0.83942400	-0.47150900
H	-0.47589700	1.08750000	0.05569800
H	0.29402700	-1.62357000	-0.83338700
H	-2.80595500	1.15458100	0.60953900
H	-6.12794000	0.62902400	-0.92418900
N	-0.57195600	0.12914900	-0.29227500
H	-4.99337300	1.86125900	-0.14071300
N	-1.86118600	-0.15609100	-0.69982500
H	-4.45754900	-1.13033500	-0.65638300
H	-1.89712900	-1.10283800	-1.08637200
C	-2.73398200	-0.78073900	1.58394800
H	-2.85236800	-1.84235800	1.34002200
H	-1.75038600	-0.64154500	2.04505000
H	-3.49234900	-0.52126000	2.32765100
C	1.84481200	-0.20301700	-0.23980000
C	2.84067900	-1.19540800	-0.35319200
C	2.21596900	1.11624200	0.09858600
C	4.17326100	-0.87979800	-0.11502800
H	2.56021400	-2.21056600	-0.62197700
C	3.54767000	1.42137300	0.33577000
H	1.47494900	1.90985500	0.16106000
C	4.52711800	0.42553000	0.23145300
H	4.93497800	-1.64850900	-0.20056400
H	3.83020800	2.43742900	0.59360200
H	5.56863300	0.67389200	0.41484000

B

Zero-point correction=	0.242593 (Hartree/Particle)
Thermal correction to Energy=	0.255396
Thermal correction to Enthalpy=	0.256340
Thermal correction to Gibbs Free Energy=	0.202520
Sum of electronic and zero-point Energies=	-537.262632
Sum of electronic and thermal Energies=	-537.249830
Sum of electronic and thermal Enthalpies=	-537.248885
Sum of electronic and thermal Free Energies=	-537.302705

C	0.37284000	-0.56043000	0.41201400
C	-2.83144900	0.28776600	-0.29737000
C	-4.16120900	-0.32134900	0.04997000
C	-4.70024200	-1.33396800	-0.62862100
H	0.09053200	-1.62073400	0.47178500
H	-2.41415700	-0.17599000	-1.19649400
H	-5.67665000	-1.73043500	-0.36700400
N	-0.49531700	0.37717400	0.57510100
H	-4.19834600	-1.79301800	-1.47751900
H	-4.69804900	0.13186100	0.88398600
H	-1.88021100	-1.14074800	0.93682200
H	-2.14818700	0.30334300	1.70524200
N	-1.83586400	-0.11335600	0.81483300
C	-2.85963700	1.80559600	-0.42450700
H	-3.23416700	2.27656400	0.49108900
H	-1.87031000	2.20766900	-0.64948100
H	-3.53874900	2.07175700	-1.23826500
C	1.77567500	-0.27963000	0.15206500
C	2.65707400	-1.36623200	0.01353800
C	2.26490500	1.03704900	0.04339200
C	4.00926600	-1.14221900	-0.22956800
H	2.27921300	-2.38233600	0.09747200
C	3.61448400	1.25202200	-0.19929600
H	1.58179800	1.87339400	0.15153300
C	4.48712100	0.16501900	-0.33532800
H	4.68798300	-1.98296700	-0.33589900
H	3.99395500	2.26607300	-0.28273200
H	5.54234500	0.34113000	-0.52455000

TS-AD

Zero-point correction=	0.241038 (Hartree/Particle)
Thermal correction to Energy=	0.252956
Thermal correction to Enthalpy=	0.253900
Thermal correction to Gibbs Free Energy=	0.202807
Sum of electronic and zero-point Energies=	-537.224875
Sum of electronic and thermal Energies=	-537.212958
Sum of electronic and thermal Enthalpies=	-537.212014
Sum of electronic and thermal Free Energies=	-537.263107

C	0.15130900	-0.41368100	-0.36968000
C	3.10425600	0.28942700	0.39833400
C	2.30761500	-0.70832700	0.99602700
C	0.95619500	-0.47059500	1.31802800
H	0.54492000	1.53535600	-0.94820300
H	0.38908700	-1.40416700	-0.75071800
H	2.89211600	1.31635800	0.70058300
H	0.40707600	-1.27746900	1.79887200
N	0.87690900	0.56711200	-1.02306600
H	0.68892700	0.51427900	1.69483600
N	2.15843900	0.32524500	-1.26629400
H	2.64461300	-1.74216900	0.91466500
C	4.52740500	0.01208200	-0.00529400
H	4.63265100	-0.98710900	-0.43507300
H	4.88593000	0.74456100	-0.73411200
H	5.18037300	0.08343400	0.87155700
H	2.56284800	1.19681800	-1.63673000
C	-1.30328100	-0.16319600	-0.16083200
C	-1.78517100	1.06168800	0.32683600
C	-2.20866600	-1.19035700	-0.46291100
C	-3.15479700	1.26307800	0.47949000
H	-1.09954500	1.86121400	0.60217300
C	-3.57786100	-0.98617600	-0.30286400
H	-1.84120400	-2.14357600	-0.83420700
C	-4.05238000	0.23998200	0.16510600
H	-3.52064000	2.21449700	0.85399600
H	-4.27273100	-1.78444900	-0.54616500
H	-5.11956800	0.39732500	0.29177900

TS-AC

Zero-point correction=	0.242853 (Hartree/Particle)
Thermal correction to Energy=	0.254118
Thermal correction to Enthalpy=	0.255063
Thermal correction to Gibbs Free Energy=	0.205748
Sum of electronic and zero-point Energies=	-537.236161
Sum of electronic and thermal Energies=	-537.224895
Sum of electronic and thermal Enthalpies=	-537.223951
Sum of electronic and thermal Free Energies=	-537.273265

C	0.12765600	-0.52232900	-0.28096700
C	3.01736200	0.41784800	0.20276600
C	2.32034000	-0.56261500	1.02558300
C	0.96643100	-0.38328000	1.36971300
H	0.69987900	1.30366900	-1.08295900
H	0.30404100	-1.57579500	-0.50131700
H	2.74293500	1.45419500	0.41376500
H	0.50127100	-1.16763500	1.96419900
N	0.91738600	0.30713600	-1.08685200
H	0.65578200	0.62016600	1.65695700
N	2.25408500	0.07224400	-1.13851500
H	2.75103100	-1.56399700	1.07665800
C	4.50699500	0.24955000	-0.01987000
H	4.76342700	-0.78581900	-0.26756500
H	4.84260200	0.89651300	-0.83345400
H	5.05122800	0.52337500	0.88809100
H	2.43132800	-0.89991000	-1.40812600
C	-1.31503000	-0.19404200	-0.13635700
C	-2.25630600	-1.22825600	-0.25079900
C	-1.75664300	1.11517300	0.11768600
C	-3.61749300	-0.95527000	-0.13303600
H	-1.92176300	-2.24512600	-0.44013900
C	-3.11689900	1.38493200	0.22919100
H	-1.04466900	1.92947000	0.23595700
C	-4.04880100	0.35053800	0.10362100
H	-4.33965500	-1.76072800	-0.22753800
H	-3.45123300	2.40023400	0.42047900
H	-5.10990900	0.56396100	0.19579300

C

Zero-point correction=	0.245679 (Hartree/Particle)
Thermal correction to Energy=	0.256804
Thermal correction to Enthalpy=	0.257748
Thermal correction to Gibbs Free Energy=	0.208340
Sum of electronic and zero-point Energies=	-537.256752
Sum of electronic and thermal Energies=	-537.245627
Sum of electronic and thermal Enthalpies=	-537.244683
Sum of electronic and thermal Free Energies=	-537.294092

C	0.07882900	-0.85349500	0.08538600
C	2.91333800	0.64583600	0.01390300
C	2.37203600	-0.49762100	0.79069500
C	0.94651600	-0.44684400	1.31595100
H	0.65991400	0.51750000	-1.40358700
H	0.02586000	-1.94645900	0.05368400
H	2.29255000	1.53978600	-0.02815000
H	0.80541500	-1.14057600	2.14712500
N	0.87215000	-0.44030500	-1.11516800
H	0.69632100	0.55723800	1.66722400
N	2.24010600	-0.49664600	-0.72198400
H	3.07026800	-1.23863600	1.17239300
C	4.38487400	0.84129900	-0.22525500
H	4.93227700	-0.10600500	-0.21837100
H	4.56355800	1.35107700	-1.17591400
H	4.78900400	1.46652400	0.57691200
H	2.81750200	-1.13460500	-1.28049700
C	-1.32788800	-0.29834400	0.03741900
C	-1.57742500	1.07844600	0.13911000
C	-2.40863800	-1.17381000	-0.11949800
C	-2.88194400	1.56627500	0.08249800
H	-0.75719000	1.78183700	0.26848700
C	-3.71491800	-0.68687100	-0.16802500
H	-2.22656700	-2.24239400	-0.20141800
C	-3.95351400	0.68377100	-0.06867700
H	-3.06203500	2.63450400	0.16215700
H	-4.54400700	-1.37878100	-0.28516800
H	-4.97014500	1.06461000	-0.10703900

TS-CE

Zero-point correction=	0.243302 (Hartree/Particle)
Thermal correction to Energy=	0.254764
Thermal correction to Enthalpy=	0.255708
Thermal correction to Gibbs Free Energy=	0.204986
Sum of electronic and zero-point Energies=	-537.207981
Sum of electronic and thermal Energies=	-537.196518
Sum of electronic and thermal Enthalpies=	-537.195574
Sum of electronic and thermal Free Energies=	-537.246296

C	0.12377400	-0.60781500	0.01114800
C	3.13392500	0.53212900	0.16354500
C	2.38018600	-0.21712800	1.06979800
C	0.95807100	0.03064400	1.28647800
H	0.61824200	0.78825700	-1.49751000
H	0.24830800	-1.69241100	0.07862100
H	2.77084200	1.52606700	-0.09751700
H	0.56511700	-0.47437700	2.17230000
N	0.86611700	-0.13914400	-1.14073600
H	0.70539700	1.09268000	1.32100200
N	2.14694000	-0.39546300	-1.22551900
H	2.81059900	-1.14236600	1.45675900
C	4.59120700	0.29026900	-0.09577000
H	4.84046800	0.52387600	-1.13508100
H	5.18719300	0.95275500	0.54440600
H	4.88481000	-0.74202300	0.12010300
H	2.31281900	-1.37994000	-0.97386800
C	-1.33407200	-0.23367400	0.00841400
C	-2.30064900	-1.24692700	0.04251300
C	-1.74514900	1.10733100	-0.03083500
C	-3.65773000	-0.92630800	0.03019700
H	-1.99090600	-2.28918500	0.07530600
C	-3.10180500	1.42542800	-0.05249100
H	-1.01341600	1.91357200	-0.04273600
C	-4.05941800	0.40919100	-0.01961100
H	-4.39955400	-1.71989100	0.05667400
H	-3.41037700	2.46673300	-0.08737100
H	-5.11700700	0.65942800	-0.02995500

R'=Boc

R1=Ph R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.281949 (Hartree/Particle)
Thermal correction to Energy=	0.298910
Thermal correction to Enthalpy=	0.299854
Thermal correction to Gibbs Free Energy=	0.236729
Sum of electronic and zero-point Energies=	-765.063479
Sum of electronic and thermal Energies=	-765.046519
Sum of electronic and thermal Enthalpies=	-765.045574
Sum of electronic and thermal Free Energies=	-765.108700

C	2.03119500	-1.02318500	-0.44803500
C	0.22337100	2.00067300	0.57403600
C	1.51410000	1.72195600	0.21136500
C	2.24155500	0.65485200	0.79193500
H	2.29963200	-0.51259900	-1.37982200
H	-0.21780300	1.41583100	1.38315300
H	3.31810500	0.61890400	0.65271300
N	0.73532900	-1.17842800	-0.14156600
H	1.88452200	0.20436200	1.71339100
N	-0.12695000	-0.46923500	-0.80051200
H	1.98324900	2.29941700	-0.58407000
C	-1.53394400	-0.52998400	-0.55031500
O	-2.28325400	0.11687600	-1.24367200
O	-1.81804600	-1.32209400	0.46340100
C	-3.23147500	-1.44929100	0.77198200
H	-3.63259600	-0.48625800	1.09361400
H	-3.77520800	-1.80827300	-0.10332000
H	-3.27840200	-2.17624000	1.58066300
H	0.11754400	0.04428100	-1.65836300
C	-0.61140200	3.08631500	0.00425300
H	-1.53874800	2.66717800	-0.41082800
H	-0.92510400	3.77420500	0.80063500
H	-0.09563200	3.65257100	-0.77438800
C	3.00971100	-1.99657000	0.07751900
C	4.28811300	-2.03646500	-0.49914300
C	2.69446700	-2.86923500	1.13204700
C	5.23890800	-2.94191700	-0.03191700
H	4.53569100	-1.36509600	-1.31844900
C	3.64884900	-3.77039700	1.59328800
H	1.70310500	-2.84579700	1.57382200
C	4.92111400	-3.80864300	1.01446500
H	6.22438400	-2.97189800	-0.48722500
H	3.39995800	-4.44778100	2.40506600
H	5.66157600	-4.51532300	1.37823100

B

Zero-point correction=	0.284497 (Hartree/Particle)
Thermal correction to Energy=	0.301774
Thermal correction to Enthalpy=	0.302719
Thermal correction to Gibbs Free Energy=	0.238342
Sum of electronic and zero-point Energies=	-765.079027
Sum of electronic and thermal Energies=	-765.061750
Sum of electronic and thermal Enthalpies=	-765.060806
Sum of electronic and thermal Free Energies=	-765.125182

C	-0.61137500	0.14156300	0.72859400
C	2.36279000	1.56731000	-0.16635800
C	1.52062200	2.78865000	0.05389500
C	0.80630000	3.36452600	-0.91198200
H	-0.47322400	0.40066900	1.78630500
H	2.36260600	1.27496700	-1.21826200
N	0.38471000	0.07832300	-0.08841700
H	0.76829700	2.95971700	-1.92012500
H	1.55059600	3.22389200	1.05339900
N	1.66957900	0.35540900	0.53548800
H	1.58217500	0.55999700	1.54955500
C	2.47532300	-0.92671800	0.47802600
O	2.74395200	-1.50506600	1.49102100
O	2.74475600	-1.20498200	-0.77015200
C	3.46387900	-2.45360300	-1.00527300
H	2.84125100	-3.29382600	-0.69406800
H	3.64023500	-2.47515300	-2.07854500
H	4.40478600	-2.44837300	-0.45307500
C	-1.97340900	-0.13060200	0.30082400
C	-3.00187900	-0.02299200	1.25375300
C	-2.28078300	-0.50461200	-1.02259700
C	-4.31972800	-0.28622000	0.89143500
H	-2.76405600	0.26422900	2.27517900
C	-3.59735900	-0.76564300	-1.37556300
H	-1.48437800	-0.58789500	-1.75515100
C	-4.61668900	-0.65727300	-0.42096300
H	-5.11170900	-0.20467800	1.62964900
H	-3.83704800	-1.05578700	-2.39423500
H	-5.64474200	-0.86539400	-0.70431000
H	0.24116300	4.27344100	-0.72810500
C	3.77987500	1.70706100	0.38380900
H	3.78304900	1.91734700	1.45852100
H	4.39630200	0.82432800	0.19231500
H	4.25674200	2.55206700	-0.11929900

A

Zero-point correction=	0.285158 (Hartree/Particle)
Thermal correction to Energy=	0.302341
Thermal correction to Enthalpy=	0.303285
Thermal correction to Gibbs Free Energy=	0.239530
Sum of electronic and zero-point Energies=	-765.100345
Sum of electronic and thermal Energies=	-765.083162
Sum of electronic and thermal Enthalpies=	-765.082218
Sum of electronic and thermal Free Energies=	-765.145974

C	-0.90993600	0.45935200	0.00615800
C	1.90535500	1.36164400	0.55808900
C	1.63040800	2.48703000	-0.41996700
C	1.34961100	2.35166700	-1.71475000
H	0.05365700	-1.35023100	0.00149000
H	-0.72115200	1.52537400	-0.06000700
H	2.98983100	1.24367100	0.62843000
H	1.20441100	3.22132800	-2.34766100
N	0.12902000	-0.32319600	0.03984700
H	1.26559800	1.37953400	-2.19507700
N	1.45942200	0.04051500	0.04561500
H	1.72565300	3.48112500	0.01476800
C	2.28470500	-1.07850600	-0.14187200
O	1.81818900	-2.18435400	-0.35383800
O	3.56755300	-0.75762200	-0.06617700
C	4.50031700	-1.84844000	-0.27543700
H	4.35729400	-2.27940600	-1.26781800
H	5.48621400	-1.39458600	-0.19122500
H	4.36290200	-2.61437900	0.48980100
C	1.38842900	1.63509700	1.97985100
H	1.88795700	2.52873600	2.36386800
H	0.31266300	1.82094300	2.03071200
H	1.63115700	0.80225000	2.64515500
C	-2.27530200	0.00062900	0.02530700
C	-3.27250300	0.98737800	0.12719600
C	-2.65164000	-1.35257000	0.17645600
C	-4.61481800	0.62854600	-0.14506300
H	-2.98511700	2.02996100	-0.23695800
C	-3.99349400	-1.69984500	0.15682500
H	-1.90669800	-2.13174700	0.31955900
C	-4.97512500	-0.71295000	-0.00573600
H	-5.37775500	1.39129400	-0.26554900
H	-4.28280200	-2.73966700	0.27342100
H	-6.02421900	-0.99484300	-0.01757200

TS-AC

Zero-point correction=	0.285440 (Hartree/Particle)
Thermal correction to Energy=	0.301092
Thermal correction to Enthalpy=	0.302036
Thermal correction to Gibbs Free Energy=	0.242259
Sum of electronic and zero-point Energies=	-765.062763
Sum of electronic and thermal Energies=	-765.047111
Sum of electronic and thermal Enthalpies=	-765.046167
Sum of electronic and thermal Free Energies=	-765.105944

C	0.55450400	-0.01264000	0.32812000
C	-1.87757500	-1.78698200	-0.17780400
C	-1.25914800	-1.59594500	1.13964000
C	0.14827100	-1.53221500	1.24496400
H	0.10067400	-0.58913300	-1.62198400
H	0.19401000	0.74616900	1.02337200
H	-1.24913600	-2.36955100	-0.85668200
H	0.55583700	-1.36632400	2.24079400
N	-0.25996100	-0.06848600	-0.82194000
H	0.70352600	-2.27101000	0.66776500
N	-1.58229100	-0.31146600	-0.59543400
H	-1.89420400	-1.20704900	1.93558500
C	-2.41511800	0.75558500	-0.15317000
O	-3.44486900	0.58163800	0.45737300
O	-1.91783000	1.92136300	-0.55716100
C	-2.72742700	3.07820500	-0.23307200
H	-3.69152000	3.01650100	-0.74143400
H	-2.88160100	3.14763200	0.84530300
H	-2.15781400	3.93195900	-0.59679900
C	2.02495300	0.05914600	0.11711500
C	2.76402700	0.99499700	0.85599100
C	2.68824400	-0.78583500	-0.78855400
C	4.14207600	1.09876200	0.67888700
H	2.25724300	1.64667900	1.56327000
C	4.06363700	-0.67562900	-0.96618600
H	2.14076100	-1.53816700	-1.35280700
C	4.79192900	0.26618200	-0.23278300
H	4.70593900	1.82934300	1.25111000
H	4.57065100	-1.32817700	-1.67063600
H	5.86661500	0.34486800	-0.36983000
C	-3.32517100	-2.22488600	-0.29447800
H	-3.96853700	-1.74385000	0.43901300
H	-3.70259300	-2.00474600	-1.29610600
H	-3.36077300	-3.30910300	-0.15184700

TS-AD

Zero-point correction=	0.282601 (Hartree/Particle)
Thermal correction to Energy=	0.299249
Thermal correction to Enthalpy=	0.300194
Thermal correction to Gibbs Free Energy=	0.237980
Sum of electronic and zero-point Energies=	-765.059714
Sum of electronic and thermal Energies=	-765.043066
Sum of electronic and thermal Enthalpies=	-765.042121
Sum of electronic and thermal Free Energies=	-765.104335

C	2.15401700	-0.76551300	-0.46987500
C	0.05918200	1.75849800	0.60621100
C	1.39913400	1.81096800	0.24982300
C	2.35302500	0.94815100	0.79124300
H	0.60827200	-1.74436800	0.52126100
H	2.29675000	-0.20582000	-1.38918700
H	-0.21420600	1.17825100	1.48832700
H	3.40346100	1.09346600	0.55698000
N	0.85946400	-1.03881800	-0.19500200
H	2.15308600	0.43602700	1.72862800
N	-0.12178600	-0.31592300	-0.66649500
H	1.68730800	2.44971100	-0.58389200
C	-1.35696500	-0.82700000	-0.14537400
O	-1.43974400	-1.72636300	0.67046200
O	-2.36234400	-0.17922300	-0.71442400
C	3.68848200	-0.60222100	-0.31035500
H	-3.83206800	-0.42905000	0.75830900
H	-4.37281500	0.01041600	-0.89485100
H	-3.82899600	-1.66064100	-0.53692600
C	-0.97175400	2.67208300	0.04925900
H	-0.63036000	3.17820200	-0.85619400
H	-1.90183300	2.13819000	-0.16483900
H	-1.21443000	3.43296000	0.80496500
C	3.22610300	-1.67702300	-0.04452800
C	4.38044800	-1.73853300	-0.84355600
C	3.14678400	-2.46692600	1.11644100
C	5.42525200	-2.59252700	-0.50088200
H	4.45103300	-1.12551900	-1.73857400
C	4.19215400	-3.32167300	1.44980100
H	2.28007300	-2.41296600	1.77232700
C	5.33177300	-3.38689100	0.64277100
H	6.31010500	-2.63929800	-1.12844400
H	4.12206500	-3.93186600	2.34518200
H	6.14768600	-4.05191800	0.91055400

C

Zero-point correction=	0.287519 (Hartree/Particle)
Thermal correction to Energy=	0.303232
Thermal correction to Enthalpy=	0.304177
Thermal correction to Gibbs Free Energy=	0.243472
Sum of electronic and zero-point Energies=	-765.077294
Sum of electronic and thermal Energies=	-765.061581
Sum of electronic and thermal Enthalpies=	-765.060637
Sum of electronic and thermal Free Energies=	-765.121342

C	0.76467700	0.01612100	0.74796400
C	-1.61505500	-1.77039100	-0.43249500
C	-1.18185600	-1.42136300	0.93441600
C	0.29658000	-1.37458000	1.27428200
H	0.14179900	0.03984500	-1.27156100
H	0.59212800	0.75256800	1.53945900
H	-0.82492200	-2.03377900	-1.13531200
H	0.45784300	-1.46315300	2.35032000
N	-0.17858500	0.36608700	-0.35751500
H	0.82857900	-2.19258200	0.78261400
N	-1.41601400	-0.26567700	-0.04800400
H	-1.93101900	-1.45208600	1.72180500
C	-2.60680200	0.60212900	0.12911400
O	-3.48887100	0.28541200	0.88148900
O	-2.50525800	1.64413900	-0.65455600
C	-3.61343900	2.58918700	-0.59290300
H	-3.70358000	2.98578100	0.41945500
H	-3.34682900	3.37544600	-1.29611700
H	-4.53834500	2.09361600	-0.89221600
C	-2.98527600	-2.27724700	-0.77850200
H	-3.73940600	-1.99374700	-0.04437500
H	-3.29158500	-1.93904800	-1.77270700
H	-2.92560000	-3.37096700	-0.80620200
C	2.20257900	0.12533200	0.28895800
C	2.99490700	1.18116600	0.75519800
C	2.75739500	-0.79336000	-0.61430100
C	4.31852100	1.31376900	0.33555600
H	2.57389500	1.90228700	1.45134100
H	4.07870500	-0.65853100	-1.03737500
C	2.16707600	-1.62553600	-0.99207100
H	4.86249100	0.39431100	-0.56141400
H	4.92269800	2.13548300	0.70925400
H	4.49729900	-1.37899700	-1.73426700
H	5.89375300	0.49514700	-0.88759100

