SUPPORTING INFORMATION

Isotope Effects and the Nature of Selectivity in Rhodium-Catalyzed Cyclopropanations

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Theoretical Structures

Starting Materials

N2 B3LYP 6-31G 5D*

E(RB+HF-LYP) = -109.520718355

Zero-point correction= 0.005600 (Hartree/Particle)
Thermal correction to Energy= 0.007961
Thermal correction to Enthalpy= 0.008905
Thermal correction to Gibbs Free Energy= -0.012849
Sum of electronic and zero-point Energies= -109.515118
Sum of electronic and thermal Energies= -109.512758
Sum of electronic and thermal Enthalpies= -109.511814
Sum of electronic and thermal Free Energies= -109.533568

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	4.995	4.970	45.786

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.552653
2	7	0	0.000000	0.000000	-0.552653

Methyl Diazoacetate B3LYP 6-31G 5D (2)*

Isomer 1

E(RB+HF-LYP) = -376.616641233

Zero-point correction= 0.077072 (Hartree/Particle)
Thermal correction to Energy= 0.084295
Thermal correction to Enthalpy= 0.085239
Thermal correction to Gibbs Free Energy= 0.045342
Sum of electronic and zero-point Energies= -376.539570
Sum of electronic and thermal Energies= -376.532346
Sum of electronic and thermal Enthalpies= -376.531402
Sum of electronic and thermal Free Energies= -376.571299

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	52.896	23.786	83.971

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	8	0	O	0.176676	1.960286	0.000000
2	6	0	C	0.000000	0.758272	0.000000
3	6	0	C	-1.319809	0.137016	0.000000
4	7	0	N	-1.456728	-1.163067	0.000000
5	8	0	O	0.994643	-0.164884	0.000000
6	6	0	C	2.324769	0.376403	0.000000

7	7	0	N	-1.564923	-2.296164	0.000000
8	1	0	H	-2.221355	0.732133	0.000000
9	1	0	H	2.989325	-0.488189	0.000000
10	1	0	H	2.491635	0.988658	0.890238
11	1	0	H	2.491635	0.988658	-0.890238

Isomer 2

E(RB+HF-LYP) = -376.616483624

Zero-point correction=	0.076916 (Hartree/Particle)
Thermal correction to Energy=	0.084217
Thermal correction to Enthalpy=	0.085161
Thermal correction to Gibbs Free Energy=	0.045127
Sum of electronic and zero-point Energies=	-376.539567
Sum of electronic and thermal Energies=	-376.532266
Sum of electronic and thermal Enthalpies=	-376.531322
Sum of electronic and thermal Free Energies=	-376.571356

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	52.847	23.861	84.259

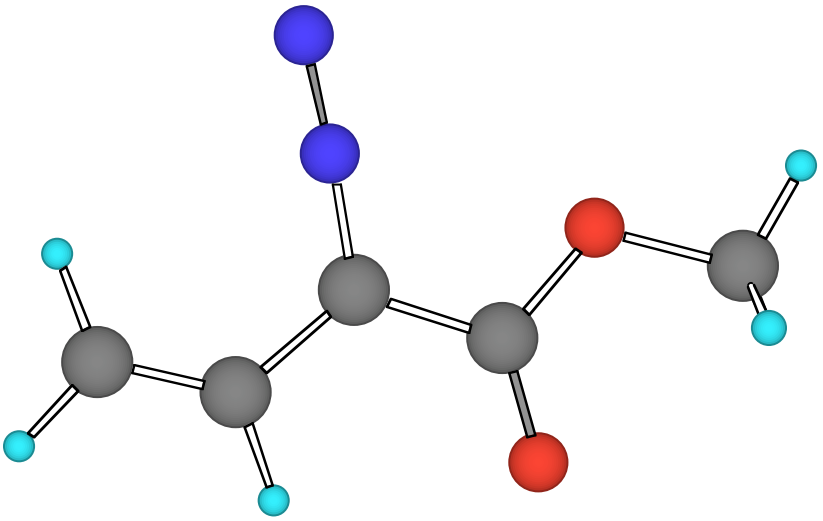
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.525794	2.632696	0.000000
2	8	0	0.984404	1.272589	0.000000
3	6	0	0.000000	0.340280	0.000000
4	6	0	0.591914	-0.993770	0.000000
5	7	0	-0.214404	-2.022755	0.000000
6	7	0	-0.927600	-2.908332	0.000000
7	8	0	-1.189742	0.592183	0.000000
8	1	0	1.653782	-1.193801	0.000000
9	1	0	1.429085	3.243664	0.000000
10	1	0	-0.076194	2.837163	0.889603
11	1	0	-0.076194	2.837163	-0.889603

Methyl vinyldiazoacetate (3)

B3LYP 6-31G*

Isomer 1 – C=O anti to N2, C=C-C=N2 s-cis



E(RB+HF-LYP) = -454.027415607

Zero-point correction=	0.110377 (Hartree/Particle)
Thermal correction to Energy=	0.119921
Thermal correction to Enthalpy=	0.120865
Thermal correction to Gibbs Free Energy=	0.075237
Sum of electronic and zero-point Energies=	-453.917039
Sum of electronic and thermal Energies=	-453.907494
Sum of electronic and thermal Enthalpies=	-453.906550
Sum of electronic and thermal Free Energies=	-453.952178

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.252	32.242	96.033

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-0.626811	-0.061720	-0.000061
2	6	0	C	0.771555	-0.509911	-0.000033
3	8	0	O	1.101887	-1.679368	-0.000197
4	8	0	O	1.639252	0.530312	0.000143
5	6	0	C	3.029350	0.165946	0.000084
6	1	0	H	3.273027	-0.418614	0.890996
7	1	0	H	3.575427	1.109541	-0.001075
8	1	0	H	3.272465	-0.420539	-0.889703
9	6	0	C	-1.738152	-1.008061	0.000005
10	6	0	C	-3.046750	-0.724886	0.000134
11	1	0	H	-1.387139	-2.036434	-0.000088
12	1	0	H	-3.781970	-1.521986	0.000155
13	1	0	H	-3.431206	0.292380	0.000241
14	7	0	N	-0.860398	1.231838	0.000103
15	7	0	N	-1.108869	2.342433	-0.000227

Isomer 2 – C=O syn to N2, C=C-C=N2 s-cis

E(RB+HF-LYP) = -454.025307587

Isomer 3 – C=O syn to N2, C=C-C=N2 s-trans

E(RB+HF-LYP) = -454.023037498

Isomer 4 C=O anti to N2, C=C-C=N2 s-trans

E(RB+HF-LYP) = -454.025745836

B3LYP 6-31G* 5D Isomer 1 – C=O anti to N2, C=C-C=N2 s-cis

E(RB+HF-LYP) = -454.018104123

Zero-point correction=	0.110444 (Hartree/Particle)
Thermal correction to Energy=	0.119965
Thermal correction to Enthalpy=	0.120909
Thermal correction to Gibbs Free Energy=	0.075384
Sum of electronic and zero-point Energies=	-453.907661
Sum of electronic and thermal Energies=	-453.898140
Sum of electronic and thermal Enthalpies=	-453.897195
Sum of electronic and thermal Free Energies=	-453.942720

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	75.279	32.214	95.814

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.629556	0.000000
2	6	0	-0.581519	-0.719190	0.000000
3	8	0	-1.777734	-0.934550	0.000000
4	8	0	0.369247	-1.683774	0.000000
5	6	0	-0.128540	-3.031394	0.000000
6	1	0	-0.735085	-3.216601	0.890389
7	1	0	0.757350	-3.666966	0.000000
8	1	0	-0.735085	-3.216601	-0.890389
9	6	0	-0.835757	1.826556	0.000000
10	6	0	-0.428922	3.102585	0.000000
11	1	0	-1.892953	1.575209	0.000000
12	1	0	-1.152314	3.910522	0.000000
13	1	0	0.620389	3.388437	0.000000
14	7	0	1.310563	0.738166	0.000000
15	7	0	2.440012	0.879535	0.000000

Styrene B3LYP 6-31G* 5D

E(RB+HF-LYP) = -309.641798718

Zero-point correction=	0.133774 (Hartree/Particle)
Thermal correction to Energy=	0.140542
Thermal correction to Enthalpy=	0.141486
Thermal correction to Gibbs Free Energy=	0.102309
Sum of electronic and zero-point Energies=	-309.508025
Sum of electronic and thermal Energies=	-309.501257
Sum of electronic and thermal Enthalpies=	-309.500313

Sum of electronic and thermal Free Energies= -309.539490

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	88.191	26.026	82.456

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	2.977797	0.335201	0.001431
2	6	0	C	1.955085	-0.529568	-0.001082
3	6	0	C	0.515275	-0.220726	-0.000632
4	1	0	H	2.840512	1.413202	0.004365
5	1	0	H	4.004804	-0.017010	0.000880
6	1	0	H	2.186775	-1.594917	-0.003604
7	6	0	C	-0.406687	-1.281795	-0.000003
8	6	0	C	-1.781388	-1.046276	0.000698
9	6	0	C	-2.265715	0.262137	0.000531
10	6	0	C	-1.362249	1.329983	-0.000291
11	6	0	C	0.009138	1.092534	-0.000925
12	1	0	H	-0.035232	-2.304219	0.000136
13	1	0	H	-2.472806	-1.884839	0.001292
14	1	0	H	-3.335797	0.450958	0.000934
15	1	0	H	-1.730308	2.352734	-0.000552
16	1	0	H	0.694526	1.935150	-0.001820

Propene B3LYP 6-31G 5D*

E(RB+HF-LYP) = -117.905219184

Zero-point correction= 0.080113 (Hartree/Particle)
Thermal correction to Energy= 0.084187
Thermal correction to Enthalpy= 0.085131
Thermal correction to Gibbs Free Energy= 0.055112
Sum of electronic and zero-point Energies= -117.825106
Sum of electronic and thermal Energies= -117.821032
Sum of electronic and thermal Enthalpies= -117.820088
Sum of electronic and thermal Free Energies= -117.850107

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	52.828	12.907	63.180

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.293589	0.150245	0.000000
2	1	0	-1.622208	-0.887505	0.000000
3	1	0	-2.074246	0.906344	0.000000
4	6	0	0.000000	0.474773	0.000000
5	6	0	1.139392	-0.504497	0.000000
6	1	0	0.278501	1.529820	0.000000
7	1	0	1.781510	-0.366302	0.880536
8	1	0	0.780121	-1.539181	0.000000
9	1	0	1.781510	-0.366302	-0.880536

trans-2-Butene B3LYP 6-31G 5D*

E(RB+HF-LYP) = -157.223861033

Zero-point correction= 0.108501 (Hartree/Particle)
Thermal correction to Energy= 0.113976
Thermal correction to Enthalpy= 0.114920
Thermal correction to Gibbs Free Energy= 0.081746
Sum of electronic and zero-point Energies= -157.115360
Sum of electronic and thermal Energies= -157.109885
Sum of electronic and thermal Enthalpies= -157.108941
Sum of electronic and thermal Free Energies= -157.142115

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	71.521	18.200	69.821

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.667862	0.000000
2	6	0	0.000000	-0.667862	0.000000
3	6	0	-1.226798	1.535579	0.000000
4	1	0	-0.958298	-1.191660	0.000000
5	6	0	1.226798	-1.535579	0.000000
6	1	0	0.958298	1.191660	0.000000
7	1	0	-2.143429	0.935529	0.000000
8	1	0	-1.252231	2.192395	0.880490
9	1	0	-1.252231	2.192395	-0.880490
10	1	0	2.143429	-0.935529	0.000000
11	1	0	1.252231	-2.192395	0.880490
12	1	0	1.252231	-2.192395	-0.880490

cis-2-Butene B3LYP 6-31G 5D*

E(RB+HF-LYP) = -157.221726146

Zero-point correction= 0.108694 (Hartree/Particle)
Thermal correction to Energy= 0.114170
Thermal correction to Enthalpy= 0.115114
Thermal correction to Gibbs Free Energy= 0.081575
Sum of electronic and zero-point Energies= -157.113032
Sum of electronic and thermal Energies= -157.107556
Sum of electronic and thermal Enthalpies= -157.106612
Sum of electronic and thermal Free Energies= -157.140151

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	71.643	18.066	70.589

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.669323	0.664396
2	6	0	0.000000	-0.669323	0.664396
3	6	0	0.000000	1.593192	-0.521986
4	1	0	0.000000	-1.169759	1.633576
5	6	0	0.000000	-1.593192	-0.521986
6	1	0	0.000000	1.169759	1.633576

7	1	0	0.000000	1.060260	-1.476876
8	1	0	-0.880156	2.250590	-0.505577
9	1	0	0.880156	2.250590	-0.505577
10	1	0	0.000000	-1.060260	-1.476876
11	1	0	0.880156	-2.250590	-0.505577
12	1	0	-0.880156	-2.250590	-0.505577

Methyl Vinyl Ether B3LYP 6-31G 5D*

E(RB+HF-LYP) = -193.110706849

Zero-point correction= 0.085830 (Hartree/Particle)
Thermal correction to Energy= 0.090557
Thermal correction to Enthalpy= 0.091502
Thermal correction to Gibbs Free Energy= 0.059135
Sum of electronic and zero-point Energies= -193.024877
Sum of electronic and thermal Energies= -193.020149
Sum of electronic and thermal Enthalpies= -193.019205
Sum of electronic and thermal Free Energies= -193.051571

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	56.826	15.750	68.120

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.453137	0.566668	-0.000110
2	6	0	0.741080	-0.565199	0.000085
3	8	0	-0.608301	-0.713978	-0.000228
4	6	0	-1.380336	0.476365	0.000135
5	1	0	1.010968	1.556128	-0.000458
6	1	0	2.535330	0.506345	0.000470
7	1	0	1.213952	-1.543753	0.000529
8	1	0	-2.426339	0.164349	0.000174
9	1	0	-1.175305	1.080740	0.893875
10	1	0	-1.175487	1.081014	-0.893428

Rh2(O2CH)4 B3LYP, lanl2dz on Rh, 6-31G on all other atoms*

E(RB+HF-LYP) = -975.812030155

Zero-point correction= 0.101583 (Hartree/Particle)
Thermal correction to Energy= 0.115523
Thermal correction to Enthalpy= 0.116467
Thermal correction to Gibbs Free Energy= 0.061081
Sum of electronic and zero-point Energies= -975.710447
Sum of electronic and thermal Energies= -975.696507
Sum of electronic and thermal Enthalpies= -975.695563
Sum of electronic and thermal Free Energies= -975.750949

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	72.492	50.336	116.569

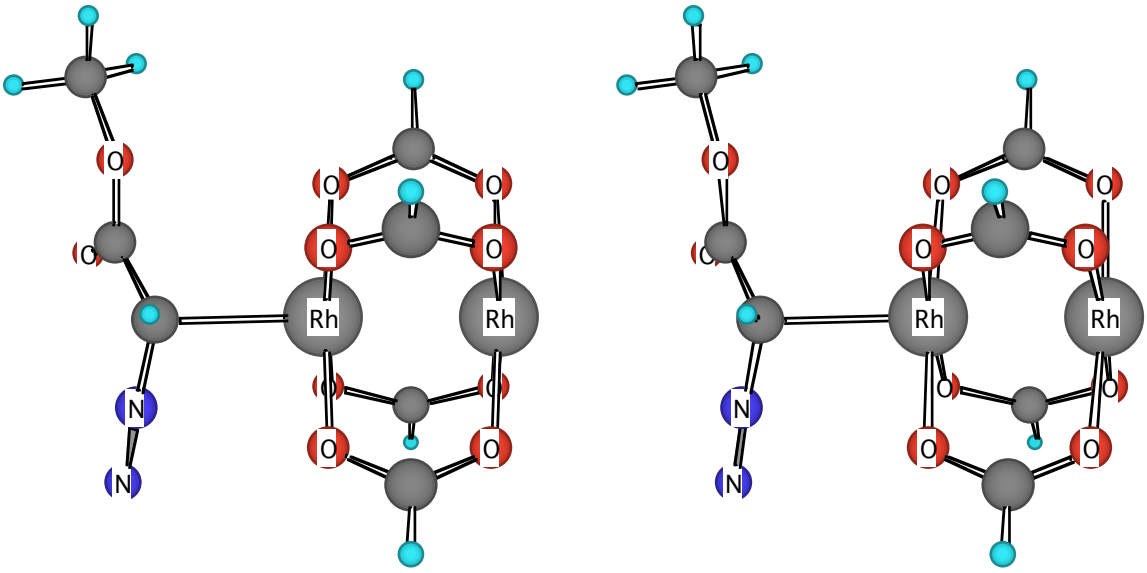
Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type		X	Y	Z
1	45	0	Rh	0.000018	0.000119	1.198735
2	45	0	Rh	-0.000041	-0.000128	-1.198733
3	8	0	O	1.464023	-1.457548	1.138851
4	6	0	C	1.855198	-1.852060	0.000143
5	8	0	O	1.460173	-1.461601	-1.138630
6	1	0	H	2.633141	-2.627532	0.000208
7	8	0	O	-1.463896	1.457879	1.138627
8	6	0	C	-1.855416	1.851857	-0.000143
9	8	0	O	-1.460172	1.461421	-1.138852
10	1	0	H	-2.632194	2.628496	-0.000207
11	8	0	O	1.457731	1.464077	1.138577
12	6	0	C	1.852091	1.855172	-0.000211
13	8	0	O	1.461511	1.460027	-1.138899
14	1	0	H	2.628023	2.632657	-0.000303
15	8	0	O	-1.457758	-1.463779	1.138900
16	6	0	C	-1.851930	-1.855337	0.000209
17	8	0	O	-1.461530	-1.460298	-1.138584
18	1	0	H	-2.628264	-2.632419	0.000303

Rh-Diazoester C-complexes, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Rh2 complex with methyl diazoacetate isomer 1 (4)



Rh-C 2.337511
E(RB+HF-LYP) = -1352.45018569

Zero-point correction=	0.179724 (Hartree/Particle)
Thermal correction to Energy=	0.202667
Thermal correction to Enthalpy=	0.203612
Thermal correction to Gibbs Free Energy=	0.126533
Sum of electronic and zero-point Energies=	-1352.270462
Sum of electronic and thermal Energies=	-1352.247518
Sum of electronic and thermal Enthalpies=	-1352.246574
Sum of electronic and thermal Free Energies=	-1352.323653

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	127.176	79.712	162.227

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.778599	-1.547052	0.754390
2	45	0	-0.221062	0.219866	-0.192053
3	6	0	-2.407048	0.851293	-0.727520
4	6	0	-3.368645	-0.011801	0.022262
5	8	0	-3.872070	0.274308	1.086238
6	8	0	-3.565910	-1.148255	-0.661480
7	6	0	-4.362257	-2.136551	0.017020
8	1	0	-3.867853	-2.439197	0.942880
9	1	0	-4.431329	-2.974612	-0.676002
10	1	0	-5.354184	-1.738375	0.244610
11	1	0	-2.324257	0.752157	-1.806521
12	45	0	2.091279	-0.400923	0.234293
13	8	0	1.392608	-2.118973	1.151172
14	6	0	0.142553	-2.294282	1.204279
15	1	0	-0.194299	-3.214146	1.703662
16	8	0	2.082681	-1.377512	-1.595018
17	6	0	1.023666	-1.347261	-2.282506
18	1	0	1.058483	-1.873407	-3.247354
19	8	0	-0.080353	-0.786476	-2.004428
20	8	0	2.643606	1.364671	-0.712219
21	6	0	1.735386	2.119863	-1.153223
22	1	0	2.067995	3.045160	-1.644968
23	8	0	0.476707	1.949177	-1.102615
24	8	0	1.944558	0.614665	2.037768
25	6	0	0.848163	1.175350	2.317514
26	1	0	0.805237	1.706182	3.279071
27	8	0	-0.217638	1.206696	1.628192
28	7	0	-2.437731	2.139515	-0.323143
29	7	0	-2.390154	3.188225	0.074696

Rh2 complex with methyl diazoacetate isomer 2 (ester turned 180°)

Rh-C 2.340
E(RB+HF-LYP) = -1352.44937699

Zero-point correction= 0.179698 (Hartree/Particle)
Thermal correction to Energy= 0.202674
Thermal correction to Enthalpy= 0.203618
Thermal correction to Gibbs Free Energy= 0.126025
Sum of electronic and zero-point Energies= -1352.269679
Sum of electronic and thermal Energies= -1352.246703
Sum of electronic and thermal Enthalpies= -1352.245759
Sum of electronic and thermal Free Energies= -1352.323352

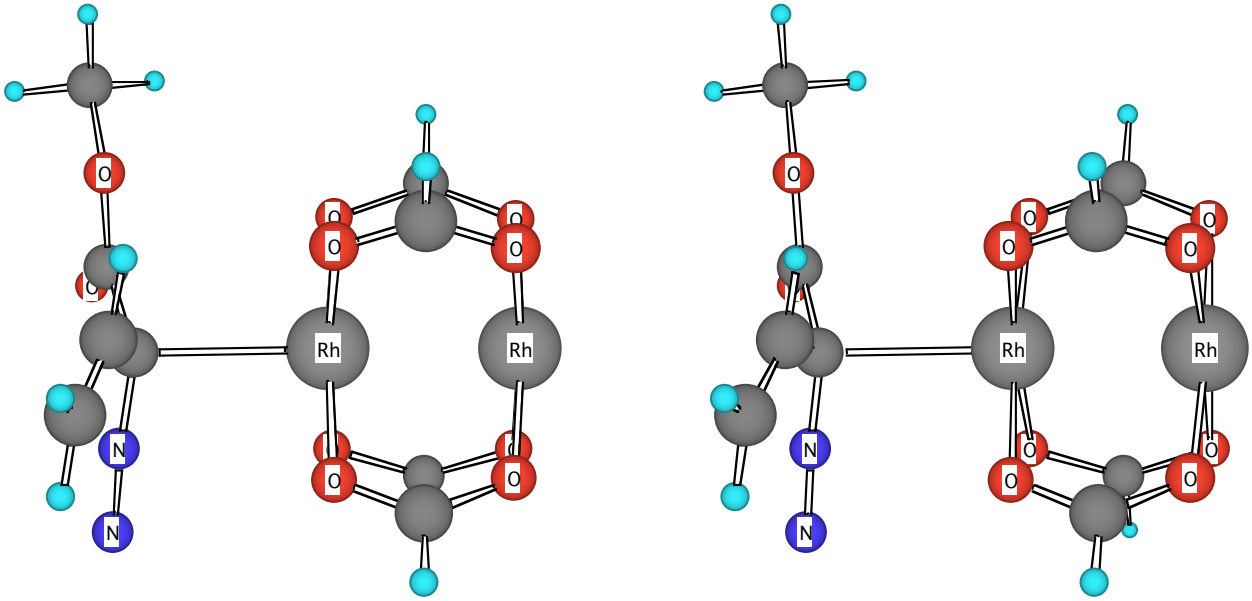
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	127.180	79.725	163.308

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.681393	-1.772513	0.138398
2	45	0	-0.193725	0.207010	-0.254513
3	6	0	-2.358734	0.779729	-0.933074

4	6	0	-3.288393	-0.345008	-0.612381
5	8	0	-3.504726	-1.252969	-1.378954
6	8	0	-3.812475	-0.217072	0.620983
7	6	0	-4.645073	-1.310767	1.049618
8	1	0	-5.493748	-1.433273	0.372109
9	1	0	-4.983954	-1.039949	2.049235
10	1	0	-4.062674	-2.234636	1.075031
11	1	0	-2.153631	0.955042	-1.985398
12	45	0	2.099926	-0.352053	0.326074
13	8	0	1.473859	-2.296883	0.661781
14	6	0	0.248614	-2.556842	0.496224
15	1	0	-0.054814	-3.596425	0.685584
16	8	0	2.414050	-0.805332	-1.670639
17	6	0	1.445232	-0.671333	-2.470741
18	1	0	1.646884	-0.925141	-3.521168
19	8	0	0.264540	-0.280119	-2.219190
20	8	0	2.580658	1.634976	-0.045406
21	6	0	1.664691	2.417502	-0.417869
22	1	0	1.962269	3.458530	-0.608949
23	8	0	0.434313	2.157818	-0.601003
24	8	0	1.637707	0.141784	2.290337
25	6	0	0.467170	0.542500	2.541569
26	1	0	0.259025	0.806220	3.588475
27	8	0	-0.507440	0.683112	1.739187
28	7	0	-2.557812	1.924657	-0.245848
29	7	0	-2.655353	2.855264	0.377393

Rh2 complex with methyl diazovinylacetate - Isomer 1



Rh-C 2.451!
E(RB+HF-LYP) = -1429.84206860

Zero-point correction=	0.212612 (Hartree/Particle)
Thermal correction to Energy=	0.238047
Thermal correction to Enthalpy=	0.238991
Thermal correction to Gibbs Free Energy=	0.157061
Sum of electronic and zero-point Energies=	-1429.629457
Sum of electronic and thermal Energies=	-1429.604022
Sum of electronic and thermal Enthalpies=	-1429.603077
Sum of electronic and thermal Free Energies=	-1429.685008

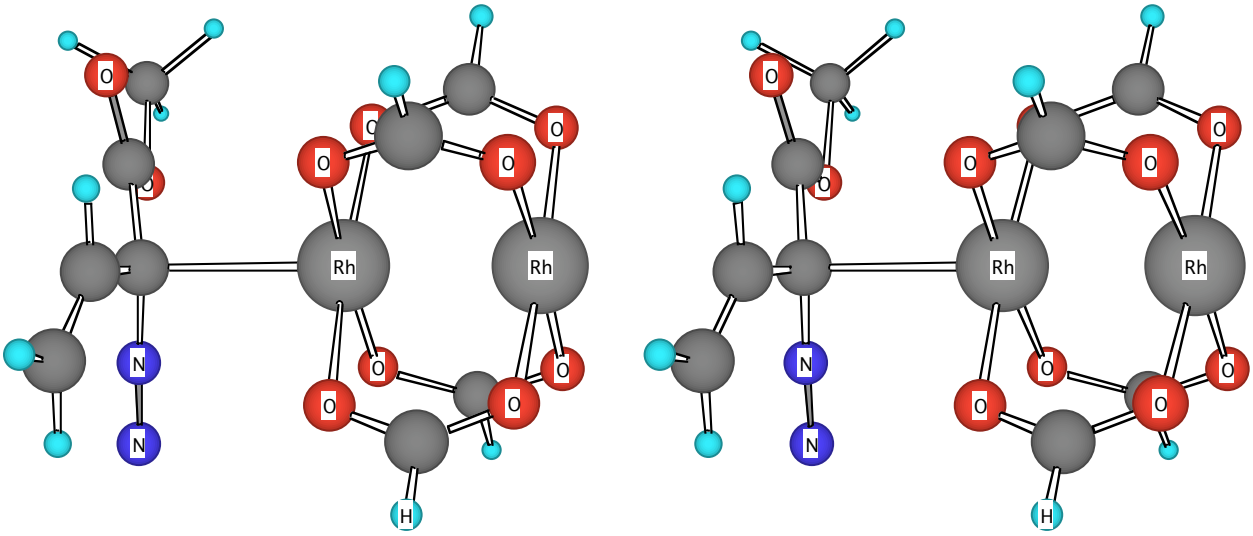
E (Thermal)	CV	S

	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	149.377	88.724	172.437

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.401730	1.873055	-0.334680
2	45	0	-0.113334	-0.160323	0.002481
3	6	0	-2.507862	-0.684807	0.024246
4	6	0	-3.090629	0.639552	-0.375103
5	8	0	-3.337616	0.957618	-1.518109
6	8	0	-3.284793	1.405567	0.707670
7	6	0	-3.720255	2.749555	0.431659
8	1	0	-2.968182	3.263323	-0.170455
9	1	0	-3.825917	3.222537	1.407815
10	1	0	-4.674675	2.740492	-0.100296
11	6	0	-2.720844	-1.285666	1.361120
12	6	0	-2.905011	-2.579836	1.637544
13	1	0	-2.684190	-0.543785	2.150658
14	1	0	-3.023472	-2.907738	2.664636
15	1	0	-2.930812	-3.354075	0.874894
16	45	0	2.275021	0.292700	0.017424
17	8	0	1.839493	2.286694	-0.332281
18	6	0	0.623380	2.614120	-0.429322
19	1	0	0.424500	3.678623	-0.619432
20	8	0	2.139281	0.618906	2.055847
21	6	0	1.003909	0.499523	2.598098
22	1	0	0.966723	0.679252	3.682204
23	8	0	-0.100757	0.198916	2.053394
24	8	0	2.579391	-1.726218	0.365031
25	6	0	1.566179	-2.477516	0.429968
26	1	0	1.765054	-3.544494	0.604720
27	8	0	0.342629	-2.159298	0.319540
28	8	0	2.272665	-0.058995	-2.026796
29	6	0	1.177265	-0.361804	-2.577011
30	1	0	1.209834	-0.540050	-3.661002
31	8	0	0.035827	-0.489118	-2.035832
32	7	0	-2.513411	-1.540228	-1.023263
33	7	0	-2.453256	-2.257882	-1.886301

Rh2 complex with methyl diazovinylacetate - Isomer 2 (8)



Rh-C 2.470!
E(RB+HF-LYP) = -1429.84347666

Zero-point correction=	0.212723 (Hartree/Particle)
Thermal correction to Energy=	0.238081
Thermal correction to Enthalpy=	0.239025
Thermal correction to Gibbs Free Energy=	0.157376
Sum of electronic and zero-point Energies=	-1429.630754
Sum of electronic and thermal Energies=	-1429.605396
Sum of electronic and thermal Enthalpies=	-1429.604451
Sum of electronic and thermal Free Energies=	-1429.686101

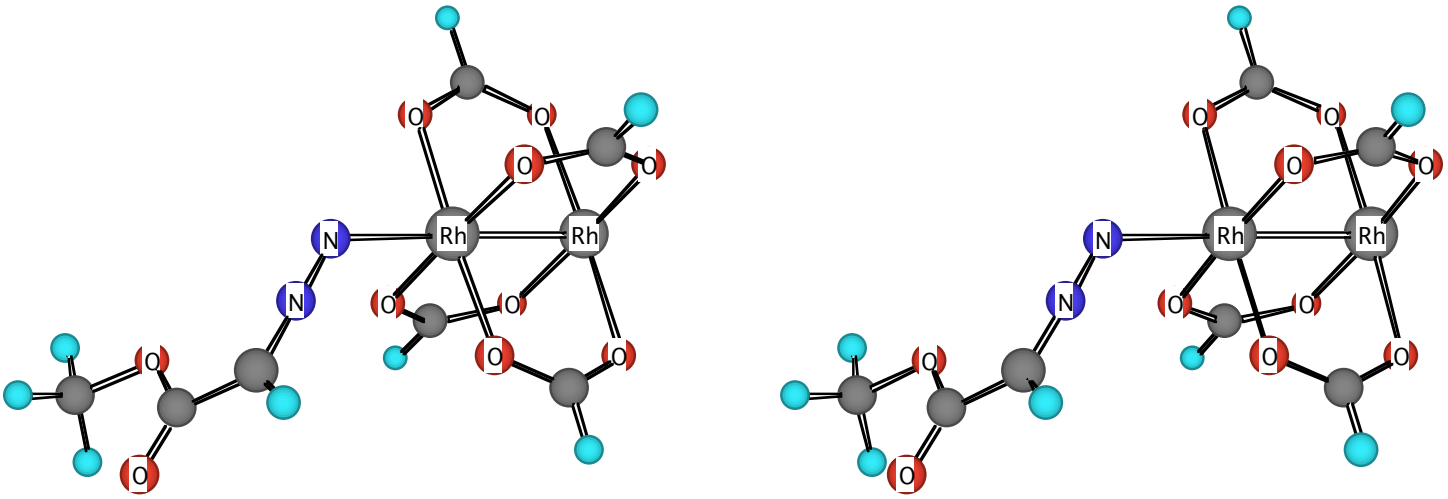
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	149.398	88.656	171.846

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.413486	-1.848981	-0.431410
2	45	0	-0.112149	0.169676	-0.016919
3	6	0	-2.515399	0.734679	-0.079269
4	6	0	-3.078665	-0.587256	-0.505380
5	8	0	-3.286313	-0.865126	-1.664009
6	8	0	-3.306315	-1.394170	0.545232
7	6	0	-3.724981	-2.730994	0.213026
8	1	0	-4.659167	-2.709214	-0.353361
9	1	0	-3.864605	-3.234224	1.169533
10	1	0	-2.947626	-3.222679	-0.375040
11	6	0	-2.613572	1.877140	-1.012367
12	6	0	-2.665239	3.173771	-0.696689
13	1	0	-2.626414	1.539609	-2.043782
14	1	0	-2.721431	3.924340	-1.477591
15	1	0	-2.637415	3.538462	0.327002
16	45	0	2.270892	-0.303264	0.005035
17	8	0	1.822870	-2.285687	-0.393454
18	6	0	0.606064	-2.597746	-0.525560
19	1	0	0.401137	-3.654493	-0.749587
20	8	0	2.304212	0.091799	-2.025244
21	6	0	1.216797	0.426955	-2.577396
22	1	0	1.266841	0.633577	-3.655856
23	8	0	0.072963	0.556447	-2.046997
24	8	0	2.592582	1.702988	0.401786
25	6	0	1.582629	2.451859	0.525008
26	1	0	1.788217	3.508122	0.749844
27	8	0	0.356697	2.142058	0.421887
28	8	0	2.100536	-0.673439	2.038790
29	6	0	0.960309	-0.565738	2.569738
30	1	0	0.905029	-0.773017	3.647874
31	8	0	-0.137132	-0.247070	2.016064
32	7	0	-2.652247	1.009180	1.232986
33	7	0	-2.706126	1.267159	2.328144

Rh-Diazoester N-complexes, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Rh2 complex with methyl diazoacetate (16)



E(RB+HF-LYP) = -1352.44611848

Zero-point correction=	0.179849 (Hartree/Particle)
Thermal correction to Energy=	0.202817
Thermal correction to Enthalpy=	0.203761
Thermal correction to Gibbs Free Energy=	0.125283
Sum of electronic and zero-point Energies=	-1352.266269
Sum of electronic and thermal Energies=	-1352.243301
Sum of electronic and thermal Enthalpies=	-1352.242357
Sum of electronic and thermal Free Energies=	-1352.320836

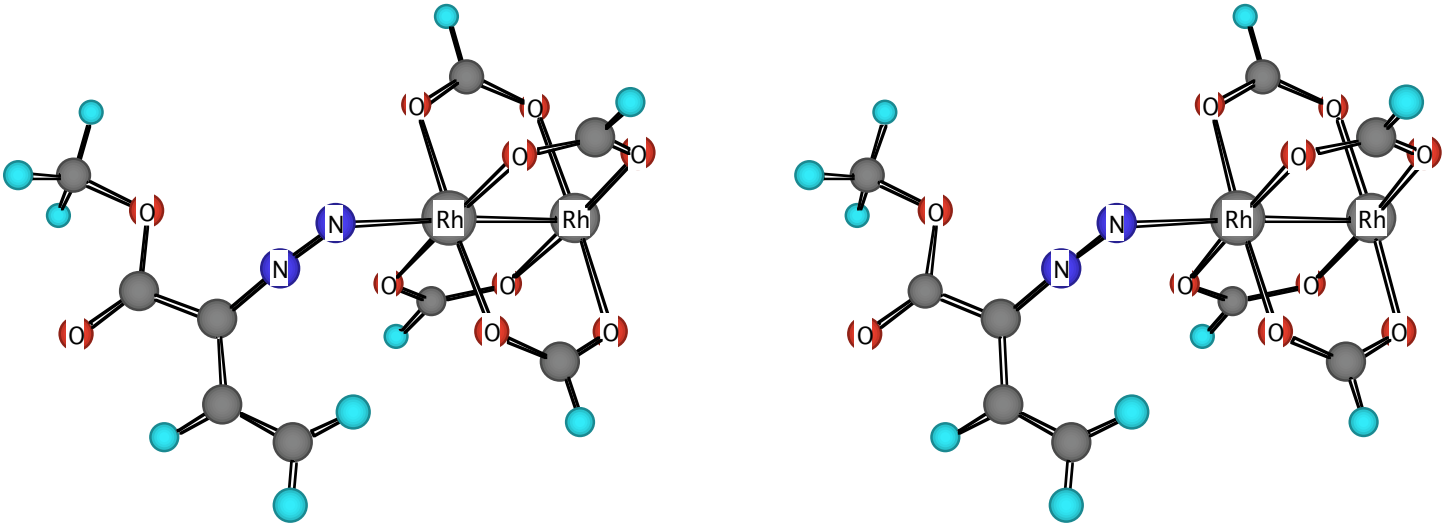
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	127.270	79.681	165.172

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.580171	1.807053	-0.154775
2	8	0	4.605971	0.766456	-0.347404
3	6	0	4.906700	-0.416536	0.224085
4	8	0	5.916206	-0.656823	0.852077
5	6	0	3.854926	-1.419447	-0.004117
6	7	0	2.778963	-1.130691	-0.660445
7	7	0	1.839918	-0.872576	-1.268982
8	45	0	-0.156567	-0.241242	-0.433452
9	8	0	-0.675583	0.892760	-2.089901
10	6	0	-1.809826	1.457916	-2.087296
11	8	0	-2.696326	1.431667	-1.185281
12	45	0	-2.299980	0.345533	0.528515
13	8	0	-3.091718	-1.342811	-0.368219
14	6	0	-2.315483	-2.063781	-1.058192
15	8	0	-1.078543	-1.895750	-1.280458
16	8	0	0.625269	1.450243	0.481776
17	6	0	-0.161315	2.172987	1.165472
18	8	0	-1.395795	2.003279	1.376821
19	8	0	0.237507	-1.336045	1.285803
20	6	0	-0.652472	-1.354628	2.190799
21	8	0	-1.778497	-0.783446	2.190156
22	1	0	3.953440	-2.424017	0.384668
23	1	0	0.291960	3.058905	1.632384

24	1	0	-0.407371	-1.943056	3.086365
25	1	0	-2.766549	-2.950404	-1.525636
26	1	0	-2.051587	2.044688	-2.984658
27	1	0	6.542362	1.512845	-0.581766
28	1	0	5.177980	2.677359	-0.672487
29	1	0	5.708077	2.015835	0.910450

Rh2 complex with methyl vinyldiazoacetate (14)



E(RB+HF-LYP) = -1429.84898561

Zero-point correction= 0.213126 (Hartree/Particle)
Thermal correction to Energy= 0.238462
Thermal correction to Enthalpy= 0.239406
Thermal correction to Gibbs Free Energy= 0.155452
Sum of electronic and zero-point Energies= -1429.635860
Sum of electronic and thermal Energies= -1429.610523
Sum of electronic and thermal Enthalpies= -1429.609579
Sum of electronic and thermal Free Energies= -1429.693534

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	149.637	88.210	176.697

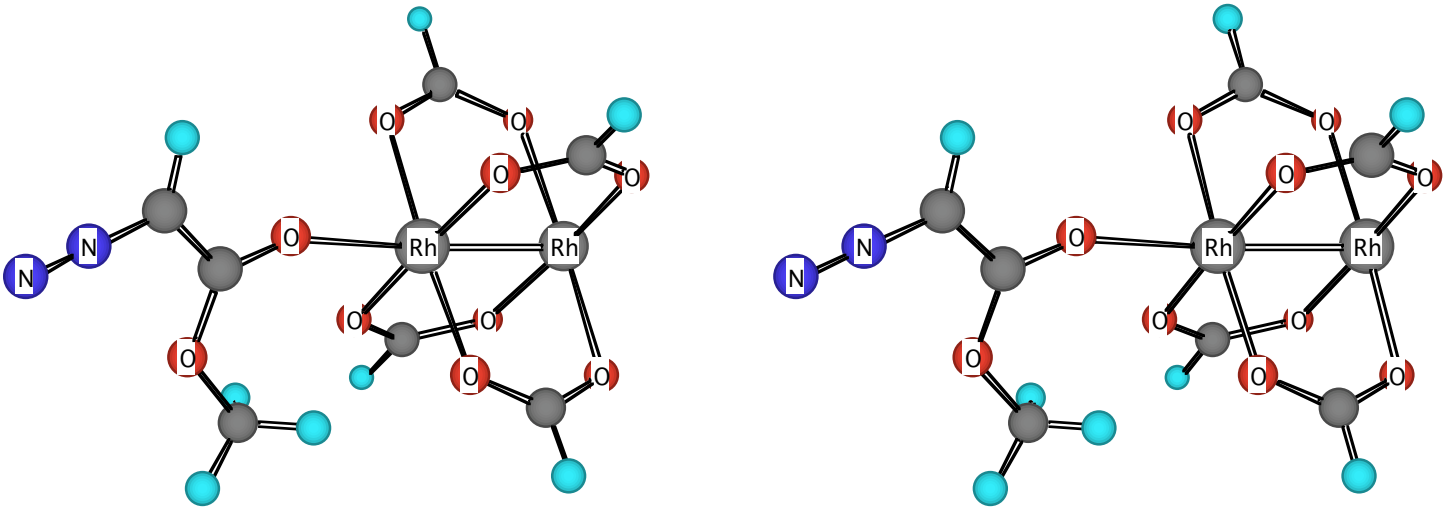
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.108659	-2.625722	0.041889
2	8	0	-4.244799	-1.515108	-0.260466
3	6	0	-4.690761	-0.310327	0.139926
4	8	0	-5.744938	-0.108259	0.705804
5	6	0	-3.739845	0.775056	-0.199438
6	7	0	-2.646228	0.455624	-0.824914
7	7	0	-1.679002	0.230452	-1.405802
8	45	0	0.346089	0.003590	-0.474931
9	8	0	1.326671	0.349234	-2.268507
10	6	0	2.593897	0.373537	-2.255882
11	8	0	3.372077	0.212880	-1.271486
12	45	0	2.522694	-0.136358	0.582376
13	8	0	2.409060	1.905582	0.922093
14	6	0	1.378414	2.518825	0.528854
15	8	0	0.364179	2.045151	-0.070254
16	8	0	0.467854	-2.039278	-0.805838

17	6	0	1.506739	-2.646358	-0.406253
18	8	0	2.513841	-2.167325	0.188940
19	8	0	-0.504090	-0.341974	1.386498
20	6	0	0.279646	-0.503855	2.371890
21	8	0	1.542446	-0.482003	2.378494
22	6	0	-4.029040	2.166260	0.143509
23	6	0	-3.183233	3.200119	0.040735
24	1	0	1.530802	-3.727259	-0.604297
25	1	0	-0.207237	-0.685226	3.340632
26	1	0	1.351269	3.599537	0.727757
27	1	0	3.075616	0.557319	-3.226596
28	1	0	-6.075438	-2.501453	-0.452478
29	1	0	-4.589974	-3.504904	-0.338976
30	1	0	-5.262533	-2.703979	1.120994
31	1	0	-5.040977	2.293331	0.517446
32	1	0	-3.507323	4.198562	0.314871
33	1	0	-2.154216	3.089677	-0.292979

Rh-Diazoester O-complexes, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Rh2 complex with methyl diazoacetate (17)



E(RB+HF-LYP) = -1352.45083526

Zero-point correction= 0.179809 (Hartree/Particle)
Thermal correction to Energy= 0.201958
Thermal correction to Enthalpy= 0.202902
Thermal correction to Gibbs Free Energy= 0.128489
Sum of electronic and zero-point Energies= -1352.271026
Sum of electronic and thermal Energies= -1352.248877
Sum of electronic and thermal Enthalpies= -1352.247933
Sum of electronic and thermal Free Energies= -1352.322347

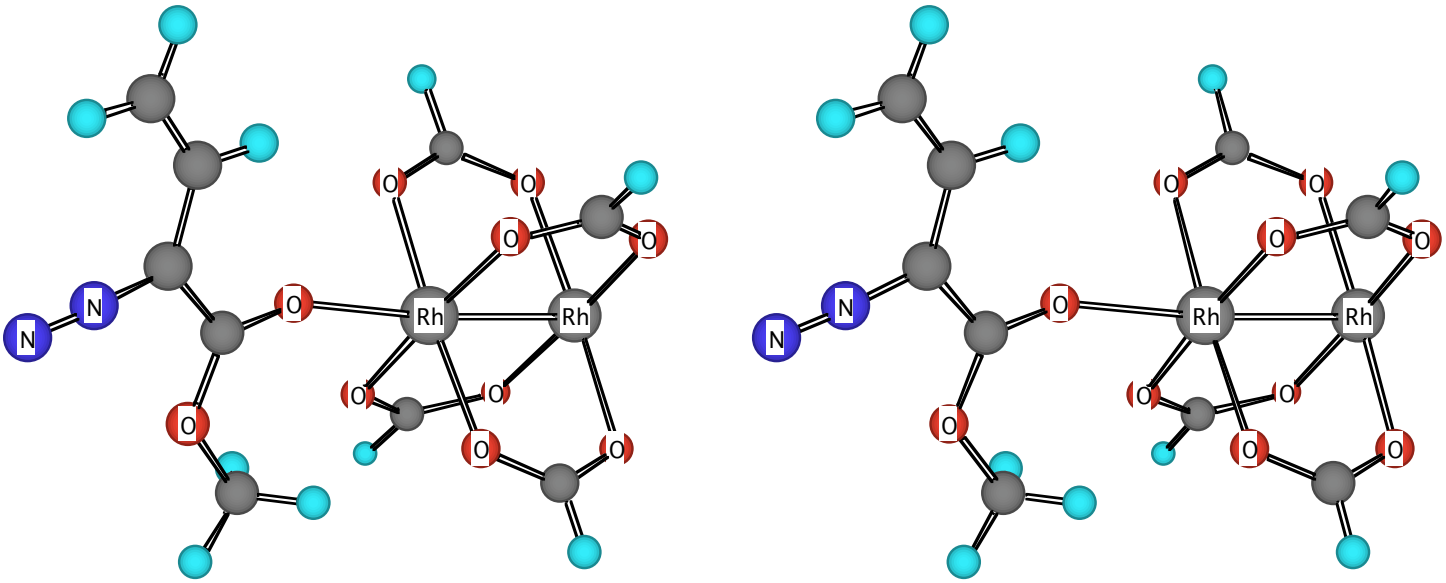
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	126.731	77.951	156.617

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.934715	2.154179	-0.010604
2	8	0	3.925561	1.102016	0.006108

3	6	0	3.483206	-0.160192	-0.017451
4	8	0	2.308641	-0.515939	-0.040771
5	45	0	0.016028	-0.155678	-0.013486
6	8	0	-0.217255	-1.565927	-1.512884
7	6	0	-1.394526	-1.835378	-1.893444
8	8	0	-2.485017	-1.346732	-1.475484
9	45	0	-2.392058	0.078093	0.016741
10	8	0	-2.454062	-1.414116	1.444578
11	6	0	-1.356274	-1.930525	1.806214
12	8	0	-0.187435	-1.646465	1.410368
13	8	0	0.060753	1.356001	-1.444275
14	6	0	-1.044165	1.858029	-1.812717
15	8	0	-2.207322	1.562681	-1.417408
16	8	0	0.090282	1.274369	1.498716
17	6	0	-1.006471	1.762754	1.908572
18	8	0	-2.176158	1.495567	1.513751
19	6	0	4.558361	-1.134478	-0.013416
20	7	0	5.809598	-0.748063	0.007825
21	7	0	6.894312	-0.410036	0.028391
22	1	0	4.363470	-2.196799	-0.028809
23	1	0	-0.979559	2.651019	-2.571718
24	1	0	-0.926365	2.512948	2.708449
25	1	0	-1.424728	-2.726702	2.561096
26	1	0	-1.478753	-2.589309	-2.689000
27	1	0	2.253928	2.049795	0.835632
28	1	0	3.508516	3.078268	0.060840
29	1	0	2.364466	2.120802	-0.940965

Rh2 complex with methyl vinyldiazoacetate (15)



E(RB+HF-LYP) = -1429.85210766

Zero-point correction=	0.213227 (Hartree/Particle)
Thermal correction to Energy=	0.237643
Thermal correction to Enthalpy=	0.238587
Thermal correction to Gibbs Free Energy=	0.158546
Sum of electronic and zero-point Energies=	-1429.638880
Sum of electronic and thermal Energies=	-1429.614464
Sum of electronic and thermal Enthalpies=	-1429.613520
Sum of electronic and thermal Free Energies=	-1429.693562

E (Thermal)	CV	S
KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN

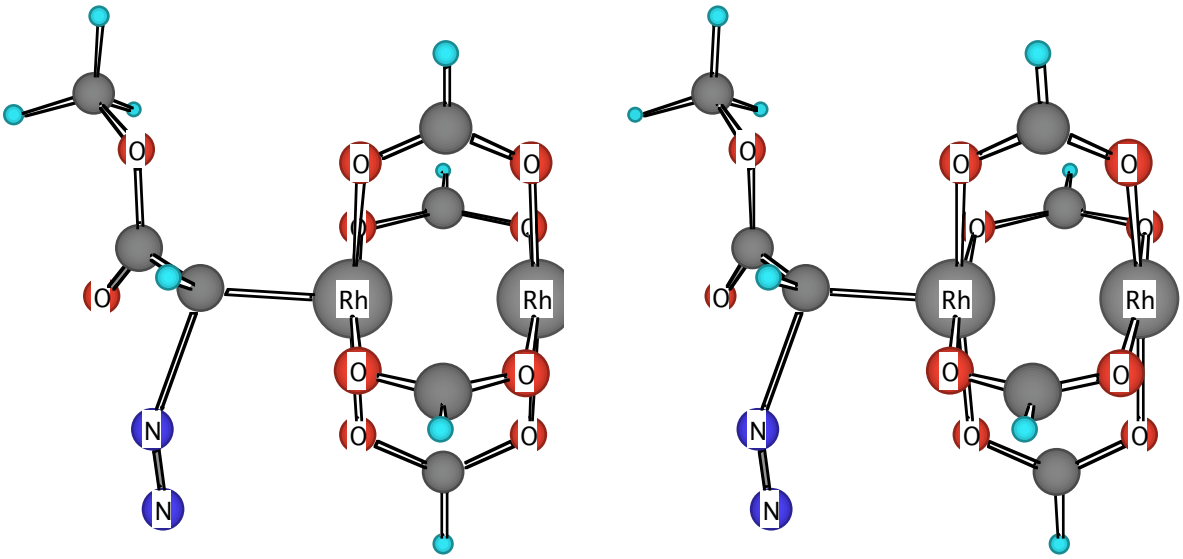
TOTAL 149.123 86.257 168.461

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.783029	1.526009	-1.585375
2	45	0	-0.242831	0.084105	-0.192898
3	45	0	-2.595792	-0.239661	0.260436
4	8	0	-2.999481	1.204250	-1.168297
5	6	0	-2.019414	1.748026	-1.754045
6	8	0	-2.459421	1.232231	1.713454
7	6	0	-1.335080	1.776884	1.898510
8	8	0	-0.241837	1.542285	1.298432
9	8	0	-2.062646	-1.666406	1.661988
10	6	0	-0.830376	-1.899040	1.828501
11	8	0	0.155173	-1.365542	1.237434
12	8	0	-2.611577	-1.689709	-1.212109
13	6	0	-1.525680	-1.929476	-1.816031
14	8	0	-0.394503	-1.387855	-1.639371
15	1	0	-2.270103	2.511395	-2.504499
16	1	0	-1.296093	2.551990	2.677369
17	1	0	-0.581259	-2.660465	2.581314
18	1	0	-1.567736	-2.705989	-2.592873
19	6	0	4.202482	-0.347508	-0.064845
20	6	0	3.108435	0.592187	-0.281497
21	8	0	2.011816	0.219499	-0.692857
22	8	0	3.438075	1.861486	-0.021491
23	6	0	2.419418	2.860943	-0.259155
24	6	0	4.050162	-1.788730	-0.259789
25	6	0	4.997324	-2.723918	-0.118248
26	7	0	5.363418	0.149591	0.313630
27	7	0	6.385636	0.528679	0.634039
28	1	0	1.617749	2.757048	0.473720
29	1	0	2.932983	3.815664	-0.146833
30	1	0	2.012213	2.752488	-1.266847
31	1	0	3.036985	-2.053843	-0.548445
32	1	0	4.765026	-3.769277	-0.288850
33	1	0	6.020735	-2.493063	0.168188

Ts's for loss of nitrogen, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Ts for loss of N2 from complex with Methyl diazoacetate Isomer 1



Key distances C-N 1.985613, N-N 1.106619
E(RB+HF-LYP) = -1352.42173492

Zero-point correction=	0.176661 (Hartree/Particle)
Thermal correction to Energy=	0.199853
Thermal correction to Enthalpy=	0.200797
Thermal correction to Gibbs Free Energy=	0.122924
Sum of electronic and zero-point Energies=	-1352.245074
Sum of electronic and thermal Energies=	-1352.221882
Sum of electronic and thermal Enthalpies=	-1352.220937
Sum of electronic and thermal Free Energies=	-1352.298811

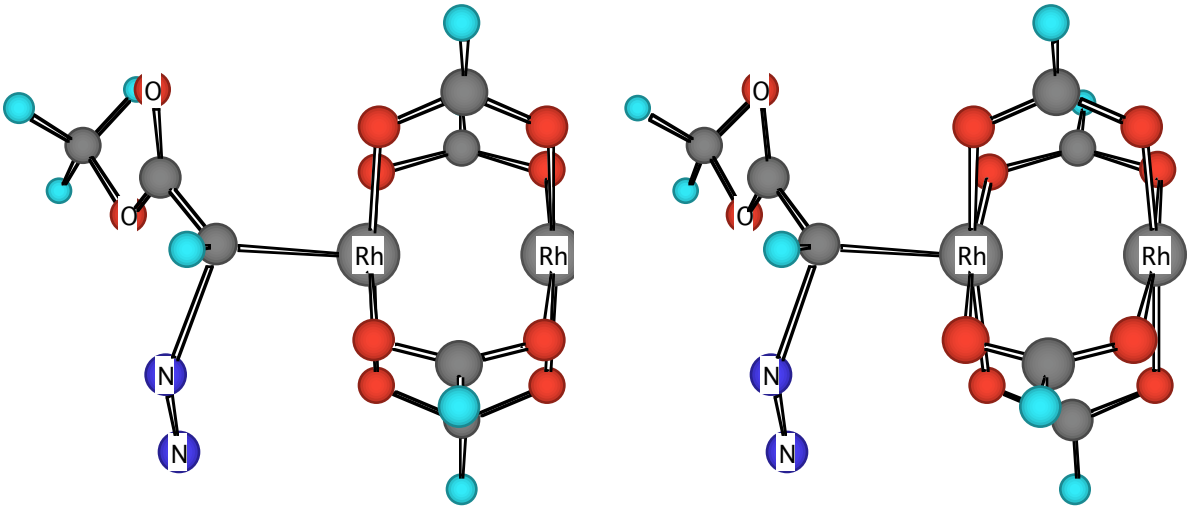
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	125.410	79.804	163.898

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	8	0	O	-0.792084	-1.188711	1.231649
2	45	0	Rh	-0.245573	0.179433	-0.238836
3	6	0	C	-2.158894	0.511567	-0.790173
4	6	0	C	-3.326650	-0.085137	-0.063387
5	8	0	O	-3.938031	0.412916	0.854585
6	8	0	O	-3.539492	-1.306700	-0.577987
7	6	0	C	-4.496342	-2.119924	0.132124
8	1	0	H	-4.178437	-2.252515	1.168735
9	1	0	H	-4.509758	-3.073092	-0.395028
10	1	0	H	-5.481862	-1.648505	0.108711
11	1	0	H	-2.322574	0.674549	-1.858702
12	45	0	Rh	2.100009	-0.364458	0.288445
13	8	0	O	1.381804	-1.693278	1.714733
14	6	0	C	0.134414	-1.793878	1.859790
15	1	0	H	-0.211819	-2.497809	2.630777
16	8	0	O	2.016256	-1.855802	-1.149269
17	6	0	C	0.933725	-2.003979	-1.774334
18	1	0	H	0.911413	-2.799068	-2.533811
19	8	0	O	-0.152391	-1.354147	-1.648997
20	8	0	O	2.630744	1.012705	-1.182442

21	6	0	C	1.718548	1.612475	-1.808013
22	1	0	H	2.041066	2.324403	-2.581694
23	8	0	O	0.456495	1.508648	-1.666765
24	8	0	O	2.046948	1.163281	1.696878
25	6	0	C	0.979291	1.815152	1.825944
26	1	0	H	0.978059	2.619214	2.575707
27	8	0	O	-0.117459	1.668676	1.194755
28	7	0	N	-2.516101	2.415277	-0.353194
29	7	0	N	-2.244263	3.359092	0.156632

Ts for loss of N2 from complex with Methyl diazoacetate Isomer 2 (5)



E(RB+HF-LYP) = -1352.42292228

Zero-point correction= 0.176828 (Hartree/Particle)
Thermal correction to Energy= 0.199976
Thermal correction to Enthalpy= 0.200920
Thermal correction to Gibbs Free Energy= 0.123325
Sum of electronic and zero-point Energies= -1352.246094
Sum of electronic and thermal Energies= -1352.222946
Sum of electronic and thermal Enthalpies= -1352.222002
Sum of electronic and thermal Free Energies= -1352.299597

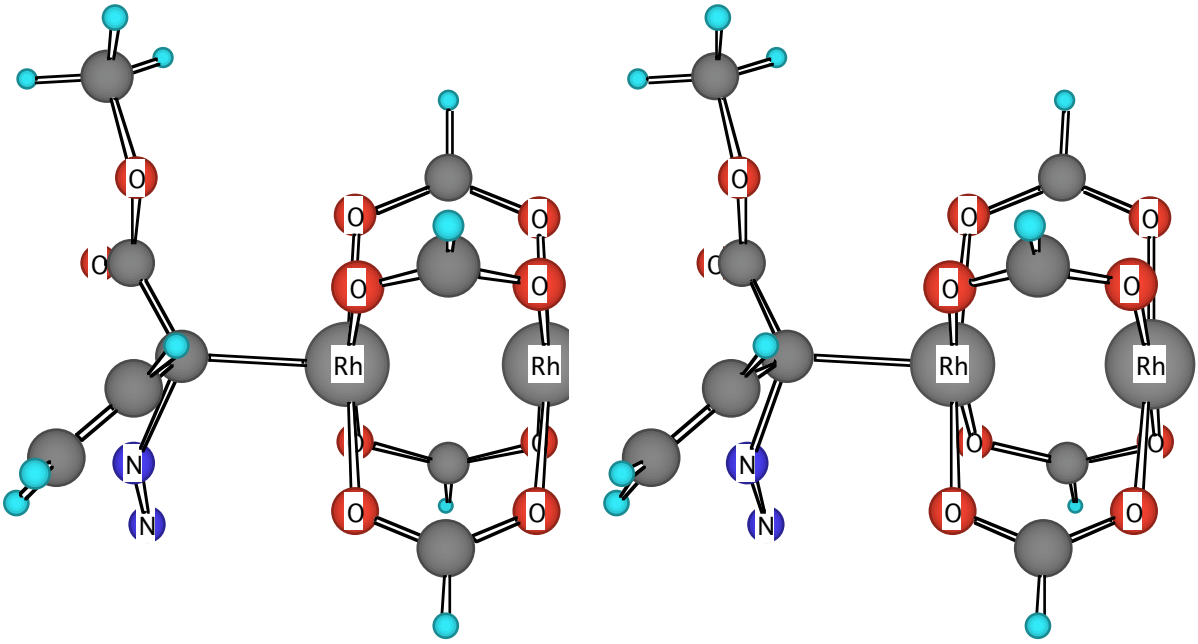
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	125.487	79.816	163.313

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.791131	-1.208031	1.177020
2	45	0	0.215396	0.138588	-0.300566
3	6	0	2.117163	0.356669	-1.008955
4	6	0	3.212598	-0.539393	-0.552216
5	8	0	3.334418	-1.610426	-1.111253
6	8	0	3.917815	-0.119956	0.502420
7	6	0	4.887334	-1.062979	1.005221
8	1	0	5.590092	-1.343773	0.217007
9	1	0	5.399844	-0.543873	1.814316
10	1	0	4.378973	-1.955264	1.377047
11	1	0	2.193754	0.610717	-2.067967
12	45	0	-2.115806	-0.263067	0.391608
13	8	0	-1.370142	-1.590981	1.806357

14	6	0	-0.122657	-1.754636	1.873340
15	1	0	0.235167	-2.462805	2.635199
16	8	0	-2.201180	-1.797550	-0.994802
17	6	0	-1.168109	-2.023990	-1.679317
18	1	0	-1.233149	-2.845187	-2.407522
19	8	0	-0.046943	-1.426732	-1.645499
20	8	0	-2.669417	1.095840	-1.087892
21	6	0	-1.769202	1.628695	-1.788148
22	1	0	-2.105261	2.334203	-2.562122
23	8	0	-0.508050	1.463200	-1.723491
24	8	0	-1.895703	1.300097	1.747297
25	6	0	-0.791719	1.900361	1.785048
26	1	0	-0.702799	2.727508	2.504140
27	8	0	0.253513	1.676112	1.091779
28	7	0	2.694422	2.105403	-0.420758
29	7	0	2.552131	3.008747	0.204714

Ts for loss of N2 from complex with vinyl substrate, Is 1



Key distances C-N 1.894374, N-N 1.107367
E(RB+HF-LYP) = -1429.81841958

Zero-point correction=	0.209499 (Hartree/Particle)
Thermal correction to Energy=	0.235041
Thermal correction to Enthalpy=	0.235985
Thermal correction to Gibbs Free Energy=	0.154068
Sum of electronic and zero-point Energies=	-1429.608921
Sum of electronic and thermal Energies=	-1429.583378
Sum of electronic and thermal Enthalpies=	-1429.582434
Sum of electronic and thermal Free Energies=	-1429.664352

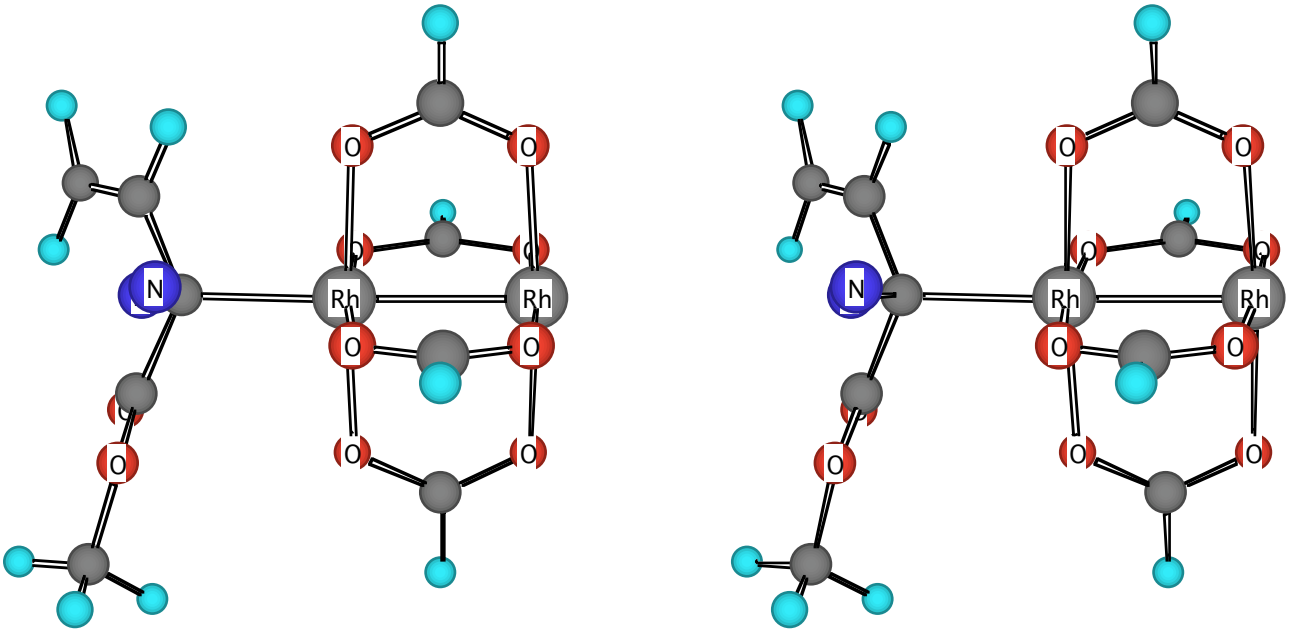
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	147.491	88.886	172.410

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.413562	1.713839	-0.784877

2	45	0	-0.125586	-0.174024	0.056359
3	6	0	-2.179230	-0.473172	0.274548
4	6	0	-3.043414	0.603378	-0.339126
5	8	0	-3.516358	0.592317	-1.452904
6	8	0	-3.154998	1.600611	0.549170
7	6	0	-3.760034	2.809497	0.048541
8	1	0	-3.160170	3.210474	-0.771428
9	1	0	-3.768454	3.496590	0.894052
10	1	0	-4.775614	2.609471	-0.300748
11	6	0	-2.612745	-1.058208	1.547462
12	6	0	-3.386494	-2.120008	1.789723
13	1	0	-2.152904	-0.513765	2.374815
14	1	0	-3.569777	-2.446480	2.807993
15	1	0	-3.832169	-2.713091	0.996080
16	45	0	2.297397	0.291137	-0.043378
17	8	0	1.827682	2.127366	-0.895694
18	6	0	0.612540	2.409494	-1.067813
19	1	0	0.400429	3.388412	-1.522744
20	8	0	2.146767	1.128234	1.851216
21	6	0	1.020740	1.114291	2.412439
22	1	0	0.971449	1.546391	3.422727
23	8	0	-0.082410	0.663272	1.966733
24	8	0	2.586646	-1.584420	0.809367
25	6	0	1.577024	-2.293947	1.061159
26	1	0	1.772960	-3.281880	1.503413
27	8	0	0.348097	-2.024325	0.872909
28	8	0	2.292361	-0.574317	-1.930666
29	6	0	1.202770	-1.005211	-2.388136
30	1	0	1.232467	-1.454703	-3.391037
31	8	0	0.054240	-0.991541	-1.838329
32	7	0	-2.571003	-1.823189	-0.995342
33	7	0	-2.306769	-2.496312	-1.834000