TS-CE

Zero-point correction=	0.284471 (Hartree/Particle)
Thermal correction to Energy=	0.300345
Thermal correction to Enthalpy=	0.301289
Thermal correction to Gibbs Free Energy=	0.241023
Sum of electronic and zero-point Energies=	-765.054694
Sum of electronic and thermal Energies=	-765.038820
Sum of electronic and thermal Enthalpies=	-765.037876
Sum of electronic and thermal Free Energies=	-765.098141

C	0.50020700	-0.09781800	0.32144800
C	-2.17064600	-2.08638300	-0.03527300
C	-1.48089200	-1.53915200	1.02876900
C	-0.01698200	-1.46192900	1.06739000
H	0.19005100	-0.66072200	-1.69771700
H	0.14144300	0.74453500	0.91494200
H	-1.59397500	-2.60736200	-0.79985100
H	0.36918400	-1.37567000	2.08626900
N	-0.23434200	-0.12532500	-0.93079400
H	0.46497400	-2.30157400	0.56385300
N	-1.52006800	-0.12287500	-0.95718600
H	-2.04752300	-1.06108000	1.82594400
C	-2.23684500	0.93282500	-0.26215000
O	-3.31825000	0.77794700	0.24225400
O	-1.58373900	2.08054200	-0.43392900
C	-2.29289000	3.26966600	0.00518500
H	-2.49192800	3.21646800	1.07707300
H	-1.62308900	4.09681800	-0.22399500
H	-3.23000000	3.36792400	-0.54556400
C	-3.64762600	-2.26567100	-0.10320100
H	-4.02761600	-1.98350200	-1.08954500
H	-3.87029300	-3.33398000	0.02473000
H	-4.17564500	-1.69681600	0.66150800
C	1.99490800	-0.04131700	0.15075200
C	2.69525300	1.06452700	0.64881900
C	2.69733000	-1.06507400	-0.50067400
C	4.07814700	1.14832300	0.49357900
H	2.15810200	1.86197600	1.15622800
C	4.07866000	-0.97463900	-0.66240600
H	2.17821300	-1.94081500	-0.88511500
C	4.77055400	0.13062300	-0.16363700
H	4.61258400	2.00910800	0.88446900
H	4.61419400	-1.77067900	-1.17121000
H	5.84802700	0.19589000	-0.28468300

R'=H

R1=CH3 R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.186458 (Hartree/Particle)
Thermal correction to Energy=	0.195878
Thermal correction to Enthalpy=	0.196822
Thermal correction to Gibbs Free Energy=	0.152938
Sum of electronic and zero-point Energies=	-345.534560
Sum of electronic and thermal Energies=	-345.525140
Sum of electronic and thermal Enthalpies=	-345.524196
Sum of electronic and thermal Free Energies=	-345.568080

C	-1.62429400	-0.25102500	0.40085600
C	1.72715500	0.31121300	-0.39037900
C	0.87939000	1.18588900	0.27697900
C	-0.36169100	1.51978400	-0.24933000
H	-1.36377900	-0.13089500	1.45878900
H	1.49735800	0.07509500	-1.42844000
H	-1.00721700	2.21926200	0.27401800
N	-0.93870800	-1.08401800	-0.36151600
H	-0.57499300	1.36695000	-1.30229700
H	1.12667000	1.49219500	1.29229300
N	0.22256700	-1.50438500	0.10247500
H	0.39051900	-1.55039700	1.11308800
H	0.63569600	-2.26048300	-0.44077800
C	-3.01010400	0.13022500	-0.02535200
H	-3.72960600	-0.55996100	0.43250800
H	-3.27283900	1.13565900	0.31336400
H	-3.12003800	0.06829200	-1.10998000
C	3.06797100	-0.09894600	0.10898800
H	3.29439700	-1.14072900	-0.13919700
H	3.82886900	0.50585600	-0.40584100
H	3.18473800	0.05650300	1.18419500

A

Zero-point correction=	0.188410 (Hartree/Particle)
Thermal correction to Energy=	0.198487
Thermal correction to Enthalpy=	0.199432
Thermal correction to Gibbs Free Energy=	0.152907
Sum of electronic and zero-point Energies=	-345.564350
Sum of electronic and thermal Energies=	-345.554272
Sum of electronic and thermal Enthalpies=	-345.553328
Sum of electronic and thermal Free Energies=	-345.599853

C	2.36493900	-0.22380400	0.41633000
C	-1.11368300	0.26853200	-0.23943500
C	-2.39306000	-0.25319700	0.36476000
C	-3.35292200	-0.86106700	-0.32773100
H	1.23660300	-0.32681800	-1.24124000
H	2.31449700	-0.22275700	1.50550700
H	-1.11691700	0.06173800	-1.31747000
H	-4.26963200	-1.19249600	0.15078500
N	1.24115000	-0.31104200	-0.21346400
H	-3.26730300	-1.04454600	-1.39614500
N	-0.00096900	-0.55462300	0.32585500
H	-2.51965900	-0.07531300	1.43367400
H	0.05177800	-0.52691900	1.34751500
C	3.67542600	-0.16074100	-0.26990000
H	3.58188700	-0.13049000	-1.35852300
H	4.22425000	0.72429900	0.07192600
H	4.27815300	-1.03361400	0.01115000
C	-0.92748600	1.77101200	0.00766500
H	-0.92987600	1.99872500	1.07929000
H	0.00964000	2.14234500	-0.42081800
H	-1.74810900	2.32557700	-0.45541400

B

Zero-point correction=	0.189151 (Hartree/Particle)
Thermal correction to Energy=	0.199098
Thermal correction to Enthalpy=	0.200042
Thermal correction to Gibbs Free Energy=	0.153823
Sum of electronic and zero-point Energies=	-345.565449
Sum of electronic and thermal Energies=	-345.555502
Sum of electronic and thermal Enthalpies=	-345.554558
Sum of electronic and thermal Free Energies=	-345.600777

C	2.20268300	-0.59090500	0.05409900
C	-1.07110500	0.30679900	-0.24827300
C	-2.35412000	-0.29787200	0.25001500
C	-2.98898800	-1.28443100	-0.38177900
H	1.94420600	-1.65535400	0.14559600
H	-0.78309100	-0.12984700	-1.20935000
H	-3.92938500	-1.67839400	-0.00823200
N	1.36191000	0.33706900	0.31020000
H	-2.60661000	-1.72395400	-1.30036700
H	-2.77360600	0.13637600	1.15821500
H	0.00636200	-1.18097800	0.80496700
H	-0.13002000	0.24161200	1.64866500
N	0.05058000	-0.15072000	0.71169600
C	3.58288200	-0.24592600	-0.37703800
H	3.72418000	0.83460600	-0.42732800
H	4.30591100	-0.68070000	0.32310000
H	3.78478500	-0.69203600	-1.35788800
H	-1.08948300	1.82893900	-0.31873200
C	-1.34310900	2.27072000	0.65119200
H	-0.13018300	2.22944100	-0.65065700
H	-1.85958200	2.13061600	-1.03305100

TS-AD

Zero-point correction=	0.188512 (Hartree/Particle)
Thermal correction to Energy=	0.197211
Thermal correction to Enthalpy=	0.198155
Thermal correction to Gibbs Free Energy=	0.155870
Sum of electronic and zero-point Energies=	-345.533152
Sum of electronic and thermal Energies=	-345.524454
Sum of electronic and thermal Enthalpies=	-345.523510
Sum of electronic and thermal Free Energies=	-345.565795

C	1.42480900	-0.10944100	-0.39610500
C	-1.51793600	0.16551000	0.38914100
C	-0.71584600	1.20220900	-0.16507900
C	0.61408300	1.39540100	0.26021100
H	0.94373600	-1.45271600	1.09522500
H	1.25214900	-0.02243300	-1.46727300
H	-1.39039600	0.01366300	1.46347100
H	1.16588800	2.20905400	-0.20833700
N	0.69250500	-1.14686500	0.14829900
H	0.82375400	1.29100900	1.32383500
N	-0.58825700	-1.24345200	-0.24448000
H	-1.01732800	1.61744800	-1.12753100
H	-1.02033000	-1.98852500	0.31819100
C	2.88103100	-0.04184500	0.01297700
H	3.32869200	0.89373100	-0.32709000
H	3.00749500	-0.11036000	1.09774300
H	3.42839300	-0.86517100	-0.45703600
C	-2.92548300	-0.04595300	-0.11549500
H	-2.96572100	0.00194200	-1.20658000
H	-3.31919600	-1.01487900	0.20429800
H	-3.58631000	0.72522300	0.29304400

TS-AC

Zero-point correction=	0.189711 (Hartree/Particle)
Thermal correction to Energy=	0.198001
Thermal correction to Enthalpy=	0.198945
Thermal correction to Gibbs Free Energy=	0.157666
Sum of electronic and zero-point Energies=	-345.544105
Sum of electronic and thermal Energies=	-345.535815
Sum of electronic and thermal Enthalpies=	-345.534870
Sum of electronic and thermal Free Energies=	-345.576150

C	1.49070800	-0.16986900	-0.38709000
C	-1.46062500	0.05961800	0.38626500
C	-0.72206500	1.16160800	-0.23490500
C	0.56755200	1.48938500	0.17120600
H	0.79408200	-1.39792100	1.10332600
H	1.38186600	-0.03501000	-1.46263800
H	-1.28955900	-0.02625600	1.46243100
H	1.09595700	2.26928200	-0.37358800
N	0.65404900	-1.12152700	0.12974700
H	0.81858000	1.42104100	1.22849500
N	-0.65839000	-1.14323300	-0.23606800
H	-1.06686500	1.49661600	-1.21481900
H	-0.73312900	-1.12818100	-1.25759100
C	2.90038500	-0.11341700	0.13103900
C	3.47644700	-0.93879900	-0.30286000
H	3.37934100	0.81852400	-0.17589600
H	2.94498100	-0.19189000	1.22107900
C	-2.92715500	-0.10262900	0.03283300
H	-3.08881600	-0.05428400	-1.04921700
H	-3.29780100	-1.06305000	0.39811200
H	-3.51215000	0.69575700	0.49714300

C

Zero-point correction=	0.183041 (Hartree/Particle)
Thermal correction to Energy=	0.191157
Thermal correction to Enthalpy=	0.192101
Thermal correction to Gibbs Free Energy=	0.150972
Sum of electronic and zero-point Energies=	-345.615964
Sum of electronic and thermal Energies=	-345.607849
Sum of electronic and thermal Enthalpies=	-345.606904
Sum of electronic and thermal Free Energies=	-345.648034

C	1.57686700	0.02201000	-0.34928200
C	-1.50183000	0.01696800	0.49807600
C	-0.67974200	0.87515100	-0.39443400
C	0.72746700	1.26560600	0.02905300
H	0.60772200	-1.46994200	0.75596900
H	1.86356600	0.10054500	-1.41729800
H	-1.09399500	-0.17689800	1.50548000
H	1.06981000	2.17275300	-0.50171600
N	0.65367100	-1.14598800	-0.23899600
H	0.77179900	1.45497000	1.111983600
N	-0.64300200	-0.63044200	-0.55922500
H	-1.18240800	1.40531800	-1.21936000
H	-1.12626300	-1.08831900	-1.41081900
C	2.82186400	-0.19726600	0.49714600
H	3.34968600	-1.10674000	0.19079200
H	3.50753000	0.64803900	0.37859300
H	2.56581600	-0.28198500	1.56075300
C	-2.99248400	-0.11654000	0.33663500
H	-3.30175800	0.03582300	-0.70329800
H	-3.33621900	-1.10045900	0.67314700
H	-3.48281800	0.64632900	0.95230800

TS-CE

Zero-point correction=	0.189958 (Hartree/Particle)
Thermal correction to Energy=	0.198209
Thermal correction to Enthalpy=	0.199153
Thermal correction to Gibbs Free Energy=	0.157821
Sum of electronic and zero-point Energies=	-345.544992
Sum of electronic and thermal Energies=	-345.536741
Sum of electronic and thermal Enthalpies=	-345.535796
Sum of electronic and thermal Free Energies=	-345.577128

C	1.50478200	-0.02501100	-0.35996000
C	-1.60284700	0.20291400	0.44293000
C	-0.76250400	1.05070400	-0.28172200
C	0.63198000	1.27748700	0.09915200
H	0.84099500	-1.41550000	1.08084700
H	1.50916300	-0.03551400	-1.45480900
H	-1.34825700	0.00597800	1.48394300
H	1.07055900	2.13617300	-0.41527000
N	0.71235100	-1.13983300	0.10294900
H	0.77050400	1.38038500	1.17880100
N	-0.53406100	-1.23619200	-0.28897400
H	-1.09186300	1.38397800	-1.26686300
H	-0.59010000	-1.05712100	-1.30132900
C	2.91597500	-0.01031500	0.20120000
H	3.48251800	-0.87237600	-0.16084500
H	3.43521800	0.89370000	-0.12570900
H	2.91590900	-0.02318500	1.29613500
C	-3.02855800	-0.06340200	0.06597500
H	-3.21119600	0.09320400	-1.00072800
H	-3.31225800	-1.08464300	0.33271000
H	-3.68091900	0.61684900	0.62570100

R'=Boc

R1=CH3 R2=CH3 R3=H R4=H

TS-BF

Zero-point correction=	0.227788 (Hartree/Particle)
Thermal correction to Energy=	0.242026
Thermal correction to Enthalpy=	0.242970
Thermal correction to Gibbs Free Energy=	0.187057
Sum of electronic and zero-point Energies=	-573.368853
Sum of electronic and thermal Energies=	-573.354616
Sum of electronic and thermal Enthalpies=	-573.353671
Sum of electronic and thermal Free Energies=	-573.409584

C	2.00154300	-1.12161600	-0.57167000
C	0.25502900	1.98951300	0.51065900
C	1.63222900	1.90897700	0.28671200
C	2.39898500	1.01406200	0.99088900
H	2.25462300	-0.56268000	-1.48161500
H	-0.15380800	1.41576700	1.34287500
H	3.46900400	0.93479800	0.81928400
N	0.79672800	-1.10700600	-0.08776500
H	1.98743200	0.44648800	1.82009000
N	-0.09370600	-0.29366700	-0.69063800
H	2.08091600	2.51011400	-0.50191500
C	-1.48167800	-0.43084100	-0.44957000
O	-2.27498300	0.17326000	-1.14160400
O	-1.74087500	-1.21199700	0.58577000
C	-3.14647200	-1.37825000	0.90042600
C	-3.57804900	-0.42644400	1.21686000
H	-3.68579000	-1.75982900	0.03192500
H	-3.16953000	-2.10026700	1.71490300
H	0.10386200	0.08355600	-1.62546100
C	3.01239600	-2.07070500	-0.01794100
H	3.99204000	-1.59587500	0.09425600
H	2.68517100	-2.47783400	0.94068600
H	3.14858900	-2.90250400	-0.72124800
C	-0.65410100	2.92364400	-0.17792000
H	-1.54038200	2.39348800	-0.55408000
H	-1.04037500	3.64085600	0.56302100
H	-0.17362500	3.47166000	-0.99050900

A

Zero-point correction=	0.231699 (Hartree/Particle)
Thermal correction to Energy=	0.245904
Thermal correction to Enthalpy=	0.246848
Thermal correction to Gibbs Free Energy=	0.190887
Sum of electronic and zero-point Energies=	-573.400781
Sum of electronic and thermal Energies=	-573.386576
Sum of electronic and thermal Enthalpies=	-573.385632
Sum of electronic and thermal Free Energies=	-573.441593

C	-2.14130900	-0.87197800	0.07663800
C	-0.15564000	1.34869900	0.45117900
C	-1.03130000	2.09199600	-0.53906300
C	-1.23407300	1.75920500	-1.81255400
H	-0.41608400	-1.94722400	-0.04844400
H	-2.54309100	0.13538000	0.10186600
H	0.83624600	1.80699300	0.42531700
H	-1.84952100	2.37760700	-2.45818900
N	-0.86090800	-1.01523900	0.03026400
H	-0.78982700	0.87536200	-2.26488000
N	0.11660800	-0.05071100	0.02885600
H	-1.48023100	2.99871900	-0.13626500
C	1.39295700	-0.63410100	-0.10709000
O	1.52270800	-1.83239800	-0.27924100
O	2.35016200	0.27241100	-0.02838600
C	3.70685200	-0.23009200	-0.16141500
H	3.84146100	-0.68604300	-1.14362900
H	4.34145000	0.64737700	-0.05280700
C	3.91474900	-0.95737000	0.62503500
C	-3.05378100	-2.03796000	0.08065800
H	-2.52661500	-2.99222900	0.00614700
H	-3.65013100	-2.02672300	1.00142700
H	-3.76177600	-1.94706700	-0.75164400
C	-0.65181100	1.42381600	1.90410500
H	-0.68503400	2.47431600	2.20544400
H	-1.65537400	1.01602200	2.05221200
H	0.03835300	0.90367900	2.57326800

B

Zero-point correction=	0.230787 (Hartree/Particle)
Thermal correction to Energy=	0.245140
Thermal correction to Enthalpy=	0.246084
Thermal correction to Gibbs Free Energy=	0.189567
Sum of electronic and zero-point Energies=	-573.382072
Sum of electronic and thermal Energies=	-573.367720
Sum of electronic and thermal Enthalpies=	-573.366775
Sum of electronic and thermal Free Energies=	-573.423293

C	1.34550200	1.59965200	0.26938300
C	0.40119700	-1.64460400	0.10594700
C	1.86199200	-1.77991100	0.41938600
C	2.81109000	-1.78806500	-0.51603800
H	1.50445800	1.55009500	1.35486900
H	0.22326700	-1.65220500	-0.97161800
H	3.85545200	-1.93342400	-0.25609500
N	0.57696400	0.78411300	-0.34765400
H	2.58144800	-1.66650600	-1.57168100
H	2.11970400	-1.91933800	1.46986200
N	-0.05677200	-0.20558800	0.52414200
H	0.17386900	-0.05906400	1.52565800
C	-1.55523200	-0.00097300	0.44849500
O	-2.16320200	0.27999000	1.44053700
O	-1.94939400	-0.18123600	-0.78335100
C	-3.37361000	0.02660100	-1.03404600
H	-3.63551700	1.05940800	-0.79993400
H	-3.50182100	-0.17748400	-2.09473300
H	-3.95963500	-0.66524000	-0.42721000
C	2.05487600	2.66340600	-0.48838000
H	1.76893600	3.64533700	-0.09292200
H	3.13601900	2.56411100	-0.33683000
H	1.82501100	2.61463400	-1.55357900
C	-0.46266300	-2.67152100	0.83199100
H	-0.35863700	-2.60122700	1.91953100
H	-1.52128300	-2.59475300	0.56938500
H	-0.12551700	-3.66667800	0.53076700

TS-AD

Zero-point correction=	0.229691 (Hartree/Particle)
Thermal correction to Energy=	0.243265
Thermal correction to Enthalpy=	0.244209
Thermal correction to Gibbs Free Energy=	0.190085
Sum of electronic and zero-point Energies=	-573.364349
Sum of electronic and thermal Energies=	-573.350775
Sum of electronic and thermal Enthalpies=	-573.349831
Sum of electronic and thermal Free Energies=	-573.403955

C	2.12896100	-0.75609500	-0.54966600
C	0.09096900	1.69654100	0.44327900
C	1.42739700	1.82496300	0.04021700
C	2.44525600	1.06630400	0.59366900
H	0.68316000	-1.64041800	0.63392800
H	2.21642000	-0.25021400	-1.50614700
H	-0.10046700	1.22612000	1.40833400
H	3.47188000	1.22716500	0.27506000
N	0.87464000	-0.99967600	-0.15718700
H	2.31976300	0.60256800	1.56868600
N	-0.14774500	-0.28237400	-0.58874800
H	1.63775700	2.41375900	-0.85191500
C	-1.34654400	-0.80585300	0.00944700
O	-1.36537000	-1.68610000	0.84858800
O	-2.39531700	-0.20377400	-0.52773100
C	-3.68812300	-0.65048000	-0.04738300
H	-3.77481300	-0.47645300	1.02717800
H	-4.41657200	-0.05429800	-0.59418600
H	-3.81942900	-1.71260200	-0.26236700
C	3.22417200	-1.67912700	-0.10881300
H	4.19120600	-1.17379300	-0.14415700
H	3.06473800	-2.06370300	0.90233600
H	3.27711000	-2.52941400	-0.80000700
C	-0.98235000	2.56659100	-0.11512700
H	-0.79191700	2.83288100	-1.15736400
H	-1.96873400	2.10925700	-0.03276900
H	-1.00690500	3.49448900	0.47456500

TS-AC

Zero-point correction=	0.232313 (Hartree/Particle)
Thermal correction to Energy=	0.244929
Thermal correction to Enthalpy=	0.245873
Thermal correction to Gibbs Free Energy=	0.194041
Sum of electronic and zero-point Energies=	-573.370910
Sum of electronic and thermal Energies=	-573.358294
Sum of electronic and thermal Enthalpies=	-573.357350
Sum of electronic and thermal Free Energies=	-573.409182

C	0.52390100	0.01985700	0.33240800
C	-1.86079600	-1.77211300	-0.17242000
C	-1.23716000	-1.64627000	1.15734200
C	0.15141200	-1.62779500	1.27696400
H	0.13211600	-0.57083300	-1.60384900
H	0.12156100	0.71051500	1.07251500
H	-1.24294200	-2.35699000	-0.85989700
H	0.57894200	-1.46590700	2.26461200
N	-0.25533300	-0.07187900	-0.80009500
H	0.72865500	-2.28887600	0.63127300
N	-1.59010400	-0.30409000	-0.62277300
H	-1.86393300	-1.26799100	1.96542900
C	-2.41536300	0.76471400	-0.17999600
O	-3.45089400	0.59793100	0.42235100
O	-1.90641000	1.92978700	-0.57787300
C	-2.71334800	3.09134500	-0.26385400
H	-3.67427800	3.03137200	-0.77834200
H	-2.87425000	3.16653900	0.81311900
H	-2.13805400	3.94136100	-0.62754900
C	-3.31016200	-2.21567600	-0.27917200
H	-3.94923700	-1.73684100	0.45963000
H	-3.69553500	-1.99405500	-1.27727700
H	-3.34265500	-3.29992200	-0.13740800
C	2.01173500	0.09870900	0.13170800
H	2.53290900	-0.03713600	1.08143600
H	2.37446700	-0.64599900	-0.58256500
H	2.26480900	1.09647100	-0.24484700

C

Zero-point correction=	0.234499 (Hartree/Particle)
Thermal correction to Energy=	0.247141
Thermal correction to Enthalpy=	0.248085
Thermal correction to Gibbs Free Energy=	0.195993
Sum of electronic and zero-point Energies=	-573.389337
Sum of electronic and thermal Energies=	-573.376695
Sum of electronic and thermal Enthalpies=	-573.375751
Sum of electronic and thermal Free Energies=	-573.427844