Ts for loss of N2 from complex with Davies' vinyl substrate, Is 2 (9)



E(RB+HF-LYP) = -1429.82283274

Zero-point correction= 0.210500 (Hartree/Particle)
Thermal correction to Energy= 0.235738
Thermal correction to Enthalpy= 0.236682
Thermal correction to Gibbs Free Energy= 0.155761

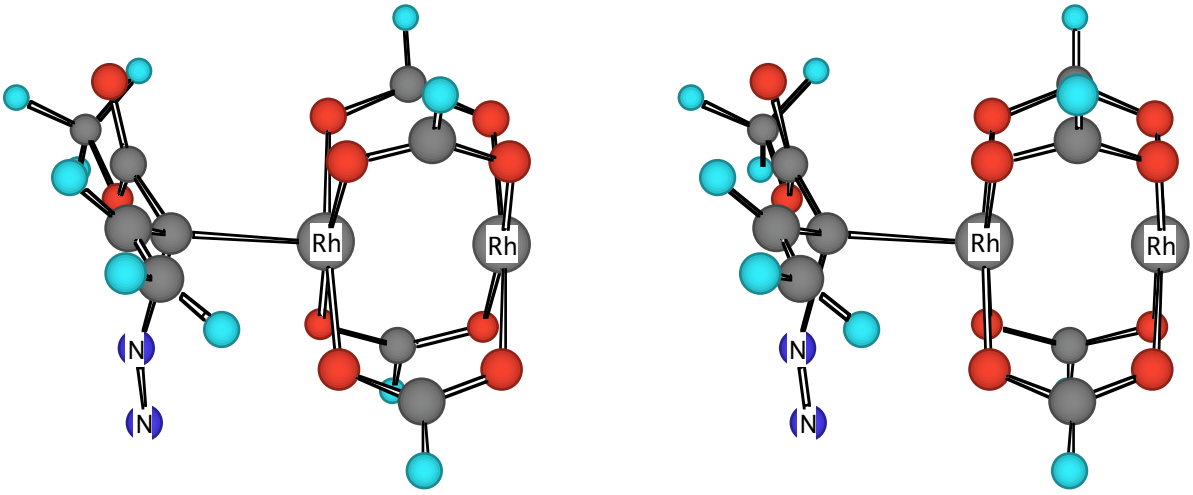
Sum of electronic and zero-point Energies= -1429.612332
Sum of electronic and thermal Energies= -1429.587095
Sum of electronic and thermal Enthalpies= -1429.586151
Sum of electronic and thermal Free Energies= -1429.667071

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	147.928	88.438	170.312

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.125037	-2.383778	-0.299722
2	8	0	-3.446901	-1.275996	0.323341
3	6	0	-3.054721	-0.303351	-0.514536
4	8	0	-3.297434	-0.277410	-1.703410
5	6	0	-2.176475	0.730116	0.122306
6	6	0	-2.433133	2.156029	-0.098114
7	6	0	-3.205284	2.655352	-1.076048
8	45	0	-0.106184	0.200266	0.071651
9	8	0	-0.021010	-0.737869	1.924980
10	6	0	1.085783	-1.237133	2.306703
11	8	0	2.189454	-1.243250	1.702912
12	45	0	2.290274	-0.328202	-0.161553
13	8	0	2.676863	1.499851	0.756303
14	6	0	1.705038	2.217878	1.108158
15	8	0	0.459887	1.986468	0.980680
16	8	0	-0.496777	-1.637501	-0.825618
17	6	0	0.491668	-2.351110	-1.184866
18	8	0	1.722534	-2.111116	-1.062186
19	8	0	0.029148	1.103050	-1.797451
20	6	0	1.149938	1.098660	-2.393680
21	8	0	2.246235	0.611239	-2.005875
22	7	0	-2.554363	0.537279	1.879231
23	7	0	-2.321386	0.403899	2.956041
24	1	0	-5.019164	-2.039390	-0.824866
25	1	0	-4.390338	-3.054137	0.517378
26	1	0	-3.452969	-2.877653	-1.004790
27	1	0	-1.821232	2.822569	0.504950
28	1	0	-3.224858	3.726293	-1.257209
29	1	0	-3.770056	2.020945	-1.748985
30	1	0	0.228540	-3.305476	-1.664530
31	1	0	1.156114	1.588299	-3.378426
32	1	0	1.954694	3.174242	1.591142
33	1	0	1.062800	-1.722525	3.293394

Ts for loss of N2 from complex with Davies' vinyl substrate, Is 3



Key distances C-N 1.786, N-N 1.110
E(RB+HF-LYP) = -1429.82071517

Zero-point correction=	0.210140 (Hartree/Particle)
Thermal correction to Energy=	0.235593
Thermal correction to Enthalpy=	0.236538
Thermal correction to Gibbs Free Energy=	0.154881
Sum of electronic and zero-point Energies=	-1429.610576
Sum of electronic and thermal Energies=	-1429.585122
Sum of electronic and thermal Enthalpies=	-1429.584177
Sum of electronic and thermal Free Energies=	-1429.665834

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	147.837	88.617	171.861

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.022153	-2.471348	0.180142
2	8	0	-3.347276	-1.241391	0.505724
3	6	0	-3.082218	-0.445873	-0.539182
4	6	0	-2.222712	0.743371	-0.227675
5	45	0	-0.142558	0.204387	-0.050196
6	8	0	0.261463	1.063991	-1.901304
7	6	0	1.444758	0.998106	-2.357938
8	8	0	2.466126	0.478949	-1.830548
9	45	0	2.241394	-0.418146	0.023913
10	8	0	1.727572	-2.195991	-0.911148
11	6	0	0.512095	-2.393612	-1.179310
12	8	0	-0.483242	-1.635024	-0.958588
13	8	0	-3.422072	-0.659641	-1.684585
14	6	0	-2.631746	1.967003	-0.938162
15	6	0	-1.969215	3.131230	-0.870409
16	8	0	-0.334797	-0.696820	1.816714
17	6	0	0.698066	-1.224780	2.338448
18	8	0	1.868763	-1.283586	1.877506
19	8	0	0.387616	1.978911	0.915536
20	6	0	1.618207	2.165456	1.188437
21	8	0	2.595106	1.408507	0.957218
22	7	0	-2.604774	1.057327	1.488804
23	7	0	-2.403181	1.330783	2.545248
24	1	0	-4.976200	-2.266089	-0.311886
25	1	0	-4.178810	-2.975082	1.133543

26	1	0	-3.393606	-3.073897	-0.479265
27	1	0	-3.512925	1.872613	-1.570663
28	1	0	-2.321519	3.997085	-1.424169
29	1	0	-1.077839	3.246941	-0.263083
30	1	0	0.270914	-3.347999	-1.670042
31	1	0	1.590412	1.460828	-3.345146
32	1	0	1.845332	3.115956	1.693670
33	1	0	0.537760	-1.688487	3.323139

Rh-Carbene complexes, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Carbomethoxy carbene from methyl diazoacetate (6)

C-Rh 1.939647
E(RB+HF-LYP) = -1242.90804704

Zero-point correction= 0.168963 (Hartree/Particle)
Thermal correction to Energy= 0.189814
Thermal correction to Enthalpy= 0.190758
Thermal correction to Gibbs Free Energy= 0.118533
Sum of electronic and zero-point Energies= -1242.739084
Sum of electronic and thermal Energies= -1242.718233
Sum of electronic and thermal Enthalpies= -1242.717289
Sum of electronic and thermal Free Energies= -1242.789514

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	119.110	72.950	152.011

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.347218	-0.442758	-0.180822
2	45	0	-1.897259	0.517853	0.223492
3	8	0	-0.129321	-1.871612	1.237163
4	6	0	-1.269559	-1.818808	1.801714
5	8	0	-2.194103	-0.985482	1.620494
6	1	0	-1.452245	-2.611335	2.541202
7	8	0	0.573062	1.102929	-1.571365
8	6	0	-0.372166	1.937140	-1.746116
9	8	0	-1.495969	1.981261	-1.184447
10	1	0	-0.161602	2.717302	-2.491833
11	8	0	-0.509976	-1.631437	-1.647656
12	6	0	-1.762176	-1.510972	-1.852440
13	8	0	-2.584501	-0.750719	-1.279439
14	1	0	-2.163976	-2.166410	-2.638659
15	8	0	1.065257	0.798261	1.319075
16	6	0	0.232203	1.566776	1.900724
17	8	0	-1.001994	1.693339	1.692182
18	1	0	0.663778	2.199851	2.689697
19	6	0	2.103694	-1.088293	-0.691021
20	1	0	2.174236	-1.867151	-1.457595
21	6	0	3.383486	-0.598669	-0.172939
22	8	0	4.000755	-1.383473	0.529211
23	8	0	3.719870	0.652212	-0.456354
24	6	0	4.932405	1.133031	0.166195
25	1	0	5.778052	0.494722	-0.100282
26	1	0	4.810795	1.149176	1.251648
27	1	0	5.070843	2.141100	-0.221942

Carbomethoxy vinylcarbene from methyl vinyldiazoacetate ls1

E(RB+HF-LYP) = -1320.32510976

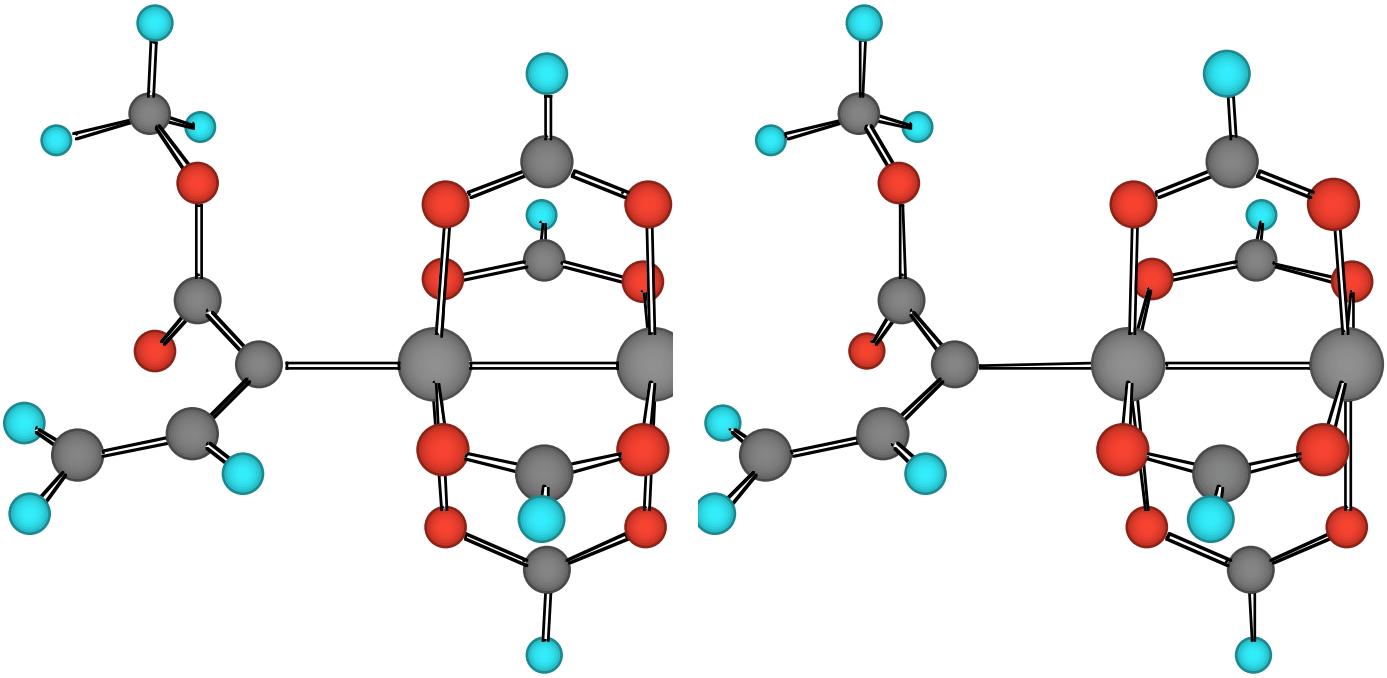
Zero-point correction= 0.202833 (Hartree/Particle)
Thermal correction to Energy= 0.226157
Thermal correction to Enthalpy= 0.227101
Thermal correction to Gibbs Free Energy= 0.149331
Sum of electronic and zero-point Energies= -1320.122277
Sum of electronic and thermal Energies= -1320.098953
Sum of electronic and thermal Enthalpies= -1320.098008
Sum of electronic and thermal Free Energies= -1320.175779

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	141.916	81.449	163.681

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.408525	-2.033536	-0.425284
2	8	0	-3.460388	-0.993280	-0.740337
3	6	0	-3.232319	-0.112793	0.232692
4	8	0	-3.774086	-0.098925	1.322783
5	6	0	-2.192159	0.906716	-0.068921
6	6	0	-2.682600	2.248487	-0.100367
7	6	0	-1.887459	3.313759	-0.376736
8	45	0	-0.276389	0.287326	-0.057049
9	8	0	-0.723774	-1.126738	1.394802
10	6	0	0.218624	-1.850790	1.851606
11	8	0	1.437795	-1.842920	1.542775
12	45	0	2.072010	-0.506009	0.083399
13	8	0	2.374296	0.939069	1.549511
14	6	0	1.412451	1.688114	1.856617
15	8	0	0.226563	1.692762	1.390737
16	8	0	-0.548718	-1.163380	-1.522237
17	6	0	0.435191	-1.903314	-1.839549
18	8	0	1.608936	-1.897888	-1.382929
19	8	0	0.389777	1.617234	-1.526397
20	6	0	1.624107	1.604047	-1.846666
21	8	0	2.546280	0.883274	-1.390808
22	1	0	-4.028363	-2.648448	0.394008
23	1	0	-4.503035	-2.621365	-1.337421
24	1	0	-5.371322	-1.602461	-0.139368
25	1	0	-3.741118	2.416604	0.103219
26	1	0	-2.303437	4.317556	-0.414964
27	1	0	-0.833693	3.189386	-0.592583
28	1	0	-0.090085	-2.575316	2.619311
29	1	0	1.607088	2.447802	2.628076
30	1	0	0.218651	-2.646549	-2.621334
31	1	0	1.905043	2.325722	-2.628251

Carbomethoxy vinylcarbene from methyl vinyldiazoacetate ls2 (10)



E(RB+HF-LYP) = -1320.32616013

Zero-point correction= 0.203052 (Hartree/Particle)
Thermal correction to Energy= 0.226317
Thermal correction to Enthalpy= 0.227261
Thermal correction to Gibbs Free Energy= 0.149639
Sum of electronic and zero-point Energies= -1320.123108
Sum of electronic and thermal Energies= -1320.099843
Sum of electronic and thermal Enthalpies= -1320.098899
Sum of electronic and thermal Free Energies= -1320.176521

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	142.016	81.270	163.369

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.233795	-2.240716	-0.368652
2	8	0	-3.366737	-1.139929	-0.709653
3	6	0	-3.168812	-0.242291	0.258626
4	8	0	-3.706818	-0.244583	1.350179
5	6	0	-2.158640	0.784549	-0.100024
6	6	0	-2.577003	2.121480	-0.391727
7	6	0	-3.834715	2.577581	-0.166799
8	45	0	-0.236727	0.274232	-0.031111
9	8	0	-0.661916	-1.577755	0.808922
10	6	0	0.315660	-2.347458	1.080348
11	8	0	1.545640	-2.152890	0.902735
12	45	0	2.160537	-0.358018	0.045839
13	8	0	2.244648	0.499513	1.934006
14	6	0	1.192242	1.008352	2.398716
15	8	0	0.040286	1.081197	1.862561
16	8	0	-0.258542	-0.583351	-1.928564
17	6	0	0.807096	-1.107438	-2.384393
18	8	0	1.940448	-1.187823	-1.843476
19	8	0	0.363640	2.081143	-0.874906
20	6	0	1.609968	2.267934	-1.067913

21	8	0	2.568671	1.496401	-0.814602
22	1	0	-3.800973	-2.810530	0.456740
23	1	0	-4.292251	-2.849121	-1.270338
24	1	0	-5.223771	-1.877126	-0.081966
25	1	0	-1.806453	2.802772	-0.743103
26	1	0	-4.088815	3.621315	-0.333047
27	1	0	-4.614544	1.938129	0.236308
28	1	0	0.031961	-3.310193	1.530700
29	1	0	1.261256	1.454386	3.401550
30	1	0	0.709499	-1.545367	-3.388779
31	1	0	1.866075	3.238769	-1.517557

Pi Complex for Interaction of vinylcarbenoid with styrene, B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

E(RB+HF-LYP) = -1629.97239114

Zero-point correction= 0.337878 (Hartree/Particle)
Thermal correction to Energy= 0.369866
Thermal correction to Enthalpy= 0.370810
Thermal correction to Gibbs Free Energy= 0.271242
Sum of electronic and zero-point Energies= -1629.634513
Sum of electronic and thermal Energies= -1629.602525
Sum of electronic and thermal Enthalpies= -1629.601581
Sum of electronic and thermal Free Energies= -1629.701149

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	232.095	113.114	209.559

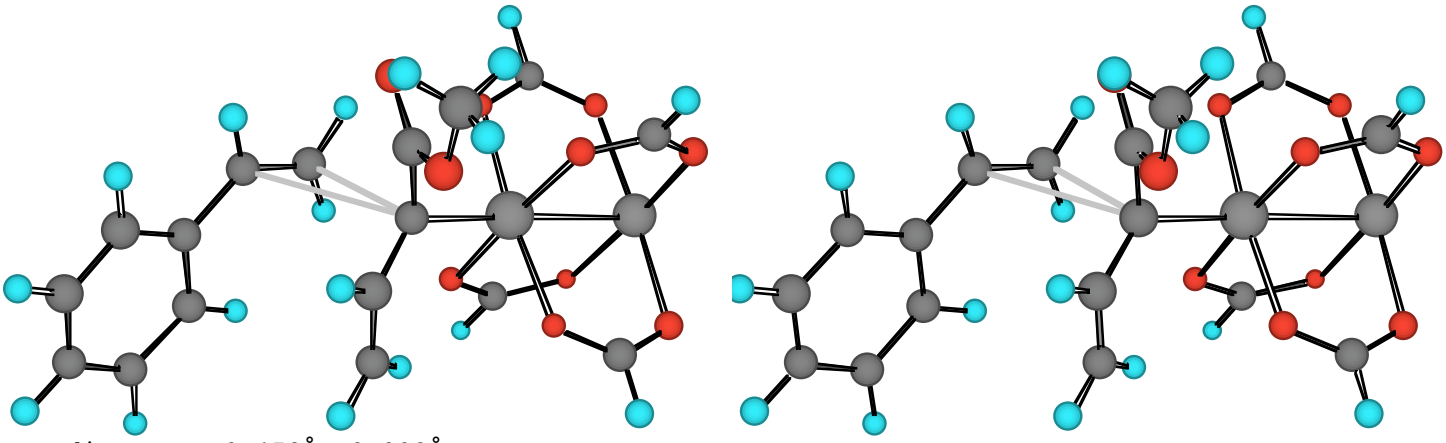
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.777755	-2.348679	0.270438
2	6	0	-4.076291	-1.346764	-0.399444
3	6	0	-4.717659	-0.148677	-0.777760
4	6	0	-6.078470	0.001097	-0.454506
5	6	0	-6.778073	-1.000293	0.216931
6	6	0	-6.129997	-2.181927	0.583075
7	6	0	-4.030889	0.941375	-1.485368
8	6	0	-2.749478	0.975880	-1.882354
9	6	0	-0.735556	1.354116	0.909548
10	6	0	-1.880604	0.973874	1.667516
11	6	0	-2.167292	-0.318739	1.977913
12	45	0	0.794358	0.188700	0.280838
13	8	0	-0.406406	-1.419910	-0.328100
14	6	0	0.163275	-2.456002	-0.810418
15	8	0	1.387962	-2.670893	-0.978749
16	45	0	2.740795	-1.187168	-0.428847
17	8	0	2.554467	-0.335960	-2.312595
18	6	0	1.626485	0.494395	-2.495805
19	8	0	0.757267	0.915794	-1.668773
20	6	0	-0.550195	2.825460	0.777861
21	8	0	-0.572927	3.296364	-0.469903
22	6	0	-0.299126	4.705078	-0.603241
23	8	0	0.996626	-0.696898	2.153669
24	6	0	1.936832	-1.537864	2.332479
25	8	0	2.795023	-1.945274	1.508793
26	8	0	2.161937	1.660412	0.793216
27	6	0	3.401693	1.426784	0.621086

28	8	0	3.952217	0.392277	0.164034
29	8	0	-0.354834	3.490006	1.779205
30	1	0	-1.024562	5.293651	-0.035707
31	1	0	-0.381897	4.913760	-1.669417
32	1	0	0.708337	4.926291	-0.243067
33	1	0	-2.552968	1.757680	2.017627
34	1	0	-3.054347	-0.566172	2.553592
35	1	0	-1.524949	-1.130585	1.662207
36	1	0	4.068834	2.249386	0.917527
37	1	0	1.991803	-1.957311	3.348068
38	1	0	-0.522855	-3.260386	-1.115579
39	1	0	1.546092	0.921640	-3.506602
40	1	0	-2.054280	0.157740	-1.722801
41	1	0	-2.346756	1.846553	-2.388977
42	1	0	-4.658560	1.807832	-1.696043
43	1	0	-6.590507	0.917612	-0.739143
44	1	0	-7.829684	-0.859190	0.452248
45	1	0	-6.672746	-2.966260	1.103499
46	1	0	-4.267007	-3.267905	0.546738
47	1	0	-3.027864	-1.495310	-0.637833

Ts's for cyclopropanation of styrene, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Vinylcarbene + styrene, Ts1a (C=O toward styrene, vinyl rotated toward Rh)



Key distances 2.478Å, 2.993Å
E(RB+HF-LYP) = -1629.96825158

Zero-point correction= 0.338231 (Hartree/Particle)
Thermal correction to Energy= 0.368823
Thermal correction to Enthalpy= 0.369767
Thermal correction to Gibbs Free Energy= 0.275663
Sum of electronic and zero-point Energies= -1629.630020
Sum of electronic and thermal Energies= -1629.599429
Sum of electronic and thermal Enthalpies= -1629.598484
Sum of electronic and thermal Free Energies= -1629.692588

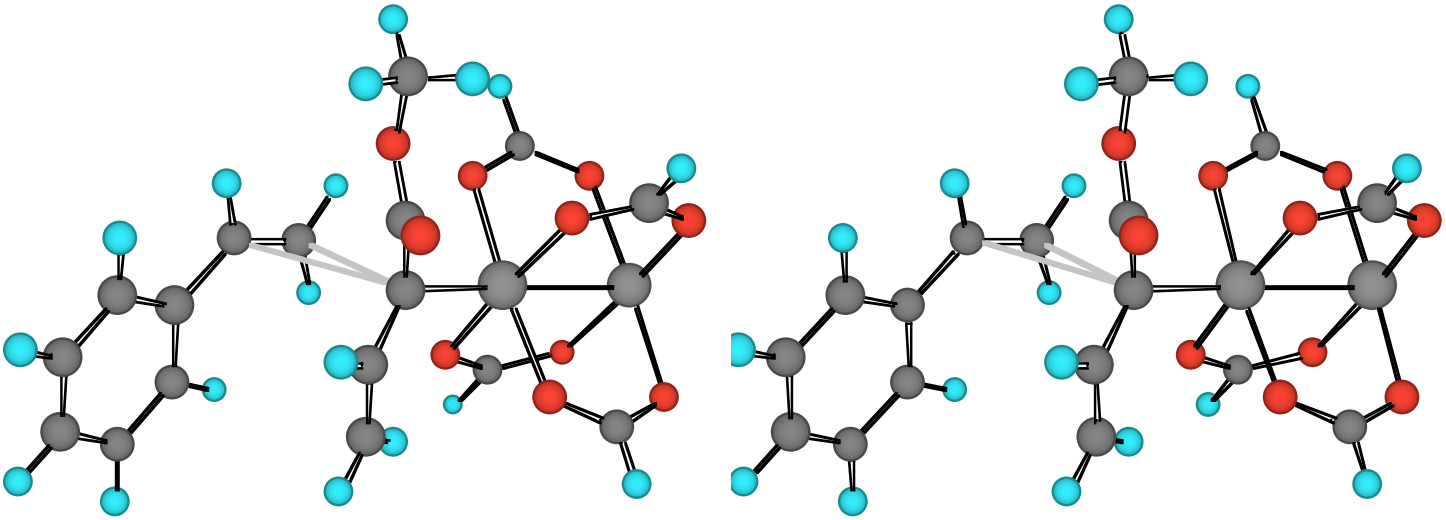
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.440	110.834	198.058

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.022305	4.507163	0.672513
2	8	0	-1.175798	3.107245	0.965153
3	6	0	-1.270657	2.298902	-0.114978
4	8	0	-1.371925	2.704221	-1.253731
5	6	0	-1.154519	0.871267	0.340184
6	6	0	-2.065669	0.466041	1.378396
7	6	0	-2.040446	-0.755919	1.958543
8	45	0	0.742190	0.078018	0.070919
9	8	0	0.778845	0.278819	-2.001675
10	6	0	1.838310	-0.034907	-2.630464
11	8	0	2.921936	-0.481857	-2.171615
12	45	0	3.079602	-0.751500	-0.119329
13	8	0	2.279585	-2.663887	-0.320264
14	6	0	1.032498	-2.806854	-0.280572
15	8	0	0.131485	-1.916443	-0.131951
16	8	0	1.565170	1.979940	0.250448
17	6	0	2.830349	2.106881	0.215004
18	8	0	3.710589	1.216769	0.086988
19	8	0	0.944935	-0.205924	2.127736
20	6	0	2.048231	-0.648307	2.579958
21	8	0	3.090042	-0.964391	1.948618
22	6	0	-2.203289	-0.174936	-1.646240
23	6	0	-3.471415	0.276504	-1.459179
24	6	0	-4.554202	-0.407138	-0.766023
25	1	0	-0.128365	4.665125	0.064514
26	1	0	-0.921388	4.996486	1.641370
27	1	0	-1.896581	4.885836	0.136573
28	1	0	-2.814067	1.185056	1.713112
29	1	0	-2.739925	-1.007040	2.751144
30	1	0	-1.329769	-1.513256	1.648971
31	1	0	3.193082	3.141083	0.312360
32	1	0	2.084760	-0.768172	3.673377
33	1	0	0.654410	-3.835064	-0.387763
34	1	0	1.789155	0.104903	-3.720588
35	1	0	-1.881249	-1.163738	-1.338161
36	1	0	-1.498656	0.398413	-2.234006
37	1	0	-3.706839	1.272633	-1.830651
38	6	0	-5.788940	0.256211	-0.607681
39	6	0	-6.849852	-0.348355	0.059065
40	6	0	-6.701591	-1.634722	0.587151
41	6	0	-5.486139	-2.309022	0.441038
42	6	0	-4.422710	-1.705607	-0.226012
43	1	0	-5.905403	1.256520	-1.017936
44	1	0	-7.793019	0.180035	0.167357
45	1	0	-7.530061	-2.110211	1.104854
46	1	0	-5.369351	-3.311623	0.843431
47	1	0	-3.492218	-2.249463	-0.351352

Vinylcarbene + styrene, Ts1b (C=O away from styrene, vinyl rotated toward Rh) (11)



Key distances 2.430, 2.938
E(RB+HF-LYP) = -1629.96893001

Zero-point correction=	0.338557 (Hartree/Particle)
Thermal correction to Energy=	0.369047
Thermal correction to Enthalpy=	0.369992
Thermal correction to Gibbs Free Energy=	0.276521
Sum of electronic and zero-point Energies=	-1629.630373
Sum of electronic and thermal Energies=	-1629.599883
Sum of electronic and thermal Enthalpies=	-1629.598938
Sum of electronic and thermal Free Energies=	-1629.692409

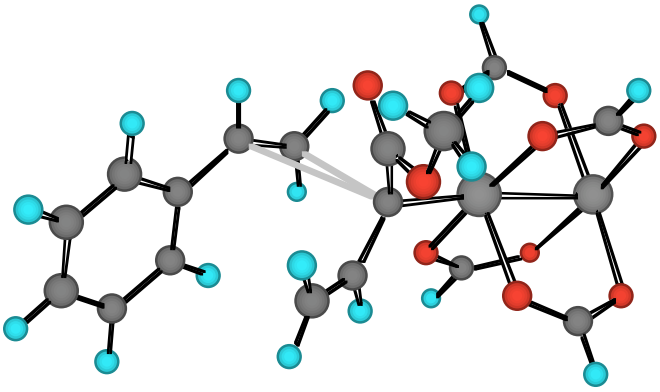
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.581	110.689	196.726

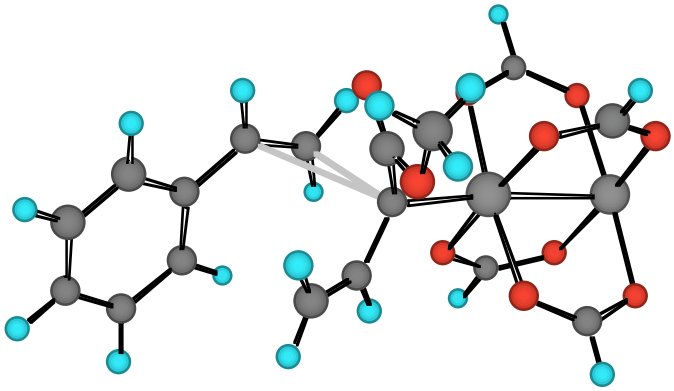
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.496221	-1.607213	-0.591702
2	6	0	-4.558171	-0.206452	-0.760525
3	6	0	-5.744965	0.456904	-0.384525
4	6	0	-6.823753	-0.244179	0.144454
5	6	0	-6.743190	-1.630681	0.307666
6	6	0	-5.578276	-2.307478	-0.064289
7	6	0	-3.449793	0.578149	-1.284214
8	6	0	-2.192164	0.140959	-1.566512
9	6	0	-1.193431	0.617752	0.596688
10	45	0	0.747550	0.030876	0.131262
11	8	0	0.938453	-0.833711	2.016149
12	6	0	2.051122	-1.353122	2.346478
13	8	0	3.113489	-1.433587	1.676572
14	45	0	3.129039	-0.597158	-0.225571
15	8	0	3.641594	1.239938	0.597756
16	6	0	2.713913	2.015406	0.946316
17	8	0	1.456638	1.835698	0.877992
18	6	0	-1.380670	2.103921	0.691218
19	8	0	-1.554267	2.638177	1.771740
20	8	0	-1.244595	2.776278	-0.462200
21	6	0	-1.218274	4.208064	-0.334639
22	6	0	-2.052741	-0.123128	1.486027
23	6	0	-1.987922	-1.463319	1.648307
24	8	0	0.804318	0.825473	-1.802279

25	6	0	1.894897	0.772766	-2.453558
26	8	0	2.998874	0.281471	-2.102250
27	8	0	0.249596	-1.842159	-0.667040
28	6	0	1.197232	-2.600462	-1.058117
29	8	0	2.435564	-2.392276	-1.025609
30	1	0	-2.139457	4.574494	0.126646
31	1	0	-1.119445	4.587041	-1.352000
32	1	0	-0.364489	4.512898	0.275192
33	1	0	-2.787892	0.443040	2.057424
34	1	0	-2.657334	-1.969523	2.338355
35	1	0	-1.276260	-2.067416	1.097126
36	1	0	3.019156	2.984393	1.368599
37	1	0	2.075419	-1.790280	3.356024
38	1	0	0.874733	-3.564956	-1.479499
39	1	0	1.857690	1.218971	-3.459019
40	1	0	-1.907532	-0.903209	-1.498633
41	1	0	-1.465009	0.800700	-2.022067
42	1	0	-3.654658	1.639440	-1.418750
43	1	0	-5.808248	1.535363	-0.508474
44	1	0	-7.727324	0.286988	0.430243
45	1	0	-7.585641	-2.180864	0.717534
46	1	0	-5.515886	-3.385949	0.052418
47	1	0	-3.607212	-2.148195	-0.898278

Vinylcarbene + styrene, Ts1c (C=O toward styrene, vinyl rotated away from Rh)





Key distances 2.463, 3.000
E(RB+HF-LYP) = -1629.96815180

Zero-point correction= 0.338356 (Hartree/Particle)
Thermal correction to Energy= 0.368973
Thermal correction to Enthalpy= 0.369917
Thermal correction to Gibbs Free Energy= 0.275343
Sum of electronic and zero-point Energies= -1629.629796
Sum of electronic and thermal Energies= -1629.599179
Sum of electronic and thermal Enthalpies= -1629.598234
Sum of electronic and thermal Free Energies= -1629.692809