C	-2.01014100	-0.86268300	0.30916400
C	-0.24621300	1.65034800	-0.59599500
C	-0.77184900	1.17961000	0.69989500
C	-2.17573500	0.60701900	0.78768600
H	-1.09938300	-0.64857900	-1.58221600
H	-1.72049000	-1.47745800	1.16925700
H	-0.93827500	1.61391800	-1.43726200
H	-2.56024000	0.66002700	1.80828000
N	-0.84321500	-0.85582500	-0.61433400
H	-2.85875300	1.15995400	0.13462300
N	0.02256400	0.17396000	-0.14746500
H	-0.23637300	1.47683600	1.59831300
C	1.38591100	-0.21645200	0.28582900
O	1.95249400	0.39878000	1.14892100
O	1.79371600	-1.23701800	-0.42337100
C	3.12802100	-1.72962800	-0.10305600
H	3.17032500	-2.02522800	0.94628600
H	3.27168800	-2.58857500	-0.75528700
H	3.86610200	-0.95319300	-0.31071700
C	-3.23136200	-1.47204500	-0.36105700
H	-3.02783200	-2.49604700	-0.68586000
H	-4.06447200	-1.50410400	0.34598700
H	-3.54886600	-0.88474800	-1.23021800
C	0.90398600	2.60311800	-0.74602000
H	1.56223300	2.61602000	0.12250500
H	1.48445400	2.38110900	-1.64627700
H	0.47656700	3.60439900	-0.86933600

TS-CE

Zero-point correction=	0.231933 (Hartree/Particle)
Thermal correction to Energy=	0.244581
Thermal correction to Enthalpy=	0.245525
Thermal correction to Gibbs Free Energy=	0.193796
Sum of electronic and zero-point Energies=	-573.365612
Sum of electronic and thermal Energies=	-573.352964
Sum of electronic and thermal Enthalpies=	-573.352020
Sum of electronic and thermal Free Energies=	-573.403749

C	0.48304900	-0.07968400	0.35865800
C	-2.14194100	-2.09916500	-0.05994900
C	-1.46811600	-1.56211900	1.02019000
C	-0.00363600	-1.45761500	1.06945100
H	0.19601100	-0.64728800	-1.65747500
H	0.10938500	0.75199500	0.96012100
H	-1.55154400	-2.59861900	-0.82848900
H	0.36785900	-1.39461500	2.09631700
N	-0.23229800	-0.10239300	-0.89875400
H	0.49835300	-2.27751900	0.54887100
N	-1.51911400	-0.11781300	-0.93529900
H	-2.04736200	-1.11023200	1.82356300
C	-2.25525600	0.92493000	-0.23948100
O	-3.33150200	0.74798500	0.26825500
O	-1.62390800	2.08358800	-0.41391700
C	-2.35341600	3.26014800	0.02764100
H	-2.54912000	3.20215300	1.09980200
H	-1.69830700	4.09881400	-0.20195200
H	-3.29296600	3.34222300	-0.52161400
C	-3.61522500	-2.29977800	-0.14394600
H	-3.99083300	-2.00435200	-1.12813000
H	-3.82157900	-3.37388800	-0.03968900
H	-4.15920700	-1.75495200	0.62701100
C	1.99073400	-0.01164100	0.18490500
H	2.47579800	-0.09499600	1.16041000
H	2.36361000	-0.82441900	-0.44724600
H	2.28529700	0.94323600	-0.25792500

R'=H

R1=CH3 R2=H R3=CH3 R4=H

TS-BF

Zero-point correction=	0.187240 (Hartree/Particle)
Thermal correction to Energy=	0.196450
Thermal correction to Enthalpy=	0.197394
Thermal correction to Gibbs Free Energy=	0.153773
Sum of electronic and zero-point Energies=	-345.527470
Sum of electronic and thermal Energies=	-345.518260
Sum of electronic and thermal Enthalpies=	-345.517315
Sum of electronic and thermal Free Energies=	-345.560937

C	-1.33472600	-0.16674800	-0.40398500
C	1.60056800	0.89187900	0.68794100
C	1.35316200	-0.42805500	0.31955800
C	0.21439500	-1.03609700	0.85947400
H	-0.85634500	-0.46354800	-1.34488300
H	1.18152500	1.29850000	1.60240600
H	2.42115100	1.45295600	0.24695600
H	-0.03225600	-2.06194800	0.59603600
N	-1.17764000	1.06972400	0.05747400
H	-0.20920500	-0.67618400	1.79110300
N	-0.14309300	1.73745400	-0.41216100
H	0.19266800	1.56834800	-1.36801400
H	-0.11820800	2.71669800	-0.12489600
C	-2.57960800	-0.90497600	-0.00477300
H	-3.38154900	-0.66341600	-0.71280500
H	-2.43159900	-1.98675100	-0.04153900
H	-2.90708500	-0.61302200	0.99530700
C	2.13363700	-1.09281800	-0.78689700
H	2.89143300	-1.75945000	-0.35928700
H	1.49362800	-1.70908500	-1.42654000
H	2.65758600	-0.36651900	-1.41432300

A

Zero-point correction=	0.189193 (Hartree/Particle)
Thermal correction to Energy=	0.199053
Thermal correction to Enthalpy=	0.199997
Thermal correction to Gibbs Free Energy=	0.154300
Sum of electronic and zero-point Energies=	-345.565552
Sum of electronic and thermal Energies=	-345.555693
Sum of electronic and thermal Enthalpies=	-345.554749
Sum of electronic and thermal Free Energies=	-345.600445

C	-2.28011200	-0.20521800	0.31286000
C	0.58998000	-0.30427800	0.39473900
C	2.07603000	-0.14798900	0.14492900
C	2.81023200	-1.20992500	-0.19425800
H	-1.97479500	0.84418600	-1.36710900
H	-1.79085700	-0.74796900	1.11598100
H	0.33100200	-1.36402500	0.48972000
H	3.88073800	-1.12839200	-0.35949600
N	-1.53261000	0.34253900	-0.58788400
H	2.37373900	-2.19757700	-0.31360400
N	-0.17384400	0.24163300	-0.73656600
H	0.30219400	0.20566600	1.32988600
H	0.18453500	1.10309900	-1.14757500
C	-3.76036300	-0.13470500	0.26501000
H	-4.17317400	-1.14866700	0.19787200
H	-4.13735300	0.29852300	1.19852400
H	-4.12962000	0.45440200	-0.57851500
C	2.65552700	1.22945300	0.33830900
H	3.72747600	1.24060100	0.12920200
H	2.18929000	1.97871900	-0.31641400
H	2.50514400	1.58046400	1.36705400

B

Zero-point correction=	0.189467 (Hartree/Particle)
Thermal correction to Energy=	0.199417
Thermal correction to Enthalpy=	0.200361
Thermal correction to Gibbs Free Energy=	0.153908
Sum of electronic and zero-point Energies=	-345.565006
Sum of electronic and thermal Energies=	-345.555057
Sum of electronic and thermal Enthalpies=	-345.554112
Sum of electronic and thermal Free Energies=	-345.600566

C	2.47026500	0.22780900	-0.34017500
C	-0.72542900	0.07761600	0.68370600
C	-2.11890000	0.18555200	0.11692500
C	-2.62093300	1.39534100	-0.15164800
H	2.22045500	0.91646400	-1.15950800
H	-0.33734200	1.03965800	1.02148900
H	-3.62667800	1.51605700	-0.54340400
N	1.59930500	-0.54337700	0.19025300
H	-2.05571800	2.30706200	0.02330100
H	-0.63985300	-0.64954800	1.49546900
H	0.22325200	0.23040000	-1.19737300
H	-0.00576500	-1.34041700	-0.70758200
N	0.26200500	-0.40211000	-0.37778300
C	3.87482300	0.20820300	0.14591000
H	4.00303900	-0.50139900	0.96445800
H	4.54531800	-0.05509200	-0.68068900
H	4.16247200	1.21264900	0.47802400
C	-2.88568700	-1.09633300	-0.08290500
H	-3.87520700	-0.90246800	-0.50192100
H	-2.37677900	-1.79218000	-0.76444300
H	-3.01569500	-1.62859400	0.86744900

TS-AD

Zero-point correction=	0.188778 (Hartree/Particle)
Thermal correction to Energy=	0.197255
Thermal correction to Enthalpy=	0.198199
Thermal correction to Gibbs Free Energy=	0.156214
Sum of electronic and zero-point Energies=	-345.538917
Sum of electronic and thermal Energies=	-345.530440
Sum of electronic and thermal Enthalpies=	-345.529496
Sum of electronic and thermal Free Energies=	-345.571480

C	-1.15341500	-0.25681300	-0.34302000
C	1.46415800	0.90587100	0.67060100
C	1.23455500	-0.44658400	0.35014700
C	-0.06466100	-0.99416200	0.69703100
H	-1.47444900	1.58395200	0.59367100
H	-0.84175600	-0.54191300	-1.35070600
H	1.06474800	1.29224600	1.60583000
H	-0.16379700	-2.06566000	0.51228200
N	-0.97867900	1.14094500	-0.18876700
H	-0.40845100	-0.73956900	1.70130400
N	0.21957000	1.60278900	-0.53678200
H	2.39657400	1.36500300	0.35089800
H	0.27808200	2.58711000	-0.23761300
C	-2.56529900	-0.72471400	-0.02610500
H	-2.62348300	-1.81357800	-0.08589600
H	-2.87713100	-0.42358200	0.97941800
H	-3.27005500	-0.30837700	-0.75111800
C	2.11244700	-1.15847500	-0.61594800
H	1.54343100	-1.82052000	-1.27733500
H	2.72083900	-0.46979000	-1.20752600
H	2.80294900	-1.80460600	-0.05259300

TS-AC

Zero-point correction=	0.189340 (Hartree/Particle)
Thermal correction to Energy=	0.197827
Thermal correction to Enthalpy=	0.198771
Thermal correction to Gibbs Free Energy=	0.156733
Sum of electronic and zero-point Energies=	-345.548445
Sum of electronic and thermal Energies=	-345.539959
Sum of electronic and thermal Enthalpies=	-345.539014
Sum of electronic and thermal Free Energies=	-345.581052

C	-1.24450200	-0.16229700	-0.42151900
C	1.30609200	0.97862000	0.62385100
C	1.20186200	-0.47368300	0.34862000
C	0.05008100	-1.13020700	0.77146600
H	-1.44276900	1.57278100	0.65115400
H	-0.83834300	-0.50687100	-1.37219000
H	1.00917200	1.26808300	1.63313100
H	-0.07799300	-2.18096200	0.51841300
N	-0.96876500	1.14237200	-0.14455200
H	-0.42544800	-0.81995900	1.69930200
N	0.30033200	1.63862600	-0.33713900
H	2.28007000	1.40953800	0.38712400
H	0.58041800	1.47945000	-1.30771200
C	-2.60868200	-0.68569200	-0.07357800
H	-3.32930700	-0.31638900	-0.81273600
H	-2.62234700	-1.77640000	-0.11629200
H	-2.93475900	-0.36543200	0.91998400
C	2.15275400	-1.09416800	-0.62194100
H	2.41183000	-0.41100300	-1.44017800
H	3.09593800	-1.30991700	-0.09975100
H	1.78043900	-2.03392500	-1.03638300

C

Zero-point correction=	0.192652 (Hartree/Particle)
Thermal correction to Energy=	0.200675
Thermal correction to Enthalpy=	0.201619
Thermal correction to Gibbs Free Energy=	0.160767
Sum of electronic and zero-point Energies=	-345.566335
Sum of electronic and thermal Energies=	-345.558311
Sum of electronic and thermal Enthalpies=	-345.557367
Sum of electronic and thermal Free Energies=	-345.598219

C	1.28586400	0.31864000	-0.36917400
C	-1.30129700	-1.02066700	0.87654300
C	-1.07551700	0.28984800	0.21798200
C	0.23513100	1.00795100	0.54091000
H	1.14451500	-1.69572300	0.20764100
H	1.24244400	0.78167700	-1.36229400
H	-0.66371600	-1.33881300	1.69675400
H	0.15593600	2.07606200	0.32518300
N	0.80936800	-1.08170100	-0.53938500
H	0.49196700	0.89325200	1.59891600
N	-0.60996600	-1.01725000	-0.45278000
H	-2.29093400	-1.46961200	0.84836400
H	-1.10790400	-1.39279400	-1.26764100
C	2.71680900	0.34704000	0.13986200
H	3.38354700	-0.18408700	-0.54527500
H	3.06735300	1.37982800	0.21427900
H	2.79991000	-0.10989500	1.13269700
C	-2.20950500	1.04425500	-0.42426700
H	-2.63062500	1.73674800	0.31136000
H	-1.85685100	1.63057100	-1.27764900
H	-3.01398900	0.38095000	-0.75471200

TS-CE

Zero-point correction=	0.189300 (Hartree/Particle)
Thermal correction to Energy=	0.197744
Thermal correction to Enthalpy=	0.198689
Thermal correction to Gibbs Free Energy=	0.156797
Sum of electronic and zero-point Energies=	-345.544370
Sum of electronic and thermal Energies=	-345.535926
Sum of electronic and thermal Enthalpies=	-345.534982
Sum of electronic and thermal Free Energies=	-345.576873

C	-1.19366000	-0.26687200	-0.31698000
C	1.59223300	0.85460300	0.78332000
C	1.24676400	-0.40570700	0.33237500
C	-0.09305500	-0.94129700	0.66226800
H	-1.42964000	1.63488400	0.59631900
H	-0.93961700	-0.55436400	-1.34367500
H	1.10945900	1.29865700	1.64753400
H	-0.16752100	-2.01864200	0.49013600
N	-0.96377100	1.15543400	-0.18222500
H	-0.39959400	-0.71662400	1.68729800
N	0.16588600	1.68552300	-0.51037400
H	2.53199300	1.31090200	0.48439700
H	0.52148600	1.22426700	-1.35923300
C	-2.61616900	-0.67373900	0.03301600
H	-3.32614900	-0.23987000	-0.67603100
H	-2.71155700	-1.76083400	-0.01704800
H	-2.88948000	-0.35732000	1.04501500
C	2.10332300	-1.15494500	-0.64156600
H	1.51834600	-1.56580000	-1.47372700
H	2.91955000	-0.54588100	-1.03666800
H	2.55031100	-2.01801600	-0.12930400

R'=Boc

R1=CH3 R2=H R3=CH3 R4=H

TS-BF

Zero-point correction=	0.228448 (Hartree/Particle)
Thermal correction to Energy=	0.242475
Thermal correction to Enthalpy=	0.243419
Thermal correction to Gibbs Free Energy=	0.187740
Sum of electronic and zero-point Energies=	-573.356812
Sum of electronic and thermal Energies=	-573.342785
Sum of electronic and thermal Enthalpies=	-573.341841
Sum of electronic and thermal Free Energies=	-573.397520

C	-1.35479300	1.42298400	-0.55064300
C	-0.50554500	-1.66186500	0.74695900
C	-1.81749700	-1.27579600	0.51672400
C	-2.21542100	-0.05844800	1.07302200
H	-1.81967300	0.87632800	-1.38006600
H	0.08378500	-1.19108600	1.52724800
H	-3.22036400	0.32468000	0.91472600
N	-0.12367500	1.15181400	-0.17597600
H	-1.64395800	0.40197200	1.87198000
N	0.42926200	0.05448800	-0.67589700
C	1.83624700	-0.19827800	-0.49720200
O	2.39753800	-0.96670700	-1.23805200
O	2.31821500	0.46231400	0.53561000
C	3.73620000	0.26943100	0.78747700
H	3.94355500	-0.78605300	0.97242300
H	4.31745100	0.62265300	-0.06605400
H	3.94891400	0.86739800	1.67162500
H	-0.08394500	-2.55116100	0.28435900
H	0.08458900	-0.35064400	-1.55780000
C	-1.95334300	2.73444200	-0.14796600
H	-3.03402100	2.65875500	-0.00242800
H	-1.48282100	3.12182300	0.75786300
H	-1.79209600	3.45847800	-0.95682000
C	-2.72208100	-2.04323900	-0.41722500
H	-3.40105600	-2.67868200	0.16245500
H	-3.34409800	-1.37678400	-1.02239800
H	-2.15630200	-2.69523200	-1.08766300

A

Zero-point correction=	0.231452 (Hartree/Particle)
Thermal correction to Energy=	0.245827
Thermal correction to Enthalpy=	0.246772
Thermal correction to Gibbs Free Energy=	0.189431
Sum of electronic and zero-point Energies=	-573.408474
Sum of electronic and thermal Energies=	-573.394099
Sum of electronic and thermal Enthalpies=	-573.393155
Sum of electronic and thermal Free Energies=	-573.450496

C	-1.75972300	1.58054400	-0.23282100
C	-0.42158800	-0.94818000	-0.78914400
C	-1.30646500	-1.68816200	0.19952700
C	-1.35862100	-1.37627200	1.49616000
H	0.15414300	2.18586200	0.13773200
H	-2.37142600	0.71319300	-0.46320200
H	0.38592900	-1.59417800	-1.14114500
H	-1.99015600	-1.93450700	2.17998700
N	-0.48703800	1.41363400	-0.11423800
H	-0.76320700	-0.57828100	1.93112100
N	0.22578800	0.25662500	-0.26906100
C	1.59590900	0.44284500	-0.00859700
O	2.02903000	1.52875200	0.32791500
O	2.26678800	-0.68174900	-0.17546600
C	3.69603500	-0.60390700	0.07439900
H	3.87746200	-0.29709100	1.10573800
H	4.06580500	-1.61270800	-0.09906700
H	4.15795900	0.10223600	-0.61747600
H	-0.99372300	-0.65900000	-1.68329100
C	-2.39195900	2.90645700	-0.04641200
H	-2.92780900	3.18461000	-0.96208000
H	-3.14398400	2.84058700	0.74903200
H	-1.67189300	3.69028100	0.20060800
C	-2.09453300	-2.81251000	-0.41910300
H	-1.43102700	-3.55187300	-0.88558700
H	-2.69978400	-3.32796100	0.32939700
H	-2.76583700	-2.45148100	-1.20890700

B

Zero-point correction=	0.230798 (Hartree/Particle)
Thermal correction to Energy=	0.245381
Thermal correction to Enthalpy=	0.246325
Thermal correction to Gibbs Free Energy=	0.188086
Sum of electronic and zero-point Energies=	-573.382442
Sum of electronic and thermal Energies=	-573.367859
Sum of electronic and thermal Enthalpies=	-573.366915
Sum of electronic and thermal Free Energies=	-573.425154

C	0.74915200	2.02591800	0.36922900
C	0.52548900	-1.26699400	-0.39959600
C	2.01946600	-1.26562600	-0.20765600
C	2.80136300	-0.75590700	-1.16517400
H	1.03585400	1.83122900	1.41135500
H	0.22506700	-1.12509500	-1.43669700
H	3.88356800	-0.75661000	-1.07090700
N	0.13746900	1.15847700	-0.34562300
H	2.39178900	-0.33386200	-2.07843400
N	-0.14079600	-0.09802500	0.35567200
H	0.18400400	-0.08256600	1.34044300
C	-1.64728200	-0.24624000	0.47486400
O	-2.15255600	-0.21990800	1.55928900
O	-2.15497000	-0.38850000	-0.71792000
C	-3.60909500	-0.51771000	-0.78550000
H	-4.07359300	0.37379800	-0.36189600
H	-3.82996600	-0.60655500	-1.84692000
H	-3.92185700	-1.41122400	-0.24323600
H	0.05485600	-2.17010800	0.00275100
C	1.09107500	3.35204900	-0.20760100
H	0.63225700	4.14187300	0.39899300
H	2.17545000	3.50534100	-0.15835700
H	0.75285700	3.43779800	-1.24109100
C	2.55091800	-1.88634000	1.06009800
H	3.63872200	-1.80642600	1.11211900
H	2.14389800	-1.41199400	1.96421300
H	2.28436900	-2.94873000	1.11939500

TS-AD

Zero-point correction=	0.230811 (Hartree/Particle)
Thermal correction to Energy=	0.243893
Thermal correction to Enthalpy=	0.244837
Thermal correction to Gibbs Free Energy=	0.191327
Sum of electronic and zero-point Energies=	-573.369788
Sum of electronic and thermal Energies=	-573.356706
Sum of electronic and thermal Enthalpies=	-573.355762
Sum of electronic and thermal Free Energies=	-573.409272

C	1.83854200	-0.89690500	-0.41461100
C	0.08844800	1.28108300	0.83629200
C	1.43702200	1.41038300	0.44757400
C	2.30603100	0.28458300	0.70768700
H	0.15385900	-1.84008000	0.46415800
H	1.99228800	-0.43272100	-1.39146000
H	-0.14255300	0.74208600	1.75258100
H	3.36144200	0.46359100	0.49792600
N	0.46391900	-1.12688400	-0.21183600
H	2.17011900	-0.18580600	1.68275400
N	-0.34820600	-0.10854600	-0.43421700
C	-1.71644500	-0.45906600	-0.07585800
O	-2.03897000	-1.55045800	0.33263400
O	-2.49646300	0.57729100	-0.32238800
C	-3.90747400	0.38105900	-0.04543100
H	-4.05591400	1.62345000	1.01405100
H	-4.38295100	1.32190000	-0.31627000
H	-4.29592400	-0.43737400	-0.65413100
H	-0.61260800	2.06577800	0.57028200
C	2.68774400	-2.14326500	-0.22099800
H	3.74680900	-1.89373100	-0.31169600
H	2.52668800	-2.59652100	0.76224300
H	2.44718800	-2.88076200	-0.99173800
C	1.81578900	2.45511700	-0.54394900
H	2.88110200	2.44968200	-0.77974800
H	1.24482200	2.29168100	-1.47189800
H	1.53413800	3.45224400	-0.18757500

TS-AC

Zero-point correction=	0.232304 (Hartree/Particle)
Thermal correction to Energy=	0.244926
Thermal correction to Enthalpy=	0.245870
Thermal correction to Gibbs Free Energy=	0.194033
Sum of electronic and zero-point Energies=	-573.384033
Sum of electronic and thermal Energies=	-573.371411
Sum of electronic and thermal Enthalpies=	-573.370467
Sum of electronic and thermal Free Energies=	-573.422304

C	-1.25653400	1.17448100	-0.32214400
C	-0.56808400	-1.28851800	1.17298200
C	-1.42537400	-1.35901900	-0.04877600
C	-2.44577700	-0.42141100	-0.16329800
H	-0.79154000	1.47880600	1.65864100
H	-0.75790300	0.89693500	-1.24967300
H	-1.12840900	-1.12870600	2.09632300
H	-3.04982700	-0.40886900	-1.06844100
N	-0.44776400	1.09088500	0.77762300
H	-2.95396700	-0.08292800	0.73727900
N	0.28182600	-0.06230200	0.93793100
C	1.52636900	-0.21853500	0.30256900
O	2.05244100	-1.30511400	0.17490000
O	2.02644600	0.95647100	-0.07651700
C	3.34854500	0.89735600	-0.66508000
H	4.06568000	0.49896300	0.05522700
H	3.34050700	0.27629400	-1.56298600
H	3.59242500	1.92888300	-0.91547800
H	0.11436500	-2.12951100	1.28329600
C	-2.18324100	2.35300800	-0.41314500
H	-1.58773800	3.24010900	-0.66059800
H	-2.91265500	2.21116600	-1.21246000
H	-2.71209900	2.53961200	0.52550500
C	-0.97055400	-2.19815900	-1.18985900
H	-1.21621600	-3.24652100	-0.96201100
H	-1.46153200	-1.93723600	-2.12985800
H	0.11946500	-2.17044200	-1.30205500

C

Zero-point correction=	0.234025 (Hartree/Particle)
Thermal correction to Energy=	0.246741
Thermal correction to Enthalpy=	0.247686
Thermal correction to Gibbs Free Energy=	0.195200
Sum of electronic and zero-point Energies=	-573.389064
Sum of electronic and thermal Energies=	-573.376347
Sum of electronic and thermal Enthalpies=	-573.375403
Sum of electronic and thermal Free Energies=	-573.427889

C	1.78118700	-0.86574500	-0.38291100
C	0.36244500	1.39019900	1.29362700
C	0.76588400	1.34442400	-0.12317600
C	2.08198400	0.65713900	-0.45403300
H	1.10932200	-1.07668700	1.59841000
H	1.32835300	-1.17306900	-1.33276000
H	1.08733700	1.18182400	2.07650200
H	2.43056000	0.94807800	-1.44781200
N	0.72895600	-1.01670200	0.65039100
H	2.85054900	0.93394800	0.27576500
N	-0.08435200	0.14088000	0.57519500
C	-1.52526900	-0.01550200	0.29092100
O	-2.28830600	0.88569000	0.52034800
O	-1.75521600	-1.19122500	-0.23530200
C	-3.14825100	-1.46178600	-0.56852600
H	-3.50061300	-0.73816500	-1.30527600
H	-3.14530800	-2.46924800	-0.97932800
H	-3.75809300	-1.41130300	0.33490300
H	-0.47291100	2.02359500	1.57847700
C	2.98021200	-1.74885600	-0.07930200
H	2.68343700	-2.79983000	-0.02448900
H	3.72569300	-1.65215300	-0.87316500
C	3.45668900	-1.46880000	0.86697500
C	0.08270300	2.18791600	-1.15873700
H	0.05311300	1.67965400	-2.12679600
H	-0.92460800	2.48571400	-0.86505000
H	0.68020600	3.09912900	-1.27997200

TS-CE

Zero-point correction=	0.230964 (Hartree/Particle)
Thermal correction to Energy=	0.244082
Thermal correction to Enthalpy=	0.245026
Thermal correction to Gibbs Free Energy=	0.191824
Sum of electronic and zero-point Energies=	-573.362781
Sum of electronic and thermal Energies=	-573.349662
Sum of electronic and thermal Enthalpies=	-573.348718
Sum of electronic and thermal Free Energies=	-573.401921

C	1.01769800	1.19201500	0.32993700
C	1.45088500	-1.82994300	-1.10557200
C	1.56983700	-1.31391800	0.13817800
C	2.13772700	0.05890300	0.33363000
H	0.93015500	1.50966900	-1.77609800
H	0.25554200	0.95336600	1.07362400
H	1.85731900	-1.32915500	-1.98012400
H	2.61631500	0.16543200	1.31349100
N	0.40840700	1.07417700	-0.99571600
H	2.87623900	0.31469000	-0.43194300
N	-0.45263600	0.25640600	-1.38342400
C	-1.42535000	-0.30716000	-0.44265200
O	-1.68845600	-1.47572500	-0.42569700
O	-2.02431000	0.69671100	0.18347100
C	-3.20897700	0.34054600	0.95560000
H	-2.93734200	-0.35209300	1.75375900
H	-3.57114900	1.28293100	1.36177000
H	-3.95271200	-0.11236500	0.29798400
H	1.00518100	-2.80531600	-1.27259900
C	1.58761900	2.58928700	0.54299500
H	0.79436500	3.34114700	0.54303400
H	2.08926200	2.62392000	1.51283600
H	2.32443800	2.84855100	-0.22473500
C	1.09359400	-2.04978300	1.36116200
H	1.94781800	-2.32096900	1.99409500
H	0.43461400	-1.43238000	1.98548100
H	0.55806800	-2.96479900	1.10288500

R'=H

R1=CH3 R2=H R3=H R4=CH3

TS-BF

Zero-point correction=	0.186728 (Hartree/Particle)
Thermal correction to Energy=	0.196022
Thermal correction to Enthalpy=	0.196967
Thermal correction to Gibbs Free Energy=	0.153455
Sum of electronic and zero-point Energies=	-345.529151
Sum of electronic and thermal Energies=	-345.519857
Sum of electronic and thermal Enthalpies=	-345.518912
Sum of electronic and thermal Free Energies=	-345.562424

C	-1.18283000	1.10734800	0.17067400
C	1.37591700	-1.13647000	-0.09611300
C	1.40826000	0.10196000	0.47952600
C	0.98082200	1.26097400	-0.21475700
H	-1.08787800	1.02093300	1.25935000
H	1.20777600	-1.26083100	-1.16129400
H	1.67398100	-2.02258600	0.45780500
N	-1.35823600	0.00166400	-0.55483100
H	0.87609600	1.17196500	-1.29471100
H	1.66643500	0.19637000	1.53388500
N	-1.09778000	-1.13538000	0.01859400
H	-1.10307700	-1.24289600	1.03779100
H	-1.30195900	-1.96628000	-0.53390300
C	1.30154300	2.62988500	0.30383200
H	2.37088800	2.80292900	0.11494900
H	0.76307400	3.41880500	-0.22220700
H	1.14252400	2.72545200	1.38152900
C	-1.78775100	2.37222300	-0.37047300
H	-1.37817300	3.25624900	0.12036200
H	-1.65416200	2.45184400	-1.45196600
H	-2.86482500	2.36450800	-0.16363400

A

Zero-point correction=	0.189035 (Hartree/Particle)
Thermal correction to Energy=	0.199092
Thermal correction to Enthalpy=	0.200036
Thermal correction to Gibbs Free Energy=	0.153735
Sum of electronic and zero-point Energies=	-345.570511
Sum of electronic and thermal Energies=	-345.560454
Sum of electronic and thermal Enthalpies=	-345.559510
Sum of electronic and thermal Free Energies=	-345.605811

C	-2.47748000	-0.56427300	-0.13203700
C	0.39738500	-0.41527800	0.14422000
C	1.79734900	0.02918300	0.45381200
C	2.80634300	-0.05085000	-0.41746700
H	-2.37646800	1.40077100	0.24231600
H	-1.89116800	-1.46210500	-0.30469800
H	0.35998300	-0.93523800	-0.81972800
N	-1.84088100	0.53653200	0.10036500
H	2.60721300	-0.44634300	-1.41501900
N	-0.48901600	0.75949700	0.06892500
H	1.96960300	0.41227300	1.46011600
H	0.02979100	-1.10650700	0.92179600
H	-0.25614100	1.51449100	0.71533400
C	4.21978200	0.35170000	-0.13709600
H	4.34295000	0.74408800	0.87625100
H	4.89906400	-0.50078100	-0.26043100
H	4.55364100	1.11817500	-0.84730200
C	-3.95888000	-0.62228800	-0.18969000
H	-4.27511100	-0.97298900	-1.17948900
H	-4.32685800	-1.35504900	0.53770800
H	-4.42752100	0.34504000	0.00980900

B

Zero-point correction=	0.189470 (Hartree/Particle)
Thermal correction to Energy=	0.199516
Thermal correction to Enthalpy=	0.200461
Thermal correction to Gibbs Free Energy=	0.153869
Sum of electronic and zero-point Energies=	-345.570756
Sum of electronic and thermal Energies=	-345.560709
Sum of electronic and thermal Enthalpies=	-345.559765
Sum of electronic and thermal Free Energies=	-345.606357

C	2.61514500	0.67964700	0.12672700
C	-0.51733500	-0.54395700	0.44014300
C	-1.85026600	-0.49361100	-0.23251600
C	-2.74747800	0.46962100	0.00929100
H	2.25075800	1.65900100	-0.21392500
H	-0.42908900	0.16426900	1.26635200
N	1.90762700	-0.38033100	0.03102500
H	-2.49479100	1.25301400	0.72692800
H	-2.07988000	-1.30003400	-0.92888900
H	-0.23915100	-1.54160400	0.78889700
H	0.43171000	0.80488700	-0.88324200
H	0.52650200	-0.77821100	-1.37048200
N	0.58821200	-0.16173000	-0.54617600
C	-4.10339100	0.56047500	-0.61258200
H	-4.88262200	0.54144800	0.15909100
H	-4.22062500	1.51196400	-1.14590100
H	-4.29246400	-0.25588800	-1.31459100
C	3.98003200	0.61075300	0.71181300
H	4.23424300	-0.40913500	1.00393700
H	4.71179900	0.98088700	-0.01563300
H	4.04027300	1.27107400	1.58500700

TS-AD

Zero-point correction=	0.188535 (Hartree/Particle)
Thermal correction to Energy=	0.197224
Thermal correction to Enthalpy=	0.198169
Thermal correction to Gibbs Free Energy=	0.155932
Sum of electronic and zero-point Energies=	-345.527234
Sum of electronic and thermal Energies=	-345.518545
Sum of electronic and thermal Enthalpies=	-345.517600
Sum of electronic and thermal Free Energies=	-345.559837

C	1.09499100	-0.95590200	-0.21681700
C	-1.14227000	1.08319800	0.18133100
C	0.13645400	1.35438400	-0.31872000
C	1.30584400	0.77906400	0.26550900
H	-0.21243800	-1.63634000	1.24698300
H	1.08221600	-0.91263100	-1.30551100
H	-1.27241200	0.98151200	1.25696100
N	-0.15849800	-1.32246500	0.27038300
H	1.26283500	0.68741800	1.35372000
N	-1.21343700	-0.74967400	-0.28824800
H	0.21560100	1.75737800	-1.32923400
H	-2.00247700	1.48579800	-0.34646700
H	-2.04053100	-1.00804000	0.26997600
C	2.65634700	1.26852000	-0.24366300
H	3.48463600	0.73257700	0.22160900
H	2.74110400	1.17264200	-1.33058600
C	2.77525500	2.32632800	0.00924500
C	2.24230800	-1.77242900	0.34998000
H	3.19494600	-1.43823500	-0.06027500
H	2.29297500	-1.71201100	1.44173500
H	2.11384300	-2.82083500	0.06332400

TS-AC

Zero-point correction=	0.189915 (Hartree/Particle)
Thermal correction to Energy=	0.198186
Thermal correction to Enthalpy=	0.199130
Thermal correction to Gibbs Free Energy=	0.157785
Sum of electronic and zero-point Energies=	-345.539856
Sum of electronic and thermal Energies=	-345.531584
Sum of electronic and thermal Enthalpies=	-345.530640
Sum of electronic and thermal Free Energies=	-345.571985

C	1.43453300	-0.43650900	-0.15914000
C	-1.45243000	0.35758900	0.27929800
C	-0.45350500	1.22053200	-0.32419600
C	0.87568300	1.27602900	0.17245600
H	0.35258700	-1.44309300	1.28420600
H	1.50321200	-0.42805400	-1.24939000
H	-1.46904700	0.31023500	1.36827000
N	0.37807200	-1.23981700	0.28326500
H	0.94103900	1.26308400	1.26459100
N	-0.86267900	-1.00454200	-0.21506300
H	-0.64943700	1.57740300	-1.33704400
H	-2.45949800	0.43877600	-0.12739700
H	-0.85552500	-1.05245000	-1.23758100
C	1.84043800	2.25211200	-0.48997700
H	1.55681000	3.27954700	-0.24365800
H	2.86324200	2.11009800	-0.13609600
H	1.83411900	2.15289600	-1.57992700
C	2.75788200	-0.70100700	0.52310400
H	3.51468300	0.01450800	0.19965200
H	2.67328600	-0.65440600	1.61331300
H	3.11207000	-1.69840200	0.24335600

C

Zero-point correction=	0.193024 (Hartree/Particle)
Thermal correction to Energy=	0.200167
Thermal correction to Enthalpy=	0.201111
Thermal correction to Gibbs Free Energy=	0.162163
Sum of electronic and zero-point Energies=	-345.557154
Sum of electronic and thermal Energies=	-345.550011
Sum of electronic and thermal Enthalpies=	-345.549067
Sum of electronic and thermal Free Energies=	-345.588015

C	1.61732900	-0.06711300	0.03837800
C	-1.31177400	0.00435400	0.75416100
C	-0.61369000	0.92860900	-0.17409700
C	0.84838500	1.29643300	0.04676700
H	0.61202500	-1.92832600	0.14983500
H	2.40881900	-0.01340800	-0.71642300
H	-0.83217800	-0.31466500	1.67359000
N	0.64817300	-1.10212600	-0.45148300
H	0.94476000	1.76199800	1.03419600
N	-0.65550100	-0.53218800	-0.48532100
H	-1.22224300	1.54652800	-0.82993100
H	-2.39664300	-0.04185800	0.73622900
H	-1.24331700	-0.87777500	-1.25255600
C	1.35625100	2.27222700	-1.02158000
H	0.80306400	3.21565200	-0.99033000
H	2.41152400	2.50300000	-0.85193300
H	1.26206900	1.85208700	-2.02857400
C	2.24972200	-0.44173400	1.37776900
H	2.73836700	-1.42001900	1.31879100
H	3.01973600	0.28894000	1.64289500
H	1.51925100	-0.47081400	2.19358300

TS-CE

Zero-point correction=	0.189785 (Hartree/Particle)
Thermal correction to Energy=	0.198096
Thermal correction to Enthalpy=	0.199040
Thermal correction to Gibbs Free Energy=	0.157601
Sum of electronic and zero-point Energies=	-345.535005
Sum of electronic and thermal Energies=	-345.526694
Sum of electronic and thermal Enthalpies=	-345.525750
Sum of electronic and thermal Free Energies=	-345.567189

C	1.07506900	-1.61730300	-0.23182000
C	1.63295100	1.45362200	0.42914000
C	1.71709200	0.74836400	-0.75763300
C	2.25678100	-0.61419300	-0.83227300
H	1.21862300	-1.19594900	1.83358100
H	0.24197600	-1.56894400	-0.94106200
H	2.28774400	1.22954400	1.26601000
N	0.66477000	-0.98777300	0.99626900
H	3.09810000	-0.74415400	-0.14235700
N	0.18085400	0.21803400	0.99053200
H	1.17982900	1.13114900	-1.62702600
H	1.16534700	2.43388900	0.45229900
C	2.63476500	-1.06219700	-2.25087300
H	3.41090900	-0.40725300	-2.65462600
H	3.03253500	-2.07848400	-2.25525600
H	1.77487500	-1.02370300	-2.92761000
H	-0.44592400	0.32986100	0.18111100
C	1.55221500	-3.04656700	-0.02950900
H	1.84285300	-3.49042400	-0.98259500
H	2.41174900	-3.09534300	0.64734200
H	0.74506300	-3.65750100	0.38410900

R'=Boc

R1=CH3 R2=H R3=H R4=CH3

TS-BF

Zero-point correction=	0.228720 (Hartree/Particle)
Thermal correction to Energy=	0.242671
Thermal correction to Enthalpy=	0.243615
Thermal correction to Gibbs Free Energy=	0.187997
Sum of electronic and zero-point Energies=	-573.360024
Sum of electronic and thermal Energies=	-573.346073
Sum of electronic and thermal Enthalpies=	-573.345129
Sum of electronic and thermal Free Energies=	-573.400747

C	1.91667600	-1.53634800	-0.63960000
C	1.21563400	1.81524600	0.23886500
C	2.38260900	1.16748400	-0.00679100
C	2.75421200	-0.02120100	0.69486100
H	2.30558900	-1.11053600	-1.57221100
H	0.55522100	1.51097800	1.04610200
N	0.65624200	-1.28162600	-0.28473600
H	2.13982000	-0.28875400	1.55317200
N	0.02189700	-0.34996700	-0.93257500
H	3.04956600	1.53229300	-0.78710500
C	-1.35113200	-0.02727900	-0.66430100
O	-1.94719000	0.69030300	-1.42888400
O	-1.77429700	-0.59266900	0.44836000
C	-3.16915100	-0.34998000	0.77300000
H	-3.33981900	0.71771300	0.92219600
H	-3.80934100	-0.72363400	-0.02808100
H	-3.34316300	-0.90159500	1.69499400
H	0.94440200	2.71627800	-0.30452700
O	0.36011800	0.02495500	-1.82929800
C	4.18975800	-0.43584700	0.76501000
H	4.67766000	0.27137800	1.45324800
H	4.32837400	-1.42827800	1.19399700
H	4.70764800	-0.36014700	-0.19496300
C	2.48565100	-2.85247700	-0.18870800
H	2.09187500	-3.64263700	-0.83937400
H	3.57199000	-2.87426700	-0.28436600
H	2.19572700	-3.08808800	0.83805700

A

Zero-point correction=	0.231888 (Hartree/Particle)
Thermal correction to Energy=	0.246134
Thermal correction to Enthalpy=	0.247078
Thermal correction to Gibbs Free Energy=	0.190610
Sum of electronic and zero-point Energies=	-573.410036
Sum of electronic and thermal Energies=	-573.395791
Sum of electronic and thermal Enthalpies=	-573.394846
Sum of electronic and thermal Free Energies=	-573.451314

C	-2.07266900	1.82005800	-0.10495500
C	-0.91204800	-0.69065500	-1.01176400
C	-1.91846300	-1.47535300	-0.20468400
C	-2.01924200	-1.49354300	1.12618900
H	-0.15688300	2.16382100	0.50941600
H	-2.72752700	1.07256900	-0.54411400
H	-0.13741500	-1.34427600	-1.41900200
N	-0.83242100	1.51478200	0.06916200
H	-1.33776200	-0.88311800	1.72166200
N	-0.20035900	0.34777900	-0.26064200
H	-2.58288000	-2.08768100	-0.81385000
C	1.15871400	0.36112500	0.10098000
O	1.65157100	1.32062000	0.66402700
O	1.75432600	-0.76446100	-0.24883500
C	3.16643100	-0.85460700	0.07915300
H	3.30166300	-0.80284100	1.16075100
H	3.48146600	-1.82407200	-0.30245200
H	3.71646700	-0.04833200	-0.40877700
H	-1.38918200	-0.20683500	-1.87635100
C	-3.00541700	-2.31694200	1.89681100
H	-2.48775000	-3.00956700	2.57176500
H	-3.64006800	-1.68384800	2.52901600
H	-3.65276800	-2.90252200	1.23824200
C	-2.60970500	3.14305300	0.28941100
H	-3.03113700	3.64008500	-0.59283700
H	-3.43687300	3.00300100	0.99553600
H	-1.85420000	3.79088100	0.74034000

B

Zero-point correction=	0.230814 (Hartree/Particle)
Thermal correction to Energy=	0.245505
Thermal correction to Enthalpy=	0.246449
Thermal correction to Gibbs Free Energy=	0.187474
Sum of electronic and zero-point Energies=	-573.388310
Sum of electronic and thermal Energies=	-573.373619
Sum of electronic and thermal Enthalpies=	-573.372674
Sum of electronic and thermal Free Energies=	-573.431649

C	1.13566000	2.17352800	-0.62973500
C	0.94857000	-1.02586700	0.36793700
C	2.39390100	-0.81888900	0.66530500
C	3.34892500	-0.95785300	-0.26258000
H	1.36558100	2.51848000	0.38687200
H	0.76549800	-1.45716400	-0.61597100
N	0.52955600	1.07020200	-0.85818100
H	3.05428400	-1.20905300	-1.28292400
H	2.65640100	-0.58523300	1.69707500
N	0.18365900	0.32303700	0.35122000
C	0.40171400	0.84736800	1.22001200
C	-1.32011300	0.14875600	0.38317100
O	-1.95507900	0.66951600	1.25386600
O	-1.68303100	-0.60246400	-0.62072000
C	-3.11679200	-0.85157900	-0.74631900
H	-3.64243300	0.09708600	-0.86302700
H	-3.21515800	-1.46502200	-1.63920300
H	-3.47382300	-1.38296600	0.13709700
H	0.44146500	-1.61938300	1.13544500
C	4.81552700	-0.82071400	-0.01245700
H	5.33483700	-1.75692100	-0.25170200
H	5.24949500	-0.05308800	-0.66492200
C	5.03529500	-0.56014900	1.02627600
H	1.54840900	3.03467700	-1.76932900
H	2.63254200	3.19350600	-1.73785200
H	1.26801000	2.58948900	-2.72502200
H	1.08090800	4.02144100	-1.66987700

TS-AD

Zero-point correction=	0.230451 (Hartree/Particle)
Thermal correction to Energy=	0.243774
Thermal correction to Enthalpy=	0.244718
Thermal correction to Gibbs Free Energy=	0.191184
Sum of electronic and zero-point Energies=	-573.359729
Sum of electronic and thermal Energies=	-573.346406
Sum of electronic and thermal Enthalpies=	-573.345461
Sum of electronic and thermal Free Energies=	-573.398995

C	2.18751500	-1.13713600	-0.50673300
C	0.69734800	1.53232300	0.27998700
C	2.02827800	1.40321400	-0.09363700
C	2.87609800	0.42302300	0.47615200
H	0.55584100	-1.69631000	0.67746500
H	2.33900000	-0.78438900	-1.52438600
H	0.38457500	1.23910200	1.27936100
N	0.86797700	-1.15871400	-0.14999100
H	2.60977700	0.09788600	1.48343700
N	0.04497300	-0.24987600	-0.61048800
H	2.36001400	1.90552300	-1.00245500
C	-1.25625700	-0.41579200	0.01825600
O	-1.49841300	-1.27049300	0.84291200
O	-2.08090400	0.48167000	-0.48246700
C	-3.43955900	0.44060600	0.02652800
H	-3.44127600	0.60850400	1.10539400
H	-3.96054700	1.24462100	-0.49006100
H	-3.89368000	-0.52497200	-0.20310900
H	0.05830900	2.24367000	-0.23210300
C	4.36439700	0.47354900	0.20469000
H	4.88522600	-0.40487100	0.58768200
H	4.58976600	0.59042100	-0.85950700
H	4.77952000	1.34215500	0.72855500
C	2.99523800	-2.34415200	-0.09173900
H	4.04492600	-2.21364800	-0.35296800
H	2.92028400	-2.55012000	0.98017400
H	2.63204300	-3.22058400	-0.63981000

TS-AC

Zero-point correction=	0.232550 (Hartree/Particle)
Thermal correction to Energy=	0.245151
Thermal correction to Enthalpy=	0.246095
Thermal correction to Gibbs Free Energy=	0.194052
Sum of electronic and zero-point Energies=	-573.371692
Sum of electronic and thermal Energies=	-573.359091
Sum of electronic and thermal Enthalpies=	-573.358147
Sum of electronic and thermal Free Energies=	-573.410189

C	1.38817600	-1.55841500	-0.23596000
C	1.25456100	1.33286800	0.62976400
C	1.76813800	0.86483800	-0.65769600
C	2.55966400	-0.31670700	-0.74836500
H	1.20268500	-1.11698700	1.78215700
H	0.71774800	-1.61186600	-1.09692000
H	1.92119200	1.23949400	1.48766600
N	0.71627900	-1.02580500	0.88724200
H	3.29406000	-0.40120800	0.06024200
N	0.20950700	0.22633100	0.71665800
H	1.28914300	1.26602600	-1.55243600
C	-1.05417200	0.44857700	0.10575600
O	-1.37803200	1.54137600	-0.30022700
O	-1.77644700	-0.66393800	0.10447800
C	-3.11052200	-0.52725500	-0.44601200
H	-3.69541200	0.17049100	0.15633600
H	-3.06083000	-0.17656800	-1.47861500
H	-3.53939000	-1.52676500	-0.39789300
H	0.74049400	2.29086200	0.61181800
C	3.11549600	-0.67671800	-2.12351900
H	3.87499900	0.05149800	-2.42120800
H	3.59500500	-1.65716100	-2.11591500
H	2.33173500	-0.67980900	-2.88739700
C	2.09483000	-2.86775600	0.03995300
H	2.63823100	-3.21243000	-0.84072800
H	2.79565300	-2.78845400	0.87684400
H	1.34720800	-3.63010500	0.28134800

C

Zero-point correction=	0.234588 (Hartree/Particle)
Thermal correction to Energy=	0.247149
Thermal correction to Enthalpy=	0.248093
Thermal correction to Gibbs Free Energy=	0.195822
Sum of electronic and zero-point Energies=	-573.383329
Sum of electronic and thermal Energies=	-573.370768
Sum of electronic and thermal Enthalpies=	-573.369823
Sum of electronic and thermal Free Energies=	-573.422095