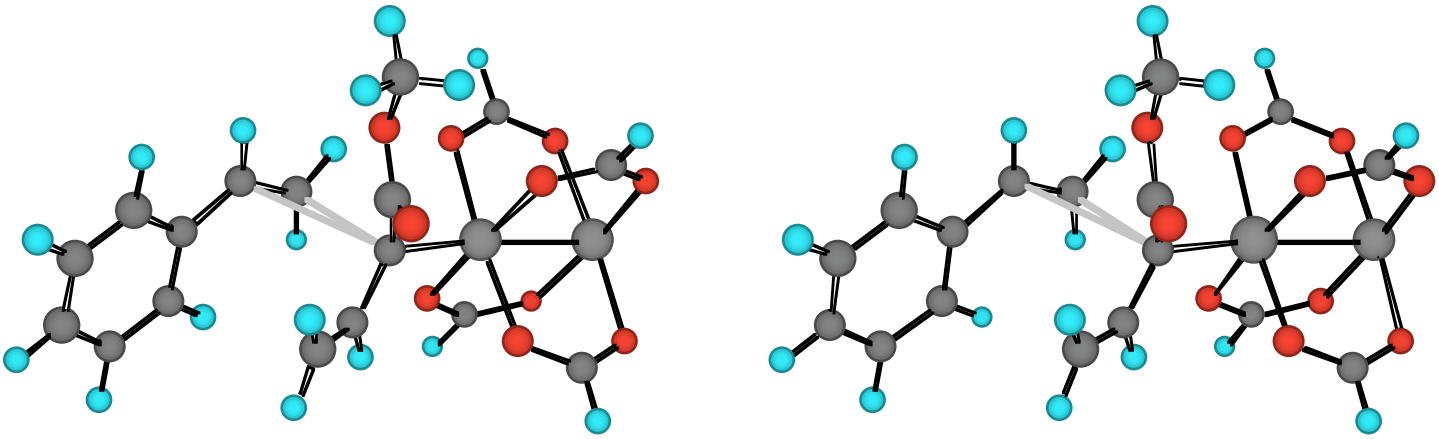
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.534	110.726	199.050

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.569707	-1.741486	0.089124
2	6	0	-4.569376	-0.621847	-0.772924

3	6	0	-5.766313	0.116093	-0.901268
4	6	0	-6.917312	-0.254143	-0.213066
5	6	0	-6.900239	-1.372786	0.625748
6	6	0	-5.723053	-2.112338	0.774529
7	6	0	-3.400727	-0.195181	-1.524880
8	6	0	-2.154999	-0.740435	-1.502035
9	6	0	-1.147960	0.637653	0.274159
10	45	0	0.806481	0.046702	0.034426
11	8	0	1.046652	0.191258	2.100803
12	6	0	2.191018	-0.043957	2.603571
13	8	0	3.254510	-0.383651	2.022347
14	45	0	3.195949	-0.629015	-0.039937
15	8	0	3.662624	1.378170	-0.294431
16	6	0	2.719559	2.212001	-0.320207
17	8	0	1.469271	2.008826	-0.206432
18	6	0	-1.452818	2.019748	-0.213562
19	8	0	-1.724075	2.346321	-1.350289
20	8	0	-1.272412	2.900524	0.797849
21	6	0	-1.222918	4.283247	0.402503
22	6	0	-1.881510	0.034295	1.354243
23	6	0	-2.953778	0.576863	1.975273
24	8	0	0.809984	-0.169158	-2.037421
25	6	0	1.880528	-0.543976	-2.614287
26	8	0	2.994100	-0.821408	-2.098713
27	8	0	0.333221	-1.969242	0.272868
28	6	0	1.294471	-2.806064	0.310656
29	8	0	2.529079	-2.592098	0.216997
30	1	0	-0.406830	4.437569	-0.307031
31	1	0	-1.043826	4.839630	1.322735
32	1	0	-2.166948	4.587931	-0.056607
33	1	0	-1.503240	-0.926112	1.696501
34	1	0	-3.418401	0.080783	2.823008
35	1	0	-3.369768	1.535061	1.680704
36	1	0	3.006031	3.265389	-0.458999
37	1	0	2.245665	0.066724	3.697090
38	1	0	0.988338	-3.854939	0.443758
39	1	0	1.809996	-0.635078	-3.708394
40	1	0	-1.921287	-1.656039	-0.968340
41	1	0	-1.381995	-0.362766	-2.159522
42	1	0	-3.538127	0.697041	-2.131161
43	1	0	-5.780972	0.982567	-1.557867
44	1	0	-7.828973	0.324890	-0.331049
45	1	0	-7.799416	-1.667295	1.159849
46	1	0	-5.706455	-2.982649	1.424853
47	1	0	-3.665999	-2.331055	0.204357

Vinylcarbene + styrene, Ts1d (C=O away from styrene, vinyl rotated away from Rh)



Key distances 2.408, 2.950
E(RB+HF-LYP) = -1629.96829250

Zero-point correction=	.338569 (Hartree/Particle)
Thermal correction to Energy=	.369131
Thermal correction to Enthalpy=	.370075
Thermal correction to Gibbs Free Energy=	.275935
Sum of electronic and zero-point Energies=	-1629.629723
Sum of electronic and thermal Energies=	-1629.599161
Sum of electronic and thermal Enthalpies=	-1629.598217
Sum of electronic and thermal Free Energies=	-1629.692357

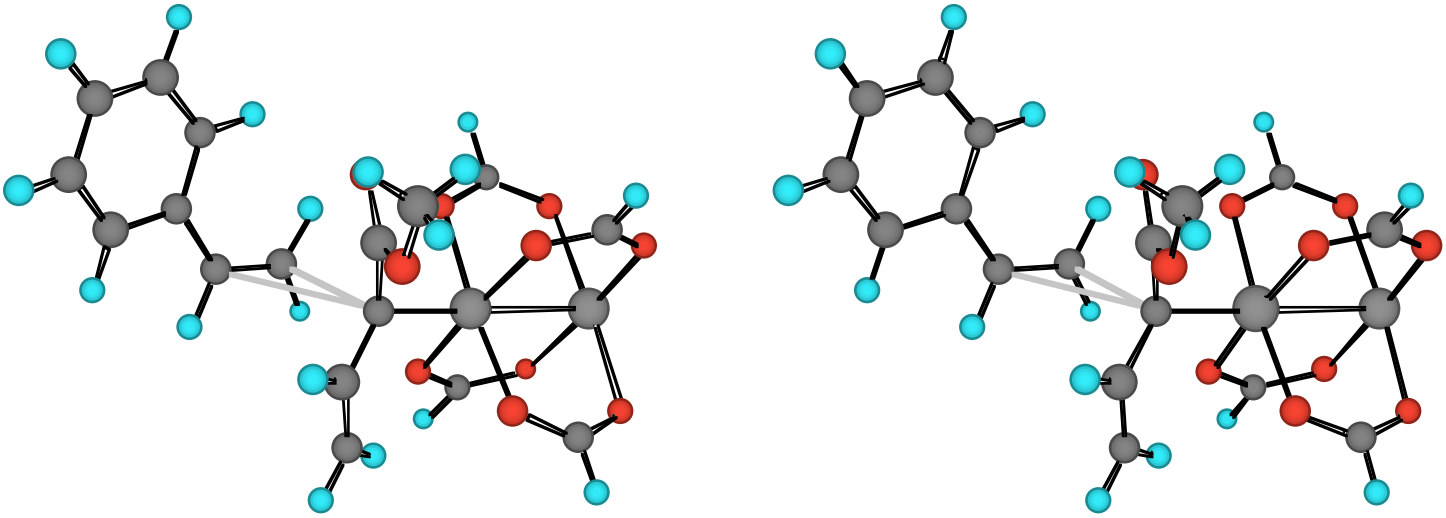
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.633	110.655	198.135

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.557248	3.952249	-.392003
2	8	0	-1.495597	2.520636	-.510780
3	6	0	-1.500551	1.854624	.658002
4	8	0	-1.643616	2.395611	1.739834
5	6	0	-1.163985	.402955	.534745
6	6	0	-1.846419	-.573270	1.346755
7	6	0	-2.884442	-.331105	2.178902
8	45	0	.813389	.008896	.101692
9	8	0	.797409	.474123	-1.937739
10	6	0	1.875709	.353044	-2.602069
11	8	0	3.007494	-.019425	-2.200695
12	45	0	3.229836	-.495173	-.188196
13	8	0	2.653302	-2.464612	-.585233
14	6	0	1.430590	-2.753570	-.567888
15	8	0	.433162	-1.995567	-.332401
16	8	0	1.382380	1.971238	.510064
17	6	0	2.621513	2.255955	.486006
18	8	0	3.601243	1.505464	.237802
19	8	0	1.079076	-.510601	2.101169
20	6	0	2.237654	-.848629	2.500910
21	8	0	3.305616	-.936757	1.841147
22	6	0	-2.140565	-.286592	-1.555112
23	6	0	-3.378091	.264747	-1.409311
24	6	0	-4.560706	-.343471	-.824884
25	1	0	-2.472657	4.262104	.119581
26	1	0	-1.541787	4.327813	-1.415347
27	1	0	-.691386	4.316217	.165718
28	1	0	-1.444299	-1.582000	1.286484
29	1	0	-3.295227	-1.125785	2.795890
30	1	0	-3.306640	.660052	2.300590
31	1	0	2.858681	3.306156	.713762
32	1	0	2.301521	-1.096813	3.570989
33	1	0	1.172823	-3.801684	-.784377
34	1	0	1.795025	.610692	-3.669026
35	1	0	-1.934892	-1.329164	-1.335474
36	1	0	-1.358987	.248947	-2.079239
37	1	0	-3.498652	1.300326	-1.720664
38	6	0	-5.728952	.437605	-.686545
39	6	0	-6.891923	-.097498	-.143147
40	6	0	-6.916648	-1.431194	.276886
41	6	0	-5.769777	-2.220832	.154109
42	6	0	-4.603203	-1.685587	-.384933
43	1	0	-5.712048	1.473008	-1.018143

44	1	0	-7.780309	.520513	-.048545
45	1	0	-7.825788	-1.853352	.695991
46	1	0	-5.786938	-3.258132	.476782
47	1	0	-3.725051	-2.313884	-.490190

Vinylcarbene + styrene, Ts2 - TS for minor product, Isomer a



Key distance 2.395, 2.974
E(RB+HF-LYP) = -1629.96492694

Zero-point correction=	0.338316 (Hartree/Particle)
Thermal correction to Energy=	0.368897
Thermal correction to Enthalpy=	0.369842
Thermal correction to Gibbs Free Energy=	0.275850
Sum of electronic and zero-point Energies=	-1629.626611
Sum of electronic and thermal Energies=	-1629.596030
Sum of electronic and thermal Enthalpies=	-1629.595085
Sum of electronic and thermal Free Energies=	-1629.689077

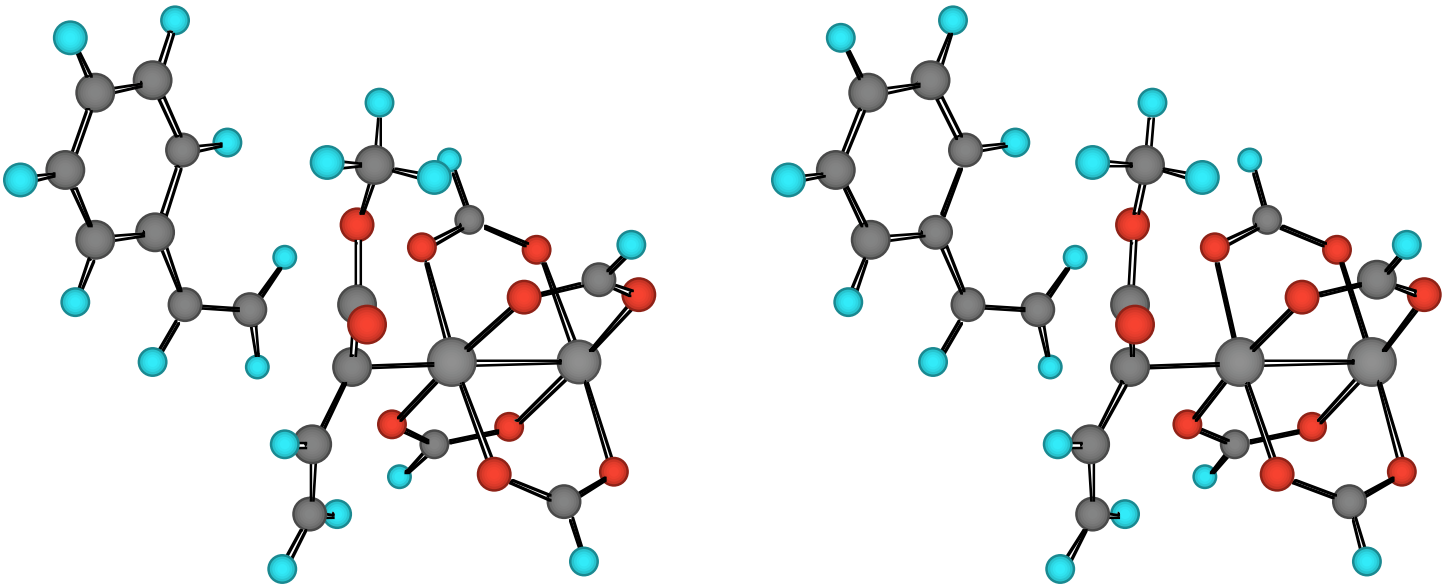
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.487	110.820	197.822

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.652625	-0.487232	-1.374929
2	6	0	-4.581092	-1.055916	-0.084604
3	6	0	-5.761083	-1.116950	0.686917
4	6	0	-6.968104	-0.630887	0.193954
5	6	0	-7.020359	-0.069877	-1.084969
6	6	0	-5.859509	0.000902	-1.863121
7	6	0	-3.356262	-1.604557	0.476809
8	6	0	-2.111222	-1.640386	-0.079962
9	6	0	-1.072682	0.226155	1.003148
10	45	0	0.841226	-0.026720	0.232639
11	8	0	1.683951	0.526501	2.058258
12	6	0	2.949801	0.598941	2.157935
13	8	0	3.824636	0.373717	1.281696
14	45	0	3.175730	-0.178023	-0.614195
15	8	0	3.022936	1.821833	-1.144280
16	6	0	1.936665	2.416432	-0.918326
17	8	0	0.876657	1.965456	-0.380395

18	6	0	-1.819667	1.323809	0.301817
19	8	0	-2.250932	1.306822	-0.831798
20	8	0	-1.867763	2.413784	1.103385
21	6	0	-2.331527	3.618458	0.469573
22	6	0	-1.412982	0.000797	2.393481
23	6	0	-0.722275	-0.824551	3.208290
24	8	0	0.245635	-0.593252	-1.684210
25	6	0	1.136266	-0.789993	-2.569301
26	8	0	2.387683	-0.707873	-2.459061
27	8	0	1.015945	-2.036746	0.771917
28	6	0	2.112844	-2.636855	0.518452
29	8	0	3.149859	-2.180783	-0.023164
30	1	0	-1.693871	3.859893	-0.384250
31	1	0	-2.263540	4.393211	1.233588
32	1	0	-3.363451	3.499300	0.129182
33	1	0	-2.258917	0.554055	2.802933
34	1	0	-1.001723	-0.931691	4.253393
35	1	0	0.117457	-1.406586	2.848153
36	1	0	1.887475	3.472611	-1.222925
37	1	0	3.318727	0.898461	3.150595
38	1	0	2.140902	-3.694987	0.819833
39	1	0	0.751136	-1.070653	-3.561110
40	1	0	-1.903236	-1.269840	-1.075699
41	1	0	-1.327029	-2.226730	0.383913
42	1	0	-3.470004	-2.037314	1.471104
43	1	0	-5.720199	-1.556759	1.680855
44	1	0	-7.866164	-0.689367	0.802582
45	1	0	-7.961000	0.309245	-1.475190
46	1	0	-5.898077	0.438980	-2.856518
47	1	0	-3.757484	-0.413789	-1.980176

Vinylcarbene + styrene, Ts2 - TS for minor product, Isomer b (12)



E(RB+HF-LYP) = -1629.96617775

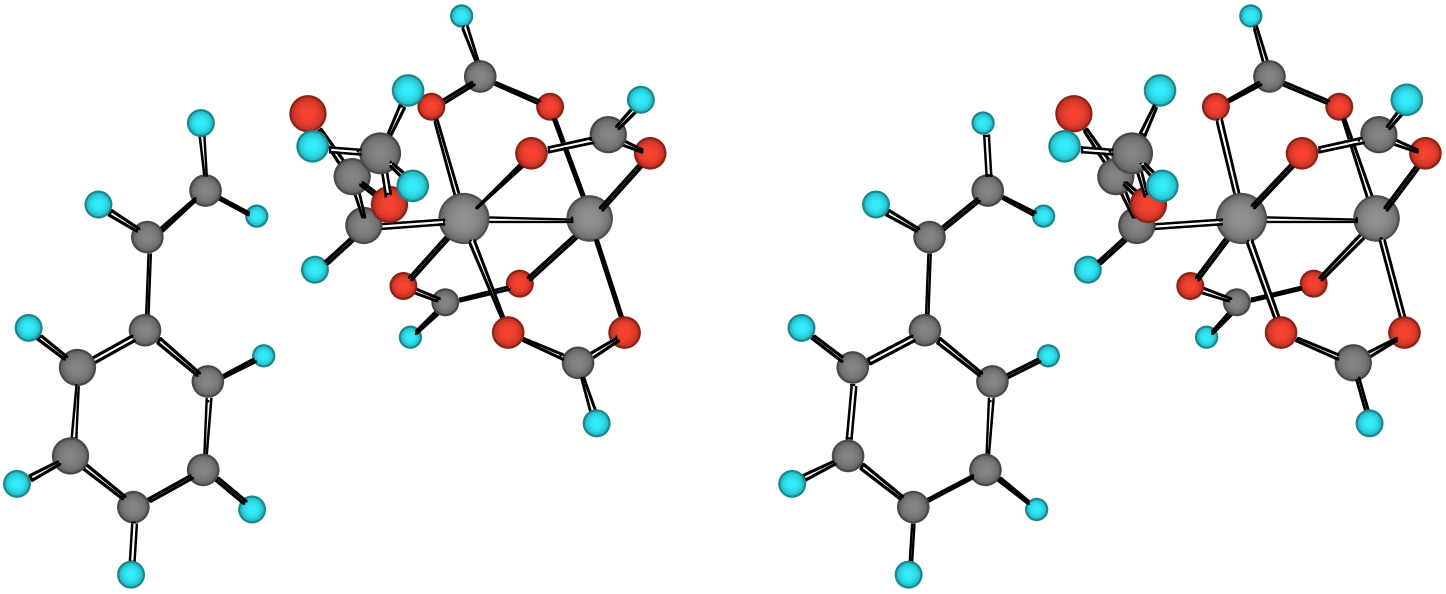
Zero-point correction= .338590 (Hartree/Particle)
Thermal correction to Energy= .369095
Thermal correction to Enthalpy= .370039
Thermal correction to Gibbs Free Energy= .276528
Sum of electronic and zero-point Energies= -1629.627588
Sum of electronic and thermal Energies= -1629.597083
Sum of electronic and thermal Enthalpies= -1629.596138
Sum of electronic and thermal Free Energies= -1629.689650

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.611	110.697	196.812

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.487009	-0.982975	-1.144554
2	6	0	4.469538	0.405273	-0.888990
3	6	0	5.633901	1.002452	-0.364010
4	6	0	6.768611	0.243900	-0.088666
5	6	0	6.765948	-1.129776	-0.342189
6	6	0	5.622274	-1.738133	-0.873122
7	6	0	3.313490	1.244752	-1.168592
8	6	0	2.056390	0.842973	-1.517738
9	6	0	1.017827	1.114301	0.573658
10	45	0	-0.835075	0.293156	0.079651
11	8	0	-1.786076	1.736170	1.242005
12	6	0	-3.047991	1.678887	1.386664
13	8	0	-3.861418	0.851019	0.899248
14	45	0	-3.103572	-0.659224	-0.305595
15	8	0	-2.809227	-1.831487	1.384225
16	6	0	-1.717074	-1.717577	1.999444
17	8	0	-0.724919	-0.968794	1.732623
18	6	0	1.838465	0.237134	1.475052
19	8	0	2.076584	0.568265	2.623399
20	8	0	2.173142	-0.950376	0.954954
21	6	0	2.769600	-1.872996	1.881459
22	6	0	1.209809	2.530579	0.828134
23	6	0	0.464607	3.505545	0.268838
24	8	0	-0.130229	-1.253283	-1.144478
25	6	0	-0.963105	-2.084836	-1.625645
26	8	0	-2.211696	-2.125881	-1.476469
27	8	0	-1.148968	1.466643	-1.623373
28	6	0	-2.258905	1.344980	-2.239194
29	8	0	-3.229542	0.595047	-1.968966
30	1	0	3.680371	-1.452933	2.315273
31	1	0	2.999416	-2.763320	1.296427
32	1	0	2.059923	-2.106318	2.678722
33	1	0	1.989026	2.799780	1.541389
34	1	0	0.644637	4.548979	0.514791
35	1	0	-0.324718	3.283676	-0.440066
36	1	0	-1.592370	-2.348855	2.892017
37	1	0	-3.475950	2.466901	2.024331
38	1	0	-2.368920	1.988569	-3.125318
39	1	0	-0.522353	-2.871759	-2.256811
40	1	0	1.793594	-0.198590	-1.656290
41	1	0	1.329238	1.562791	-1.871852
42	1	0	3.489737	2.315490	-1.067343
43	1	0	5.637868	2.072229	-0.169059
44	1	0	7.654021	0.722029	0.320538
45	1	0	7.651310	-1.724192	-0.134051
46	1	0	5.622187	-2.804613	-1.081181
47	1	0	3.608532	-1.462259	-1.562680

Unsubstituted carbene + styrene, Approximate Ts1 (7)



E(RB+HF-LYP) = -1552.55485432

Zero-point correction= 0.303480 (Hartree/Particle)
Thermal correction to Energy= 0.332452
Thermal correction to Enthalpy= 0.333396
Thermal correction to Gibbs Free Energy= 0.239736
Sum of electronic and zero-point Energies= -1552.251374
Sum of electronic and thermal Energies= -1552.222402
Sum of electronic and thermal Enthalpies= -1552.221458
Sum of electronic and thermal Free Energies= -1552.315118

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	208.617	102.825	197.125

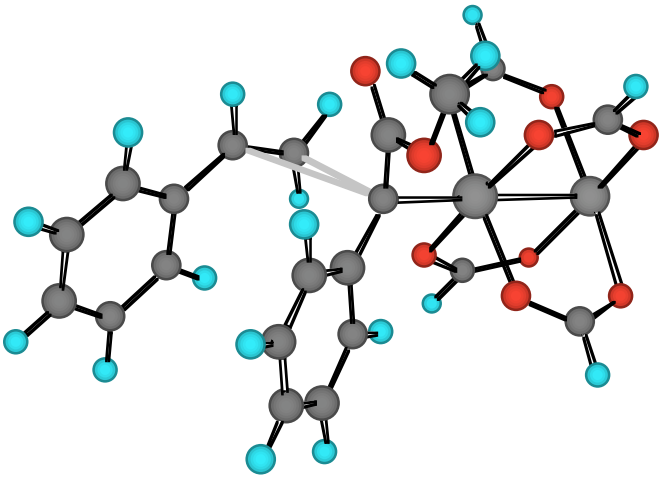
Standard orientation:

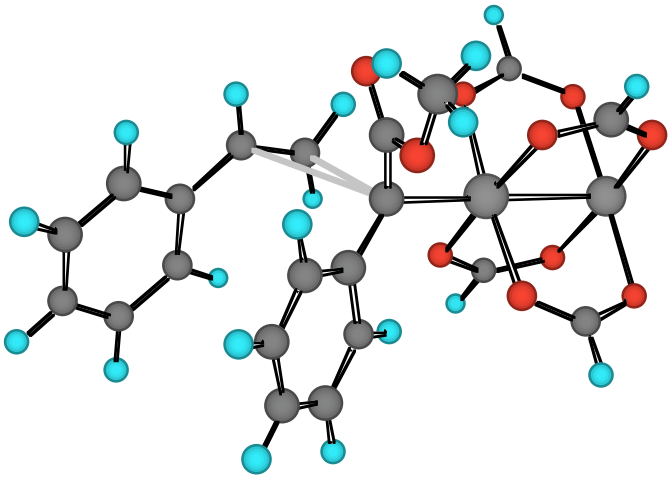
Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	1.049347	1.242838	-0.068594
2	6	0	C	1.178169	2.704788	-0.012068
3	8	0	O	0.971332	3.352169	-1.154631
4	6	0	C	1.030856	4.794078	-1.075669
5	45	0	Rh	-0.633083	0.255854	0.010215
6	8	0	O	-0.969059	0.481233	2.043495
7	6	0	C	-2.015509	-0.030715	2.557151
8	8	0	O	-2.921966	-0.695243	1.992252
9	45	0	Rh	-2.748577	-1.030875	-0.047806
10	8	0	O	-1.602613	-2.733240	0.327620
11	6	0	C	-0.358256	-2.607013	0.444862
12	8	0	O	0.346467	-1.545443	0.368248
13	8	0	O	-1.758327	1.964463	-0.340686
14	6	0	C	-3.018886	1.828398	-0.465582
15	8	0	O	-3.707865	0.777337	-0.411173
16	8	0	O	-0.526385	-0.115366	-2.041769
17	6	0	C	-1.445666	-0.795430	-2.601216
18	8	0	O	-2.471080	-1.306621	-2.083734
19	8	0	O	1.442972	3.200039	1.068630
20	6	0	C	2.828678	-0.020206	2.407028
21	6	0	C	4.033844	0.162053	1.842915
22	6	0	C	4.607168	-0.558599	0.694380

23	1	0	H	0.256050	5.162972	-0.399790
24	1	0	H	0.854946	5.142468	-2.092396
25	1	0	H	2.012581	5.115705	-0.719973
26	1	0	H	-3.566312	2.765090	-0.645879
27	1	0	H	-1.309283	-0.947284	-3.681779
28	1	0	H	0.213716	-3.525864	0.639939
29	1	0	H	-2.125790	0.139072	3.637805
30	1	0	H	2.120171	-0.769577	2.066349
31	1	0	H	2.515348	0.590814	3.247592
32	1	0	H	4.683939	0.929145	2.264261
33	1	0	H	1.991311	0.695699	-0.169611
34	6	0	C	5.936187	-0.290386	0.319203
35	6	0	C	6.527426	-0.940960	-0.762794
36	6	0	C	5.797228	-1.873755	-1.501356
37	6	0	C	4.472840	-2.147632	-1.146356
38	6	0	C	3.882362	-1.501160	-0.062799
39	1	0	H	6.510024	0.436273	0.890009
40	1	0	H	7.557138	-0.718364	-1.029876
41	1	0	H	6.253063	-2.381146	-2.347236
42	1	0	H	3.895349	-2.868787	-1.719160
43	1	0	H	2.849908	-1.722664	0.190667

Ts's for cyclopropanation using phenylcarbene, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Phenyl Carbene + Styrene, Isomer 1





E(RB+HF-LYP) = -1783.62129072

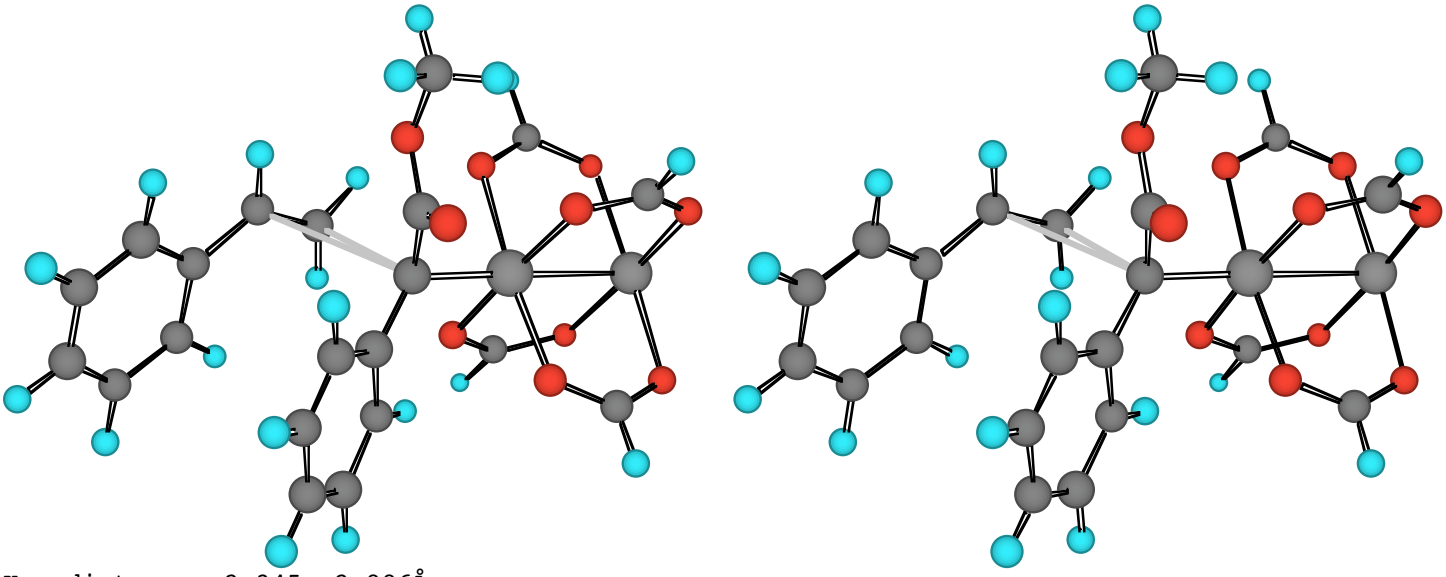
Zero-point correction=	0.386437 (Hartree/Particle)
Thermal correction to Energy=	0.419351
Thermal correction to Enthalpy=	0.420295
Thermal correction to Gibbs Free Energy=	0.321132
Sum of electronic and zero-point Energies=	-1783.234854
Sum of electronic and thermal Energies=	-1783.201940
Sum of electronic and thermal Enthalpies=	-1783.200996
Sum of electronic and thermal Free Energies=	-1783.300159

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	263.146	121.182	208.706

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.277827	-1.506207	-1.157709
2	6	0	-4.195221	-0.146526	-1.527915
3	6	0	-5.366780	0.637139	-1.452113
4	6	0	-6.569527	0.091459	-1.014283
5	6	0	-6.628376	-1.254212	-0.641382
6	6	0	-5.479511	-2.049315	-0.717134
7	6	0	-2.961877	0.481689	-1.970803
8	6	0	-1.712113	-0.060490	-1.980669
9	6	0	-0.964738	0.715270	0.149144
10	45	0	1.042040	0.062456	-0.055469
11	8	0	1.078692	-0.474142	1.959977
12	6	0	2.160227	-0.917700	2.458098
13	8	0	3.270774	-1.105734	1.894774
14	45	0	3.429095	-0.641814	-0.122240
15	8	0	3.939054	1.305653	0.369770
16	6	0	3.008931	2.140029	0.523336
17	8	0	1.754138	1.962244	0.431794
18	6	0	-1.040519	2.197255	-0.086214
19	8	0	-1.111254	2.769382	-1.154920
20	8	0	-0.909827	2.844001	1.096039
21	6	0	-0.652251	4.254842	0.998063
22	6	0	-1.922862	0.098109	1.047453
23	8	0	1.261873	0.544985	-2.070208
24	6	0	2.385311	0.349357	-2.632473
25	8	0	3.442159	-0.121368	-2.135986
26	8	0	0.572851	-1.907438	-0.592090
27	6	0	1.525432	-2.741232	-0.741292
28	8	0	2.761067	-2.552854	-0.616776
29	1	0	0.261442	4.427024	0.425286
30	1	0	-0.533383	4.598209	2.026038
31	1	0	-1.487533	4.767758	0.513714
32	1	0	3.314660	3.167223	0.773349
33	1	0	2.107974	-1.170382	3.527970
34	1	0	1.211108	-3.759581	-1.016733
35	1	0	2.427560	0.631147	-3.695168
36	1	0	-1.519981	-1.100424	-1.738354
37	1	0	-0.891083	0.486968	-2.424619
38	1	0	-3.047653	1.523663	-2.270982
39	1	0	-5.318600	1.684148	-1.741759
40	1	0	-7.460154	0.711649	-0.963181
41	1	0	-7.566290	-1.684620	-0.301041
42	1	0	-5.525943	-3.097718	-0.435877
43	1	0	-3.397269	-2.136244	-1.224197
44	6	0	-1.769945	-1.258279	1.430988
45	6	0	-2.651176	-1.851562	2.328218
46	6	0	-3.710317	-1.115458	2.865841
47	6	0	-3.897578	0.217838	2.486667
48	6	0	-3.027488	0.812445	1.582388
49	1	0	-0.951556	-1.828943	1.013193
50	1	0	-2.509331	-2.889852	2.615207
51	1	0	-4.392311	-1.579351	3.573643
52	1	0	-4.727670	0.788811	2.892645
53	1	0	-3.182043	1.847074	1.299543