C	1.82525500	-1.42839500	-0.20883200
C	1.05241400	1.47929100	0.79151900
C	1.34565700	0.91954700	-0.53489700
C	2.46874700	-0.09576200	-0.71249300
H	1.15011000	-0.96434800	1.73537700
H	1.29549100	-1.88903100	-1.05254400
H	1.73427400	1.29785300	1.61778400
N	0.78913100	-1.04496300	0.78201000
H	3.29136900	0.17610700	-0.03855000
N	0.29762500	0.22654000	0.38394900
H	0.89092300	1.40062700	-1.39817700
C	-1.14071200	0.38960800	0.04386700
O	-1.55233200	1.47504200	-0.26527500
O	-1.75634900	-0.75782100	0.12973600
C	-3.17787000	-0.72861700	-0.19774100
H	-3.31430300	-0.36820500	-1.21842900
H	-3.50646100	-1.76118400	-0.10034300
H	-3.70282700	-0.08335300	0.50831200
H	0.40806200	2.34931200	0.86771800
C	2.98784400	-0.17105900	-2.15006900
H	3.43146400	0.77842600	-2.46263900
H	3.76389900	-0.93675900	-2.23491300
H	2.18698400	-0.42310800	-2.85320600
C	2.79281200	-2.43524900	0.39317700
H	2.26160700	-3.32934800	0.73096700
H	3.52524100	-2.74756400	-0.35558800
H	3.33806100	-2.00991900	1.24330500

TS-CE

Zero-point correction=	0.203278 (Hartree/Particle)
Thermal correction to Energy=	0.214786
Thermal correction to Enthalpy=	0.215730
Thermal correction to Gibbs Free Energy=	0.165656
Sum of electronic and zero-point Energies=	-534.063382
Sum of electronic and thermal Energies=	-534.051873
Sum of electronic and thermal Enthalpies=	-534.050929
Sum of electronic and thermal Free Energies=	-534.101004

C	1.03925300	-1.57217400	-0.30402100
C	1.75291300	1.55312800	0.32760400
C	1.72853400	0.77337600	-0.79259000
C	2.24360500	-0.60914600	-0.83239400
H	1.21906100	-1.30957800	1.77891800
H	0.21056600	-1.54902600	-1.01110100
H	1.41499200	-2.58888000	-0.17917400
H	2.35387700	1.29195000	1.19427800
N	0.64969900	-1.03536500	0.96640400
H	3.06276700	-0.74582400	-0.11826800
N	0.08751000	0.09857600	1.10971100
H	1.17525300	1.12754900	-1.66261900
C	-1.03478900	0.47702500	0.25325800
O	-1.22055800	1.60496500	-0.11380000
O	-1.84389200	-0.57015400	0.13316300
C	-3.13720000	-0.29268700	-0.47465900
H	-3.00105800	0.09659900	-1.48496800
H	-3.65030400	-1.25247000	-0.49159300
H	-3.68316600	0.42847700	0.13594800
H	1.29334000	2.53530200	0.33204700
C	2.65082600	-1.11250100	-2.22450200
H	3.51815500	-0.55000000	-2.57922300
H	2.92687400	-2.16974000	-2.19400100
H	1.84202800	-0.98632600	-2.95084300

R'=H

R1=CH3 R2=CH3 R3=H R4=CH3

TS-BF

Zero-point correction=	0.214620 (Hartree/Particle)
Thermal correction to Energy=	0.225540
Thermal correction to Enthalpy=	0.226484
Thermal correction to Gibbs Free Energy=	0.179218
Sum of electronic and zero-point Energies=	-384.829051
Sum of electronic and thermal Energies=	-384.818130
Sum of electronic and thermal Enthalpies=	-384.817186
Sum of electronic and thermal Free Energies=	-384.864452

C	-1.23081400	1.13328300	0.12546800
C	1.43915300	-1.15817400	-0.01604100
C	1.36234200	0.08076100	0.56320000
C	0.94818200	1.23139200	-0.15279100
H	-1.18977900	1.04064600	1.21714400
H	1.26955700	-1.23743500	-1.08915100
N	-1.38380800	0.03409700	-0.61208900
H	0.89144100	1.13860300	-1.23554800
H	1.57963900	0.18568800	1.62651300
N	-1.17643000	-1.11152000	-0.03509100
H	-1.22134300	-1.22270900	0.98179400
H	-1.35970000	-1.93442400	-0.60425300
C	1.26240600	2.60151600	0.37129500
H	2.34071000	2.76137200	0.22886400
H	0.75597300	3.39362400	-0.18076700
H	1.05801400	2.70509200	1.44062600
C	-1.79268500	2.40843900	-0.43898100
H	-1.39203400	3.28592200	0.07091500
H	-1.60666900	2.48816800	-1.51292600
H	-2.87831800	2.41901000	-0.28359600
C	1.91642700	-2.38643100	0.67779000
H	1.27108500	-3.24492200	0.45996300
H	2.91074000	-2.65544000	0.29492900
H	1.98935400	-2.25678400	1.76026800

A

Zero-point correction=	0.217212 (Hartree/Particle)
Thermal correction to Energy=	0.228598
Thermal correction to Enthalpy=	0.229542
Thermal correction to Gibbs Free Energy=	0.180404
Sum of electronic and zero-point Energies=	-384.858242
Sum of electronic and thermal Energies=	-384.846856
Sum of electronic and thermal Enthalpies=	-384.845912
Sum of electronic and thermal Free Energies=	-384.895049

C	-2.54480000	-0.58545100	0.01160800
C	0.39607800	-0.51406600	-0.25751100
C	1.72343800	-0.03942300	0.28717900
C	2.88400400	-0.02363400	-0.37356700
H	-2.31254200	1.39234900	0.17935300
H	-2.03939300	-1.52277800	-0.19646000
N	-1.83850800	0.49733300	0.01190900
H	2.92318100	-0.37232700	-1.40452500
N	-0.51294400	0.66428400	-0.28540100
H	1.69445000	0.29871800	1.32408900
H	-0.01661000	-1.23221700	0.47172000
H	-0.16277200	1.49354400	0.19320600
C	4.18595300	0.43538500	0.20622200
H	4.08058300	0.77602200	1.24009100
H	4.92809800	-0.37231400	0.18471400
H	4.60671200	1.25683500	-0.38682700
C	-4.00521800	-0.57566700	0.27249200
H	-4.53920700	-0.97507800	-0.59808700
H	-4.23181300	-1.23950300	1.11474900
H	-4.38769900	0.42405400	0.49507100
C	0.44576600	-1.16468600	-1.64185800
H	0.84672600	-0.47078100	-2.38447200
H	1.07197600	-2.06014300	-1.61614700
H	-0.54907800	-1.46668200	-1.98283100

B

Zero-point correction=	0.217489 (Hartree/Particle)
Thermal correction to Energy=	0.228886
Thermal correction to Enthalpy=	0.229830
Thermal correction to Gibbs Free Energy=	0.180294
Sum of electronic and zero-point Energies=	-384.861531
Sum of electronic and thermal Energies=	-384.850135
Sum of electronic and thermal Enthalpies=	-384.849191
Sum of electronic and thermal Free Energies=	-384.898727

C	2.70172900	0.66567700	0.04709800
C	-0.56164500	-0.43654200	0.58487600
C	-1.84438400	-0.38570600	-0.20042800
C	-2.84495400	0.47873800	-0.00176700
H	2.41047400	1.62307800	-0.40722300
N	1.88941100	-0.31641900	0.14408500
H	-2.76518500	1.22587400	0.78746100
H	-1.94133200	-1.14533900	-0.97777600
H	-0.31277200	-1.47264300	0.83988500
H	0.42967000	0.92422100	-0.71707100
H	0.47463100	-0.64985600	-1.23763700
N	0.56630900	-0.05318800	-0.40169800
C	-4.11951500	0.49667300	-0.78458700
H	-4.98047300	0.33977200	-0.12348000
H	-4.26808500	1.47485400	-1.25834700
H	-4.13777900	-0.27151800	-1.56224900
C	4.09365600	0.53122900	0.55226400
H	4.26347400	-0.45504400	0.98667600
H	4.79946000	0.69893700	-0.26988200
H	4.29188300	1.30579200	1.30220900
C	-0.45639100	0.44356200	1.81955500
H	0.50722800	0.30779300	2.31509100
H	-0.58493500	1.50571700	1.58603700
H	-1.23713500	0.15678300	2.52771200

TS-AD

Zero-point correction=	0.216219 (Hartree/Particle)
Thermal correction to Energy=	0.226651
Thermal correction to Enthalpy=	0.227596
Thermal correction to Gibbs Free Energy=	0.181401
Sum of electronic and zero-point Energies=	-384.823531
Sum of electronic and thermal Energies=	-384.813099
Sum of electronic and thermal Enthalpies=	-384.812154
Sum of electronic and thermal Free Energies=	-384.858349

C	1.08747100	-0.99935800	-0.20827600
C	-1.15454700	1.10358000	0.14189700
C	0.14294300	1.34012800	-0.35370500
C	1.30658300	0.80047700	0.25116400
H	-0.19492400	-1.61856400	1.28880500
H	1.06572300	-0.95436300	-1.29581200
H	-1.24458000	1.02223800	1.22640200
N	-0.15358900	-1.32607800	0.30561900
H	1.26067700	0.70629500	1.33812200
N	-1.21606200	-0.75052700	-0.24675300
H	0.23070800	1.70871600	-1.37771100
H	-2.02769200	-0.98910500	0.34047600
C	2.66048900	1.26400100	-0.26571300
H	3.48313800	0.71773900	0.19785500
H	2.73895700	1.16389700	-1.35268000
H	2.79741900	2.32102700	-0.01696100
C	2.24500600	-1.78906300	0.36667100
H	3.19225400	-1.44869400	-0.05090800
H	2.29754500	-1.71464400	1.45728700
H	2.13030600	-2.84326100	0.09402700
C	-2.36039900	1.66353700	-0.56686300
H	-3.27129800	1.12782500	-0.28478700
H	-2.50248600	2.71249900	-0.28495700
H	-2.24679300	1.60785800	-1.65215200

TS-AC

Zero-point correction=	0.217701 (Hartree/Particle)
Thermal correction to Energy=	0.227515
Thermal correction to Enthalpy=	0.228459
Thermal correction to Gibbs Free Energy=	0.183858
Sum of electronic and zero-point Energies=	-384.835332
Sum of electronic and thermal Energies=	-384.825518
Sum of electronic and thermal Enthalpies=	-384.824574
Sum of electronic and thermal Free Energies=	-384.869175

C	1.44470900	-0.46883600	-0.14734300
C	-1.46259500	0.36706600	0.24336300
C	-0.44431000	1.21440200	-0.36284900
C	0.86685000	1.30711400	0.15194200
H	0.33840200	-1.43583800	1.29581700
H	1.52197500	-0.45295600	-1.23600900
H	-1.41653400	0.32493400	1.33414700
N	0.37757300	-1.23882400	0.29432400
H	0.93168000	1.29276600	1.24308800
N	-0.85544200	-1.01261100	-0.22766200
H	-0.62441000	1.53912400	-1.39055500
H	-0.82220300	-1.06280000	-1.25032000
C	1.84658700	2.25570200	-0.52170200
H	1.58116400	3.29102200	-0.28647400
H	2.86796200	2.10166100	-0.16795600
H	1.83655300	2.14576900	-1.61054500
C	2.75544900	-0.71007500	0.56094700
H	3.50836200	0.01403500	0.24741500
H	2.64964900	-0.66007000	1.64899800
H	3.12944500	-1.70382400	0.29267500
C	-2.88634600	0.48023600	-0.26572300
H	-2.92445400	0.47834200	-1.36010900
H	-3.48510700	-0.35444200	0.10560600
H	-3.33496600	1.41316300	0.08575300

C

Zero-point correction=	0.220799 (Hartree/Particle)
Thermal correction to Energy=	0.230366
Thermal correction to Enthalpy=	0.231310
Thermal correction to Gibbs Free Energy=	0.186805
Sum of electronic and zero-point Energies=	-384.858684
Sum of electronic and thermal Energies=	-384.849117
Sum of electronic and thermal Enthalpies=	-384.848173
Sum of electronic and thermal Free Energies=	-384.892678

C	1.55597900	-0.17661900	-0.00586700
C	-1.55801600	0.09406500	0.65760700
C	-0.64163200	0.79376600	-0.27650400
C	0.77378800	1.16302300	0.17048700
H	0.45134400	-1.57812800	1.10019500
H	1.92913100	-0.22049400	-1.03713700
H	-1.20822200	-0.01857100	1.68319700
N	0.55569500	-1.26894600	0.13054700
H	0.74816200	1.41927500	1.23716700
N	-0.69194000	-0.71929300	-0.28555100
H	-1.06548100	1.25783900	-1.16498300
H	-1.13795400	-1.21285300	-1.06658400
C	1.37160700	2.33064100	-0.61696700
H	0.79828700	3.24921600	-0.46240400
H	2.39704200	2.52723100	-0.29148400
H	1.39493300	2.11941600	-1.69144500
C	2.71209200	-0.38799100	0.96069900
H	3.19506600	-1.35406400	0.78802900
H	3.46829200	0.38907800	0.82095100
H	2.37573100	-0.34717600	2.00319600
C	-3.04575600	0.03814300	0.44864600
H	-3.46828400	-0.87614100	0.87428400
H	-3.50209300	0.89219500	0.95867700
H	-3.31655900	0.09781200	-0.60975800

TS-CE

Zero-point correction=	0.217564 (Hartree/Particle)
Thermal correction to Energy=	0.227503
Thermal correction to Enthalpy=	0.228448
Thermal correction to Gibbs Free Energy=	0.183231
Sum of electronic and zero-point Energies=	-384.833573
Sum of electronic and thermal Energies=	-384.823634
Sum of electronic and thermal Enthalpies=	-384.822690
Sum of electronic and thermal Free Energies=	-384.867907

C	1.08950100	-1.64919000	-0.21602900
C	1.59497600	1.46844200	0.40227700
C	1.64413200	0.73079000	-0.77917200
C	2.21052300	-0.62249100	-0.86314100
H	1.23293500	-1.14981900	1.82806100
H	0.24857200	-1.66626000	-0.91804100
H	2.27867800	1.19067800	1.20365000
N	0.66130300	-0.99279000	0.99320400
H	3.08321000	-0.72198600	-0.20784100
N	0.18659800	0.22418000	0.92642200
H	1.08059700	1.10142400	-1.63830800
C	2.54960400	-1.06129000	-2.29526200
H	3.30691600	-0.40039600	-2.72411800
H	2.95376000	-2.07518600	-2.31479300
H	1.66739400	-1.02973900	-2.94311800
H	-0.46736000	0.29382200	0.13436600
C	1.62525200	-3.04911800	0.03751900
H	1.94632400	-3.51167700	-0.89707200
H	2.47874500	-3.03796400	0.72374700
H	0.84189200	-3.68129400	0.46453200
C	1.02691900	2.85252900	0.49012600
H	0.55231500	3.01078200	1.46195900
H	1.84020600	3.58186000	0.39831800
H	0.29953300	3.05407000	-0.30113800

R'=Boc

R1=CH3 R2=CH3 R3=H R4=CH3

TS-BF

Zero-point correction=	0.257203 (Hartree/Particle)
Thermal correction to Energy=	0.272423
Thermal correction to Enthalpy=	0.273367
Thermal correction to Gibbs Free Energy=	0.215724
Sum of electronic and zero-point Energies=	-612.661468
Sum of electronic and thermal Energies=	-612.646249
Sum of electronic and thermal Enthalpies=	-612.645304
Sum of electronic and thermal Free Energies=	-612.702947

C	1.93193300	-1.58077400	-0.56946000
C	1.23061600	1.83119600	0.22111100
C	2.35665600	1.13599100	-0.10303600
C	2.75154000	-0.05765900	0.58515500
H	2.30261700	-1.22661100	-1.53913400
H	0.63351100	1.47784300	1.06326700
N	0.65354900	-1.33156900	-0.24640400
H	2.20498900	-0.27939200	1.50069100
N	0.03033900	-0.43290700	-0.93842900
H	2.98657400	1.48558100	-0.92154600
C	-1.31844500	-0.03195500	-0.66686100
O	-1.85588400	0.75436300	-1.41004600
O	-1.79193700	-0.60599800	0.41914900
C	-3.16303300	-0.26041000	0.75319800
H	-3.24211700	0.81038800	0.94911400
H	-3.82913400	-0.54298500	-0.06379000
H	-3.38732900	-0.83506500	1.64988300
C	0.39470600	-0.06911900	-1.82973500
C	4.20969200	-0.42804200	0.60874600
H	4.71551300	0.33195200	1.22058800
H	4.39732800	-1.38986700	1.08525200
H	4.67154700	-0.40584600	-0.38234400
C	2.48574500	-2.89016100	-0.06797200
H	2.04387600	-3.70552600	-0.65179900
H	3.56586300	-2.94447300	-0.20765000
H	2.23921400	-3.05845300	0.98330000
C	0.78180100	3.09203100	-0.42563300
H	1.43207000	3.39953900	-1.24779400
H	-0.24343100	2.97917800	-0.80349000
H	0.74162200	3.90002200	0.31638900

A

Zero-point correction=	0.259540 (Hartree/Particle)
Thermal correction to Energy=	0.275535
Thermal correction to Enthalpy=	0.276479
Thermal correction to Gibbs Free Energy=	0.215485
Sum of electronic and zero-point Energies=	-612.697541
Sum of electronic and thermal Energies=	-612.681545
Sum of electronic and thermal Enthalpies=	-612.680601
Sum of electronic and thermal Free Energies=	-612.741596

C	-2.12667900	1.76205400	0.11469400
C	-0.89177200	-0.75110300	-0.97239200
C	-2.02890300	-1.40584100	-0.20925400
C	-2.13398900	-1.49351200	1.11956700
H	-0.17033000	2.16143800	0.51427300
H	-2.80946200	0.99319700	-0.23103600
H	-0.09377000	-1.48714900	-1.09508500
N	-0.86828700	1.48396400	0.15803400
N	-1.36920300	-1.02894200	1.74527900
H	-0.22456200	0.32220300	-0.18614500
H	-2.77684000	-1.87998700	-0.84414400
C	1.15954500	0.42931900	0.05300700
O	1.63716600	1.42778500	0.56084800
O	1.80315200	-0.66021500	-0.32668100
C	3.23687900	-0.65668600	-0.09367900
H	3.44034900	-0.57129300	0.97503100
H	3.58486300	-1.61428200	-0.47665900
H	3.70277300	0.16909000	-0.63368600
C	-3.23378500	-2.20484300	1.84639200
H	-2.82511400	-3.00850800	2.47116200
H	-3.76396400	-1.52539900	2.52501400
H	-3.96310300	-2.64383800	1.16002000
C	-2.64188500	3.08411700	0.54149500
H	-3.16932400	3.55582000	-0.29654100
H	-3.38223600	2.94416000	1.33829000
H	-1.85441500	3.75476700	0.89399300
C	-1.28002500	-0.26309600	-2.37635600
H	-1.64251600	-1.11710300	-2.95516000
H	-2.07453200	0.48818300	-2.37768100
H	-0.41021700	0.15003700	-2.89356500

B

Zero-point correction=	0.258834 (Hartree/Particle)
Thermal correction to Energy=	0.274818
Thermal correction to Enthalpy=	0.275762
Thermal correction to Gibbs Free Energy=	0.214956
Sum of electronic and zero-point Energies=	-612.680261
Sum of electronic and thermal Energies=	-612.664277
Sum of electronic and thermal Enthalpies=	-612.663333
Sum of electronic and thermal Free Energies=	-612.724138

C	1.07843100	2.15317100	-0.60752200
C	0.94348100	-1.08889200	0.47323600
C	2.39697100	-0.80454400	0.68548800
C	3.32062900	-0.97113000	-0.26797000
H	1.17872900	2.56364600	0.40617100
H	0.76181200	-1.53190500	-0.50819900
N	0.58810300	0.99313400	-0.83108900
H	2.99770300	-1.29374800	-1.25899000
H	2.69047400	-0.49861600	1.69091200
N	0.17660800	0.28243100	0.37904100
H	0.36685200	0.82691100	1.24173500
C	-1.32851900	0.15082100	0.34414900
O	-1.98754700	0.68646400	1.18850600
O	-1.67410700	-0.57411300	-0.68671500
C	-3.11008100	-0.74820100	-0.88770900
H	-3.58271000	0.22815900	-1.00355200
H	-3.19422600	-1.33354300	-1.80077500
H	-3.53758200	-1.28314600	-0.03829800
C	4.79028700	-0.76898700	-0.08574500
H	5.33468100	-1.69942000	-0.28921900
H	5.17071400	-0.02815000	-0.79976400
H	5.04105000	-0.43796900	0.92562400
C	1.53459600	2.99355500	-1.74597300
H	2.59271100	3.24796600	-1.61429600
H	1.39360200	2.48240800	-2.69930300
H	0.97999200	3.93946300	-1.74784700
C	0.32075400	-1.91858800	1.59259900
H	0.40984400	-1.42697400	2.56688500
H	-0.73026100	-2.15825100	1.40872900
H	0.86459400	-2.86500900	1.64944500

TS-AD

Zero-point correction=	0.257555 (Hartree/Particle)
Thermal correction to Energy=	0.272763
Thermal correction to Enthalpy=	0.273708
Thermal correction to Gibbs Free Energy=	0.215897
Sum of electronic and zero-point Energies=	-612.659073
Sum of electronic and thermal Energies=	-612.643865
Sum of electronic and thermal Enthalpies=	-612.642921
Sum of electronic and thermal Free Energies=	-612.700731

C	2.12119800	-1.25396200	-0.55184000
C	0.78156400	1.78835600	0.21385800
C	2.05770200	1.45832100	-0.19476200
C	2.85633300	0.49969500	0.46082200
H	0.53795900	-1.71003900	0.70747100
H	2.28144900	-0.85902700	-1.55103300
H	0.44245000	1.42650800	1.18491300
N	0.83796000	-1.20112800	-0.14631500
N	2.53214700	0.19107200	1.45513700
H	-0.02806100	-0.37361500	-0.65948400
H	2.43337900	1.89219200	-1.12174600
C	-1.26251800	-0.49011600	0.06343900
O	-1.42534000	-1.20365500	1.03566100
O	-2.17062100	0.27857500	-0.51738700
C	-3.49552000	0.23550900	0.06839800
H	-3.46304600	0.57417200	1.10600400
H	-4.09772400	0.90926200	-0.53874500
H	-3.89050300	-0.78107500	0.02198400
C	4.33785100	0.43730700	0.21386600
H	4.79775800	-0.45827000	0.63384100
H	4.59246400	0.51888300	-0.84680900
H	4.79654200	1.29336200	0.72688000
C	2.94651600	-2.42548800	-0.10200300
H	4.00175000	-2.26148600	-0.31998400
H	2.83361400	-2.63534400	0.96606800
H	2.63932200	-3.31792100	-0.66095400
C	-0.05021500	2.82763900	-0.45000000
C	0.34211700	3.10628700	-1.43050100
H	-1.08522400	2.49086900	-0.55996900
H	-0.07913900	3.72529500	0.18314700

TS-AC

Zero-point correction=	0.260650 (Hartree/Particle)
Thermal correction to Energy=	0.274648
Thermal correction to Enthalpy=	0.275592
Thermal correction to Gibbs Free Energy=	0.221027
Sum of electronic and zero-point Energies=	-612.661884
Sum of electronic and thermal Energies=	-612.647887
Sum of electronic and thermal Enthalpies=	-612.646942
Sum of electronic and thermal Free Energies=	-612.701508

C	1.31898600	-1.53689600	-0.19713300
C	1.23175700	1.37644900	0.61176400
C	1.72500700	0.90428500	-0.68778200
C	2.52478900	-0.25863000	-0.78865600
H	1.14669100	-1.03987200	1.80392700
H	0.66235700	-1.59438000	-1.06705700
H	1.90634600	1.12407500	1.43403300
N	0.67215000	-0.96542000	0.90186800
H	3.25875200	-0.35960100	0.01687200
N	0.13503200	0.27132300	0.70280000
H	1.23340600	1.30530400	-1.57602400
C	-1.09286400	0.38676400	-0.00660500
O	-1.43730100	1.39929200	-0.57128300
O	-1.78909000	-0.74247200	0.09720000
C	-3.09410700	-0.71664700	-0.53058200
H	-3.72494600	0.03898500	-0.05872100
H	-2.99989200	-0.50631200	-1.59776000
H	-3.50421600	-1.71249700	-0.37002100
C	3.04137000	-0.66215700	-2.16219600
H	3.83191300	0.02508900	-2.47787000
H	3.47501500	-1.66412200	-2.15138600
H	2.24999900	-0.63572400	-2.91755200
C	2.04873200	-2.82524300	0.09840600
H	2.61748400	-3.16178300	-0.76919200
H	2.72936700	-2.72666900	0.94963900
H	1.31371900	-3.60380500	0.32851600
C	0.73543300	2.80338100	0.76138800
H	0.14736700	3.13451000	-0.09201100
H	0.12877100	2.89356900	1.66585200
H	1.60760500	3.45408900	0.87485000

C

Zero-point correction=	0.262571 (Hartree/Particle)
Thermal correction to Energy=	0.276674
Thermal correction to Enthalpy=	0.277619
Thermal correction to Gibbs Free Energy=	0.222453
Sum of electronic and zero-point Energies=	-612.679355
Sum of electronic and thermal Energies=	-612.665251
Sum of electronic and thermal Enthalpies=	-612.664307
Sum of electronic and thermal Free Energies=	-612.719472

C	1.85520300	-1.43163800	-0.29315600
C	0.95591300	1.44178900	0.77262300
C	1.33489000	0.91281600	-0.55131300
C	2.49860800	-0.06612000	-0.69068500
H	1.00935200	-1.06311400	1.60395700
H	1.40871800	-1.87305400	-1.19379500
H	1.58186500	1.13095900	1.60912600
N	0.73054400	-1.11484000	0.62174600
H	3.26215400	0.19356500	0.05359600
N	0.24361500	0.16249400	0.22320700
H	0.94330900	1.42436800	-1.42827900
C	-1.16166500	0.25315500	-0.24177000
O	-1.48585100	1.08474100	-1.04675600
O	-1.88531300	-0.64655500	0.37230300
C	-3.29655800	-0.66940300	0.00722800
H	-3.39836200	-0.85982300	-1.06224300
H	-3.72137400	-1.48420700	0.58982300
H	-3.76039800	0.28252800	0.27071500
C	3.12666100	-0.06575000	-2.08552900
H	3.56682800	0.90694100	-2.32276900
H	3.92724600	-0.80857100	-2.14391800
H	2.38836200	-0.30463800	-2.85831100
C	2.79930200	-2.43504800	0.34878100
H	2.27051000	-3.35506100	0.61283000
H	3.59817200	-2.69962900	-0.34875600
H	3.26320900	-2.02700100	1.25404400
C	0.16536500	2.69948400	0.99108900
H	-0.43020800	2.98316400	0.12378800
H	-0.47999700	2.60931000	1.86968700
H	0.88519600	3.50038400	1.19272600

TS-CE

Zero-point correction=	0.259768 (Hartree/Particle)
Thermal correction to Energy=	0.274005
Thermal correction to Enthalpy=	0.274949
Thermal correction to Gibbs Free Energy=	0.219818
Sum of electronic and zero-point Energies=	-612.653884
Sum of electronic and thermal Energies=	-612.639647
Sum of electronic and thermal Enthalpies=	-612.638703
Sum of electronic and thermal Free Energies=	-612.693834

C	1.03187200	-1.61701100	-0.27687300
C	1.74264700	1.59872700	0.32322500
C	1.65562700	0.78503200	-0.78472300
C	2.18709100	-0.59144500	-0.83707600
H	1.19993600	-1.19853700	1.78750200
H	0.19879100	-1.57996000	-0.98236500
H	2.33613400	1.24873800	1.16805700
N	0.62021700	-1.00062900	0.96219900
H	3.02835400	-0.70964500	-0.14501200
N	0.07895600	0.16232100	0.99899300
H	1.11001800	1.15076600	-1.65468100
C	-1.07411300	0.43466300	0.15652800
O	-1.30908600	1.52002600	-0.30550900
O	-1.86327900	-0.63760100	0.14393300
C	-3.16441100	-0.44221400	-0.47225100
H	-3.04580200	-0.17935100	-1.52502200
H	-3.67248300	-1.39933600	-0.36655800
H	-3.70981400	0.34526000	0.05068700
C	2.59581000	-1.02469800	-2.25518100
H	3.36589200	-0.35140200	-2.63977300
H	3.01320100	-2.03314900	-2.25913700
H	1.74669600	-0.99592000	-2.94554000
C	1.52540800	-3.04062000	-0.07257400
H	1.83692600	-3.47333000	-1.02410800
H	2.37629300	-3.08148400	0.61588100
H	0.72161300	-3.66586200	0.32528100
C	1.30579700	3.02184900	0.38283500
H	0.75574400	3.22002600	1.30759600
H	2.20083400	3.65818200	0.40870400
H	0.68942500	3.30843300	-0.46908700

R²=H

R1=CH3 R2=H R3=CH3 R4=CH3

TS-BF

Zero-point correction=	0.214871 (Hartree/Particle)
Thermal correction to Energy=	0.225597
Thermal correction to Enthalpy=	0.226541
Thermal correction to Gibbs Free Energy=	0.179927
Sum of electronic and zero-point Energies=	-384.821908
Sum of electronic and thermal Energies=	-384.811183
Sum of electronic and thermal Enthalpies=	-384.810238
Sum of electronic and thermal Free Energies=	-384.856852

C	-1.18619100	1.11029600	0.16171500
C	1.34243000	-1.11114990	-0.11508100
C	1.40942000	0.09975700	0.52831800
C	0.97332300	1.25584800	-0.18497000
H	-1.10219100	1.03673500	1.25303000
H	1.16033700	-1.17348200	-1.18260200
H	1.64113400	-2.03205300	0.37988300
N	-1.37191700	-0.00254000	-0.54981200
H	0.88470600	1.14371000	-1.26307700
N	-1.09739800	-1.13322800	0.03190400
H	-1.11122300	-1.23437700	1.05189800
H	-1.30749300	-1.96940800	-0.51056000
C	1.27727200	2.64361400	0.29592200
H	2.36384000	2.79051400	0.20963100
H	0.80828000	3.40766400	-0.32443400
H	1.01520000	2.81148000	1.34373200
C	-1.78677800	2.37054600	-0.39660100
H	-1.37642200	3.26027600	0.08292400
H	-1.64752000	2.43510200	-1.47841800
H	-2.86479200	2.36807900	-0.19537900
C	1.81684700	0.19599100	1.97750500
H	2.71538500	0.81324900	2.08933000
H	1.03786000	0.65944300	2.59521500
H	2.03624600	-0.78913100	2.39467600

A

Zero-point correction=	0.216890 (Hartree/Particle)
Thermal correction to Energy=	0.228605
Thermal correction to Enthalpy=	0.229549
Thermal correction to Gibbs Free Energy=	0.178751
Sum of electronic and zero-point Energies=	-384.860443
Sum of electronic and thermal Energies=	-384.848728
Sum of electronic and thermal Enthalpies=	-384.847784
Sum of electronic and thermal Free Energies=	-384.898581

C	-2.45496100	-0.53044400	-0.13004500
C	0.40479200	-0.40445900	0.23794400
C	1.81287400	0.03332100	0.58173700
C	2.76172200	-0.02869400	-0.36512000
H	-2.32390300	1.46553100	-0.02017400
H	-1.88259200	-1.45303400	-0.15477900
H	0.39708500	-1.02432500	-0.66487200
N	-1.80336000	0.58068600	-0.01868800
H	2.46119600	-0.38518600	-1.35126600
N	-0.44624100	0.77142900	-0.01668100
H	-0.02270700	-0.99801500	1.06378800
H	-0.22470600	1.60504100	0.52666900
C	4.21163900	0.32417800	-0.24604300
H	4.49816400	0.67525300	0.74710400
H	4.83586900	-0.54531000	-0.48719600
H	4.47670800	1.10364600	-0.97131100
C	-3.93325300	-0.57319200	-0.24677000
H	-4.21400300	-1.04717400	-1.19503100
H	-4.34624500	-1.19855600	0.55311500
H	-4.39106600	0.41826100	-0.19655400
C	2.01879600	0.47347900	2.00996900
H	3.00259800	0.91373300	2.17654400
H	1.27688000	1.22109600	2.32192600
H	1.91018200	-0.37275300	2.70066000

B

Zero-point correction=	0.217334 (Hartree/Particle)
Thermal correction to Energy=	0.229059
Thermal correction to Enthalpy=	0.230003
Thermal correction to Gibbs Free Energy=	0.178946
Sum of electronic and zero-point Energies=	-384.860599
Sum of electronic and thermal Energies=	-384.848874
Sum of electronic and thermal Enthalpies=	-384.847930
Sum of electronic and thermal Free Energies=	-384.898987

C	2.56923700	0.72907900	0.10877700
C	-0.50921600	-0.64165900	0.35828800
C	-1.85928500	-0.58975200	-0.30700200
C	-2.68607000	0.42054500	0.01577900
H	2.17044200	1.68401500	-0.26152600
H	-0.42683600	0.04116300	1.20525500
N	1.91281900	-0.36361200	0.01488500
H	-2.32355100	1.15260600	0.73933000
H	-0.21898800	-1.64594200	0.67890000
H	0.40938700	0.74557200	-0.94645300
H	0.60445700	-0.83074400	-1.42773100
N	0.60178200	-0.21274300	-0.60413500
C	-4.07625500	0.67136100	-0.47495200
H	-4.78135300	0.66230800	0.36556700
H	-4.14640300	1.67002400	-0.92339700
H	-4.42155800	-0.05544600	-1.21209000
C	3.91909600	0.73649800	0.73151500
H	4.21062200	-0.26159400	1.06128900
H	4.65335700	1.11752800	0.01209600
H	3.92619900	1.42525500	1.58449000
C	-2.17676400	-1.72445700	-1.24970400
H	-3.15898700	-1.62058000	-1.71123500
H	-1.45104000	-1.80473100	-2.07144100
H	-2.15618300	-2.68587100	-0.72170500

TS-AD

Zero-point correction=	0.216955 (Hartree/Particle)
Thermal correction to Energy=	0.226879
Thermal correction to Enthalpy=	0.227823
Thermal correction to Gibbs Free Energy=	0.182748
Sum of electronic and zero-point Energies=	-384.826503
Sum of electronic and thermal Energies=	-384.816579
Sum of electronic and thermal Enthalpies=	-384.815635
Sum of electronic and thermal Free Energies=	-384.860710

C	1.12276200	-0.92021400	-0.21206200
C	-1.12597000	1.08129900	0.21752500
C	0.11847900	1.35664600	-0.37245400
C	1.29544800	0.72686700	0.21983500
H	-0.22165400	-1.64533900	1.21462700
H	1.13143100	-0.92617700	-1.30519400
H	-1.17795100	0.94686500	1.29549900
N	-0.15144500	-1.33546200	0.23851500
H	1.22898700	0.70268500	1.31136200
N	-1.18793200	-0.73430400	-0.32621500
H	-2.02341700	1.49611400	-0.23412000
H	-2.03394900	-1.00247100	0.19818600
C	2.66477400	1.23174800	-0.23827500
H	3.46452800	0.76595200	0.33939300
H	2.85135500	1.03864400	-1.29871500
H	2.73753900	2.31101200	-0.07413900
C	2.24925000	-1.76019200	0.37436000
H	3.21336400	-1.45287700	-0.03099700
H	2.29347000	-1.68118600	1.46562100
H	2.09990100	-2.80995500	0.10628800
C	0.18623500	1.94566900	-1.73786600
H	0.85584800	2.81509600	-1.75015800
H	0.61476400	1.22560400	-2.45010300
H	-0.79370000	2.25554400	-2.10328100

TS-AC

Zero-point correction=	0.217624 (Hartree/Particle)
Thermal correction to Energy=	0.227587
Thermal correction to Enthalpy=	0.228531
Thermal correction to Gibbs Free Energy=	0.183337
Sum of electronic and zero-point Energies=	-384.838581
Sum of electronic and thermal Energies=	-384.828618
Sum of electronic and thermal Enthalpies=	-384.827674
Sum of electronic and thermal Free Energies=	-384.872868

C	1.39368200	-0.50654000	-0.16709600
C	-1.41029800	0.34650900	0.25984400
C	-0.43915000	1.23640900	-0.40293100
C	0.85506600	1.32717600	0.15319300
H	0.39214100	-1.46940100	1.34585000
H	1.40278000	-0.48763500	-1.25877200
H	-1.41138500	0.39835300	1.34957300
N	0.36641200	-1.26830600	0.34521400
H	0.88446800	1.26066500	1.24250900
N	-0.91282900	-1.06621500	-0.10799000
H	-2.42976300	0.42984700	-0.11862000
H	-0.94473300	-1.20598300	-1.12055600
C	1.90235100	2.24697600	-0.44673100
H	1.54710000	3.28317700	-0.44096700
H	2.82491500	2.22145200	0.13622100
H	2.14801200	1.99285800	-1.48287500
C	2.74892300	-0.71225900	0.46123600
H	3.47424000	0.00204300	0.07066700
H	2.71500500	-0.62609100	1.55140800
H	3.10713900	-1.71499100	0.20342500
C	-0.74765500	1.76298700	-1.76394800
H	-0.93374500	2.84504600	-1.68473300
H	0.08638500	1.65327700	-2.46533900
H	-1.64581900	1.31354800	-2.19463400

C

Zero-point correction=	0.218337 (Hartree/Particle)
Thermal correction to Energy=	0.228612
Thermal correction to Enthalpy=	0.229556
Thermal correction to Gibbs Free Energy=	0.183730
Sum of electronic and zero-point Energies=	-384.839659
Sum of electronic and thermal Energies=	-384.829384
Sum of electronic and thermal Enthalpies=	-384.828440
Sum of electronic and thermal Free Energies=	-384.874266

C	1.45746900	-0.38022500	-0.15259800
C	-1.43826800	0.36440100	0.28796400
C	-0.45931700	1.17177200	-0.42870200
C	0.91513200	1.16578500	0.09296400
H	0.36962500	-1.39804600	1.29695000
H	1.57068300	-0.47866000	-1.23913200
H	-1.38732700	0.37087700	1.37665900
N	0.40436800	-1.26054300	0.28514600
H	0.89454600	1.26196900	1.18574700
N	-0.83981000	-0.96594800	-0.19369000
H	-2.46854700	0.43084800	-0.06095100
H	-0.91470000	-1.11801000	-1.20091700
C	1.88508000	2.18229000	-0.52032200
H	1.48185900	3.19684500	-0.45641500
H	2.82890400	2.17746600	0.02843300
H	2.10729800	1.97046800	-1.57044400
C	2.77330800	-0.66581600	0.55158000
H	3.56703200	-0.01755100	0.17648700
H	2.69295200	-0.52278100	1.63450200
H	3.07376200	-1.69960000	0.35930700
C	-0.79129700	1.74834600	-1.75639200
H	-0.85598500	2.84198900	-1.63471700
H	-0.01340700	1.57684000	-2.50753500
H	-1.75903300	1.41056200	-2.13413000

TS-CE

Zero-point correction=	0.217880 (Hartree/Particle)
Thermal correction to Energy=	0.227586
Thermal correction to Enthalpy=	0.228530
Thermal correction to Gibbs Free Energy=	0.184187
Sum of electronic and zero-point Energies=	-384.830903
Sum of electronic and thermal Energies=	-384.821196
Sum of electronic and thermal Enthalpies=	-384.820252
Sum of electronic and thermal Free Energies=	-384.864595

C	1.06168800	-1.59996800	-0.23356800
C	1.65303000	1.47930600	0.39252200
C	1.65542500	0.78297200	-0.80022500
C	2.21836700	-0.59562100	-0.82514000
H	1.26320200	-1.26841600	1.84942800
H	0.19859400	-1.52967000	-0.90622500
H	2.32804400	1.21999000	1.20145500
N	0.69187000	-1.01687200	1.03499000
H	3.04483500	-0.67261400	-0.11053400
N	0.17331800	0.16052600	1.11612500
H	1.19105700	2.46036800	0.46165100
C	2.67904400	-1.09801600	-2.20133500
H	3.38603900	-0.38823500	-2.63952200
H	3.19889400	-2.05325000	-2.10923800
H	1.84910400	-1.22679500	-2.90193700
H	-0.46603800	0.30202200	0.32202900
C	1.52365500	-3.04229100	-0.08441300
H	1.74720900	-3.47357100	-1.06094800
H	2.42256000	-3.11800000	0.53663200
H	0.73264300	-3.64668100	0.36781800
C	0.94120200	1.31524100	-2.00573700
H	1.67052500	1.53364600	-2.79712700
H	0.24008300	0.58860200	-2.43473000
H	0.40305700	2.24021900	-1.78736000

R'=Boc

R1=CH3 R2=H R3=CH3 R4=CH3

TS-BF

Zero-point correction=	0.256973 (Hartree/Particle)
Thermal correction to Energy=	0.272272
Thermal correction to Enthalpy=	0.273216
Thermal correction to Gibbs Free Energy=	0.214937
Sum of electronic and zero-point Energies=	-612.652706
Sum of electronic and thermal Energies=	-612.637407
Sum of electronic and thermal Enthalpies=	-612.636463
Sum of electronic and thermal Free Energies=	-612.694742

C	1.91996900	-1.53850800	-0.61988600
C	1.20226300	1.75345700	0.25982100
C	2.40172100	1.17960300	-0.04397200
C	2.77088500	-0.01490500	0.66964000
H	2.30937700	-1.12868600	-1.55998100
H	0.59213500	1.38770800	1.07986200
N	0.65463300	-1.28591100	-0.27909700
H	2.15357600	-0.25473700	1.53290900
N	0.03026100	-0.34899400	-0.92891400
C	-1.34564000	-0.02353600	-0.67196700
O	-1.93562400	0.68886100	-1.44582200
O	-1.77528000	-0.57987900	0.44224700
C	-3.17257000	-0.33673800	0.75704700
H	-3.34307400	0.73093900	0.90663900
H	-3.80708200	-0.70868600	-0.04926400
H	-3.35359500	-0.88944100	1.67700400
H	0.86081000	2.65632600	-0.23988300
H	0.36722000	0.01442000	-1.83081900
C	4.19736700	-0.46053800	0.76408300
H	4.71987600	0.29358700	1.37262400
H	4.30237600	-1.41029800	1.28843600
H	4.71274600	-0.50722700	-0.19808100
C	2.48331900	-2.85471500	-0.15965900
H	2.09023600	-3.64746100	-0.80732000
H	3.57007100	-2.88027200	-0.24856600
H	2.18783400	-3.08286200	0.86718400
C	3.30029200	1.73665900	-1.11867400
H	4.25930800	2.06050000	-0.69923900
H	3.52794900	0.99233100	-1.89118800
H	2.84243900	2.59904800	-1.60754100

A

Zero-point correction=	0.260134 (Hartree/Particle)
Thermal correction to Energy=	0.275816
Thermal correction to Enthalpy=	0.276760
Thermal correction to Gibbs Free Energy=	0.217270
Sum of electronic and zero-point Energies=	-612.701385
Sum of electronic and thermal Energies=	-612.685703
Sum of electronic and thermal Enthalpies=	-612.684759
Sum of electronic and thermal Free Energies=	-612.744249

C	-2.07541900	1.83194300	-0.11209000
C	-0.93373700	-0.69311200	-1.01415400
C	-1.96293900	-1.51061700	-0.24740700
C	-2.04541600	-1.46675100	1.08962700
H	-0.15491100	2.15799900	0.49607700
H	-2.74186500	1.08426400	-0.53260300
H	-0.15770200	-1.34074300	-1.42871100
N	-0.83984700	1.51148100	0.06672300
H	-1.35075000	-0.81447700	1.62033400
N	-0.22632500	0.32856800	-0.23917300
C	1.12755700	0.32269600	0.14279300
O	1.62837300	1.27952400	0.70366100
O	1.70832300	-0.81609000	-0.18837100
C	3.11539200	-0.92597300	0.15423500
H	3.24156500	-0.86162400	1.23620100
H	3.41716700	-1.90589900	-0.21116600
H	3.68375200	-0.13624100	-0.33970200
H	-1.39934800	-0.18739900	-1.87346600
C	-2.97569200	-2.23136200	1.98224300
H	-2.40658100	-2.87013100	2.66918400
H	-3.55811200	-1.54585000	2.61018400
H	-3.67909500	-2.86658200	1.44083800
C	-2.59026200	3.17256900	0.25034700
H	-3.00805800	3.65336000	-0.64258400
H	-3.41548000	3.06451400	0.96428500
H	-1.82207300	3.81977600	0.68033600
C	-2.80060700	-2.36594100	-1.16317400
H	-2.16594100	-2.99371400	-1.80195500
H	-3.47241700	-3.02872200	-0.61735200
H	-3.41290600	-1.75272700	-1.83751800

B

Zero-point correction=	0.259256 (Hartree/Particle)
Thermal correction to Energy=	0.275227
Thermal correction to Enthalpy=	0.276171
Thermal correction to Gibbs Free Energy=	0.214764
Sum of electronic and zero-point Energies=	-612.680942
Sum of electronic and thermal Energies=	-612.664972
Sum of electronic and thermal Enthalpies=	-612.664028
Sum of electronic and thermal Free Energies=	-612.725434

C	1.05609900	2.16225400	-0.67458300
C	0.92766100	-1.06643100	0.34222200
C	2.38361300	-0.87741400	0.59038300
C	3.36543800	-0.97474900	-0.32694200
H	1.27499800	2.53289200	0.33547900
H	0.67671400	-1.51410800	-0.61693800
N	0.49535100	1.03094300	-0.88166600
H	2.65650600	-0.69513800	1.62894100
N	0.18002600	0.29490100	0.34223200
H	0.44059600	0.81940100	1.19888500
C	-1.32401600	0.14702100	0.42838500
O	-1.92002000	0.67968700	1.31941900
O	-1.73535700	-0.59809500	-0.56170500
C	-3.17764100	-0.81402300	-0.64221500
H	-3.68299200	0.14547700	-0.76069700
H	-3.31619100	-1.43986400	-1.52098200
H	-3.52240600	-1.32148900	0.25995400
H	0.44941300	-1.63589600	1.14543600
C	4.80482600	-0.83649700	0.09268100
H	5.36625200	-1.74648700	-0.15306800
H	5.29145500	-0.01799500	-0.45191800
H	4.91117000	-0.64924900	1.16381300
C	1.42858300	3.02134500	-1.82916400
H	2.50528100	3.22596300	-1.80479300
H	1.16316200	2.55032000	-2.77675700
H	0.92092200	3.98930800	-1.74293700
C	3.15845800	-1.24208500	-1.79317500
H	2.11290100	-1.25578500	-2.10342100
H	3.67072100	-0.47794200	-2.38982900
H	3.61173600	-2.20205800	-2.06965700

TS-AD

Zero-point correction=	0.258934 (Hartree/Particle)
Thermal correction to Energy=	0.273463
Thermal correction to Enthalpy=	0.274407
Thermal correction to Gibbs Free Energy=	0.218094
Sum of electronic and zero-point Energies=	-612.657791
Sum of electronic and thermal Energies=	-612.643463
Sum of electronic and thermal Enthalpies=	-612.642518
Sum of electronic and thermal Free Energies=	-612.698832