Phenyl Carbene + Styrene, Isomer 2 (18)



Key distances 2.345, 2.886Å
E(RB+HF-LYP) = -1783.62187363

Zero-point correction=	0.386969 (Hartree/Particle)
Thermal correction to Energy=	0.419610
Thermal correction to Enthalpy=	0.420554
Thermal correction to Gibbs Free Energy=	0.322722
Sum of electronic and zero-point Energies=	-1783.234905
Sum of electronic and thermal Energies=	-1783.202264
Sum of electronic and thermal Enthalpies=	-1783.201320
Sum of electronic and thermal Free Energies=	-1783.299151

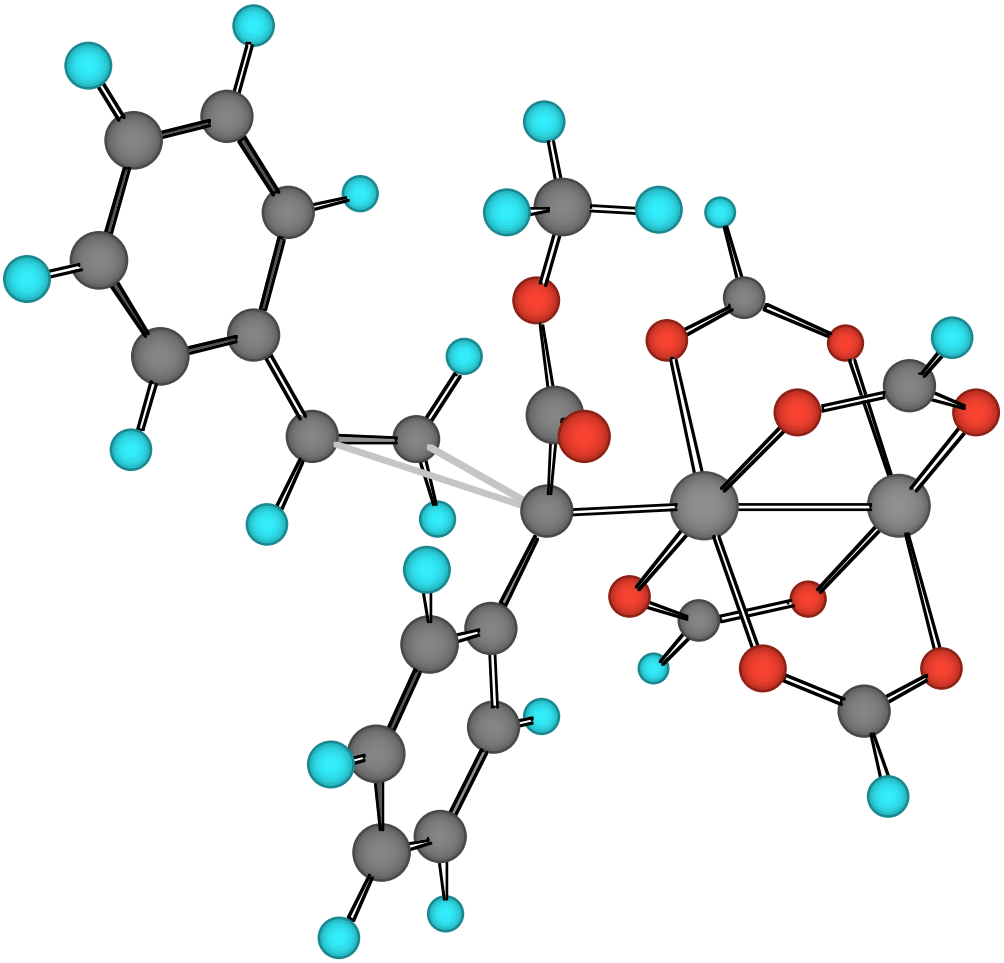
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	263.309	120.896	205.904

Standard orientation:

Center Number	Atomic Number	Atomic Type		Coordinates (Angstroms) X	Y	Z
1	6	0	C	-3.019481	-0.315025	1.818039
2	6	0	C	-1.915745	-0.592420	0.968642
3	6	0	C	-1.721880	-1.936034	0.561080
4	6	0	C	-2.567747	-2.948197	1.001580
5	6	0	C	-3.629844	-2.652923	1.860444
6	6	0	C	-3.853302	-1.332707	2.263610
7	6	0	C	-0.992266	0.438370	0.518458
8	6	0	C	-1.083527	1.783169	1.174047
9	8	0	O	-0.928185	2.832633	0.344127
10	6	0	C	-0.742513	4.098452	0.999090
11	45	0	Rh	1.041047	0.037296	0.023818
12	8	0	O	0.652922	-1.406682	-1.447286
13	6	0	C	1.641797	-1.998907	-1.990395
14	8	0	O	2.868988	-1.841418	-1.770807
15	45	0	Rh	3.453646	-0.438849	-0.346661
16	8	0	O	3.451134	1.037824	-1.807635
17	6	0	C	2.371629	1.643979	-2.033087
18	8	0	O	1.239505	1.482852	-1.477796
19	8	0	O	1.104667	-1.444177	1.483708
20	6	0	C	2.203756	-2.041960	1.705603
21	8	0	O	3.318460	-1.880238	1.141730
22	8	0	O	1.668440	1.443977	1.423502

23	6	0	C	2.913114	1.590635	1.633316
24	8	0	O	3.880421	0.992775	1.092678
25	8	0	O	-1.166878	1.899389	2.383726
26	6	0	C	-1.726367	0.820905	-1.676064
27	6	0	C	-2.950288	1.354498	-1.393799
28	6	0	C	-4.217290	0.653832	-1.278582
29	6	0	C	-4.371359	-0.713742	-1.591987
30	6	0	C	-5.604970	-1.338644	-1.448148
31	6	0	C	-6.714778	-0.615726	-0.997438
32	6	0	C	-6.584641	0.741972	-0.691691
33	6	0	C	-5.349929	1.367632	-0.831003
34	1	0	H	-1.613413	4.353302	1.609470
35	1	0	H	-0.611626	4.822921	0.194786
36	1	0	H	0.144569	4.061753	1.635213
37	1	0	H	3.168719	2.345007	2.392356
38	1	0	H	2.163960	-2.804166	2.498195
39	1	0	H	1.373973	-2.746041	-2.753131
40	1	0	H	2.401819	2.419385	-2.813603
41	1	0	H	-1.596257	-0.216788	-1.962823
42	1	0	H	-0.877263	1.469879	-1.845370
43	1	0	H	-2.987727	2.420522	-1.178952
44	1	0	H	-5.246347	2.423331	-0.591558
45	1	0	H	-7.444350	1.308899	-0.345633
46	1	0	H	-7.677939	-1.107471	-0.891907
47	1	0	H	-5.706583	-2.392256	-1.692491
48	1	0	H	-3.521977	-1.283298	-1.953222
49	1	0	H	-0.898740	-2.166685	-0.102191
50	1	0	H	-2.393631	-3.972182	0.682460
51	1	0	H	-4.283725	-3.446783	2.212219
52	1	0	H	-4.682579	-1.097618	2.924725
53	1	0	H	-3.194103	0.699745	2.151495

Phenyl Carbene + Styrene, Isomer 3 - gives minor enantiomer



E(RB+HF-LYP) = -1783.61891667

Zero-point correction=	.386842 (Hartree/Particle)
Thermal correction to Energy=	.419636
Thermal correction to Enthalpy=	.420580
Thermal correction to Gibbs Free Energy=	.321767
Sum of electronic and zero-point Energies=	-1783.232075
Sum of electronic and thermal Energies=	-1783.199281
Sum of electronic and thermal Enthalpies=	-1783.198337
Sum of electronic and thermal Free Energies=	-1783.297150

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	263.326	120.971	207.970

C,0,2.4361728453,2.6513922224,1.0454033519
C,0,1.3935276027,2.0946960912,0.2612530379
C,0,0.7119889469,2.9540109897,-0.6325336917
C,0,1.0557078529,4.2980124806,-0.7399542107
C,0,2.0793117454,4.8268749338,0.0495012995
C,0,2.7647530635,3.9977569165,0.9442009433
C,0,1.020607306,0.6798154354,0.3285663093
C,0,1.6411090422,-0.1527833726,1.4079348648
O,0,1.9415057349,-1.4102329338,1.0440392758
C,0,2.3268832598,-2.2758268201,2.1242568433
Rh,0,-0.9810481272,0.0191459369,0.0083769615
O,0,-1.1718955891,0.7883518758,-1.9328441976
C,0,-2.3045770314,0.7047437519,-2.510833779
O,0,-3.3710896534,0.2041203806,-2.07563307
Rh,0,-3.3730755088,-0.646032542,-0.1757159626

```
O,0,-2.7359368816,-2.4448550058,-0.9957557698
C,0,-1.4975993398,-2.6321380118,-1.1231539203
O,0,-0.538883538,-1.8556537661,-0.8178182832
O,0,-1.6708511237,1.804645311,0.8194422218
C,0,-2.9224879501,1.9720940819,0.9613596426
O,0,-3.8628571524,1.1912249948,0.6575659004
O,0,-1.024007526,-0.846321166,1.899538228
C,0,-2.1048957963,-1.3699792285,2.3138411706
O,0,-3.2162632007,-1.4572369467,1.7280888262
O,0,1.7398069269,0.2519242784,2.5532262336
C,0,1.8649340668,-0.1690317341,-1.6353877008
C,0,3.1731225965,0.1866365042,-1.4560740771
C,0,4.2832715536,-0.6516429374,-1.0364656381
C,0,4.200220345,-2.0592945824,-0.9640016096
C,0,5.3005389961,-2.8127116238,-0.5719959069
C,0,6.5081545804,-2.184029435,-0.2447472275
C,0,6.6110339792,-0.7928552813,-0.3183449114
C,0,5.5114104891,-0.0366976142,-0.7148360967
H,0,2.9652304372,2.0242343848,1.7509717215
H,0,-0.0821185573,2.5488794996,-1.2457832359
H,0,0.5186731414,4.9365197816,-1.4360009058
H,0,2.3423809308,5.8785178966,-0.0295296887
H,0,3.5586233694,4.4051461214,1.5642895916
H,0,3.2167988612,-1.8920538025,2.6297060876
H,0,2.5371793629,-3.2398448883,1.6610548223
H,0,1.5086676252,-2.360647909,2.8427918901
H,0,-2.3412825545,1.1298847044,-3.525327117
H,0,-1.1951608126,-3.5975516424,-1.5573788488
H,0,-3.2125153272,2.9343952327,1.4090279992
H,0,-2.050766352,-1.8037738342,3.3235669882
H,0,1.187913071,0.5012679131,-2.1502749124
H,0,1.5150694657,-1.1864917243,-1.5136925566
H,0,3.4317139603,1.2324835076,-1.6187578742
H,0,3.2714753332,-2.5546031743,-1.2252921801
H,0,5.2241973623,-3.8956750211,-0.5273035693
H,0,7.3658281667,-2.7784012944,0.0580047853
H,0,7.547041974,-0.3003821719,-0.0704410548
H,0,5.5912612634,1.0460008737,-0.7761039755
```

Phenyl Carbene + Propene, Isomer 1 – gives major enantiomer

```
E(RB+HF-LYP) =  -1591.88140594

 Zero-point correction=                           0.333201 (Hartree/Particle)
 Thermal correction to Energy=                    0.363035
 Thermal correction to Enthalpy=                  0.363979
 Thermal correction to Gibbs Free Energy=         0.273443
 Sum of electronic and zero-point Energies=          -1591.548204
 Sum of electronic and thermal Energies=             -1591.518371
 Sum of electronic and thermal Enthalpies=           -1591.517426
 Sum of electronic and thermal Free Energies=        -1591.607963

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 227.808            107.939           190.549

 C,0,3.8364497539,-0.5111787689,-1.112755849
 C,0,2.6724852199,-0.6637573958,-0.315912251
 C,0,2.4282595517,-1.9357297017,0.2554048023
 C,0,3.2985610151,-2.9981315801,0.0389754235
 C,0,4.426863527,-2.8313370816,-0.7695905556
 C,0,4.6888797915,-1.5860371934,-1.3467624222
 C,0,1.7247045564,0.4236454569,-0.0783779942
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C,0,1.9361846702,1.7139985917,-0.8130528694
O,0,1.6785490948,2.8252243117,-0.0972615454
C,0,1.6155004254,4.0380471153,-0.8673764238
Rh,0,-0.3848876356,0.0490240335,0.0579584298
O,0,-0.3103158347,-1.2758521053,1.6837061806
C,0,-1.388823111,-1.847275024,2.0488185846
O,0,-2.5426358955,-1.7299369328,1.5644217665
Rh,0,-2.821953793,-0.4294407326,-0.0380623668
O,0,-3.1047633429,1.1383345256,1.2969788616
C,0,-2.0922822227,1.7746892453,1.6896367678
O,0,-0.8717436432,1.5921411289,1.3848174621
O,0,-0.1544972589,-1.5330847524,-1.2725674906
C,0,-1.1865411955,-2.153260876,-1.6772199679
O,0,-2.3935925651,-1.9584377613,-1.3739051297
O,0,-0.7161622753,1.3544668816,-1.5284931162
C,0,-1.8912550041,1.4714225489,-1.9971277357
O,0,-2.949028638,0.8981138829,-1.6256679498
O,0,2.1973777144,1.7357976037,-2.0025012964
H,0,4.0406577298,0.4430133101,-1.5811952594
H,0,1.5483603654,-2.0719321903,0.871406424
H,0,3.0905021697,-3.964385539,0.4902402826
H,0,5.0979086587,-3.6671800209,-0.9493799406
H,0,5.5620755219,-1.4506249648,-1.9789531247
H,0,2.5670603618,4.229718679,-1.3706848083
H,0,1.3958244725,4.82597738,-0.1465946214
H,0,0.8213795278,3.9631232762,-1.613435219
H,0,-1.2855712615,-2.5320966645,2.9043076194
H,0,-2.2788018375,2.6010750922,2.3922460125
H,0,-0.9879923361,-2.9700435066,-2.3870791983
H,0,-1.986337549,2.1710351909,-2.8408479969
C,0,2.0037425313,0.9606366323,2.1404799919
C,0,3.2945186072,1.3635532235,1.9963355417
C,0,4.4934488417,0.4971840608,2.170408471
H,0,1.7652477766,-0.0318264802,2.51071754
H,0,1.1871924065,1.6699828602,2.1004812502
H,0,3.4777865888,2.3906147995,1.6856035699
H,0,4.9913548335,0.3379928871,1.2009251845
H,0,4.2413360449,-0.4821002633,2.5859308277
H,0,5.2302002231,0.9834578333,2.823465596
```

Phenyl Carbene + Propene, Isomer 2 – gives minor enantiomer

```
E(RB+HF-LYP) =  -1591.87840901

 Zero-point correction=                           0.333265 (Hartree/Particle)
 Thermal correction to Energy=                    0.363099
 Thermal correction to Enthalpy=                  0.364043
 Thermal correction to Gibbs Free Energy=         0.273254
 Sum of electronic and zero-point Energies=          -1591.545144
 Sum of electronic and thermal Energies=             -1591.515310
 Sum of electronic and thermal Enthalpies=           -1591.514366
 Sum of electronic and thermal Free Energies=        -1591.605155

                    E (Thermal)             CV                S
                     KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                 227.848            107.909           191.082

 C,0,3.8178115827,-0.9600391034,-0.9714459876
 C,0,2.6368482328,-0.9497819745,-0.1890675408
 C,0,2.2873759648,-2.1382067995,0.4921568436
 C,0,3.0799830408,-3.2781809425,0.4006683623
 C,0,4.2331727772,-3.2709964412,-0.3873927255
 C,0,4.5945620514,-2.1085370067,-1.075498505
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```
C,0,1.7775494902,0.2347592856,-0.0555551391
C,0,2.0843141928,1.4306610294,-0.9046466372
O,0,1.8442723959,2.6160985202,-0.3139633399
C,0,1.8752244669,3.7496952946,-1.1970238266
Rh,0,-0.3650865208,0.0288422021,0.0536218913
O,0,-0.4076724233,-1.0780411263,1.8336590039
C,0,-1.5320115608,-1.4968308651,2.2628518558
O,0,-2.6704528151,-1.3443479408,1.7534989543
Rh,0,-2.8262904512,-0.2913110912,-0.0346057516
O,0,-3.0187150719,1.4844643744,1.0283709962
C,0,-1.9684055708,2.0865898827,1.3746120559
O,0,-0.7583399054,1.7682754326,1.1525934228
O,0,-0.2305105965,-1.7277959536,-1.0561721694
C,0,-1.2967471975,-2.3443535881,-1.3661054772
O,0,-2.489770705,-2.0439592779,-1.0941567562
O,0,-0.5775409467,1.1314491654,-1.6973807686
C,0,-1.7300934925,1.2387812798,-2.221061164
O,0,-2.8280685723,0.7760238307,-1.8130267717
O,0,2.3951399836,1.3259484017,-2.0779402646
H,0,4.1024414631,-0.0722916589,-1.5210268659
H,0,1.388905927,-2.1528248695,1.0959993953
H,0,2.7909627689,-4.1783922043,0.9361049625
H,0,4.8460148474,-4.1649901778,-0.4679906717
H,0,5.4873114148,-2.0976894096,-1.6948731234
H,0,2.8547043821,3.8467366651,-1.6730598462
H,0,1.6671387331,4.6135539687,-0.5650596486
H,0,1.1087601473,3.6411125053,-1.9674370497
H,0,-1.4888865647,-2.0644796828,3.2046919269
H,0,-2.1082971975,3.015975335,1.9477406052
H,0,-1.1471823494,-3.2656138548,-1.9486951572
H,0,-1.7620902564,1.8164415368,-3.1568300187
C,0,2.0294774391,0.9022975591,2.0633092917
C,0,3.3745024366,1.0918313304,1.9512978874
C,0,4.069090629,2.3977533733,1.7599129381
H,0,1.6286087815,-0.0454198579,2.4024413188
H,0,1.3403299226,1.7386777004,2.0584266488
H,0,4.020830392,0.2155607886,1.9976368488
H,0,4.7796530138,2.5553952139,2.5842704253
H,0,3.371000374,3.2356303402,1.7273187248
H,0,4.6691002988,2.3961403822,0.8386833941
```

Phenyl Carbene + Methyl Vinyl Ether, Isomer 1 – gives major enantiomer

```
E(RB+HF-LYP) =  -1667.09323106

 Zero-point correction=                           0.338793 (Hartree/Particle)
 Thermal correction to Energy=                    0.369541
 Thermal correction to Enthalpy=                  0.370485
 Thermal correction to Gibbs Free Energy=         0.277739
 Sum of electronic and zero-point Energies=          -1666.754438
 Sum of electronic and thermal Energies=             -1666.723690
 Sum of electronic and thermal Enthalpies=           -1666.722746
 Sum of electronic and thermal Free Energies=        -1666.815492

                     E (Thermal)             CV                S
                      KCAL/MOL        CAL/MOL-KELVIN    CAL/MOL-KELVIN
 TOTAL                  231.891            110.923           195.201

 C                     0     4.70751  -1.29554  -1.51478
 C                     0     3.77044  -0.30511  -1.24754
 C                     0     2.51108  -0.6242   -0.67487
 C                     0     2.24598  -1.98394  -0.3774
 C                     0     3.18993  -2.96986  -0.64297
```

C	0	4.4218	-2.6309	-1.21233
C	0	1.51312	0.39474	-0.38654
Rh	0	-0.52935	0.02739	-0.05646
O	0	-1.05632	1.42658	-1.50501
C	0	-2.28645	1.58919	-1.78101
O	0	-3.2894	1.00943	-1.28849
Rh	0	-2.9671	-0.41969	0.18086
O	0	-2.76214	-1.87174	-1.28967
C	0	-1.61931	-2.0534	-1.78536
O	0	-0.52561	-1.4697	-1.50228
C	0	1.70131	1.73266	-1.02864
O	0	1.90219	1.81907	-2.22699
O	0	1.50133	2.79637	-0.23087
C	0	1.41481	4.05837	-0.91673
O	0	-0.23792	-1.40438	1.44502
C	0	-1.26209	-1.98458	1.93356
O	0	-2.47293	-1.81913	1.64337
O	0	-0.80195	1.4964	1.40887
C	0	-1.96101	1.67043	1.9022
O	0	-3.03036	1.06647	1.62981
C	0	2.11935	0.84914	1.99074
C	0	3.34548	1.37777	1.75883
O	0	4.53702	0.76741	1.80483
H	0	3.99905	0.72355	-1.49777
H	0	1.29879	-2.24653	0.07198
H	0	2.96525	-4.00722	-0.41094
H	0	5.15665	-3.40416	-1.42088
H	0	5.66284	-1.02858	-1.95752
H	0	2.34571	4.27791	-1.44665
H	0	1.23257	4.79792	-0.13675
H	0	0.58897	4.03672	-1.63103
H	0	-1.04415	-2.72873	2.715
H	0	-2.02671	2.45713	2.6691
H	0	-1.54284	-2.82128	-2.56978
H	0	-2.49001	2.34111	-2.55807
H	0	1.96546	-0.17251	2.31567
H	0	1.26143	1.50669	2.01236
H	0	3.46322	2.41005	1.44442
C	0	4.60149	-0.55469	2.35287
H	0	5.66259	-0.80139	2.40303
H	0	4.16549	-0.56932	3.35837
H	0	4.08427	-1.273	1.71253

Phenyl Carbene + Methyl Vinyl Ether, Isomer 2 – gives minor enantiomer

E(RB+HF-LYP) = -1667.09056832

Zero-point correction=	0.338813 (Hartree/Particle)
Thermal correction to Energy=	0.369577
Thermal correction to Enthalpy=	0.370521
Thermal correction to Gibbs Free Energy=	0.277226
Sum of electronic and zero-point Energies=	-1666.751755
Sum of electronic and thermal Energies=	-1666.720991
Sum of electronic and thermal Enthalpies=	-1666.720047
Sum of electronic and thermal Free Energies=	-1666.813342

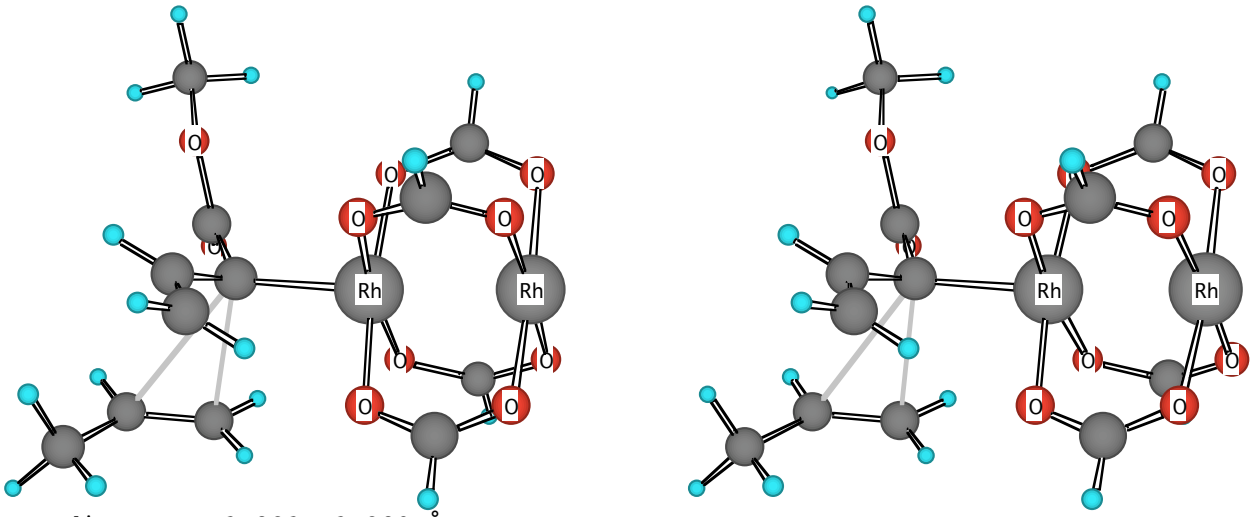
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	231.913	110.897	196.357

C	0	4.52574	2.60585	0.6292
C	0	3.7663	1.45125	0.77051
C	0	2.4843	1.34081	0.17265

C	0	2.01247	2.44293	-0.57945
C	0	2.77919	3.59501	-0.7214
C	0	4.03574	3.68291	-0.11756
C	0	1.66489	0.13597	0.2973
Rh	0	-0.43159	0.08275	0.04324
O	0	-0.68949	-0.80702	1.90874
C	0	-1.87036	-1.01523	2.33016
O	0	-2.96728	-0.76547	1.76399
Rh	0	-2.91674	0.11649	-0.11248
O	0	-2.86542	1.98651	0.78517
C	0	-1.74151	2.46449	1.09122
O	0	-0.58709	1.9605	0.91759
C	0	2.06936	-0.83851	1.35642
O	0	2.31739	-0.45868	2.48754
O	0	2.00856	-2.13592	1.01336
C	0	2.19044	-3.05434	2.10516
O	0	-0.41982	0.94592	-1.863
C	0	-1.53628	1.20056	-2.42233
O	0	-2.69758	0.99924	-1.98727
O	0	-0.53782	-1.8185	-0.84507
C	0	-1.68193	-2.28728	-1.14721
O	0	-2.81469	-1.76426	-0.99153
C	0	2.20338	-0.82728	-1.85709
C	0	3.41893	-1.36301	-1.56198
O	0	3.71951	-2.64476	-1.35458
H	0	4.15172	0.63184	1.36501
H	0	1.04494	2.37378	-1.0571
H	0	2.39466	4.42856	-1.30255
H	0	4.63246	4.58454	-0.22804
H	0	5.50178	2.66992	1.10199
H	0	3.1705	-2.91549	2.56888
H	0	2.11358	-4.04843	1.66387
H	0	1.41059	-2.9026	2.85445
H	0	-1.46066	1.65761	-3.42088
H	0	-1.66843	-3.28723	-1.60816
H	0	-1.74547	3.45339	1.57344
H	0	-1.93058	-1.47853	3.32645
H	0	2.15362	0.19702	-2.1938
H	0	1.31932	-1.43359	-1.99758
H	0	4.30199	-0.74125	-1.43389
C	0	2.70384	-3.6211	-1.62725
H	0	3.15723	-4.58644	-1.39917
H	0	1.82703	-3.44692	-1.00059
H	0	2.42316	-3.58074	-2.6861

Ts's for cyclopropanation of propene, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Vinylcarbene + propene TS2a



Key distances 2.832, 2.389 Å
E(RB+HF-LYP) = -1438.22701828

Zero-point correction=	0.284815 (Hartree/Particle)
Thermal correction to Energy=	0.312438
Thermal correction to Enthalpy=	0.313382
Thermal correction to Gibbs Free Energy=	0.227711
Sum of electronic and zero-point Energies=	-1437.942203
Sum of electronic and thermal Energies=	-1437.914581
Sum of electronic and thermal Enthalpies=	-1437.913636
Sum of electronic and thermal Free Energies=	-1437.999307

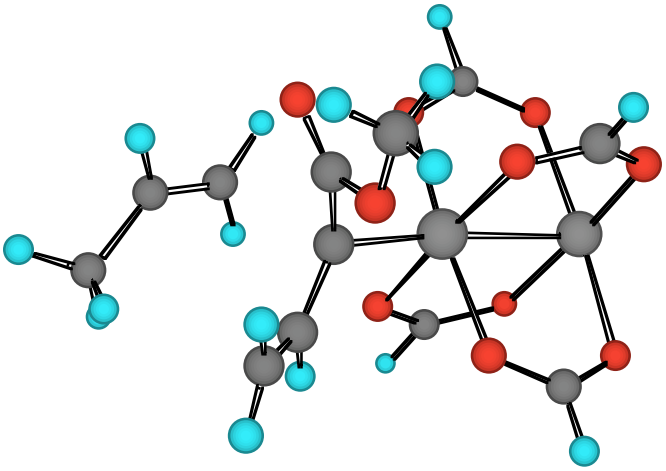
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	196.058	97.650	180.309

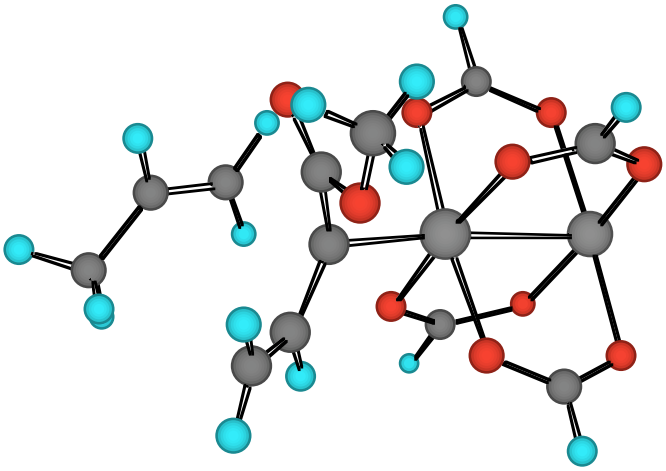
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.086821	2.010557	-0.119087
2	45	0	0.016453	-0.065916	0.059609
3	6	0	-2.055424	0.011484	0.342369
4	6	0	-2.673791	1.249894	-0.248888
5	8	0	-2.951996	1.460178	-1.410566
6	8	0	-2.811010	2.167613	0.735102
7	6	0	-3.138068	3.497369	0.295106
8	1	0	-2.370812	3.860272	-0.392501
9	1	0	-3.163361	4.103720	1.200697
10	1	0	-4.109880	3.507973	-0.205294
11	6	0	-2.698033	-0.498371	1.537130
12	6	0	-2.206874	-1.515717	2.275179
13	1	0	-3.613414	-0.006475	1.868886
14	1	0	-2.712160	-1.836378	3.182690
15	1	0	-1.307618	-2.044817	1.982307
16	45	0	2.495318	-0.019232	-0.121398
17	8	0	2.362486	2.043309	-0.293718
18	6	0	1.219795	2.570360	-0.258711
19	1	0	1.185646	3.665377	-0.360600
20	8	0	2.572761	0.156002	1.949853

21	6	0	1.481546	0.176278	2.576282
22	1	0	1.548558	0.270646	3.670655
23	8	0	0.297809	0.099892	2.117906
24	8	0	2.449211	-2.097010	0.052886
25	6	0	1.336046	-2.667245	0.168510
26	1	0	1.354138	-3.764785	0.248341
27	8	0	0.172753	-2.145902	0.206778
28	8	0	2.273254	-0.191763	-2.174494
29	6	0	1.106028	-0.238213	-2.644980
30	1	0	1.022974	-0.311860	-3.739535
31	8	0	-0.001835	-0.213479	-2.022694
32	6	0	-2.636438	-1.511737	-1.403467
33	1	0	-1.986520	-2.315678	-1.069833
34	1	0	-2.216987	-0.796186	-2.098765
35	6	0	-3.957887	-1.508556	-1.102594
36	6	0	-4.641296	-2.526171	-0.250672
37	1	0	-4.569384	-0.691575	-1.482991
38	1	0	-5.520463	-2.935542	-0.765885
39	1	0	-3.975077	-3.352480	0.013917
40	1	0	-5.010994	-2.071979	0.681133

Vinylcarbene + propene TS2b (rotated vinyl)





E(RB+HF-LYP) = -1438.22849366

Zero-point correction= 0.284635 (Hartree/Particle)
Thermal correction to Energy= 0.312305
Thermal correction to Enthalpy= 0.313249
Thermal correction to Gibbs Free Energy= 0.227198
Sum of electronic and zero-point Energies= -1437.943859
Sum of electronic and thermal Energies= -1437.916189
Sum of electronic and thermal Enthalpies= -1437.915245
Sum of electronic and thermal Free Energies= -1438.001296

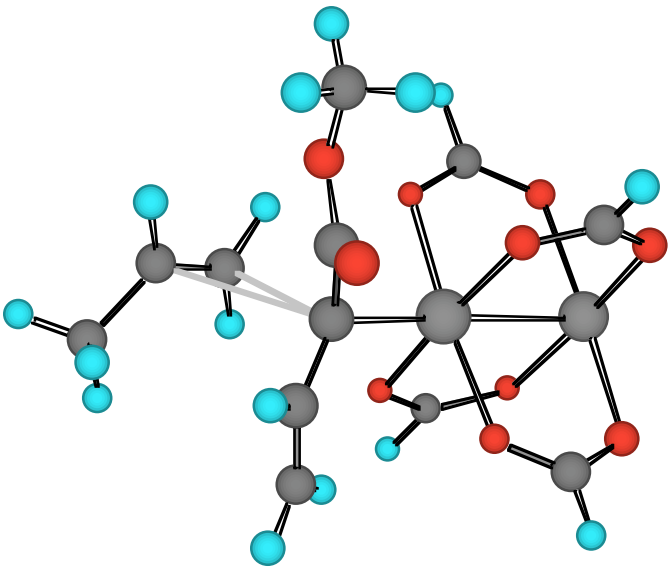
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	195.974	97.678	181.110