C	2.25137300	-1.09244500	-0.40973100
C	0.68583900	1.40593400	0.38442300
C	2.00409400	1.37890500	-0.10685200
C	2.88080200	0.32747300	0.37846200
H	0.58776100	-1.70404200	0.74606100
H	2.36975800	-0.86745000	-1.47264700
H	0.49787800	1.08443500	1.40656500
N	0.88998400	-1.18064900	-0.08841700
H	2.70543000	0.10157600	1.43342200
N	0.10125100	-0.21312000	-0.51504400
C	-1.25076700	-0.40384900	-0.01121400
O	-1.58073800	-1.35133300	0.66473200
O	-2.01327100	0.57618200	-0.45909400
C	-3.41150100	0.50570000	-0.07864600
H	-3.50797200	0.52314000	1.00874600
H	-3.87148800	1.38765900	-0.52058100
H	-3.86042600	-0.40537200	-0.47839000
H	-0.00357200	2.14905200	-0.00248800
C	4.37086500	0.44147100	0.06187300
H	4.93801900	-0.34910600	0.55534700
H	4.57884600	0.39727100	-1.01115800
H	4.75471800	1.39498100	0.43794800
C	3.02776700	-2.32771600	0.02175400
H	4.06780500	-2.26104100	-0.29672100
H	3.00430600	-2.46883200	1.10688700
H	2.59554400	-3.21224700	-0.45527600
C	2.36339400	2.16682100	-1.31836300
H	3.28113500	2.74334100	-1.14987500
H	2.57896600	1.49624700	-2.16408200
H	1.56798500	2.85108800	-1.61626700

TS-AC

Zero-point correction=	0.260193 (Hartree/Particle)
Thermal correction to Energy=	0.274446
Thermal correction to Enthalpy=	0.275390
Thermal correction to Gibbs Free Energy=	0.219736
Sum of electronic and zero-point Energies=	-612.674637
Sum of electronic and thermal Energies=	-612.660384
Sum of electronic and thermal Enthalpies=	-612.659440
Sum of electronic and thermal Free Energies=	-612.715094

C	1.30714700	-1.54215200	-0.30546000
C	1.17695000	1.29009800	0.47605200
C	1.79037300	0.85857100	-0.81112100
C	2.62760400	-0.28149200	-0.77458300
H	1.09993500	-1.19280300	1.71518400
H	0.67901600	-1.51676600	-1.19791800
H	1.86027800	1.26583200	1.32718700
N	0.64725400	-1.04089500	0.81180300
H	3.21256800	-0.36292500	0.14473600
N	0.13211100	0.22548900	0.69587100
C	-1.16669300	0.44257200	0.20684600
O	-1.53997200	1.53665400	-0.16702400
O	-1.89420000	-0.67155900	0.25545400
C	-3.27312100	-0.52144700	-0.15719600
H	-3.79371500	0.17244800	0.50570600
H	-3.32792000	-0.16007900	-1.18585200
H	-3.70286800	-1.51893100	-0.07757000
H	0.66388200	2.24885800	0.42115000
C	3.35368100	-0.75851600	-2.02157800
H	3.96704200	0.04699800	-2.43766800
H	4.02639900	-1.58378900	-1.78211800
H	2.67032600	-1.09452900	-2.80781100
C	2.00641600	-2.86284700	-0.08699200
H	2.53905300	-3.18104600	-0.98332100
H	2.70890600	-2.82517600	0.75094900
H	1.24691200	-3.62206000	0.12994300
C	1.29063900	1.47051000	-2.06576900
H	1.43864400	0.84867000	-2.94983200
H	0.24273300	1.77435400	-1.97421300
H	1.86064100	2.40160600	-2.22356900

C

Zero-point correction=	0.262293 (Hartree/Particle)
Thermal correction to Energy=	0.276386
Thermal correction to Enthalpy=	0.277331
Thermal correction to Gibbs Free Energy=	0.222220
Sum of electronic and zero-point Energies=	-612.676968
Sum of electronic and thermal Energies=	-612.662874
Sum of electronic and thermal Enthalpies=	-612.661930
Sum of electronic and thermal Free Energies=	-612.717041

C	1.76866200	-1.40298900	-0.20251000
C	1.06416500	1.51560000	0.72744100
C	1.31765800	0.96278800	-0.61761600
C	2.43152200	-0.09374700	-0.73276900
H	1.20671900	-0.86789100	1.74690600
H	1.19475300	-1.85115900	-1.02395600
H	1.78381600	1.35926000	1.52694300
N	0.78712500	-0.98526300	0.82118900
H	3.22893000	0.19262200	-0.03411900
N	0.27536500	0.27141200	0.41033000
C	-1.18343500	0.40524700	0.20791800
O	-1.70027000	1.49115700	0.21419600
O	-1.71512700	-0.77357300	0.00791300
C	-3.15733000	-0.78256300	-0.20189900
H	-3.41038600	-0.17144700	-1.06976800
H	-3.40604000	-1.82771500	-0.37444300
H	-3.66035500	-0.40444700	0.68955200
H	0.43147700	2.39323800	0.82467300
C	3.03738500	-0.25350700	-2.12915700
H	3.49203400	0.67560300	-2.48326800
H	3.83009800	-1.00600700	-2.09877400
H	2.29996200	-0.58160900	-2.86769600
C	2.72481900	-2.43660400	0.37130400
H	2.17298600	-3.30249900	0.74745900
H	3.41187700	-2.79166800	-0.40066200
H	3.32161100	-2.02055100	1.19103900
C	0.74352200	1.63232900	-1.83387800
H	0.44852300	0.90731400	-2.59640300
H	-0.10765300	2.26921100	-1.59043100
H	1.52325400	2.26993700	-2.26424200

TS-CE

Zero-point correction=	0.259482 (Hartree/Particle)
Thermal correction to Energy=	0.273874
Thermal correction to Enthalpy=	0.274818
Thermal correction to Gibbs Free Energy=	0.219171
Sum of electronic and zero-point Energies=	-612.648735
Sum of electronic and thermal Energies=	-612.634343
Sum of electronic and thermal Enthalpies=	-612.633399
Sum of electronic and thermal Free Energies=	-612.689046

C	1.02506000	-1.55464200	-0.30409200
C	1.89210000	1.68082800	0.14110500
C	1.68287200	0.83858500	-0.89182800
C	2.19665400	-0.57809500	-0.81832400
H	1.33799700	-1.35451100	1.78882700
H	0.14647700	-1.42546800	-0.93710800
H	2.49659000	1.40081400	1.00001800
N	0.70124200	-1.05183200	1.03135700
H	2.99246800	-0.63496000	-0.06621100
N	-0.02891900	-0.10042200	1.37596200
C	-1.11741400	0.38462900	0.52606300
O	-1.33197400	1.55855900	0.41405500
O	-1.84836000	-0.64049800	0.11181100
C	-3.11646200	-0.28964200	-0.51842600
H	-2.93701900	0.33923300	-1.39144600
H	-3.55934000	-1.24112600	-0.80576600
H	-3.74866100	0.23277500	0.20143400
H	1.51588200	2.69888600	0.12895700
C	2.74593700	-1.11692900	-2.15144700
H	3.48765200	-0.41331700	-2.53973300
H	3.24943500	-2.07605700	-2.01726000
H	1.96569900	-1.23706400	-2.90825600
C	0.90641700	1.26340000	-2.11194900
H	0.42676100	2.23175600	-1.95847600
H	1.56823300	1.35225300	-2.98190400
H	0.13061000	0.53973600	-2.39283500
C	1.42597100	-3.02498400	-0.20310400
H	1.59875800	-3.42599600	-1.20255500
H	2.34153500	-3.15944900	0.38267600
H	0.62422600	-3.61231400	0.25231400

R1=CH3 R2=CH2SiH3 R3=H R4=CH3

Reactant

Zero-point correction=	0.274527 (Hartree/Particle)
Thermal correction to Energy=	0.292752
Thermal correction to Enthalpy=	0.293696
Thermal correction to Gibbs Free Energy=	0.227172
Sum of electronic and zero-point Energies=	-903.373943
Sum of electronic and thermal Energies=	-903.355717
Sum of electronic and thermal Enthalpies=	-903.354773
Sum of electronic and thermal Free Energies=	-903.421298

C	-2.13530000	1.77856000	0.08482900
C	-0.95526700	-0.78541700	-0.94467200
C	-2.06883200	-1.41679100	-0.12601500
C	-2.10660700	-1.49718400	1.20743200
H	-0.16723000	2.17016200	0.42654300
H	-2.83516200	1.00008300	-0.19996200
H	-0.15634600	-1.52043700	-1.06960100
N	-0.88001600	1.48564700	0.11700600
H	-1.30065600	-1.04830200	1.79123900
N	-0.26186600	0.29973000	-0.18538700
H	-2.86377000	-1.87275300	-0.71440300
C	1.12247200	0.38155400	0.06013700
O	1.62268300	1.38630600	0.53333100
O	1.74104300	-0.73840400	-0.27118400
C	3.17143900	-0.76409900	-0.02127000
H	3.36371300	-0.66621000	1.04851800
H	3.50184500	-1.73570300	-0.38419500
H	3.66295000	0.04216900	-0.56781700
C	-3.18535300	-2.17824100	1.99263600
H	-2.76499200	-2.98912600	2.60005700
H	-3.66375900	-1.48335100	2.69373000
H	-3.95883700	-2.60233800	1.34634200
C	-2.62343200	3.13106500	0.44204000
H	-3.15171400	3.56398400	-0.41632600
H	-3.35731300	3.05035500	1.25267900
H	-1.82040500	3.80675900	0.74658800
C	-1.38018800	-0.30879500	-2.34861000
H	-2.24043300	0.36973400	-2.31688400
H	-0.55199700	0.25724700	-2.79246300
Si	-1.79127400	-1.69851900	-3.59510600
H	-3.02175900	-2.42791200	-3.20034500
H	-1.99605000	-1.06709600	-4.92070900
H	-0.65507200	-2.65211200	-3.65494900

amine-H+

Zero-point correction=	0.272383 (Hartree/Particle)
Thermal correction to Energy=	0.289957
Thermal correction to Enthalpy=	0.290902
Thermal correction to Gibbs Free Energy=	0.226552
Sum of electronic and zero-point Energies=	-903.343524
Sum of electronic and thermal Energies=	-903.325950
Sum of electronic and thermal Enthalpies=	-903.325006
Sum of electronic and thermal Free Energies=	-903.389356

C	1.91318300	-1.55697100	-0.51831900
C	1.12826300	1.84588100	0.24245300
C	2.25646000	1.15514500	-0.10261900
C	2.68161700	-0.03352900	0.57832700
H	2.26396700	-1.21575500	-1.49993700
H	0.55272300	1.48425500	1.09658600
N	0.61940100	-1.35536200	-0.20527100
H	2.16358600	-0.24838800	1.51217600
N	-0.02690000	-0.47728900	-0.89786700
H	2.86224600	1.50737800	-0.93826600
C	-1.38862700	-0.11701100	-0.62618200
O	-1.94459400	0.66834400	-1.35572600
O	-1.85000500	-0.72902500	0.44461500
C	-3.23765000	-0.44974800	0.77042200
H	-3.37183300	0.61629400	0.96255000
H	-3.88482500	-0.76708300	-0.04918500
H	-3.43847500	-1.03247500	1.66746300
H	0.33191600	-0.09219300	-1.78234300
C	4.15693100	-0.35348100	0.59210200
H	4.64755000	0.43348100	1.17999000
H	4.38160600	-1.30030900	1.08245900
H	4.60334000	-0.33954600	-0.40632300
C	2.49308700	-2.85588000	-0.01168700
H	2.05153500	-3.68476800	-0.57563700
H	3.57119200	-2.89764500	-0.16873100
H	2.26837100	-3.01277800	1.04636700
C	0.67408400	3.10842500	-0.36935300
H	1.11267300	3.26902900	-1.36025500
H	-0.41929300	3.12089000	-0.46384900
Si	1.12082000	4.63976900	0.71578900
H	0.53054100	5.83687000	0.07250100
H	0.55910600	4.45325700	2.07543000
H	2.59575300	4.76325100	0.79310300

imine-H+

Zero-point correction=	0.272695 (Hartree/Particle)
Thermal correction to Energy=	0.290207
Thermal correction to Enthalpy=	0.291151
Thermal correction to Gibbs Free Energy=	0.227090
Sum of electronic and zero-point Energies=	-903.341492
Sum of electronic and thermal Energies=	-903.323980
Sum of electronic and thermal Enthalpies=	-903.323036
Sum of electronic and thermal Free Energies=	-903.387096

C	2.13621400	-1.24810000	-0.54365800
C	0.70438300	1.77370400	0.31248100
C	1.97215400	1.46568800	-0.14793900
C	2.80388500	0.50375200	0.46175300
H	0.53551200	-1.77194500	0.66811600
H	2.30366000	-0.85115800	-1.54113700
H	0.39603500	1.35147000	1.26989500
N	0.84057900	-1.23891400	-0.16870100
H	2.51292200	0.17381900	1.45958400
N	-0.03281200	-0.42442200	-0.68593600
H	2.31579400	1.93261100	-1.07135200
C	-1.27866000	-0.57266600	0.00428600
O	-1.46165500	-1.32220200	0.94627700
O	-2.17702300	0.21738700	-0.56567000
C	-3.51227900	0.14894000	-0.00919400
H	-3.50181500	0.44424400	1.04217900
H	-4.10426800	0.84624600	-0.59967400
H	-3.90589900	-0.86503200	-0.10373200
C	4.28482100	0.50083500	0.18751300
H	4.78439600	-0.38465800	0.58232500
H	4.51518000	0.60680300	-0.87658400
H	4.72309500	1.36438300	0.70468000
C	2.97758700	-2.40516800	-0.08173900
H	4.03284800	-2.21955400	-0.28104200
H	2.85187000	-2.61595200	0.98478800
H	2.69908700	-3.30445400	-0.64434900
C	-0.15151200	2.82467900	-0.26231100
H	0.05112700	2.97822300	-1.32739700
H	-1.21174000	2.58061700	-0.14027000
Si	0.11647500	4.51732600	0.62594600
H	-0.85096500	5.48225900	0.05348100
H	-0.11957900	4.34787600	2.07991700
H	1.50807600	4.97075200	0.39245300

R1=CH3 R2=H R3=CH2SiH3 R4=CH3

Reactant

Zero-point correction=	0.275096 (Hartree/Particle)
Thermal correction to Energy=	0.293059
Thermal correction to Enthalpy=	0.294004
Thermal correction to Gibbs Free Energy=	0.228375
Sum of electronic and zero-point Energies=	-903.379769
Sum of electronic and thermal Energies=	-903.361806
Sum of electronic and thermal Enthalpies=	-903.360862
Sum of electronic and thermal Free Energies=	-903.426491

C	-2.07812400	1.83293400	-0.11297100
C	-0.94763800	-0.69737900	-1.00886900
C	-1.96716100	-1.51061900	-0.22172700
C	-2.05154600	-1.42958600	1.11555000
H	-0.14816400	2.16675800	0.46100700
H	-2.75125200	1.07852500	-0.51080000
H	-0.17753500	-1.34304700	-1.43635700
N	-0.83959000	1.51503600	0.05042500
H	-1.36825000	-0.75540800	1.63215000
N	-0.23140000	0.32725800	-0.24831300
C	1.12665900	0.32138800	0.11864000
O	1.63696500	1.28328100	0.66183200
O	1.69852400	-0.82426600	-0.20408600
C	3.10757900	-0.93866800	0.12896700
H	3.24139900	-0.86894200	1.20970900
H	3.40213600	-1.92206900	-0.23292600
H	3.67612300	-0.15439900	-0.37330800
H	-1.42952300	-0.19327800	-1.85976100
C	-2.97457100	-2.19448100	2.01590300
H	-2.40210600	-2.84761700	2.68660300
H	-3.54268100	-1.51235400	2.66013400
H	-3.68801800	-2.82126800	1.47711500
C	-2.58689200	3.17834100	0.24015000
H	-3.01927200	3.64778700	-0.65185100
H	-3.40029800	3.07975300	0.96888800
H	-1.81192400	3.83092800	0.64941200
C	-2.78965900	-2.42326400	-1.10046000
H	-3.76890700	-2.62322400	-0.65447900
H	-2.99306000	-1.94715600	-2.06892700
Si	-1.96219800	-4.11125800	-1.44891400
H	-2.77533100	-4.87313700	-2.43035700
H	-0.60162600	-3.89755200	-2.00926100
H	-1.84281800	-4.88651700	-0.18942500

amine-H+

Zero-point correction=	0.272221 (Hartree/Particle)
Thermal correction to Energy=	0.289755
Thermal correction to Enthalpy=	0.290700
Thermal correction to Gibbs Free Energy=	0.226440
Sum of electronic and zero-point Energies=	-903.330586
Sum of electronic and thermal Energies=	-903.313052
Sum of electronic and thermal Enthalpies=	-903.312108
Sum of electronic and thermal Free Energies=	-903.376368

C	1.93946000	-1.49764100	-0.64324900
C	1.11672100	1.72457600	0.28410000
C	2.33918200	1.20858500	-0.04859100
C	2.75086700	0.01044100	0.64221000
H	2.31150200	-1.06770700	-1.58152900
H	0.54171600	1.32400600	1.11250600
N	0.66332000	-1.29114100	-0.29942300
H	2.14831000	-0.24511300	1.51150000
N	0.01787700	-0.35672000	-0.92778600
C	-1.36229400	-0.06021500	-0.65167100
O	-1.98051100	0.63255700	-1.42077700
O	-1.75820100	-0.61383800	0.47602200
C	-3.15294000	-0.39268100	0.81769000
H	-3.34161500	0.67438400	0.94883400
H	-3.79754100	-0.79432300	0.03396800
H	-3.30156000	-0.92925300	1.75289200
H	0.72563400	2.61821500	-0.19604000
H	0.34117600	0.02863700	-1.82602800
C	4.18805600	-0.40624400	0.74073200
H	4.69637900	0.34867900	1.35765600
H	4.30310300	-1.35961400	1.25655000
H	4.71064100	-0.44292300	-0.21785900
C	2.53005600	-2.81229800	-0.21006600
H	2.14281700	-3.60156800	-0.86516100
H	3.61592500	-2.81837100	-0.31035200
H	2.24969300	-3.06067300	0.81641700
C	3.18791500	1.83444600	-1.12506400
H	3.84378200	1.10049500	-1.60521100
H	2.55059600	2.24827400	-1.91518600
Si	4.28517100	3.28465000	-0.50980500
H	5.16500900	2.82419500	0.59220000
H	5.10794900	3.76157700	-1.64677100
H	3.40633100	4.37188800	-0.01580900

imine-H+

Zero-point correction=	0.274665 (Hartree/Particle)
Thermal correction to Energy=	0.291180
Thermal correction to Enthalpy=	0.292124
Thermal correction to Gibbs Free Energy=	0.230683
Sum of electronic and zero-point Energies=	-903.340141
Sum of electronic and thermal Energies=	-903.323626
Sum of electronic and thermal Enthalpies=	-903.322682
Sum of electronic and thermal Free Energies=	-903.384123

C	2.27461900	-1.08506100	-0.45688600
C	0.73288600	1.44309100	0.43169500
C	2.01952700	1.37304400	-0.12086500
C	2.88154000	0.27032600	0.33609500
H	0.60291200	-1.71979300	0.69714700
H	2.37588600	-0.85928500	-1.52241700
H	0.56129800	1.07790900	1.44115800
N	0.89692800	-1.18918900	-0.13649400
H	2.70603900	0.05779700	1.39490500
N	0.10885700	-0.22439000	-0.54241700
C	-1.22326300	-0.39229000	0.03044600
O	-1.51626800	-1.28946600	0.78780200
O	-2.01067500	0.54844300	-0.45465400
C	-3.38952500	0.50525000	-0.00530600
H	-3.43542400	0.62348500	1.07919200
H	-3.87811000	1.33943300	-0.50557100
H	-3.84670100	-0.44165700	-0.29814400
H	0.03458900	2.19345300	0.07449600
C	4.38316400	0.38409900	0.05518500
H	4.92986500	-0.41326500	0.56110700
H	4.62195500	0.33455600	-1.01125500
H	4.76507300	1.33231000	0.44250300
C	3.02929300	-2.34974200	-0.06350100
H	4.06727700	-2.29848600	-0.39199200
H	3.01655200	-2.51168400	1.01931100
H	2.57394100	-3.21623800	-0.55115700
C	2.35702600	2.18984500	-1.29853600
H	3.11903000	1.72989300	-1.93471800
H	1.46413400	2.39319900	-1.90256800
Si	3.02261800	3.94984000	-0.82018300
H	4.22082200	3.81639600	0.03858000
H	3.35675900	4.63362100	-2.08943200
H	1.94867900	4.66360600	-0.09272700

R1=CO2CH3 R2=H R3=H R4=CH3

Reactant

Zero-point correction=	0.246717 (Hartree/Particle)
Thermal correction to Energy=	0.264011
Thermal correction to Enthalpy=	0.264955
Thermal correction to Gibbs Free Energy=	0.199719
Sum of electronic and zero-point Energies=	-761.939053
Sum of electronic and thermal Energies=	-761.921759
Sum of electronic and thermal Enthalpies=	-761.920815
Sum of electronic and thermal Free Energies=	-761.986051

C	2.32398300	-0.59514600	-0.31050000
C	0.21303000	1.25935200	-1.03304400
C	0.85688500	2.31648500	-0.16797600
C	0.96647500	2.28559800	1.16183600
H	0.77031000	-1.72789100	0.32396500
H	2.66414700	0.34588700	-0.72756100
H	-0.77702600	1.56674000	-1.37594900
N	1.07239900	-0.82930800	-0.10106200
H	0.57646500	1.42739300	1.71272300
N	0.01802600	-0.03393500	-0.36294800
H	1.23278900	3.16926300	-0.73204700
C	-1.21268800	-0.62447300	0.03211900
O	-1.23520000	-1.71989900	0.55260900
O	-2.22013300	0.17304800	-0.24917800
C	-3.53949700	-0.32578100	0.10936700
H	-3.58566900	-0.51034900	1.18356700
H	-4.22570100	0.46827700	-0.17794500
H	-3.75056100	-1.24222300	-0.44397700
H	0.81018400	1.06957500	-1.93618100
C	3.34157500	-1.63460200	0.03289600
O	4.51646100	-1.45135800	-0.18265500
O	2.77518600	-2.71328000	0.57111500
C	3.66990500	-3.79983100	0.92988200
H	3.02713100	-4.57786700	1.33721200
H	4.19538300	-4.15457600	0.04150400
H	4.38702900	-3.45738900	1.67815400
C	1.58881400	3.36573700	1.99210000
H	0.86458900	3.76761500	2.71118000
H	2.42705700	2.97405000	2.58097000
H	1.95726100	4.19283000	1.37927600

amine-H+

Zero-point correction=	0.243423 (Hartree/Particle)
Thermal correction to Energy=	0.260456
Thermal correction to Enthalpy=	0.261400
Thermal correction to Gibbs Free Energy=	0.197655
Sum of electronic and zero-point Energies=	-761.897210
Sum of electronic and thermal Energies=	-761.880177
Sum of electronic and thermal Enthalpies=	-761.879233
Sum of electronic and thermal Free Energies=	-761.942978

C	-1.79732700	-0.90551400	0.53422800
C	-0.52975200	2.20588600	-0.44405000
C	-1.77640300	1.84086100	-0.05273700
C	-2.48309100	0.76326200	-0.67676900
H	-2.10676300	-0.49939900	1.50143000
H	-0.03376700	1.72762200	-1.28488800
N	-0.51910100	-0.90914900	0.16290400
N	-2.05259000	0.36117100	-1.59310900
N	0.29708000	-0.14915000	0.81532000
H	-2.25980700	2.35988000	0.77403600
C	1.70980200	-0.10406800	0.52921800
O	2.43716300	0.48340000	1.28912800
O	1.99545500	-0.73855200	-0.58627700
C	3.40675300	-0.77779800	-0.93329900
H	3.79168800	0.23665700	-1.05119500
H	3.96461400	-1.30475800	-0.15726400
H	3.44982100	-1.32119900	-1.87520900
H	-0.01333200	3.03960800	0.02409500
H	0.04756900	0.29681500	1.71078700
C	-2.66350800	-2.02898200	0.03628300
O	-3.64573800	-2.37752700	0.65628900
O	-2.23510200	-2.54306400	-1.111480500
C	-2.98558600	-3.67633800	-1.61554000
H	-4.01699300	-3.38689100	-1.82795200
H	-2.47595700	-3.97739700	-2.52940100
H	-2.97487400	-4.48704700	-0.88437600
C	-3.96756300	0.66394400	-0.53746700
H	-4.38345000	1.44805900	-1.18941700
H	-4.37505400	-0.28469400	-0.88663500
H	-4.31514600	0.86609900	0.47860800

imine-H+

Zero-point correction=	0.244934 (Hartree/Particle)
Thermal correction to Energy=	0.261362
Thermal correction to Enthalpy=	0.262306
Thermal correction to Gibbs Free Energy=	0.200715
Sum of electronic and zero-point Energies=	-761.898913
Sum of electronic and thermal Energies=	-761.882484
Sum of electronic and thermal Enthalpies=	-761.881540
Sum of electronic and thermal Free Energies=	-761.943131

C	2.06053600	-0.48264900	-0.54251300
C	0.08489000	1.82907300	0.38170600
C	1.39155000	2.00269100	-0.03975100
C	2.46045400	1.24262700	0.48865000
H	0.61970300	-1.43816700	0.57960500
H	2.22300600	-0.10599800	-1.54731000
H	-0.12635100	1.39683600	1.35696600
N	0.78132400	-0.77362700	-0.20349200
H	2.30490800	0.81045000	1.47846200
N	-0.21070400	-0.05485000	-0.63748300
H	1.57413800	2.59576400	-0.93561000
C	-1.45412500	-0.54219100	-0.05701700
O	-1.51791700	-1.50220600	0.67775800
O	-2.43780300	0.21804500	-0.49222100
C	-3.76664000	-0.15056100	-0.03882200
H	-3.81052300	-0.13189400	1.05191000
H	-4.43094500	0.59799200	-0.46648400
H	-4.01993200	-1.14687700	-0.40596400
H	-0.71710600	2.39355200	-0.08166900
C	3.02702500	-1.49132600	0.02554500
O	2.75314300	-2.17164700	0.99260200
O	4.15897700	-1.50695500	-0.66510200
C	5.17134500	-2.44267900	-0.20813900
H	4.80532100	-3.46563300	-0.31409000
H	6.03001100	-2.27236200	-0.85498200
H	5.42405500	-2.24420800	0.83510900
C	3.88609900	1.59847500	0.15246800
H	4.58732400	0.79974700	0.39585300
H	4.00779200	1.87113000	-0.89927500
H	4.16392600	2.46968700	0.75878600

R1=CO2CH3 R2=CH3 R3=H R4=CH3

Reactant

Zero-point correction= 0.274820 (Hartree/Particle)
Thermal correction to Energy= 0.293564
Thermal correction to Enthalpy= 0.294508
Thermal correction to Gibbs Free Energy= 0.226864
Sum of electronic and zero-point Energies= -801.226570
Sum of electronic and thermal Energies= -801.207826
Sum of electronic and thermal Enthalpies= -801.206882
Sum of electronic and thermal Free Energies= -801.274526

C	2.36298100	-0.52503800	-0.15343000
C	0.15945600	1.33935100	-0.96238900
C	1.01233800	2.29257700	-0.14467800
C	1.10226800	2.31368700	1.18829600
H	0.79447700	-1.69773800	0.33063900
H	2.72797200	0.42531300	-0.51888200
N	1.10206900	-0.77583400	-0.03925600
H	0.55603500	1.56943100	1.77195900
N	0.03401000	-0.00022700	-0.31386000
H	1.54396300	3.03696800	-0.73641200
C	-1.18031200	-0.70096200	-0.06448300
O	-1.16383800	-1.83222500	0.37595600
O	-2.22467200	0.03967500	-0.36692900
C	-3.52461100	-0.57162900	-0.13233300
H	-3.64254100	-0.79214700	0.92980800
H	-4.24615200	0.17601200	-0.45565500
H	-3.61764100	-1.48396800	-0.72307700
C	3.35931000	-1.57018300	0.23502600
O	4.54464500	-1.38719500	0.08524800
O	2.76529800	-2.65440100	0.73191000
C	3.63813200	-3.75146100	1.11021900
H	2.97721400	-4.52062900	1.50529600
H	4.17624100	-4.11476600	0.23275200
H	4.34495900	-3.41745200	1.87173700
C	1.90254200	3.30518400	1.97479400
H	1.25482900	3.86040600	2.66414700
H	2.65553000	2.80257800	2.59421100
H	2.41222700	4.02503200	1.32867200
C	0.60607500	1.19956700	-2.42448200
H	1.63059300	0.83452800	-2.53652600
H	-0.06386900	0.53064900	-2.97048400
H	0.55811900	2.18442600	-2.89738800
H	-0.87169300	1.70002200	-0.96377000

imine-H+

Zero-point correction= 0.272084 (Hartree/Particle)
Thermal correction to Energy= 0.290423
Thermal correction to Enthalpy= 0.291367
Thermal correction to Gibbs Free Energy= 0.224915
Sum of electronic and zero-point Energies= -801.200086
Sum of electronic and thermal Energies= -801.181748
Sum of electronic and thermal Enthalpies= -801.180804
Sum of electronic and thermal Free Energies= -801.247256

C	2.01916200	-0.58713200	-0.54052200
C	0.14133100	2.18447400	0.25698500
C	1.41752100	2.09816900	-0.25085100
C	2.44313100	1.34955300	0.36840200
H	0.62526800	-1.36601500	0.74196200
H	2.15448700	-0.25265300	-1.56282900
H	-0.05531400	1.74647700	1.23682700
N	0.75747100	-0.79234000	-0.11883900
H	2.25165900	0.98987700	1.37991100
N	-0.26417800	-0.19018800	-0.62368200
H	1.63767100	2.58290900	-1.20182700
C	-1.44766900	-0.56165700	0.11321500
O	-1.45118900	-1.29537300	1.08004100
O	-2.48830200	0.02323800	-0.45546900
C	-3.77578900	-0.26162400	0.14854800
H	-3.79613600	0.09881400	1.17912800
H	-4.50154100	0.27256900	-0.46186700
H	-3.96824500	-1.33595800	0.12702100
C	3.00214600	-1.51759200	0.09720600
O	2.75759400	-2.12369900	1.12197500
O	4.13416600	-1.56311300	-0.59837500
C	5.16686300	-2.43975100	-0.07902000
H	4.83132000	-3.47759300	-0.12617400
H	6.02680800	-2.28491300	-0.72825800
H	5.40626600	-2.17548400	0.95278700
C	3.88153700	1.58700900	0.01586800
H	4.54087800	0.78437800	0.34659300
H	4.02783900	1.76081900	-1.05335400
H	4.19538400	2.49788300	0.54514200
C	-0.93651800	3.01417200	-0.33796900
H	-0.66648000	3.40620700	-1.32055400
H	-1.86533900	2.44012600	-0.42266900
H	-1.15426800	3.85717700	0.33254100

amine-H+

Zero-point correction=	0.271459 (Hartree/Particle)
Thermal correction to Energy=	0.290082
Thermal correction to Enthalpy=	0.291026
Thermal correction to Gibbs Free Energy=	0.223842
Sum of electronic and zero-point Energies=	-801.199566
Sum of electronic and thermal Energies=	-801.180944
Sum of electronic and thermal Enthalpies=	-801.180000
Sum of electronic and thermal Free Energies=	-801.247183

C	-1.81147000	-0.93835400	0.53940500
C	-0.53212400	2.22883200	-0.42478600
C	-1.73915100	1.78996900	0.02951300
C	-2.43418800	0.68450300	-0.56549100
H	-2.10759500	-0.58375800	1.53125400
H	-0.07964200	1.70835000	-1.27102900
N	-0.51945200	-0.96664000	0.18840700
H	-2.03800300	0.32273000	-1.51337700
N	0.29109800	-0.23343700	0.86840600
H	-2.21542100	2.29908100	0.86761200
C	1.69161100	-0.11863100	0.55604200
O	2.39130800	0.55489800	1.27199800
O	2.00280400	-0.78781000	-0.53147300
C	3.40183900	-0.71953700	-0.92135700
H	3.68707500	0.31746500	-1.10700800
H	4.02780900	-1.14824300	-0.13700400
H	3.46832800	-1.30869200	-1.83394300
H	0.02676300	0.21883700	1.75655900
C	-2.66410100	-2.07130400	0.02748600
O	-3.58268500	-2.50957800	0.68484600
O	-2.29806300	-2.48080300	-1.18582200
C	-3.04232400	-3.60174500	-1.72230100
H	-4.10242800	-3.35254500	-1.80240400
H	-2.61577800	-3.78538900	-2.70712700
H	-2.91810400	-4.47703700	-1.08161200
C	-3.92981300	0.61609800	-0.42057700
H	-4.33838300	1.43044700	-1.03521000
H	-4.35827500	-0.31271200	-0.79705500
H	-4.26282900	0.78164300	0.60721300
C	0.19668300	3.41643600	0.09157400
H	-0.32355100	3.90436800	0.91879600
H	1.20462900	3.13037900	0.42160900
H	0.34259200	4.14468900	-0.71689000

R1=CO2CH3 R2=H R3=CH3 R4=CH3

Reactant

Zero-point correction=	0.274918 (Hartree/Particle)
Thermal correction to Energy=	0.293683
Thermal correction to Enthalpy=	0.294627
Thermal correction to Gibbs Free Energy=	0.226589
Sum of electronic and zero-point Energies=	-801.230410
Sum of electronic and thermal Energies=	-801.211645
Sum of electronic and thermal Enthalpies=	-801.210701
Sum of electronic and thermal Free Energies=	-801.278739

C	2.37729900	-0.60105800	-0.28318300
C	0.27875500	1.26070700	-1.05193600
C	0.84020100	2.38418100	-0.19167200
C	0.95001600	2.27318300	1.13929200
H	0.80478600	-1.72570200	0.31775200
H	2.73170700	0.34092900	-0.68552200
H	-0.69572200	1.53270000	-1.46325000
N	1.12035800	-0.82697700	-0.09734300
H	0.62466800	1.34153600	1.60425300
N	0.07631700	-0.02232800	-0.36996200
C	-1.16334200	-0.59555200	0.02510200
O	-1.20193400	-1.68983400	0.54683400
O	-2.15728100	0.21850900	-0.25584700
C	-3.48429400	-0.24914500	0.11535800
H	-3.52260200	-0.43791200	1.18912800
H	-4.15339800	0.56385000	-0.15934400
H	-3.72588600	-1.15671200	-0.44009400
H	0.93226700	1.06534500	-1.91482100
C	3.38005600	-1.65383200	0.06404500
O	4.55895800	-1.48377200	-0.13987300
O	2.79539600	-2.72784700	0.59178500
C	3.67007900	-3.83165400	0.94657900
H	3.01239900	-4.60054200	1.34759500
H	4.19134900	-4.19059900	0.05737900
H	4.39090300	-3.50623600	1.69876400
C	1.46070500	3.29517300	2.10962700
H	0.68026700	3.55730400	2.83457700
H	2.29784400	2.88783500	2.68956700
H	1.80086800	4.21707200	1.63500500
C	1.19899000	3.59231900	-1.01760200
H	1.52908400	4.43159200	-0.40543000
H	2.00064500	3.36612000	-1.73272200
H	0.33855700	3.93268600	-1.60796000

imine-H+

Zero-point correction=	0.273695 (Hartree/Particle)
Thermal correction to Energy=	0.291241
Thermal correction to Enthalpy=	0.292185
Thermal correction to Gibbs Free Energy=	0.228103
Sum of electronic and zero-point Energies=	-801.196781
Sum of electronic and thermal Energies=	-801.179235
Sum of electronic and thermal Enthalpies=	-801.178291
Sum of electronic and thermal Free Energies=	-801.242374

C	2.12324700	-0.35983700	-0.42149700
C	0.04477500	1.68203600	0.37337400
C	1.35370900	1.96828600	-0.06143000
C	2.42388300	1.12023800	0.43837200
H	0.67602000	-1.39776000	0.68083100
H	2.26320600	-0.11816300	-1.47591500
H	-0.09919400	1.31279700	1.38665500
N	0.82399500	-0.77939000	-0.13271400
H	2.26052700	0.80978200	1.47350400
N	-0.16027800	-0.00671100	-0.54155900
C	-1.43880900	-0.52321500	-0.06967400
O	-1.55003500	-1.56320100	0.53571000
O	-2.39503000	0.29849100	-0.45952500
C	-3.74364100	-0.08712500	-0.08588200
H	-3.83249800	-0.13227100	1.00144300
H	-4.38463200	0.69231900	-0.49376200
H	-3.98816700	-1.05695700	-0.52244600
H	-0.77939500	2.26075900	-0.02998700
C	3.10835500	-1.40015800	0.10373400
O	2.91213000	-2.00366000	1.13611600
O	4.15228000	-1.52306800	-0.70363700
C	5.16550300	-2.47928100	-0.29317900
H	4.72876500	-3.47675300	-0.21810800
H	5.92230100	-2.44741300	-1.07492400
H	5.58950400	-2.18574600	0.66910000
C	3.86697200	1.55089100	0.19146700
H	4.56829600	0.84750000	0.64372900
H	4.10814000	1.63562900	-0.87102700
H	4.03923900	2.52539700	0.65847900
C	1.57926200	2.86290600	-1.22976800
H	2.31573900	3.63880000	-0.98463100
H	2.00515600	2.30160100	-2.07497400
H	0.66010400	3.34599000	-1.56344900

amine-H+

Zero-point correction=	0.271424 (Hartree/Particle)
Thermal correction to Energy=	0.289998
Thermal correction to Enthalpy=	0.290942
Thermal correction to Gibbs Free Energy=	0.223433
Sum of electronic and zero-point Energies=	-801.190208
Sum of electronic and thermal Energies=	-801.171634
Sum of electronic and thermal Enthalpies=	-801.170690
Sum of electronic and thermal Free Energies=	-801.238200

C	-1.78088000	-0.89895300	0.55465200
C	-0.53743000	2.18256800	-0.40516000
C	-1.79778200	1.86604900	0.00529200
C	-2.45699200	0.76014300	-0.64785900
H	-2.08161500	-0.50152200	1.52869200
H	-0.06279800	1.66471800	-1.23351900
N	-0.50247800	-0.91431100	0.18244600
H	-1.97718800	0.38642600	-1.55014300
N	0.32167400	-0.16102400	0.83254300
C	1.73154100	-0.12094700	0.53062300
O	2.47098800	0.45766200	1.28549900
O	2.00005300	-0.74927100	-0.59272800
C	3.40616000	-0.79323400	-0.95939800
H	3.79362400	0.22009300	-1.07895000
H	3.97292700	-1.32589600	-0.19386900
H	3.43340200	-1.33263200	-1.90424600
H	0.00697400	3.01889600	0.02573600
H	0.08611100	0.27582000	1.73601100
C	-2.65271900	-2.02154500	0.06244400
O	-3.61398800	-2.38901300	0.70318300
O	-2.25311200	-2.51067500	-1.11003600
C	-3.01056200	-3.63851200	-1.61237100
H	-4.05599200	-3.36095800	-1.76255600
H	-2.54302000	-3.89967600	-2.56033200
H	-2.94982400	-4.47391100	-0.91192600
C	-3.94348000	0.60381700	-0.59135400
H	-4.36283900	1.45326500	-1.15296700
H	-4.28987200	-0.30328800	-1.08574900
H	-4.35440700	0.65104800	0.41934000
C	-2.49790900	2.62901200	1.10113700
H	-3.38418300	3.14371600	0.71376700
H	-2.84094300	1.97066500	1.90795900
H	-1.83864900	3.38159400	1.53823200

1,5-hexadiene

Reactant

Zero-point correction=	0.142062 (Hartree/Particle)
Thermal correction to Energy=	0.149428
Thermal correction to Enthalpy=	0.150372
Thermal correction to Gibbs Free Energy=	0.110427
Sum of electronic and zero-point Energies=	-234.488437
Sum of electronic and thermal Energies=	-234.481071
Sum of electronic and thermal Enthalpies=	-234.480127
Sum of electronic and thermal Free Energies=	-234.520072

C	-2.99854100	0.19871400	0.15342900
H	-3.92095600	-0.33652000	0.36213700
H	-3.03743000	1.28329700	0.23286200
C	-1.87913400	-0.43938600	-0.18737900
H	-1.89088800	-1.52917700	-0.25163300
C	-0.56093100	0.21937500	-0.48574500
H	-0.24609200	-0.03111000	-1.50856200
H	-0.67464400	1.30989100	-0.44974800
C	0.56093100	-0.21937500	0.48574500
H	0.24609200	0.03111000	1.50856300
H	0.67464400	-1.30989000	0.44974800
C	2.99854100	-0.19871300	-0.15342900
H	3.92095600	0.33652000	-0.36213600
C	1.87913400	0.43938600	0.18737900
H	1.89088800	1.52917700	0.25163300
H	3.03743000	-1.28329600	-0.23286200

parent N-allylhydrazone

Reactant

Zero-point correction=	0.119088 (Hartree/Particle)
Thermal correction to Energy=	0.125934
Thermal correction to Enthalpy=	0.126878
Thermal correction to Gibbs Free Energy=	0.088437
Sum of electronic and zero-point Energies=	-266.558769
Sum of electronic and thermal Energies=	-266.551924
Sum of electronic and thermal Enthalpies=	-266.550980
Sum of electronic and thermal Free Energies=	-266.589421

C	2.45233000	0.61416200	0.06550500
C	-0.34768100	0.36460200	0.22157700
C	-1.72920200	-0.20569700	0.37132900
C	-2.80685100	0.24432400	-0.26852100
H	1.90904700	1.55248300	0.18878900
H	-0.36747600	1.23398000	-0.44812200
H	-3.78745300	-0.19520400	-0.10893300
N	1.91895900	-0.53034100	-0.16554200
H	-2.75236800	1.07201500	-0.97205000
N	0.57357400	-0.64592100	-0.30195100
H	-1.82556200	-1.03906200	1.06911700
H	0.01781100	0.72280400	1.20158200
H	0.28621800	-1.60662000	-0.15344700
H	3.53682200	0.64715200	0.11965700

TS

Zero-point correction=	0.141754 (Hartree/Particle)
Thermal correction to Energy=	0.147625
Thermal correction to Enthalpy=	0.148569
Thermal correction to Gibbs Free Energy=	0.112938
Sum of electronic and zero-point Energies=	-234.435100
Sum of electronic and thermal Energies=	-234.429229
Sum of electronic and thermal Enthalpies=	-234.428285
Sum of electronic and thermal Free Energies=	-234.463916

C	0.93470700	-1.21844600	0.24803400
C	1.42516600	-0.00000100	-0.26303300
C	0.93470800	1.21844500	0.24803400
C	-0.93470700	1.21844600	-0.24803400
C	-1.42516600	0.00000000	0.26303300
C	-0.93470800	-1.21844500	-0.24803400
H	1.30098000	2.14286300	-0.19810200
H	1.81468400	-0.00000100	-1.28135300
H	0.81120600	-1.30393400	1.32613600
H	1.30097800	-2.14286400	-0.19810200
H	-0.81120600	1.30393400	-1.32613600
H	-1.30097800	2.14286400	0.19810200
H	-1.81468400	0.00000100	1.28135300
H	-1.30098000	-2.14286300	0.19810200
H	0.81120700	1.30393300	1.32613600
H	-0.81120700	-1.30393400	-1.32613600

TS

Zero-point correction=	0.119130 (Hartree/Particle)
Thermal correction to Energy=	0.124503
Thermal correction to Enthalpy=	0.125447
Thermal correction to Gibbs Free Energy=	0.090691
Sum of electronic and zero-point Energies=	-266.509267
Sum of electronic and thermal Energies=	-266.503894
Sum of electronic and thermal Enthalpies=	-266.502950
Sum of electronic and thermal Free Energies=	-266.537706

C	-1.48947200	0.19233000	0.17823800
C	1.47427200	-0.38177600	-0.26554500
C	1.04403500	0.85585200	0.28353200
C	-0.12925300	1.47112800	-0.20655100
H	-1.50800600	0.26510900	1.27523100
H	1.41379100	-0.52655500	-1.34108500
H	2.34434100	-0.86146000	0.17913800
H	-0.47133500	2.37370200	0.29955300
N	-0.94085700	-0.89634300	-0.41066500
H	-0.27067600	1.51249400	-1.28440200
H	1.36116900	1.09044400	1.29898700
N	0.10675700	-1.38899100	0.23273900
H	0.07916300	-1.15032700	1.24385100
H	-2.39400900	0.57550400	-0.29786700

parent Boc-protected N-allylhydrazone

Reactant

Zero-point correction=	0.162491 (Hartree/Particle)
Thermal correction to Energy=	0.173314
Thermal correction to Enthalpy=	0.174259
Thermal correction to Gibbs Free Energy=	0.125832
Sum of electronic and zero-point Energies=	-494.404232
Sum of electronic and thermal Energies=	-494.393409
Sum of electronic and thermal Enthalpies=	-494.392465
Sum of electronic and thermal Free Energies=	-494.440891

TS

Zero-point correction=	0.160465 (Hartree/Particle)
Thermal correction to Energy=	0.170783
Thermal correction to Enthalpy=	0.171727
Thermal correction to Gibbs Free Energy=	0.124136
Sum of electronic and zero-point Energies=	-494.345161
Sum of electronic and thermal Energies=	-494.334842
Sum of electronic and thermal Enthalpies=	-494.333898
Sum of electronic and thermal Free Energies=	-494.381489

C	-1.51009900	2.13630600	-0.12544800
C	-1.29094700	-0.54627100	-0.96604800
C	-2.30387700	-1.07800200	0.01726000
C	-2.23227900	-0.97921100	1.34240800
H	-2.43867700	1.65094500	-0.42563700
H	-0.80755300	-1.37698800	-1.48580300
H	-2.99907200	-1.40776500	1.98053100
N	-0.36360500	1.57795300	-0.03939400
H	-1.40916800	-0.47134600	1.83789000
N	-0.22047700	0.25909500	-0.37809900
C	-3.14491600	-1.59400500	-0.44629300
C	1.03466200	-0.31860200	-0.22300900
O	1.27330000	-1.47382500	-0.53505500
O	1.93359800	0.52703600	0.30467400
C	3.24626700	-0.03206900	0.47944700
H	3.66022500	-0.36509400	-0.47542200
H	3.85040900	0.77698900	0.89073500
H	3.22228000	-0.87490900	1.17490500
H	-1.55037200	3.18869100	0.14211400
H	-1.78865300	0.05990900	-1.73523800

C	1.65427700	-1.55406700	-0.27470200
C	1.26200300	1.48297500	0.09304000
C	2.51940100	0.94084600	-0.19008500
C	2.97897800	-0.16670000	0.51519500
H	1.92641200	-1.39498600	-1.31828400
H	0.90932700	1.49207000	1.12002200
H	3.92390100	-0.63024200	0.24159500
N	0.50505900	-1.09770600	0.22188500
H	2.68421900	-0.31136800	1.54991200
N	0.05505700	-0.03664000	-0.44637300
H	2.96265400	1.15499600	-1.16101900
C	-1.25563900	0.32456100	-0.04681700
O	-2.08881200	-0.41955800	0.42951200
O	-1.50531900	1.60338500	-0.40632800
C	-2.85143700	2.04591700	-0.17654900
H	-3.10381400	1.99721000	0.88602800
H	-2.88211000	3.07951500	-0.52304000
H	-3.56325200	1.43757100	-0.74052600
H	2.03608200	-2.45840600	0.19418500
H	0.86599700	2.27558900	-0.52959200