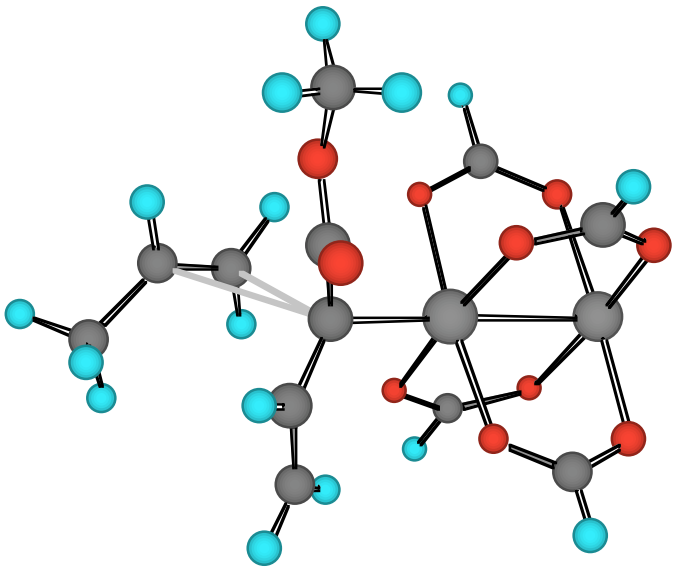
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.063522	3.457342	-0.225068
2	8	0	-2.717103	2.216114	0.418351
3	6	0	-2.677987	1.139301	-0.398341
4	8	0	-3.065217	1.150166	-1.548061

5	6	0	-1.991799	0.004055	0.297536
6	6	0	-2.504311	-0.573260	1.515844
7	6	0	-3.535493	-0.084600	2.240492
8	45	0	0.054010	-0.060093	0.051131
9	8	0	0.091544	-0.471869	-1.989513
10	6	0	1.217559	-0.565785	-2.573701
11	8	0	2.370003	-0.454356	-2.080708
12	45	0	2.536749	-0.051631	-0.051042
13	8	0	2.450819	-2.092205	0.366845
14	6	0	1.328607	-2.627332	0.549624
15	8	0	0.172394	-2.093011	0.499729
16	8	0	0.143383	1.972402	-0.402363
17	6	0	1.286725	2.508807	-0.552238
18	8	0	2.425850	1.980994	-0.462199
19	8	0	0.267414	0.356460	2.084306
20	6	0	1.437762	0.466768	2.569401
21	8	0	2.547582	0.356901	1.986391
22	6	0	-2.532284	-1.848293	-1.238396
23	6	0	-3.869103	-1.788194	-1.034129
24	6	0	-4.621922	-2.593356	-0.032211
25	1	0	-2.343881	3.677366	-1.016654
26	1	0	-3.014935	4.211481	0.560446
27	1	0	-4.068911	3.404063	-0.650214
28	1	0	-1.938019	-1.417713	1.902550
29	1	0	-3.779303	-0.507406	3.211754
30	1	0	-4.107972	0.779916	1.920691
31	1	0	1.265726	3.582548	-0.792104
32	1	0	1.471884	0.687531	3.646912
33	1	0	1.331303	-3.702426	0.784666
34	1	0	1.164016	-0.773612	-3.652666
35	1	0	-1.910799	-2.572130	-0.718408
36	1	0	-2.056834	-1.266481	-2.018276
37	1	0	-4.439599	-1.056165	-1.602987
38	1	0	-5.536499	-3.017111	-0.465712
39	1	0	-4.017408	-3.403227	0.388213
40	1	0	-4.941683	-1.944513	0.802709

Vinylcarbene + propene TS2c (rotated ester from 2a)





E(RB+HF-LYP) = -1438.22802786

Zero-point correction= .285085 (Hartree/Particle)
Thermal correction to Energy= .312635

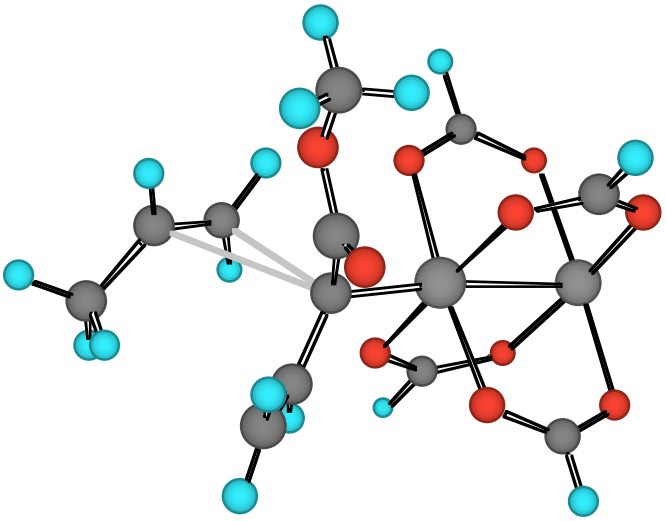
Thermal correction to Enthalpy= .313579
Thermal correction to Gibbs Free Energy= .228234
Sum of electronic and zero-point Energies= -1437.942943
Sum of electronic and thermal Energies= -1437.915393
Sum of electronic and thermal Enthalpies= -1437.914449
Sum of electronic and thermal Free Energies= -1437.999794

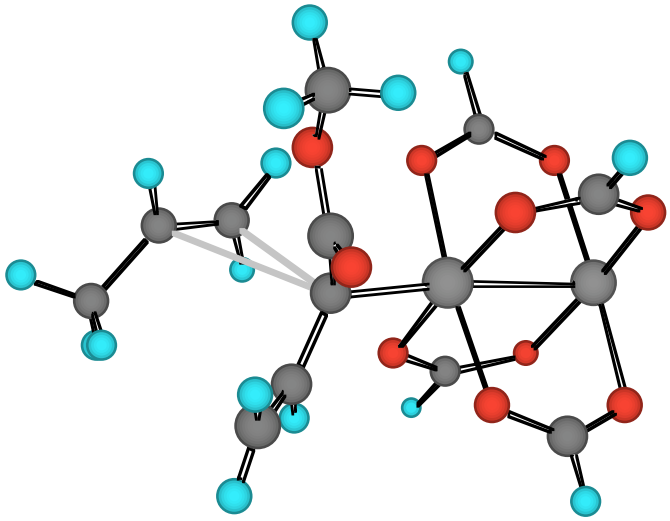
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	196.181	97.554	179.624

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.143753	3.232093	-.243122
2	8	0	-2.747576	1.863936	-.439751
3	6	0	-2.669339	1.126218	.679654
4	8	0	-2.987591	1.532126	1.782649
5	6	0	-2.036429	-.225944	.517189
6	6	0	-2.577125	-1.224117	1.422718
7	6	0	-2.069602	-2.464899	1.561928
8	45	0	.029176	-.115576	.102470
9	8	0	-.141755	.721860	-1.805547
10	6	0	.917090	1.042562	-2.432337
11	8	0	2.114501	.919576	-2.066478
12	45	0	2.487062	.081091	-.201769
13	8	0	2.436519	-1.823534	-1.047336
14	6	0	1.334725	-2.423140	-1.119859
15	8	0	.183517	-2.023004	-.746687
16	8	0	.095714	1.801412	.909555
17	6	0	1.222625	2.381229	1.010513
18	8	0	2.358977	1.963038	.665564
19	8	0	.465329	-.926904	1.972648
20	6	0	1.680120	-1.053619	2.323236
21	8	0	2.721742	-.756683	1.680607
22	6	0	-2.695904	-.875652	-1.594228
23	6	0	-4.021218	-.829695	-1.298242
24	6	0	-4.841334	-1.988861	-.839726
25	1	0	-4.133035	3.287662	.219340
26	1	0	-3.159079	3.674031	-1.239562
27	1	0	-2.418270	3.742396	.394532
28	1	0	-3.423012	-.922394	2.040813
29	1	0	-2.504771	-3.164795	2.270642
30	1	0	-1.224044	-2.803005	.973423
31	1	0	1.188144	3.384377	1.461066
32	1	0	1.831085	-1.484156	3.324533
33	1	0	1.354536	-3.430144	-1.563741
34	1	0	.753477	1.485375	-3.426481
35	1	0	-2.149219	-1.813641	-1.578150
36	1	0	-2.185174	-.026887	-2.030944
37	1	0	-4.533973	.127729	-1.379363
38	1	0	-5.675564	-2.159150	-1.534683
39	1	0	-4.252801	-2.907761	-.773452
40	1	0	-5.293129	-1.789467	.142343

Vinylcarbene + propene TS2d (rotated ester and vinyl from 2a) (13)





Key distances 2.400, 2.856
E(RB+HF-LYP) = -1438.22918651

Zero-point correction= .284987 (Hartree/Particle)
Thermal correction to Energy= .312515
Thermal correction to Enthalpy= .313460
Thermal correction to Gibbs Free Energy= .227889
Sum of electronic and zero-point Energies= -1437.944199
Sum of electronic and thermal Energies= -1437.916671
Sum of electronic and thermal Enthalpies= -1437.915727
Sum of electronic and thermal Free Energies= -1438.001298

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	196.106	97.512	180.099

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.311264	3.095490	-.625284
2	8	0	-2.875265	1.724914	-.680795
3	6	0	-2.654092	1.151496	.514301
4	8	0	-2.877036	1.701390	1.577819
5	6	0	-1.973233	-.177252	.446956
6	6	0	-2.393867	-1.262473	1.304395
7	6	0	-3.288802	-1.179330	2.313300
8	45	0	.065685	-.085228	.073860
9	8	0	.010317	.302900	-1.978510
10	6	0	1.108609	.440221	-2.605572
11	8	0	2.282432	.370722	-2.158412
12	45	0	2.538812	.009496	-.130455
13	8	0	2.480067	-2.046851	-.484067
14	6	0	1.365552	-2.627586	-.486667
15	8	0	.206638	-2.130697	-.301052
16	8	0	.117738	1.967722	.417483
17	6	0	1.250395	2.545620	.424803
18	8	0	2.392447	2.048138	.242607
19	8	0	.382367	-.458019	2.097322
20	6	0	1.573525	-.495330	2.540281
21	8	0	2.654065	-.346114	1.911721
22	6	0	-2.626026	-1.108025	-1.666279
23	6	0	-3.954862	-1.085691	-1.397750
24	6	0	-4.729373	-2.202645	-.789062

25	1	0	-4.250769	3.181893	-.073039
26	1	0	-3.445529	3.396842	-1.664179
27	1	0	-2.548530	3.708649	-.140184
28	1	0	-1.850262	-2.193137	1.156479
29	1	0	-3.448175	-2.027472	2.974293
30	1	0	-3.809550	-.257274	2.546080
31	1	0	1.216099	3.628434	.617079
32	1	0	1.658315	-.685889	3.620526
33	1	0	1.379176	-3.711879	-.674819
34	1	0	1.006772	.645500	-3.681903
35	1	0	-2.039766	-2.013732	-1.534935
36	1	0	-2.133349	-.284746	-2.167796
37	1	0	-4.501001	-.163070	-1.588469
38	1	0	-5.691263	-2.343110	-1.297339
39	1	0	-4.175925	-3.146477	-.803620
40	1	0	-4.958138	-1.966392	.265124

Structure 13 calculated BP86 instead of B3LYP

E(RB-P86) = -1438.41760240

Zero-point correction= 0.275275 (Hartree/Particle)
Thermal correction to Energy= 0.303359
Thermal correction to Enthalpy= 0.304303
Thermal correction to Gibbs Free Energy= 0.217350
Sum of electronic and zero-point Energies= -1438.142327
Sum of electronic and thermal Energies= -1438.114244
Sum of electronic and thermal Enthalpies= -1438.113299
Sum of electronic and thermal Free Energies= -1438.200253

	E (Thermal)	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	190.361	99.665	183.009

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.293377	3.129572	-0.548227
2	8	0	-2.823724	1.765270	-0.666985
3	6	0	-2.636838	1.138019	0.525978
4	8	0	-2.902233	1.656945	1.609946
5	6	0	-1.955527	-0.190338	0.417392
6	6	0	-2.364693	-1.298642	1.263172
7	6	0	-3.258987	-1.255309	2.288648
8	45	0	0.054106	-0.087631	0.067243
9	8	0	0.003763	0.326051	-1.982307
10	6	0	1.119262	0.467649	-2.601468
11	8	0	2.303481	0.389509	-2.145069
12	45	0	2.528366	0.009062	-0.126049
13	8	0	2.498468	-2.036424	-0.498971
14	6	0	1.371791	-2.622607	-0.516943
15	8	0	0.197093	-2.132619	-0.334646
16	8	0	0.108704	1.969523	0.436969
17	6	0	1.257167	2.540090	0.447236
18	8	0	2.411672	2.038332	0.259437
19	8	0	0.373669	-0.485721	2.094175
20	6	0	1.577989	-0.524755	2.532251
21	8	0	2.671960	-0.361914	1.901605
22	6	0	-2.639441	-1.054248	-1.649500
23	6	0	-3.987488	-1.048714	-1.414607
24	6	0	-4.757042	-2.174445	-0.810766

25	1	0	-4.259485	3.168073	-0.017935
26	1	0	-3.401435	3.487272	-1.581784
27	1	0	-2.555601	3.736197	0.000599
28	1	0	-1.822107	-2.234669	1.074592
29	1	0	-3.416599	-2.136833	2.920771
30	1	0	-3.776869	-0.331662	2.561851
31	1	0	1.229888	3.630233	0.650633
32	1	0	1.667147	-0.731166	3.618301
33	1	0	1.391372	-3.713252	-0.719586
34	1	0	1.025421	0.687319	-3.684622
35	1	0	-2.051075	-1.972449	-1.536067
36	1	0	-2.144568	-0.221628	-2.154990
37	1	0	-4.539012	-0.116864	-1.599902
38	1	0	-5.753959	-2.286019	-1.275072
39	1	0	-4.216100	-3.133822	-0.873755
40	1	0	-4.927955	-1.964379	0.270998

Structure 13 calculated with acetate ligands on Rh instead of formate

E(RB+HF-LYP) = -1595.52546230

Zero-point correction= 0.395172 (Hartree/Particle)
Thermal correction to Energy= 0.430213
Thermal correction to Enthalpy= 0.431158
Thermal correction to Gibbs Free Energy= 0.326148
Sum of electronic and zero-point Energies= -1595.130290
Sum of electronic and thermal Energies= -1595.095249
Sum of electronic and thermal Enthalpies= -1595.094305
Sum of electronic and thermal Free Energies= -1595.199314

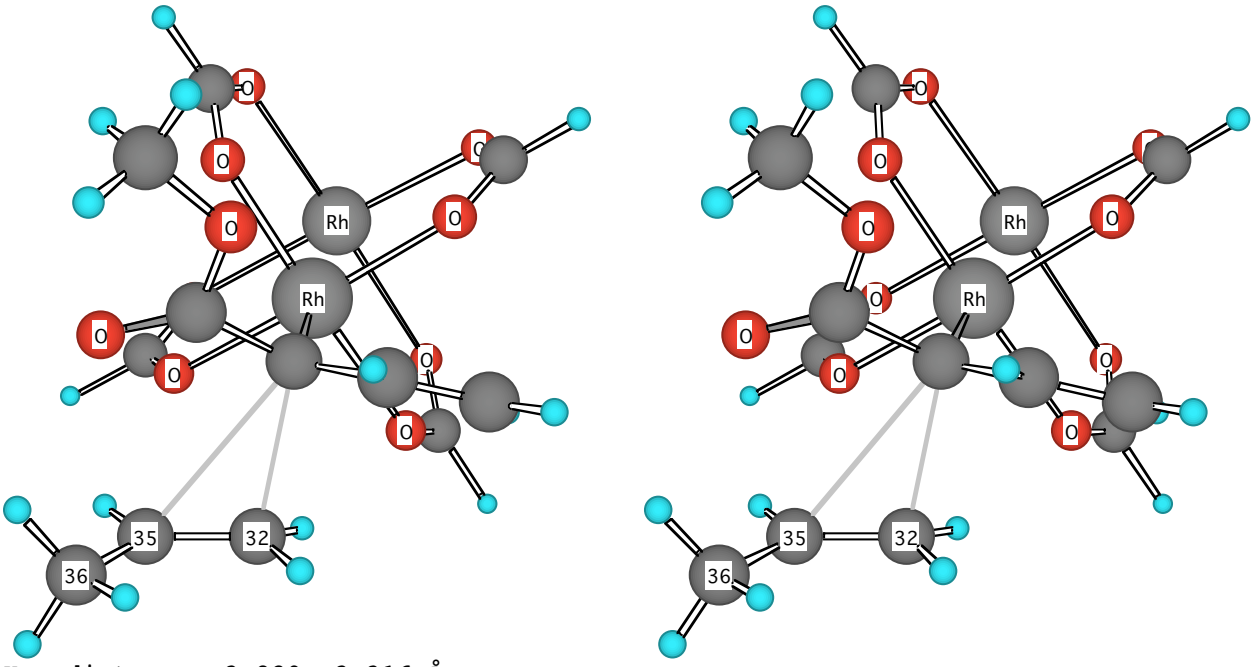
	E (Thermal)	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	269.963	120.903	221.011

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.548653	3.018354	-0.500030
2	8	0	-3.090559	1.658098	-0.580982
3	6	0	-2.803956	1.085667	0.603723
4	6	0	-2.101521	-0.228076	0.503240
5	45	0	-0.069916	-0.087450	0.074686
6	8	0	0.311872	-0.481753	2.080485
7	6	0	1.513652	-0.498550	2.513937
8	8	0	2.563837	-0.312405	1.833290
9	45	0	2.375807	0.067363	-0.192248
10	8	0	2.201740	2.092089	0.216903
11	6	0	1.058178	2.586003	0.438700
12	8	0	-0.055193	1.959269	0.445585
13	8	0	-2.992332	1.634592	1.674865
14	6	0	-2.467140	-1.320741	1.380327
15	6	0	-3.318706	-1.255994	2.426267
16	8	0	-0.190688	0.326636	-1.966238
17	6	0	0.879116	0.506760	-2.643231
18	8	0	2.063018	0.452917	-2.203911
19	8	0	0.105701	-2.122279	-0.332533
20	6	0	1.266509	-2.611310	-0.565752
21	8	0	2.360080	-1.979953	-0.576246
22	6	0	-2.770202	-1.151175	-1.560070
23	6	0	-4.094542	-1.174469	-1.264489
24	6	0	-4.818030	-2.317300	-0.640692
25	1	0	-4.462428	3.087239	0.096471

26	1	0	-3.738522	3.320738	-1.530211
27	1	0	-2.775848	3.645488	-0.049672
28	1	0	-1.912861	-2.240824	1.206877
29	1	0	-3.433509	-2.107214	3.092737
30	1	0	-3.846915	-0.344323	2.682061
31	6	0	0.979321	4.076170	0.702463
32	6	0	1.673503	-0.767245	3.996297
33	6	0	1.308164	-4.093410	-0.880102
34	6	0	0.686134	0.816205	-4.114144
35	1	0	-2.151450	-2.037353	-1.446214
36	1	0	-2.318267	-0.314798	-2.078220
37	1	0	-4.674704	-0.269893	-1.440006
38	1	0	-5.788148	-2.485563	-1.124458
39	1	0	-4.236100	-3.243450	-0.674972
40	1	0	-5.024684	-2.093421	0.420589
41	1	0	2.729818	-0.793054	4.267895
42	1	0	1.162008	0.016440	4.564696
43	1	0	1.198176	-1.719900	4.251007
44	1	0	0.694950	-4.647443	-0.163614
45	1	0	0.886855	-4.262165	-1.877847
46	1	0	2.336421	-4.457605	-0.860230
47	1	0	1.651047	0.924449	-4.611408
48	1	0	0.110375	0.014245	-4.587485
49	1	0	0.108863	1.740766	-4.219992
50	1	0	1.967013	4.471959	0.944682
51	1	0	0.605712	4.580600	-0.196375
52	1	0	0.276304	4.275971	1.515519

Vinylcarbene + propene TS1



Key distances 2.839, 2.216 Å
E(RB+HF-LYP) = -1438.22258109

Zero-point correction=	0.284849 (Hartree/Particle)
Thermal correction to Energy=	0.312401
Thermal correction to Enthalpy=	0.313346
Thermal correction to Gibbs Free Energy=	0.227873
Sum of electronic and zero-point Energies=	-1437.937732
Sum of electronic and thermal Energies=	-1437.910180
Sum of electronic and thermal Enthalpies=	-1437.909235

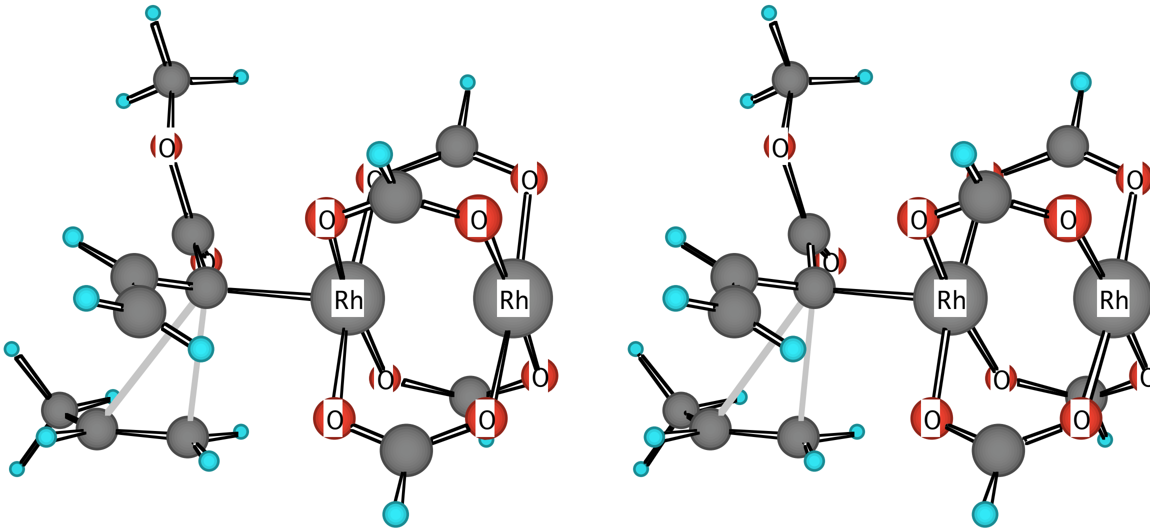
Sum of electronic and thermal Free Energies= -1437.994708

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	196.035	97.556	179.892

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.152168	1.760791	-0.832097
2	45	0	0.023296	-0.036193	0.208195
3	6	0	-2.013521	-0.014869	0.753725
4	6	0	-2.800925	0.842655	-0.198632
5	8	0	-3.181178	0.582710	-1.322868
6	8	0	-2.943376	2.065794	0.363085
7	6	0	-3.412321	3.097730	-0.521184
8	1	0	-2.713373	3.220412	-1.351389
9	1	0	-3.452724	4.002134	0.086238
10	1	0	-4.402679	2.848238	-0.911168
11	6	0	-2.435817	0.057718	2.148026
12	6	0	-1.721201	-0.430293	3.181246
13	1	0	-3.380750	0.560117	2.358916
14	1	0	-2.079210	-0.321104	4.201723
15	1	0	-0.781713	-0.948406	3.029575
16	45	0	2.434791	0.014210	-0.398272
17	8	0	2.070232	1.820883	-1.353901
18	6	0	0.891025	2.262336	-1.358324
19	1	0	0.730581	3.213834	-1.887564
20	8	0	2.778449	1.031583	1.379993
21	6	0	1.786352	1.303277	2.105976
22	1	0	1.998194	1.859758	3.031590
23	8	0	0.560612	1.020954	1.920399
24	8	0	2.625590	-1.806875	0.602875
25	6	0	1.609832	-2.301730	1.149925
26	1	0	1.750759	-3.260830	1.671076
27	8	0	0.420331	-1.840575	1.187148
28	8	0	1.931060	-0.999145	-2.142932
29	6	0	0.725933	-1.312692	-2.322312
30	1	0	0.496867	-1.852426	-3.253895
31	8	0	-0.275525	-1.093267	-1.568766
32	6	0	-2.677392	-2.100520	0.406488
33	1	0	-3.370838	-2.214774	1.235250
34	1	0	-1.649029	-2.387084	0.592159
35	6	0	-3.170298	-2.037996	-0.867932
36	6	0	-4.616958	-2.027728	-1.217290
37	1	0	-2.458126	-1.995937	-1.686675
38	1	0	-4.856369	-2.929066	-1.800834
39	1	0	-5.259551	-2.010485	-0.331241
40	1	0	-4.846416	-1.165287	-1.852049

Vinylcarbene + propene TS3a (gives minor product)



E(RB+HF-LYP) = -1438.22531863

Zero-point correction= 0.284959 (Hartree/Particle)
Thermal correction to Energy= 0.312501
Thermal correction to Enthalpy= 0.313445
Thermal correction to Gibbs Free Energy= 0.228108
Sum of electronic and zero-point Energies= -1437.940359
Sum of electronic and thermal Energies= -1437.912818
Sum of electronic and thermal Enthalpies= -1437.911874
Sum of electronic and thermal Free Energies= -1437.997210

	E (Thermal)	CV	S
	KCAL/MOL	CAL/MOL-KELVIN	CAL/MOL-KELVIN
TOTAL	196.097	97.588	179.606

Standard orientation:

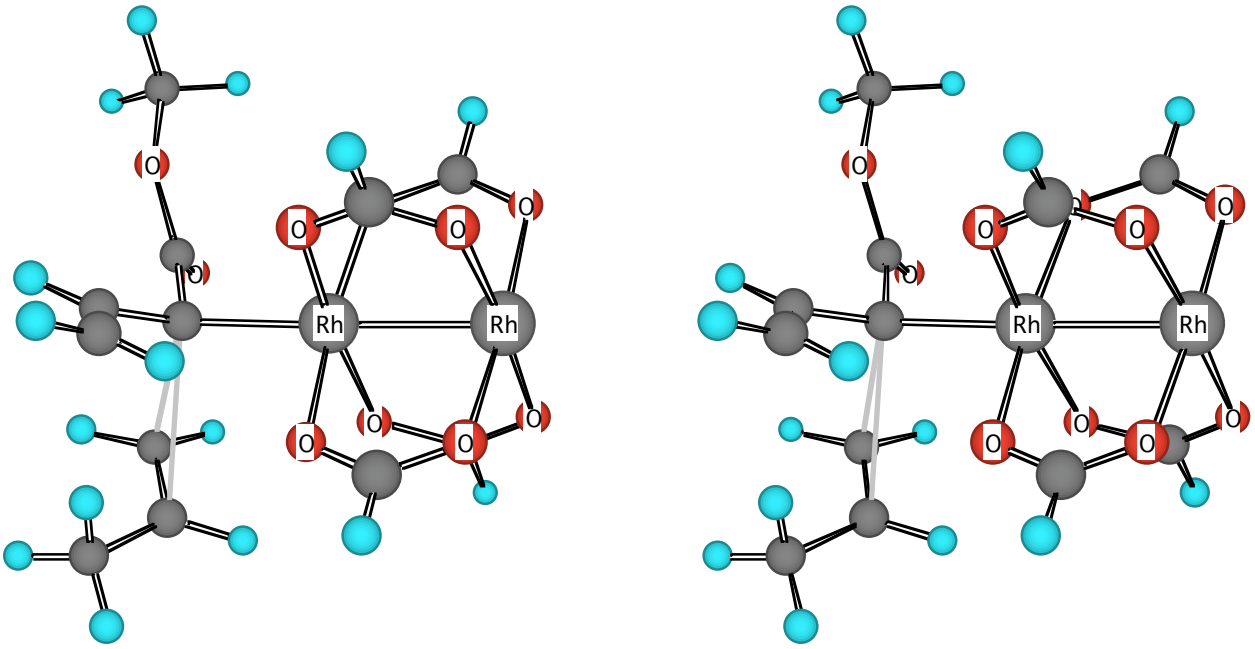
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.090624	1.927579	-0.254107
2	45	0	0.047083	-0.115157	0.135388
3	6	0	-2.009958	-0.188421	0.576720
4	6	0	-2.745587	0.930811	-0.105497
5	8	0	-3.033434	1.017709	-1.280501
6	8	0	-2.965359	1.917936	0.794804
7	6	0	-3.396302	3.171377	0.236973
8	1	0	-2.651937	3.536426	-0.474344
9	1	0	-3.485982	3.850642	1.084958
10	1	0	-4.357741	3.056102	-0.270234
11	6	0	-2.511020	-0.589974	1.881632
12	6	0	-1.864538	-1.447382	2.695828
13	1	0	-3.446861	-0.145456	2.222772
14	1	0	-2.266972	-1.692399	3.675439
15	1	0	-0.935944	-1.920161	2.398358
16	45	0	2.481689	0.117180	-0.287758
17	8	0	2.150205	2.133496	-0.636589
18	6	0	0.970392	2.564060	-0.546339
19	1	0	0.827941	3.636940	-0.744395
20	8	0	2.726096	0.511944	1.734742
21	6	0	1.697314	0.520532	2.460784
22	1	0	1.855474	0.740814	3.527354
23	8	0	0.488525	0.305397	2.131754
24	8	0	2.645353	-1.927489	0.087868

25	6	0	1.605912	-2.569039	0.381976
26	1	0	1.732059	-3.645039	0.575435
27	8	0	0.409148	-2.141049	0.489316
28	8	0	2.101824	-0.279473	-2.290173
29	6	0	0.908362	-0.491410	-2.631072
30	1	0	0.733558	-0.693924	-3.698263
31	8	0	-0.134079	-0.505468	-1.903965
32	6	0	-2.540238	-1.954239	-0.812324
33	1	0	-1.833669	-2.563611	-0.260082
34	1	0	-2.175062	-1.486680	-1.719612
35	6	0	-3.866937	-1.976619	-0.514930
36	6	0	-4.952876	-1.357841	-1.330323
37	1	0	-4.182868	-2.493290	0.392253
38	1	0	-5.569020	-0.680265	-0.723674
39	1	0	-4.556182	-0.802009	-2.180942
40	1	0	-5.629915	-2.144916	-1.694140

Vinylcarbene + propene TS3d (gives minor product, rotated both vinyl and ester from 3a)

E(RB+HF-LYP) = -1438.22599048

Vinylcarbene + propene TS4 = reversed ts1 for vinyl carbene



E(RB+HF-LYP) = -1438.22185556

Zero-point correction= 0.284717 (Hartree/Particle)
Thermal correction to Energy= 0.311974
Thermal correction to Enthalpy= 0.312918
Thermal correction to Gibbs Free Energy= 0.228706
Sum of electronic and zero-point Energies= -1437.937139
Sum of electronic and thermal Energies= -1437.909882
Sum of electronic and thermal Enthalpies= -1437.908938
Sum of electronic and thermal Free Energies= -1437.993149

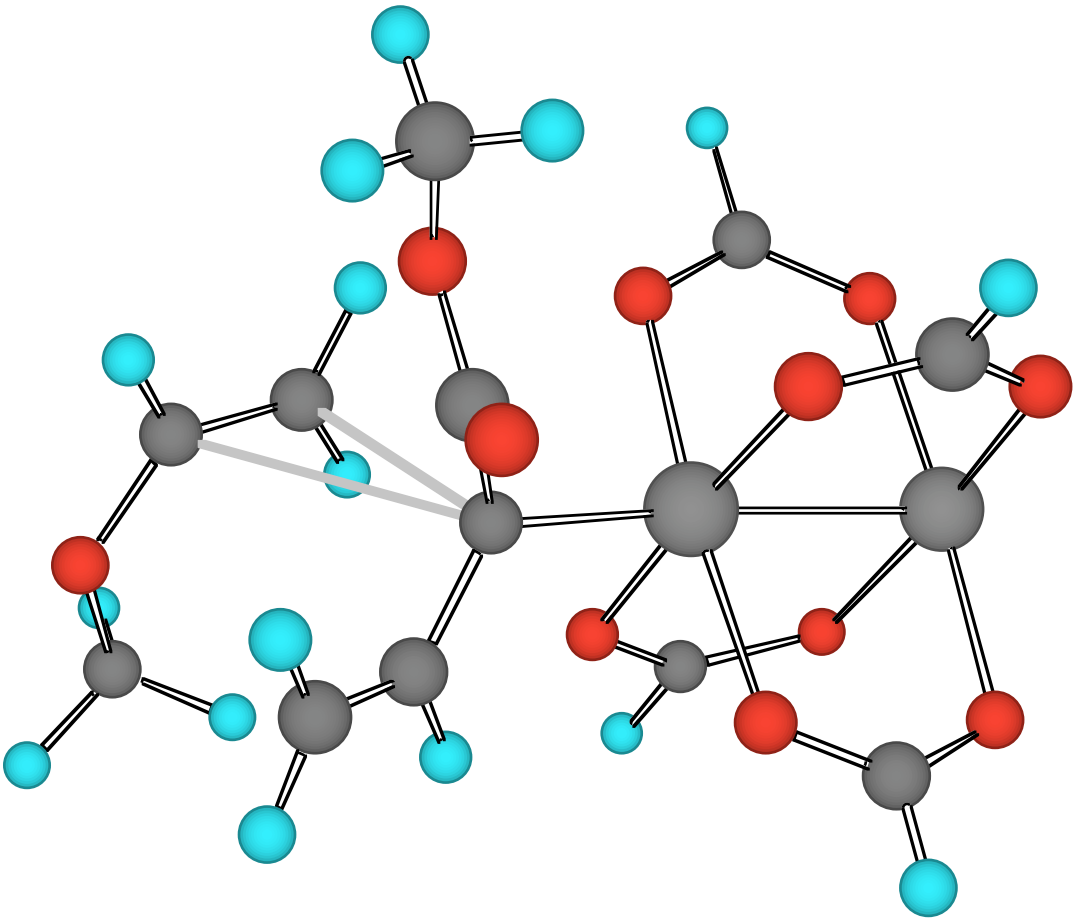
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	195.767	97.335	177.238

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.065410	-2.020215	-0.365082
2	45	0	0.077340	0.019831	0.051524
3	6	0	2.207293	0.064981	0.162367
4	6	0	2.763823	-1.225601	-0.401624
5	8	0	2.973665	-1.517610	-1.560819
6	8	0	2.936324	-2.090563	0.624570
7	6	0	3.215249	-3.446678	0.237916
8	1	0	2.398813	-3.832617	-0.376273
9	1	0	3.292524	-4.003083	1.172361
10	1	0	4.151197	-3.501878	-0.324482
11	6	0	2.912627	0.536607	1.356963
12	6	0	2.395641	1.373456	2.279947
13	1	0	3.926470	0.163261	1.516802
14	1	0	2.972646	1.646195	3.160402
15	1	0	1.384551	1.754520	2.200742
16	45	0	-2.407571	-0.090178	-0.064589
17	8	0	-2.213150	-2.113787	-0.465231
18	6	0	-1.053436	-2.600738	-0.527101
19	1	0	-0.989899	-3.676261	-0.750985
20	8	0	-2.397926	-0.494398	1.974690
21	6	0	-1.284472	-0.564211	2.559429
22	1	0	-1.314957	-0.792587	3.635780
23	8	0	-0.118385	-0.403883	2.079878
24	8	0	-2.418515	1.959101	0.343955
25	6	0	-1.322432	2.546252	0.510751
26	1	0	-1.374101	3.623889	0.732114
27	8	0	-0.141108	2.064865	0.457568
28	8	0	-2.227756	0.310931	-2.101087
29	6	0	-1.080210	0.483748	-2.584928
30	1	0	-1.031668	0.691346	-3.664855
31	8	0	0.046283	0.456092	-1.991991
32	6	0	2.915414	1.242295	-1.334956
33	1	0	3.981507	1.098030	-1.172025
34	1	0	2.455896	0.613624	-2.089757
35	6	0	2.363683	2.475008	-1.067233
36	6	0	2.998029	3.499734	-0.221786
37	1	0	1.339124	2.643476	-1.383797
38	1	0	2.604864	4.504625	-0.398949
39	1	0	4.090317	3.495214	-0.286979
40	1	0	2.747108	3.224496	0.827771

Ts's for cyclopropanation of methyl vinyl ether, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Vinylcarbene + methyl vinyl ether TS1d (21)



E(RB+HF-LYP) = -1513.43857617

Zero-point correction=	0.290171 (Hartree/Particle)
Thermal correction to Energy=	0.318953
Thermal correction to Enthalpy=	0.319897
Thermal correction to Gibbs Free Energy=	0.229777
Sum of electronic and zero-point Energies=	-1513.148405
Sum of electronic and thermal Energies=	-1513.119623
Sum of electronic and thermal Enthalpies=	-1513.118679
Sum of electronic and thermal Free Energies=	-1513.208799

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	200.146	100.719	189.672

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.915513	3.450013	-1.043074
2	8	0	-2.561753	2.068752	-0.840772
3	6	0	-2.325718	1.723367	0.434879
4	6	0	-1.764697	0.355243	0.625864
5	45	0	0.195689	0.073715	0.170011
6	8	0	0.598784	-0.239104	2.189870
7	6	0	1.800035	-0.459870	2.546909

8	8	0	2.833135	-0.537173	1.833184
9	45	0	2.623235	-0.278024	-0.218782
10	8	0	2.858720	1.773527	0.017674
11	6	0	1.834834	2.469959	0.242936
12	8	0	0.624197	2.096031	0.361633
13	8	0	-2.454613	2.480284	1.380311
14	6	0	-2.362483	-0.537590	1.583761
15	6	0	-3.475648	-0.279241	2.307375
16	8	0	0.037891	0.352888	-1.891779
17	6	0	1.086184	0.257270	-2.605887
18	8	0	2.265712	0.009031	-2.245579
19	8	0	-0.038128	-1.992897	-0.047657
20	6	0	1.002605	-2.691492	-0.283733
21	8	0	2.191670	-2.311571	-0.420378
22	6	0	-2.728157	-0.890466	-1.589960
23	6	0	-3.991582	-0.854106	-1.121005
24	8	0	-4.638860	-1.802029	-0.418651
25	1	0	-3.826701	3.700926	-0.493612
26	1	0	-3.072967	3.551326	-2.116819
27	1	0	-2.102422	4.098441	-0.708751
28	1	0	-1.825268	-1.467299	1.752543
29	1	0	-3.826364	-0.980942	3.059472
30	1	0	-4.030351	0.647208	2.201564
31	1	0	1.994771	3.552621	0.355095
32	1	0	1.939786	-0.602151	3.628990
33	1	0	0.820531	-3.773018	-0.379795
34	1	0	0.927271	0.413676	-3.683706
35	1	0	-2.073428	-1.744475	-1.474058
36	1	0	-2.348728	-0.051907	-2.155136
37	1	0	-4.623768	0.021365	-1.239820
38	6	0	-3.993712	-3.070845	-0.288050
39	1	0	-4.678487	-3.698979	0.282899
40	1	0	-3.817036	-3.510444	-1.276886
41	1	0	-3.039367	-2.977817	0.239829

Vinylcarbene + methyl vinyl ether TS1d with anti-arrangement of OMe

E(RB+HF-LYP) = -1513.43690680

Zero-point correction=	0.289446 (Hartree/Particle)
Thermal correction to Energy=	0.318499
Thermal correction to Enthalpy=	0.319443
Thermal correction to Gibbs Free Energy=	0.229053
Sum of electronic and zero-point Energies=	-1513.147461
Sum of electronic and thermal Energies=	-1513.118408
Sum of electronic and thermal Enthalpies=	-1513.117464
Sum of electronic and thermal Free Energies=	-1513.207854

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	199.861	101.072	190.241

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.880838	3.242977	-0.844323
2	8	0	-2.475494	1.869653	-0.700743
3	6	0	-2.297436	1.458853	0.564662
4	8	0	-2.534539	2.142743	1.544606

5	6	0	-1.659659	0.117640	0.689169
6	6	0	-2.241186	-0.889490	1.524743
7	6	0	-3.407841	-0.757492	2.201310
8	45	0	0.294617	-0.015881	0.190634
9	8	0	0.198881	-2.083777	-0.063291
10	6	0	1.276416	-2.700655	-0.351995
11	8	0	2.432043	-2.233928	-0.515833
12	45	0	2.728821	-0.185232	-0.272009
13	8	0	2.295726	0.124004	-2.282014
14	6	0	1.090310	0.279526	-2.605562
15	8	0	0.057338	0.274173	-1.862100
16	8	0	0.775377	-0.330867	2.191042
17	6	0	1.997998	-0.484987	2.508364
18	8	0	3.012531	-0.479848	1.764385
19	8	0	0.581000	2.030070	0.410253
20	6	0	1.760060	2.491669	0.277934
21	8	0	2.825494	1.875449	0.015673
22	6	0	-2.692955	-1.283516	-1.495305
23	6	0	-3.962741	-0.923753	-1.248137
24	8	0	-4.751147	-1.615056	-0.391285
25	6	0	-6.131225	-1.255313	-0.387236
26	1	0	-3.841018	3.419417	-0.351509
27	1	0	-2.963554	3.407579	-1.918688
28	1	0	-2.126852	3.903391	-0.409898
29	1	0	-1.673625	-1.811997	1.616230
30	1	0	-3.768903	-1.552027	2.848598
31	1	0	-3.990438	0.156855	2.166061
32	1	0	1.845394	3.580208	0.414304
33	1	0	2.177634	-0.644106	3.582126
34	1	0	1.166473	-3.789081	-0.472680
35	1	0	0.888394	0.442592	-3.675185
36	1	0	-2.265747	-2.189398	-1.081221
37	1	0	-2.076370	-0.682829	-2.150831
38	1	0	-4.403407	-0.021454	-1.671665
39	1	0	-6.589990	-1.792050	0.444534
40	1	0	-6.261026	-0.175231	-0.240754
41	1	0	-6.614787	-1.555454	-1.324846

Vinylcarbene + methyl vinyl ether TS1c

E(RB+HF-LYP) = -1513.43790537

Zero-point correction= 0.290403 (Hartree/Particle)
Thermal correction to Energy= 0.319016
Thermal correction to Enthalpy= 0.319960
Thermal correction to Gibbs Free Energy= 0.230422
Sum of electronic and zero-point Energies= -1513.147503
Sum of electronic and thermal Energies= -1513.118890
Sum of electronic and thermal Enthalpies= -1513.117945
Sum of electronic and thermal Free Energies= -1513.207483

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	200.185	100.620	188.448

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.591824	3.673496	-0.653843

2	8	0	-2.342717	2.256571	-0.601487
3	6	0	-2.267648	1.739256	0.631611
4	8	0	-2.470122	2.373584	1.652141
5	6	0	-1.794370	0.322442	0.733184
6	6	0	-2.515138	-0.448927	1.718873
7	6	0	-2.118829	-1.663075	2.159619
8	45	0	0.167573	0.024292	0.194555
9	8	0	-0.054174	-2.014046	-0.229379
10	6	0	0.984417	-2.673280	-0.567279
11	8	0	2.167148	-2.269916	-0.691208
12	45	0	2.583634	-0.261084	-0.321952
13	8	0	2.149386	0.192677	-2.301571
14	6	0	0.953612	0.457396	-2.591718
15	8	0	-0.065711	0.475994	-1.831690
16	8	0	0.658846	-0.453542	2.160225
17	6	0	1.876407	-0.686422	2.448399
18	8	0	2.879027	-0.688339	1.688509
19	8	0	0.602681	2.024636	0.556234
20	6	0	1.804058	2.422170	0.421875
21	8	0	2.820954	1.762442	0.083559
22	6	0	-2.882271	-0.600281	-1.487548
23	6	0	-4.139535	-0.473815	-1.011339
24	8	0	-4.919384	-1.427196	-0.470894
25	6	0	-4.473372	-2.781675	-0.578403
26	1	0	-3.537114	3.919066	-0.162630
27	1	0	-2.632835	3.919461	-1.714830
28	1	0	-1.778422	4.212424	-0.162669
29	1	0	-3.404162	0.004450	2.157146
30	1	0	-2.684712	-2.180024	2.930721
31	1	0	-1.241730	-2.155968	1.758995
32	1	0	1.961918	3.490258	0.633190
33	1	0	2.063485	-0.917815	3.507672
34	1	0	0.807108	-3.739537	-0.776062
35	1	0	0.750982	0.707108	-3.644321
36	1	0	-2.345675	-1.540811	-1.500041
37	1	0	-2.396407	0.247758	-1.946842
38	1	0	-4.653775	0.483507	-0.998758
39	1	0	-5.262085	-3.391069	-0.135215
40	1	0	-4.336052	-3.054168	-1.631857
41	1	0	-3.535322	-2.935621	-0.037741

Vinylcarbene + methyl vinyl ether TS1c with anti-arrangement of OMe

E(RB+HF-LYP) = -1513.43617134

Zero-point correction= 0.289059 (Hartree/Particle)
Thermal correction to Energy= 0.318313
Thermal correction to Enthalpy= 0.319257
Thermal correction to Gibbs Free Energy= 0.228093
Sum of electronic and zero-point Energies= -1513.147112
Sum of electronic and thermal Energies= -1513.117858
Sum of electronic and thermal Enthalpies= -1513.116914
Sum of electronic and thermal Free Energies= -1513.208079

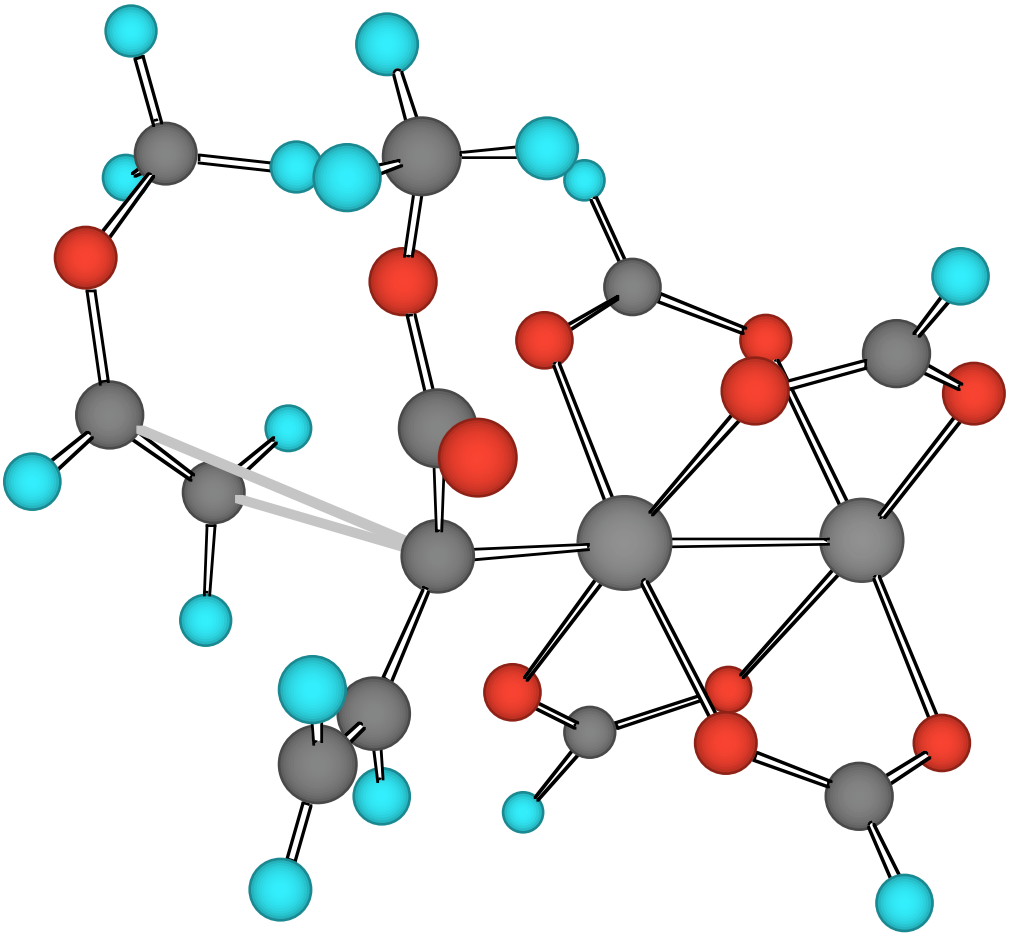
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	199.745	101.309	191.872

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.329950	3.849427	-0.688050
2	8	0	-2.115339	2.428589	-0.605112
3	6	0	-2.085661	1.931566	0.634429
4	6	0	-1.696094	0.491875	0.745234
5	45	0	0.213973	0.045749	0.207974
6	8	0	0.791131	1.996244	0.643967
7	6	0	2.018149	2.310483	0.522647
8	8	0	2.984573	1.589747	0.164646
9	45	0	2.607722	-0.398886	-0.303390
10	8	0	2.844743	-0.913624	1.698026
11	6	0	1.832991	-0.880239	2.445012
12	8	0	0.637659	-0.552759	2.154833
13	8	0	-2.284329	2.581425	1.645975
14	6	0	-2.543661	-0.266346	1.610177
15	6	0	-2.397898	-1.598544	1.817456
16	8	0	-0.141159	-1.953132	-0.304244
17	6	0	0.848836	-2.678269	-0.652308
18	8	0	2.060186	-2.361703	-0.742801
19	8	0	0.021512	0.573530	-1.800076
20	6	0	1.041729	0.502419	-2.554970
21	8	0	2.215620	0.147492	-2.268779
22	6	0	-2.974913	-0.518389	-1.732168
23	6	0	-4.185049	-0.758201	-1.211272
24	8	0	-4.450213	-1.890006	-0.507319
25	6	0	-5.795823	-2.037860	-0.066743
26	1	0	-3.277615	4.126520	-0.218473
27	1	0	-2.345875	4.076785	-1.753720
28	1	0	-1.513116	4.379093	-0.191990
29	1	0	-3.356835	0.262905	2.108517
30	1	0	-3.079722	-2.134676	2.471931
31	1	0	-1.620840	-2.164753	1.317889
32	1	0	2.251247	3.357539	0.767138
33	1	0	1.988300	-1.173027	3.494202
34	1	0	0.592245	-3.718325	-0.904457
35	1	0	0.862645	0.792830	-3.601437
36	1	0	-2.166769	-1.233767	-1.636504
37	1	0	-2.785768	0.397605	-2.275032
38	1	0	-5.013656	-0.053909	-1.297100
39	1	0	-5.839319	-2.974528	0.491620
40	1	0	-6.095611	-1.209798	0.589344
41	1	0	-6.486601	-2.093280	-0.917805

Vinylcarbene + methyl vinyl ether TS2d (22)



E(RB+HF-LYP) = -1513.43766840

Zero-point correction=	0.290740 (Hartree/Particle)
Thermal correction to Energy=	0.319193
Thermal correction to Enthalpy=	0.320137
Thermal correction to Gibbs Free Energy=	0.231910
Sum of electronic and zero-point Energies=	-1513.146929
Sum of electronic and thermal Energies=	-1513.118476
Sum of electronic and thermal Enthalpies=	-1513.117532
Sum of electronic and thermal Free Energies=	-1513.205759

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	200.296	100.436	185.689

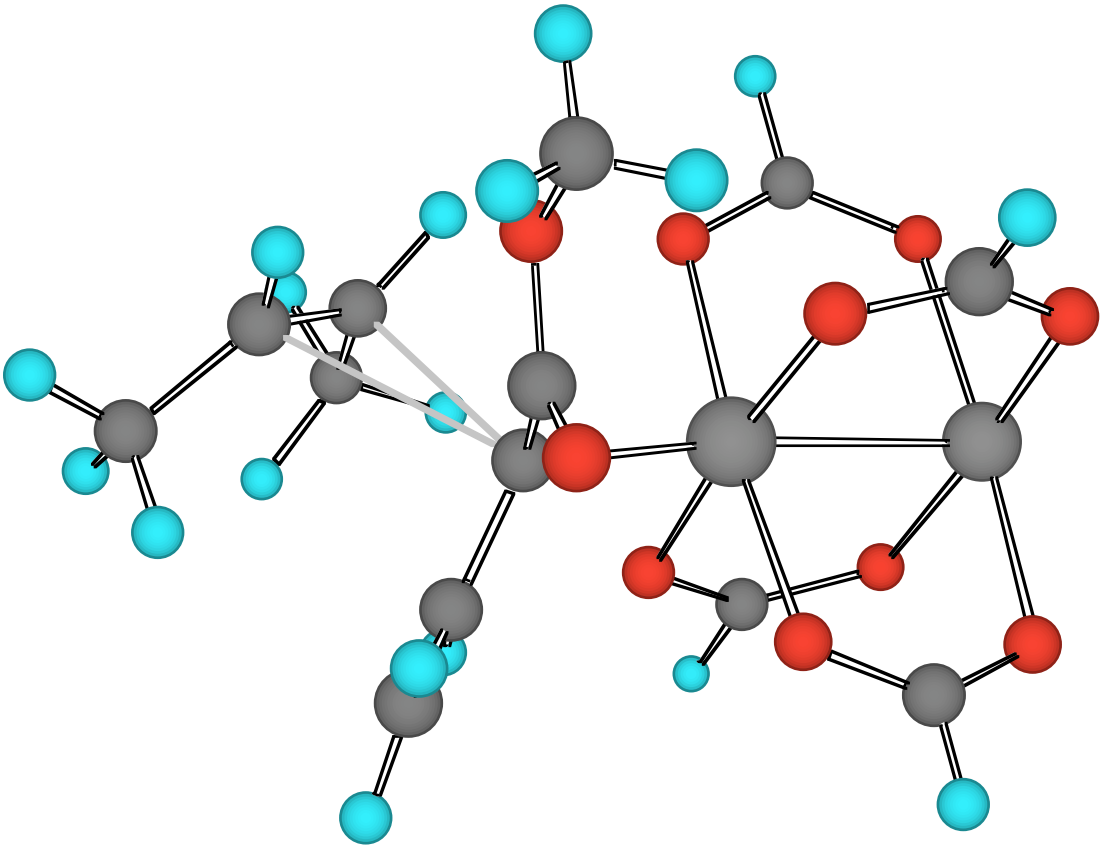
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.545356	-0.160574	2.593559
2	8	0	2.895815	-0.131890	1.310467
3	6	0	2.493809	1.081024	0.905864
4	6	0	1.659058	1.072795	-0.332594
5	45	0	-0.214898	0.282505	-0.119300
6	8	0	-1.003165	2.200938	-0.259082
7	6	0	-2.263427	2.353210	-0.173883
8	8	0	-3.154201	1.479588	-0.012635
9	45	0	-2.559304	-0.502706	0.157945
10	8	0	-2.297672	-0.246726	2.205245
11	6	0	-1.179270	0.152538	2.622076

12	8	0	-0.134590	0.441177	1.955780
13	8	0	2.684976	2.102229	1.542814
14	6	0	1.835046	2.101575	-1.333731
15	6	0	2.646290	3.177402	-1.235876
16	8	0	0.339050	-1.735277	0.044883
17	6	0	-0.572770	-2.605850	0.227981
18	8	0	-1.814287	-2.438081	0.319478
19	8	0	-0.488013	0.069381	-2.175022
20	6	0	-1.613868	-0.361387	-2.588976
21	8	0	-2.626374	-0.690232	-1.920729
22	6	0	2.593309	-0.725698	-1.892334
23	6	0	3.895679	-0.701330	-1.513677
24	8	0	4.531124	-1.551487	-0.703794
25	1	0	4.430576	0.480372	2.594024
26	1	0	3.826308	-1.201715	2.751930
27	1	0	2.853335	0.175287	3.369196
28	1	0	1.170899	2.018861	-2.191315
29	1	0	2.631956	3.945525	-2.004852
30	1	0	3.286000	3.341213	-0.376296
31	1	0	-1.078830	0.270966	3.711460
32	1	0	-2.607057	3.395086	-0.255652
33	1	0	-1.697779	-0.454873	-3.682479
34	1	0	-0.212973	-3.642615	0.316276
35	1	0	1.903002	-1.496109	-1.578474
36	1	0	2.266090	-0.059344	-2.677642
37	1	0	4.575679	0.078389	-1.849441
38	6	0	3.808887	-2.707533	-0.258974
39	1	0	4.499694	-3.256753	0.382060
40	1	0	2.914925	-2.412846	0.295540
41	1	0	3.527342	-3.326437	-1.119169

Ts's for cyclopropanation of *cis* or *trans*-2-butene, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

Vinylcarbene + cis-2-butene TS1d (20)



E(RB+HF-LYP) = -1477.54245905

Zero-point correction=	0.313553 (Hartree/Particle)
Thermal correction to Energy=	0.342518
Thermal correction to Enthalpy=	0.343462
Thermal correction to Gibbs Free Energy=	0.255327
Sum of electronic and zero-point Energies=	-1477.228906
Sum of electronic and thermal Energies=	-1477.199941
Sum of electronic and thermal Enthalpies=	-1477.198997
Sum of electronic and thermal Free Energies=	-1477.287132

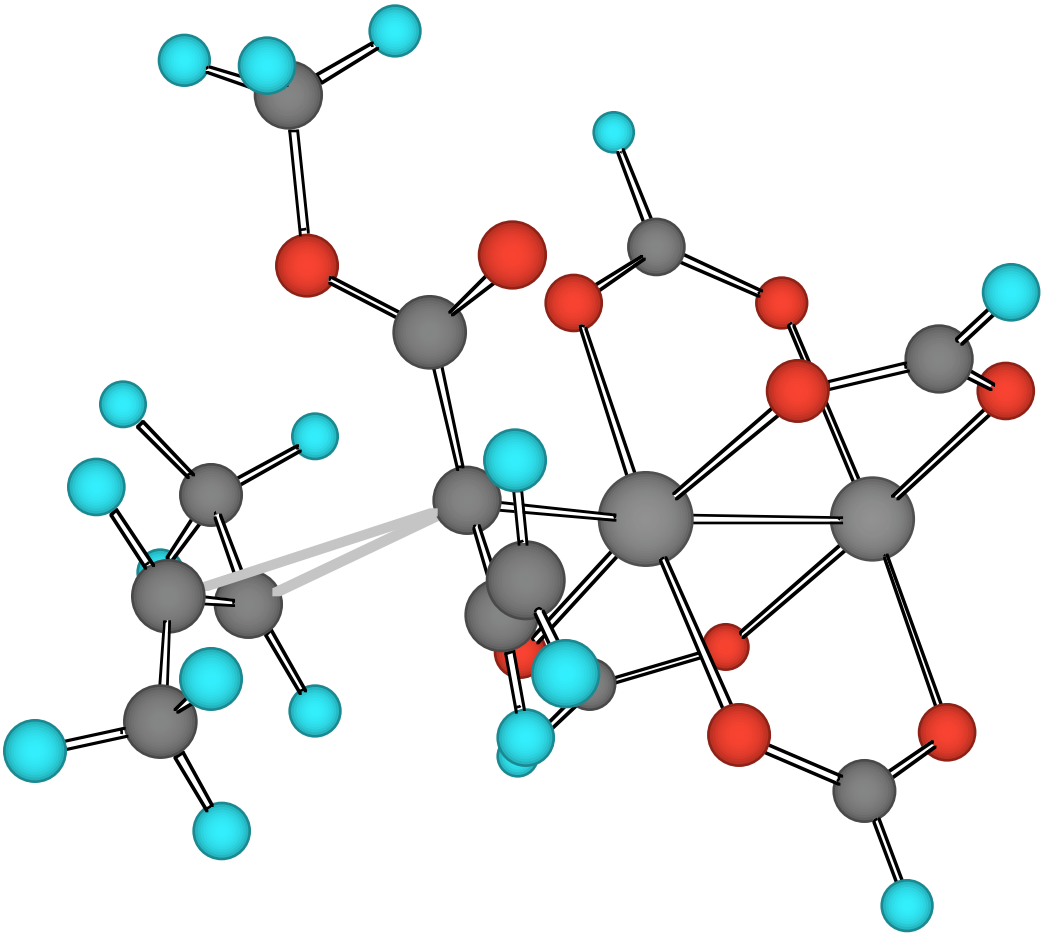
	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	214.933	102.830	185.497

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.896400	3.163109	-1.173261
2	8	0	-2.653146	1.760435	-0.974962
3	6	0	-2.487344	1.383569	0.309721
4	6	0	-1.972619	-0.013728	0.468064
5	45	0	0.127866	-0.060869	0.087800
6	8	0	0.412702	0.397128	2.097717
7	6	0	1.596249	0.530517	2.538326
8	8	0	2.687848	0.422246	1.917464
9	45	0	2.602250	-0.013202	-0.109024

10	8	0	2.452099	2.010802	-0.531988
11	6	0	1.303644	2.526325	-0.570234
12	8	0	0.175106	1.973197	-0.384273
13	8	0	-2.627645	2.145189	1.249034
14	6	0	-2.366452	-0.827406	1.600685
15	6	0	-3.100490	-0.431465	2.662598
16	8	0	0.088887	-0.509550	-1.952302
17	6	0	1.194449	-0.589128	-2.576788
18	8	0	2.361633	-0.446914	-2.129510
19	8	0	0.317416	-2.086126	0.565444
20	6	0	1.483599	-2.598455	0.578640
21	8	0	2.587316	-2.047172	0.336949
22	6	0	-2.793249	-1.245822	-1.320129
23	6	0	-4.033145	-0.819393	-0.917817
24	6	0	-5.028182	-1.572650	-0.107062
25	1	0	-3.804546	3.478861	-0.652519
26	1	0	-3.008605	3.286241	-2.250807
27	1	0	-2.046661	3.741281	-0.805085
28	1	0	-1.929745	-1.824008	1.610952
29	1	0	-3.236052	-1.098186	3.510596
30	1	0	-3.496809	0.573931	2.744012
31	1	0	1.262831	3.602210	-0.797961
32	1	0	1.667239	0.771939	3.609298
33	1	0	1.517857	-3.668067	0.835631
34	1	0	1.107709	-0.814260	-3.650669
35	6	0	-2.296002	-2.659700	-1.212481
36	1	0	-2.231182	-0.602062	-1.989172
37	1	0	-4.317101	0.190155	-1.195933
38	1	0	-6.046560	-1.353181	-0.447252
39	1	0	-4.875147	-2.654352	-0.117756
40	1	0	-4.964504	-1.241402	0.945939
41	1	0	-1.226375	-2.683679	-1.003580
42	1	0	-2.812755	-3.239789	-0.443418
43	1	0	-2.456902	-3.160950	-2.177353

Vinylcarbene + trans-2-butene TS1d (19)



E(RB+HF-LYP) = -1477.53757340

Zero-point correction=	0.313794 (Hartree/Particle)
Thermal correction to Energy=	0.342487
Thermal correction to Enthalpy=	0.343431
Thermal correction to Gibbs Free Energy=	0.255998
Sum of electronic and zero-point Energies=	-1477.223779
Sum of electronic and thermal Energies=	-1477.195086
Sum of electronic and thermal Enthalpies=	-1477.194142
Sum of electronic and thermal Free Energies=	-1477.281575

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	214.914	102.763	184.018

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.478259	3.039223	-0.345643
2	8	0	-3.103010	1.656620	-0.465071
3	6	0	-2.601857	1.105080	0.655970
4	6	0	-1.986900	-0.249824	0.489483
5	45	0	0.141274	-0.148415	0.083368
6	8	0	0.316539	0.857369	1.891942
7	6	0	1.461336	1.244888	2.276875
8	8	0	2.575696	1.108271	1.701832
9	45	0	2.597661	0.120633	-0.116003
10	8	0	2.222055	1.925645	-1.083717
11	6	0	1.026550	2.282539	-1.245859

12	8	0	-0.039379	1.678887	-0.901348
13	8	0	-2.559797	1.695698	1.719795
14	6	0	-2.265304	-1.272505	1.481890
15	6	0	-2.894265	-1.098844	2.663142
16	8	0	0.246230	-1.196549	-1.728022
17	6	0	1.374380	-1.323851	-2.299696
18	8	0	2.496132	-0.891264	-1.928237
19	8	0	0.545983	-1.965194	1.041076
20	6	0	1.758301	-2.307988	1.206310
21	8	0	2.805372	-1.696796	0.863790
22	6	0	-2.697202	-1.098134	-1.531359
23	6	0	-3.941521	-1.186532	-0.965830
24	6	0	-4.489133	-2.338834	-0.198852
25	1	0	-4.257575	3.167569	0.410125
26	1	0	-3.848122	3.323597	-1.331243
27	1	0	-2.609255	3.642406	-0.072598
28	1	0	-1.808142	-2.237710	1.280620
29	1	0	-2.926526	-1.910727	3.385274
30	1	0	-3.304922	-0.142602	2.965521
31	1	0	0.871325	3.245391	-1.755844
32	1	0	1.472680	1.769363	3.243640
33	1	0	1.905327	-3.271199	1.718012
34	1	0	1.358791	-1.887445	-3.245090
35	1	0	-2.018204	-1.941451	-1.435221
36	6	0	-2.377458	-0.121227	-2.632688
37	1	0	-4.625128	-0.354746	-1.131224
38	1	0	-5.427929	-2.668625	-0.664952
39	1	0	-3.799388	-3.186738	-0.166068
40	1	0	-4.731168	-2.051938	0.835721
41	1	0	-2.188097	-0.695986	-3.548859
42	1	0	-3.211011	0.560619	-2.814853
43	1	0	-1.483285	0.464979	-2.423168

Ts's for cyclopropanations with vinyldiazoacetonitrile, All B3LYP, lanl2dz on Rh, 6-31G* on all other atoms

vinyl cyano carbene + styrene TS1a

E(RB+HF-LYP) = -1494.33949025

Zero-point correction= 0.294394 (Hartree/Particle)
Thermal correction to Energy= 0.321971
Thermal correction to Enthalpy= 0.322915
Thermal correction to Gibbs Free Energy= 0.236125
Sum of electronic and zero-point Energies= -1494.045097
Sum of electronic and thermal Energies= -1494.017519
Sum of electronic and thermal Enthalpies= -1494.016575
Sum of electronic and thermal Free Energies= -1494.103365

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	202.040	101.127	182.665

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.651675	-1.175176	0.623977
2	6	0	4.617751	0.236333	0.699668

3	6	0	5.763436	0.956940	0.293641
4	6	0	6.893901	0.298133	-0.174828
5	6	0	6.908380	-1.099286	-0.244704
6	6	0	5.787007	-1.831230	0.157495
7	6	0	3.459566	0.974279	1.156577
8	6	0	2.207859	0.479730	1.423038
9	6	0	1.299723	0.780627	-0.625260
10	6	0	2.145451	0.019371	-1.529881
11	6	0	1.451557	2.199340	-0.715059
12	7	0	1.532508	3.362692	-0.769115
13	45	0	-0.671778	0.182441	-0.148983
14	8	0	-0.149904	-1.578191	0.861136
15	6	0	-1.094129	-2.314024	1.300032
16	8	0	-2.334542	-2.130889	1.217455
17	45	0	-3.041186	-0.423862	0.248847
18	8	0	-2.926281	0.646369	2.028227
19	6	0	-1.841303	1.215007	2.314362
20	8	0	-0.751145	1.216700	1.657425
21	8	0	-0.822710	-0.910284	-1.920481
22	6	0	-1.935071	-1.452595	-2.210907
23	8	0	-3.010890	-1.442993	-1.556710
24	8	0	-1.395440	1.860587	-1.127176
25	6	0	-2.651066	2.040455	-1.194181
26	8	0	-3.577007	1.314174	-0.741687
27	1	0	-1.949262	-2.004066	-3.162968
28	1	0	-2.960309	2.955649	-1.719292
29	1	0	-1.819758	1.786241	3.254105
30	1	0	-0.768669	-3.228749	1.818644
31	1	0	1.991624	-0.582592	1.441513
32	1	0	1.459521	1.113490	1.884702
33	1	0	3.593018	2.052918	1.225136
34	1	0	5.748651	2.042685	0.345516
35	1	0	7.764223	0.868780	-0.485766
36	1	0	7.793349	-1.615803	-0.605728
37	1	0	5.802195	-2.916499	0.112659
38	1	0	3.796794	-1.753583	0.957620
39	6	0	2.105663	-1.326747	-1.615302
40	1	0	2.844053	0.566294	-2.163406
41	1	0	2.743886	-1.857301	-2.316105
42	1	0	1.437447	-1.913106	-0.994207

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vinyl cyano carbene + styrene TS1d

E(RB+HF-LYP) = -1494.34205193

Zero-point correction= 0.294427 (Hartree/Particle)
Thermal correction to Energy= 0.322039
Thermal correction to Enthalpy= 0.322983
Thermal correction to Gibbs Free Energy= 0.235487
Sum of electronic and zero-point Energies= -1494.047625
Sum of electronic and thermal Energies= -1494.020013
Sum of electronic and thermal Enthalpies= -1494.019069
Sum of electronic and thermal Free Energies= -1494.106565

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	202.082	101.043	184.150

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.651892	1.925725	0.550802
2	6	0	-1.288183	0.545864	0.519925
3	45	0	0.713464	0.132707	0.113439
4	8	0	0.885885	-0.827569	1.957564
5	6	0	2.022583	-1.279883	2.304701
6	8	0	3.112065	-1.241172	1.675485
7	45	0	3.126786	-0.325876	-0.188238
8	8	0	3.509061	1.504217	0.707700
9	6	0	2.522356	2.195977	1.077505
10	8	0	1.284075	1.927998	0.984580
11	6	0	-1.990820	-0.357392	1.409575
12	6	0	-2.990634	0.003812	2.242324
13	8	0	0.750882	1.041028	-1.759386
14	6	0	1.858852	1.083104	-2.386008
15	8	0	2.976121	0.627109	-2.032111
16	8	0	0.344312	-1.724294	-0.769668
17	6	0	1.345736	-2.414682	-1.147257
18	8	0	2.568485	-2.133878	-1.065899
19	7	0	-1.895976	3.067255	0.562515
20	1	0	2.045517	-1.770316	3.289449
21	1	0	2.752343	3.164539	1.544794
22	1	0	-1.630455	-1.382516	1.413620
23	1	0	-3.430076	-0.708531	2.934973
24	1	0	-3.368472	1.022207	2.273159
25	1	0	1.820847	1.584386	-3.364419
26	1	0	1.096360	-3.384264	-1.604569
27	6	0	-2.166430	-0.107729	-1.492461
28	6	0	-3.379483	0.523461	-1.400609
29	6	0	-4.603406	0.018816	-0.817146
30	6	0	-5.707057	0.894354	-0.698410
31	6	0	-6.909694	0.460441	-0.153086
32	6	0	-7.039918	-0.861122	0.286905
33	6	0	-5.959186	-1.742642	0.183291
34	6	0	-4.752263	-1.310539	-0.357147
35	1	0	-2.031577	-1.158886	-1.262523
36	1	0	-1.359397	0.359028	-2.044996
37	1	0	-3.425737	1.556228	-1.742473
38	1	0	-5.604037	1.920302	-1.042167
39	1	0	-7.746986	1.147401	-0.071400
40	1	0	-7.981360	-1.203461	0.707440
41	1	0	-6.061024	-2.769587	0.522479
42	1	0	-3.925816	-2.007629	-0.448563

vinyl cyano carbene + styrene TS2d

E(RB+HF-LYP) = -1494.34108307

Zero-point correction= 0.294010 (Hartree/Particle)
Thermal correction to Energy= 0.321809
Thermal correction to Enthalpy= 0.322753
Thermal correction to Gibbs Free Energy= 0.234379
Sum of electronic and zero-point Energies= -1494.047073
Sum of electronic and thermal Energies= -1494.019274
Sum of electronic and thermal Enthalpies= -1494.018330
Sum of electronic and thermal Free Energies= -1494.106704

	E (Thermal) KCAL/MOL	CV CAL/MOL-KELVIN	S CAL/MOL-KELVIN
TOTAL	201.938	101.305	185.998

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.982863	0.430079	1.323130
2	6	0	1.179888	1.042922	0.328745
3	45	0	-0.719166	0.258708	0.063172
4	8	0	-1.546044	2.148493	0.368588
5	6	0	-2.812700	2.265096	0.378659
6	8	0	-3.688299	1.374896	0.218890
7	45	0	-3.047176	-0.572505	-0.108698
8	8	0	-3.000363	-0.901473	1.937847
9	6	0	-1.939889	-0.616380	2.555858
10	8	0	-0.857337	-0.133407	2.097809
11	6	0	1.376864	2.455332	0.054576
12	6	0	2.113973	3.280476	0.825593
13	8	0	-0.100415	-1.704488	-0.260070
14	6	0	-0.993342	-2.598856	-0.415407
15	8	0	-2.244187	-2.467011	-0.415815
16	8	0	-0.793026	0.606748	-1.993342
17	6	0	-1.864679	0.307231	-2.614181
18	8	0	-2.924950	-0.185998	-2.153783
19	7	0	2.612919	-0.129831	2.133599
20	1	0	-3.182187	3.287107	0.550511
21	1	0	-1.939240	-0.806090	3.639131
22	1	0	0.789702	2.859377	-0.765705
23	1	0	2.128682	4.351850	0.645103
24	1	0	2.687420	2.912365	1.672350
25	1	0	-0.608259	-3.617550	-0.571353
26	1	0	-1.847350	0.510564	-3.695433
27	6	0	2.214942	-0.043873	-1.530232
28	6	0	3.483157	0.456402	-1.452530
29	6	0	4.626194	-0.118051	-0.771173
30	6	0	5.852349	0.583181	-0.799660
31	6	0	6.983397	0.072452	-0.174510
32	6	0	6.913339	-1.151744	0.498940
33	6	0	5.707727	-1.858519	0.542881
34	6	0	4.574497	-1.352394	-0.083859
35	1	0	1.477332	0.424842	-2.171243
36	1	0	1.946294	-1.022071	-1.147551
37	1	0	3.671592	1.418676	-1.928576
38	1	0	5.904266	1.534212	-1.324361
39	1	0	7.918679	0.623856	-0.208465
40	1	0	7.795954	-1.552994	0.989211
41	1	0	5.651283	-2.805446	1.071399
42	1	0	3.646246	-1.911190	-0.043504

Structures related to 28. B3LYP using lanl2dz on Rh and 3-21G on the lighter atoms

28, Isomer 1

E(RB+HF-LYP) = -2074.76988136
Single point calculation using 6-31G* on all of the light atoms
E(RB+HF-LYP) = -2084.73168202

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	1.472372	-0.166620	1.249576
2	45	0	2.478207	0.413777	-0.840573
3	8	0	-0.122273	1.032964	0.758193
4	8	0	0.856642	1.600397	-1.237240
5	8	0	1.484390	-1.151185	-1.685553
6	8	0	0.516052	-1.702888	0.313365
7	8	0	2.452051	1.432066	2.112117
8	8	0	3.431466	1.984634	0.098081
9	8	0	3.087833	-1.367342	1.650917
10	8	0	4.048926	-0.826732	-0.372433
11	6	0	-0.134734	1.597041	-0.409553
12	6	0	0.666135	-1.861636	-0.970230
13	6	0	3.216394	2.153434	1.360029
14	6	0	4.020983	-1.444960	0.760102
15	6	0	-1.362932	2.374796	-0.836029
16	6	0	-1.393160	3.816208	-0.269504
17	6	0	-3.650383	2.882563	-0.067742
18	6	0	-2.892134	4.198830	-0.405348
19	7	0	-2.588956	1.814328	-0.203960
20	16	0	-3.142777	0.304469	-1.002644
21	8	0	-1.818250	-0.223468	-1.738093
22	8	0	-4.460832	0.513016	-1.878610
23	6	0	-3.618067	-0.668570	0.480768
24	6	0	-0.190624	-2.898994	-1.672948
25	6	0	-4.822978	-1.349475	0.417063
26	6	0	-5.194182	-2.133328	1.510593
27	6	0	-4.353916	-2.211928	2.625743
28	6	0	-3.148257	-1.503244	2.660592
29	6	0	-2.766771	-0.713663	1.573349
30	6	0	-0.572335	-4.040060	-0.710359
31	6	0	0.503721	-3.409423	-2.949647
32	1	0	3.731136	2.988630	1.839763
33	1	0	4.867522	-2.094771	0.989320
34	1	0	-1.383324	2.381661	-1.929261
35	1	0	-1.099915	3.781399	0.783759
36	1	0	-0.725470	4.478924	-0.823823
37	1	0	-4.020915	2.873270	0.959149
38	1	0	-4.469570	2.682874	-0.766091
39	1	0	-3.103075	4.499383	-1.436135
40	1	0	-3.171495	5.012921	0.267070
41	1	0	-1.092684	-2.332003	-1.947030
42	1	0	-5.442658	-1.244326	-0.464934
43	1	0	-6.131110	-2.676499	1.492637
44	1	0	-4.641474	-2.824014	3.472466
45	1	0	-2.506611	-1.560926	3.531886
46	1	0	-1.854153	-0.130695	1.567676
47	1	0	-1.071775	-3.644891	0.176645
48	1	0	0.322324	-4.586581	-0.391951
49	1	0	-1.245080	-4.739412	-1.217351
50	1	0	0.761181	-2.575562	-3.605643
51	1	0	-0.163846	-4.092369	-3.484907
52	1	0	1.423422	-3.948137	-2.695582

28, Isomer 2

E(RB+HF-LYP) = -2074.76829618
Single point calculation using 6-31G* on all of the light atoms
E(RB+HF-LYP) = -2084.71919249

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.858746	1.767403	-1.189282
2	6	0	2.962628	1.454672	-0.179928
3	6	0	1.987416	2.328222	0.266157
4	6	0	1.906322	3.587579	-0.334334
5	6	0	2.796043	3.935797	-1.354368
6	6	0	3.769194	3.027627	-1.783504
7	16	0	3.105101	-0.182115	0.650540
8	8	0	1.797428	-0.472530	1.537089
9	7	0	3.150874	-1.296481	-0.862588
10	6	0	1.882511	-2.109433	-0.947546
11	6	0	2.067110	-3.283827	0.036346
12	6	0	3.560623	-3.656473	-0.160326
13	6	0	4.243161	-2.332510	-0.646480
14	6	0	0.590137	-1.343642	-0.755056
15	8	0	-0.423007	-2.058746	-0.385252
16	45	0	-2.234781	-1.144827	-0.123033
17	8	0	-4.010514	-0.143545	0.138745
18	6	0	-4.030214	1.127253	-0.089698
19	8	0	-3.032841	1.850894	-0.480701
20	45	0	-1.221874	0.924490	-0.769211
21	8	0	-0.767240	1.241564	1.205134
22	6	0	-1.023165	0.309409	2.081772
23	8	0	-1.701751	-0.758740	1.807599
24	8	0	0.543433	-0.088723	-1.059144
25	8	0	-1.737582	0.526425	-2.722471
26	6	0	-2.363603	-0.577069	-2.967892
27	8	0	-2.700869	-1.475333	-2.103456
28	8	0	4.523489	-0.339832	1.367412
29	1	0	-2.633633	-0.768124	-4.008394
30	6	0	-0.463349	0.490381	3.481337
31	1	0	-4.981817	1.640885	0.059067
32	1	0	1.872776	-2.487297	-1.980322
33	1	0	1.878688	-2.899908	1.041866
34	1	0	1.384398	-4.106411	-0.176844
35	1	0	4.937121	-1.923985	0.092871
36	1	0	4.749360	-2.459514	-1.605767
37	1	0	3.661099	-4.432209	-0.925490
38	1	0	4.009376	-4.016290	0.768163
39	1	0	1.271696	2.012201	1.013363
40	1	0	1.146705	4.288177	-0.006836
41	1	0	2.729543	4.912706	-1.818517
42	1	0	4.452136	3.294866	-2.580608
43	1	0	4.587130	1.040717	-1.523129
44	6	0	-1.048104	-0.542863	4.458033
45	1	0	0.614074	0.314167	3.349378
46	6	0	-0.690028	1.941499	3.964095
47	1	0	-0.188851	2.093532	4.925191
48	1	0	-0.294638	2.656577	3.239561
49	1	0	-1.760809	2.133195	4.096953
50	1	0	-0.586410	-0.420059	5.443113
51	1	0	-2.129689	-0.404993	4.557281
52	1	0	-0.863414	-1.559511	4.103989

Structures related to 29. B3LYP using lanl2dz on Rh, 6-31G* on the reacting carbenoid and olefinic carbons, 6-31G on the rest of the lighter atoms

29, Isomer 1 (gives major isomer)

```
E(RB+HF-LYP) =  -3655.15772010
 C,0,7.2320334023,0.0108403411,1.8091343474
 C,0,6.0439284248,0.1449058439,1.0978569321
 C,0,4.9005015574,0.7486227638,1.6123173673
 C,0,4.9615345504,1.2467475464,2.9201565518
 C,0,6.1429307938,1.1304563447,3.6662011836
 C,0,7.2729117154,0.5122297861,3.1163702371
 S,0,6.0446906967,-0.4536353797,-0.6707500996
 O,0,7.3816684993,-1.3916591691,-0.8611019836
 N,0,4.4533409574,-1.5000315433,-0.6959759042
 C,0,3.6837903272,-1.2464743687,-1.9587606019
 C,0,3.5508448285,-2.6334406428,-2.665784606
 C,0,4.7039711591,-3.46929701,-2.0717911869
 C,0,4.7842422498,-2.962095966,-0.6230078232
 C,0,2.3339278035,-0.6202960441,-1.6566390326
 O,0,1.7221182452,-0.9755988192,-0.5647859869
 Rh,0,0.00393458,0.0531059328,0.0070618488
 O,0,-1.2436982767,-1.3937155184,-0.8765036599
 C,0,-1.4911480012,-1.3565957972,-2.1637104428
 C,0,-2.4601199366,-2.3901394359,-2.7227669808
 C,0,-2.4806979052,-2.3846292441,-4.2599883484
 O,0,-0.9931046462,-0.4812242451,-2.9611709383
 Rh,0,0.0413745094,1.1500703656,-2.2229031818
 O,0,1.0603740417,2.7380778921,-1.3631224619
 C,0,1.5124584509,2.6246071084,-0.1643037605
 C,0,2.3851294902,3.7420548198,0.3816134031
 C,0,3.5817257748,3.999585406,-0.5595084301
 O,0,-1.7723765067,2.0180298518,-1.7156912462
 C,0,-2.3025510766,1.7934154709,-0.5646989627
 O,0,-1.7563174203,1.1176825448,0.3985145388
 C,0,-3.6535122275,2.4483985228,-0.3377198503
 N,0,-4.5635666855,1.6409962624,0.5407982102
 C,0,-5.3515844177,2.5613217044,1.4394038571
 C,0,-4.9674961993,3.9852889803,0.9948933842
 C,0,-3.5518687574,3.802983217,0.4115589389
 S,0,-5.6778664762,0.5286859808,-0.4925549428
 O,0,-4.8776079591,0.2997311398,-1.9060246042
 C,0,-5.6977634322,-1.0647914311,0.4810024905
 C,0,-4.503109669,-1.7527345013,0.6679094776
 C,0,-4.5638400222,-2.9778049426,1.3455936142
 C,0,-5.7920382138,-3.4727436431,1.8054836712
 C,0,-6.973962806,-2.7500151629,1.5970367105
 C,0,-6.9352526207,-1.5244951599,0.9202438683
 O,0,-7.2189745923,1.1007110856,-0.5103220408
 O,0,1.8726672836,0.193701997,-2.5365437857
 C,0,-2.182778628,-3.7963704577,-2.152774678
 C,0,0.1423227386,-0.6578350545,1.9448147535
 C,0,1.4859126929,-0.8361060856,2.4556296404
 C,0,1.8799682472,-0.6193761803,3.7342390728
 O,0,1.2697487357,1.6111078543,0.6241591104
 C,0,-0.9250826073,-0.1875428374,2.8595931326
 O,0,-0.807358281,0.8677612479,3.507845285
 O,0,-2.078295262,-0.9288606422,2.867906883
 C,0,-3.2262987373,-0.3228172998,3.5731180211
 O,0,5.7883192547,0.7955041239,-1.7050484407
 C,0,1.5325405243,5.0179390855,0.5752444154
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C,0,-0.3339199201,-2.9802354108,1.479978732
C,0,-0.3242857981,-3.4118938099,2.7634407182
C,0,0.8641232285,-3.9656593375,3.4740147487
H,0,8.0852142465,-0.4733871376,1.3483551491
H,0,3.9869459239,0.8179866933,1.0340070783
H,0,4.0852478947,1.7217693371,3.3476765762
H,0,6.1820073695,1.5236166915,4.6768227683
H,0,8.1848108457,0.4225430186,3.6966739023
H,0,4.2246111032,-0.5285585675,-2.5850815638
H,0,2.5848483375,-3.0866530228,-2.4148666665
H,0,3.6060652238,-2.527797072,-3.7516418918
H,0,5.6481621654,-3.2559582708,-2.586156241
H,0,4.5159721205,-4.5456316693,-2.1328988117
H,0,4.0161598824,-3.4197150149,0.0109581186
H,0,5.7637947803,-3.1108212074,-0.1634765631
H,0,-3.4483570457,-2.0573778458,-2.3662319743
H,0,-2.7128959813,-1.3902211634,-4.6469155307
H,0,-3.2392716113,-3.0880730588,-4.620841926
H,0,-1.5088017422,-2.6852029132,-4.6673416722
H,0,2.7467233447,3.4067868518,1.35989872
H,0,4.1929759469,3.1018556991,-0.7030476656
H,0,4.2208453086,4.7857807713,-0.1418648183
H,0,3.2257175577,4.3232237874,-1.5421155668
H,0,-4.083542736,2.598967024,-1.3332870022
H,0,-5.0377273481,2.3603253167,2.4688567268
H,0,-6.4231057081,2.3628796442,1.3450401517
H,0,-5.6570391997,4.3370483045,0.2186060166
H,0,-4.9934110754,4.6993359598,1.8232031947
H,0,-2.8087856618,3.7245556753,1.2131450452
H,0,-3.2508192727,4.603993399,-0.2681040289
H,0,-3.5570492302,-1.3545032102,0.3189819972
H,0,-3.6501054907,-3.5370740753,1.5130230198
H,0,-5.8281988681,-4.4248108081,2.3250335649
H,0,-7.9228639286,-3.1378608761,1.951431452
H,0,-7.8274632992,-0.9402887733,0.7267163774
H,0,-2.2044583269,-3.7979127558,-1.0603307814
H,0,-1.1996378744,-4.160051334,-2.4760730409
H,0,-2.9387657176,-4.5003025247,-2.5172193808
H,0,2.2233423088,-1.1116003789,1.7052010979
H,0,2.9272555995,-0.6976652217,4.0104984809
H,0,1.1898784698,-0.2932740089,4.5051459247
H,0,-3.9496111577,-1.129068248,3.6692319368
H,0,-2.9123551813,0.0554054518,4.5471323899
H,0,-3.6202396463,0.4853540388,2.9559737682
H,0,0.7007728956,4.8403865739,1.2662700947
H,0,1.1242378421,5.3498534034,-0.3848248318
H,0,2.1536526029,5.8216824644,0.9859149445
H,0,-1.2353231311,-2.6314507889,0.9948816316
H,0,0.5323984325,-3.101597161,0.8350432058
H,0,-1.2310569247,-3.2861315391,3.3522692949
H,0,1.2788756326,-3.2030943653,4.1587685799
H,0,0.5986276855,-4.833390993,4.0902083586
H,0,1.6629993559,-4.2504096326,2.7820821679
```

29, Isomer 2 (gives minor isomer)

```
E(RB+HF-LYP) =  -3655.15346914
 C           7.536136    1.559363    -.695749
 C           6.205706    1.413834    -.316717
 C           5.349406    2.487693    -.092999
 C           5.866642    3.779671    -.249007
 C           7.203273    3.962293    -.630047
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C	8.035455	2.858269	-.853218
S	5.557984	-.329794	-.141337
O	6.874745	-1.310001	-.054855
N	4.693764	-.168220	1.489778
C	3.832913	-1.350526	1.788161
C	3.872917	-1.415711	3.337664
C	5.329301	-1.035791	3.664261
C	5.661646	.062144	2.632264
C	2.409594	-1.282951	1.262610
O	1.948664	-.209805	.710087
Rh	.016279	-.227110	-.113402
O	-.796825	.408161	1.697477
C	-1.200869	-.464557	2.579928
C	-2.014935	.046726	3.760645
C	-1.777067	-.810786	5.018099
O	-.991854	-1.733513	2.488052
Rh	-.199274	-2.550959	.754826
O	.606975	-3.249180	-1.022650
C	.970758	-2.406134	-1.925754
C	1.715714	-2.908695	-3.155484
C	1.799727	-4.442133	-3.196190
O	-2.110802	-2.563651	-.033926
C	-2.601858	-1.512624	-.589433
O	-1.960016	-.409277	-.819687
C	-4.031009	-1.678757	-1.076895
N	-4.831035	-.413189	-1.096263
C	-5.759712	-.409927	-2.285422
C	-5.540974	-1.776106	-2.965817
C	-4.104972	-2.154811	-2.550657
S	-5.743916	-.171405	.516363
O	-4.756480	-.819532	1.653418
C	-5.819239	1.687193	.635690
C	-4.636110	2.410560	.546437
C	-4.717664	3.802994	.672148
C	-5.955872	4.418771	.896088
C	-7.126953	3.654000	.989028
C	-7.067613	2.261649	.857649
O	-7.293251	-.710677	.409380
O	1.751027	-2.371737	1.456777
C	-1.791391	1.545344	4.023419
C	.197745	1.771579	-.665735
C	1.029347	2.585321	.196176
C	.802471	3.875371	.544604
O	.766561	-1.120981	-1.847633
C	-1.028625	2.334535	-1.271405
O	-1.842618	3.021394	-.620078
O	-1.278710	1.947980	-2.559025
C	-2.649366	2.179913	-3.050424
O	4.401345	-.683090	-1.246279
C	1.103049	-2.328205	-4.448438
C	1.698647	1.540812	-2.524321
C	1.603563	2.840306	-2.908655
C	2.519580	3.935996	-2.485530
H	8.152772	.680428	-.844994
H	4.323791	2.316822	.210980
H	5.227545	4.638088	-.071883
H	7.595987	4.966458	-.750500
H	9.069568	3.003312	-1.145943
H	4.267787	-2.277385	1.389112
H	3.174019	-.681351	3.754073
H	3.581547	-2.405995	3.691887
H	5.986480	-1.900735	3.519925

H	5.452856	-.683145	4.692112
H	5.477734	1.067792	3.021051
H	6.699008	-.001392	2.290632
H	-3.059947	-.100025	3.439144
H	-1.948686	-1.868332	4.807216
H	-2.455731	-.494361	5.817903
H	-.747494	-.696583	5.379886
H	2.732309	-2.497693	-3.048235
H	2.254368	-4.839604	-2.285535
H	2.401339	-4.757634	-4.056137
H	.802497	-4.886130	-3.289999
H	-4.478714	-2.434441	-.422821
H	-5.468024	.421928	-2.934636
H	-6.795464	-.265961	-1.964393
H	-6.253395	-2.510429	-2.572289
H	-5.669224	-1.724473	-4.050913
H	-3.367723	-1.608625	-3.150062
H	-3.892130	-3.223813	-2.627466
H	-3.683757	1.929342	.364780
H	-3.808423	4.384972	.583574
H	-6.010290	5.498175	.995922
H	-8.083541	4.135575	1.161440
H	-7.950163	1.635528	.916557
H	-1.995622	2.138934	3.129433
H	-.755439	1.739329	4.327589
H	-2.452049	1.882517	4.830124
H	1.860704	2.047296	.645416
H	1.430910	4.367385	1.281960
H	-.050877	4.432619	.174993
H	-2.631149	1.826085	-4.079395
H	-3.343687	1.601103	-2.439345
H	-2.897319	3.242296	-3.002855
H	1.069969	-1.236562	-4.414411
H	.081498	-2.700488	-4.594412
H	1.701193	-2.633696	-5.313934
H	2.543270	1.163816	-1.951762
H	1.030626	.788855	-2.923539
H	.753030	3.127395	-3.524029
H	2.685926	4.658540	-3.293173
H	2.061183	4.490717	-1.643328
H	3.485248	3.557261	-2.139110

Additional Experimental Results

NMR Results

For the ^{13}C spectra of styrene the integrations of the *para* carbons were set at 1000. The average integrations for the other carbons are shown in Table 1 along with the number of spectra recorded for each sample (n).

Table 1. Average ^{13}C integrations for *styrene*.

% conversion	C_1	α-olefinic	meta	para	ortho	β-olefinic	n
Reaction with ethyl diazoacetate							
Standard	975.53	989.96	1993.44	1000	1995.94	1002.21	6

80.3 ± 1 %	982.39	995.07	1994.64	1000	1995.18	1021.95	6
81.1 ± 1 %	984.58	999.30	1999.23	1000	1999.90	1027.19	6
87.8 ± 1 %	983.79	999.12	1996.96	1000	1997.61	1027.35	6
Reactions with Rh_2(octanoate)$_4$ and phenyldiazoacetate							
Standard	976.40	985.23	1997.14	1000	2002.57	1011.30	6
83.9 ± 1 %	974.56	991.03	1994.60	1000	1999.27	1054.75	6
82.8 ± 1 %	976.52	991.40	1998.38	1000	2000.83	1053.99	6
Reaction with Rh_2(S-DOSP)$_4$ and phenyldiazoacetate							
Standard	986.06	991.51	1997.64	1000	2000.52	1005.35	6
84.2 ± 1 %	984.55	996.40	1997.99	1000	2000.84	1045.77	6

The values for R/R_O, calculated as the ratio of average integrations in Table 1 relative to standard, are shown in Table 2. The standard deviations were calculated from the formula:

$$\Delta R / R_0 = R / R_0 \times ((\Delta \text{IntSample} / \text{IntSample})^2 + (\Delta \text{IntStandard} / \text{IntStandard})^2)^{1/2} \quad (1)$$

Table 2. R/R_O for ^{13}C.

R/R_0 and stand dev	C_1	α-olefinic	meta	ortho	β-olefinic
Reaction with ethyl diazoacetate					
80.3 ± 1 % R/R_0	1.007	1.005	1.001	1.000	1.020
stand dev	0.003	0.003	0.003	0.003	0.004
81.1 ± 1 % R/R_0	1.009	1.009	1.003	1.002	1.025
stand dev	0.004	0.003	0.003	0.003	0.004
87.8 ± 1 % R/R_0	1.008	1.009	1.002	1.001	1.025
stand dev	0.003	0.004	0.003	0.003	0.003
Reactions with Rh_2(octanoate)$_4$ and phenyldiazoacetate					
83.9 ± 1 % R/R_0	0.998	1.006	0.999	0.998	1.043
stand dev	0.004	0.003	0.003	0.003	0.004
82.8 ± 1 % R/R_0	1.000	1.006	1.001	0.999	1.042

stand dev	0.004	0.003	0.003	0.003	0.003
Reaction with Rh_2(S-DOSP)$_4$ and phenyldiazoacetate					
84.2 ± 1 % R/R_0	0.998	1.005	1.000	1.000	1.040
stand dev	0.003	0.003	0.002	0.002	0.005

The ^{13}C KIEs for styrene were then calculated from eq. 2, with the standard deviations calculated from eq. 3, 4, and 5. All of these equations are taken from: Singleton, D. A.; Thomas, A. A. *J. Am. Chem. Soc*. **1995**, *117*, 9357, its Supporting Information, and references therein.

$$KIE_{calcd} = \frac{\ln(1 - F)}{\ln[(1 - F)R/R_0]} \quad (2)$$

$$\Delta KIE_F = \frac{\partial KIE}{\partial F}\Delta F = \frac{-\ln(R/R_0)}{(1 - F)\ln^2[(1 - F)R/R_0]}\Delta F \quad (3)$$

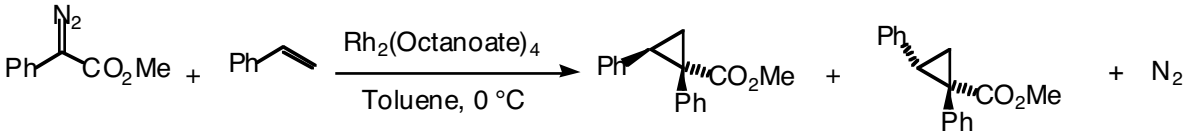
$$\Delta KIE_R = \frac{\partial KIE}{\partial (R/R_0)}\Delta(R/R_0) = \frac{-\ln(1 - F)}{(R/R_0)\ln^2[(1 - F)R/R_0]}\Delta(R/R_0) \quad (4)$$

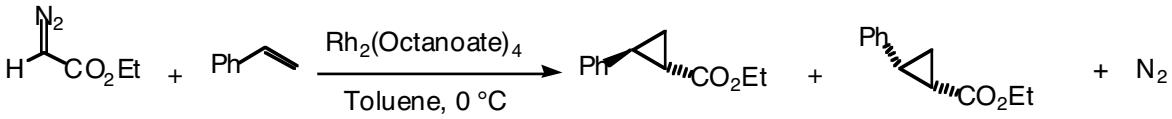
$$\Delta KIE = KIE*((\Delta KIE_R/KIE)^2 + (\Delta KIE_F/KIE)^2)^{1/2} \quad (5)$$

Table 3. ^{13}C KIEs**.**

sample	C_1	α-olefinic	meta	ortho	β-olefinic
Reaction with ethyl diazoacetate					
80.3 ± 1 %	1.004(2)	1.003(2)	1.000(2)	1.000(2)	1.012(3)
81.1 ± 1 %	1.006(3)	1.006(2)	1.002(2)	1.001(2)	1.015(3)
87.8 ± 1 %	1.004(2)	1.004(2)	1.001(1)	1.000(2)	1.012(2)
Reactions with Rh_2(octanoate)$_4$ and phenyldiazoacetate					
83.9 ± 1 %	0.999(2)	1.003(1)	0.999(2)	0.999(1)	1.024(3)
82.8 ± 1 %	1.000(2)	1.004(2)	1.000(2)	1.000(2)	1.024(2)
Reaction with Rh_2(S-DOSP)$_4$ and phenyldiazoacetate					
84.2 ± 1 %	0.999(2)	1.003(2)	1.000(1)	1.000(1)	1.022(3)

Kinetics Study of Cyclopropanation Reactions using Methyl Phenyldiazoacetate versus Ethyl Diazoacetate





General Procedure: Styrene (2.08 g, 20 mmol) and the diazo (2 mmol) were dissolved in toluene and cooled on ice/water. The flasks were fitted with septa and 1/8" teflon tubes leading to inverted grad. Cylinders filled with water. At time = 0, a solution of $Rh_2(Octanoate)_4$ (0.6 μmol) in toluene (100 μl) was added by syringe through the septum of each. Nitrogen evolution displacing water was recorded until no further bubbling from the tubes was observed (250 minutes). The results are summarized in the graph below. The ethyl diazoacetate reaction gave 73% yield of crude mixture of diastereomer products after evaporation of volatiles.